

National Aeronautics and Space Administration

High-End Computing Capability

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Script Checks Wall-Time Availability on Nodes

- Time-Wizard is a script created and maintained by NAS Control Room Analysts that performs checks to ensure requested wall-time extensions for jobs will not impact reserved nodes. The Time-Wizard script:
  - Checks the nodes in the currently running job requesting a wall-time increase for any nodes scheduled for reservation.
  - Calculates the maximum safe wall-time increase for the current job if there are nodes scheduled for reservation.
  - Outputs the maximum safe wall-time increase without cutting into any reservations.
  - If there are no reservation conflicts, returns the maximum time requested.
- The PBS scheduler allocates nodes to reservations with the assumption that jobs use the wall-time assigned for each reservation. Prior to the Time-Wizard script, when a wall-time increase for a job was requested there was no easy way to know the impact to scheduled reservations; increasing wall-time on jobs could cause nodes to continue being used for a job when they should be switching over to a reservation.
- The new script now allows wall-time increases without impacting reservations, improving user satisfaction and reducing wasted SBUs in idle reservations.

IMPACT: The new script can analyze wall-time and automatically extend HECC job wall-times without disrupting reserved nodes and reduces waste of reservation resources.

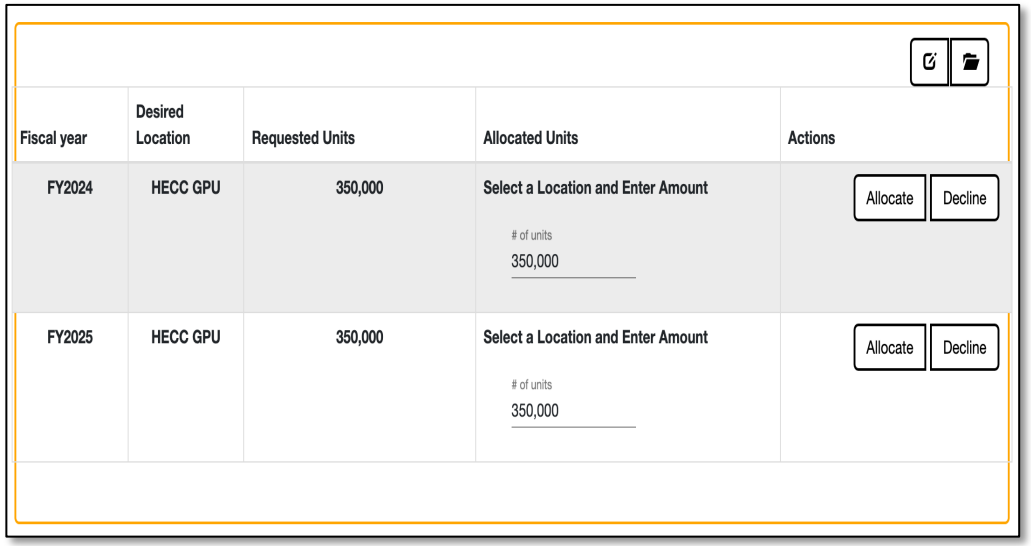
```
kzhang9@pfe20:~> ./time-wizard.sh
Usage: time-wizard.sh [job ID] [requested walltime increment in H:M:S]
kzhang9@pfe20:~> ./time-wizard.sh 17019108 144:0:0
Generating node list..
New requested job end date: Tue Oct 3 10:12:46 PDT 2023
Reservation R17031075 start time: Fri Sep 29 08:00:00 2023
Maximum possible walltime increment: 44 hours, 47 minutes, 14 seconds
Executable command: qalter -l walltime=92:47:14 17019108
```

Screenshot of the new Time-Wizard interface.

RMS Adds New Admin Features

- The Request Management System (RMS) application development team released a significant update and corrected a vulnerability in September.
- RMS 3.8 added the ability to allocate GPU resources. This includes:
  - Administrator User Interface (UI) for allocating GPU resources.
  - Email notifications for requests to increase or decrease GPU resources.
  - Ability to move GPU requests between centers.
  - Addition of GPU requests to allocation workbooks.
  - New GPU requests Included in the RMS Weekly Admin Digest.
  - Updates to the view pages displaying GPU resources.
- RMS 3.8.1 corrected a URL vulnerability. The new version uses a randomization algorithm to create links to requests and limits access to view links to authorized users only.
- Upcoming versions will focus on the opening views in new tabs and updates to the Security section of the RMS form.

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

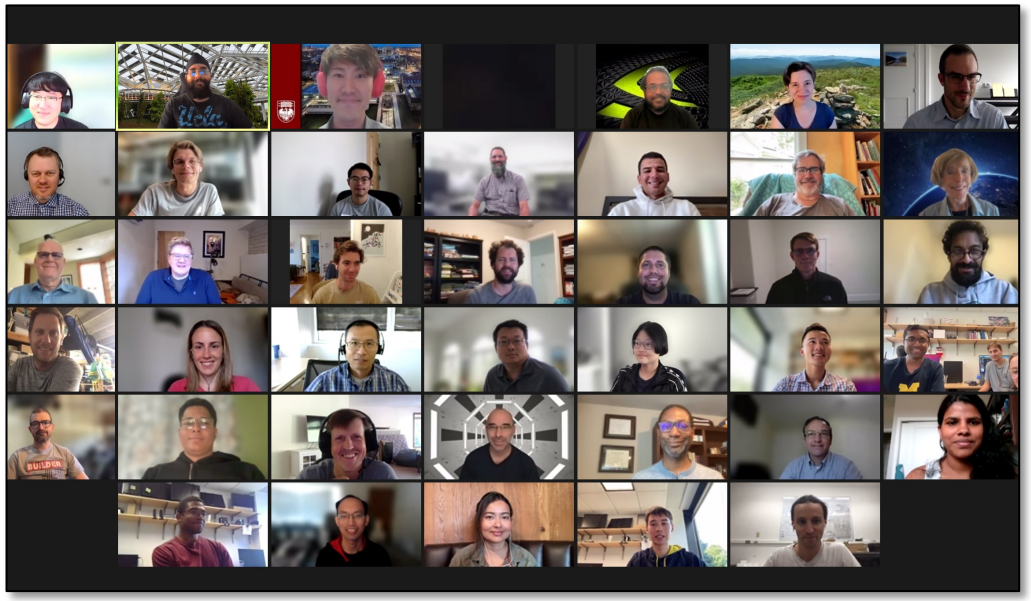


Screenshot of new Allocate Resource ability for GPU resources in the Request Management System.

HECC Hosts Successful 2023 NASA GPU Hackathon

- HECC, NASA Langley, and NVIDIA jointly organized the 2023 NASA GPU Hackathon to bring together application developers and computer experts to help get important applications used by NASA running effectively on GPU nodes. The virtual event took place over four days on September 12 and 19–21.
  - 42 members representing 9 teams from NASA and academic institutions participated in the hackathon. The teams were selected through a review process from 20 submissions and 8 of the selected teams are NASA-affiliated.
  - The teams brought a variety of scientific applications including CFD and AI/ML codes 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 V100 and A100 GPUs for the teams to use.
- By the end of the Hackathon, most teams had made good progress and achieved considerable performance improvements on the GPUs that will be documented in the final report:
  - A key to the success was the pairing of teams with 22 expert mentors from industry (including NVIDIA) and NASA application optimization and data analytics groups.
  - With optimization techniques and performance tools, teams were able to achieve significant performance improvements over their original codes prior to the hackathon.
  - All teams expressed appreciation for the opportunity and desire to continue working on their GPU projects after the hackathon. The Hackathon received a 4.6 out of 5 overall feedback score.
- HECC will coordinate with NVIDIA for next year's GPU hackathon.

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



GPU Hackathon group photo showing 39 of approximately 70 team members, mentors, and supporting staff. *Image courtesy of NVIDIA*

HECC Successfully Completes 2023 Annual Inventory

- Property custodians responsible for HECC/NAS property completed the 2023 Annual Equipment Inventory of more than 1,060 pieces of decaled equipment with a 100% scan rate.
- The Property staff's active tracking and updating of the HECC/NAS data created an efficient and successful inventory.
- Ongoing tracking and management of equipment during FY23 included:
  - Tagged 83 new pieces of equipment.
  - Excessed 154 controlled pieces of equipment.
  - Closed 221 tickets, most relating to equipment location and ownership updates.

IMPACT: Accurate tracking of assets through their life cycle and removal of NASA data prior to system disposal ensures control of government equipment and prevents loss of NASA data.



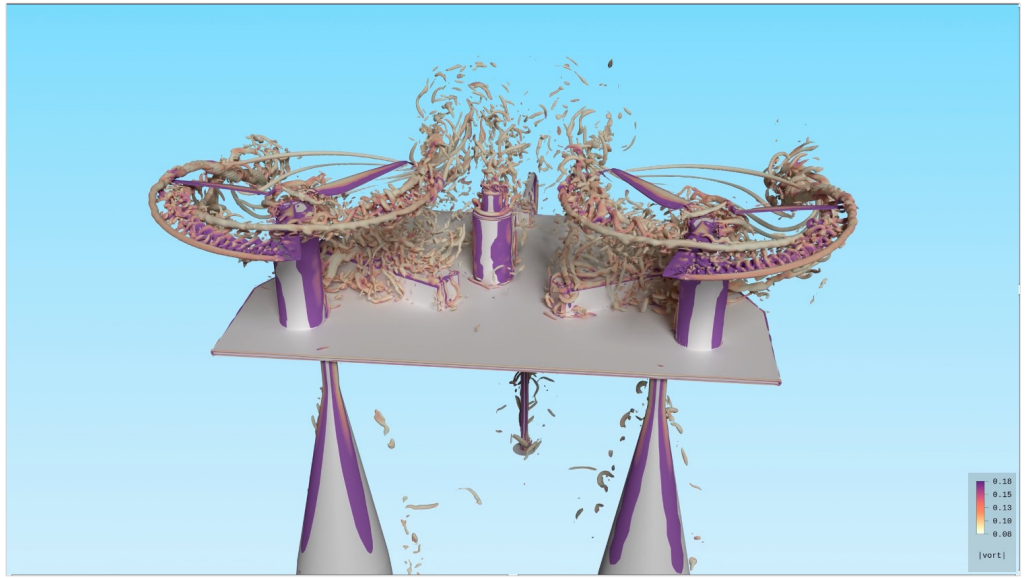
During the annual equipment inventory, HECC property custodians account for all equipment associated with the NASA Advanced Supercomputing (NAS) facility, including all components of the Pleiades supercomputer. *NASA*

