

National Aeronautics and Space Administration

High-End Computing Capability

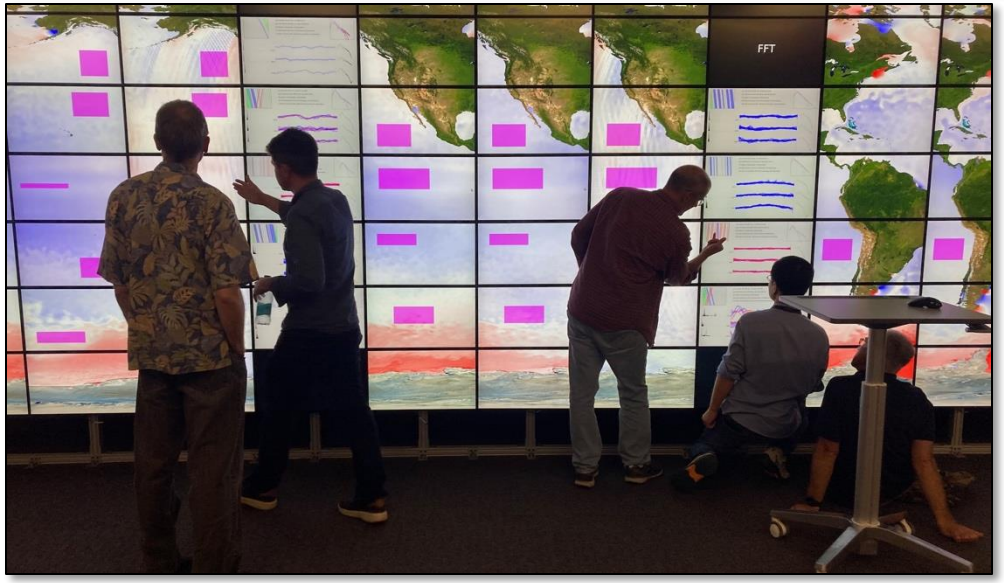
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October 10, 2024

SWOT and ECCO Scientists Utilize New hyperwall

- The HECC Visualization team leverages high-performance computing (HPC) to develop large-scale data access and manipulation strategies, new analysis capabilities, and interactive implementations of techniques to aide in the exploration of large data sets that are otherwise long-term efforts for domain scientists.
  - The Visualization Lab and hyperwall located at the NAS facility at Ames Research Center, with the new 128-LED-monitor displays and 128 nodes with 512 teraflops of compute capacity, provides a powerful tool for NASA scientists and engineers to leverage at no cost to their projects.
- Recently, the hyperwall was used to enable synoptic views and rapid analysis of recently downlinked data from the Surface Water and Ocean Topography (SWOT) mission as well as comparative analysis of SWOT and Estimating the Circulation and Climate of the Ocean (ECCO) model data.
  - Key SWOT mission and ECCO scientists from NASA's Jet Propulsion Laboratory, Ames, and other collaborating research institutions joined the HECC visualization experts to conduct analysis in the Visualization Lab for several days in August and September.
  - The visiting scientists commented that the hyperwall utility enabled months of data exploration and processing, interactively; that they were amazed by the powerful collaborative dynamic that the hyperwall and Vis Lab promoted; and that time really flies in the lab. Future visits have already been scheduled.

IMPACT: With the new hyperwall, HECC provides new analysis capabilities and interactive implementations of techniques for NASA's Earth observing missions, paving the way for future advancements in the understanding and production of mission data products.

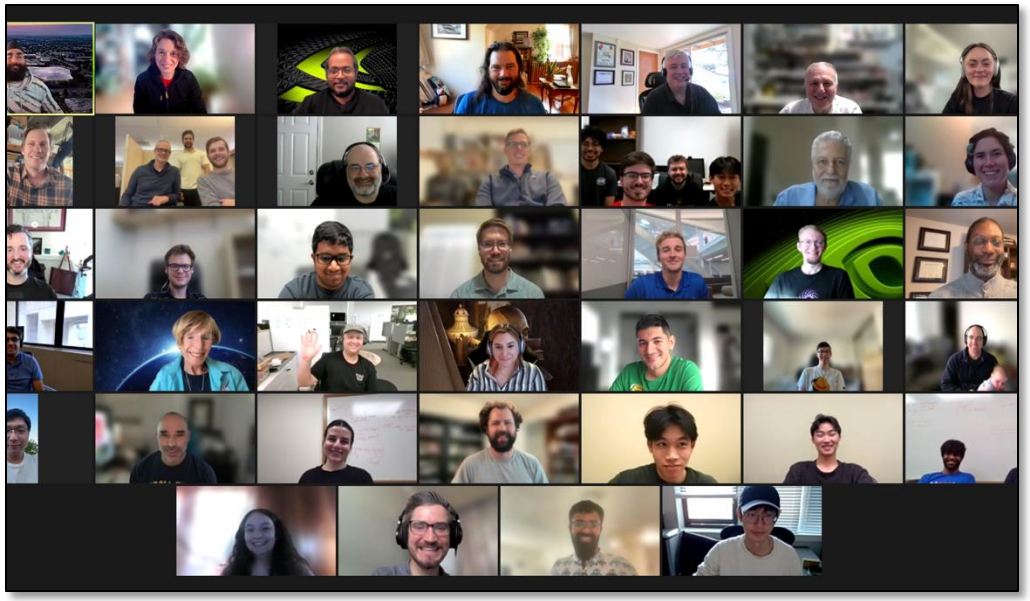


The NAS Visualization team and and members of the SWOT and ECCO science teams analyzing data in front of the hyperwall at the NASA Advanced Supercomputing (NAS) Facility. *Nina McCurdy, NASA/Ames*

HECC Hosts Successful 2024 NASA GPU Hackathon

- HECC and NVIDIA jointly organized the 2024 NASA GPU Hackathon, bringing together application developers and computer experts to help get important applications from NASA and academics running effectively on GPU nodes. The virtual event took place over four days on September 10 and 17-19.
  - Thirty-four members representing eight teams from two NASA centers (two teams from Ames and one team from Goddard) and academic institutions participated in the hackathon. The teams were selected from 14 submissions through a review process.
  - Teams brought a variety of CFD and AI/ML applications and applied several GPU acceleration techniques, including OpenACC, CUDA, CuPy, and CuML.
  - The participants used Zoom and Slack for collaboration. All the teams met together in a daily "scrum" session to present their progress.
  - HECC and NVIDIA provided nodes containing NVIDIA A100 and H100 GPUs for the teams to use.
  - A key to the success was the pairing of teams with 14 expert mentors from NASA, industry, and national labs.
  - With optimization techniques and performance tools, teams were able to achieve application performance improvement ranging from 10% up to 250X compared to original codes prior to the hackathon.
- HECC will coordinate with NASA Langley for next year's GPU Hackathon, and will explore ways to increase NASA participation at future events.

IMPACT: The NASA GPU Hackathon allowed the participating teams to gain experience porting and optimizing their codes for GPUs and increasing the performance of their applications.

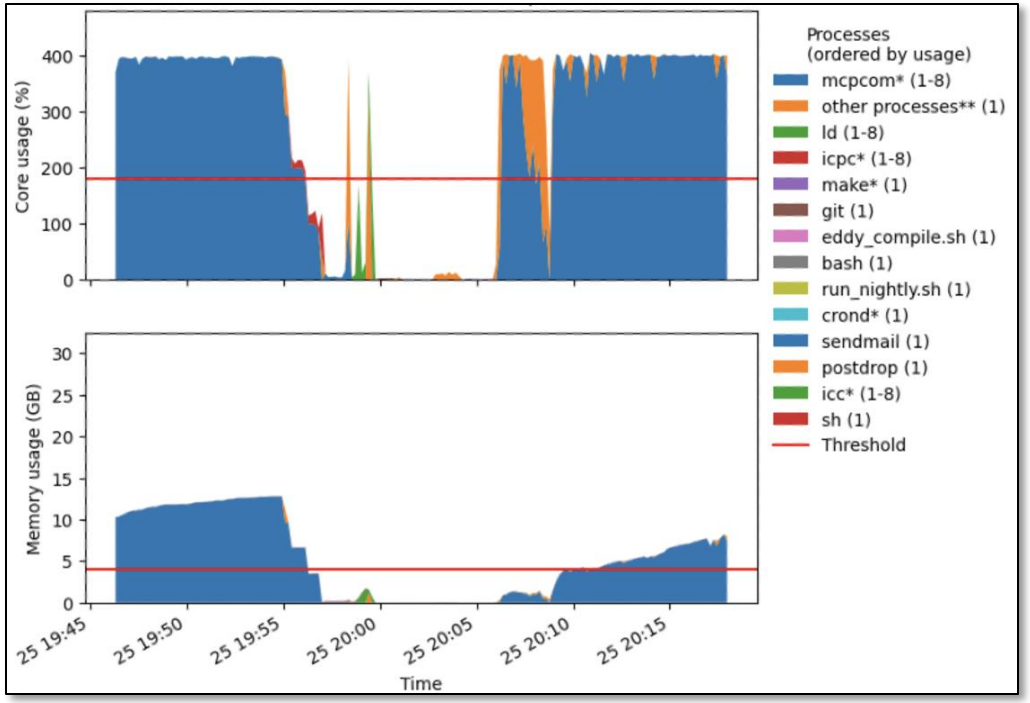


GPU Hackathon group photo showing 39 of the 54 team members, mentors, and supporting staff. *Image courtesy of NVIDIA*

HECC Deploys Arbiter Login Node Monitor

- In any shared HPC environment, multi-user login nodes are susceptible to poor performance due to user behavior. To enhance the availability and performance of front-end systems, the Systems and Control Room teams implemented Arbiter, a software solution developed by the University of Utah's Center for High Performance Computing.
- Arbiter is a cgroups-based service—a collection of processes that are bound by the same criteria and associated with a set of parameters or limits—designed to prevent overuse of scarce shared resources on login nodes. Arbiter implements tiered penalty statuses for users who exceed resource usage limits. If a user violates these limits, they are placed in a penalty status, which progressively reduces their CPU and memory allowances. Repeat offenses further reduces these allowances.
- Users receive email notifications detailing their violations and any changes in their penalty status. Providing this information to users helps educate them to make more informed choices to execute their applications on HECC compute resources, thus increasing the performance and stability of login nodes.

IMPACT: Installing the Arbiter software will help increase the stability of HECC login nodes while informing users on how to reduce harmful impacts to those nodes.



Example analysis report of intensive processes, generated by the Arbiter software and emailed to an individual user. The report shows each individual process and its resource usage over time. The red lines indicate the assigned limits.

Compute Module 2 Nears Completion

- Compute Module 2 at the NASA Ames Modular Supercomputing Facility (MSF) is entering the final stages of its installation. Module 2 is scheduled to have all its infrastructure running by the end of October 2024.
- Primary completed tasks are the installation of the pumps and piping for the cooling water to cool the compute racks.
  - The compute racks used Module 2 are nearly 100% water cooled.
  - At 108 kilowatts per rack, water cooling is the only way to keep the processors operational within their temperature limits.
- The 25-kilovolt (kV) – 480volt transformer that provides power to the module and racks was delivered on site on September 20, after being reworked at the factory to install 25kV overcurrent protection fuses.
  - The transformer was originally delivered in June 2024 without fuses, necessitating the rework. While the transformer is now at specification, the rework activity resulted in a six-week schedule delay.
- Compute Module 2, which has a capacity of 24 racks consuming a total of 3 megawatts of power, will house the 512-node AMD Milan expansion of Aitken supercomputer. In addition, a larger system is planned for deployment in FY2025.

IMPACT: Compute Module 2 provides increased capacity to install additional supercomputing resources for HECC users in the near future.

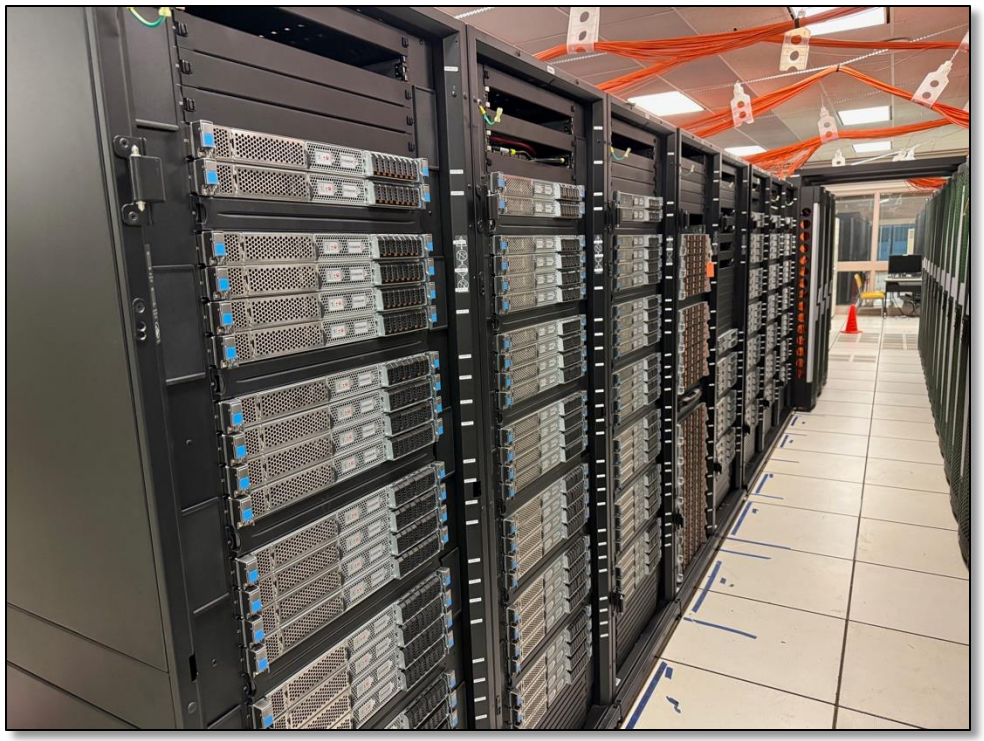


Compute Module 2 and support infrastructure during installation at the Modular Supercomputing Facility at NASA's Ames Research Center.
Chris Tanner, NASA/Ames

Grace Hopper Supercomputer Delivered

- Supermicro delivered the Grace Hopper system to the NASA Advanced Supercomputing facility on September 30, 2024. The system will provide additional graphics processing unit (GPU) capacity for HECC users.
- The system is configured with:
  - 350 compute nodes, each with one NVIDIA GH200 Grace CPU and one H100 GPU.
  - Two login nodes, each one NVIDIA GH200 Grace Hopper superchip.
  - An InfiniBand NDR200 interconnect.
- System installation by Supermicro is planned for completion by mid-October; and the system will be turned over to HECC Systems experts for software installation, system configuration, and system benchmarking. Early user access is targeted for December 2024 with general user access targeted for the first quarter of calendar year 2025.

IMPACT: Additional GPU capacity from the Grace Hopper system will provide more computational capacity to support HECC users requirements.

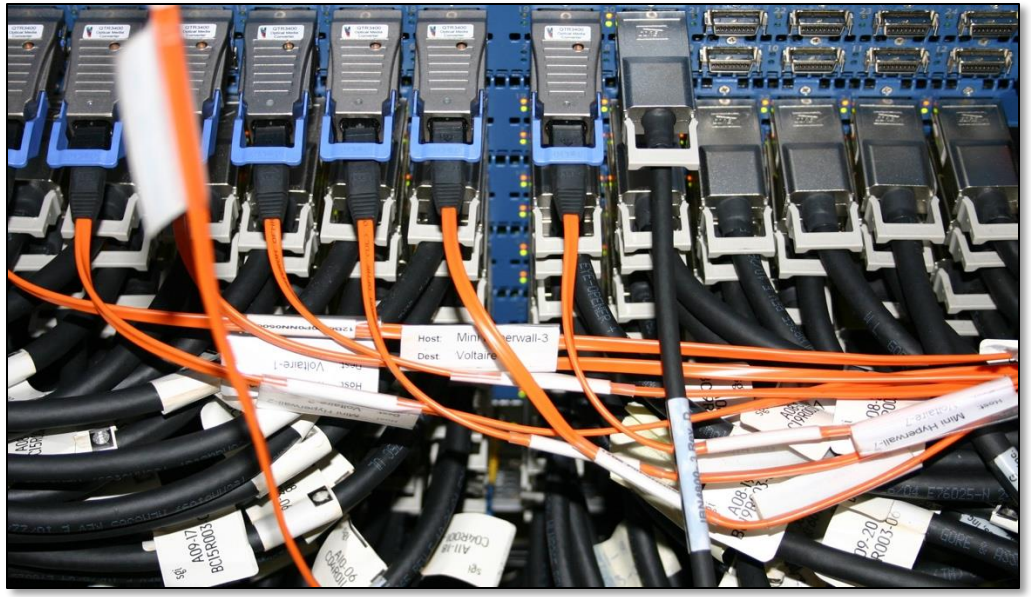


One of the two rows of the Grace Hopper racks being installed at the NASA Advanced Supercomputing facility. *Davin Chan, NASA/Ames*

InfiniBand Redesign Plan Gets First-Round Approval

- The HECC Systems team proposed an InfiniBand (IB) redesign that will better position the NAS facility systems for organic growth in the future.
  - The proposed IB redesign provides a robust topology that separates the storage and infrastructure servers from the compute clusters.
  - This modular design approach enables more flexibility, less downtime, and better supportability.
  - The approach also opens up the ability to support future compute capabilities with a wider array of technologies, architectures, and vendors to provide cutting-edge performance.
- The team proposed a phased implementation schedule over the next nine months.
  - Following hardware procurement, the majority of the implementation will be conducted during monthly dedicated times, limiting user impacts.
  - HECC and NAS Division senior leaders reviewed and approved the approach and transition plans.

IMPACT: Redesigning the InfiniBand infrastructure at NASA's premiere supercomputing facility lays the groundwork for a more modular approach to systems deployment, with better sustainability and flexibility to deploy more powerful systems for the users with less downtime.



Representative InfiniBand cables in the HECC supercomputing environment. *NAS Division Archive*

Total Solar Eclipse: A Lens to Understand the Sun*

- A team of researchers at Predictive Science, Inc. ran simulations to predict the April 8, 2024 total solar eclipse, using their Magnetohydrodynamic Algorithm Outside a Sphere (MAS) code on NASA's Pleiades, Electra, and Aitken supercomputers.
  - During a total solar eclipse, the magnetized solar atmosphere is revealed, presenting a perfect opportunity to study the complex structure and interconnected physics that link the Sun to the Earth and beyond—critical for accurately forecasting our space environment, including space weather events such as immense solar storms, which can damage critical infrastructure.
- Results of the team's simulations over the years have led to interesting discoveries such as how complexity in the surface magnetic field can lead to the sharp, complex features far from the Sun observed during eclipses.
  - By tracing magnetic field lines at extremely high resolution, the researchers can calculate a 3D map of the so-called squashing factor (Q) - a scientific measure designed to indicate the presence of complex structuring in the magnetic field.
  - They can then integrate the map along the line-of-sight, with weightings to create a composite that resembles eclipse images—highlighting the complexity of the Sun's magnetic field and its connection to visible emission in the corona.
- The predictions for the April 8, 2024 eclipse tested the latest advances in the model, including the ability to drive the simulation with continuously updated measurements to the moment of the event.

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

IMPACT: These predictive models improve our understanding of the physics of the corona and provide key insights into solar events that could impact Earth, in addition to providing planning data for observations.



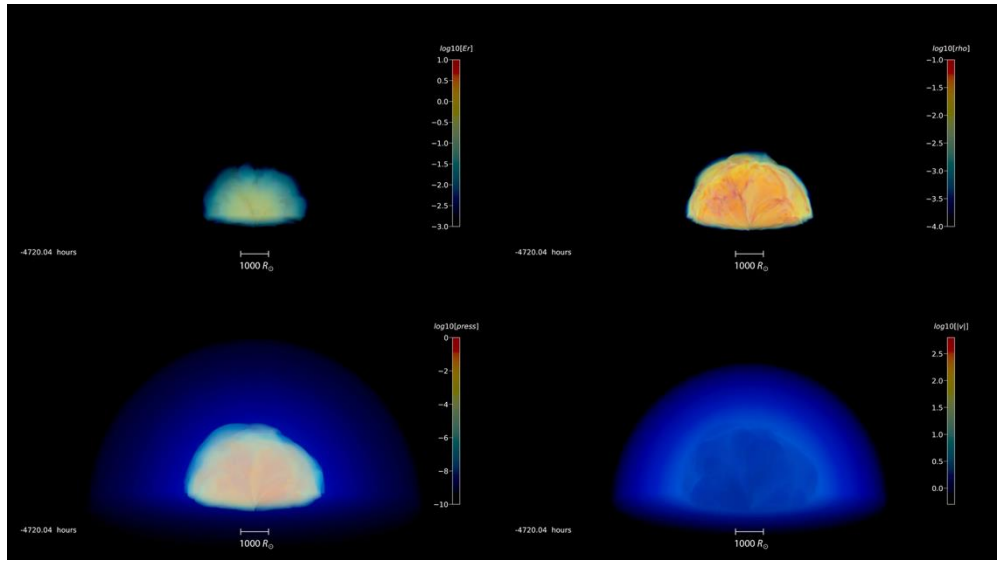
Simulation of the April 8, 2024 total solar eclipse, run on HECC systems. *Predictive Science, Inc.*

Simulating Supernova Shock Breakouts in 3D*

- By observing the "shock breakout" of a red supergiant star—a bright flash that occurs when the supernova's shock reaches the surface of the star—astrophysicists can discover a lot of information about the star's properties and about the collapse of its core.
- To help improve our understanding of these observations, researchers from the Flatiron Institute's Center for Computational Astrophysics ran 3D radiation hydrodynamic simulations of red supergiant stars' convective envelope, then simulated the propagation of a strong shock from the collapse of the star through the convective envelope.
- Results showed that convection in the envelope of red supergiant stars can cause significant fluctuations of the stellar photosphere, significantly broadening the number of shock breakout signatures available to help astrophysicists interpret future observations.
- The light curves generated from the simulations can be directly compared with shock breakout observations and constrain the properties of the original star.
- Each 3D simulation ran across 150 Skylake nodes of HECC's Electra supercomputer for a month to obtain the 3D structures of the stellar envelopes.

