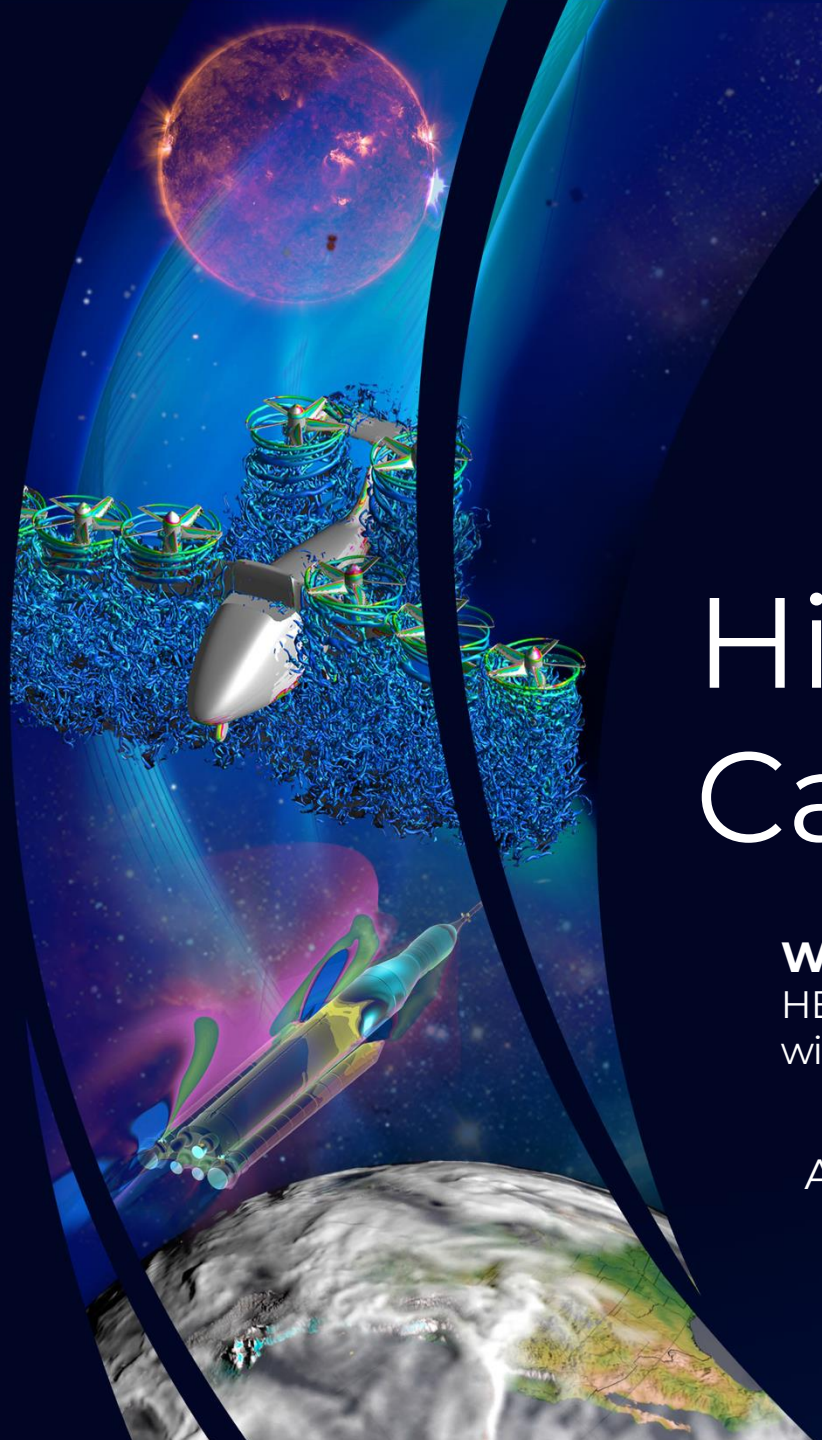


National Aeronautics and Space Administration

High-End Computing Capability

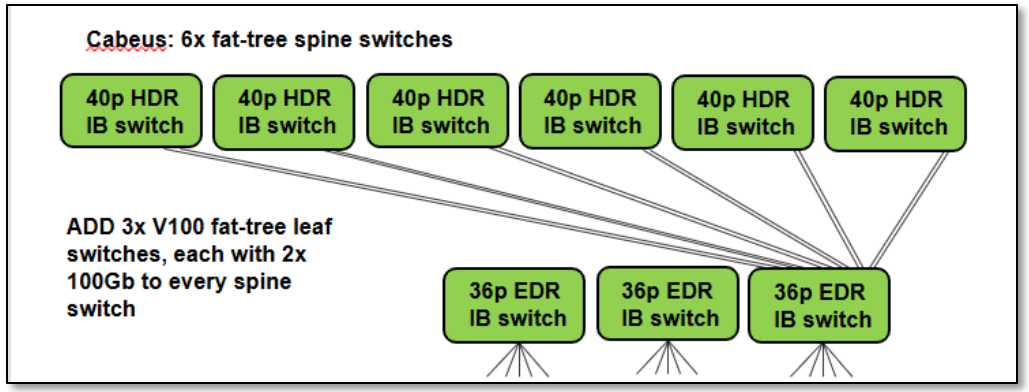
William Thigpen
HECC Component Manager
william.w.thigpen@nasa.gov

April 10, 2025

Systems Team Migrates V100 GPU Nodes to Cabeus

- The HECC Systems team worked with HPE staff and the Application Performance and Productivity (APP) team to complete the migration of the NVIDIA V100 graphics processing unit (GPU) nodes from the Pleiades HyperCube topology to the Cabeus Fat Tree topology.
- The teams also simplified the InfiniBand (IB) cabling:
  - Reduced the number of Enhanced Data Rate (EDR) IB switches from 16 to 6, leaving 10 free for reuse.
  - Reduced the number of connections per node from three to two, reducing cabling and port requirements.
- The V100 GPUs are now consolidated on the Cabeus network with the NVIDIA A100 GPUs on same front-end systems and PBS server. As a result:
  - Multi-node jobs across the V100s and A100s are now possible.
  - System administration for Cabeus is more efficient.

IMPACT: Integrating the NVIDIA V100 graphics processing units with the Cabeus supercomputer simplifies the user experience and improves the efficiency of system administration.

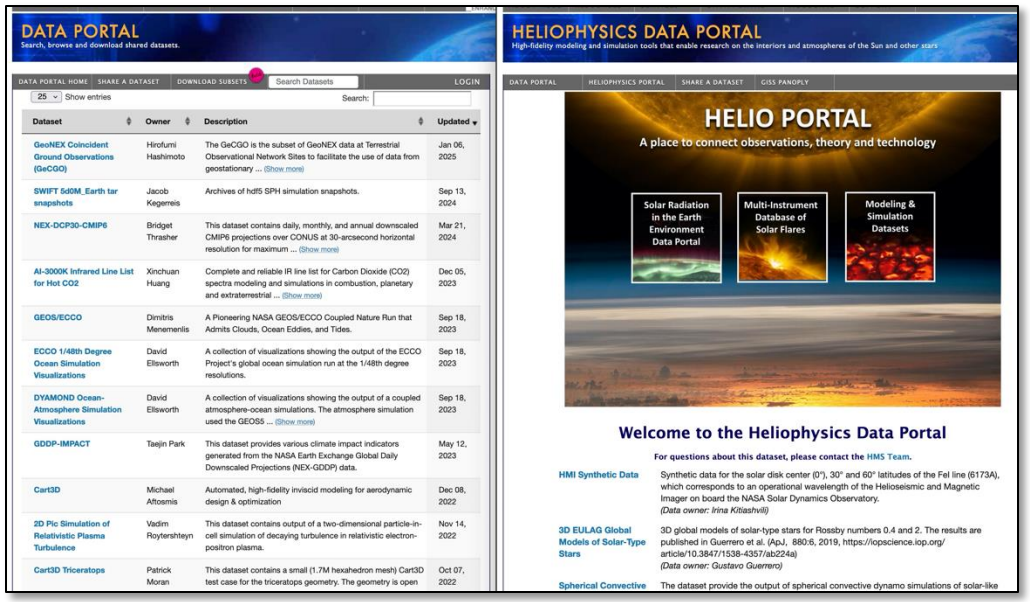


The Cabeus InfiniBand Fat Tree topology with consolidated EDR switches for connection with the V100 GPU nodes.

Data Portal Code Modernization

- The Data Portal team implemented GitLab CI and Ansible to automatically provision code changes between environments. In the past, updates to code for the Data Portal involved manually copying code between development and production servers. The process was time consuming and error prone due to the large number of hosted datasets.
- The benefits are:
  - Reduces work required to update the Data Portal and deploy new datasets.
  - Enables workflow automation for applications developed by teams such as the Mars Climate Modeling Center (MCMC) and the HECC Visualization team to automate updates and provide failover.
- The Data Portal codebase has now been updated into a more modular, dynamic workflow with the following advantages:
  - Over time, individual Data Portal code repositories were created for each dataset, with code repetitions. The team reduced 30 different codebases down to one template to simplify maintenance and addition of new portals.
  - Most codebases were refactored into one common codebase that dynamically loads pages for the Data Portal, significantly reducing the complexity of updates and bug fixes for the application.
  - Public dataset pages are now dynamically created and presented using PHP scripts. The dynamic workflow for private datasets also includes user validation to ensure secure access only to the dataset pages and files that the user is authorized to view.

IMPACT: A new codebase for the Data Portal provides significant advantages for automating and streamlining updates and new dataset deployments.

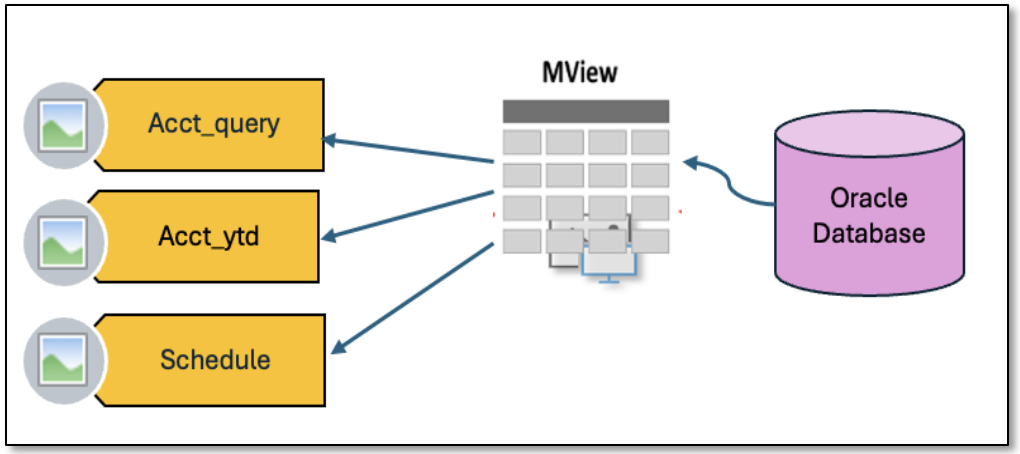


Left: The Data Portal provides scientists with access to a variety of shared datasets. Right: The Heliophysics Portal provides access to one of the publicly available downloadable datasets.

New User Usage and Allocation Reporting Tools

- The Tools team completed a major milestone, developing and implementing a new usage, allocation, and schedule tool written in Python, replacing a legacy tools written in an old programming language. The new tool connecting to high performance Oracle normalized data view with a simplified SQL database query.
- **Acct_query Program**: Displays the SBU usage data for the user/GID with different options by querying account data generated by the Portable Batch System (PBS).
- **Acct_ytd Program**: Displays allocation limit, used and remaining allocation for a user's GIDs with different options by querying account data generated by PBS.
- **Schedule Program**: Queries the Remedy database to display the scheduled downtime of all NAS hosts.
- To achieve this milestone, the team investigated and documented requirements and all options for the above programs. They tested the Python code for all three scripts and their associated options; created binaries; and developed support and user documentation for all three programs.

IMPACT: SBU usage and allocation data is now available in real time for HECC users by leveraging Python to eliminate technical debt and improve support and maintainability.

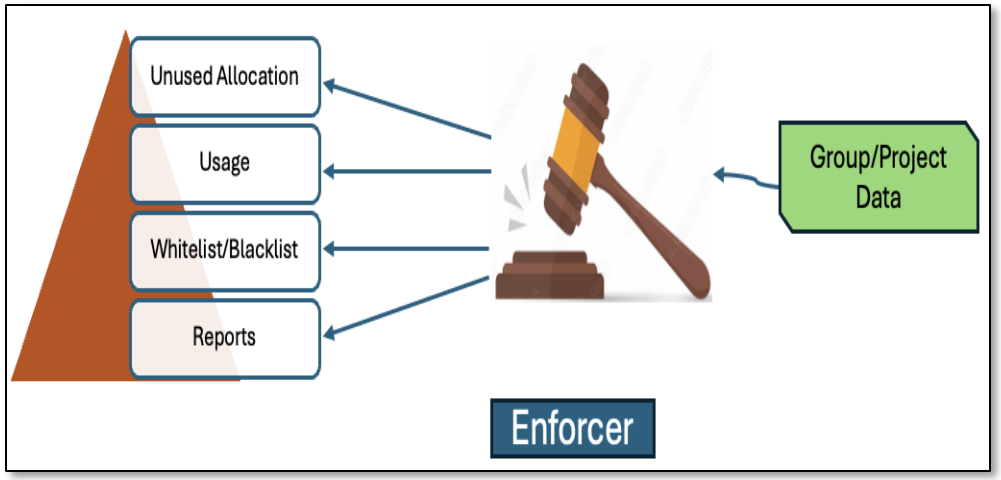


The working flow of three Python scripts supporting the NAS secure enclave.

Tools Team Develops PBS Public Queue Allocation Enforcer

- At NAS, HECC system users are awarded computer time via group allocations, with which they run jobs using public queues managed by the PBS server. Previously, a legacy Systems team-managed Perl script determined whether users of a group are permitted to run provided the group's accumulated computer time usage falls within its allocation limit.
- Now, in support of the Cabeus system's Grace Hopper queues, the Tools team took over responsibility for policing queues and developed Enforcer, a new Python script that is more efficient, reliable, and replete with features than its predecessor. It has three modes:
  - **Normal mode**: This option evaluates each valid group, determines its allocation budget, its current allocation usage to date, and other factors (such as blacklist, whitelist).
  - **Specific Group report mode**: This option reports detailed information about one specific group; most useful when trying to determine if a group is on an ACL or not.
  - **Daily Allocation Usage report mode**: This option generates a report detailing the allocation and usage for all groups for the current Fiscal Year (the New Operational Period).
- To implement the new Python script, the Tools team investigated and documented requirements, tested the code and its features, and deployed the script on the Cabeus Grace Hopper PBS server.
- The team is working to deploy the script on the remaining PBS servers at NAS to support remaining systems and create support and user documentation.

IMPACT: NAS staff experts develop tools such as Enforcer, which improves HECC operational efficiency, data accuracy, and reporting while simplifying maintenance and support.



The working flow of the Enforcer script that reports various details and status of HECC user groups.

Nagios Implemented on HECC Tools Hosts

- The Tools team augmented out implementation of Nagios, an open-source system monitoring platform, to include approximately 50 Tools system hosts to monitor events in real time for servers, switches, applications, and services. Nagios provides a clear indication of any environment issue as green, red, or yellow.
- The team grouped the hosts by environment, allowing for a quick view of alerts ranging from high-level to very detailed status for a service on the host to highlight issue urgency. Nagios also alerts the team when an implemented check fails and when an event has resolved.
  - For example: a red alert on a host for the Apache service can notify the Control Room that a website is unavailable before an end user reports the issue. Nagios can also page the team about the issue before the end user reports, delivering better service and reliability. Further thresholds can be set to identify an issue before it occurs.
- As part of the Nagios implementation work, the Tools team:
  - Identified the minimum level of Nagios alerts for every Tools host, creating a standardized set of services.
  - Identified additional unique services a particular host may require in addition to the standardized minimum set, resulting in 20-plus Nagios checks implemented on each Tools host.
  - Wrote scripts for custom plugin checks where Nagios checks did not exist.

IMPACT: Providing thorough, customized monitoring of all services on all HECC Tools hosts enables proactive team notification of host system events and resolutions



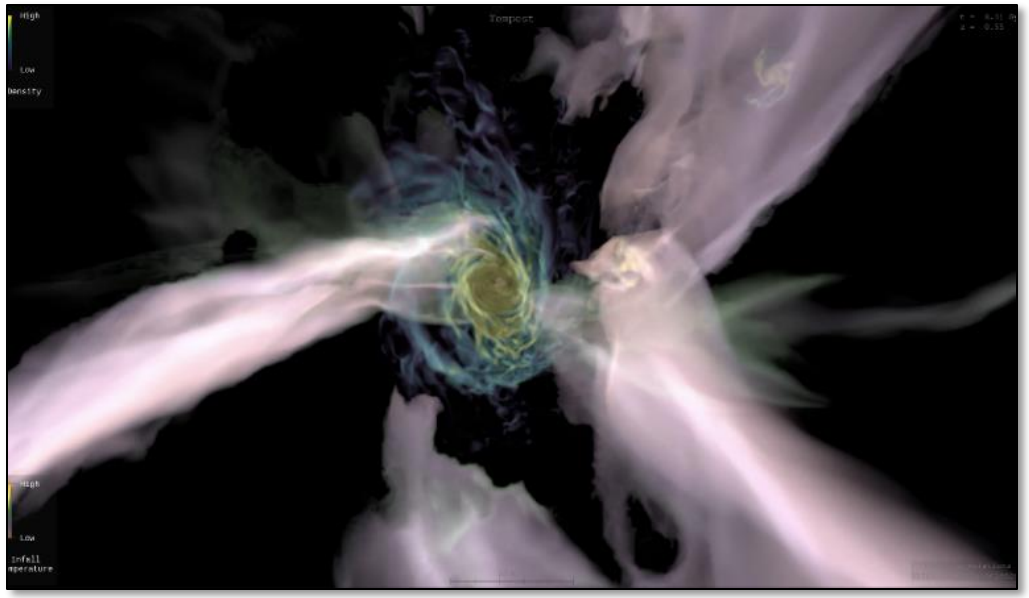
The Nagios open-source monitoring platform helps identify and resolve problems before they impact operational processes, providing real-time insights and proactive alerts. *Logo provided with permission from Nagios.*

Simulations to Track the Fuel for Galaxy Growth *

- Researchers at the Space Telescope Science Institute (STScI) use their "FOGGIE" (Figuring Out Gas & Galaxies In Enzo) code to shine a light through the circumgalactic medium (CGM) by simulating galaxy evolution across 13.7 billion years of cosmic time. Because the creation of new stars is fueled by gas flowing into galaxies from the CGM, understanding this material is essential for astrophysicists studying how galaxies evolve.
- The FOGGIE simulations revealed that most of the gas falling through the CGM onto a galaxy is predominantly cooler than the CGM gas that is not flowing inward.
  - They also show that the accreting gas was not affected by the heavy elements that are formed in stars, suggesting that it is nearly pristine gas that has never been located near another galaxy.
  - The simulations helped reveal how this fresh gas reaches the galaxy and what happens to it along the way through the CGM.
- Each of the six galaxies simulated in the FOGGIE suite ran on 512 Intel Xeon Haswell nodes on Pleiades and took 12–18 months of wall-clock time (several million node-hours).
- The team also heavily relied on support from the HECC visualization team to produce beautiful images and movies used for scientific analysis.

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

IMPACT: Coupled with observational data from space-based observatories, these simulations help reveal the physics of the complex circumgalactic medium—a crucial step to understand how galaxies form and evolve—addressing NASA's strategic goal to understand the universe.

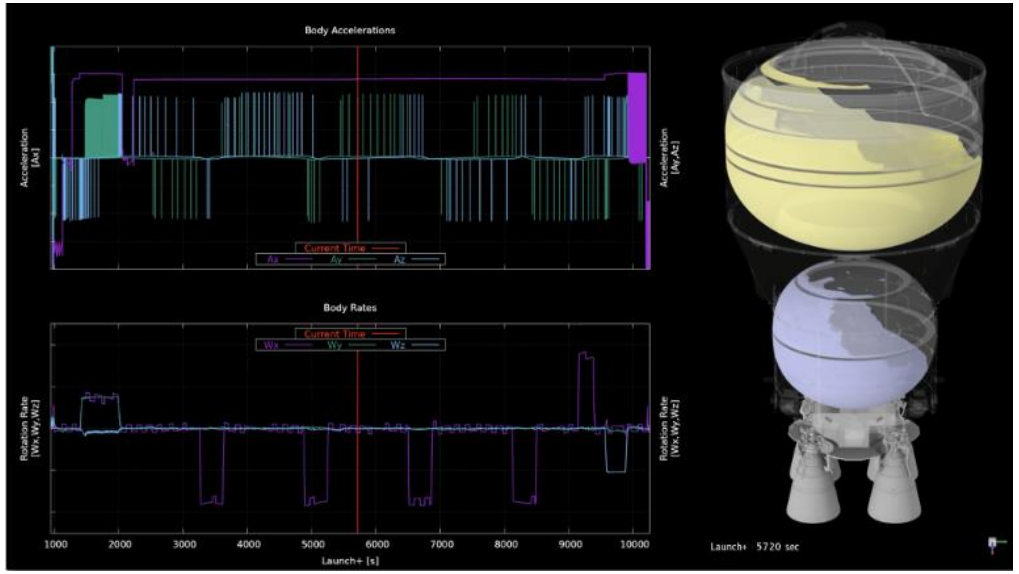


Many galaxies merge over time to make one of the FOGGIE galaxies.
Cassi Lochhaas, Center for Astrophysics Harvard & Smithsonian; Chris Henze, NASA/Ames

Long-Duration SLS Slosh Dynamics Simulations *

- Using the Aitken, Pleiades, and Electra supercomputers, engineers at NASA Marshall completed a parametric analysis consisting of 28 primary simulations of the Space Launch System (SLS) Exploration Upper Stage to support an assessment of hydrazine propellant mass usage by its Reaction Control System during two coast phases.
  - First, the team evaluated open-loop stability control with loose coupling to the vehicle model. Next, they determined sensitivity using a more tightly coupled closed-loop model linking the computational fluid dynamics (CFD) solver and vehicle model.
  - Each case simulated several thousands of seconds of mission time and required continuous run times over two months.
- This analysis successfully produced useful estimates of hydrazine usage employing CFD as the most trusted method of low-gravity slosh modeling despite the high computational resource cost.
- Successful coupling of the CFD solver and vehicle model is a significant capability improvement that can be carried forward to a wide range of future analyses, bolstered by the plug-and-play flexibility for both tools should other models be preferred.
- Visualizations of the tank dynamics provided further insights for evaluating propellant settling maneuvers.