Computational Analysis for Design of NASA's Side-By-Side Concept Vehicle

- As part of NASA's Revolutionary Vertical Lift Technology (RVLT) Project, aerospace engineers in the NAS Division tested a unique side-by-side (SBS) rotor Urban Air Mobility (UAM) concept vehicle design in the 7x10-foot wind tunnel at NASA Ames and analyzed results using HECC supercomputers.
  - The NAS team used experimental data and computational fluid dynamic (CFD) analysis to determine how changes in the position and orientation of multiple rotors affected the aerodynamic characteristics of the SBS concept vehicle.
- Researchers ran large simulations on the Pleiades, Electra, and Aitken supercomputers to capture the rotor blade aerodynamics and performance and rotor-body interactions, and then compared them with the wind tunnel data.
  - The CFD work captured the complex rotor blade aerodynamics, rotor performance, and rotor-rotor interactions, where the blade-tip vortices interact with each other.
  - Lower-order methods, like the rotor disk model, are important tools that help reduce the time requirements needed to explore many new vehicle concepts. It is also important to validate the computation with experiment.
  - Detailed comparison and validation were done on the SBS using both methods.
- Results enabled engineers to understand the flight characteristics of such concept UAM vehicles in urban settings.

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

IMPACT: HECC resources are required for the large simulation effort of this new concept vehicle. The rotor-rotor interactions and interactions with other components of the wind tunnel test section are an important aspect of the CFD validation effort.



A flow visualization of NASA's side-by-side rotor. The flowfield is colored by vorticity magnitude, the surfaces are colored by pressure coefficient.
Jasim Ahmad, Tim Sandstrom, NASA/Ames

Papers

- "**TESS Discovery of a Super-Earth Orbiting the M-Dwarf Star TOI-1680**," M. Ghachoui, et al., *Astronomy & Astrophysics*, vol. 677, September 2023. *
  https://www.aanda.org/articles/aa/full_html/2023/09/aa47040-23/aa47040-23.html
- "**Interhemispheric Observations of ULF Waves Caused by Foreshock Transients Under Quiet Solar Wind Conditions**," S. J. Noh, et al., *Journal of Geophysical Research: Space Physics*, vol. 128, issue 9, published online September 2, 2023. *
  https://agupubs.onlinelibrary.wiley.com/doi/full/10.1029/2023JA031596
- "**Disk Wind Feedback from High-Mass Protostars. III. Synthetic CO Line Emission**," D. Xu, et al., arXiv:2309.03868 [astro-ph.GA], September 7, 2023. *
  https://arxiv.org/abs/2309.03868
- "**The Thesan Project: Public Data Release of Radiation-Hydrodynamic Simulations Matching Reionization-Era JWST Observations**," E. Garaldi, et al., arXiv:2309.06475 [astro-ph.CO], September 12, 2023. *
  https://arxiv.org/abs/2309.06475
- "**Solar Atmospheric Heating Due to Small-Scale Events in an Emerging Flux Region**," R. Yadav, et al., arXiv:2309.06452 [astro-ph.SR], September 12, 2023. *
  https://arxiv.org/abs/2309.06452
- "**Reynolds-Number Effects on the Acoustic Disturbance Environment in a Mach 6 Nozzle**," N. Hildebrand, et al., *AIAA Journal of Aeronautics and Astronautics*, published online September 12, 2023. *
  https://arc.aiaa.org/doi/full/10.2514/1.J062631

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

Papers (cont.)

- "**Microstructural Mechanisms of Hysteresis and Transformation Width in NiTi Alloy from Molecular Dynamics Simulations**," G. Plummer, et al., *Journal of Physics: Condensed Matter*, vol. 35, no. 49, published online September 13, 2023. * *https://iopscience.iop.org/article/10.1088/1361-648X/acf6a3/meta*
- "**Spectro-Polarimetric Properties of Sunquake Sources in X1.5 Flare and Evidence for Electron and Proton Beam Impacts**," A. Kosovichev, V. Sadykov, J. Stefan, arXiv:2309.07346 [astro-ph.SR], September 13, 2023. * *https://arxiv.org/abs/2309.07346*
- "**Force Balances in Strong-Field Magnetoconvection Simulations**," I. Cresswell, et al., *Physical Review Fluids*, vol. 8, issue 9, published online September 14, 2023. * *https://journals.aps.org/prfluids/abstract/10.1103/PhysRevFluids.8.093503*
- "**Shining Light on the Hosts of the Nano-Hertz Gravitational Wave Sources: A Theoretical Perspective**," V. Saeedzadeh, et al., arXiv:2309.08683 [astro-ph.GA], September 15, 2023. * *https://arxiv.org/abs/2309.08683*
- "**TESS Spots a Super-Puff: The Remarkably Low Density of TOI-1420b**," S. Yoshida, et al., arXiv:2309.09945 [astro-ph.EP], September 18, 2023. * *https://arxiv.org/abs/2309.09945*
- "**Impacts of Abiotic and Biotic Factors on Tundra Productivity near Utqiagvik, Alaska**," Q. Zhang, et al., *Environmental Research Letters*, vol. 18, no. 9, published online September 18, 2023. * *https://iopscience.iop.org/article/10.1088/1748-9326/acf7d6/meta*

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

Papers (cont.)

- "**Orbit-Spin Coupling, the Solar Dynamo, and the Planetary Theory of Sunspots**," J. Shirley, arXiv:2309.13076 [astro-ph.SR], September 20, 2023. *
  https://arxiv.org/abs/2309.13076
- "**ICM-SHOX. Paper I: Methodology Overview and Discovery of a Baryon—Dark Matter Velocity Decoupling in the MACS J0018.5+1626 Merger**," E. Silich, et al., arXiv:2309.12533 [astro-ph.CO], September 21, 2023. *
  https://arxiv.org/abs/2309.12533
- "**Anharmonic IR Absorption Spectra of the Prototypical Interstellar PAHs Phenanthrene, Pyrene, and Pentacene in their Neutral and Cation States**," V. Esposito, et al., *An International Journal at the Interface Between Chemistry and Physics*, published online September 21, 2023. *
  https://www.tandfonline.com/doi/abs/10.1080/00268976.2023.2252936
- "**Ice-Front Retreat Controls on Ocean Dynamics Under Larsen C Ice Shelf, Antarctica**," M. Poinelli, et al., *Geophysical Research Letters*, vol. 50, issue 18, September 21, 2023. *
  https://agupubs.onlinelibrary.wiley.com/doi/full/10.1029/2023GL104588
- "**Anharmonicity and Deuteration in the IR Absorption and Emission Spectrum of Phenylacetylene**," V. Esposito, et al., *An International Journal at the Interface Between Chemistry and Physics*, published online September 25, 2023. *
  https://www.tandfonline.com/doi/abs/10.1080/00268976.2023.2261570
- "**101 Eclipsing Quadruple Star Candidates Discovered in TESS Full Frame Images**," V. Kostov, et al., arXiv:2309.14600 [astro-ph.SR], September 25, 2023. *
  https://arxiv.org/abs/2309.14200

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

Papers (cont.)

- "**Quantum Chemical Exploration of the Binding Motifs and Binding Energies of Neutral Molecules, Radicals, and Ions with Small Water Clusters: Characterisation and Astrochemical Implications**," J. Hendrix, et al., *An International Journal at the Interface Between Chemistry and Physics*, published online September 25, 2023. *
https://www.tandfonline.com/doi/abs/10.1080/00268976.2023.2252100
- "**The Properties and Origin of Kuiper Belt Object Arrokoth's Large Mounds**," S. Stern, et al., *The Planetary Science Journal*, vol. 4, no. 9, published online September 26, 2023. *
https://iopscience.iop.org/article/10.3847/PSJ/acf317
- "**Little Change in Apparent Hydrological Sensitivity at Large CO2 Forcing**," D. Raiter, et al., *Geophysical Research Letters*, vol. 50, issue 18, published online September 28, 2023. *
https://agupubs.onlinelibrary.wiley.com/doi/full/10.1029/2023GL104954
- "**Particle-in-Cell Simulations — Ion Beam Instability and the Generation of Alfvén and Whistler Waves in Low β Plasma**," H. Che, et al., *Monthly Notices of the Royal Astronomical Society*, vol. 526, issue 2, published online September 28, 2023. *
https://academic.oup.com/mnras/article-abstract/526/2/2110/7285821