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

IMPACT: These 3D simulation results—which would be impossible without the supercomputing resources provided by HECC—have important implications for future observations of shock breakouts.



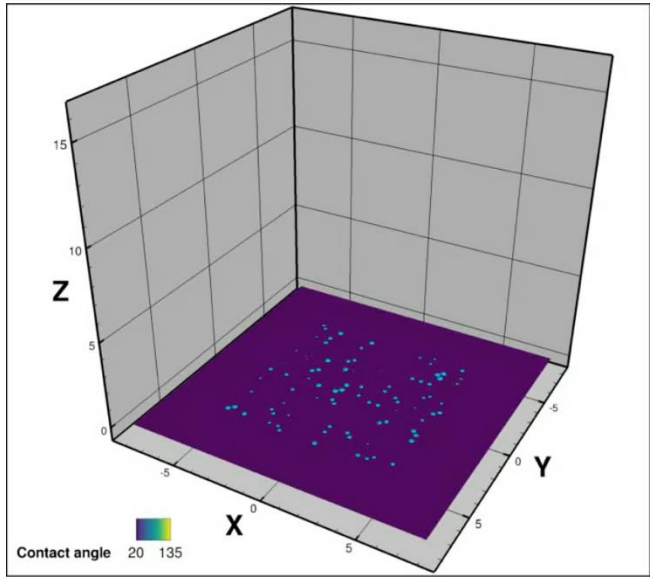
Volume renderings of a supernova shock breakout showing radiation energy density (top left); gas density (top right); gas pressure (bottom left); and magnitude of the velocity field (bottom right). After the shock passes through the envelope for 20 hours, the star is rotated to demonstrate very anisotropic shock breakout emission. *Yan-Fei Jiang, Flatiron Institute; Nina McCurdy, NASA/Ames*

Biphilic Surfaces for Electronics Cooling*

- As more powerful electronics are developed, it is vital to also improve systems that keep them cool. Researchers from the University of Maryland, College Park are using HECC supercomputers to simulate liquid cooling behavior on biphilic surfaces—patterned with areas that repel water (hydrophobic) and attract water (hydrophilic).
- Experiments have shown that biphilic surfaces have increased cooling properties compared to normal surfaces. Using numerical experiments and an in-house multiphase solver, the team simulated pool boiling (vaporization) of coolant liquid under normal gravity on a simple model of a heater surface with a uniform pattern of hydrophobic and hydrophilic surfaces, varying the ratio to understand its effects on heat flux and thermo-fluid characteristics.
- Three cases were considered, with hydrophobic surface ratios of 0.01, 0.25, and 0.75. The 0.25 case showed the highest average heat flux at steady state, and the team was able to identify the different heat transfer mechanisms and their contributions to overall cooling, which have been difficult to understand in real-world experiments.
- Using the FLASH multiphase computational fluid dynamics solver, these simulations required a total of 1.2 million wall-clock core hours on Pleiades' Broadwell nodes and 4 terabytes of storage.
- These simulations can also be applied to low-gravity conditions, helping to design better cooling systems for future space missions.

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

IMPACT: As more powerful electronics are developed, it is vital to improve the systems that keep them cool, especially to reduce energy consumption and increase efficiency for electronics used in future space missions.



Animation showing the pool boiling simulation for the A* = 0.25 case. The blue surfaces denote vapor bubbles that are naturally growing due to wall superheat. The bubbles keep increasing until the buoyant force is substantive enough for its departure from the heater surface. Subsequently, a new vapor nucleus is generated and the process repeats again. *Shantanu Vachhani, University of Maryland, College Park*

Papers

- "**The Contribution of Solar Magnetic Regions to the Residual Meridional and Zonal Flows**," D. C. Braun, *The Astrophysical Journal*, vol. 972, no. 2, published online September 4, 2024. *
  https://iopscience.iop.org/article/10.3847/1538-4357/ad5fea/meta
- "**Source of Drift-Dispersed Electrons in Martian Crustal Magnetic Fields**," C. Zhang, et al., *The Astrophysical Journal*, vol. 972, no. 2, published online September 4, 2024. *
  https://iopscience.iop.org/article/10.3847/1538-4357/ad64d5/meta
- "**TOI-3568 b: A Super-Neptune in the Sub-Jovian Desert**," E. Martioli, et al., arXiv:2409.03704 [astro-ph.EP], September 5, 2024. *
  https://arxiv.org/abs/2409.03704
- "**Aircraft Ducted Heat Exchanger Aerodynamic Shape Thermal Optimization**," E. Adler, et al., *Journal of Heat Mass Transfer*, published online September 6, 2024. *
  https://asmedigitalcollection.asme.org/heattransfer/article-abstract/147/1/011902/1205259
- "**Transformer Approach to Nowcasting Solar Energy Using Geostationary Satellite Data**," R. Li, et al., *Applied Energy*, vol. 377, Part A, published online September 10, 2024. *
  https://www.sciencedirect.com/science/article/abs/pii/S0306261924017707
- "**The Inflated, Eccentric Warm Jupiter TOI-4914 b Orbiting a Metal-Poor Star, and the Hot Jupiters TOI-2714 b and TOI-2981 b**," G. Mantovan, et al., arXiv:2409.07520 [astro-ph.EP], September 11, 2024. *
  https://arxiv.org/abs/2409.07520

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

Papers (cont.)

- "**Confirming the Tidal Tails of the Young Open Cluster Blanco 1 TESS Rotation**," L. Sha, et al., arXiv:2409.07550 [astro-ph.SR], September 11, 2024. *
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- "**Three Atmospheric Patterns Dominate Decadal North Atlantic Overturning Variability**," D. Stephenson, et al., *Geophysical Research Letters*, vol. 51, issue 8, published online September 11, 2024. *
  https://agupubs.onlinelibrary.wiley.com/doi/full/10.1029/2024GL109193
- "**Mapping the Sun's Coronal Magnetic Field Using the Zeeman Effect**," T. Schad, et al., *Science Advances*, vol. 10, issue 37, September 11, 2024. *
  https://www.science.org/doi/full/10.1126/sciadv.adq1604
- "**Identification of Internal Tides in ECCO Estimates of Sea Surface Salinity of Andaman Sea**," B. Subrahmanyam, et al., *Remote Sensing*, vol. 16, issue 18, published online September 13, 2024. *
  https://www.mdpi.com/2072-4292/16/18/3408
- "**3D Radiation-Hydrodynamical Simulation of Shadows on Transition Disks**," S. Zhang, Z. Zhu, arXiv:2409.08373 [astro-ph.EP], September 17, 2024. *
  https://arxiv.org/abs/2409.08373
- "**The K2 and TESS Synergy. III. Search and Rescue of the Lost Ephemeris for K2's First Planet**," E. Thygesen, et al., *The Astronomical Journal*, vol. 168, no. 4, published online September 17, 2024. *
  https://iopscience.iop.org/article/10.3847/1538-3881/ad60bf/meta

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

Papers (cont.)

- "**The Debiased Near-Earth Object Population from ATLAS Telescopes**," R. Deienno, et al., *Icarus*, vol. 425, published online September 17, 2024. *
  https://www.sciencedirect.com/science/article/abs/pii/S0019103524003762
- "**Characterization of TOI-406 as Showcase of the THIRSTEE Program: A 2-Planet System Straddling the M-Dwarf Density Gap**," G. Lacedelli, et al., arXiv:2409.11083 [astro-ph.EP], September 17, 2024. *
  https://arxiv.org/abs/2409.11083
- "**Prithvi WxC: Foundation Model for Weather and Climate**," J. Schmude, et al., arXiv:2409.13598 [cs.LG], September 20, 2024. *
  https://arxiv.org/abs/2409.13598
- "**Quartz Clouds in the Dayside Atmosphere of the Quintessential Hot Jupiter HD 189733 b**," J. Inglis, et al., *The Astrophysical Journal Letters*, vol. 973, no. 2, published online 23, 2024. *
  https://iopscience.iop.org/article/10.3847/2041-8213/ad725e/meta
- "**Deriving Seasonal and Annual Surface Mass Balance for Debris-Covered Glaciers from Flow-Corrected Satellite Stereo DEM Time Series**," S. Bhushan, et al., *Journal of Glaciology*, published online September 25, 2024. *
  https://www.cambridge.org/core/journals/journal-of-glaciology/article/deriving-seasonal-and-annual-surface-mass-balance-for-debriscovered-glaciers-from-flowcorrected-satellite-stereo-dem-time-series/C58CFCE164F14E4F7D7DD895B8193660
- "**A Data-Driven MHD Simulation of the 2011-02-15 Coronal Mass Ejection from Active Region NOAA 11158**," Y. Fan, et al., arXiv:2409.17507 [astro-ph.SR], September 26, 2024. *
  https://arxiv.org/abs/2409.17507

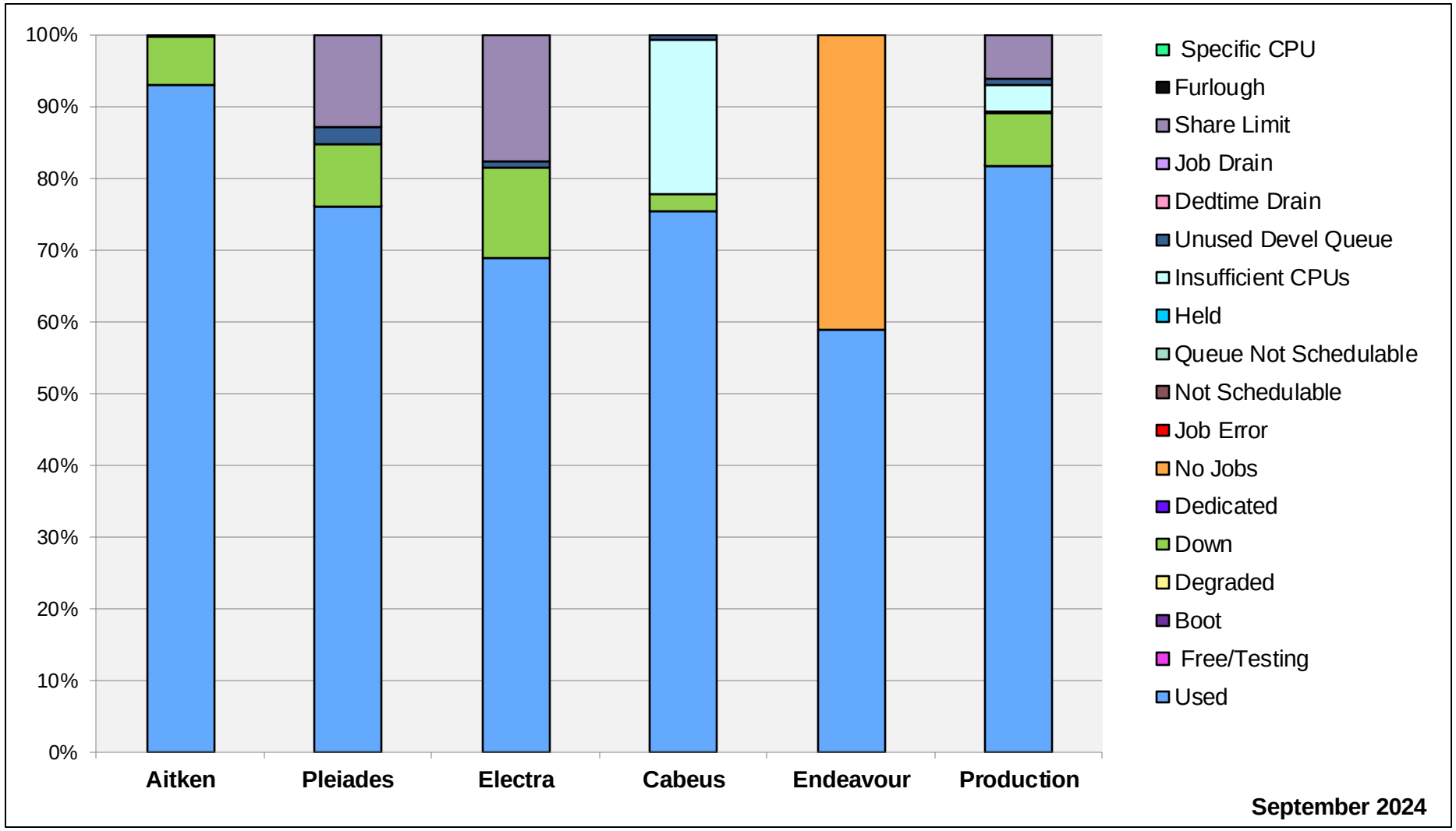
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Papers (cont.)

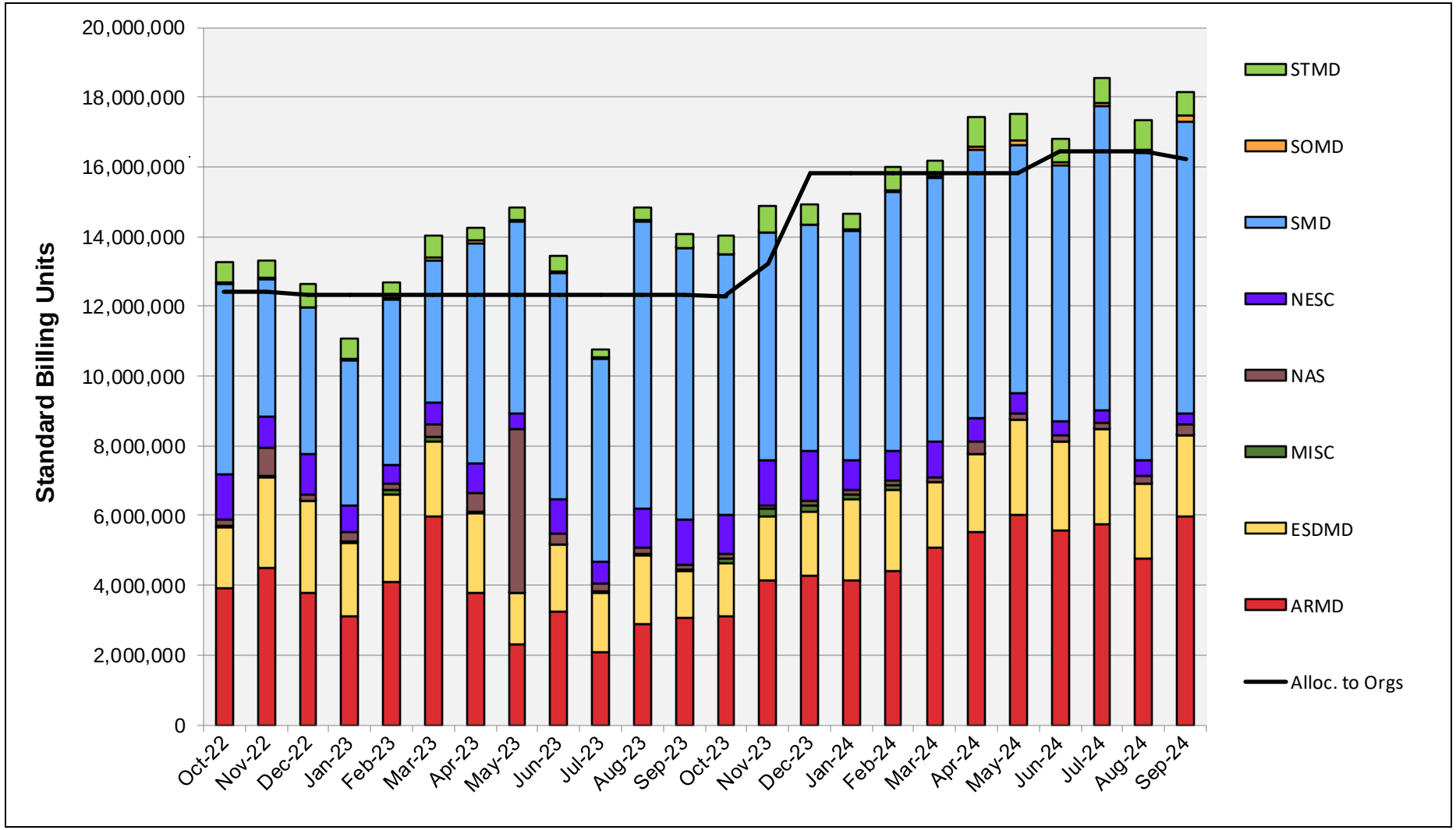
- "**TOI-5005 b: A Super-Neptune in the Savanna Near the Ridge**," A. Castro-González, et al., arXiv:2409.18129 [astro-ph.EP], September 26, 2024. *
  https://arxiv.org/abs/2409.18129
- "**TOI-2458 b: A Mini-Neptune Consistent with In Situ Hot Jupiter Formation**," J. Subjak, et al., arXiv:2409.17532 [astro-ph.EP], September 26, 2024. *
  https://arxiv.org/abs/2409.17532

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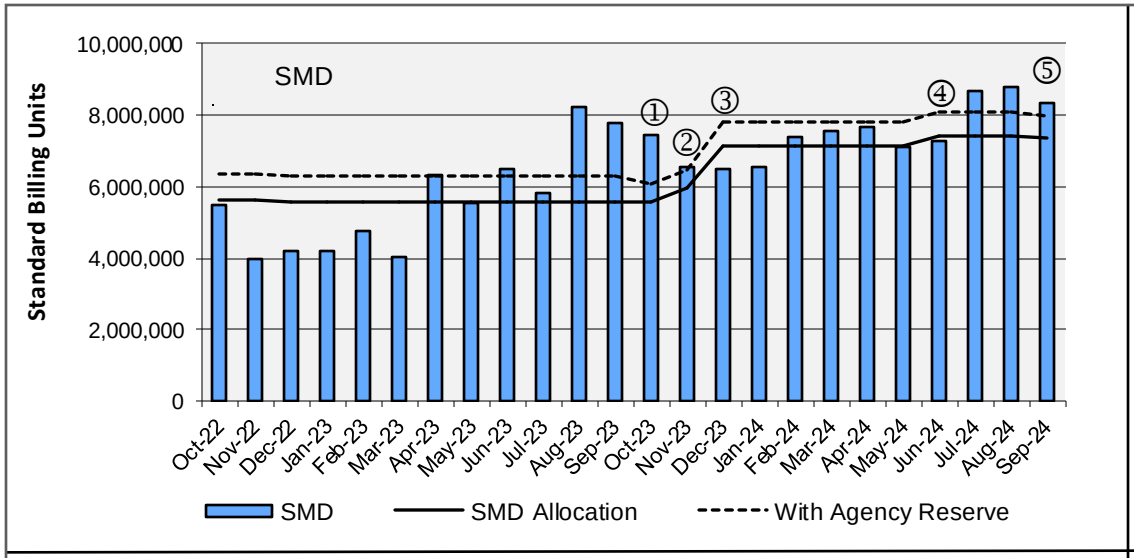
HECC Utilization

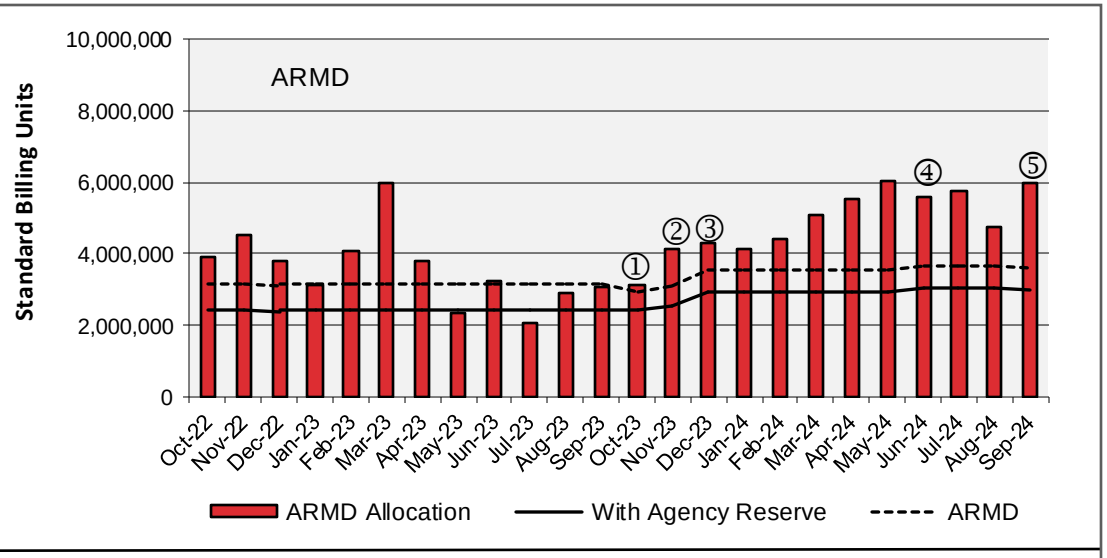


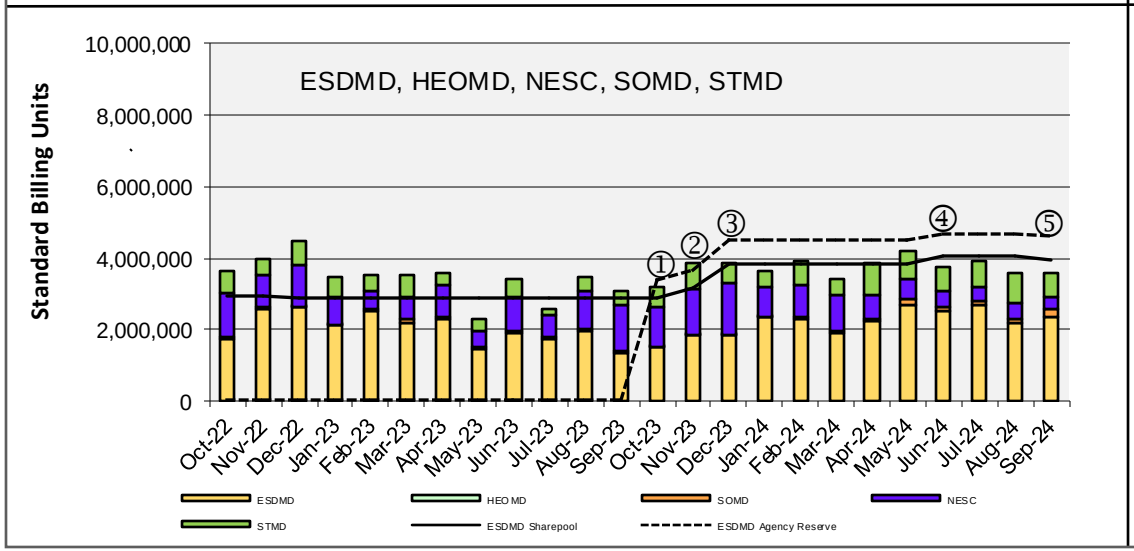
HECC Utilization Normalized to 30-Day Month