IMPACT: Simulating propellant control for entire mission phases using coupled CFD and vehicle model analysis is a necessary capability to ensure safety of flagship NASA missions, such as the Space Launch System.



"Fishbowl" style animation of the two Space Launch System Exploration Upper Stage propellant tanks. The simulations depict where the fluid interface is located, and on what side the liquid resides, using a combination of isosurface and wall thresholding to allow for better understanding of the fluid motion in low gravity. (See Notes for more details). *Marco Sansone, NASA/Marshall*

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

Papers

- "**Orbital and Absolute Magnitude Distribution of Hilda Population**," D. Vokrouhlicky, et al., arXiv:2503.04403 [astro-ph.EP], March 6, 2025. *
  https://arxiv.org/abs/2503.04403
- "**Probing Conditions for Strong Clumping by the Streaming Instability: Small Dust Grains and Low Dust-to-Gas Density Ratio**," J. Lim, et al., *The Astrophysical Journal*, vol. 981, no. 2, published online March 6, 2025. *
  https://iopscience.iop.org/article/10.3847/1538-4357/adb311
- "**An Oasis in the Brown Dwarf Desert: Confirmation of Two Low-Mass Transiting Brown Dwarfs Discovered by TESS**," E. Zhang, et al., arXiv:2503.05115 [astro-ph.SR], March 7, 2025. *
  https://arxiv.org/abs/2503.05115
- "**BATSRUS GPU: Faster-than-real-time Magnetospheric Simulations with a Block-Adaptive Grid Code**," Y. An, et al., *The Astrophysical Journal*, vol. 981, no. 2, published online March 7, 2025. *
  https://iopscience.iop.org/article/10.3847/1538-4357/adaf15
- "**Predicting Internal Tides with a Global Ocean Forecast System: Insights from SWOT CalVal Orbit**," B. Yadidya, et al., *ESS Open Archive*, published online March 10, 2025. *
  https://essopenarchive.org/doi/full/10.22541/essoar.174164232.20506498
- "**TESS and HARPS-N Unveil Two Planets Transiting TOI-1453. A Super-Earth and One of the Lowest Mass Sub-Neptunes**," M. Stalport, et al., arXiv:2503.07529 [astro-ph.EP], March 10, 2025. *
  https://arxiv.org/abs/2503.07529

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

Papers (cont.)

- "**Interplanetary Magnetic Field B_y Controlled Alfvén Wings at Earth During an Encounter of a Coronal Mass Ejection**," Y. Chen, et al., *Geophysical Research Letters*, vol. 52, issue 6, published online March 13, 2025. *
  https://agupubs.onlinelibrary.wiley.com/doi/10.1029/2024GL113416
- "**Forecasting the 8 April 2024 Total Solar Eclipse with Multiple Solar Photospheric Magnetograms**," X. Liu, et al., arXiv:2503.10974 [astro-ph.SR], March 14, 2025. *
  https://arxiv.org/abs/2503.10974
- "**Zonal and Adaptive Mesh Refinement for RANS-based Transition Models in FUN3D**," N. Hildebrand, et al., *Computers & Fluids*, vol. 293, published online March 24, 2025. *
  https://www.sciencedirect.com/science/article/abs/pii/S0045793025000672
- "**Transit Ephemerides and Timing Variations from Kepler and K2 to TESS**," L. Kaye, S. Aigrain, *Monthly Notices of the Royal Astronomical Society*, vol. 538, issue 4, published online March 25, 2025. *
  https://academic.oup.com/mnras/article/538/4/2283/8093570
- "**Simulations of Global Solar Connectivity with a Fully Compressible CHORUS++ Code**," K. Hayashi, A. Kosovichev, C. Liang, arXiv:2503.21043 [astro-ph.SR], March 26, 2025. *
  https://arxiv.org/abs/2503.21043
- "**3D Simulations Demonstrate Propagating Thermohaline Convection for Polluted White Dwarfs**," I. Cresswell, et al., arXiv:2503.20885 [astro-ph.SR], March 26, 2025. *
  https://arxiv.org/abs/2503.20885

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

Papers (cont.)

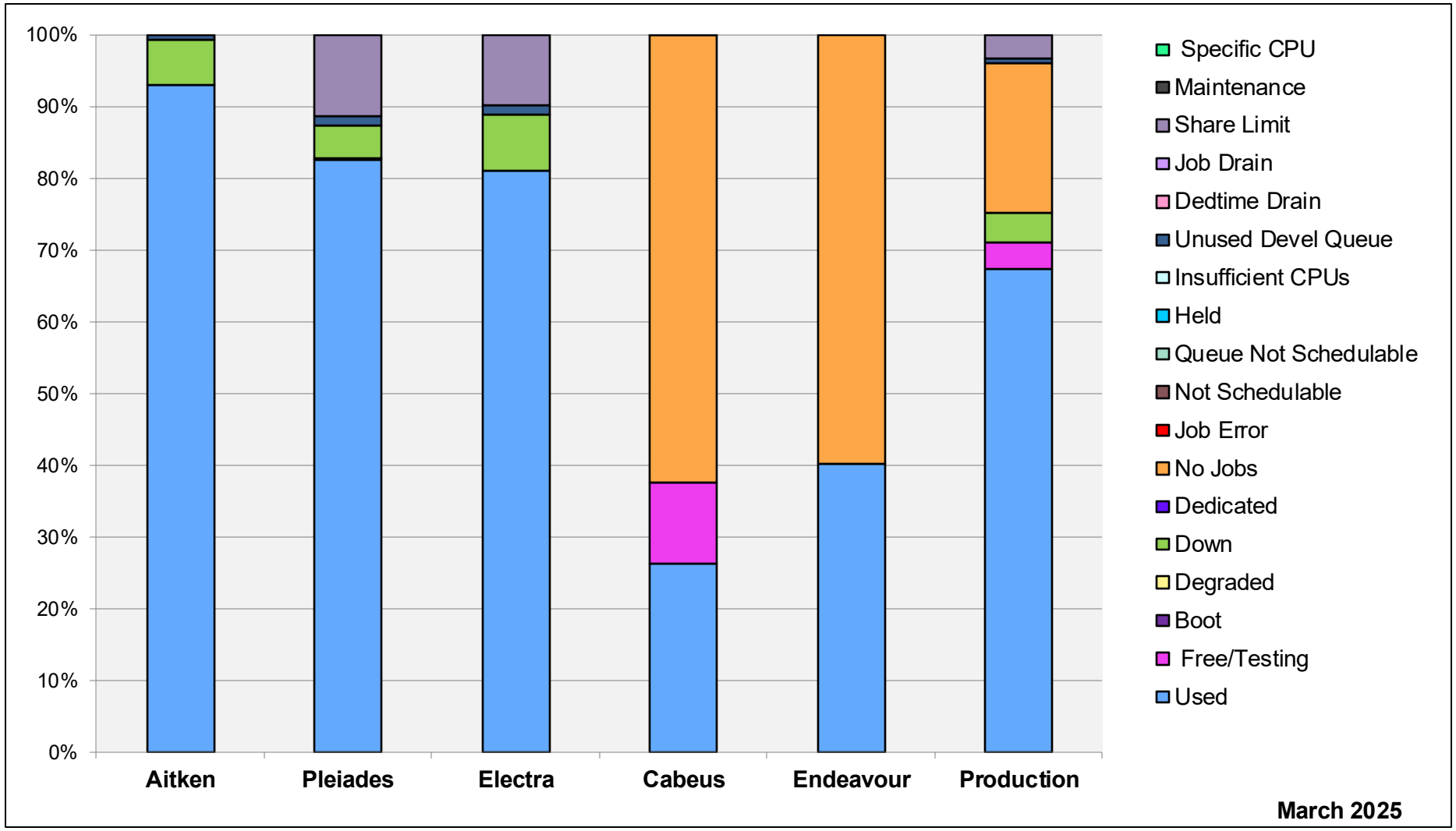
- "**Limits on the Efficacy of Wave-Particle Interaction on the Energization and Transport of Atomic and Molecular Heavy Ionospheric Ions**," M.-Y. Lin, R. Ilie, A. Glocer, *Journal of Geophysical Research: Space Physics*, vol. 130, issue 4, published online March 28, 2025. *
  https://agupubs.onlinelibrary.wiley.com/doi/full/10.1029/2024JA033523
- "**Molecular Dynamics Simulations for the Prediction of the Conformational, Dynamic, and Thermal Properties of Poly(phenylsulfone) (PPSU) and Their Dependence on Molecular Weight**," E. Skountzos, et al., *Industrial & Engineering Chemistry Research*, published online March 28, 2025. *
  https://pubs.acs.org/doi/abs/10.1021/acs.iecr.4c04601

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

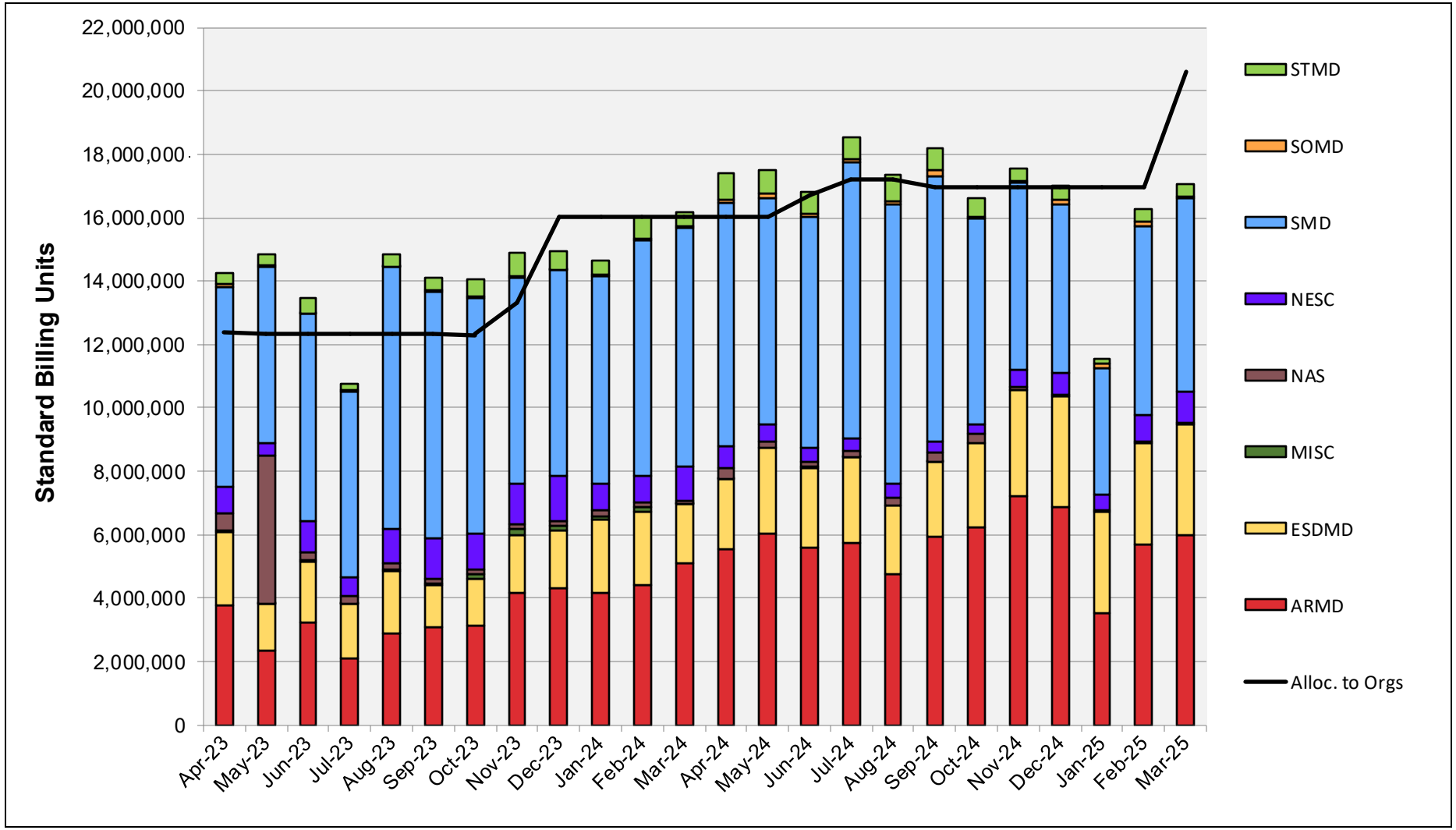
News & Events

- Continued coverage of the role of the Pleiades supercomputer in scientists' discovery of a spiral structure on the edge of our solar system composed of billions of icy bodies surrounded by a shell of comets called the Oort cloud.
  - **NASA Supercomputer Reveals Strange Spiral Structure at the Edge of Our Solar System**, *MSN*, March 22, 2025—When the scientists ran this model through NASA's Pleiades supercomputer, it spit out a structure for the inner part of the cloud (the most densely populated region, located 1,000 to 10,000 AU from the sun) that resembles the spiral disk of the Milky Way. https://www.msn.com/en-gb/news/techandscience/nasa-supercomputer-reveals-strange-spiral-structure-at-the-edge-of-our-solar-system/ar-AA1zCuc2?cvid=AA3C5035FDBB4FEAB2C86A73BF79D845&ocid=iehp
  - **Scientists Discover a New Twist at the Edge of Solar System**," The *Business Standard*, March 7, 2025. https://www.tbsnews.net/tech/scientists-discover-new-twist-edge-solar-system-1086881

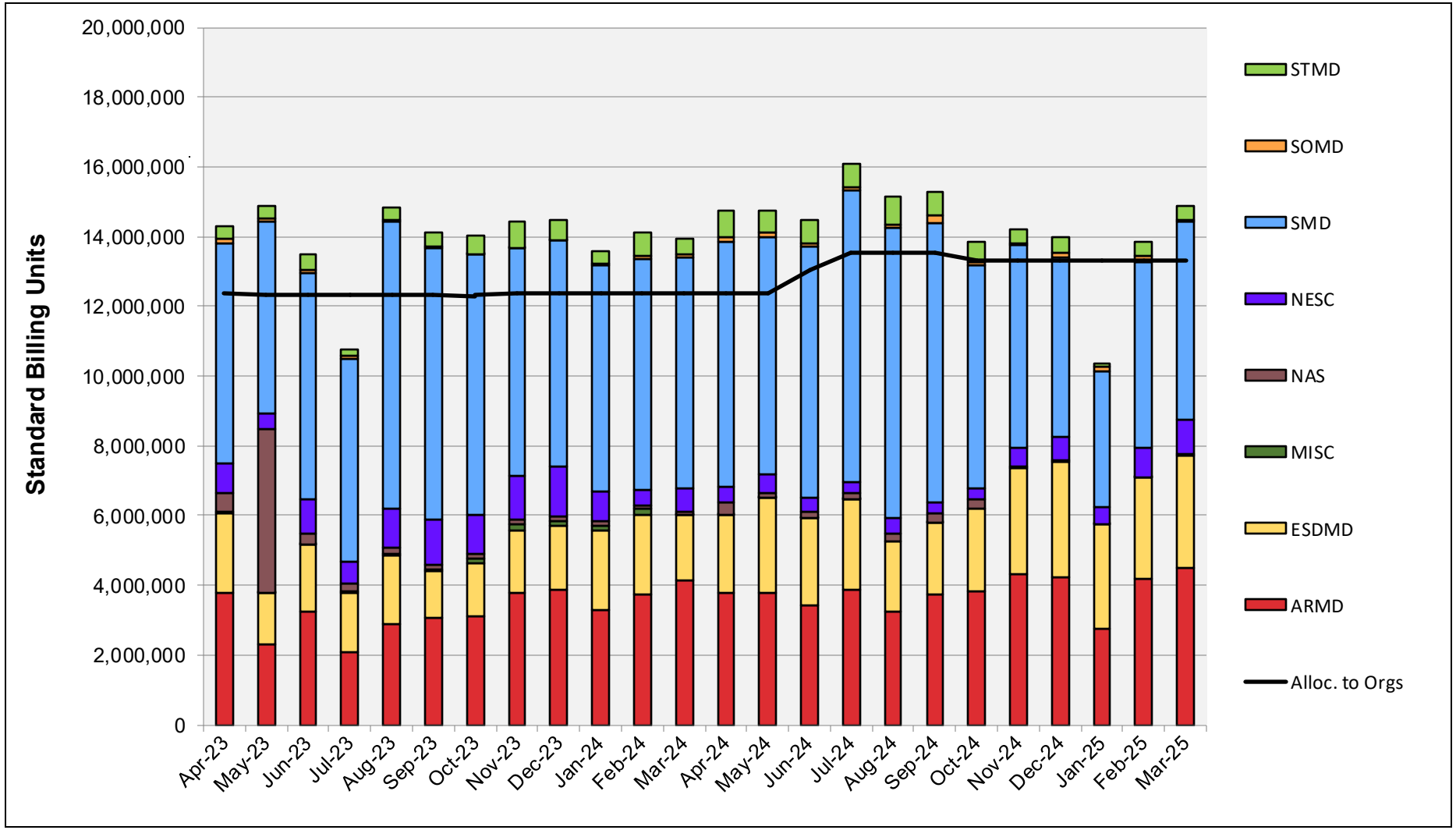
HECC Utilization



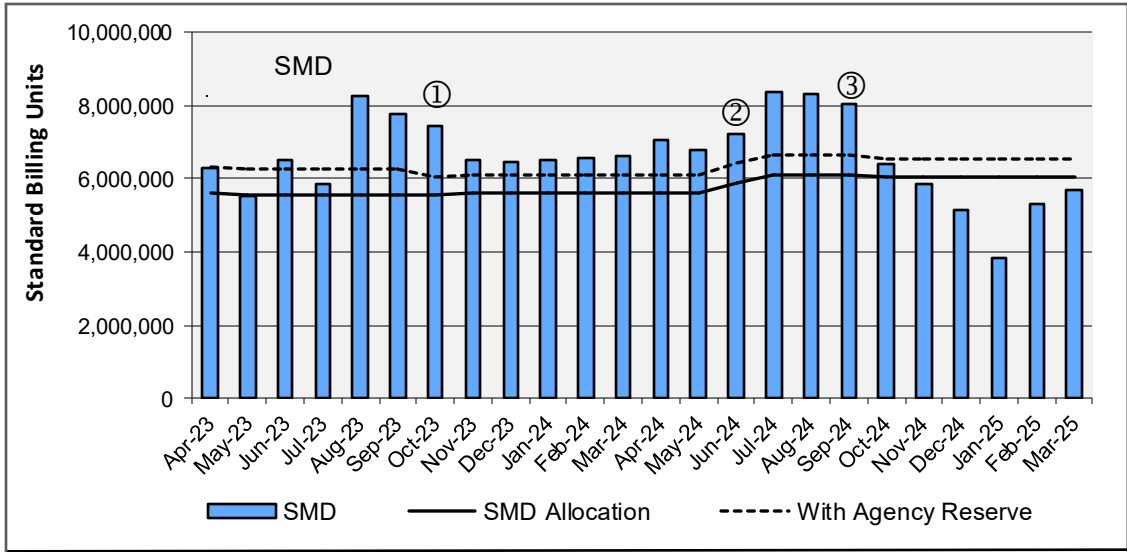
HECC Utilization Normalized to 30-Day Month