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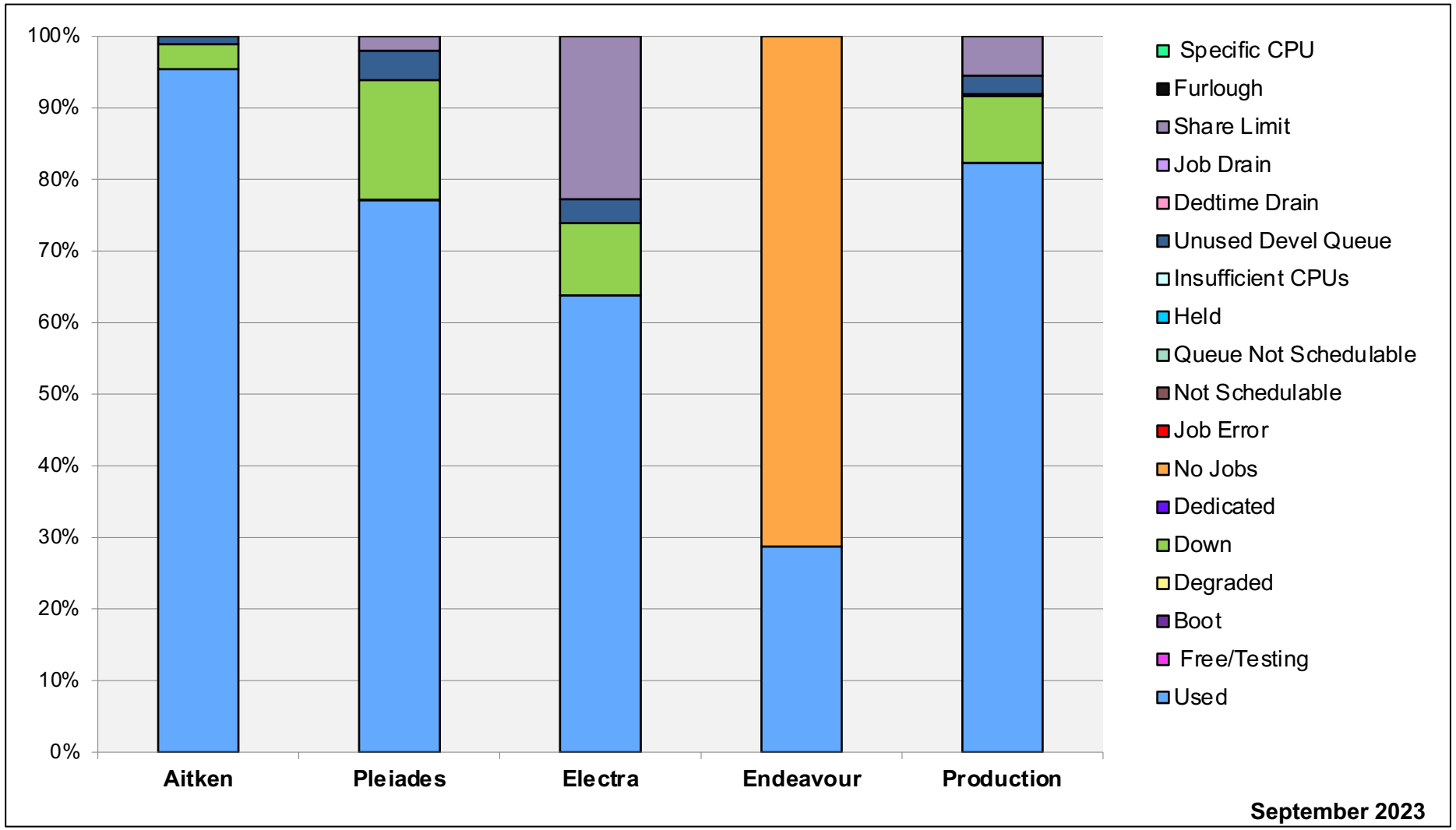
Presentations

- "**Effect of Turbulence Modeling on Rotor Performance for NASA's Tiltwing Air Taxi Concept**," D. Garcia Perez, P. Ventura Diaz, S. Yoon, presented at the 18th European Turbulence Conference, Valencia, Spain, September 4-6, 2023.
- "**Sustainability: NASA Advanced Supercomputing Facility at Ames Research Center**," P. Mehrotra, presented at the High Performance Computing User Forum Fall Meeting, Tucson, AZ, September 6-7, 2023.
- "**Modular HPC Centers NASA Advanced Supercomputing Facility at Ames Research Center**," C. Tanner, presented at the Energy Efficient HPC Working Group Workshop, Virtual Meeting, September 14, 2023.
- "**Photometric Properties of Quiet Sun Observed with DKIST and HINODE**," I. Kitiashvili, presented at the Sun in Science Society, Venice, Italy, September 11-15, 2023.
- "**Acoustic Signature Uncertainty Quantification for the X-59**," M. Nemec, presented as part of NASA's ARMD Technical Seminars, Virtual Meeting, September 19, 2023.
- "**Turning Noise into Data: Characterization of the Van Allen Radiation Belt Using SDO Spikes Data**," S. Kasapis, presented at the Lockheed Martin Solar and Astrophysics Laboratory Seminar, Palo Alto, CA, September 21, 2023.
- **6th NAOJ Symposium HINODE-16/IRIS-13 Meeting**, Niigata, Japan, September 25-29, 2023.
  - "**3D Radiative MHD Modeling of the Solar Transition Zone and Corona**," I. Kitiashvili, et al.
  - "**3D Radiative Hydrodynamic Modeling of Multi-Scale Flows Driven by Subsurface Turbulent Convection**," ," I. Kitiashvili, et al.
  - "**Acoustic Wave Excitation and Small-Scale Eruptive Activity in Quiet-Sun Regions**," ," I. Kitiashvili, et al.
- "**A Study on Flow Solutions Computed on Automatically and Manually Generated Structured Overset Meshes**," A. Chuen, W. Chan, presented as part of the Advanced Modeling and Simulation Seminar series, September 27, 2023.

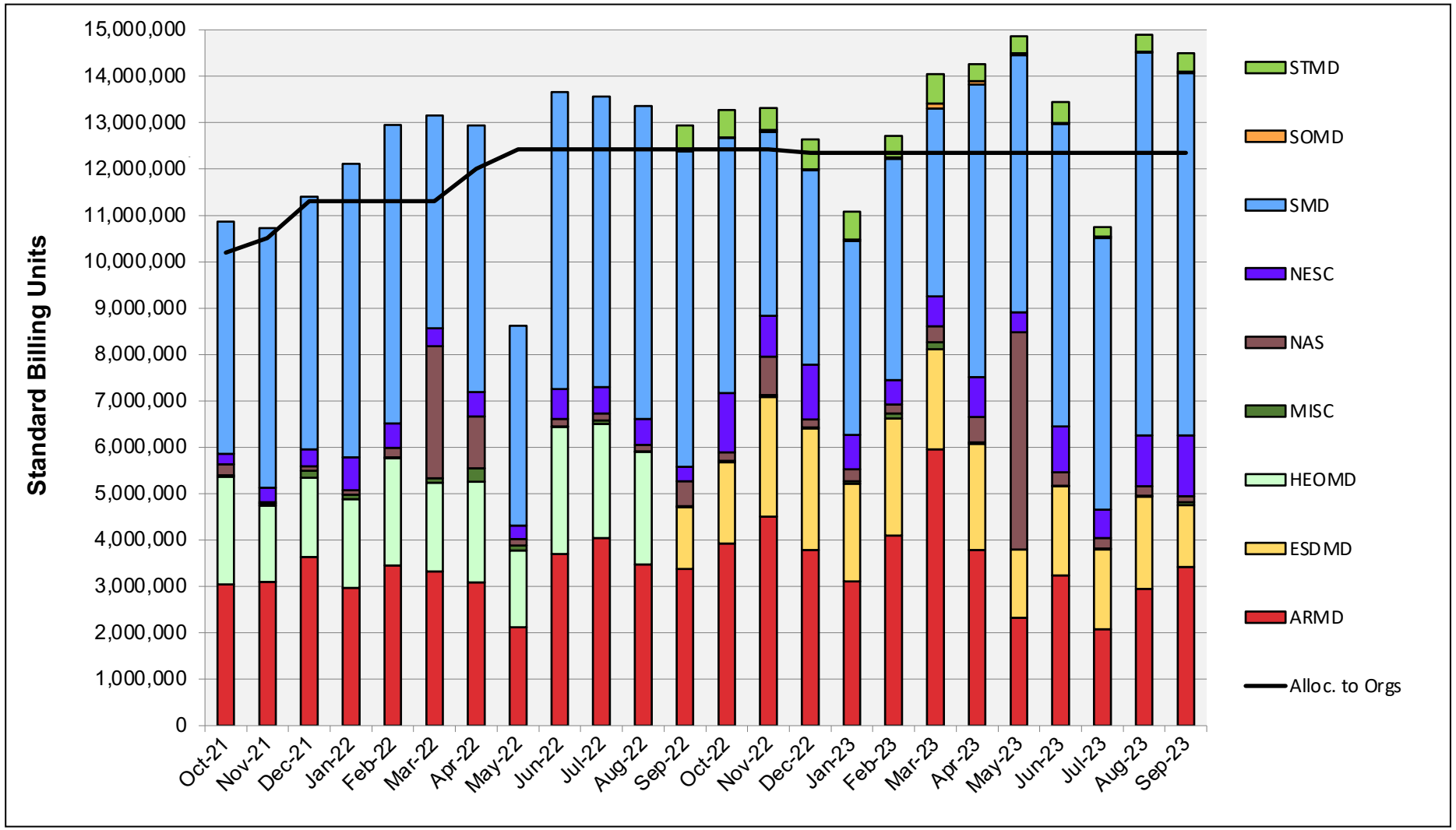
News and Events

- **NASA's Steve Yoon on the Latest Research to Help Shape the eVTOL Industry**, *Vertical Magazine*, September 1, 2023—NAS Division Computational Physics Branch Chief, Steve (Seokkwan) Yoon, discusses how computational tools are being used to support the design of advanced air mobility (AAM) vehicles. NASA work helps guide industry's development of electric air taxis and drones and will assist the Federal Aviation Administration in safely integrating these vehicles into the national airspace. *https://verticalmag.com/q-and-a/nasas-steve-yoon-on-the-latest-research-to-help-shape-the-evtol-industry/*
- **NASA Ames Data Processing Software Receives Honorable Mention**, *NASA Advanced Supercomputing Division,* September 13, 2023—NASA management has announced that the Unsteady Pressure-Sensitive Paint (uPSP) Data Processing Software received an honorable mention in the 2023 NASA Software of the Year Award competition. Developed by several teams across NASA's Ames Research Center in Silicon Valley—including visualization and aerodynamics experts in the NASA Advanced Supercomputing (NAS) Division—the uPSP software is a collection of applications that processes raw data from wind tunnel-based testing systems. *https://www.nas.nasa.gov/pubs/stories/2023/news_09-13-23_uPSP_Honorable_Mention.html*