HECC Utilization Normalized to 30-Day Month







① 4 Rome Apollo Racks added to Aitken

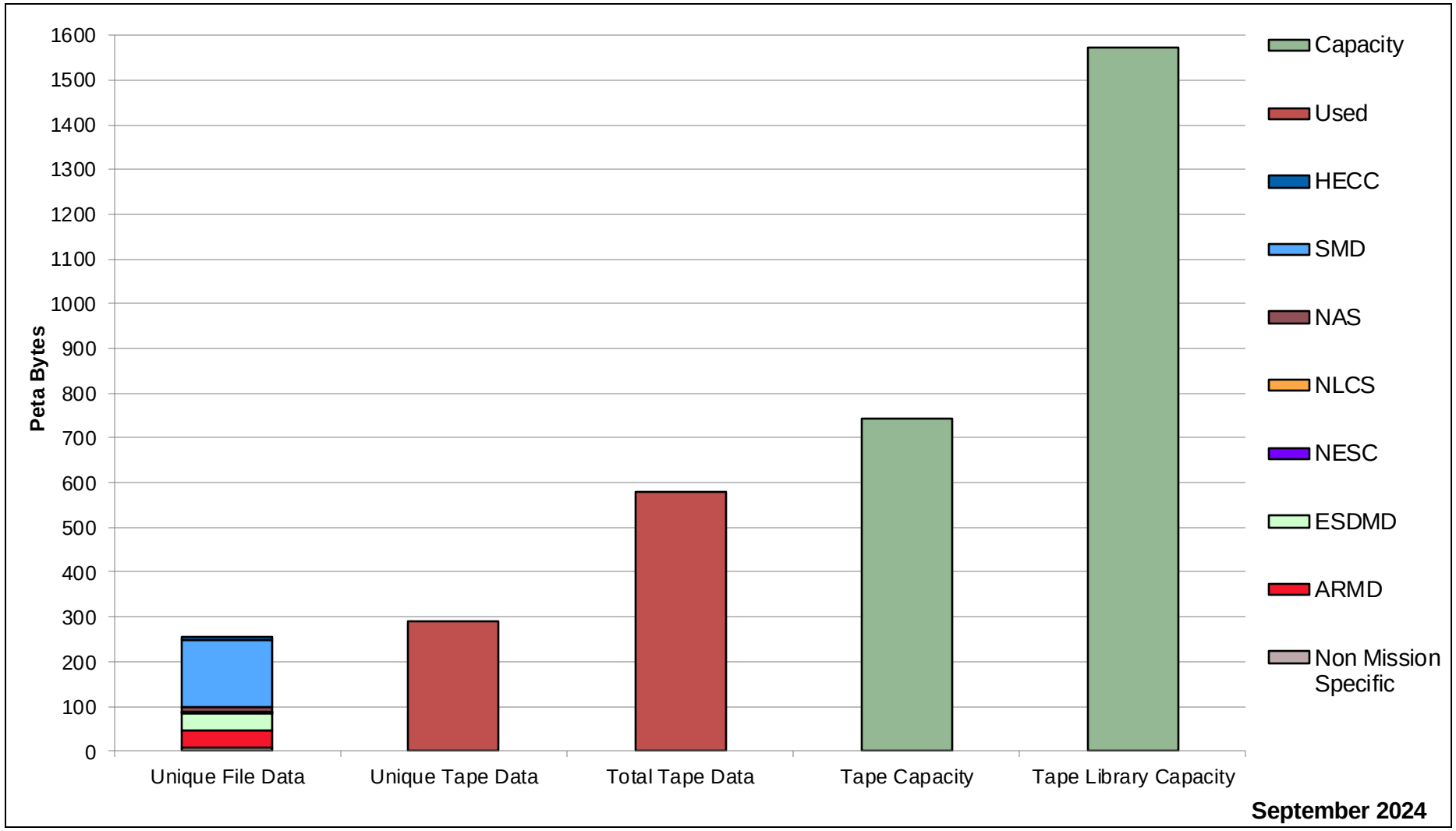
② Cabeus v100 nodes added

③ Cabeus Milan a100 nodes added

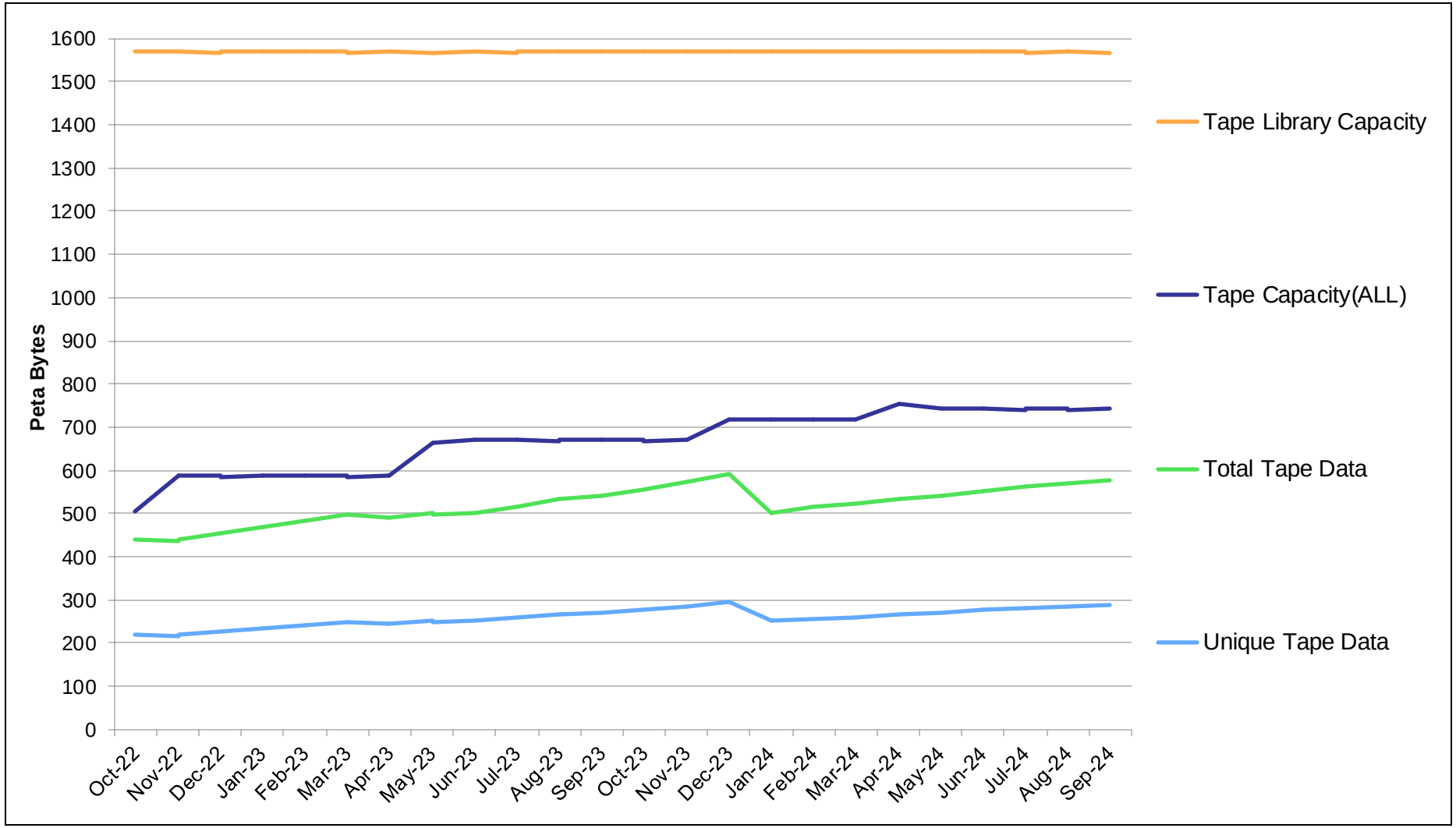
④ Aitken Milan Nodes added

⑤ Sandy Bridge temporarily removed

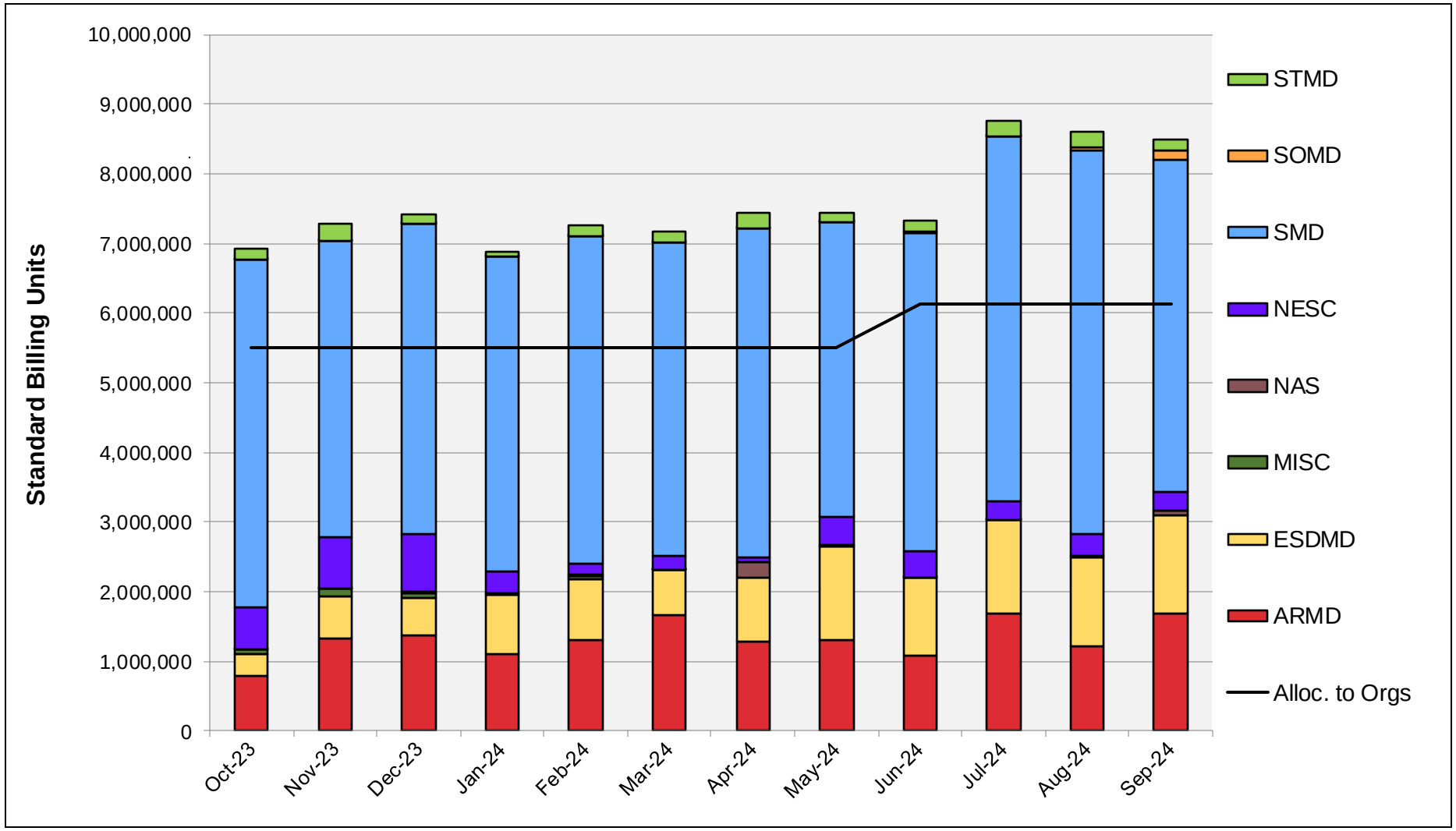
Tape Archive Status



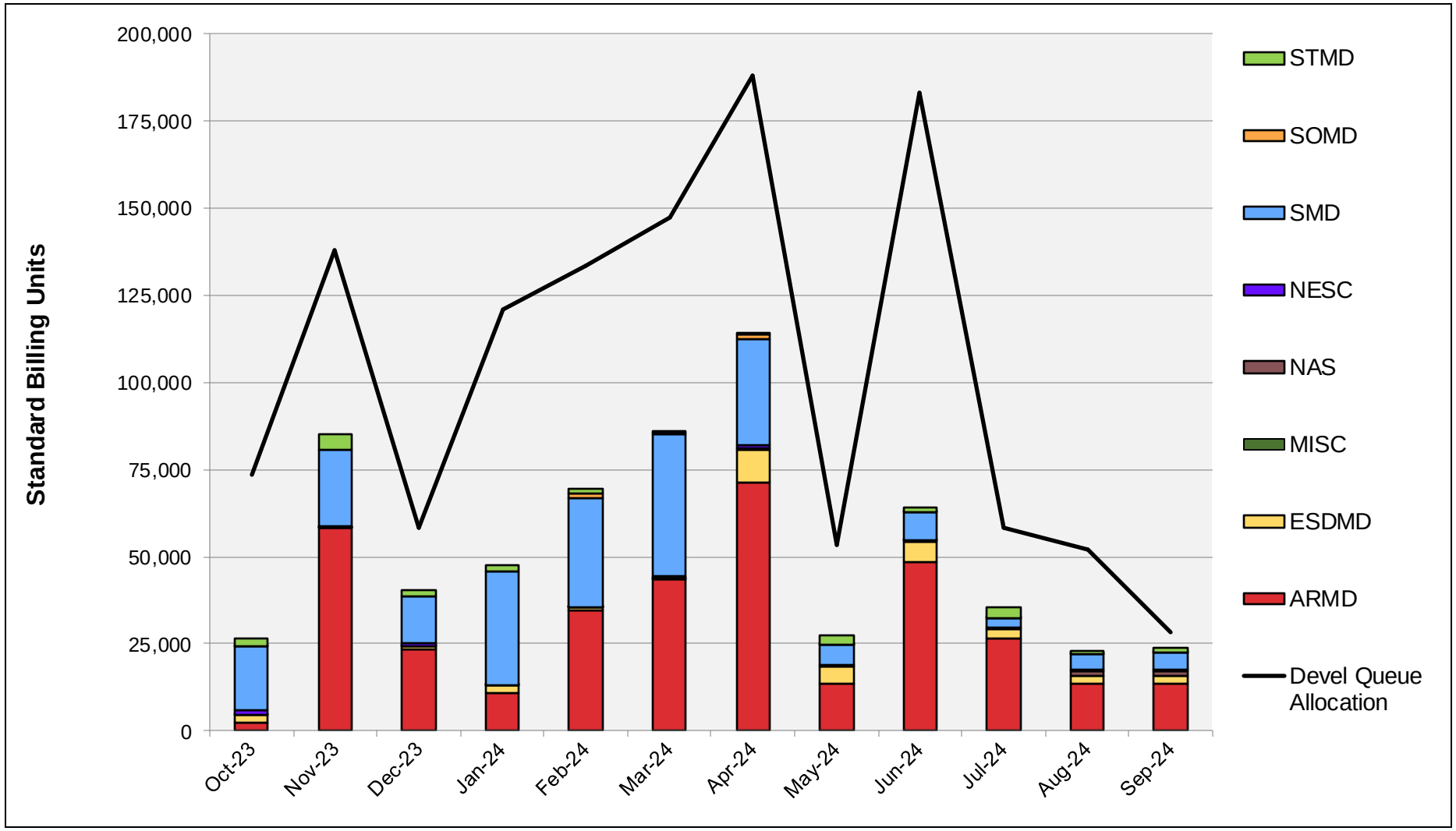
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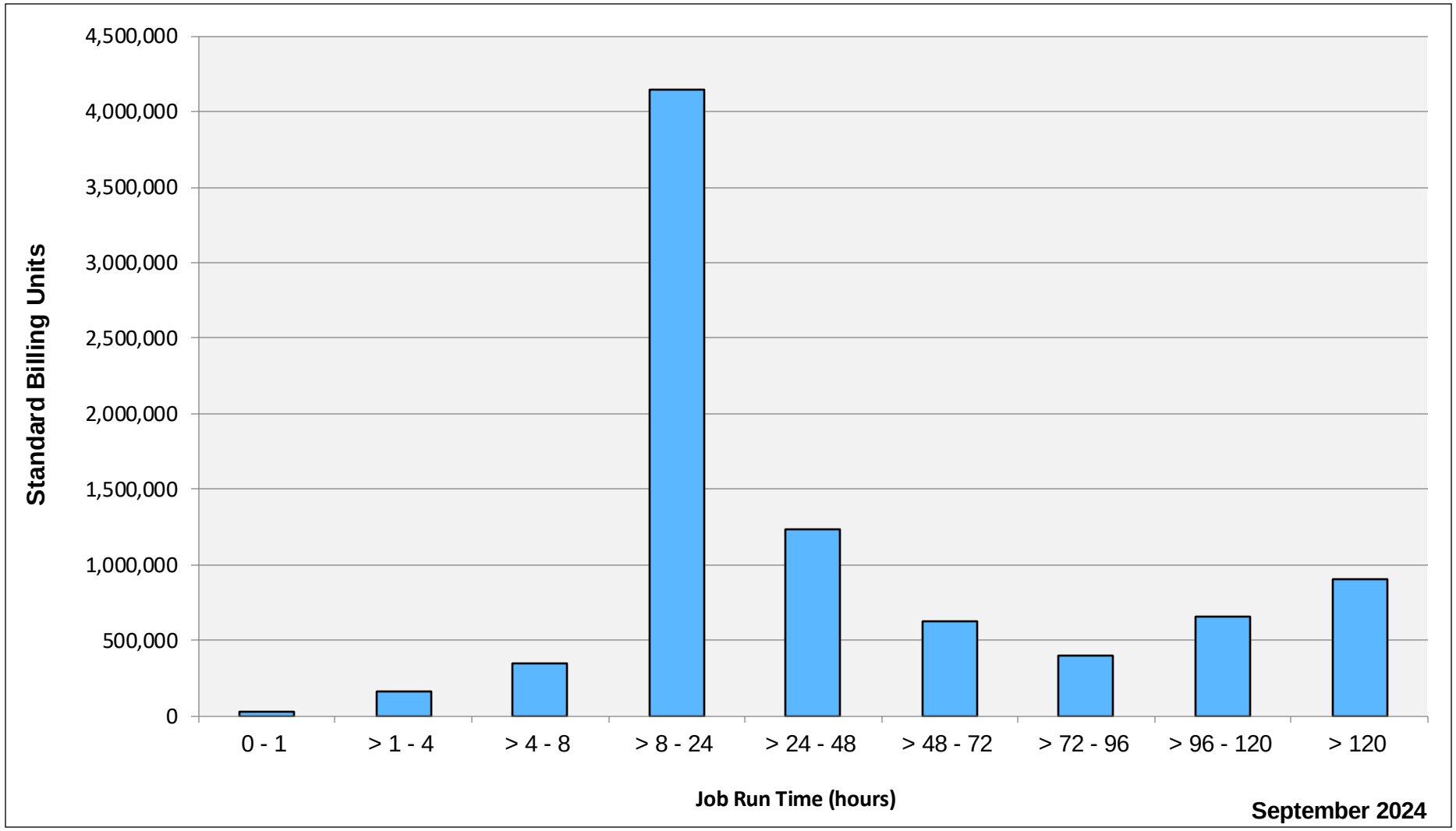
Aitken: SBUs Reported, Normalized to 30-Day Month