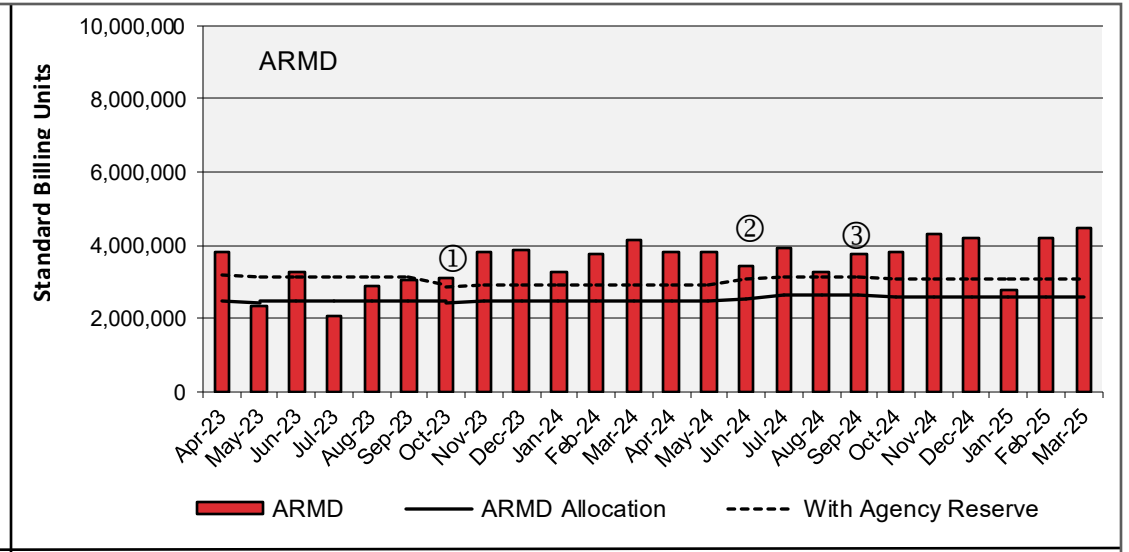


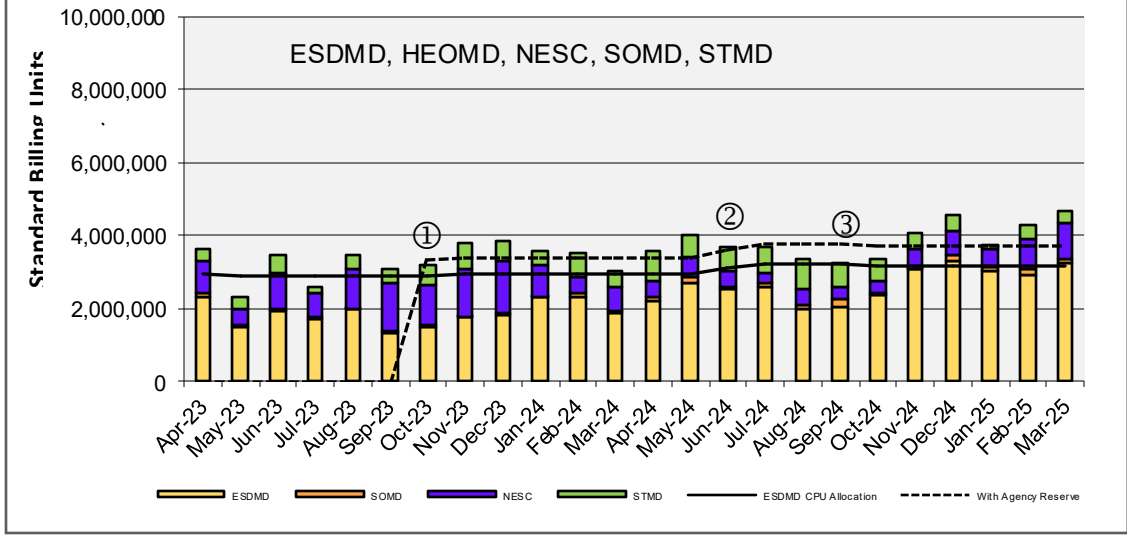
CPU Only Normalized Data



CPU Only by Mission Directorate





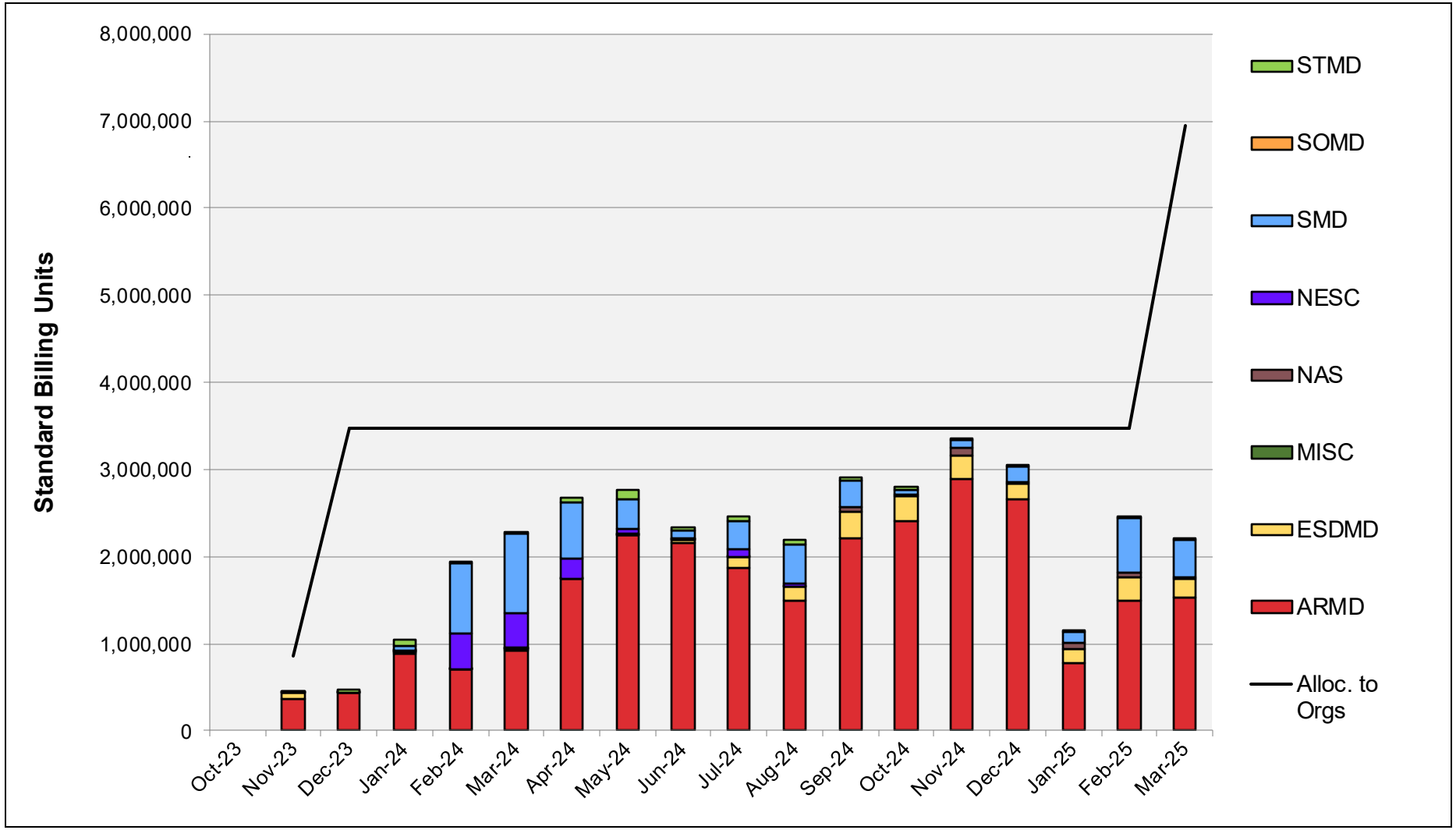


① 4 Rome Apollo Racks added to Aitken

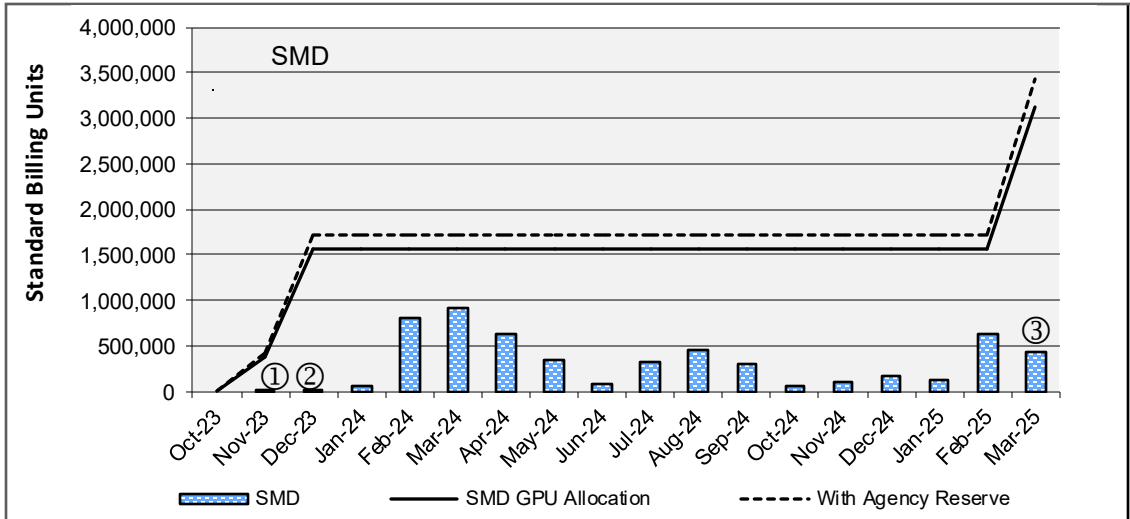
② Aitken Milan nodes added

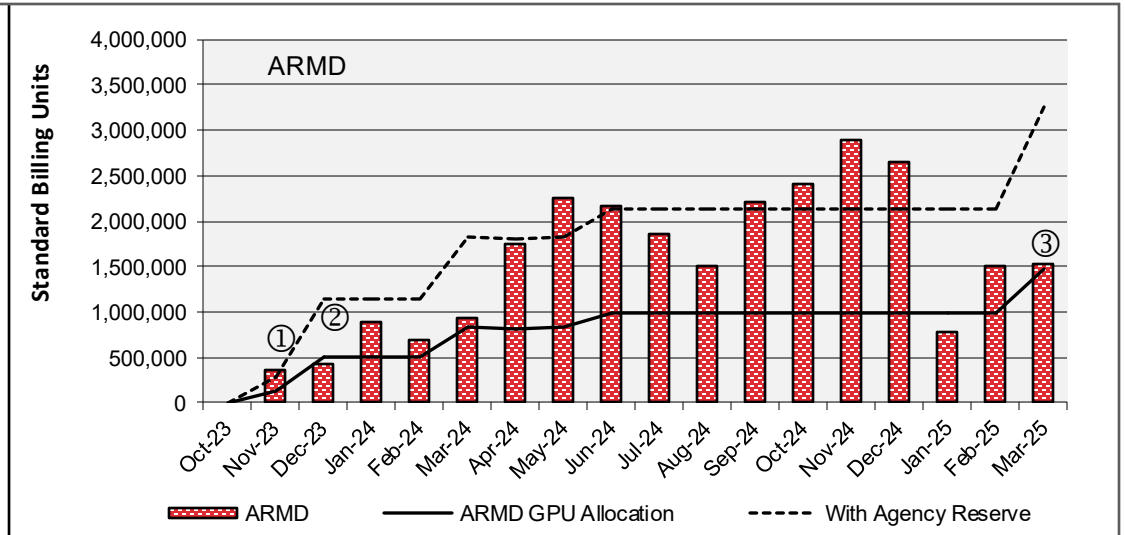
③ Sandy Bridge temporarily removed

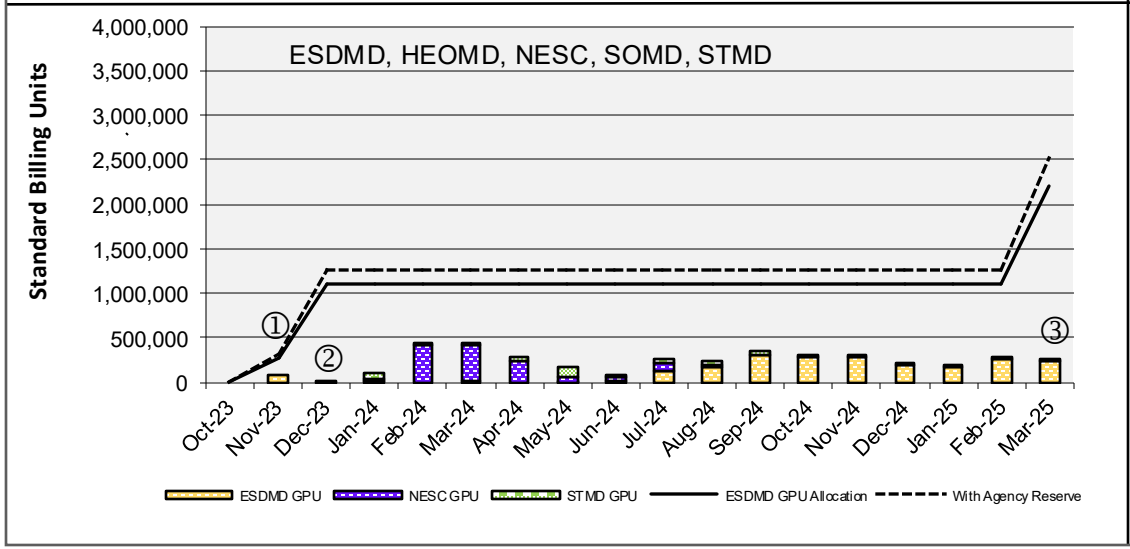
GPU Only Normalized Data



GPU Only Normalized Data





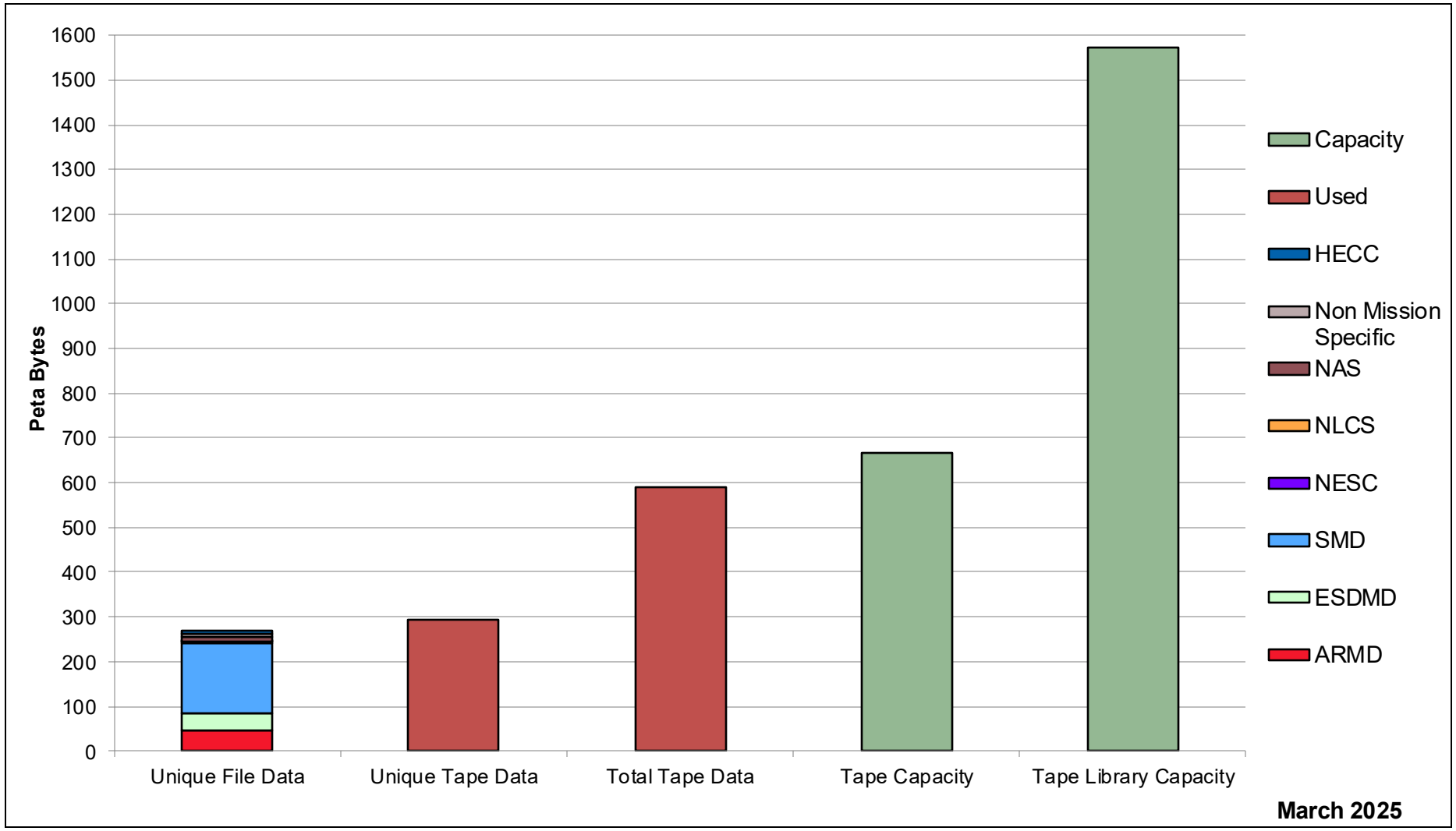


① Cabeus v100 nodes added

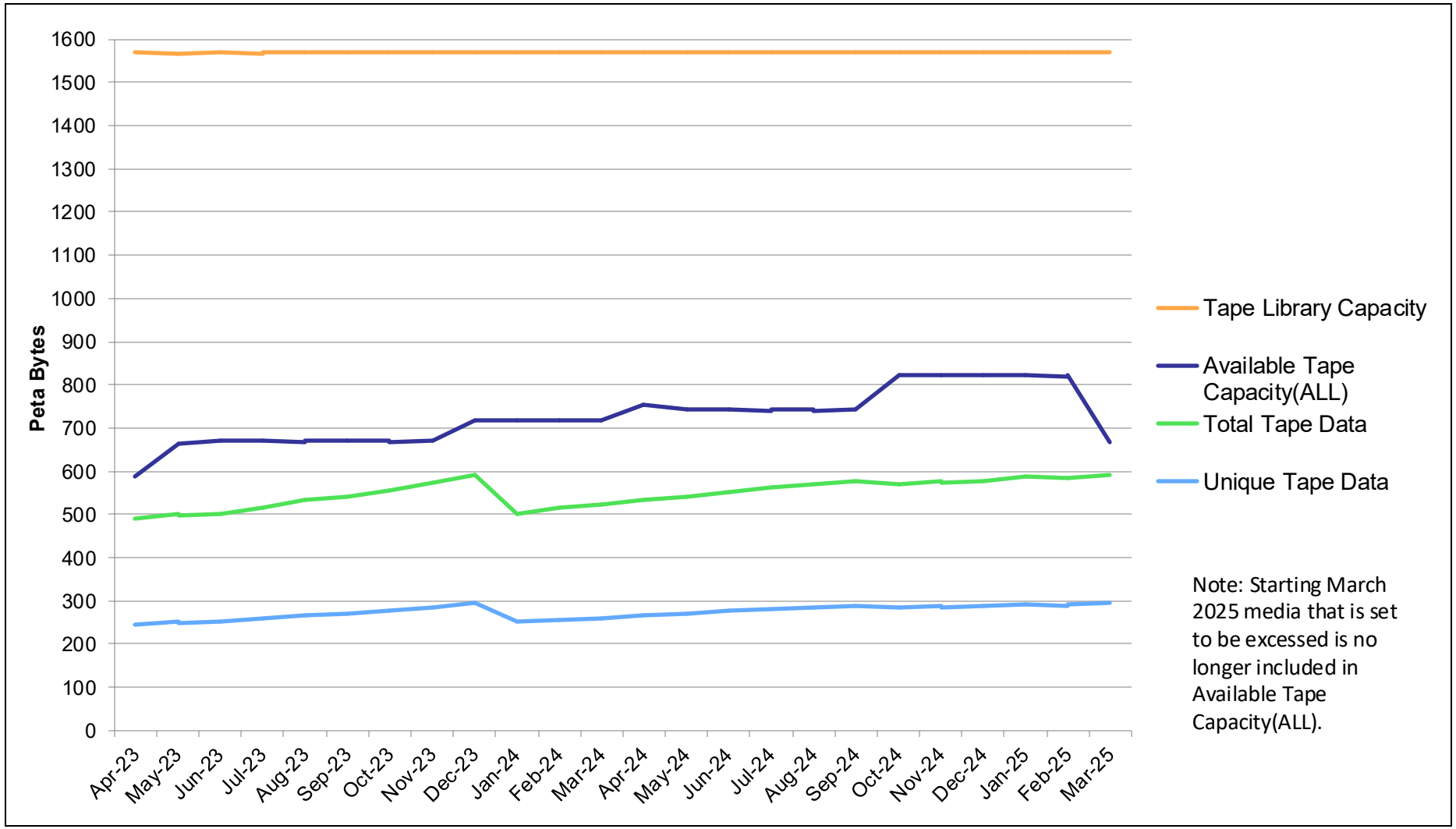
② Cabeus a100 nodes added