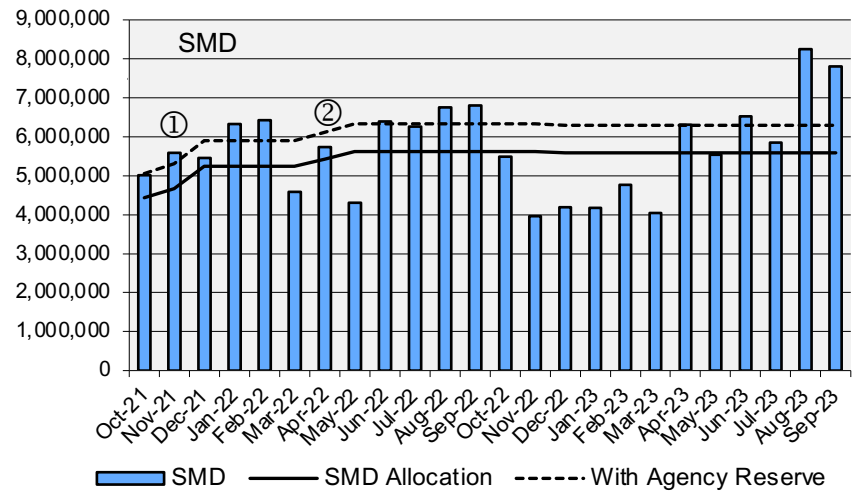
HECC Utilization

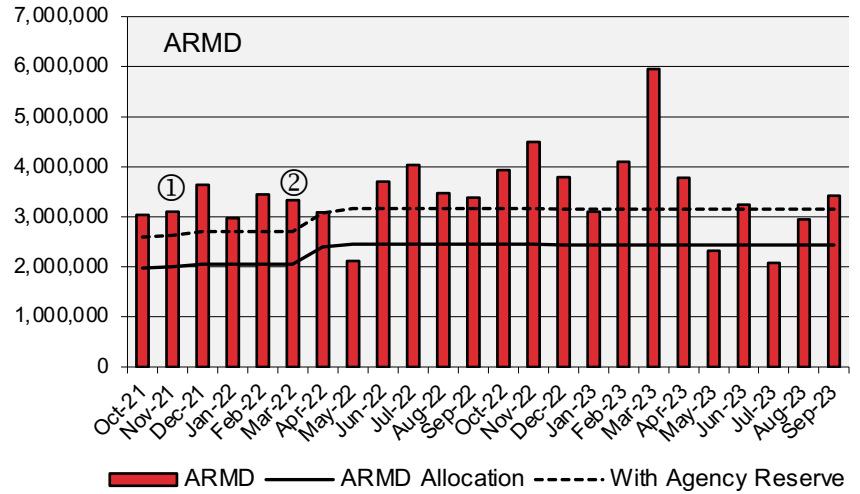


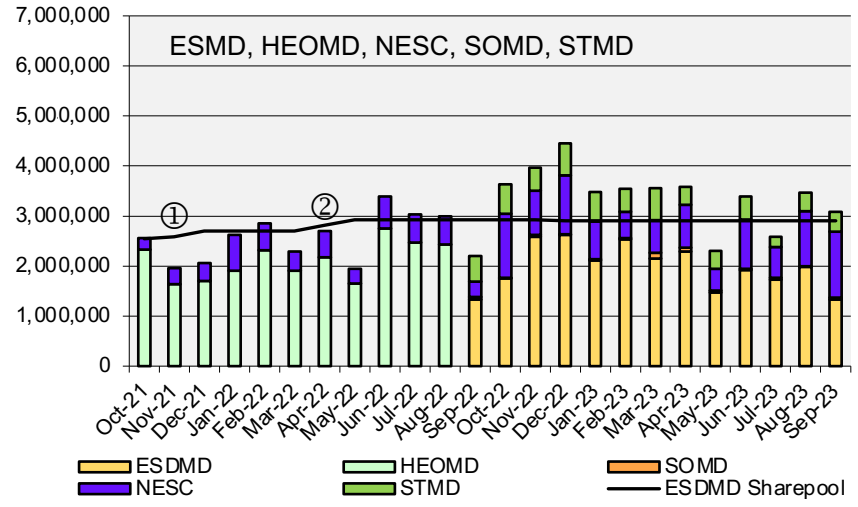
HECC Utilization Normalized to 30-Day Month