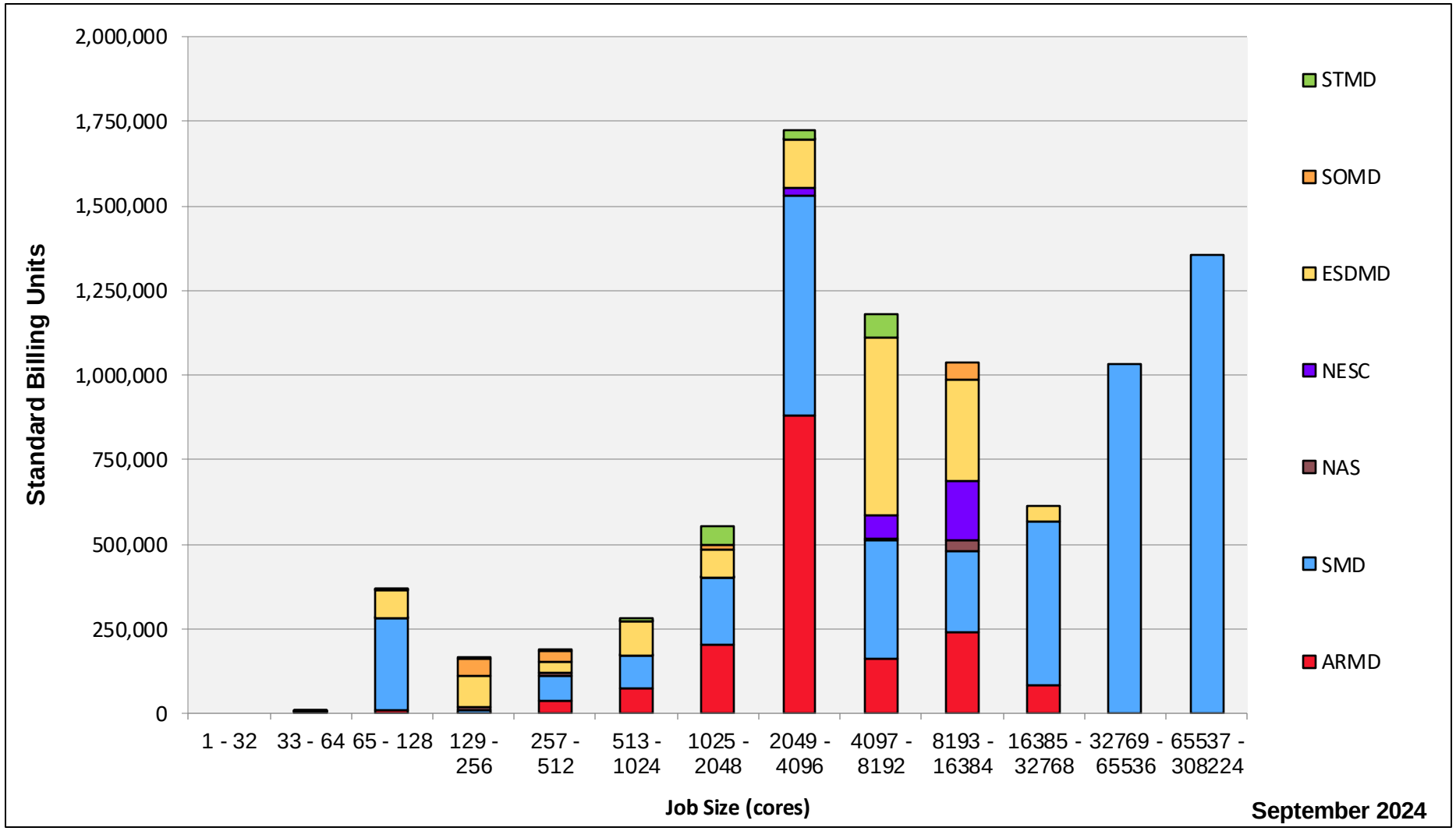
Aitken: Devel Queue Utilization



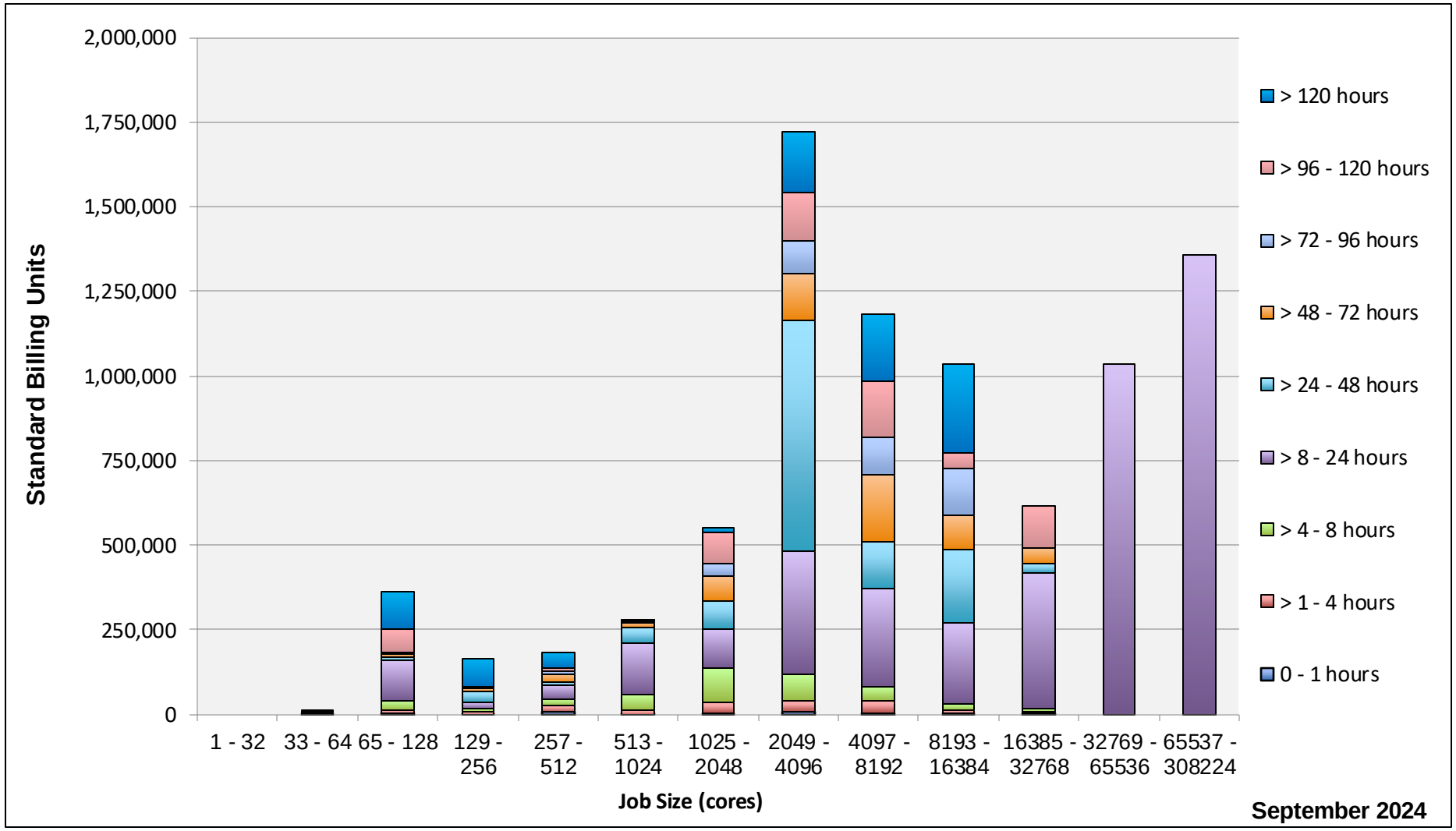
Aitken: Monthly Utilization by Job Length



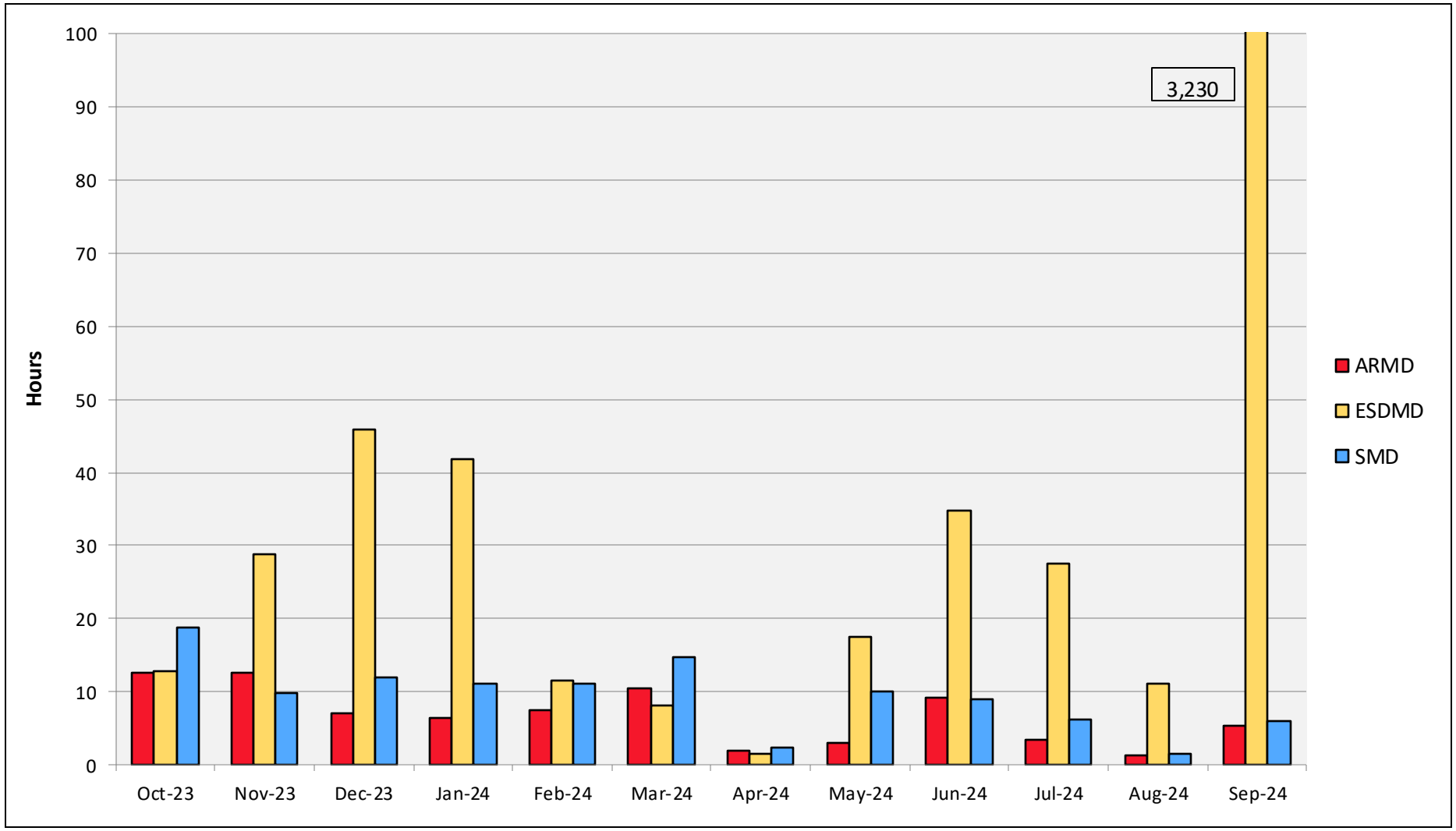
Aitken: Monthly Utilization by Job Size



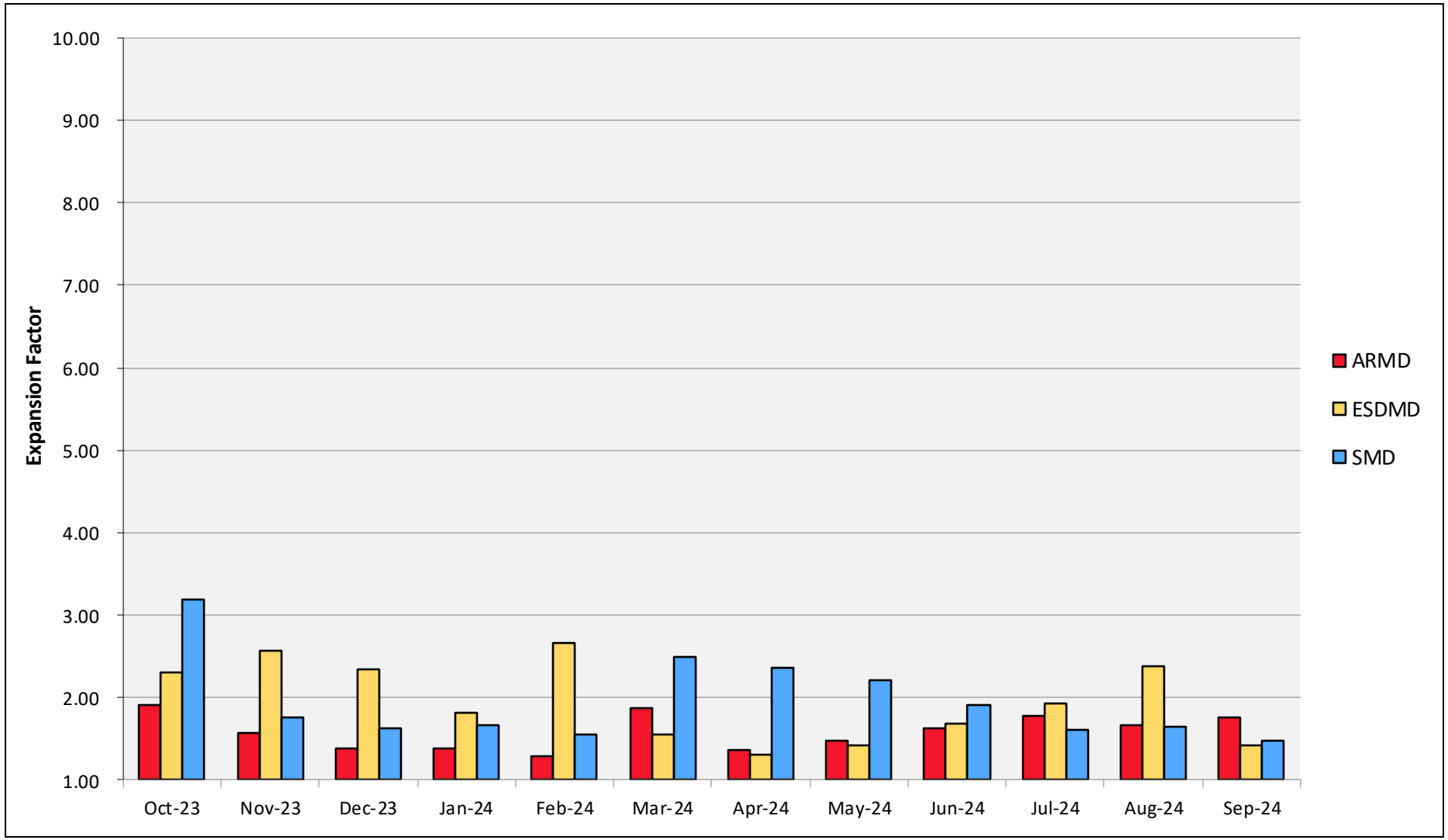
Aitken: Monthly Utilization by Size and Length



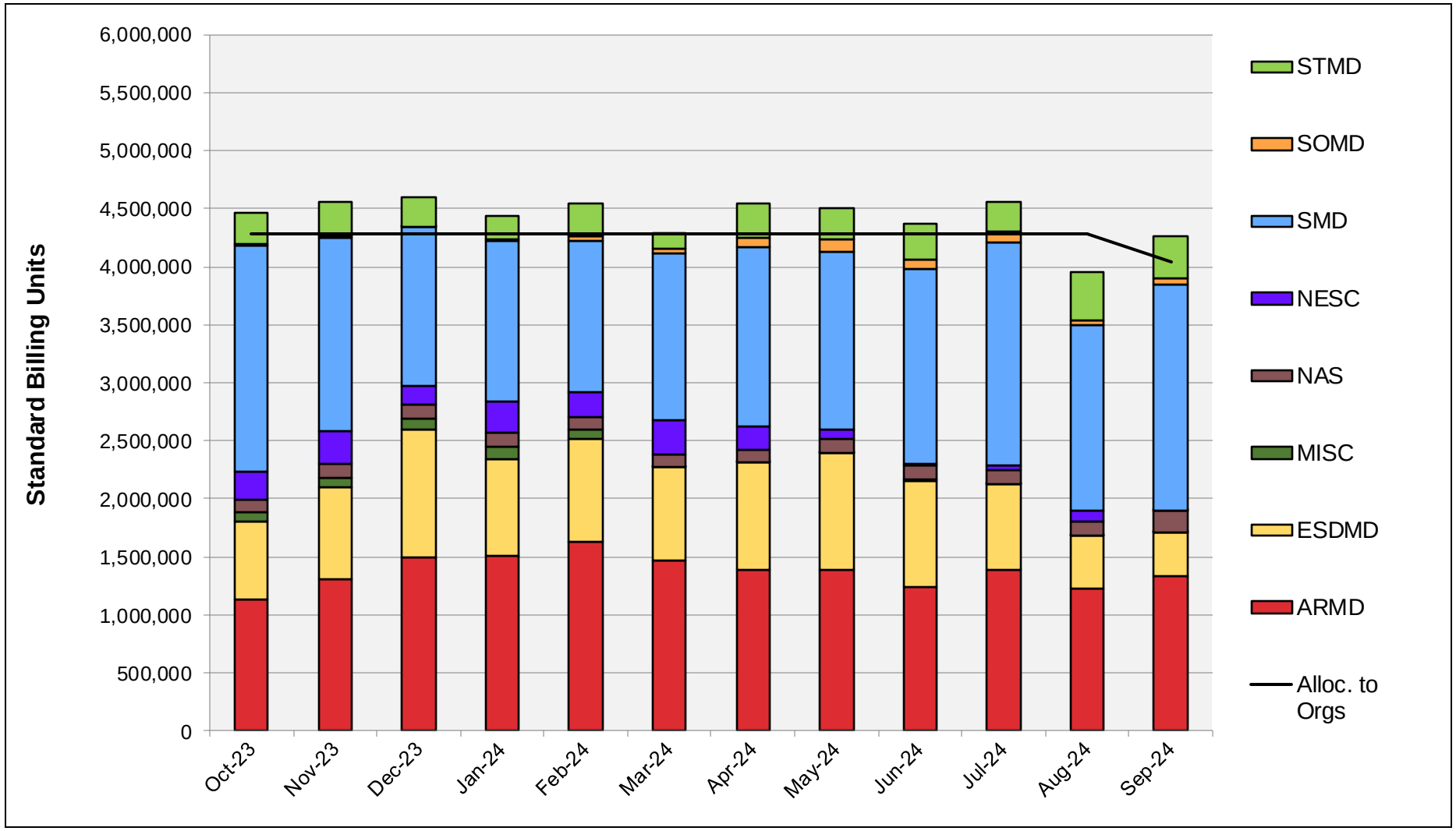
Aitken: Average Time to Clear All Jobs



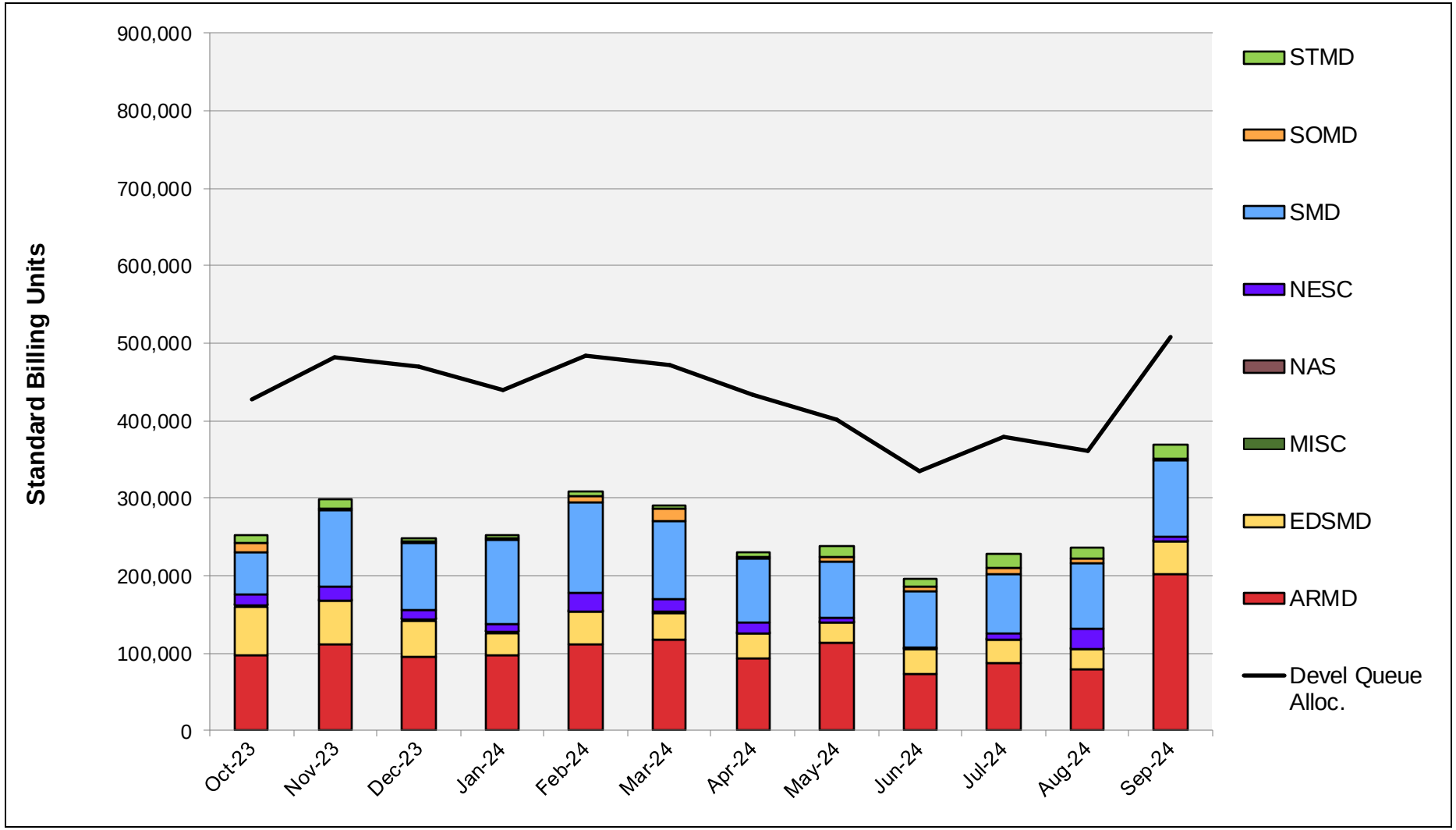
Aitken: Average Expansion Factor



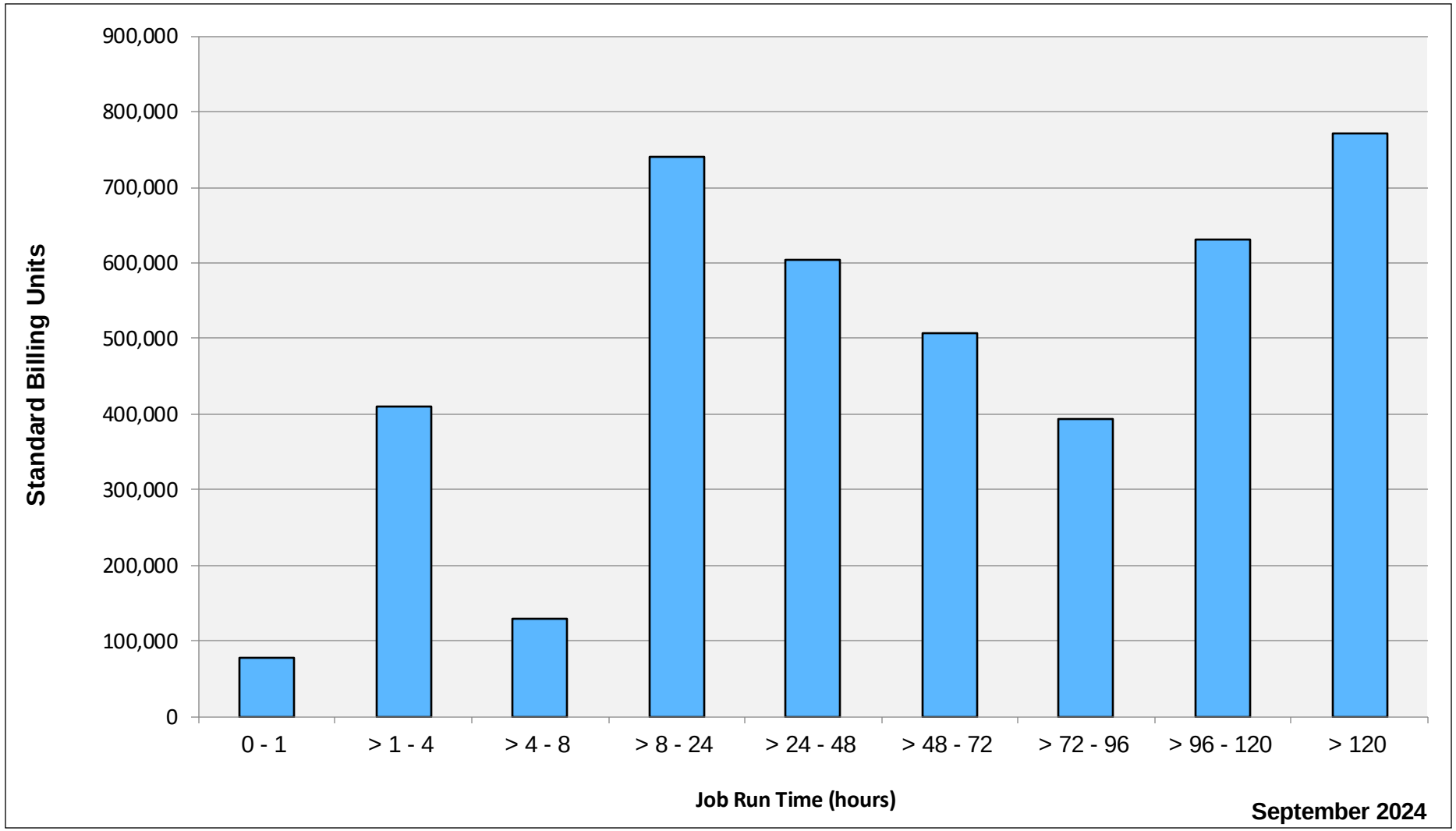
Pleiades: SBUs Reported, Normalized to 30-Day Month