③ Cabeus Grace Hopper nodes added

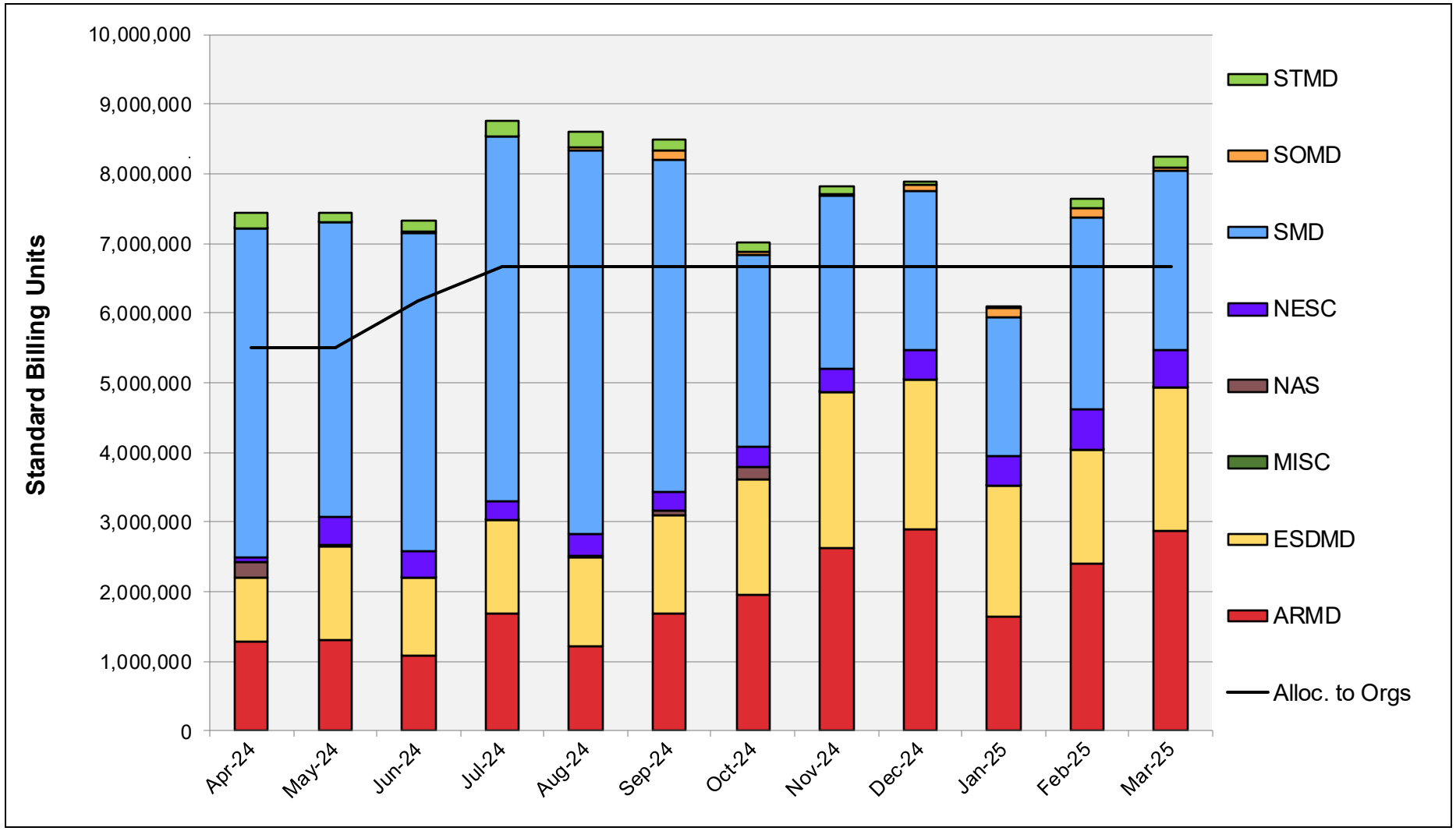
Tape Archive Status



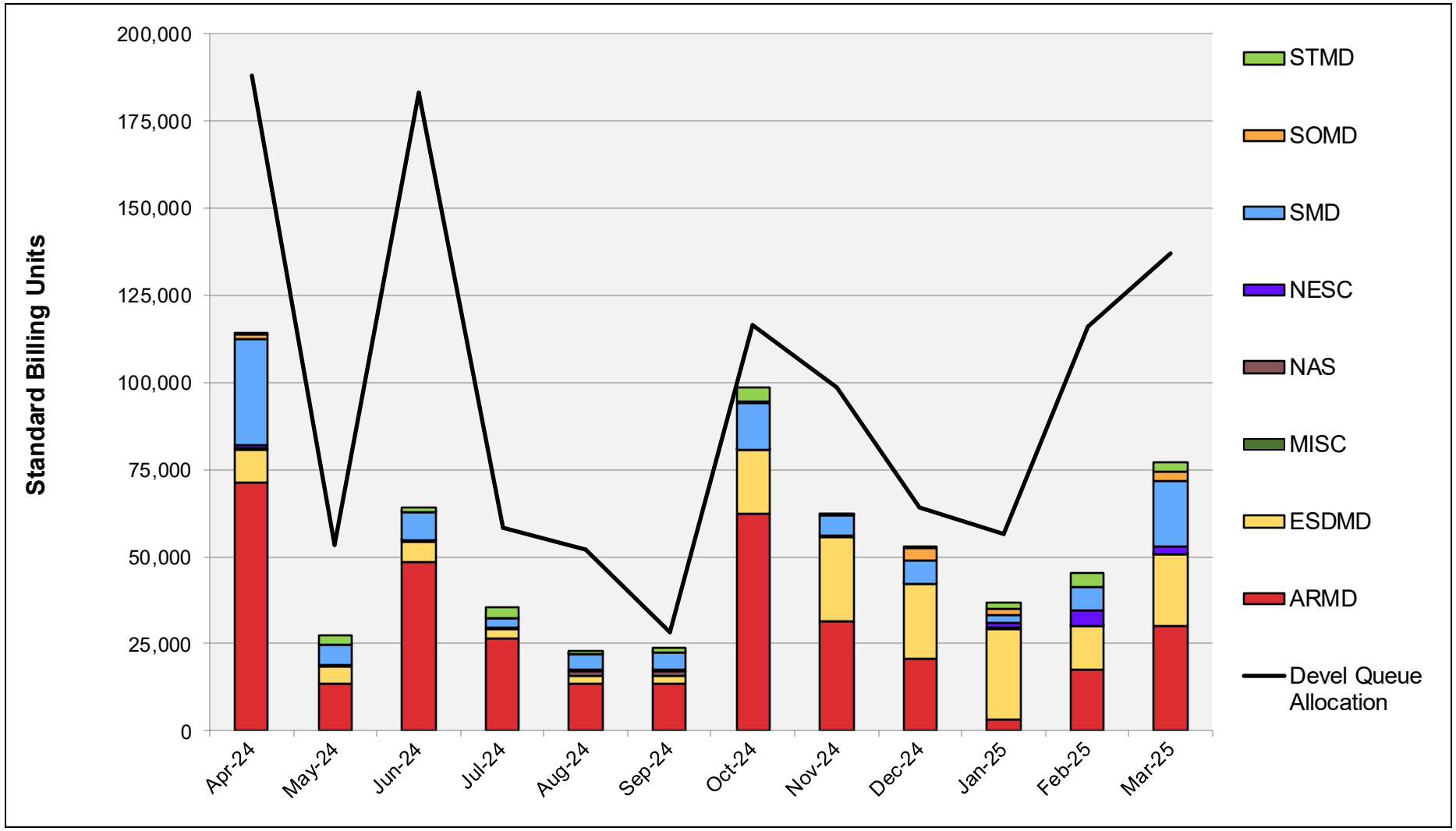
Tape Archive Status



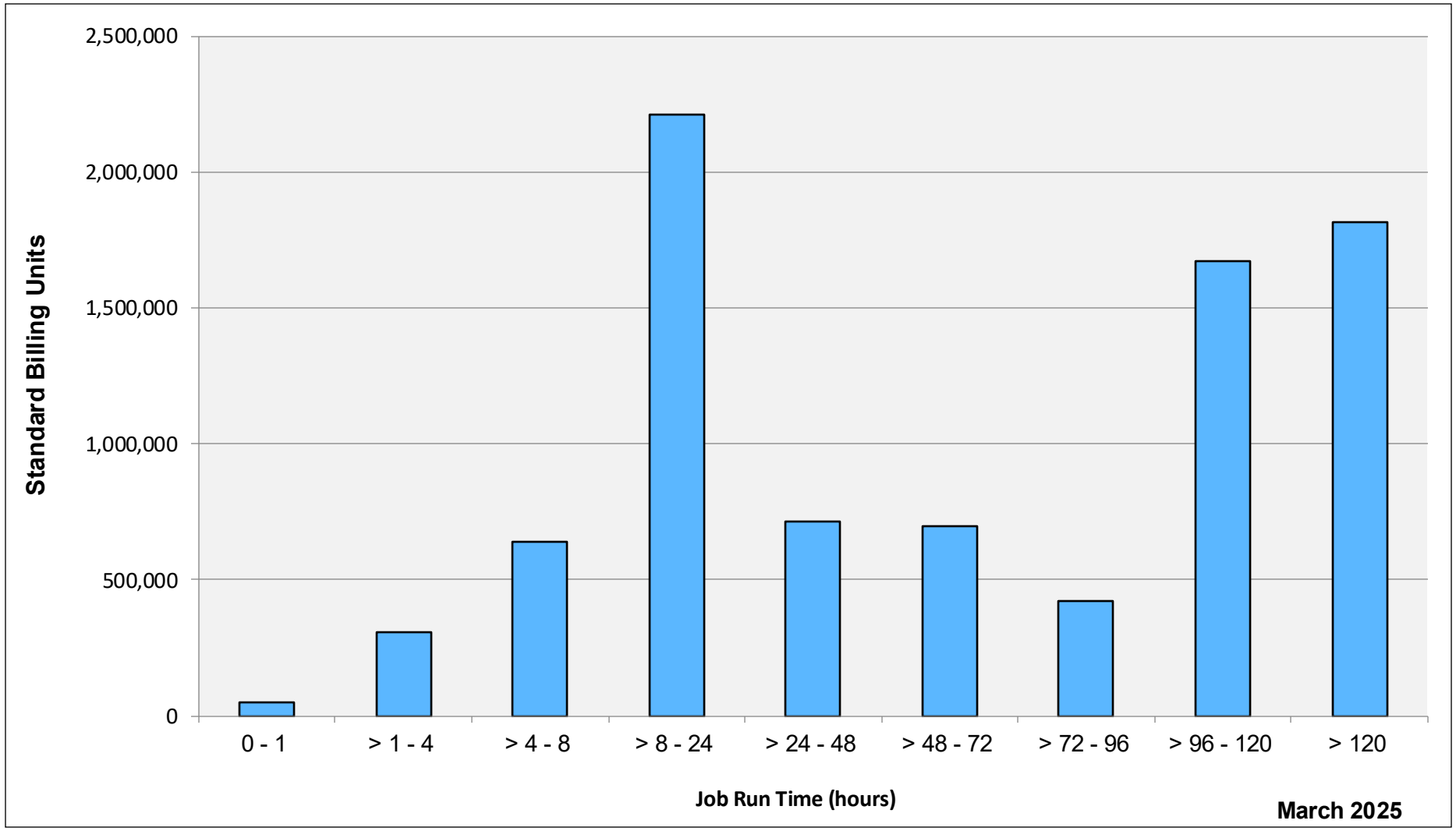
Aitken: SBUs Reported, Normalized to 30-Day Month



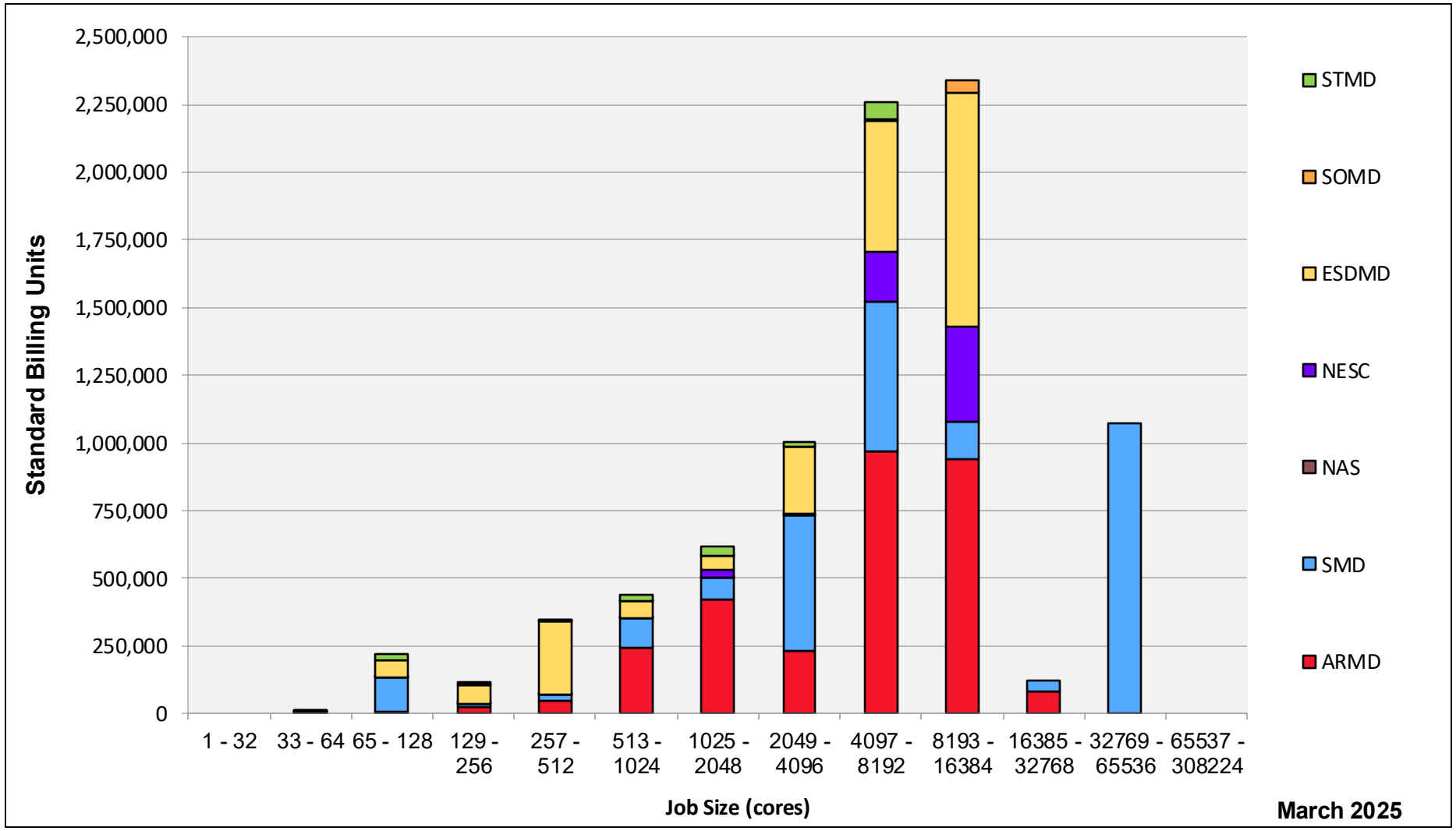
Aitken: Devel Queue Utilization



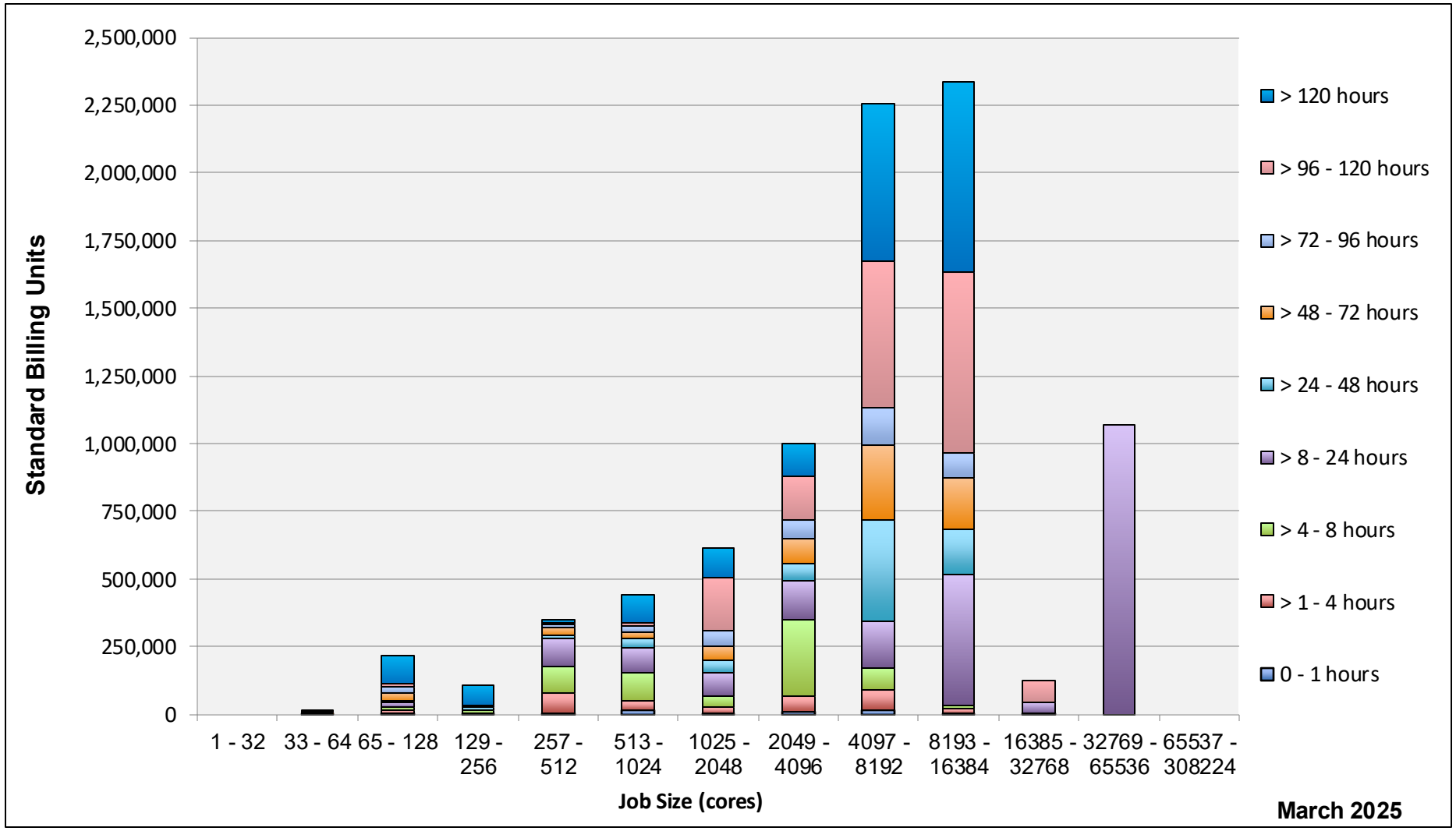
Aitken: Monthly Utilization by Job Length



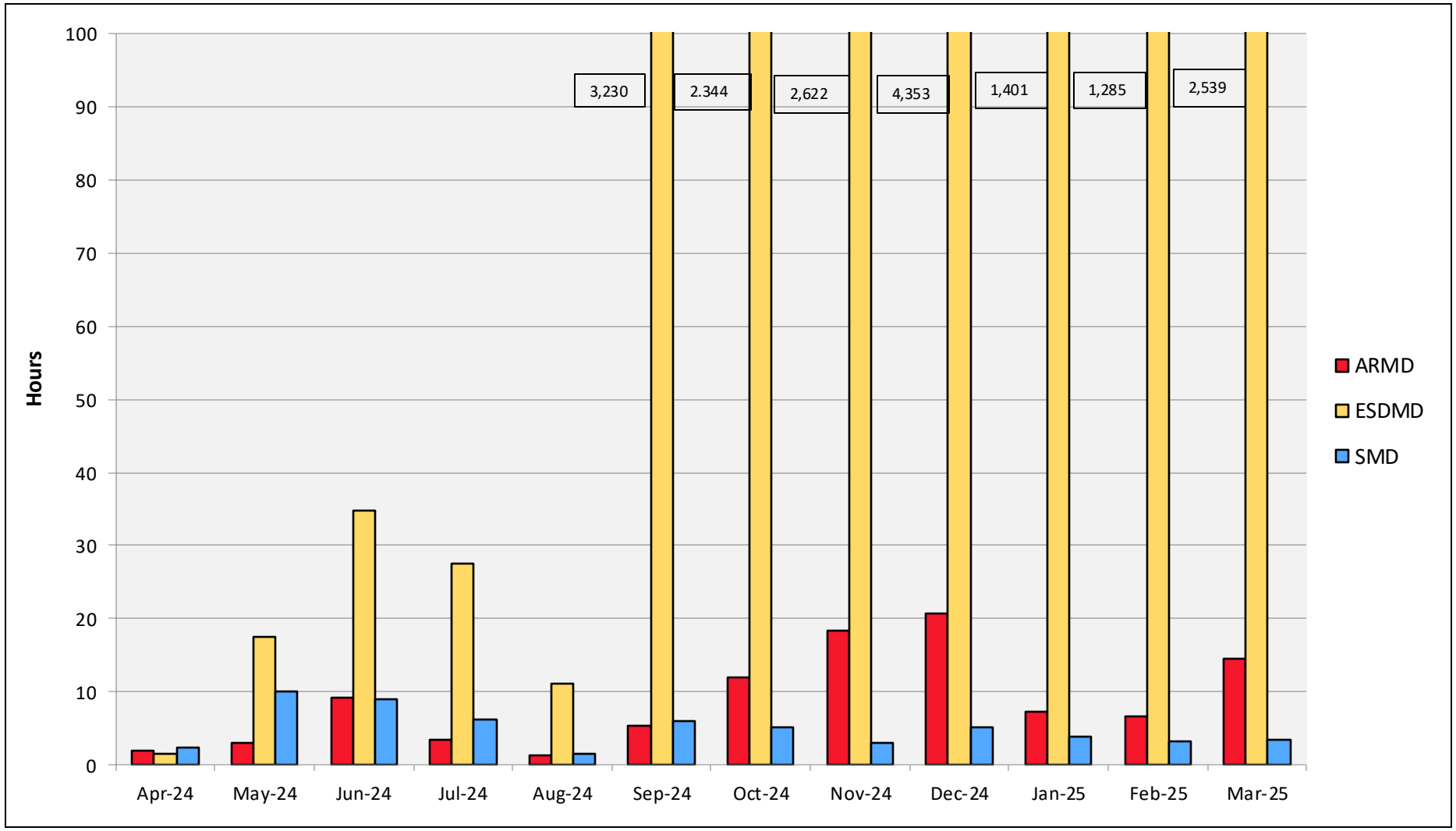
Aitken: Monthly Utilization by Job Size



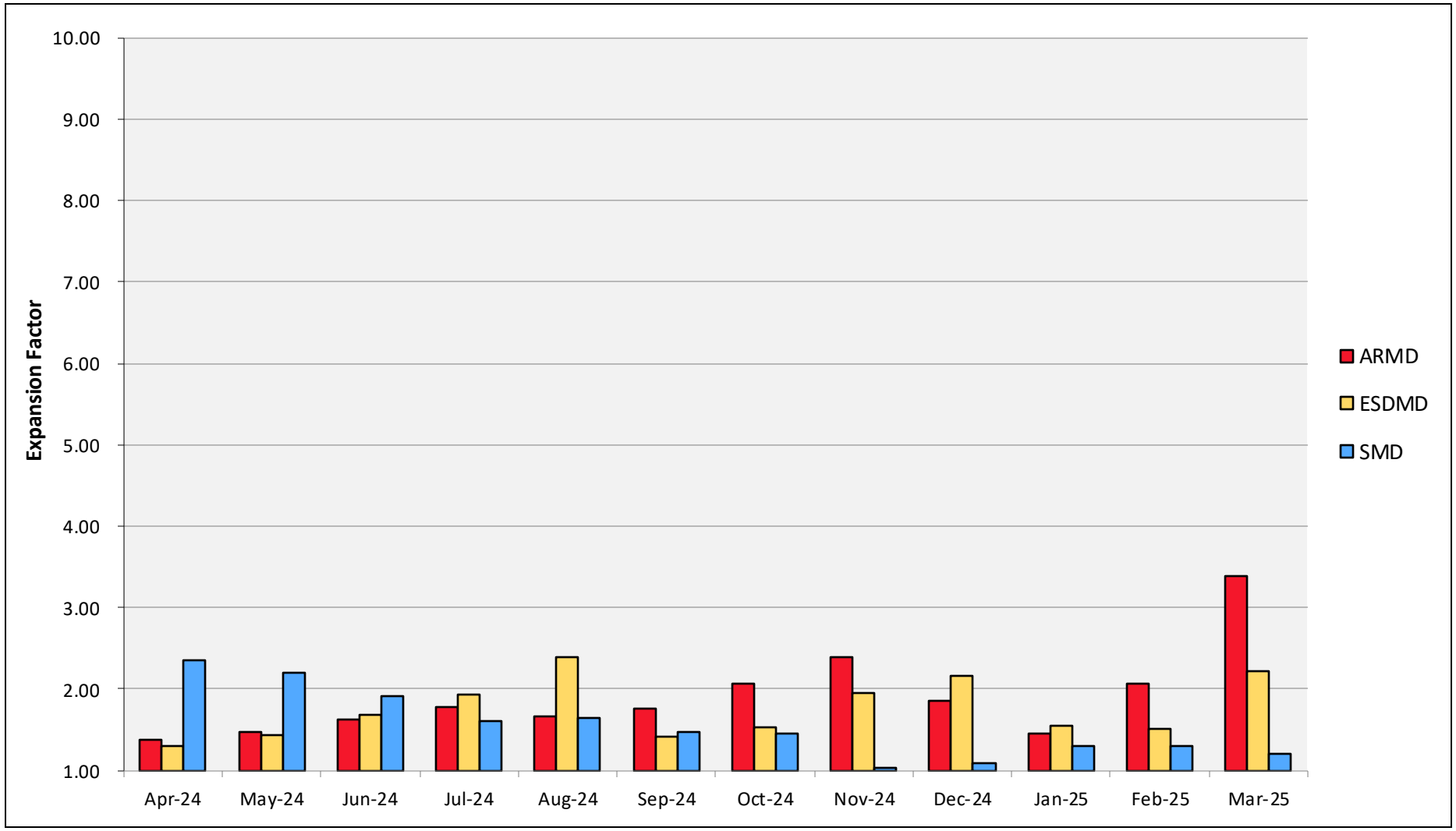
Aitken: Monthly Utilization by Size and Length