HECC Utilization Normalized to 30-Day Month



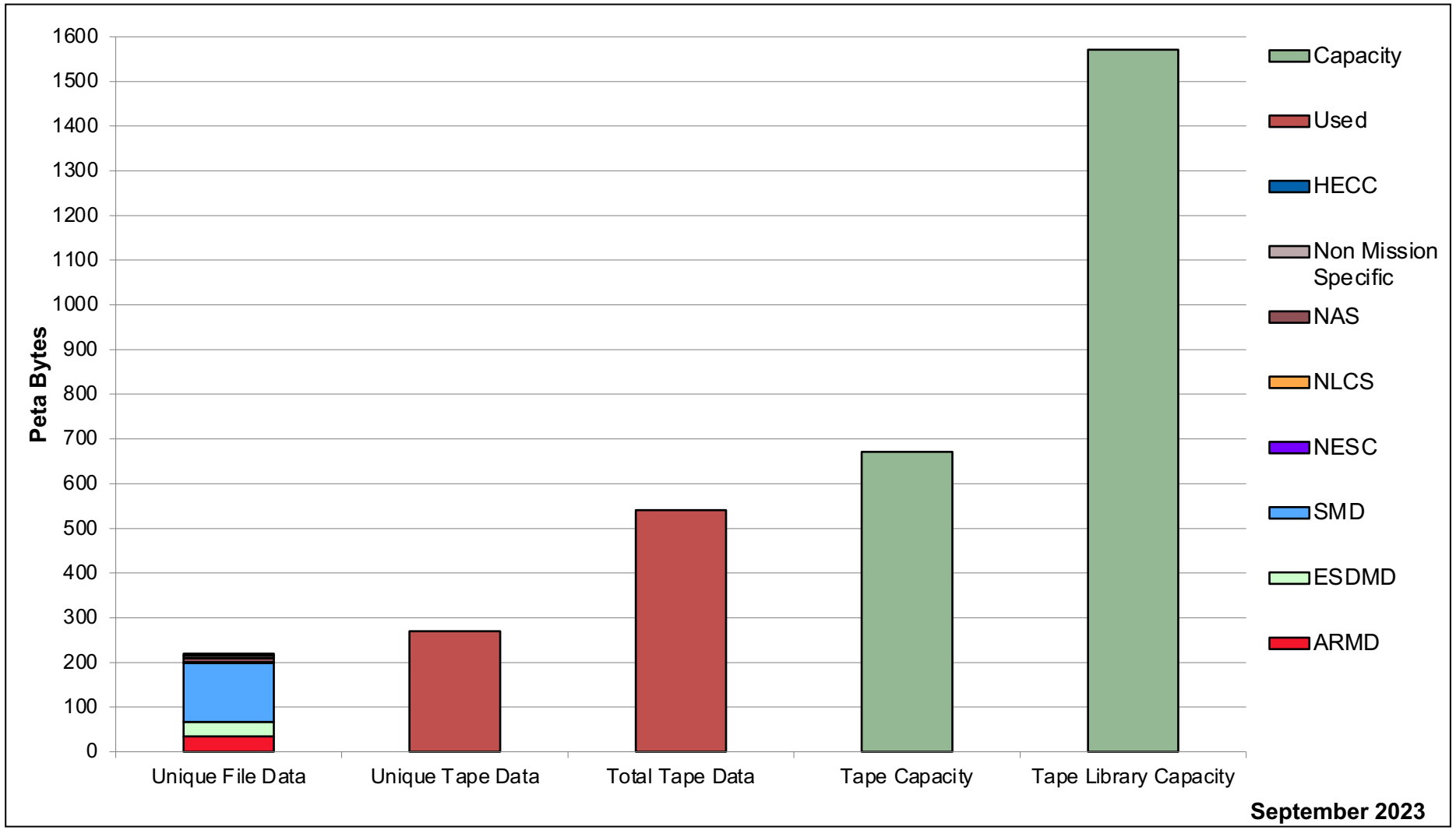




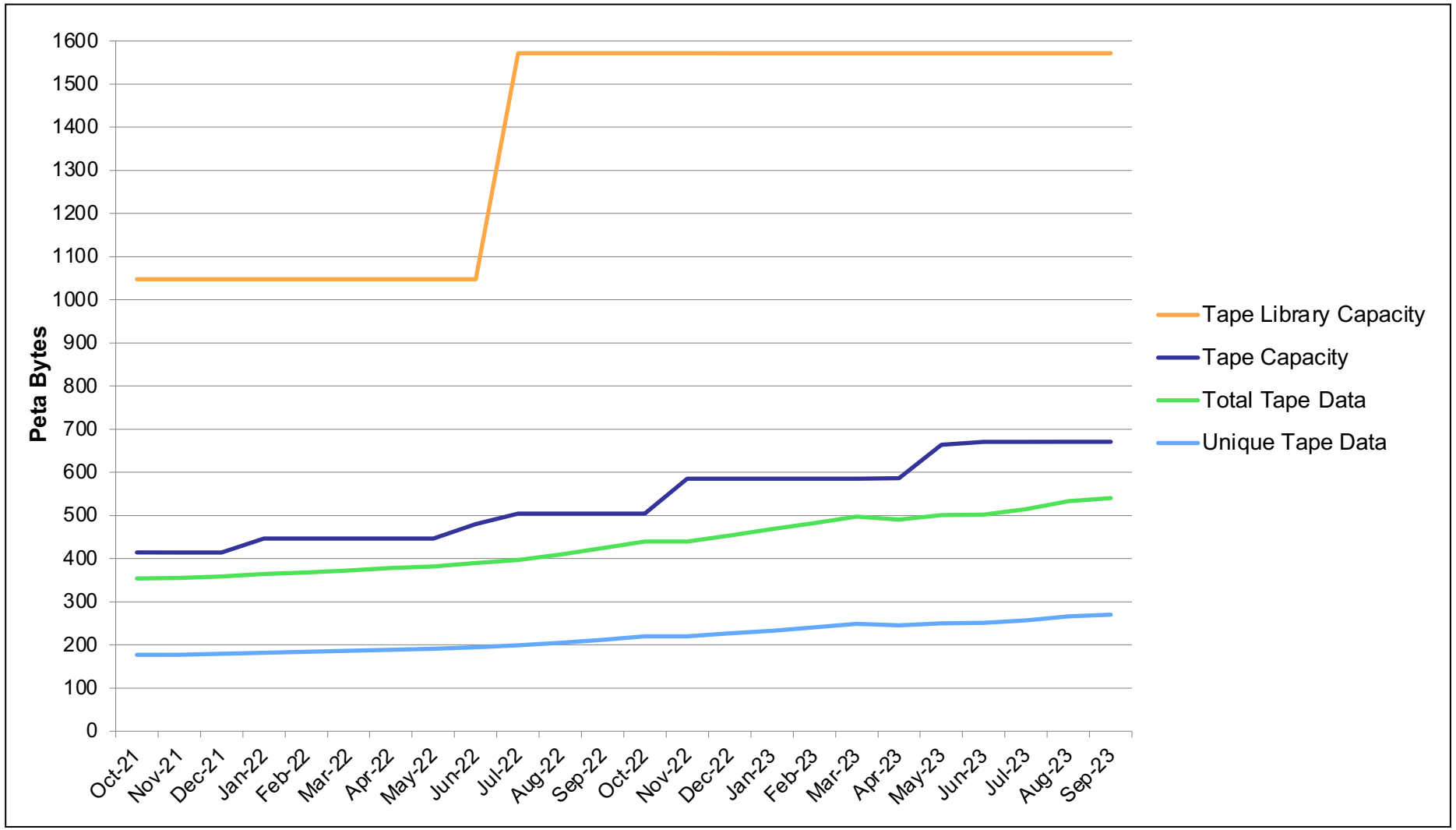
① 4 Rome Apollo Racks added to Aitken

② 4 Rome Apollo Racks added to Aitken

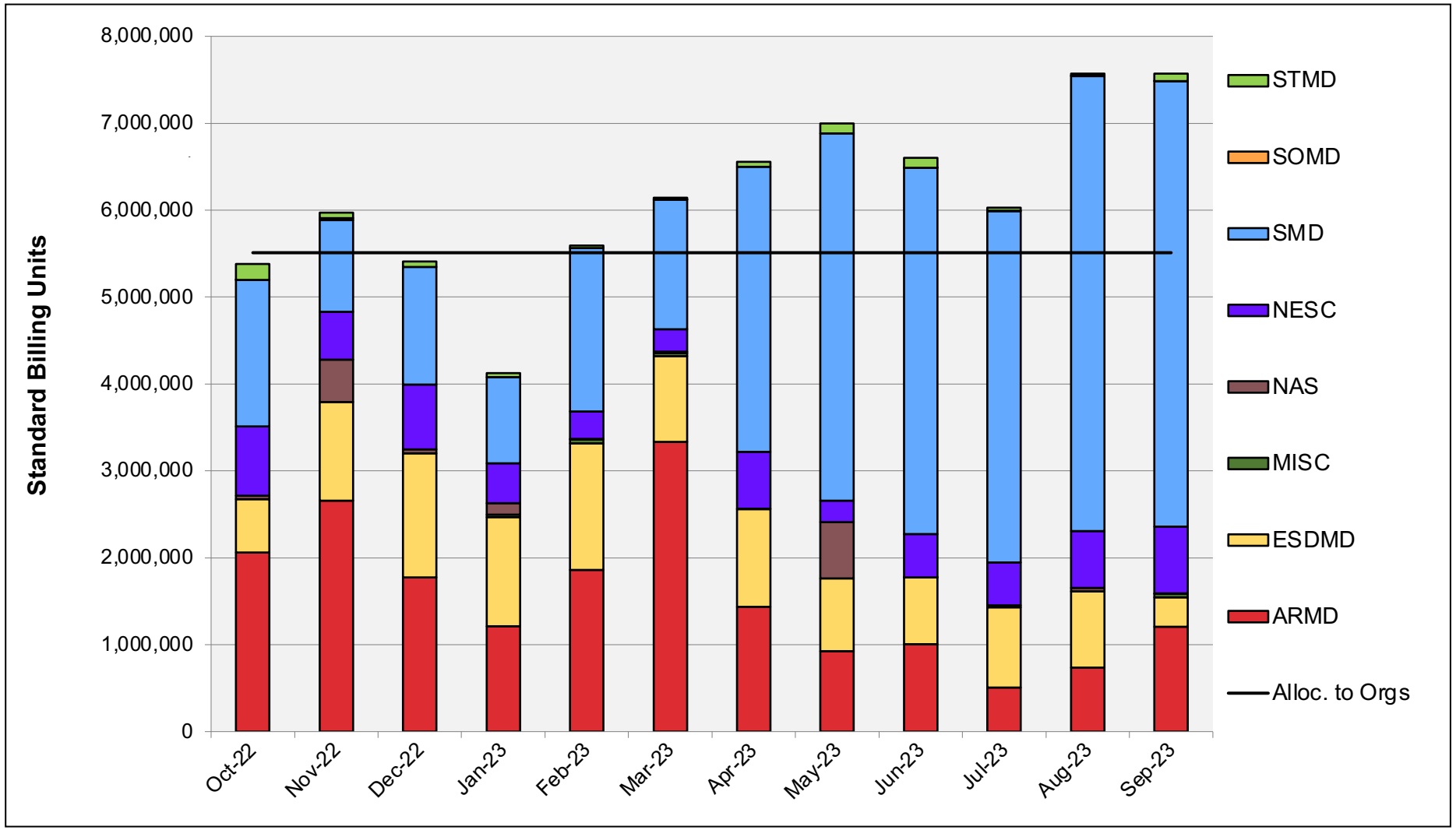
Tape Archive Status



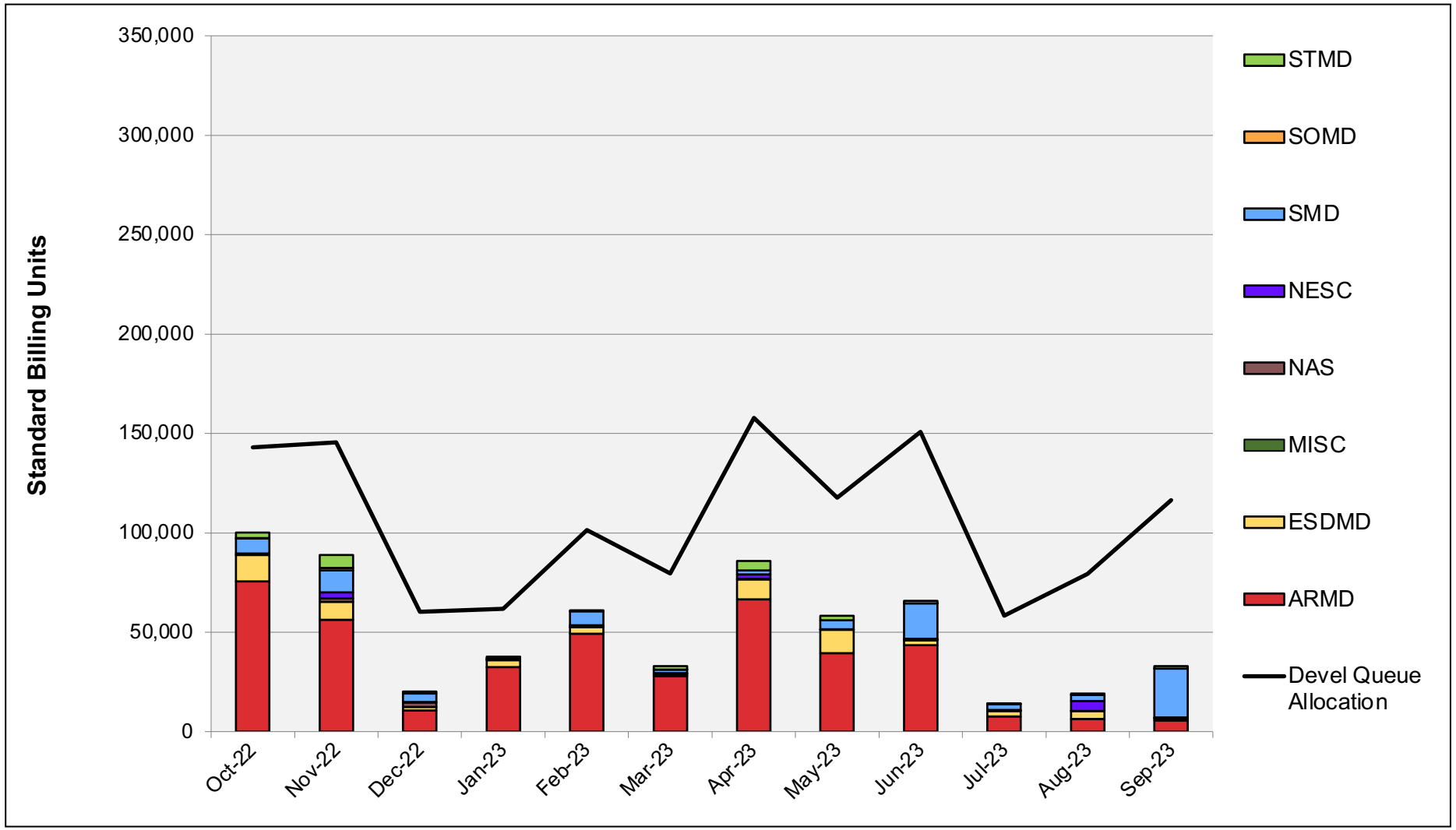
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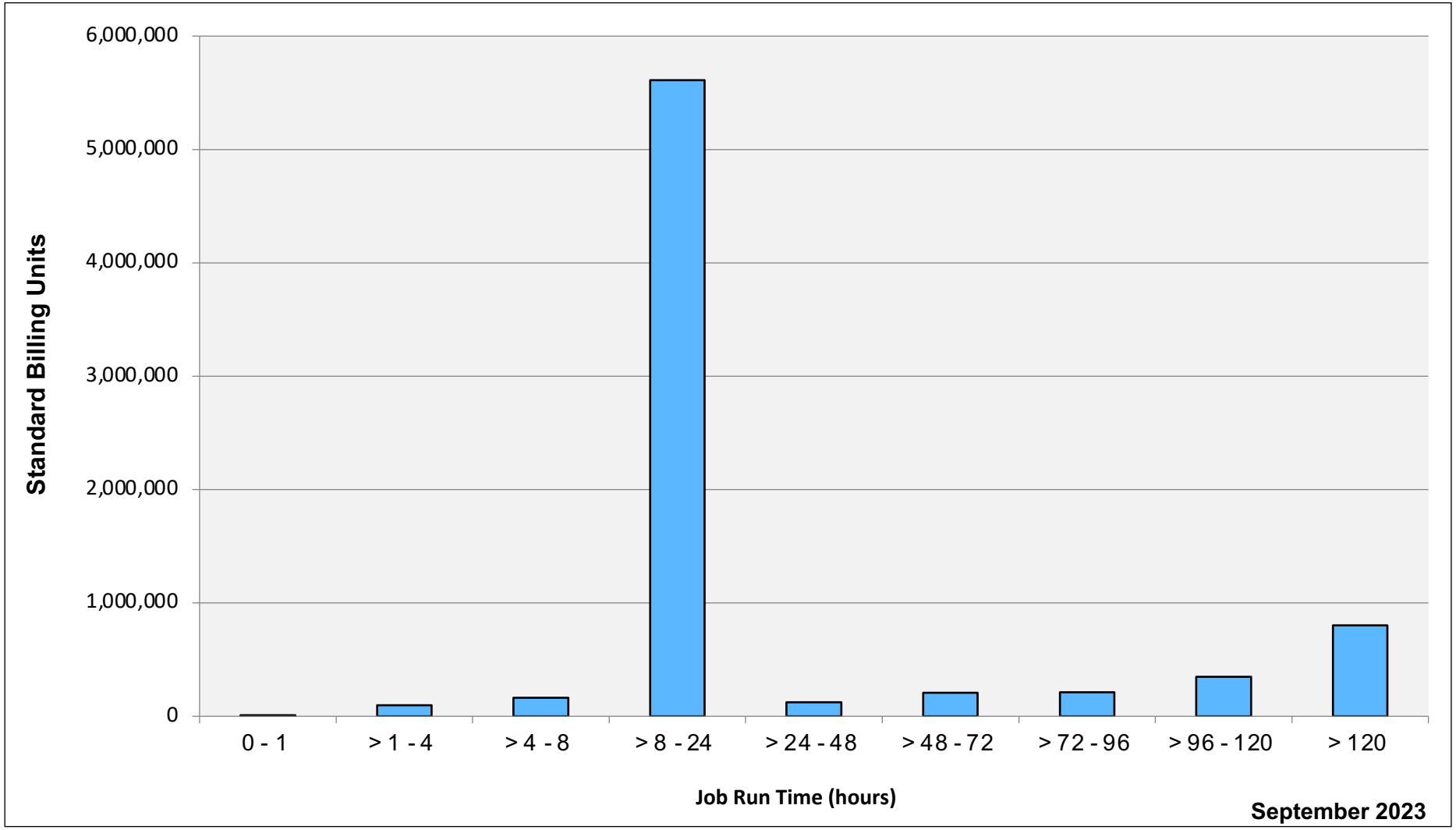
Aitken: SBUs Reported, Normalized to 30-Day Month