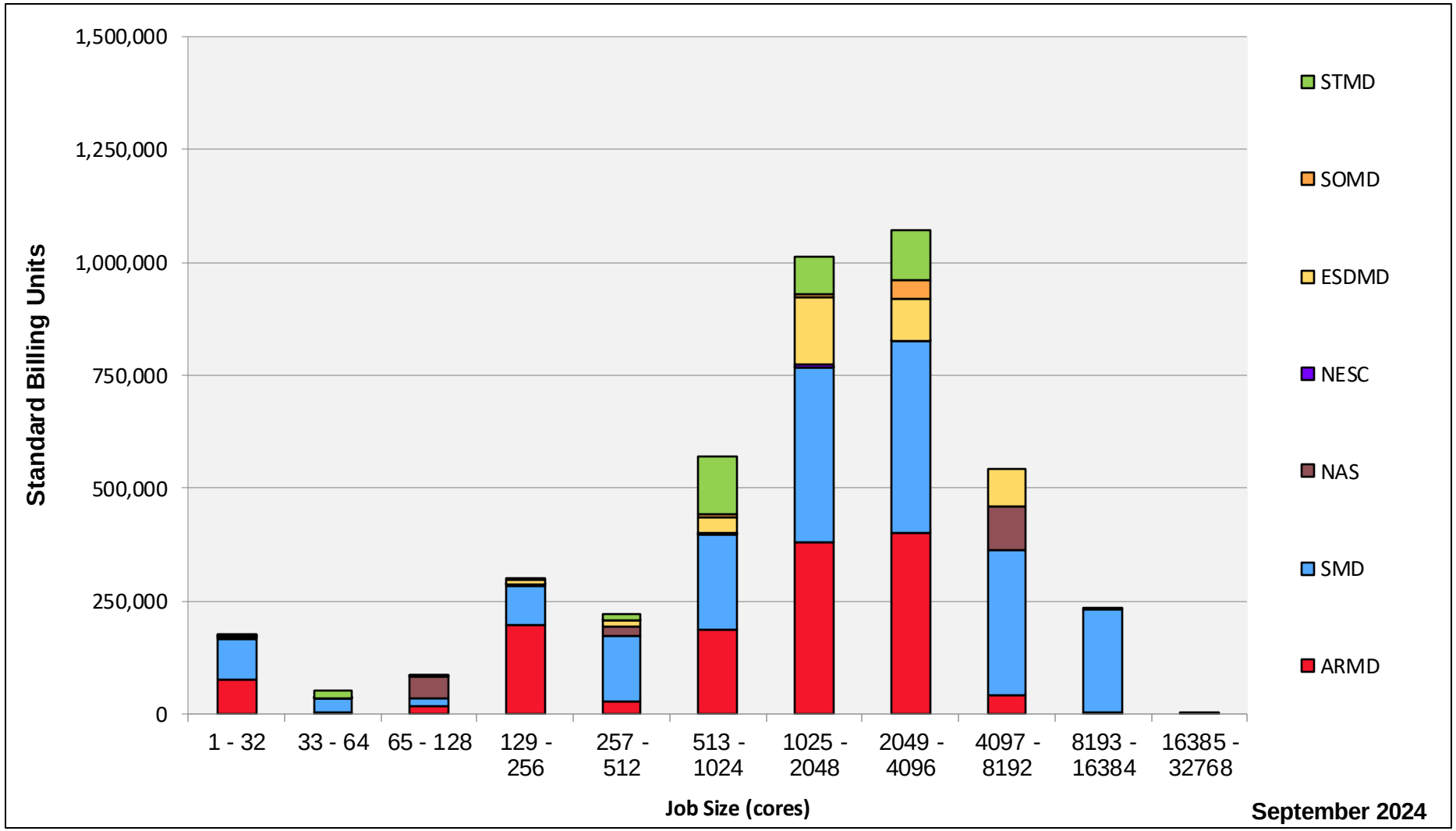
Pleiades: Devel Queue Utilization



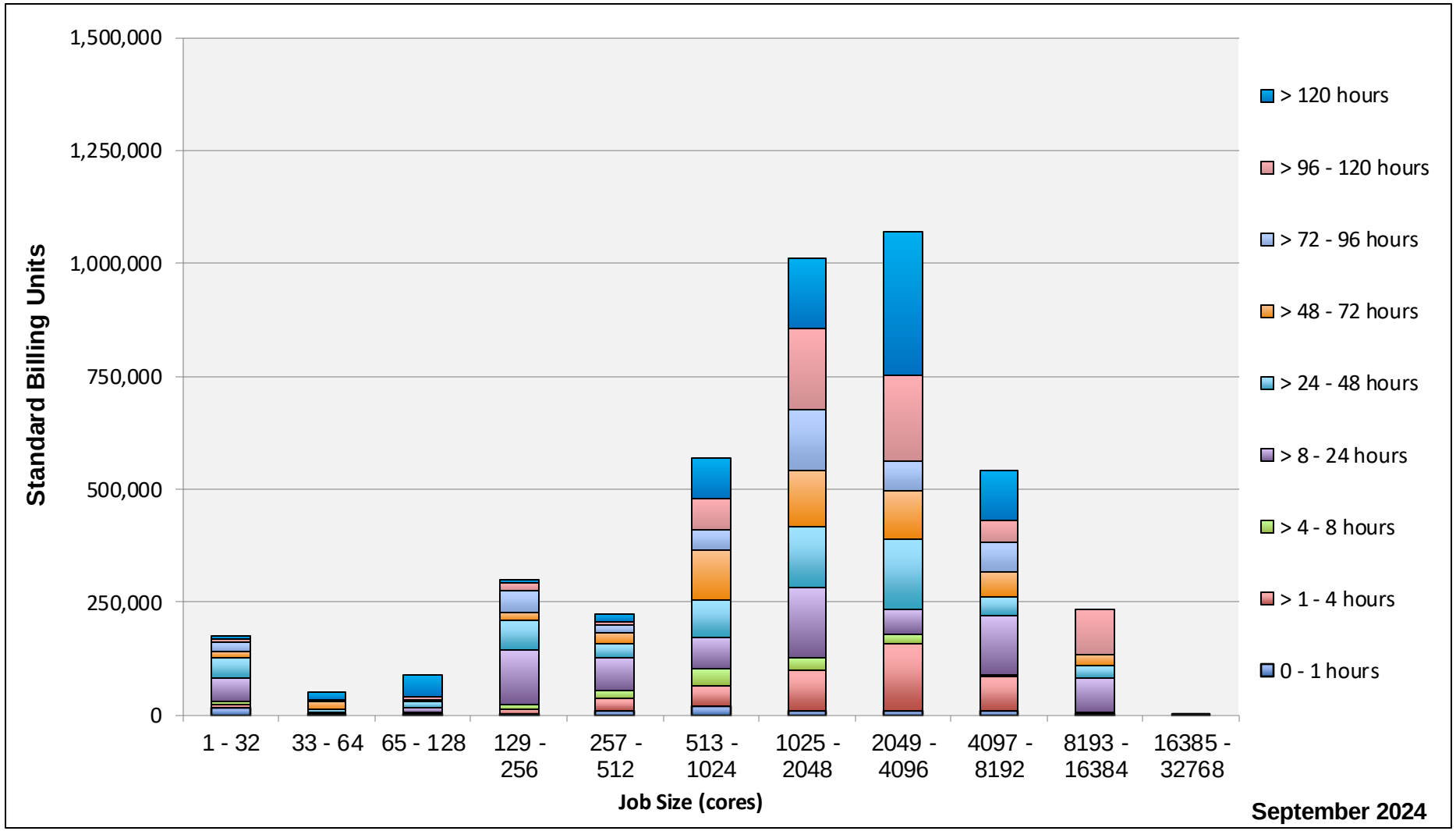
Pleiades: Monthly Utilization by Job Length



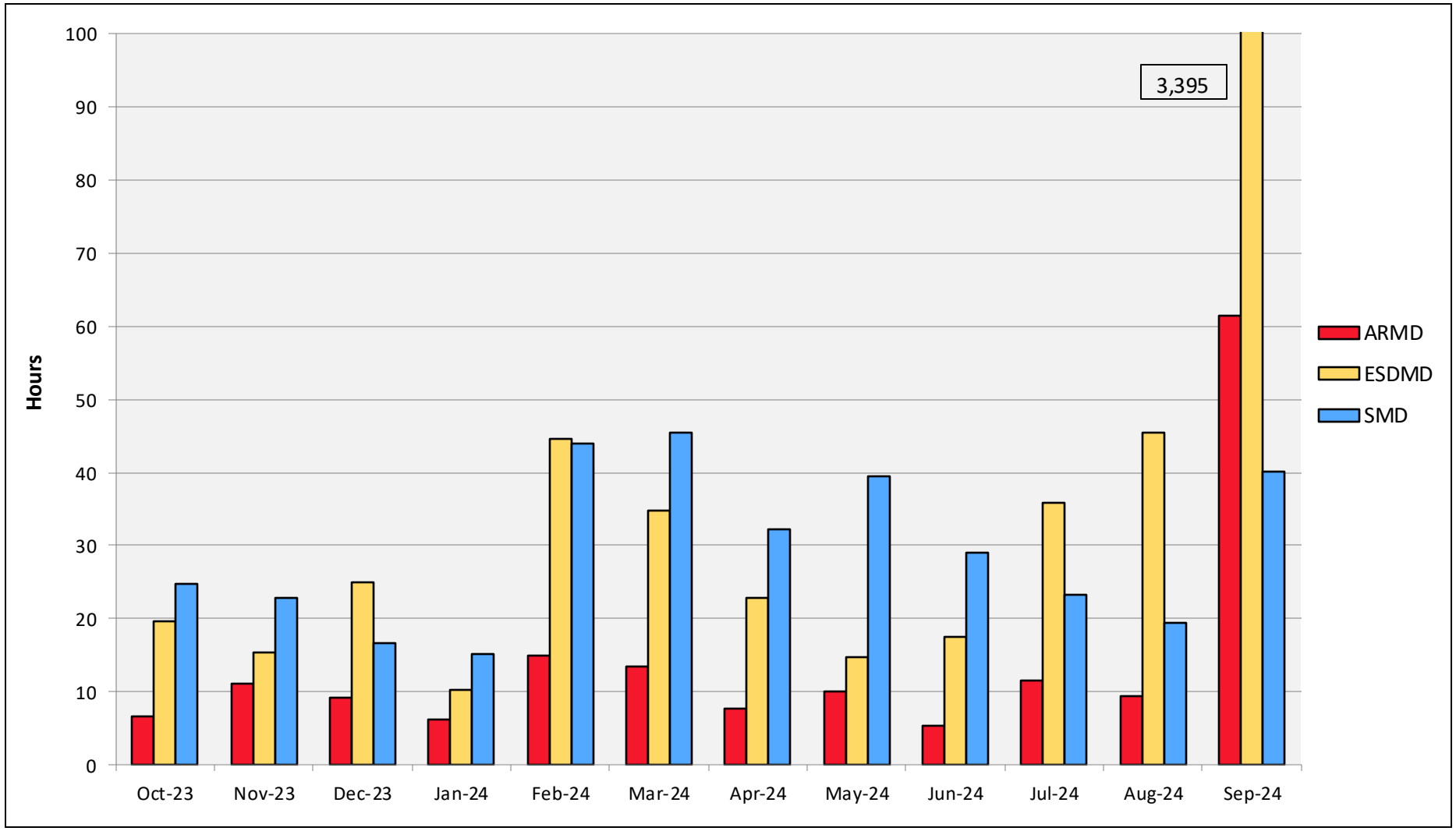
Pleiades: Monthly Utilization by Job Size



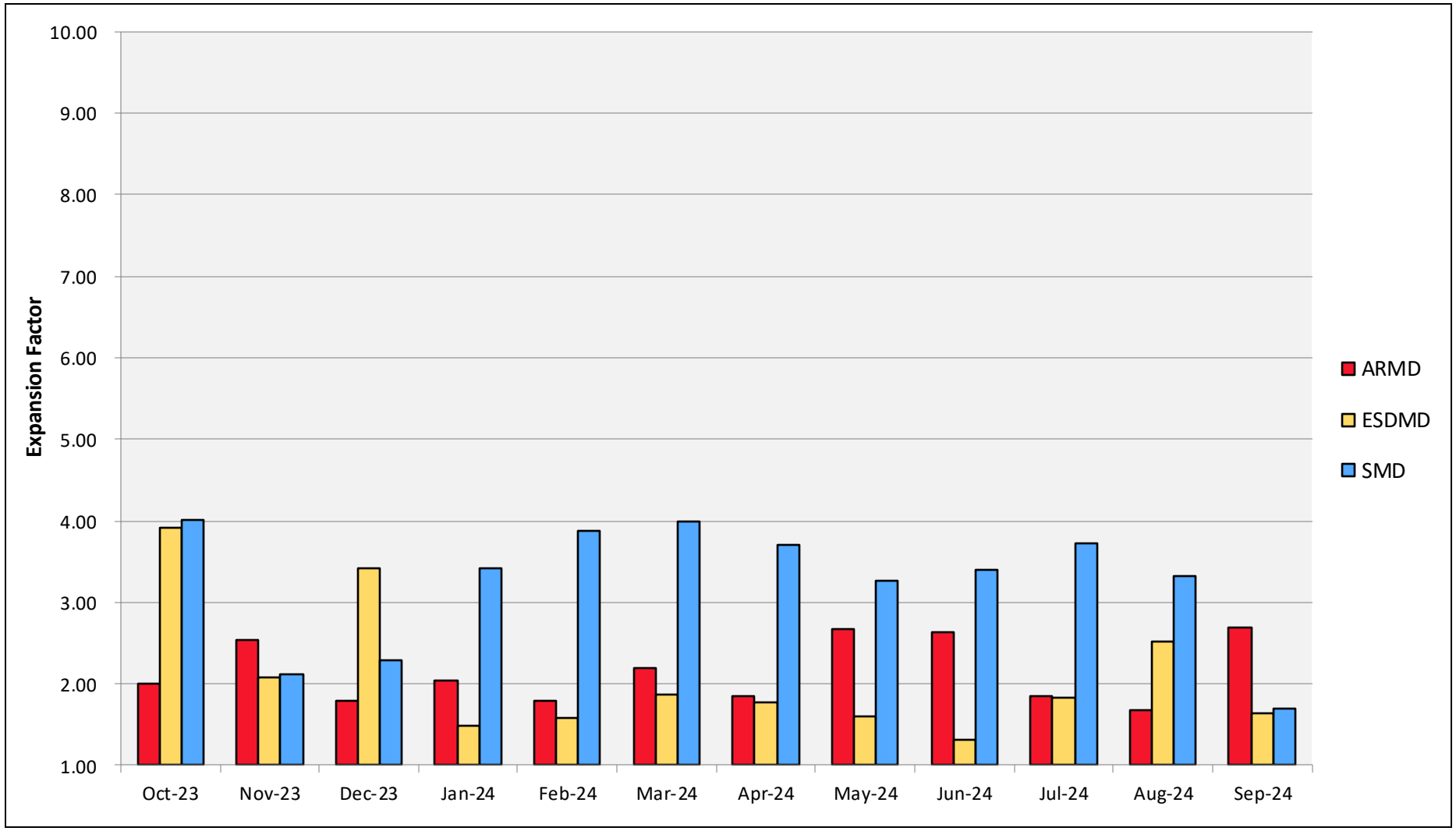
Pleiades: Monthly Utilization by Size and Length



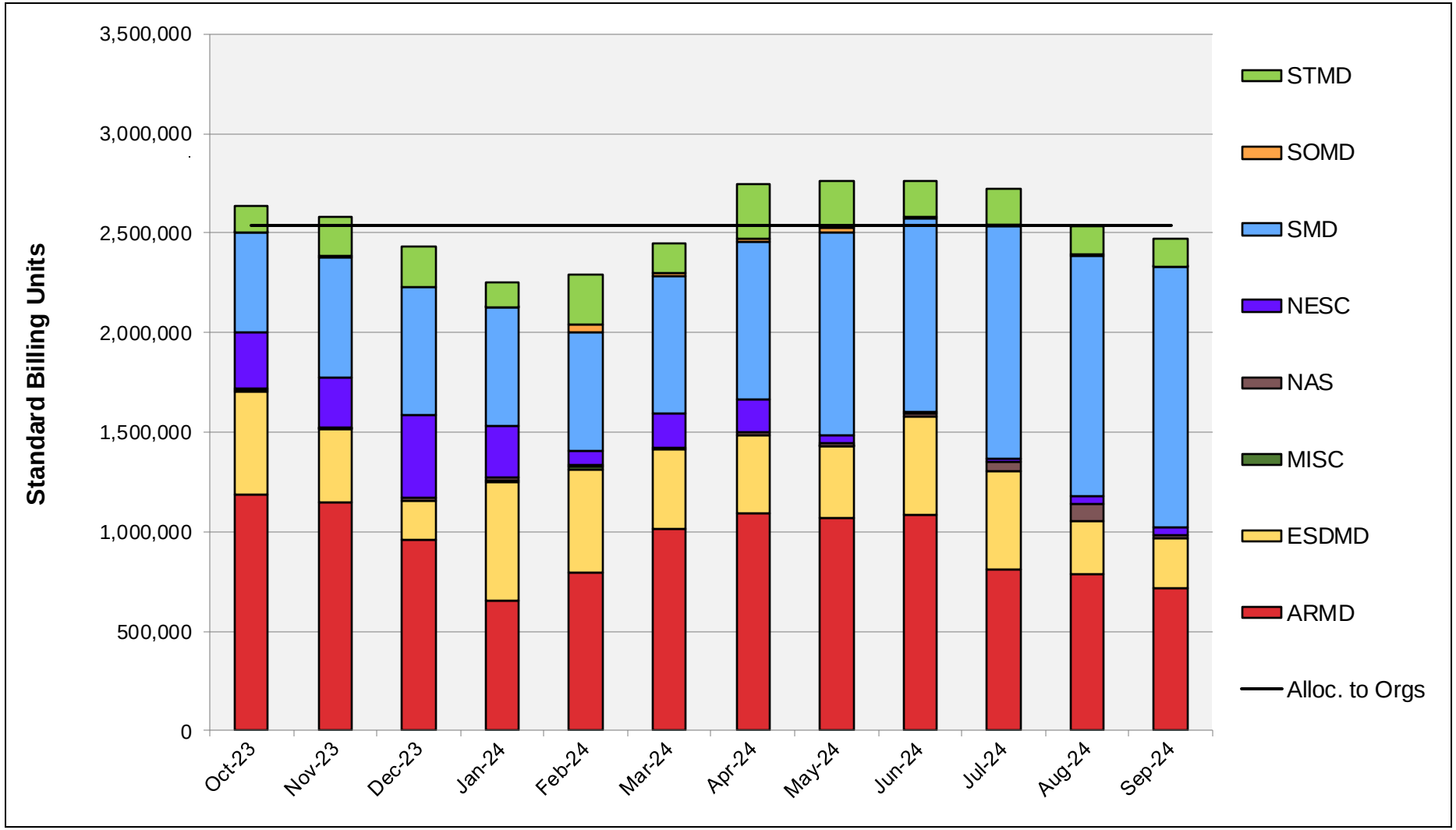
Pleiades: Average Time to Clear All Jobs