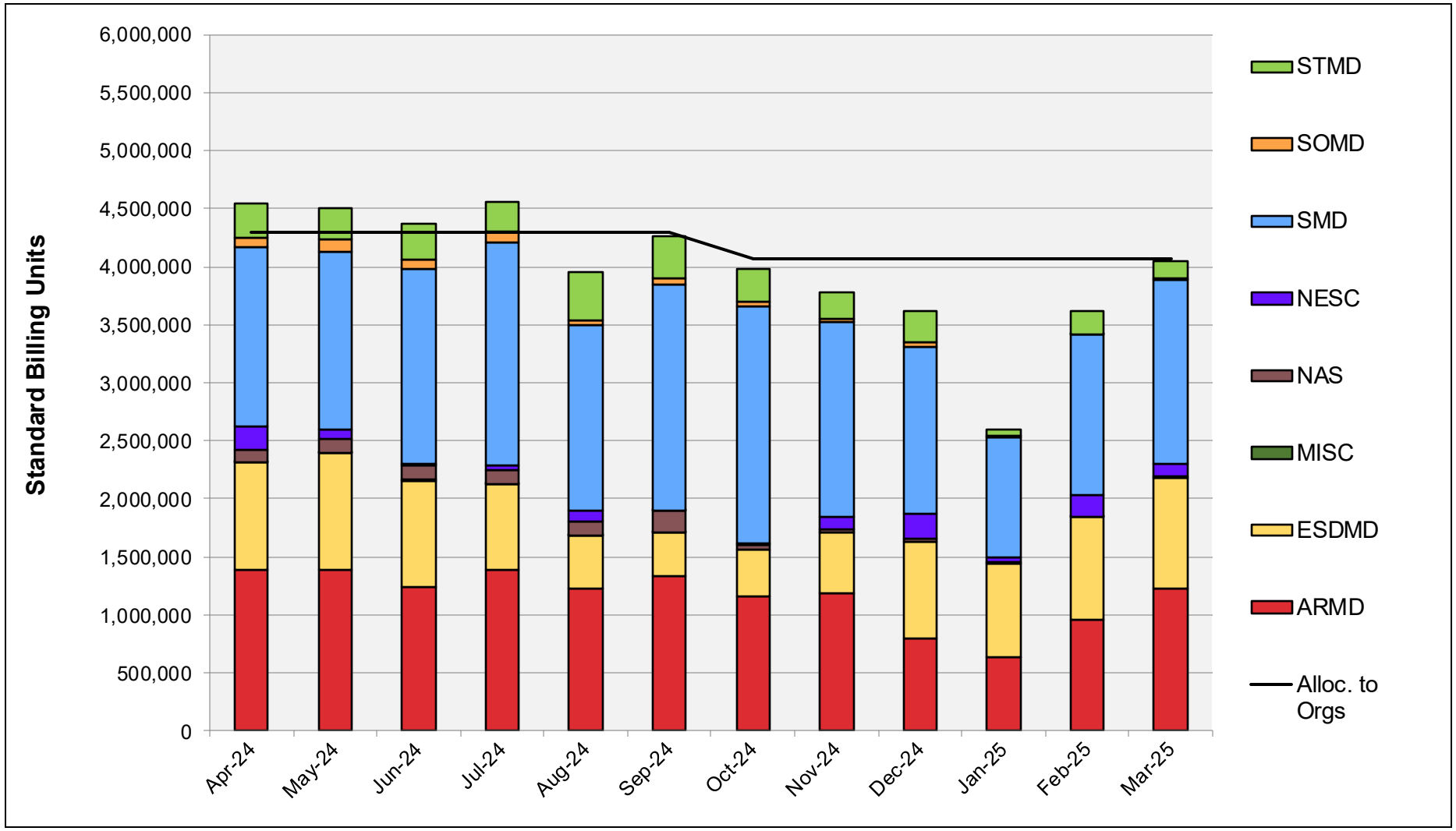
Aitken: Average Time to Clear All Jobs



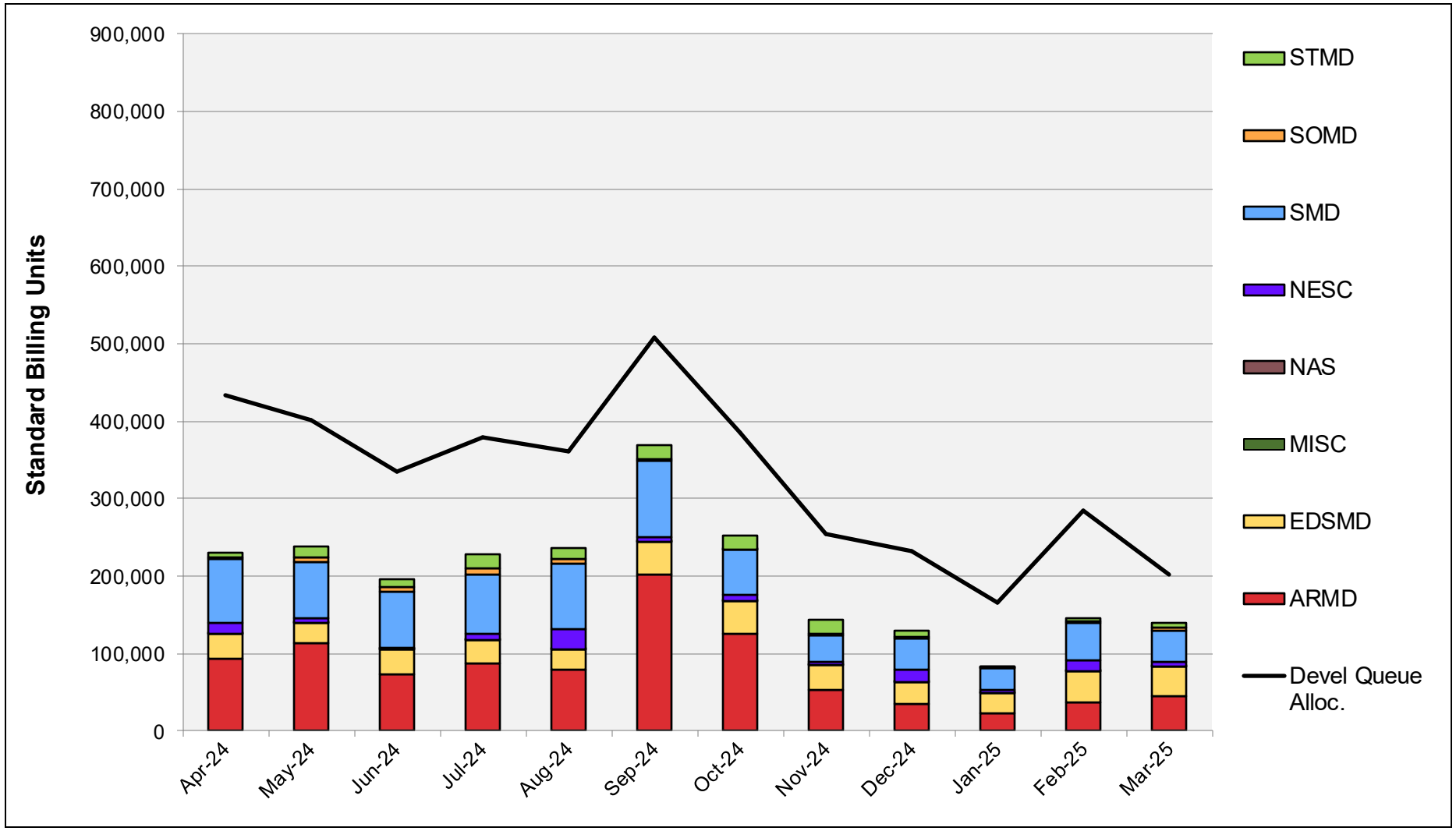
Aitken: Average Expansion Factor



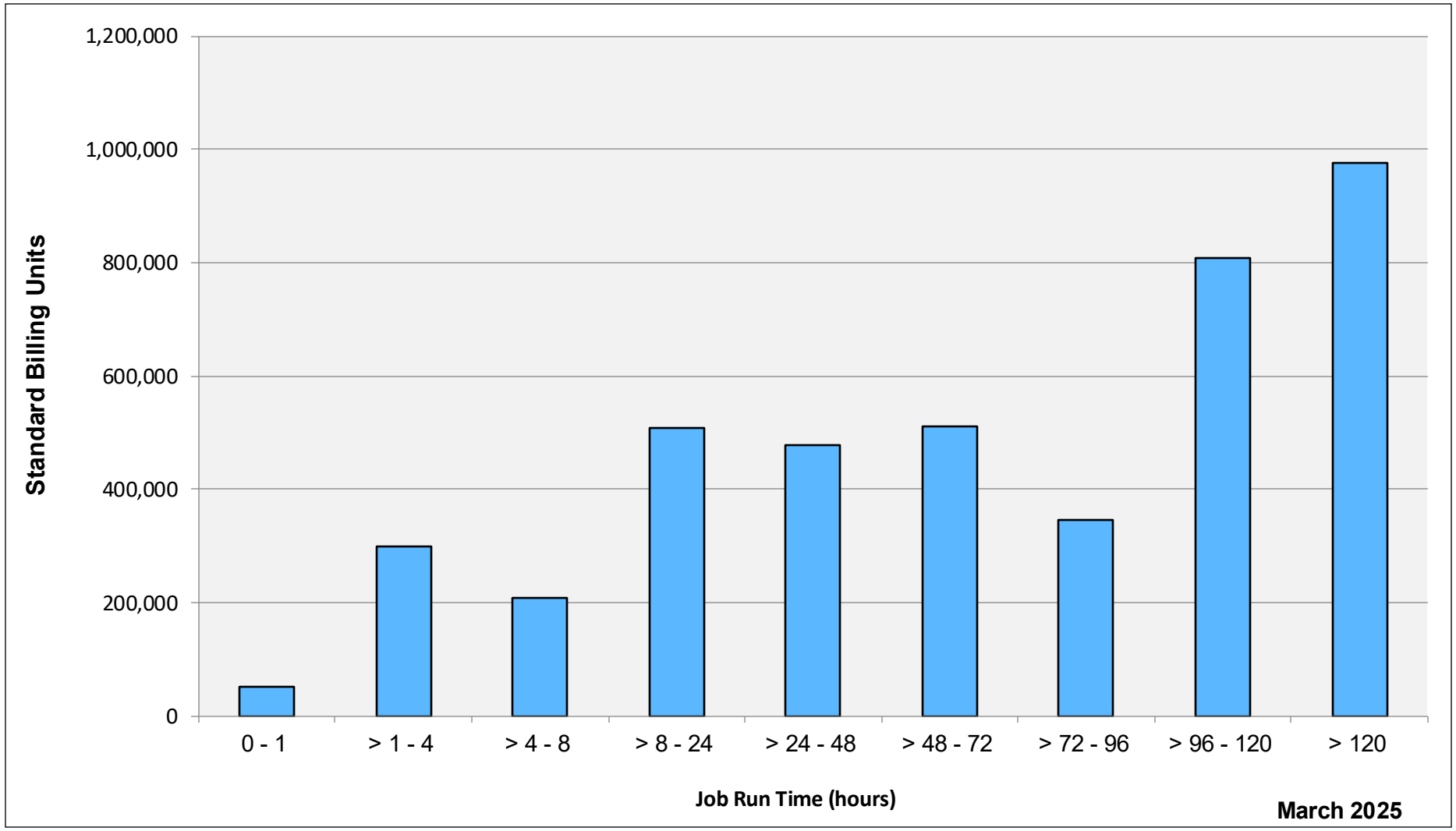
Pleiades: SBUs Reported, Normalized to 30-Day Month



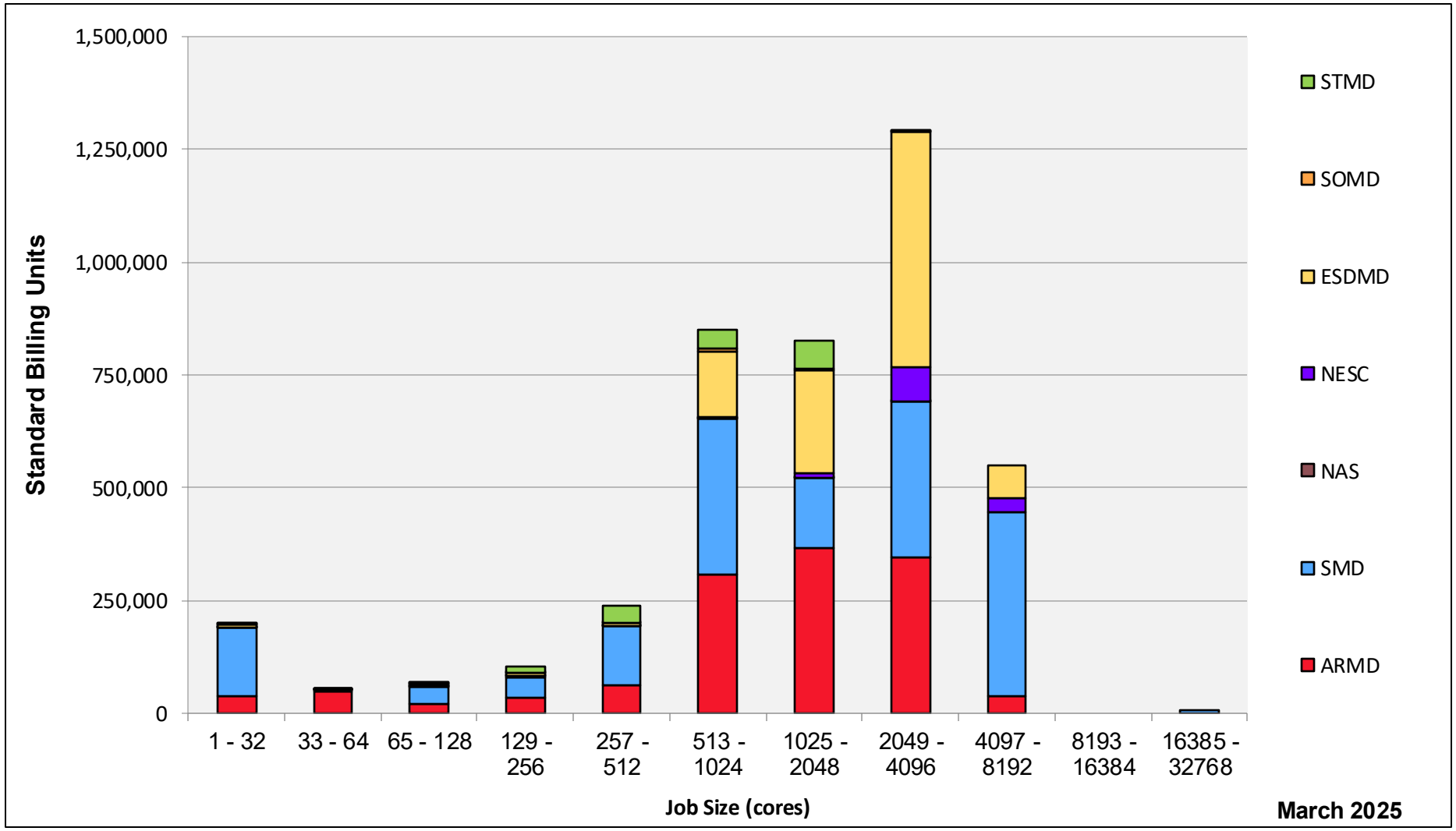
Pleiades: Devel Queue Utilization



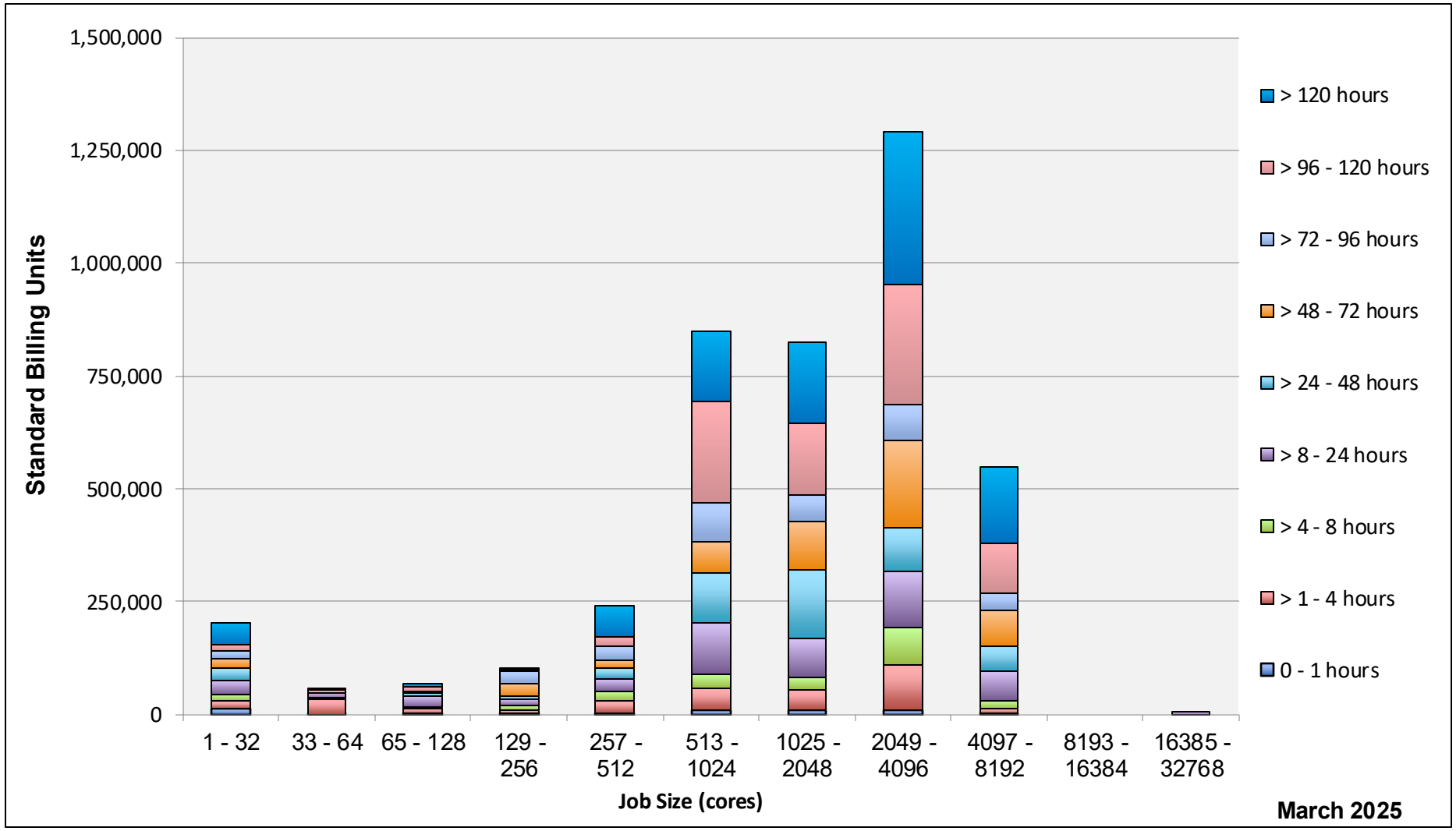
Pleiades: Monthly Utilization by Job Length



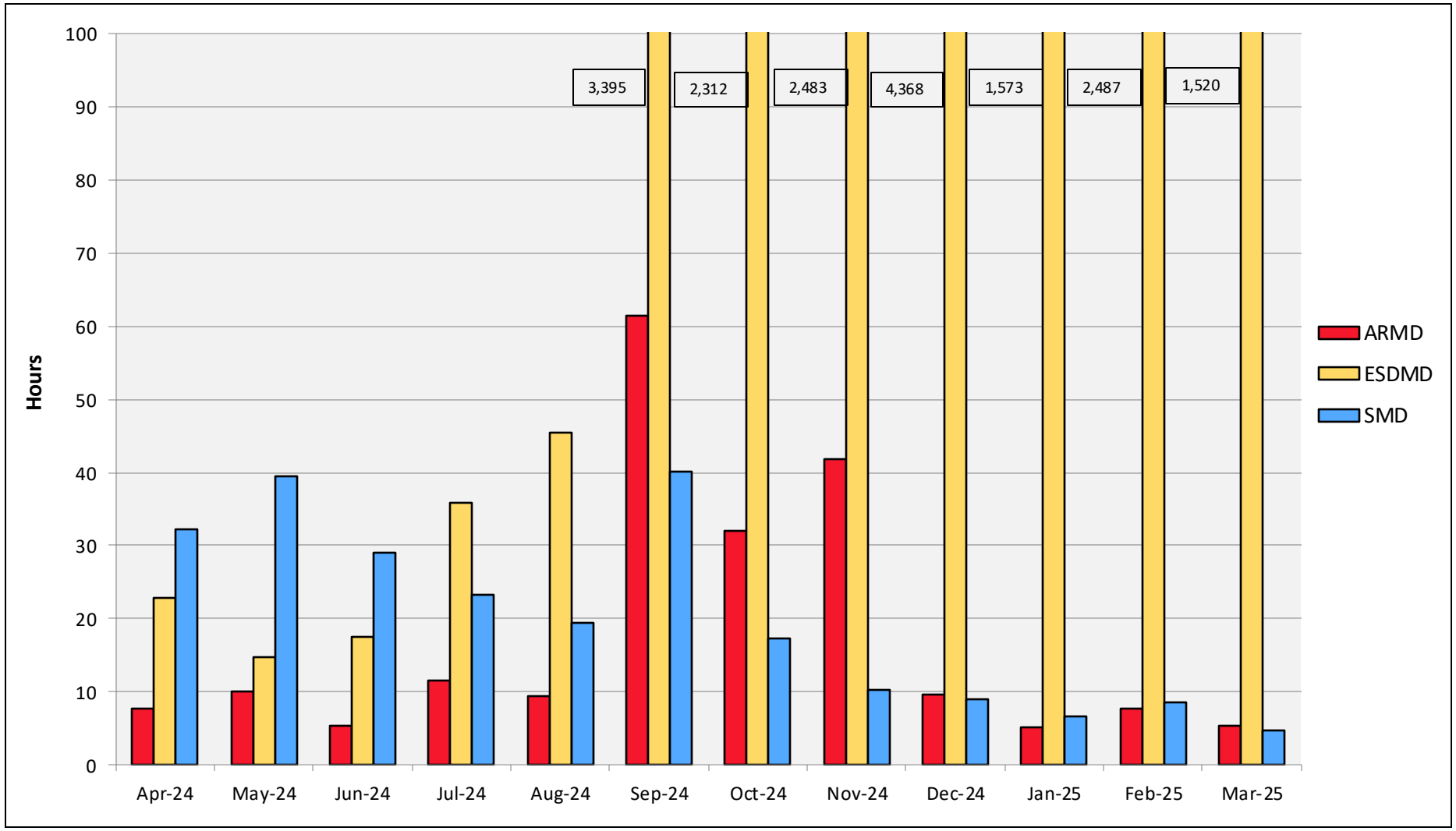
Pleiades: Monthly Utilization by Job Size