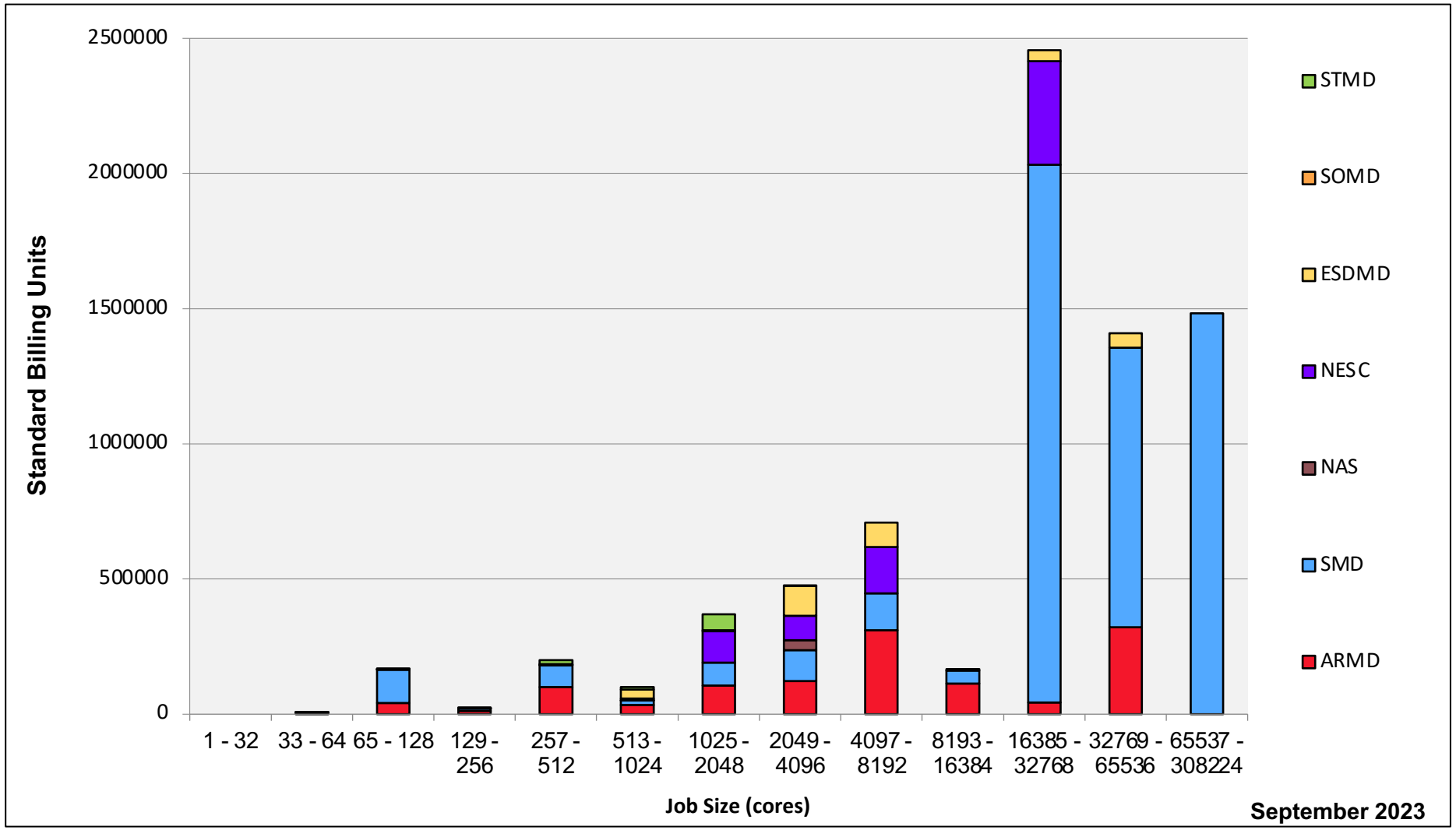
Aitken: Devel Queue Utilization



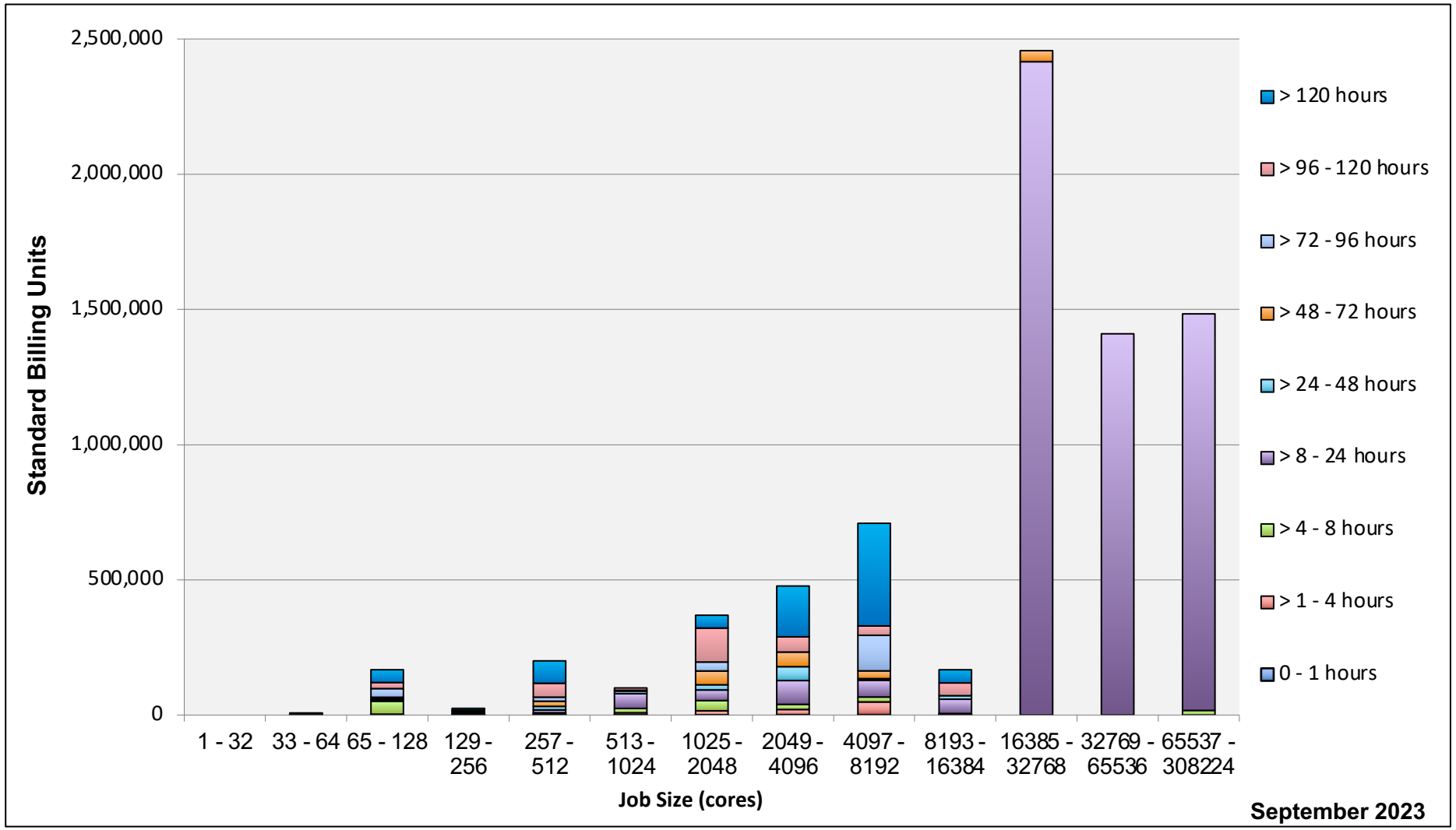
Aitken: Monthly Utilization by Job Length