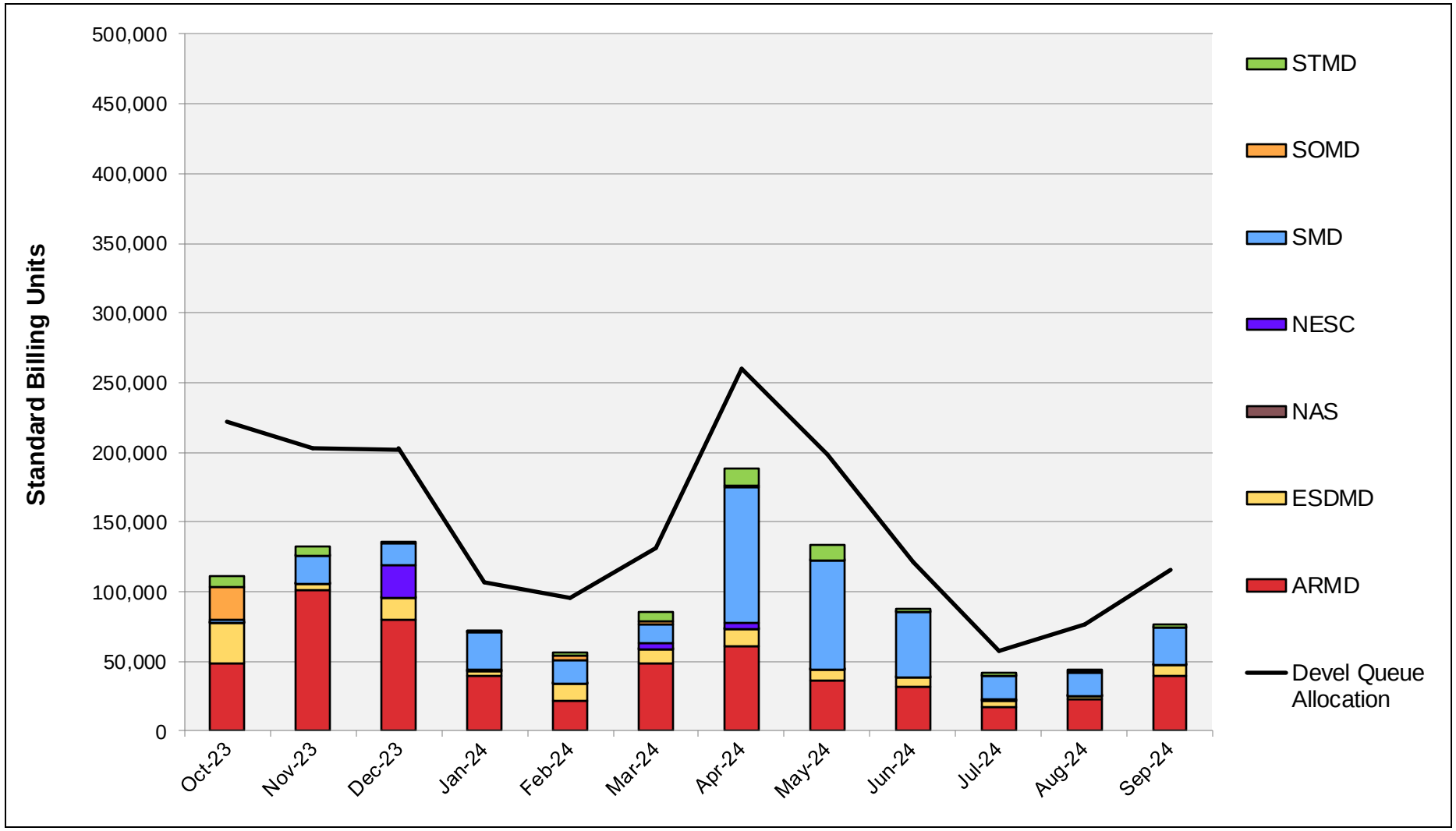
Pleiades: Average Expansion Factor



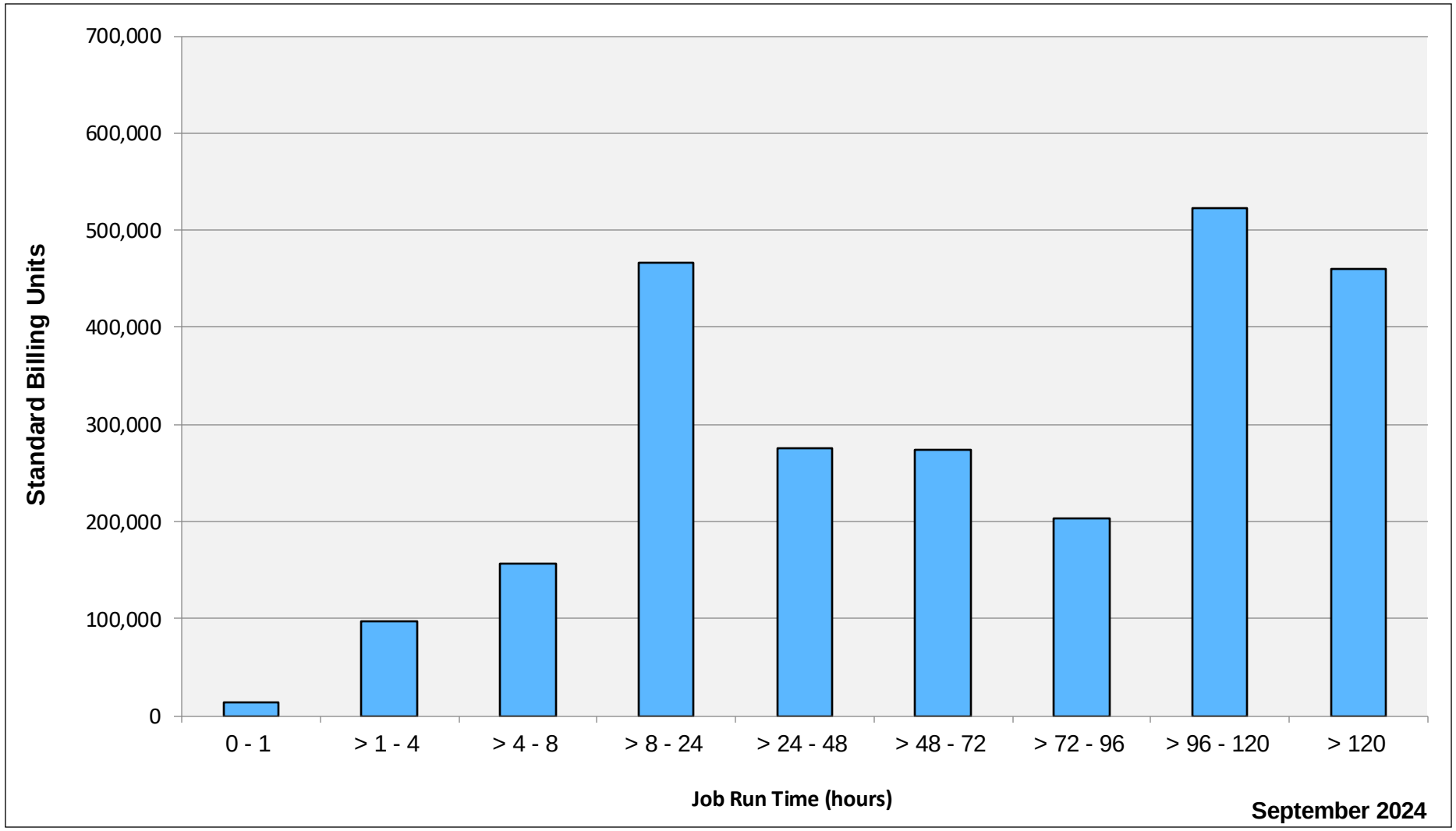
Electra: SBUs Reported, Normalized to 30-Day Month



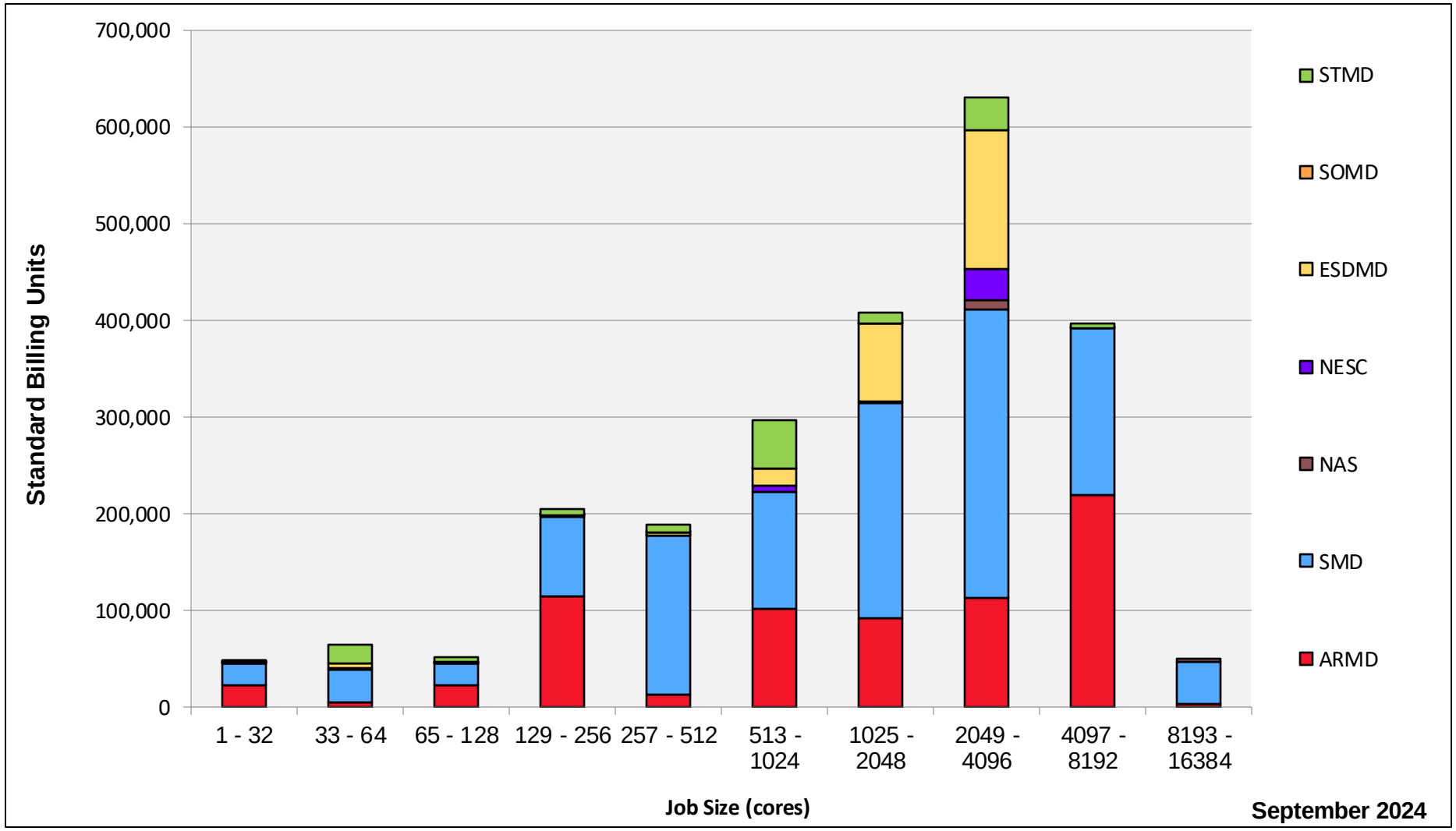
Electra: Devel Queue Utilization



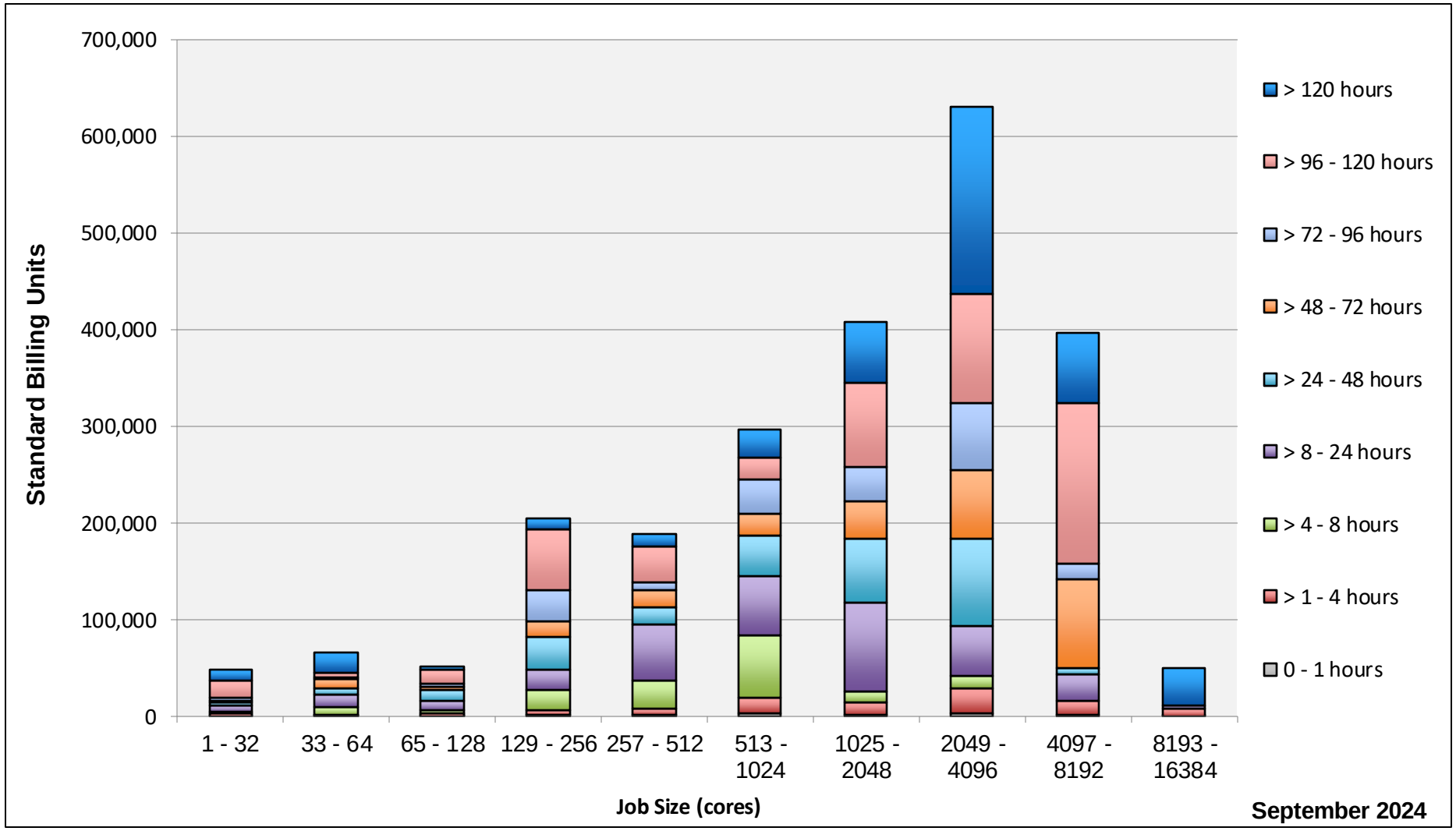
Electra: Monthly Utilization by Job Length



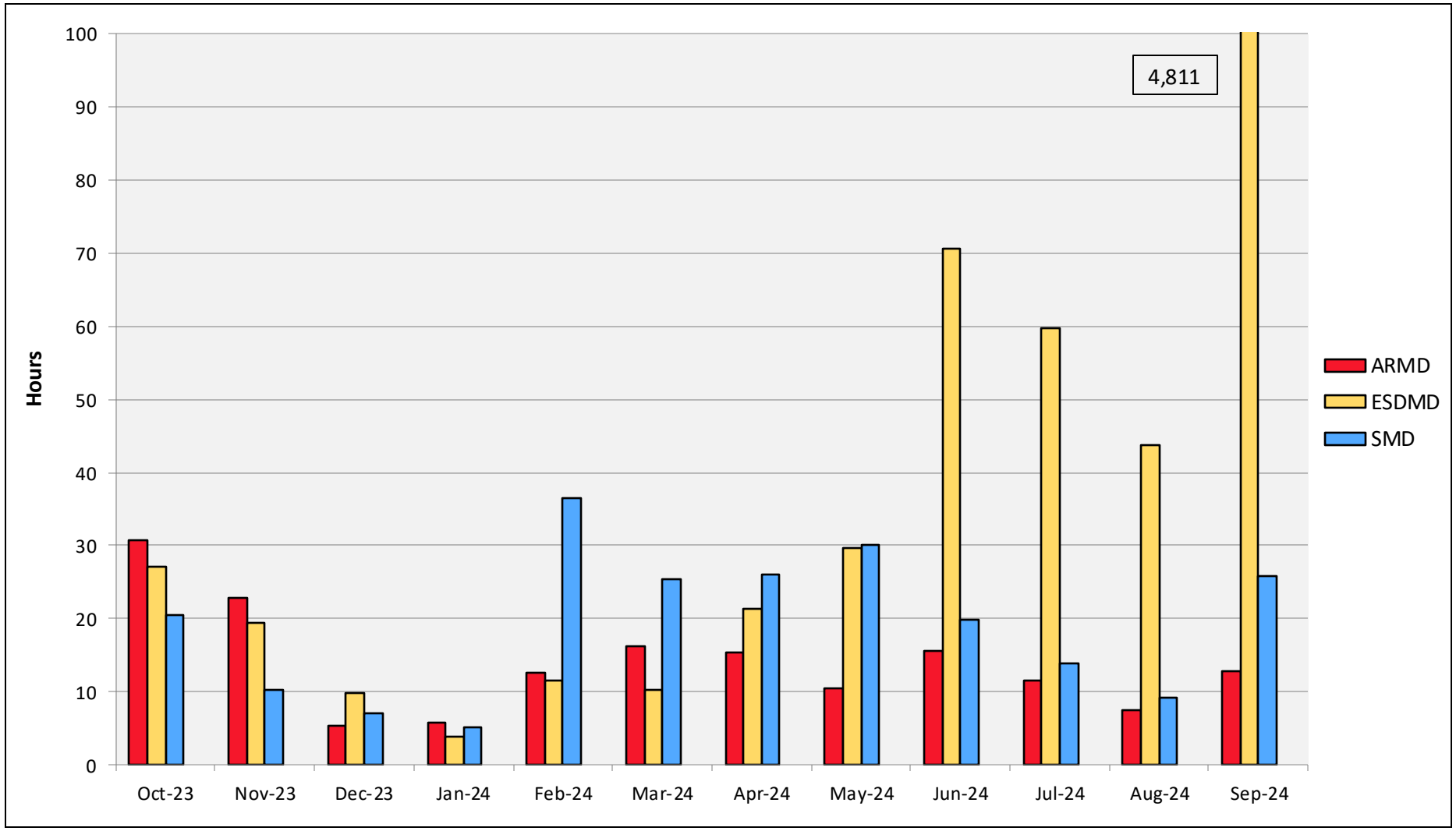
Electra: Monthly Utilization by Job Size



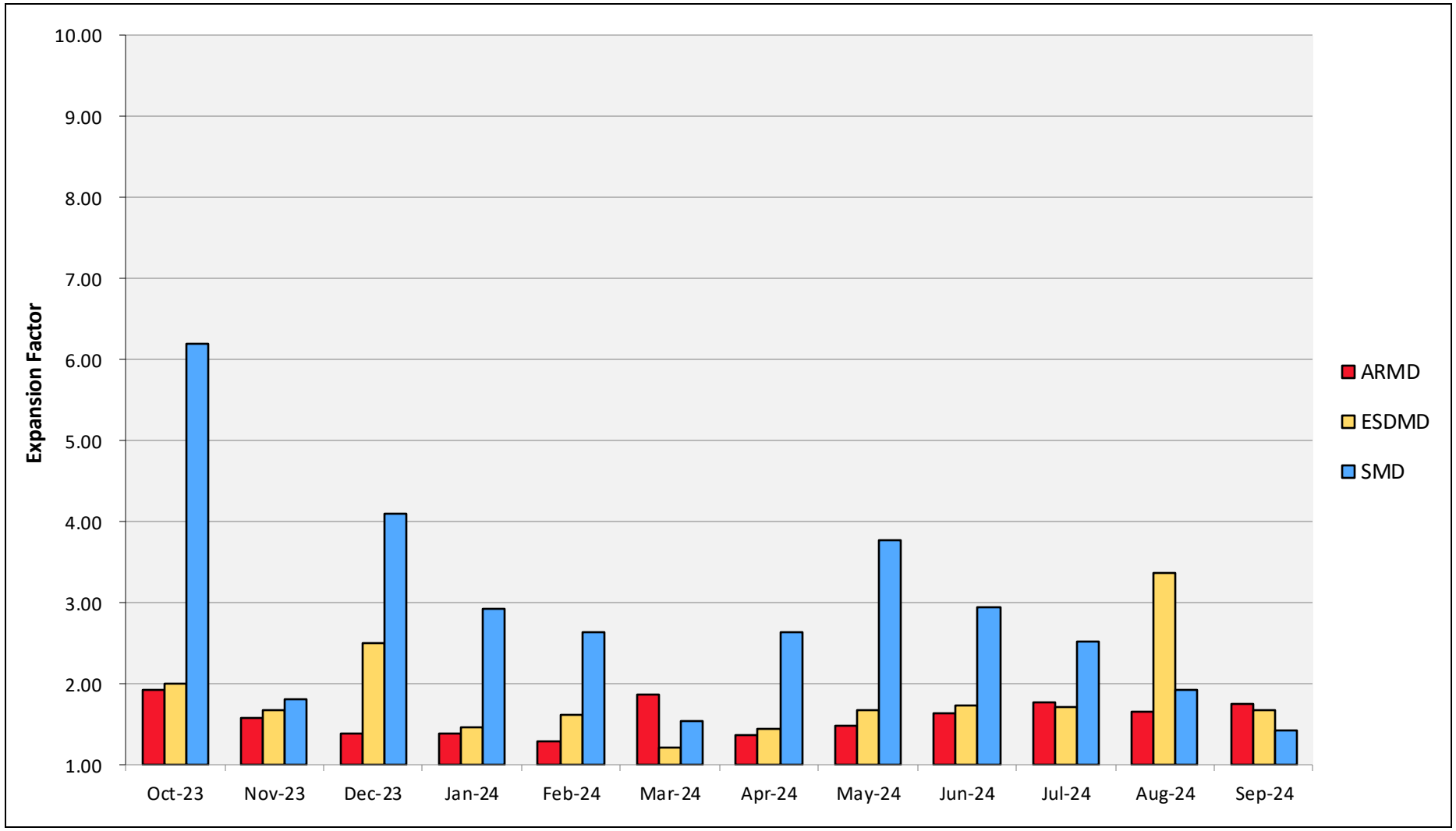
Electra: Monthly Utilization by Size and Length