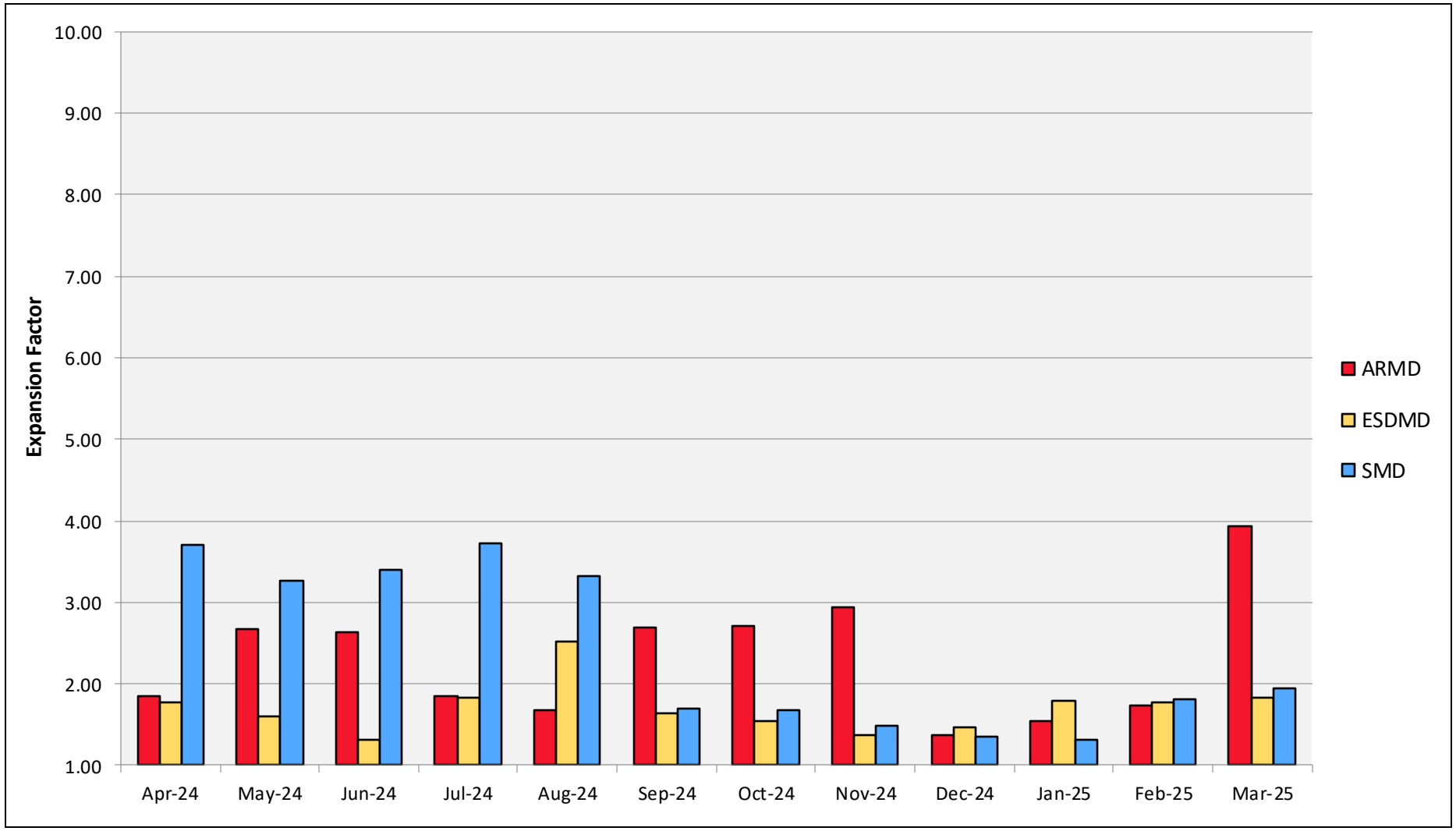
Pleiades: Monthly Utilization by Size and Length



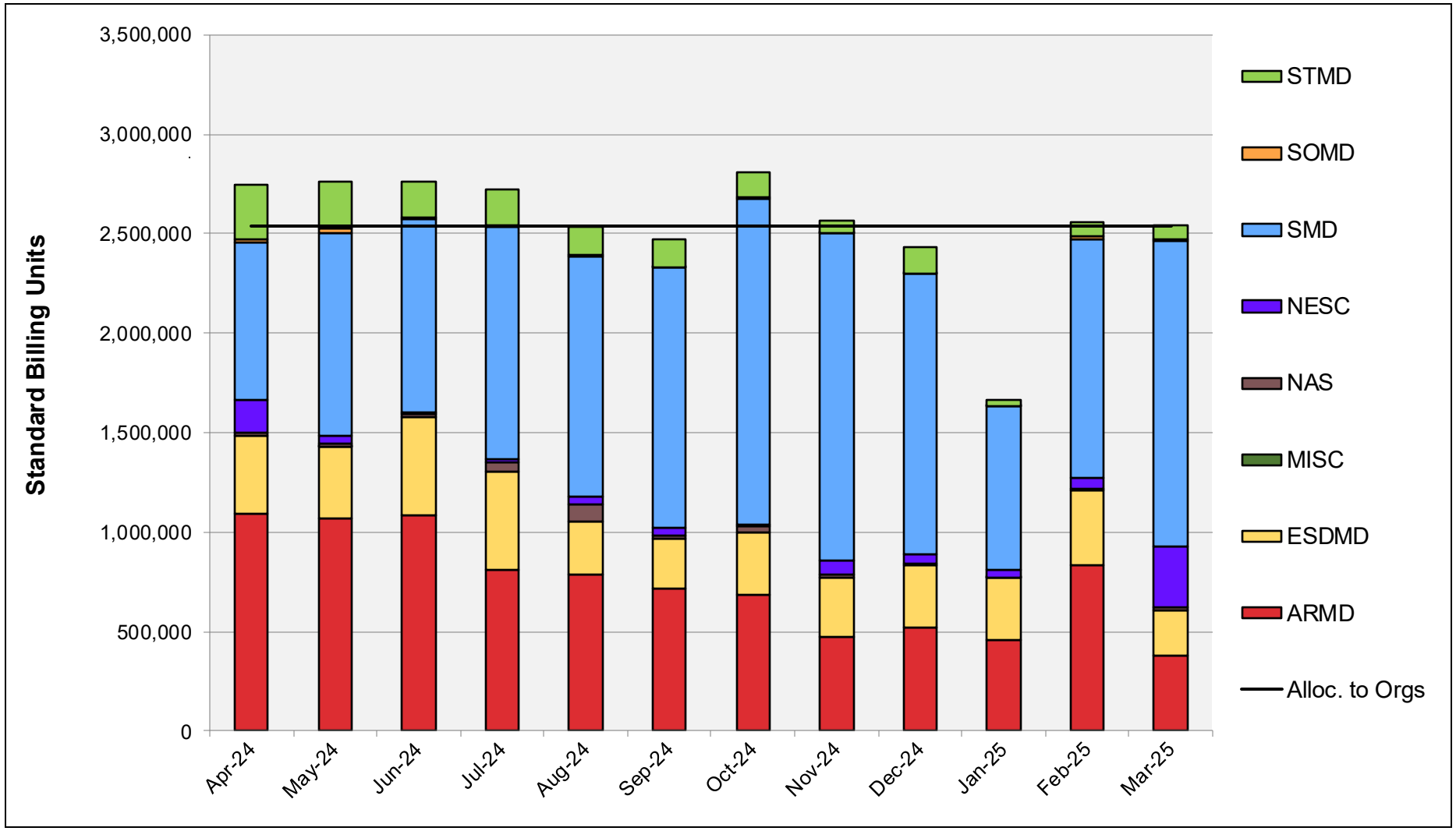
Pleiades: Average Time to Clear All Jobs



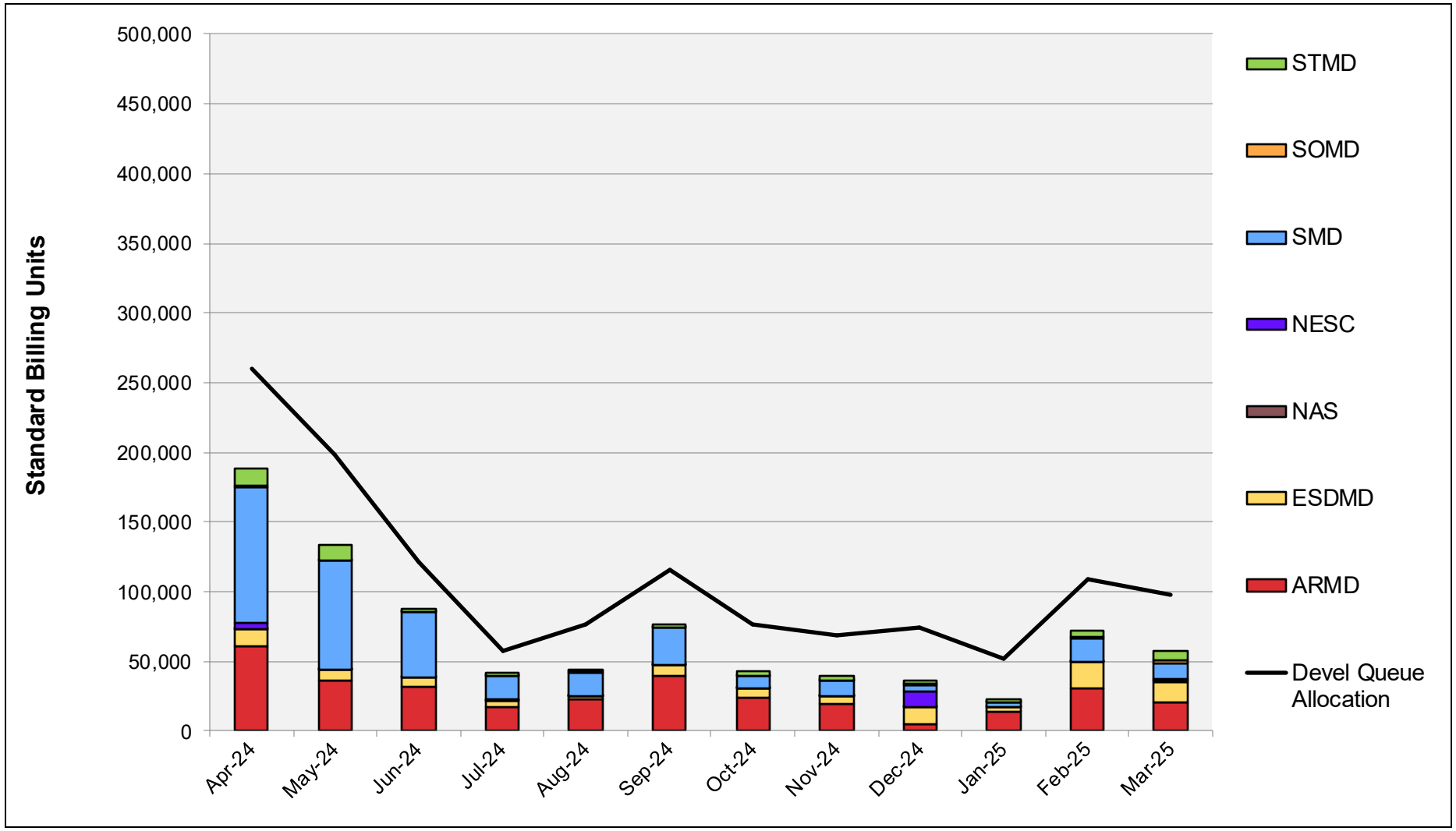
Pleiades: Average Expansion Factor



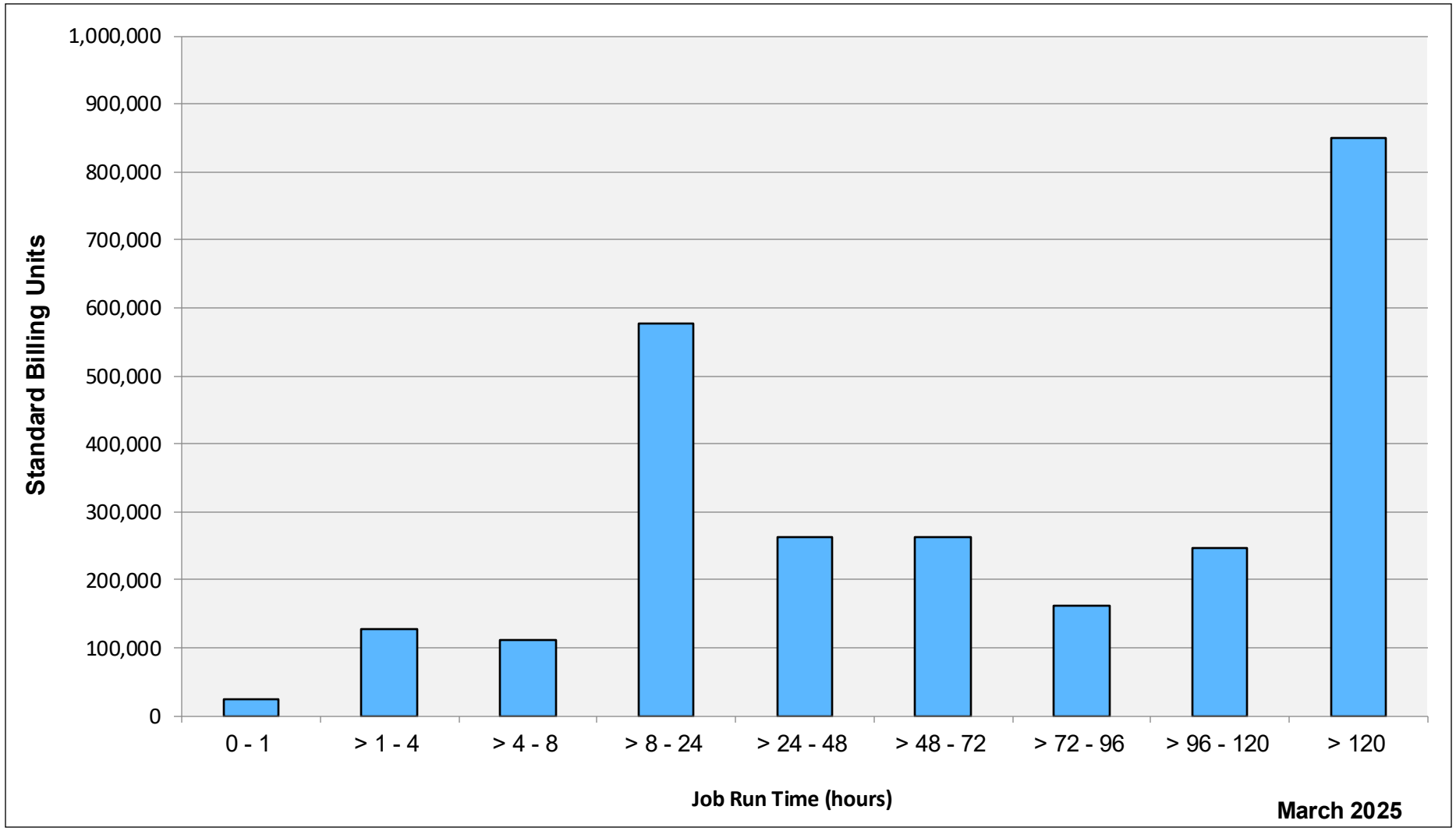
Electra: SBUs Reported, Normalized to 30-Day Month



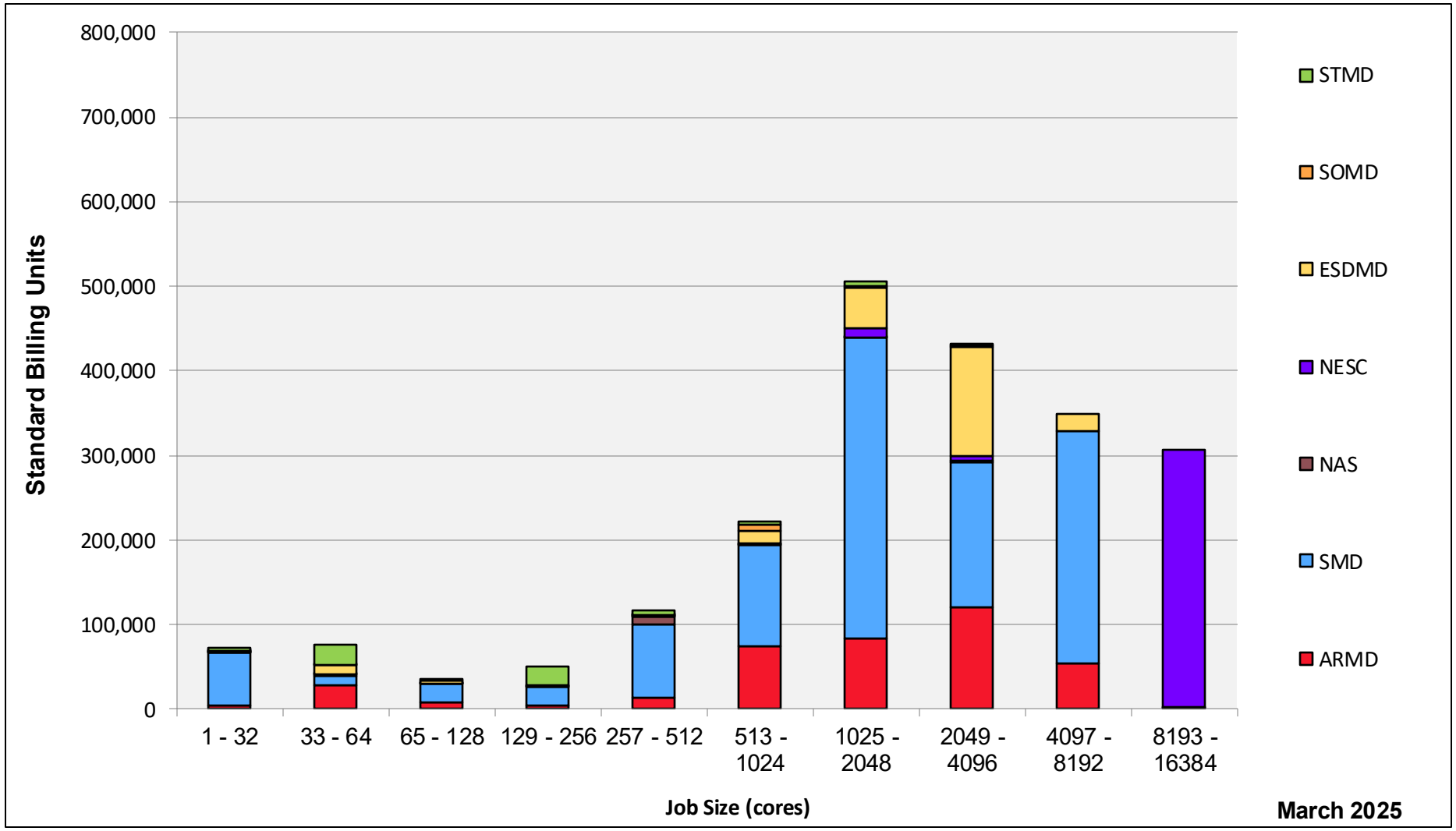
Electra: Devel Queue Utilization



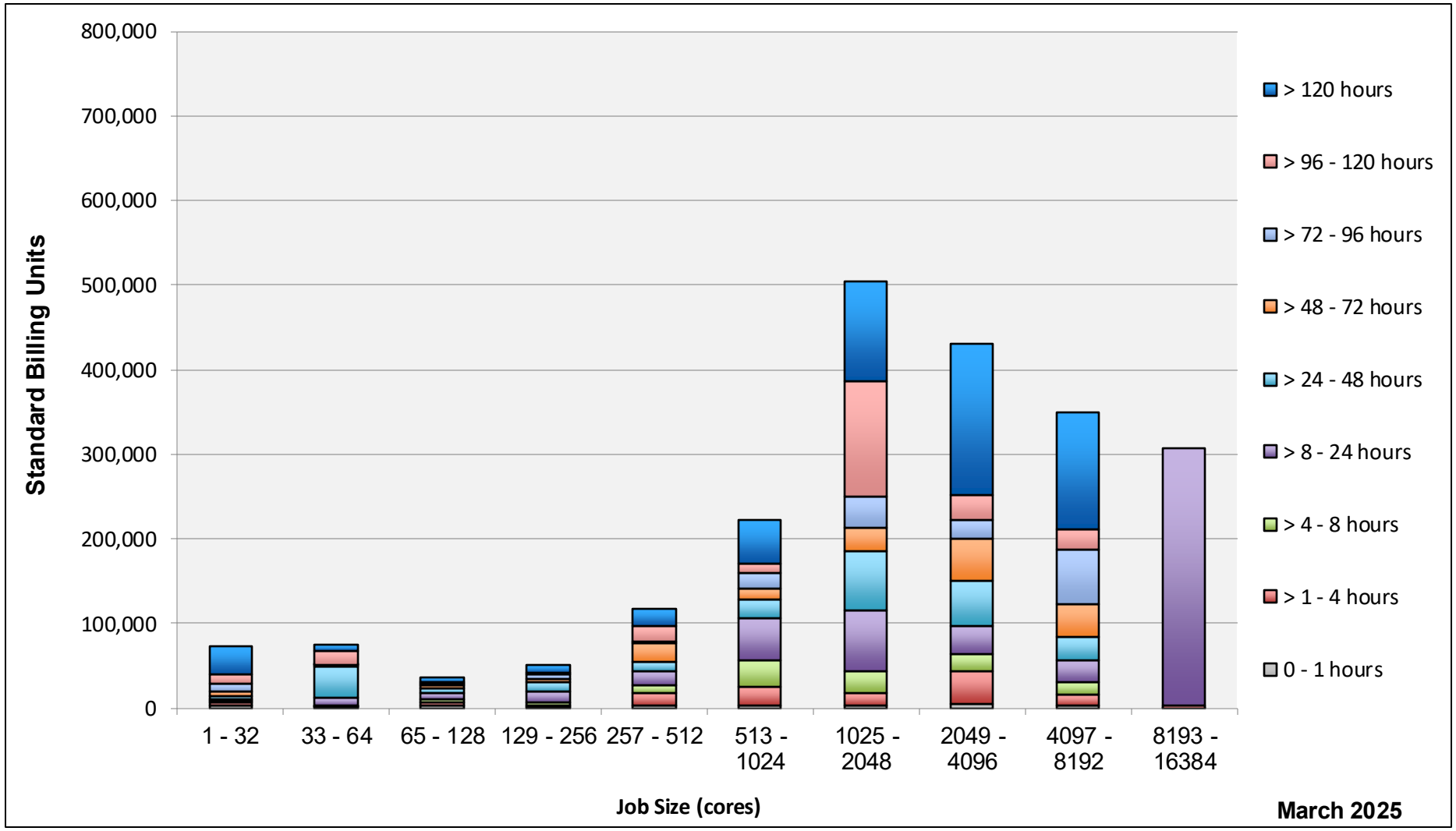
Electra: Monthly Utilization by Job Length