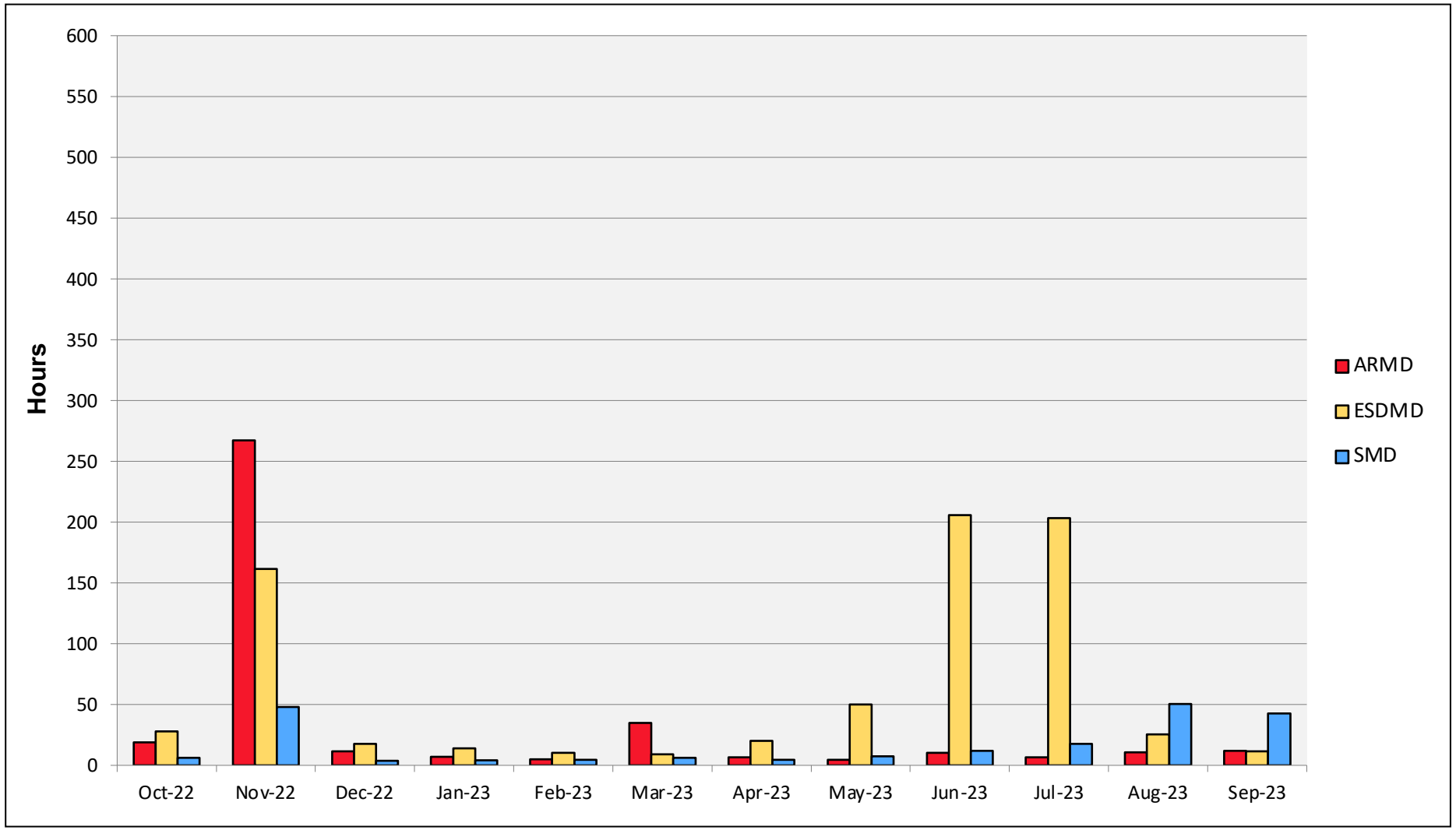
Aitken: Monthly Utilization by Job Size



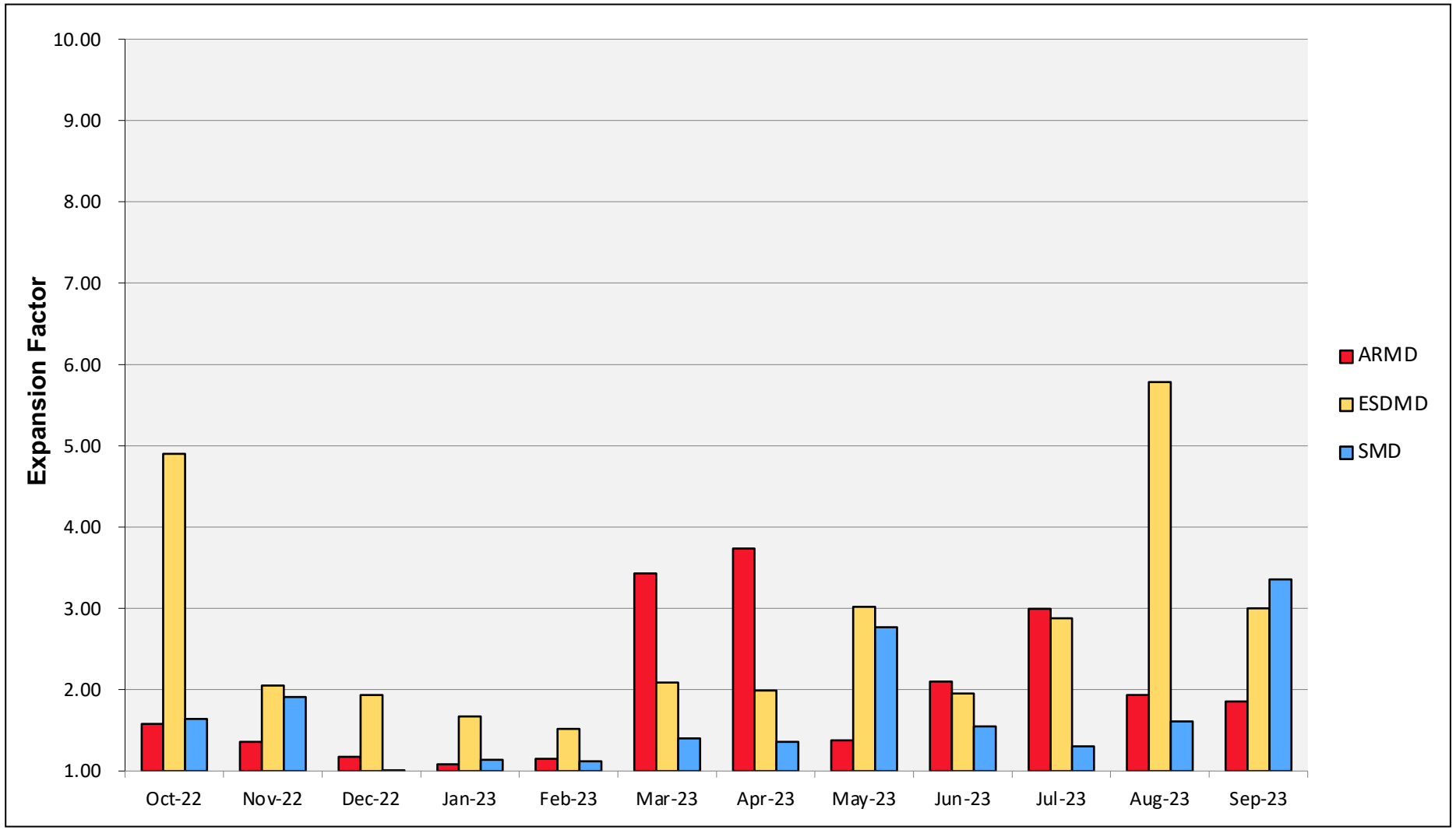
Aitken: Monthly Utilization by Size and Length