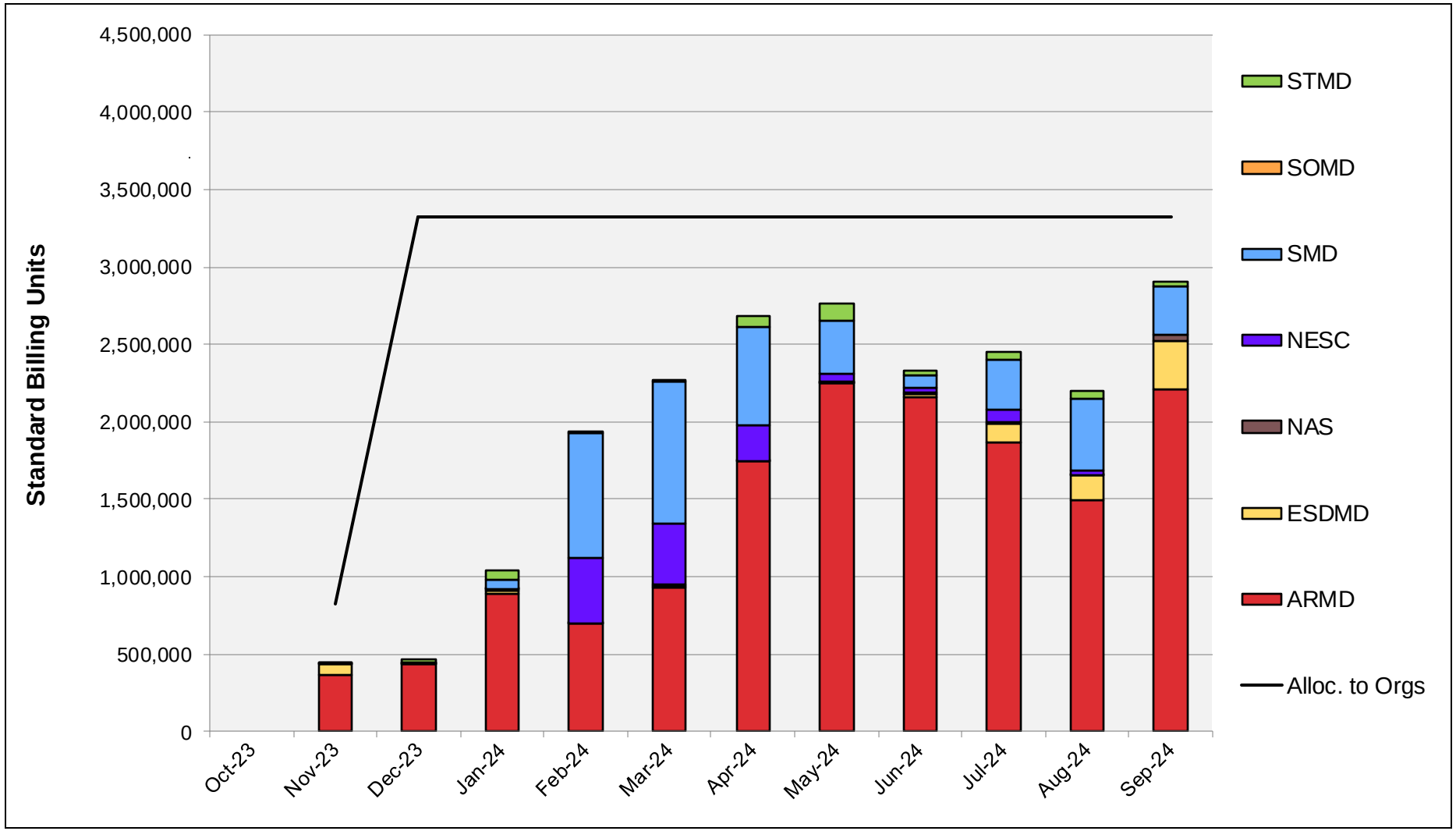
Electra: Average Time to Clear All Jobs



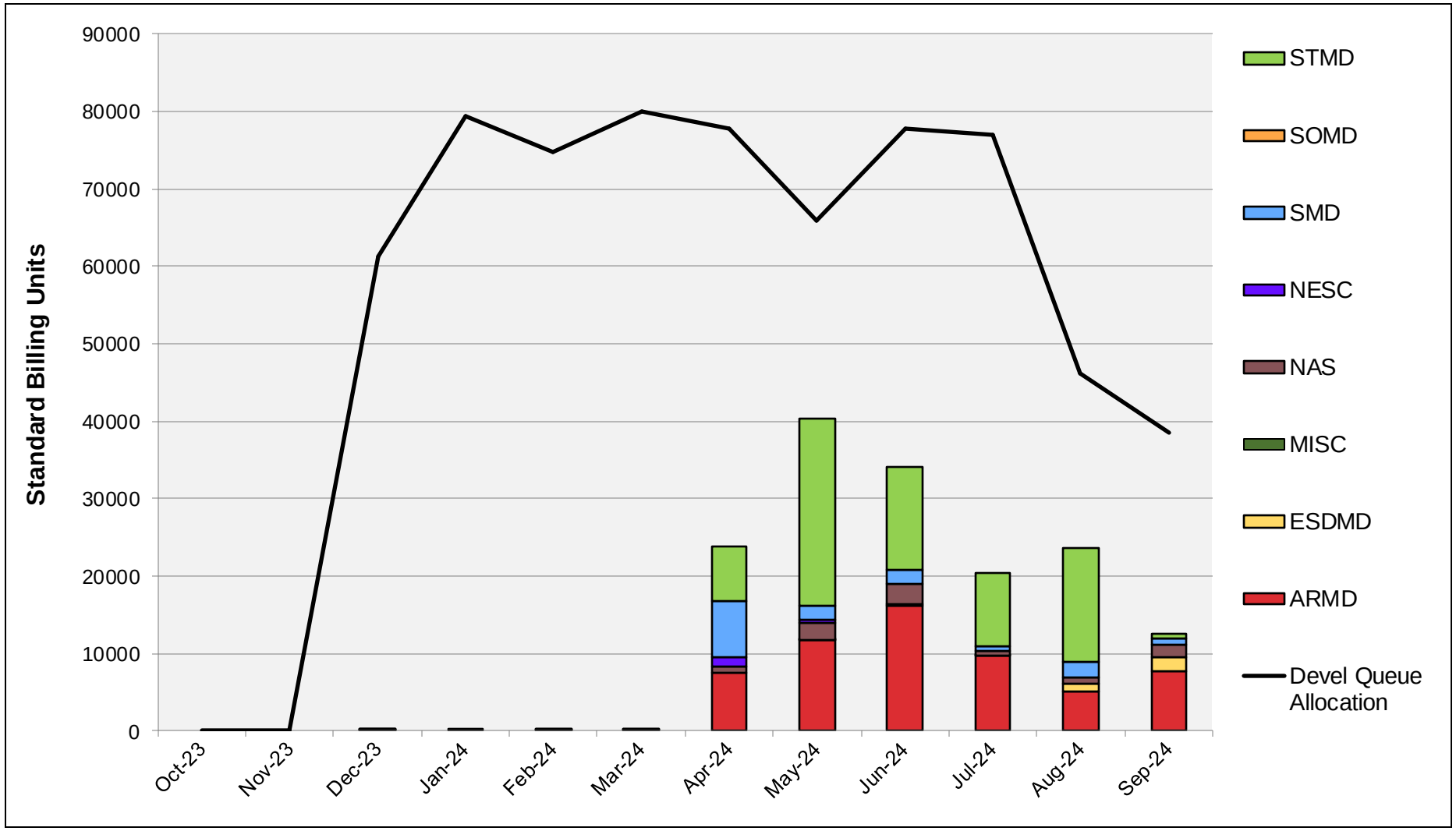
Electra: Average Expansion Factor



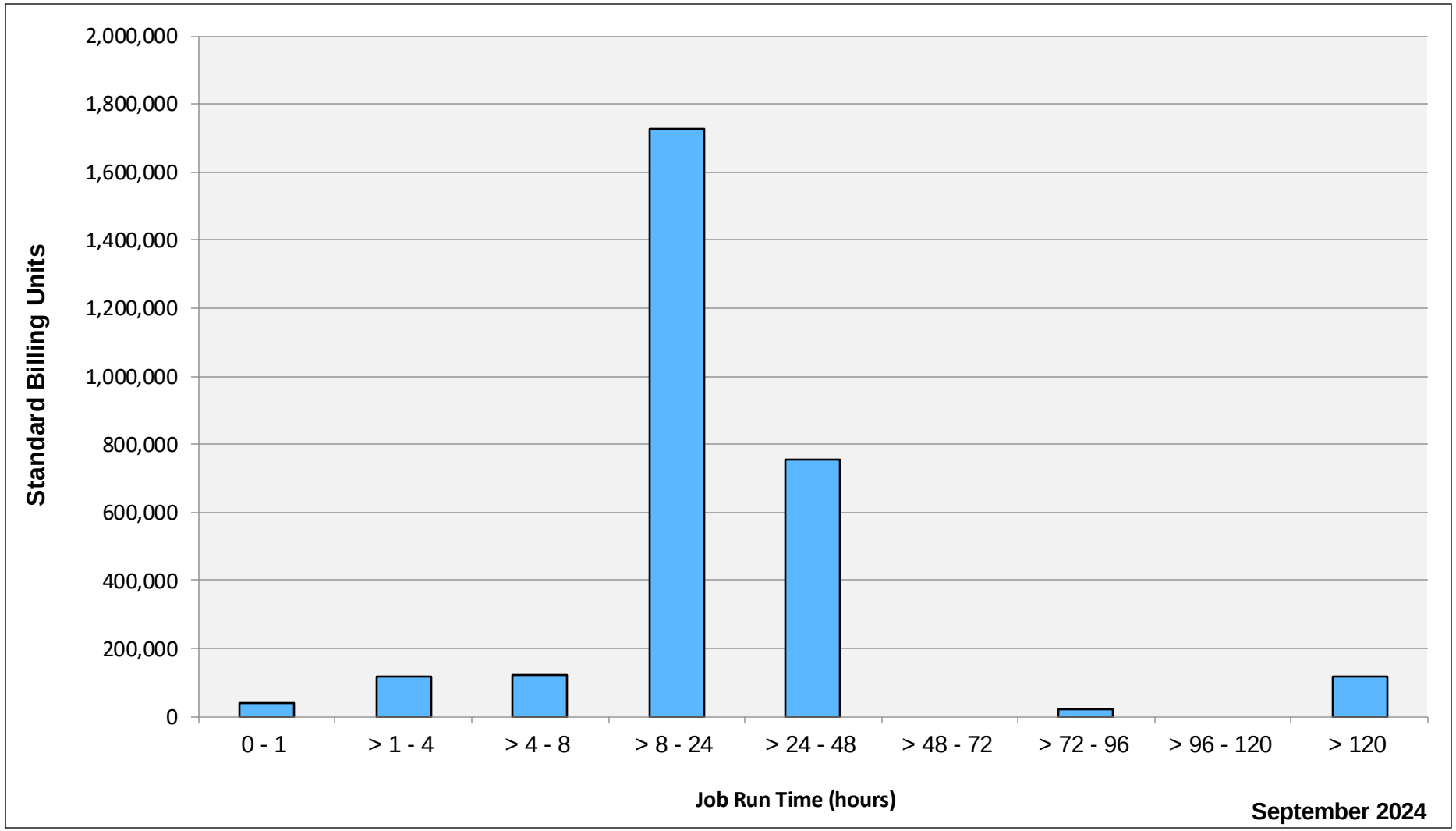
Cabeus: SBUs Reported, Normalized to 30-Day Month



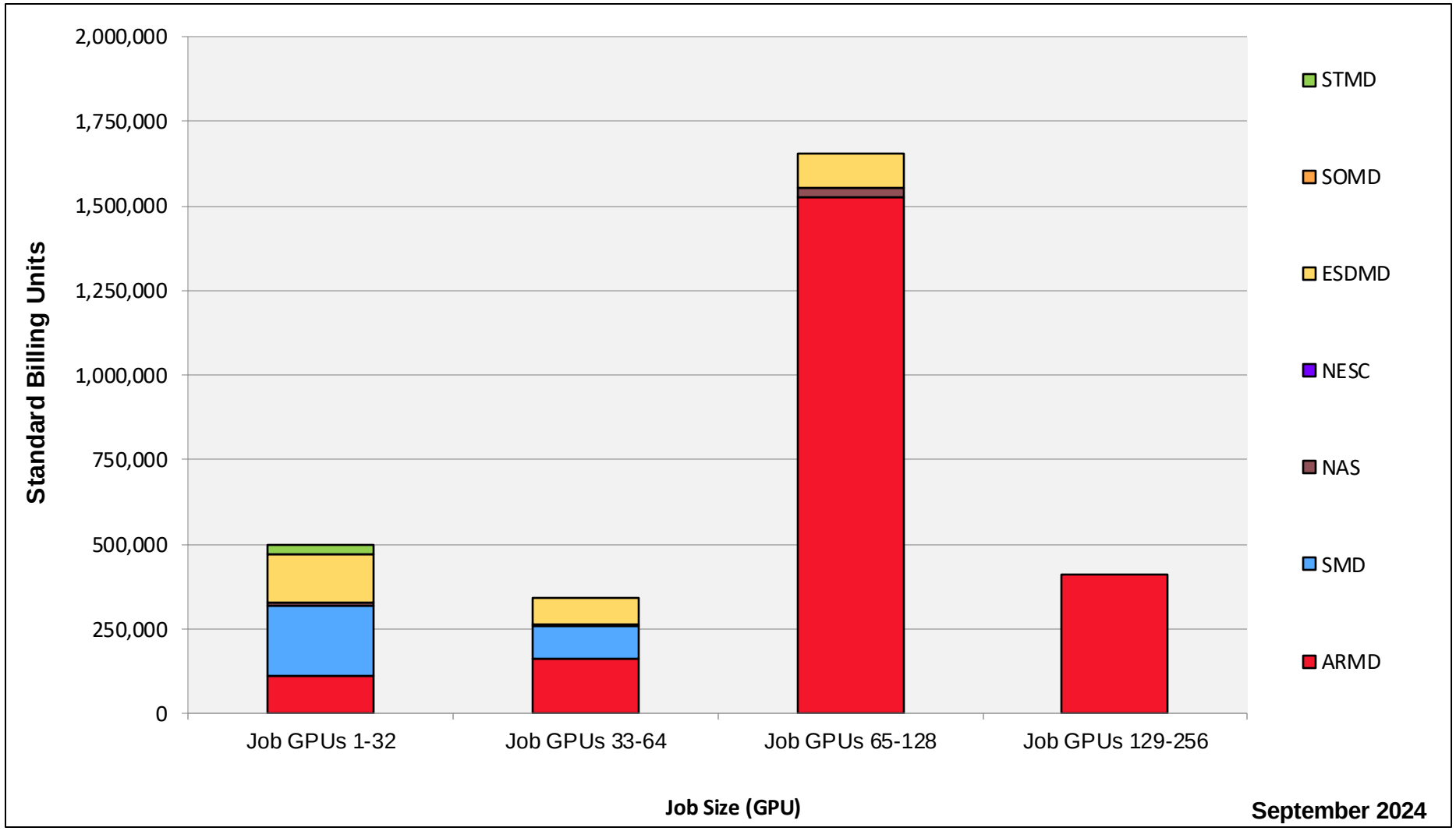
Cabeus: Devel Queue Utilization



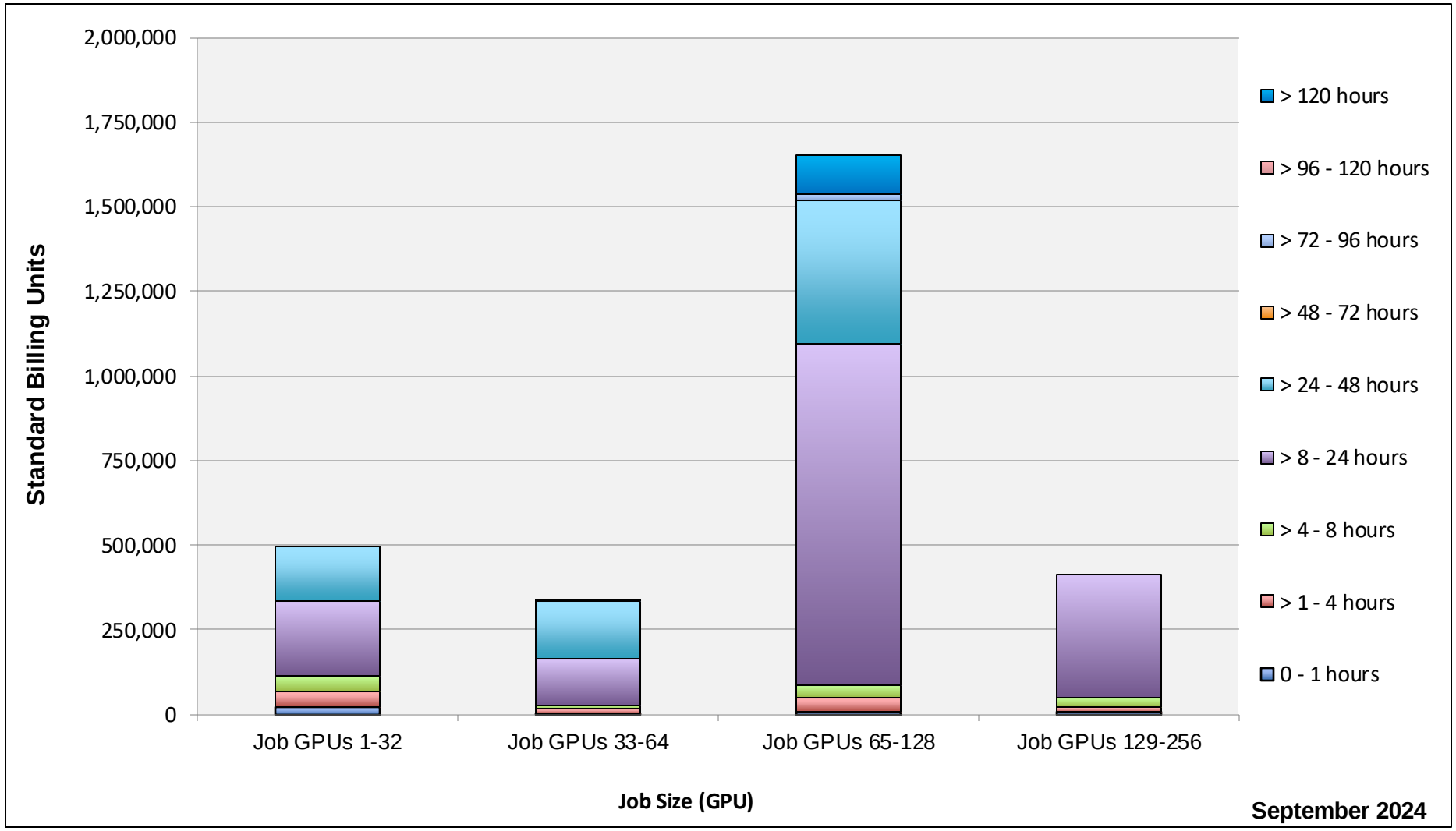
Cabeus: Monthly Utilization by Job Length