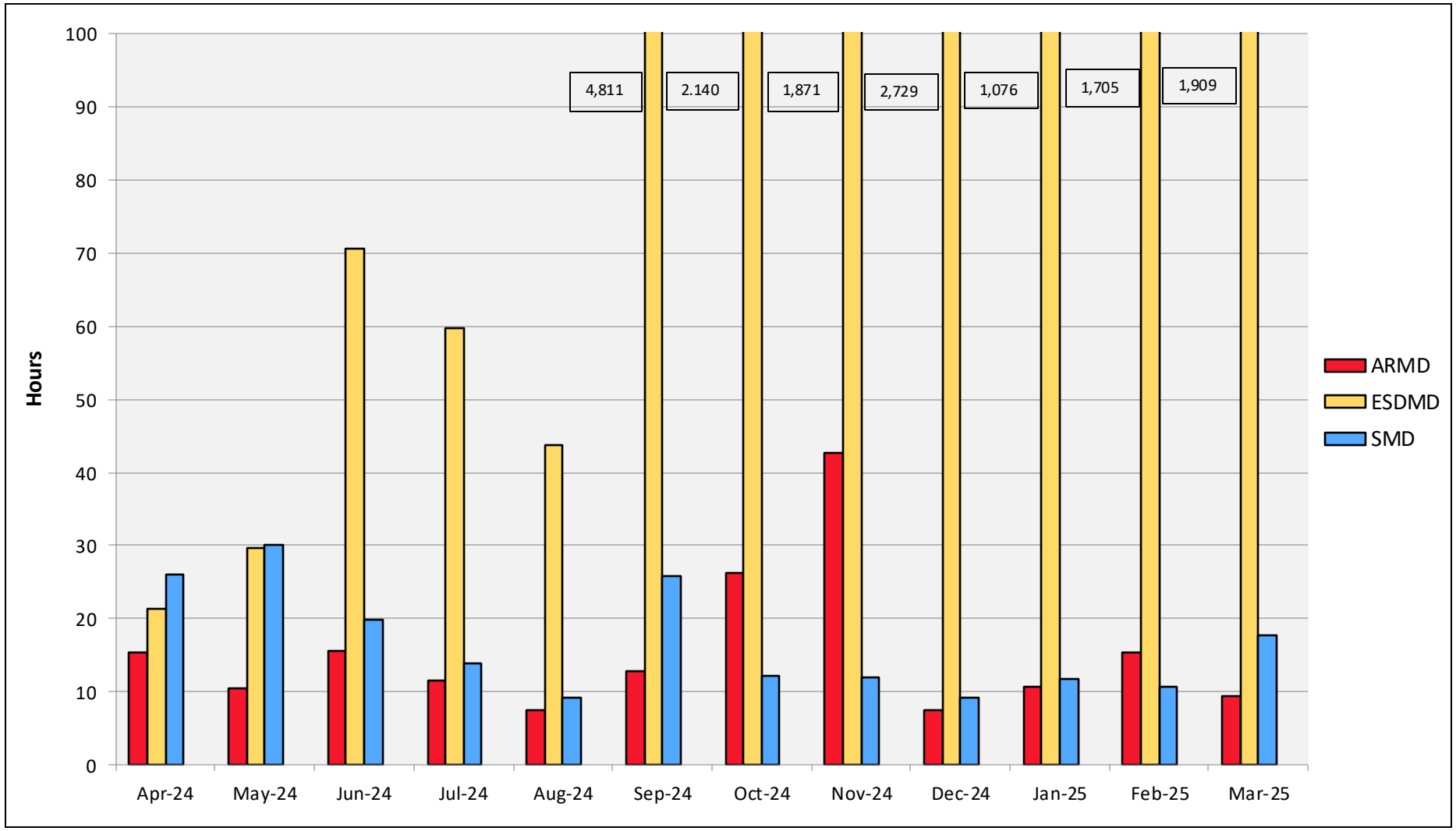
Electra: Monthly Utilization by Job Size



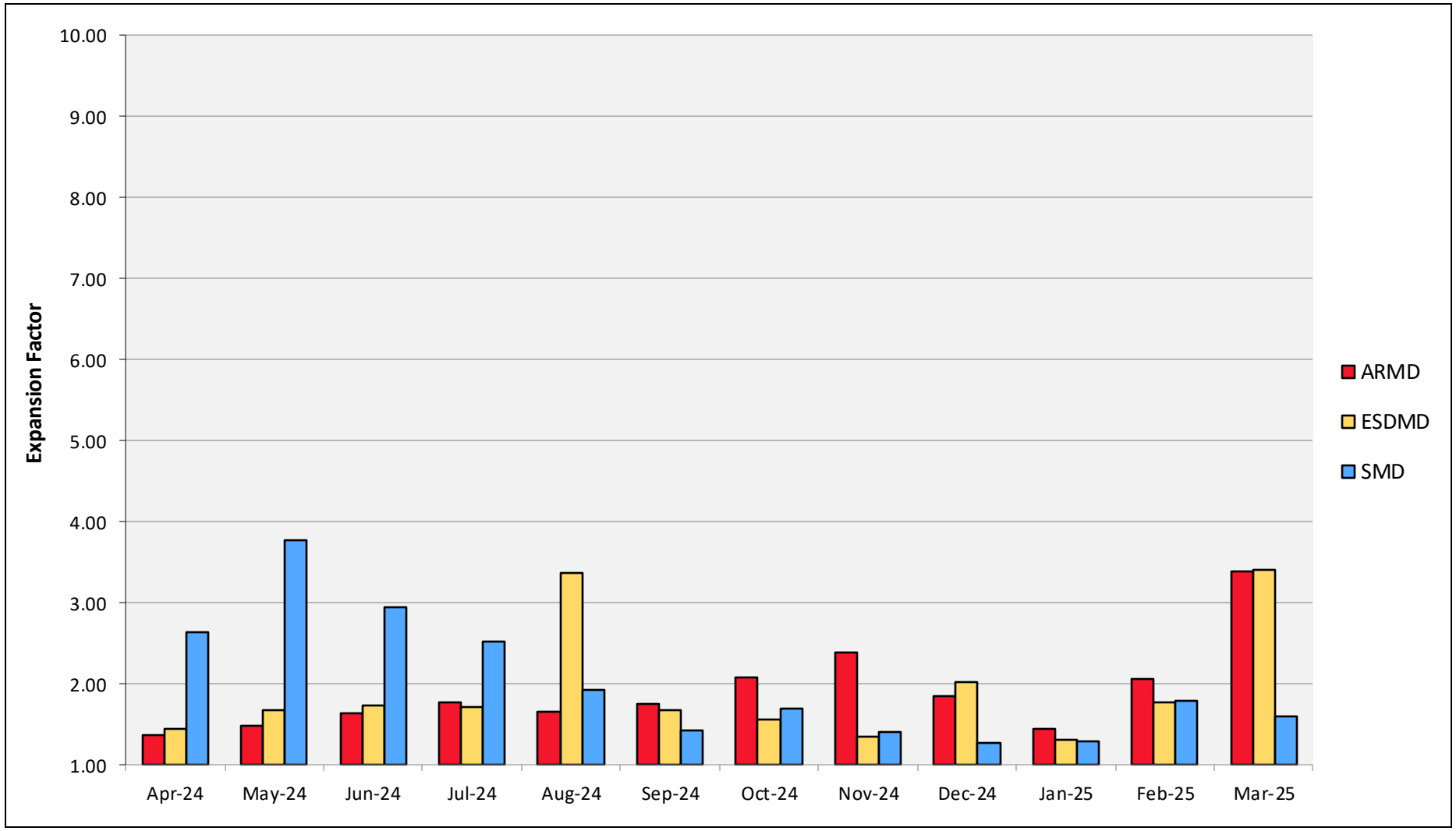
Electra: Monthly Utilization by Size and Length



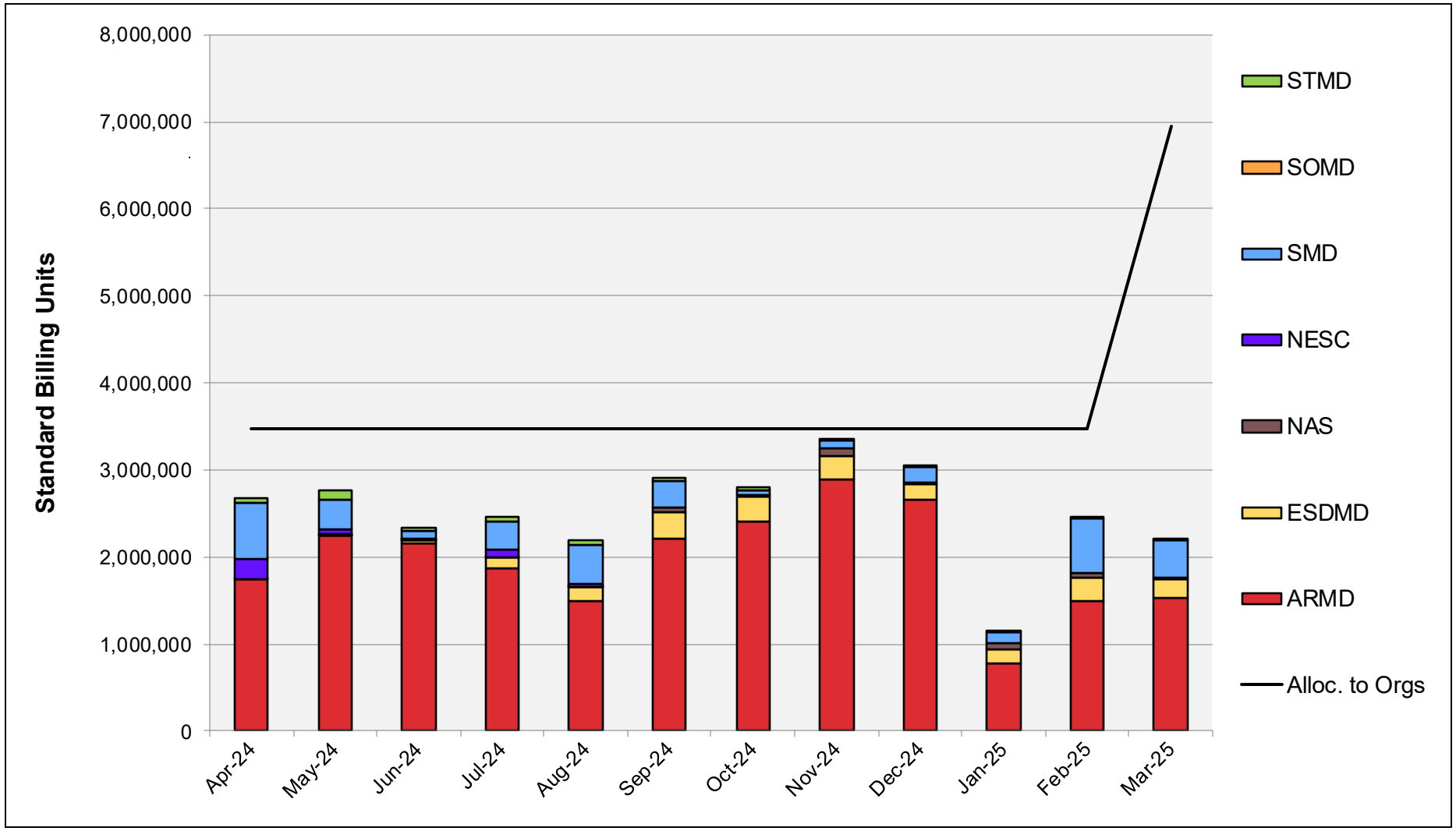
Electra: Average Time to Clear All Jobs



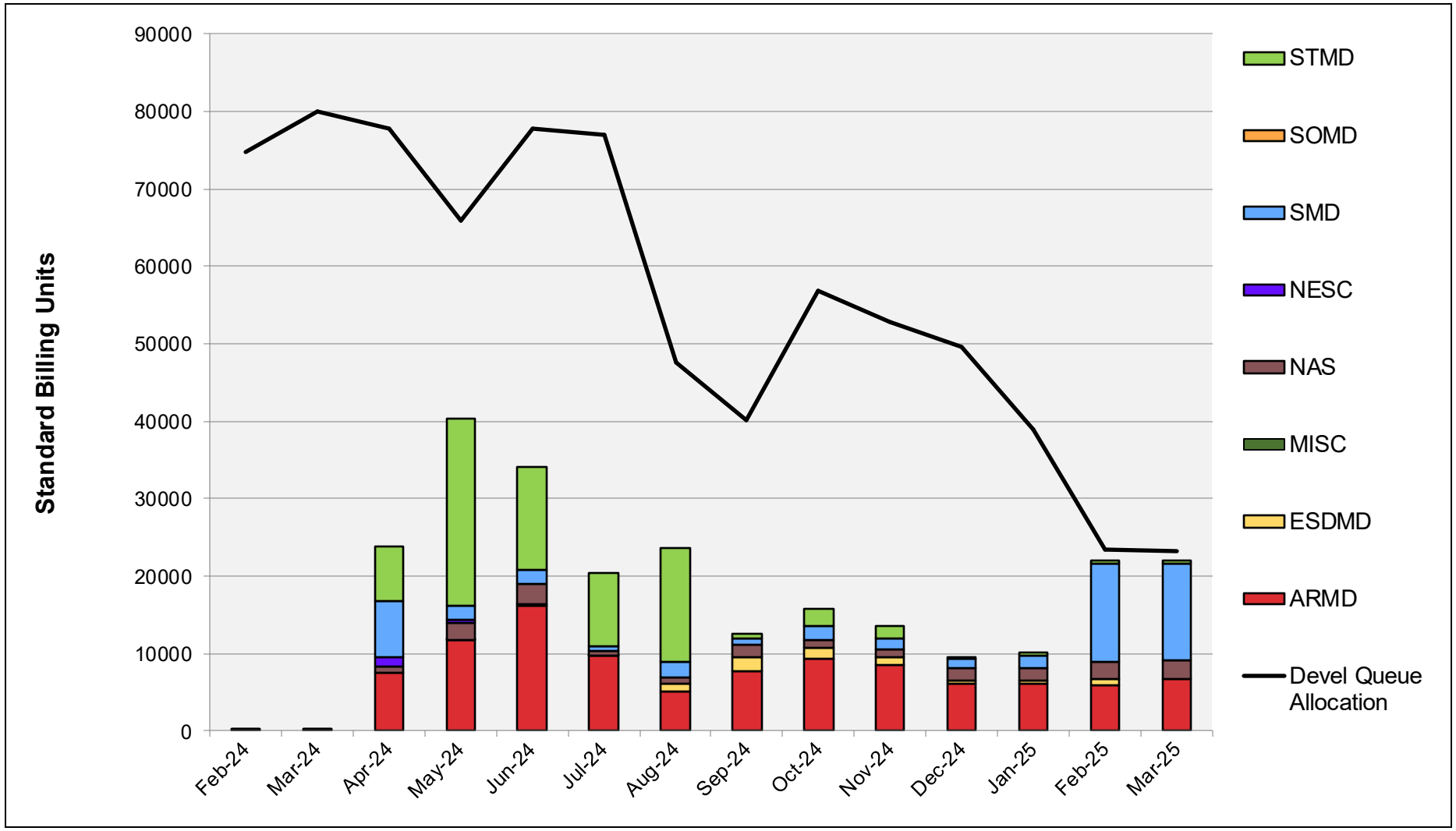
Electra: Average Expansion Factor



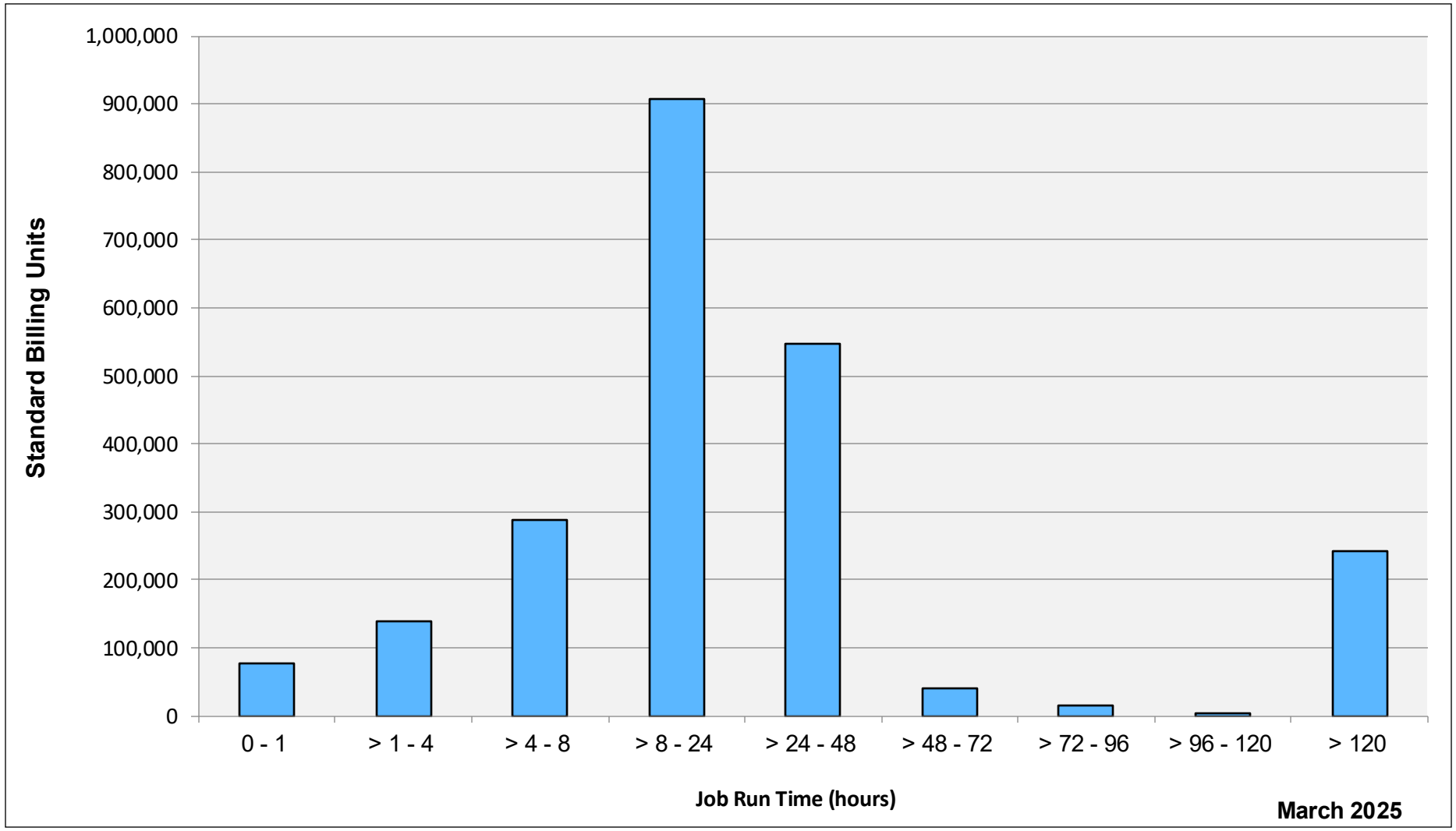
Cabeus: SBUs Reported, Normalized to 30-Day Month



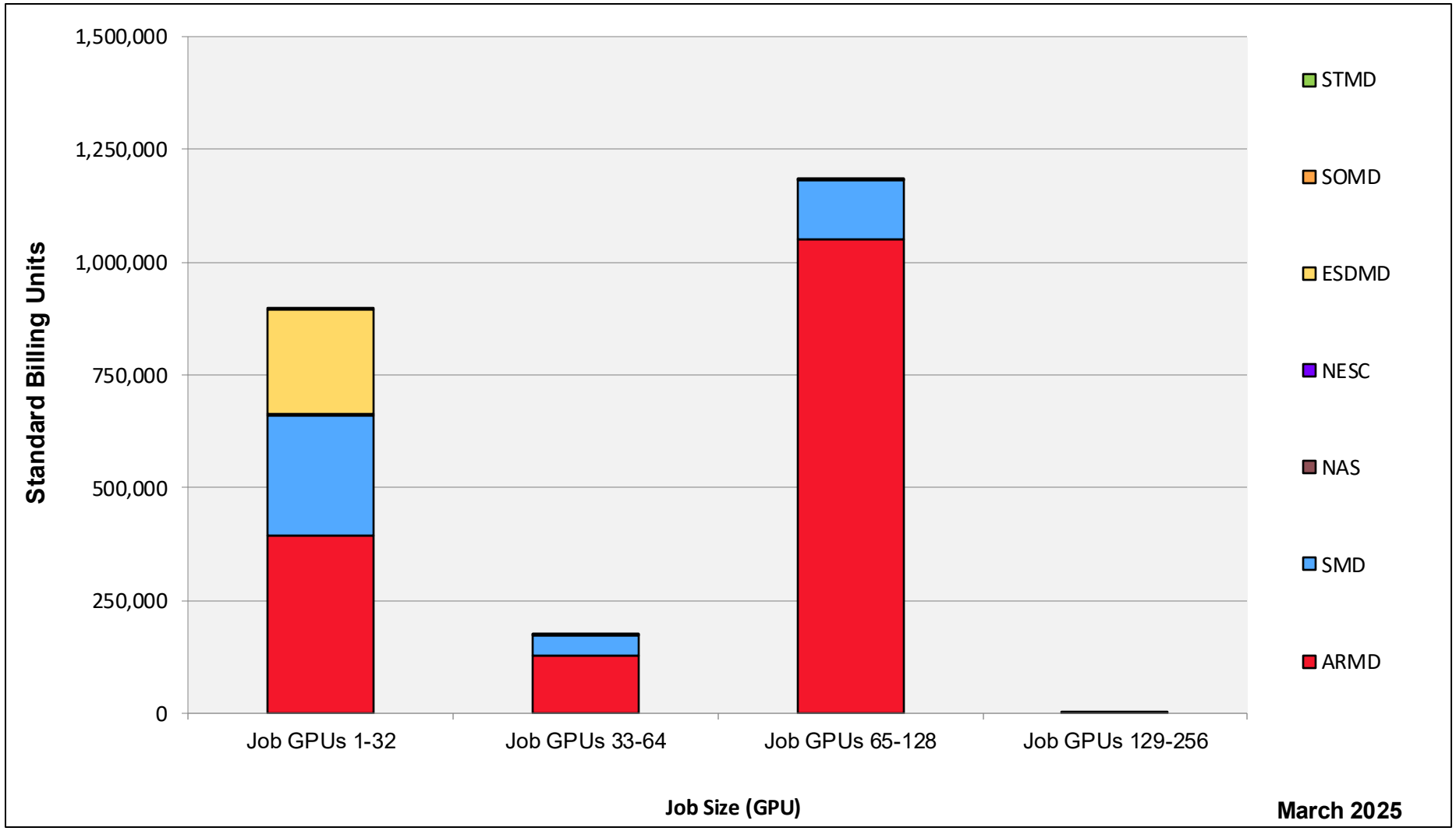
Cabeus: Devel Queue Utilization



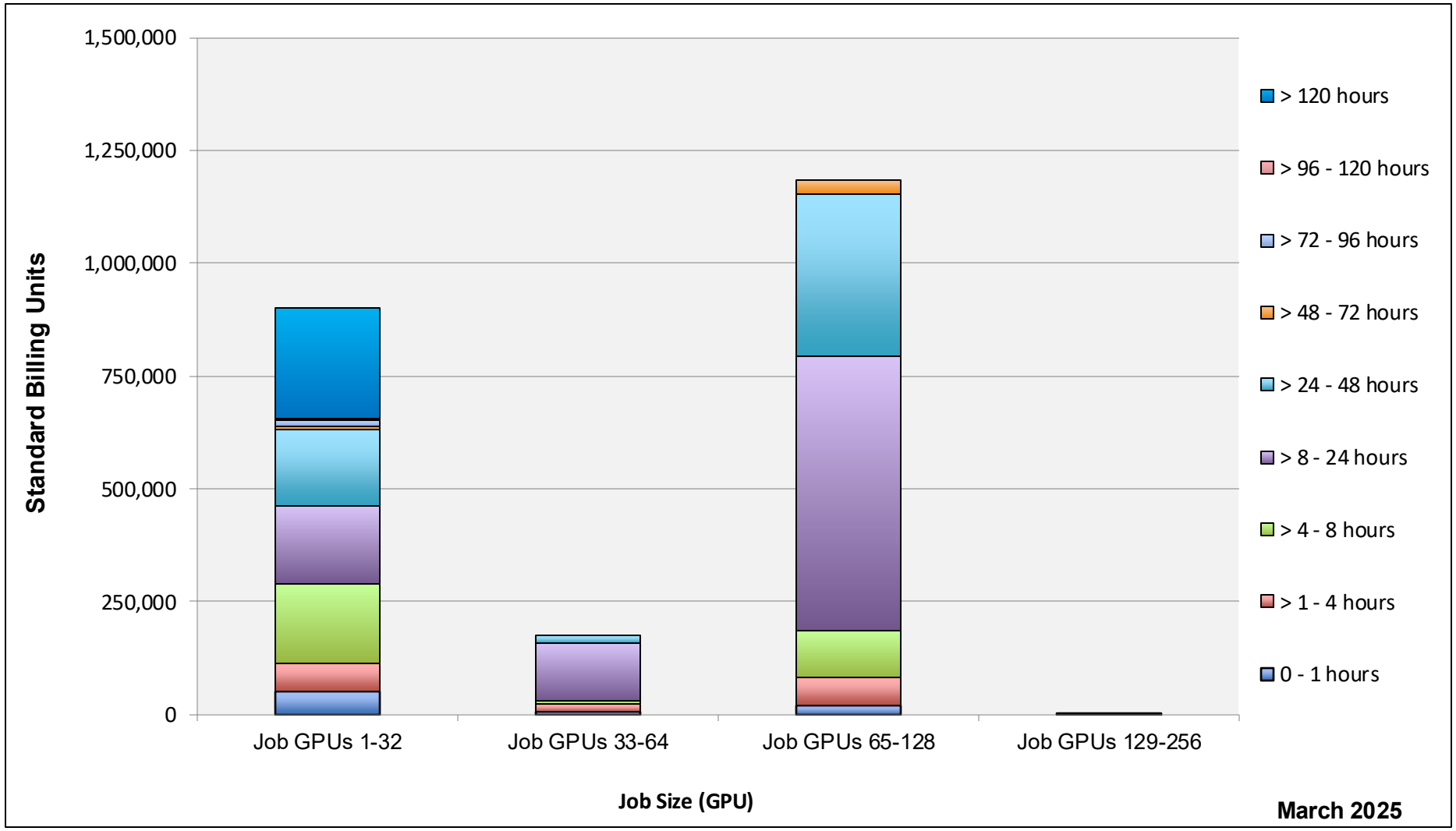
Cabeus: Monthly Utilization by Job Length



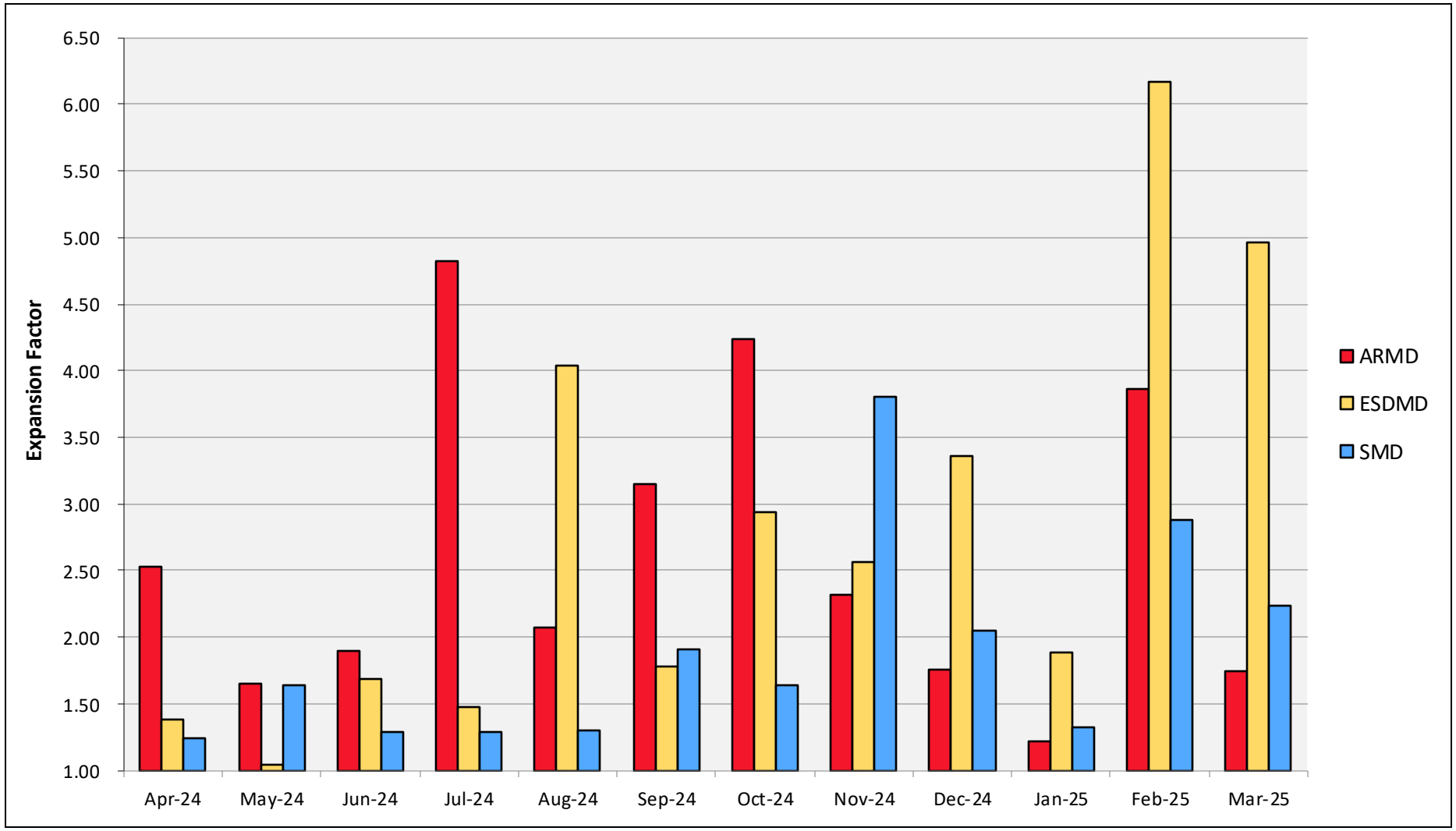
Cabeus: Monthly Utilization by Job Size



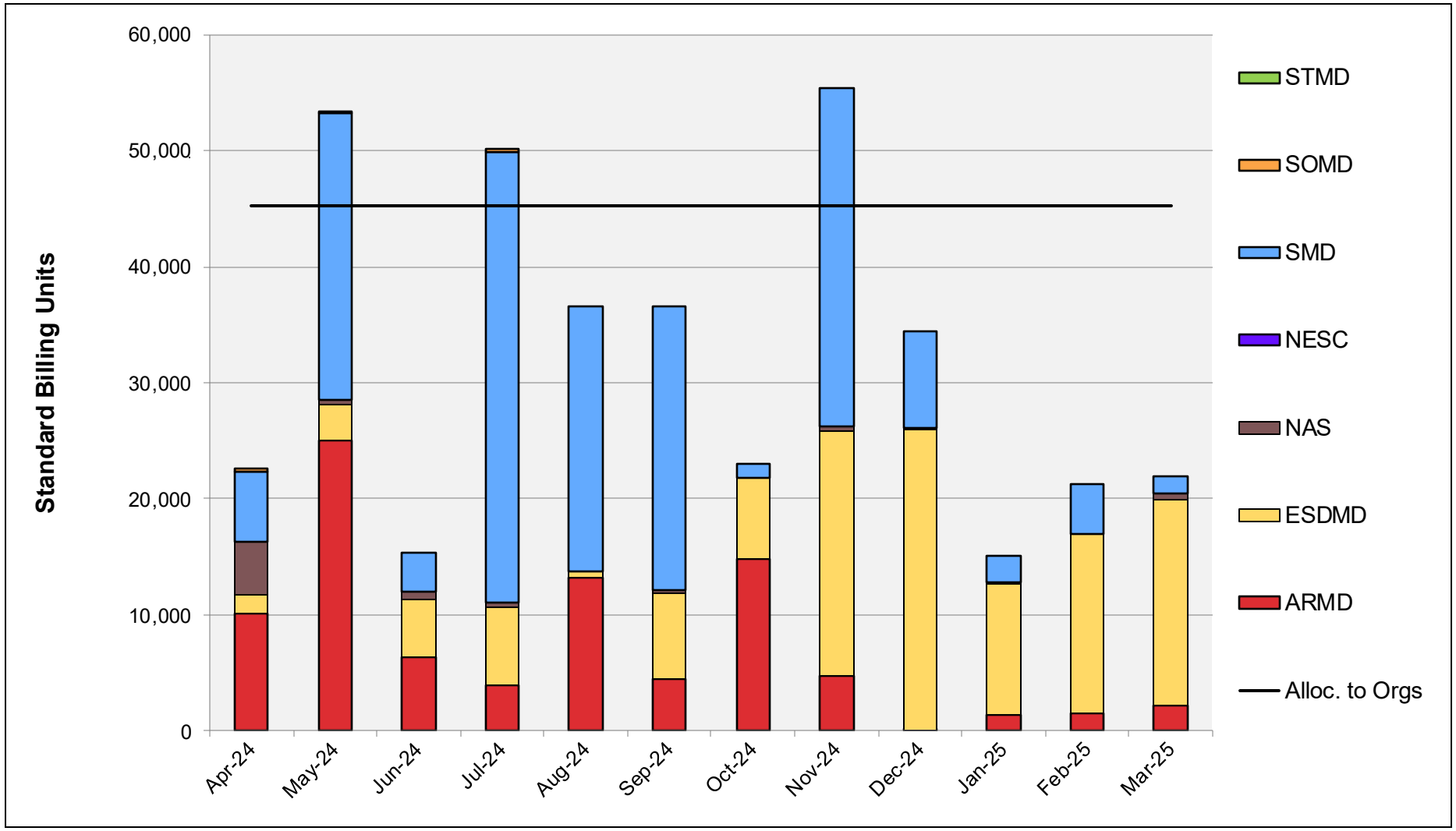
Cabeus: Monthly Utilization by Size and Length



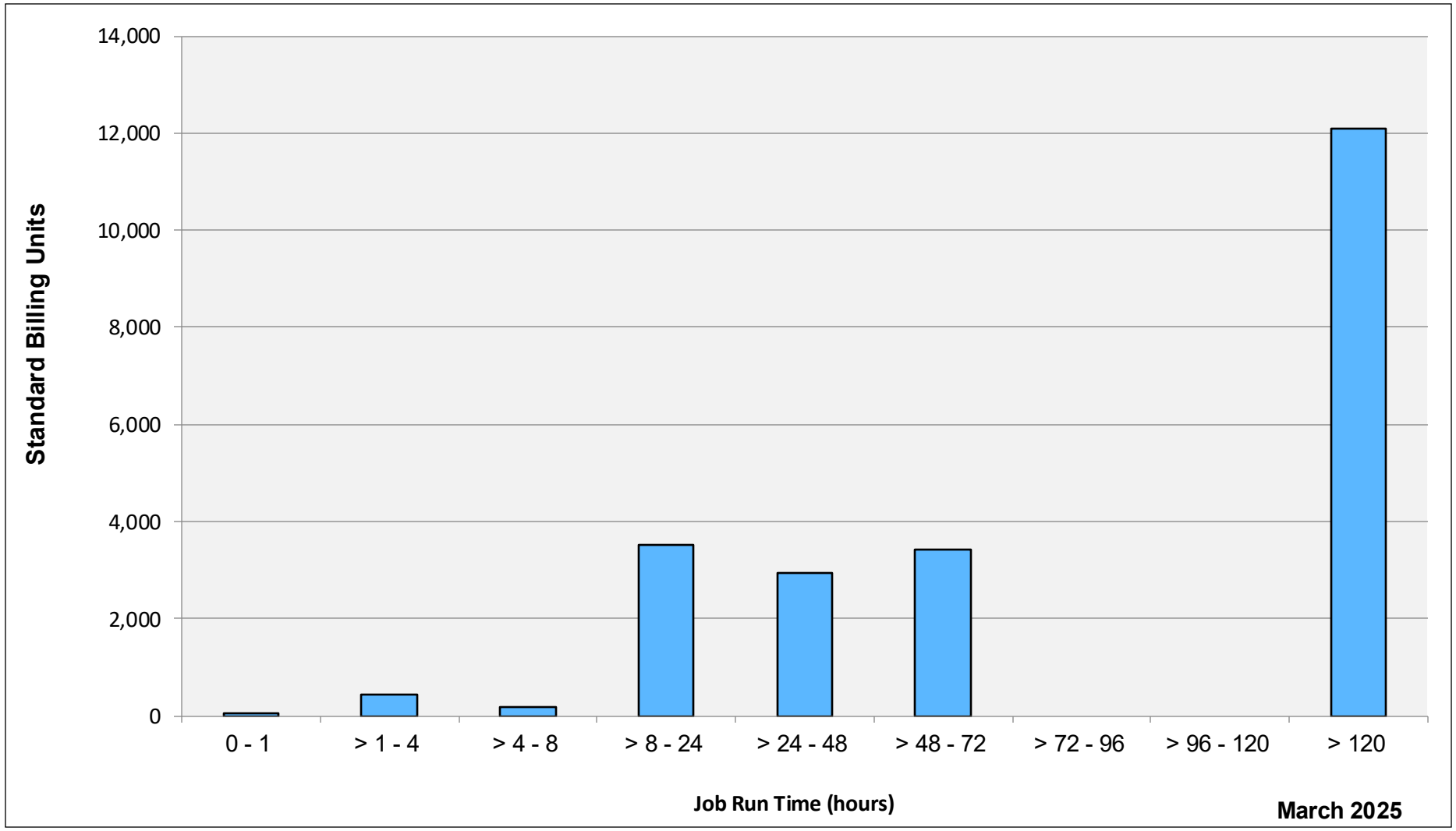
Cabeus: Average Expansion Factor



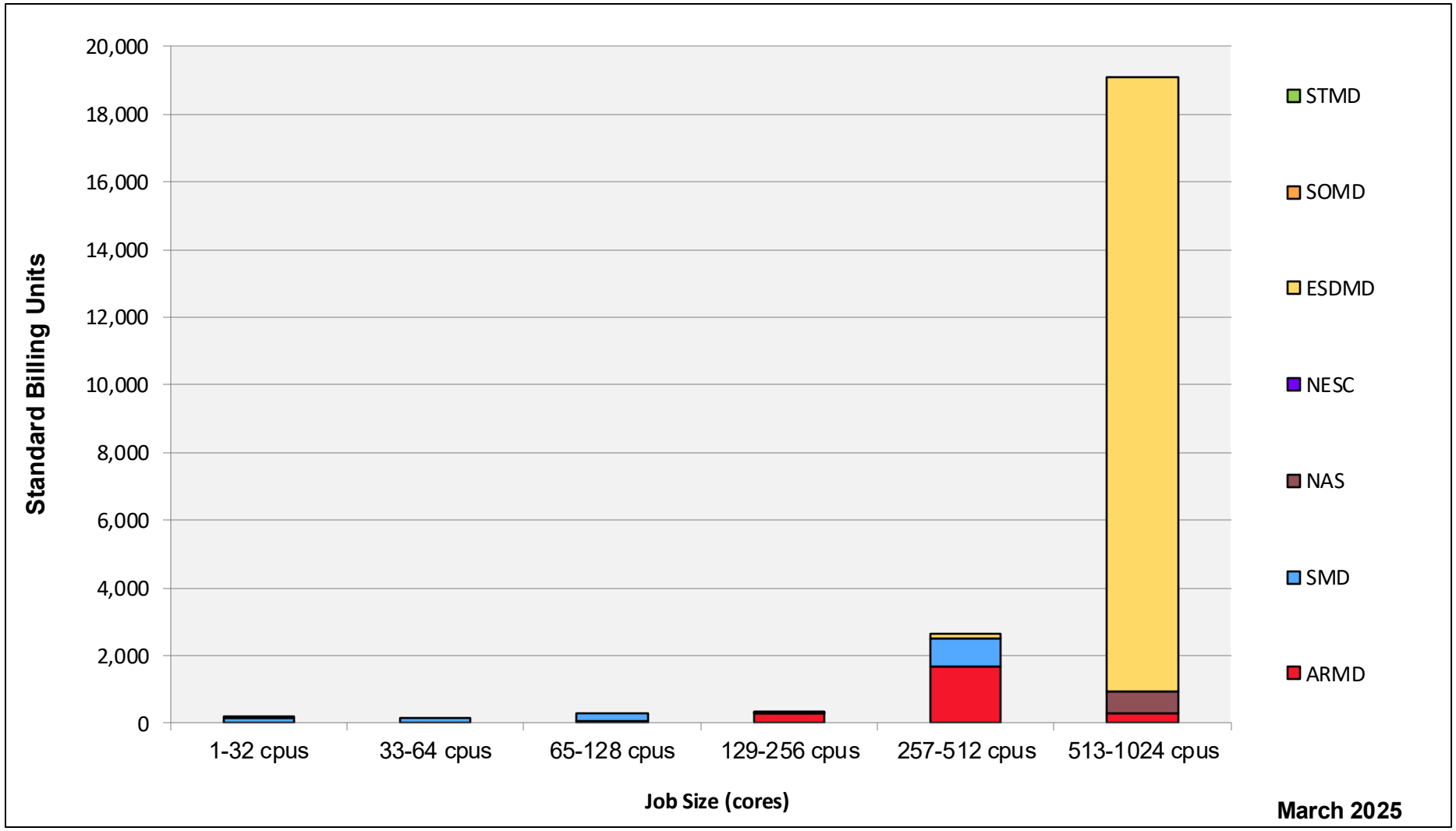
Endeavour: SBUs Reported, Normalized to 30-Day Month



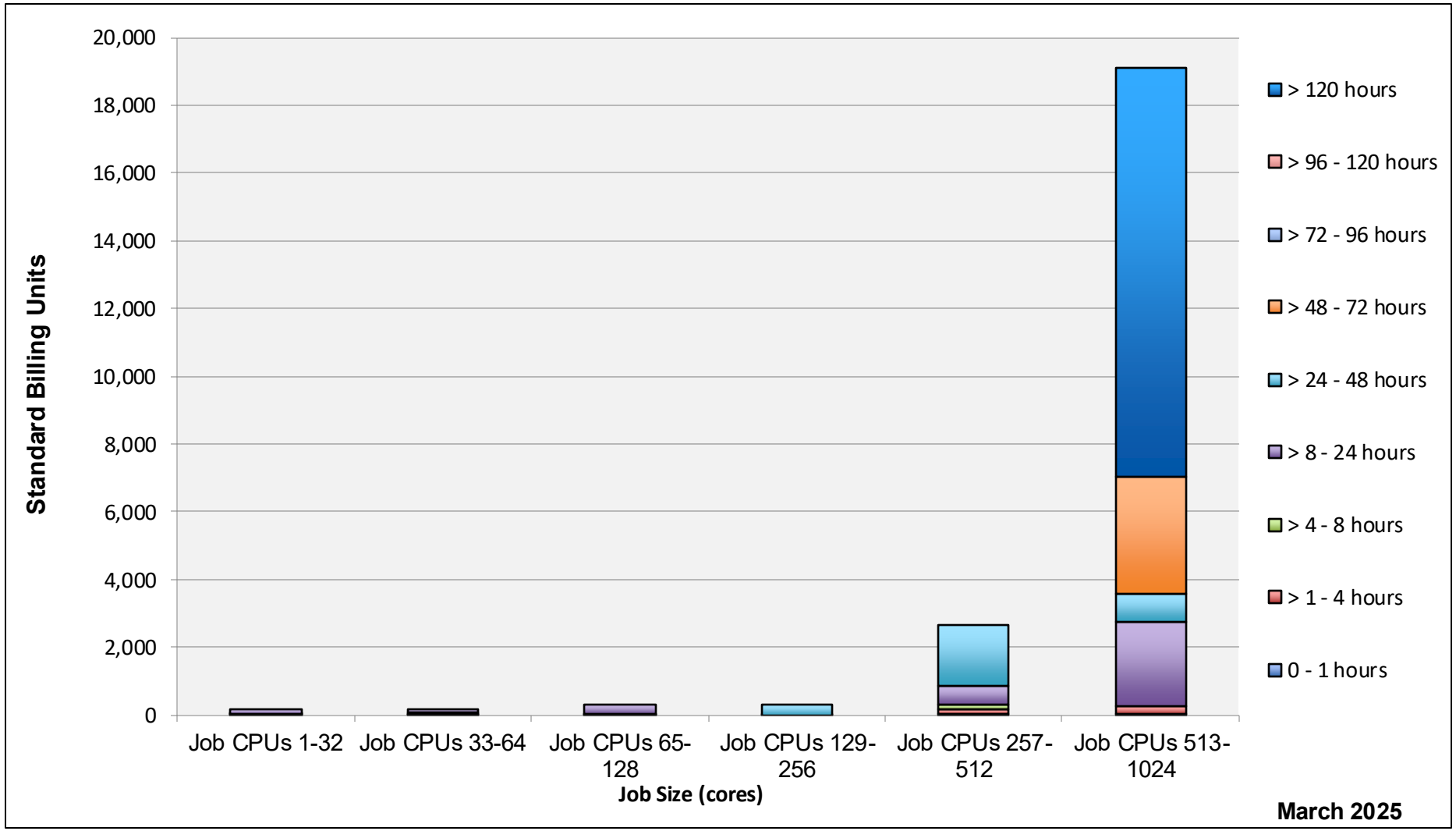
Endeavour: Monthly Utilization by Job Length



Endeavour: Monthly Utilization by Job Size



Endeavour: Monthly Utilization by Size and Length



Endeavour: Average Expansion Factor