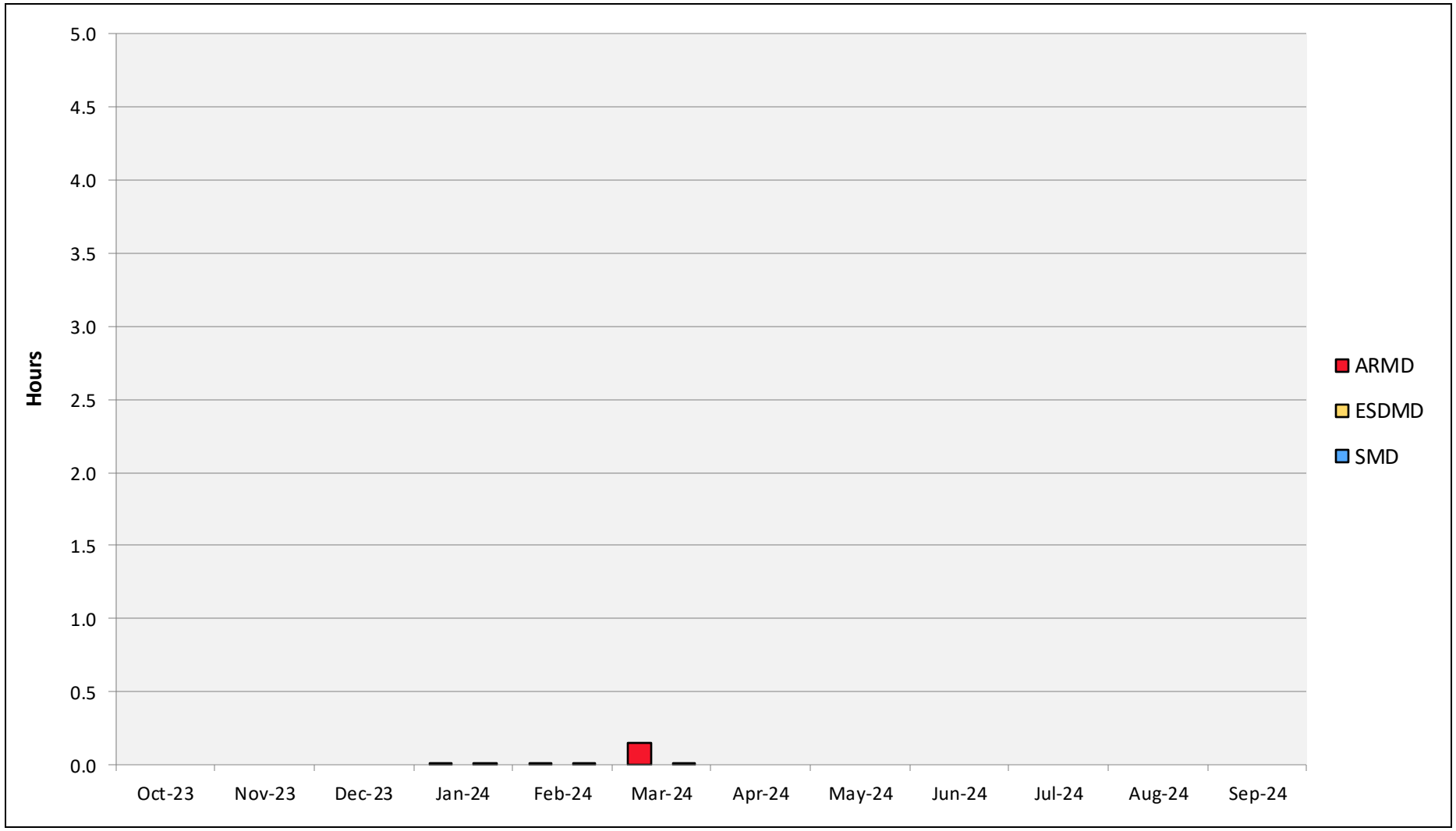
Cabeus: Monthly Utilization by Job Size



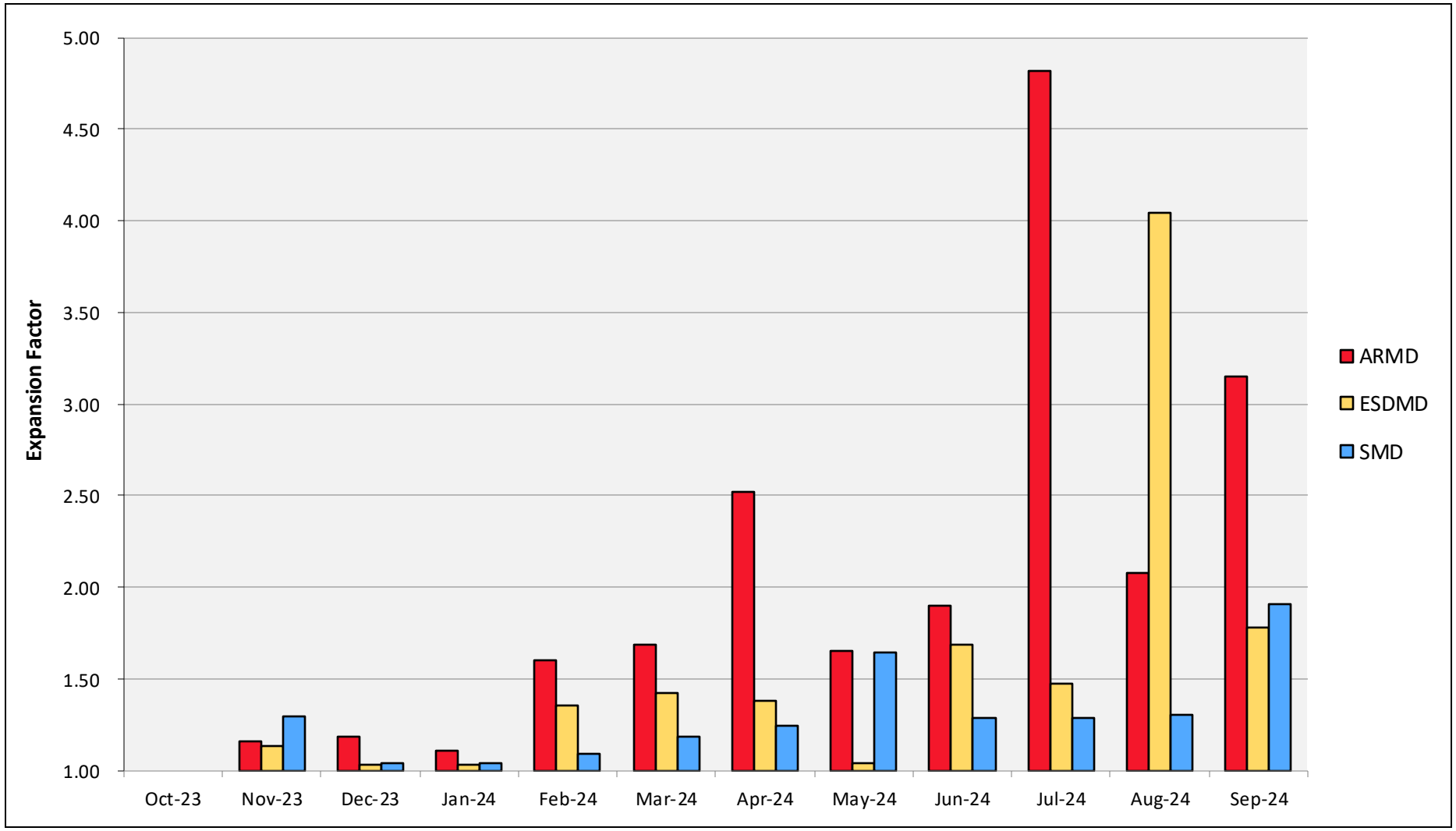
Cabeus: Monthly Utilization by Size and Length



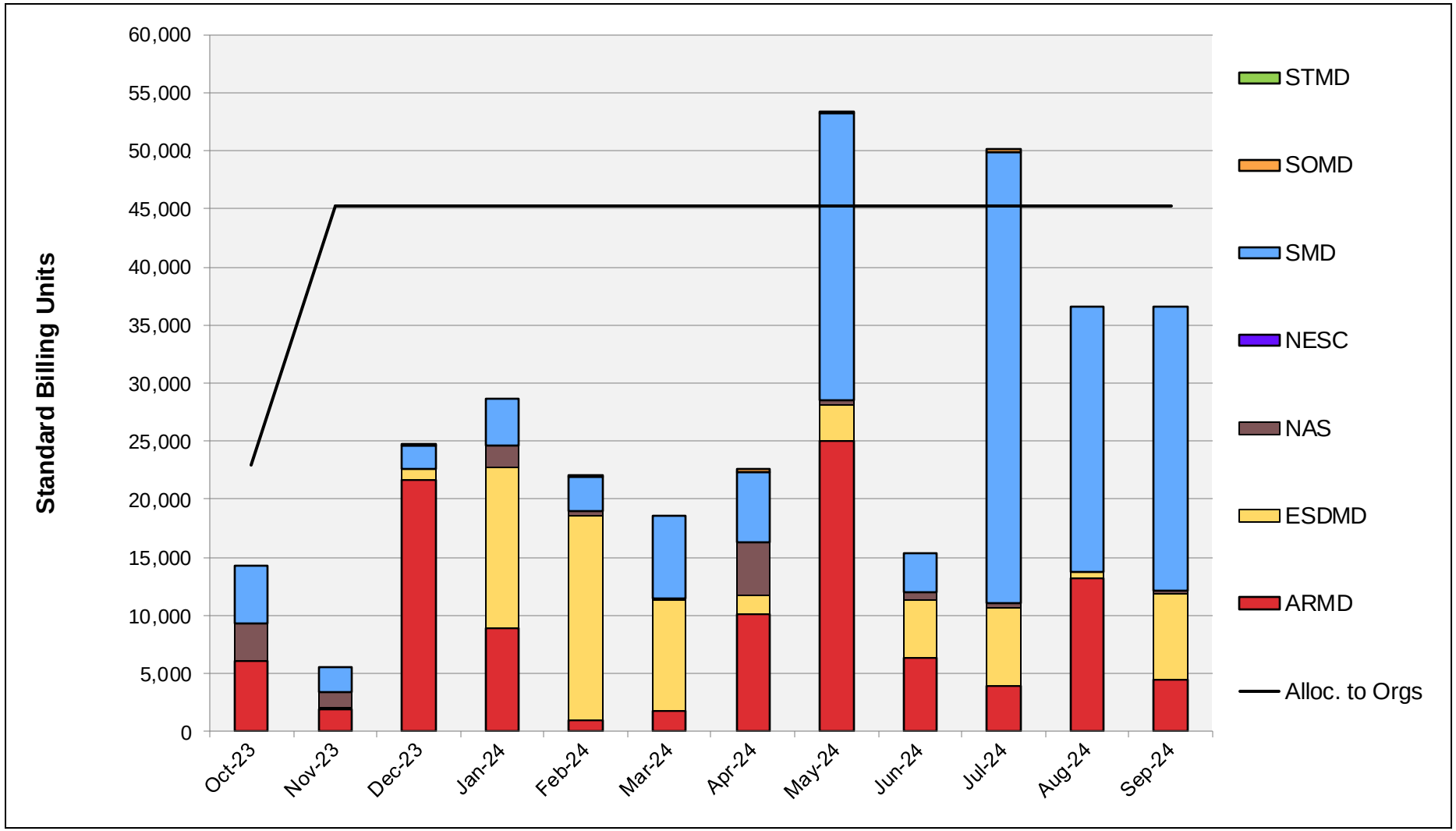
Cabeus: Average Time to Clear All Jobs



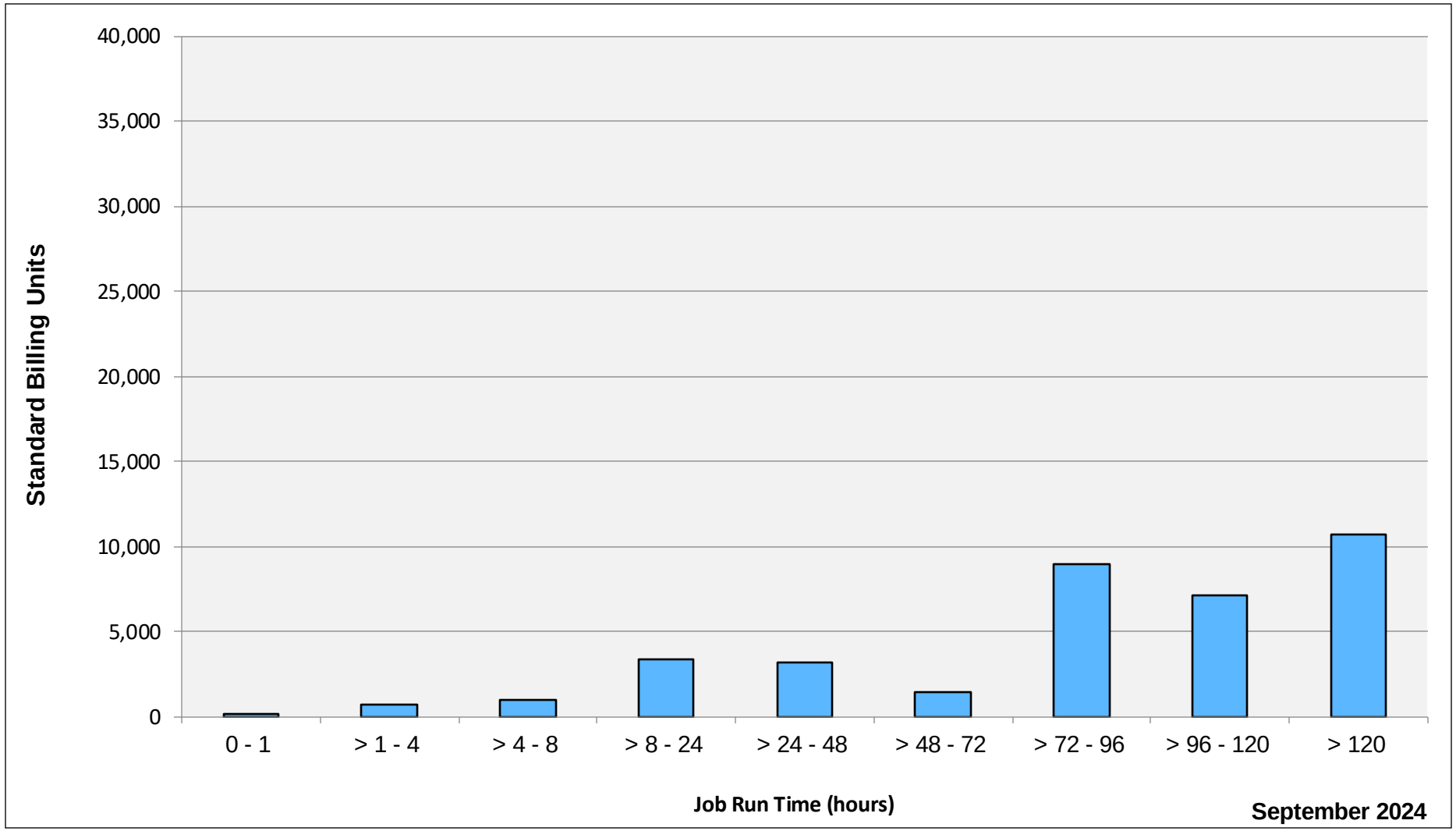
Cabeus: Average Expansion Factor



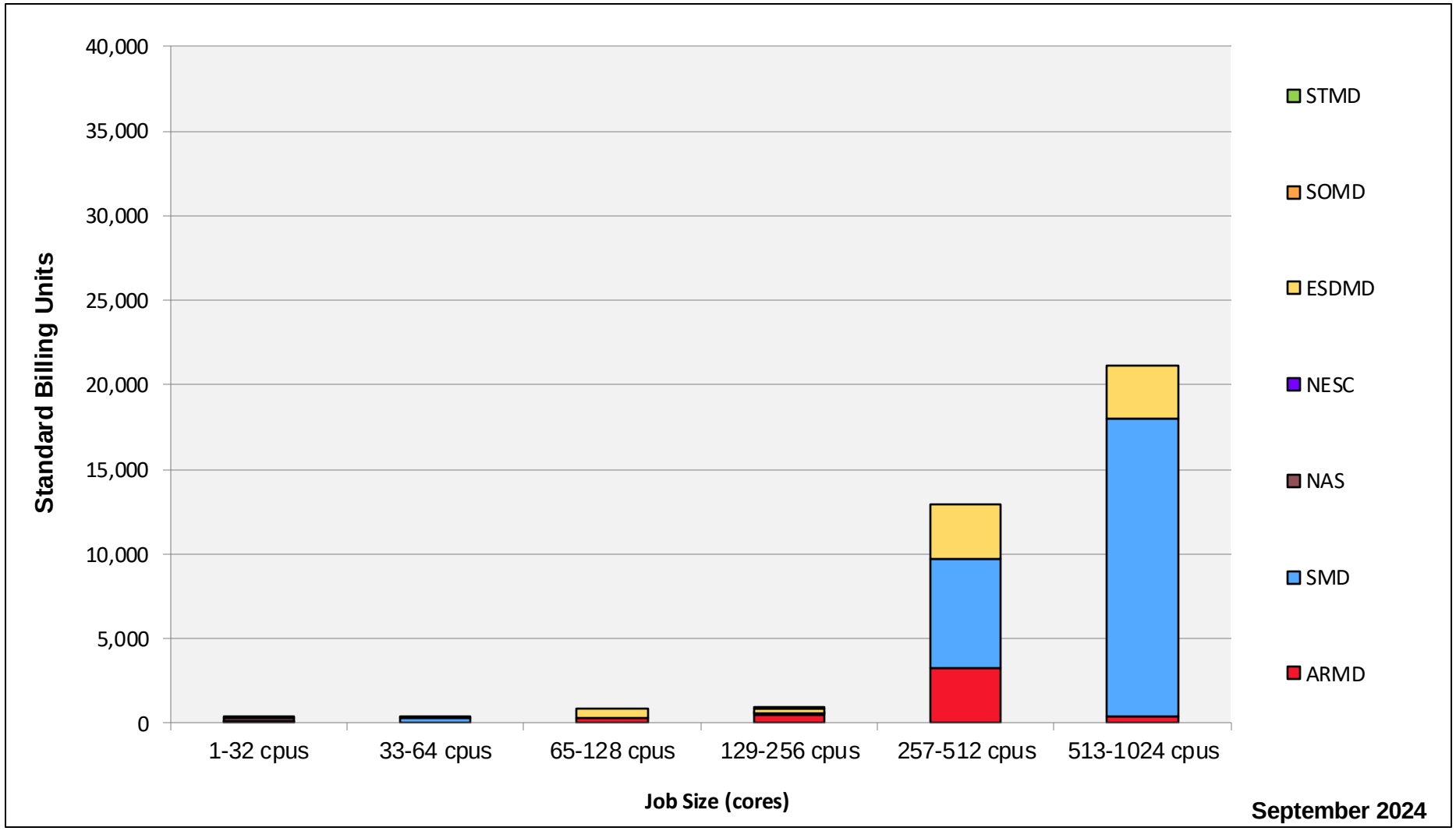
Endeavour: SBUs Reported, Normalized to 30-Day Month



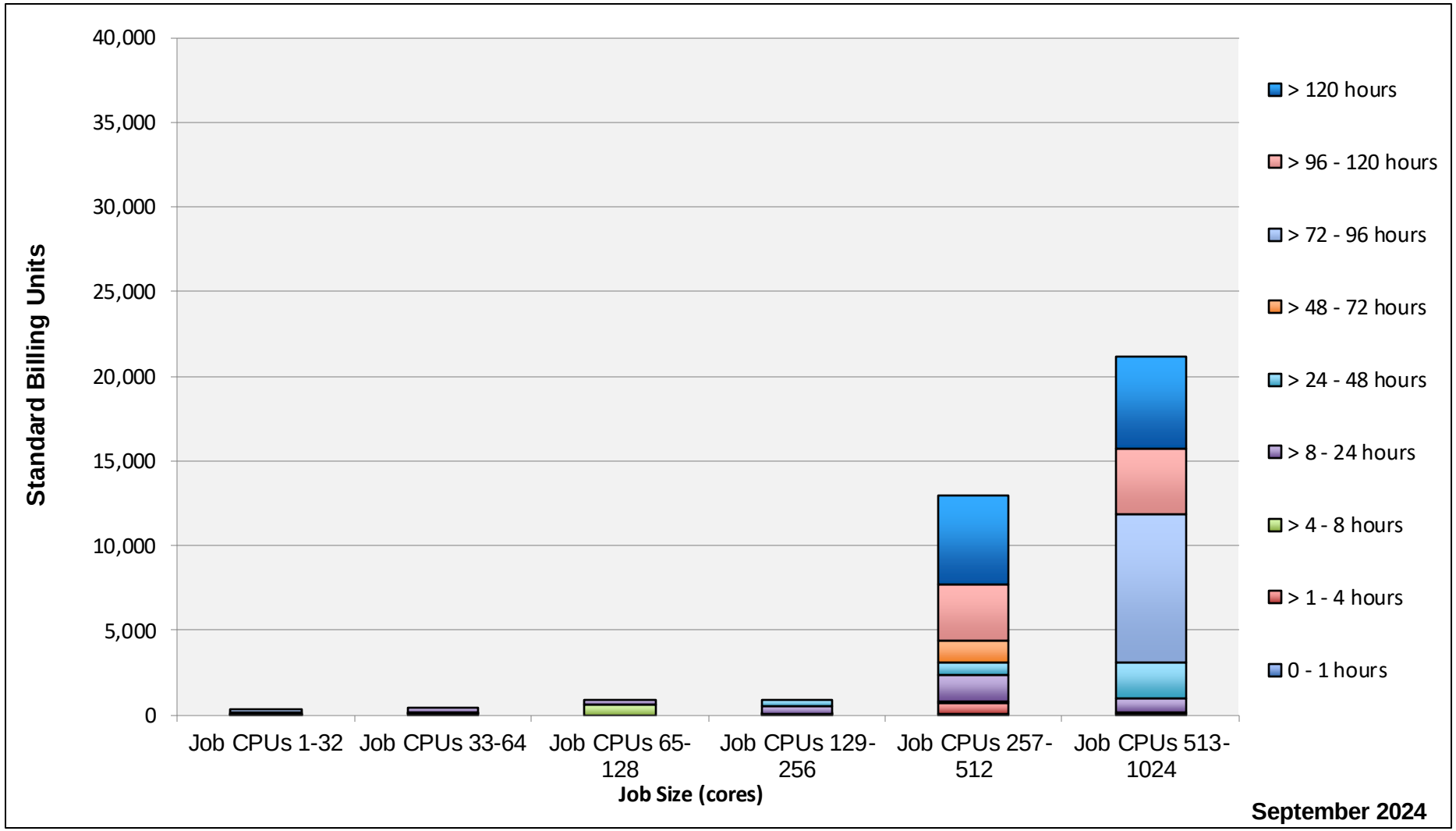
Endeavour: Monthly Utilization by Job Length



Endeavour: Monthly Utilization by Job Size



Endeavour: Monthly Utilization by Size and Length



Endeavour: Average Expansion Factor