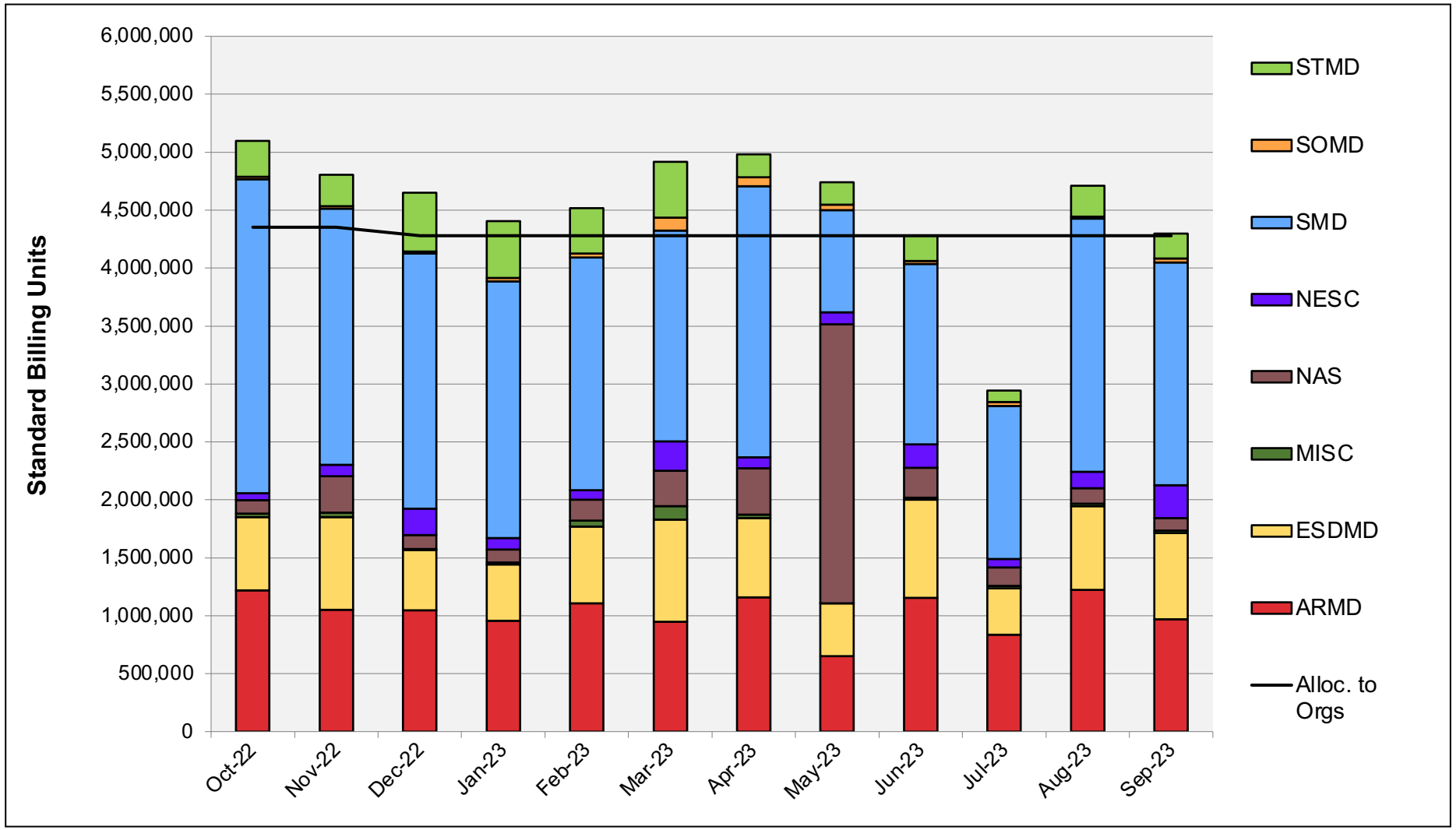
Aitken: Average Time to Clear All Jobs



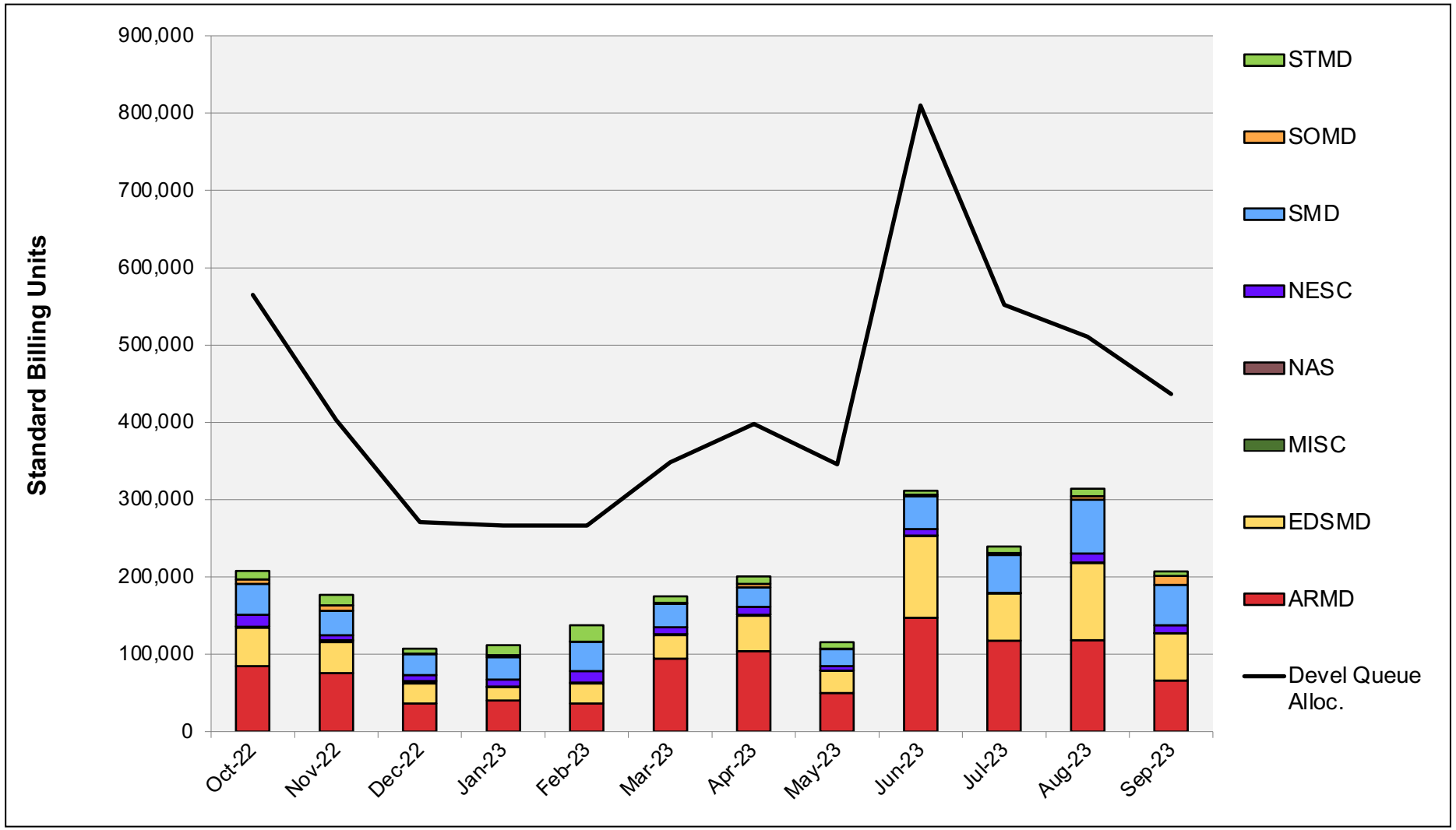
Aitken: Average Expansion Factor



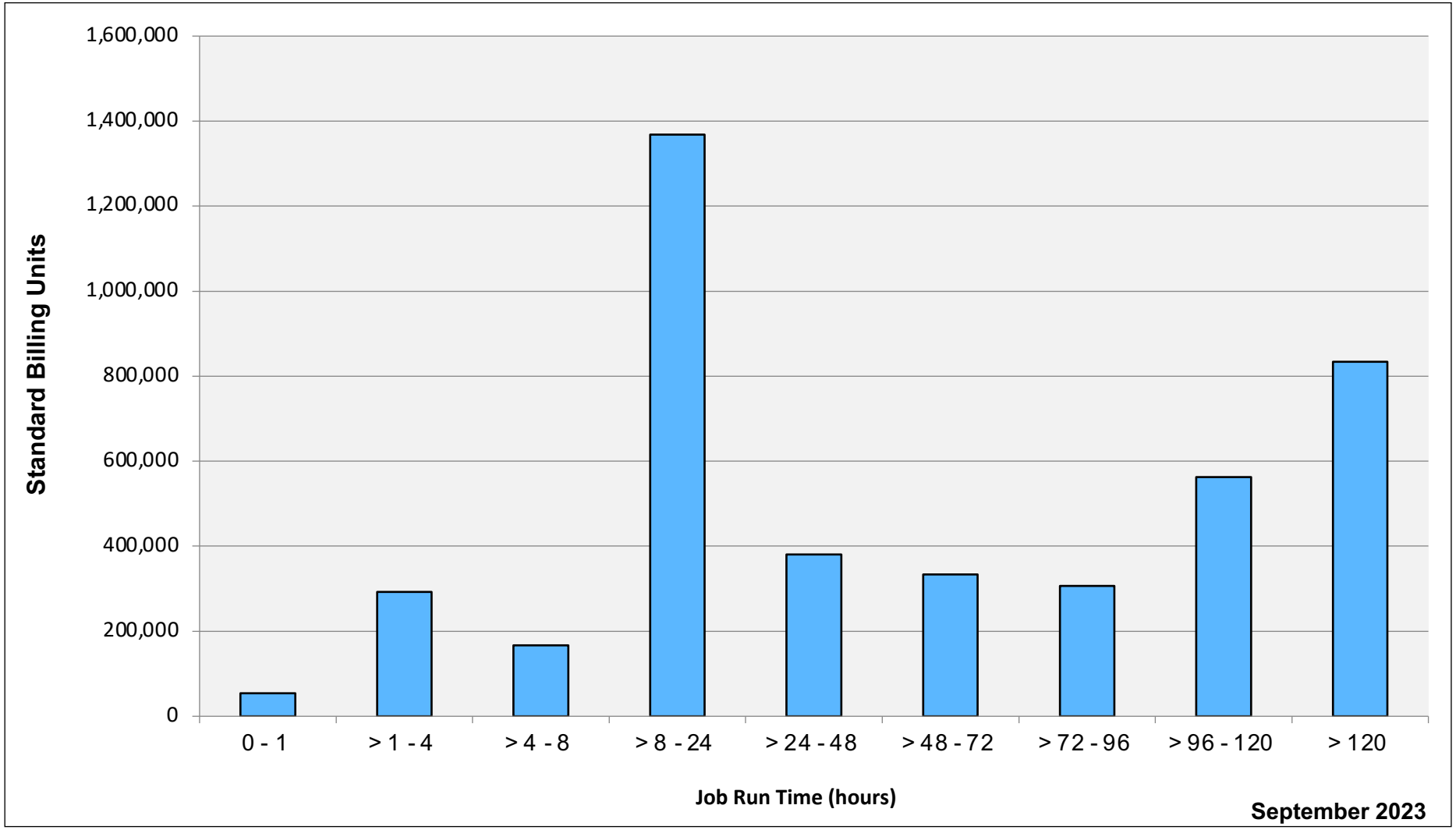
Pleiades: SBUs Reported, Normalized to 30-Day Month



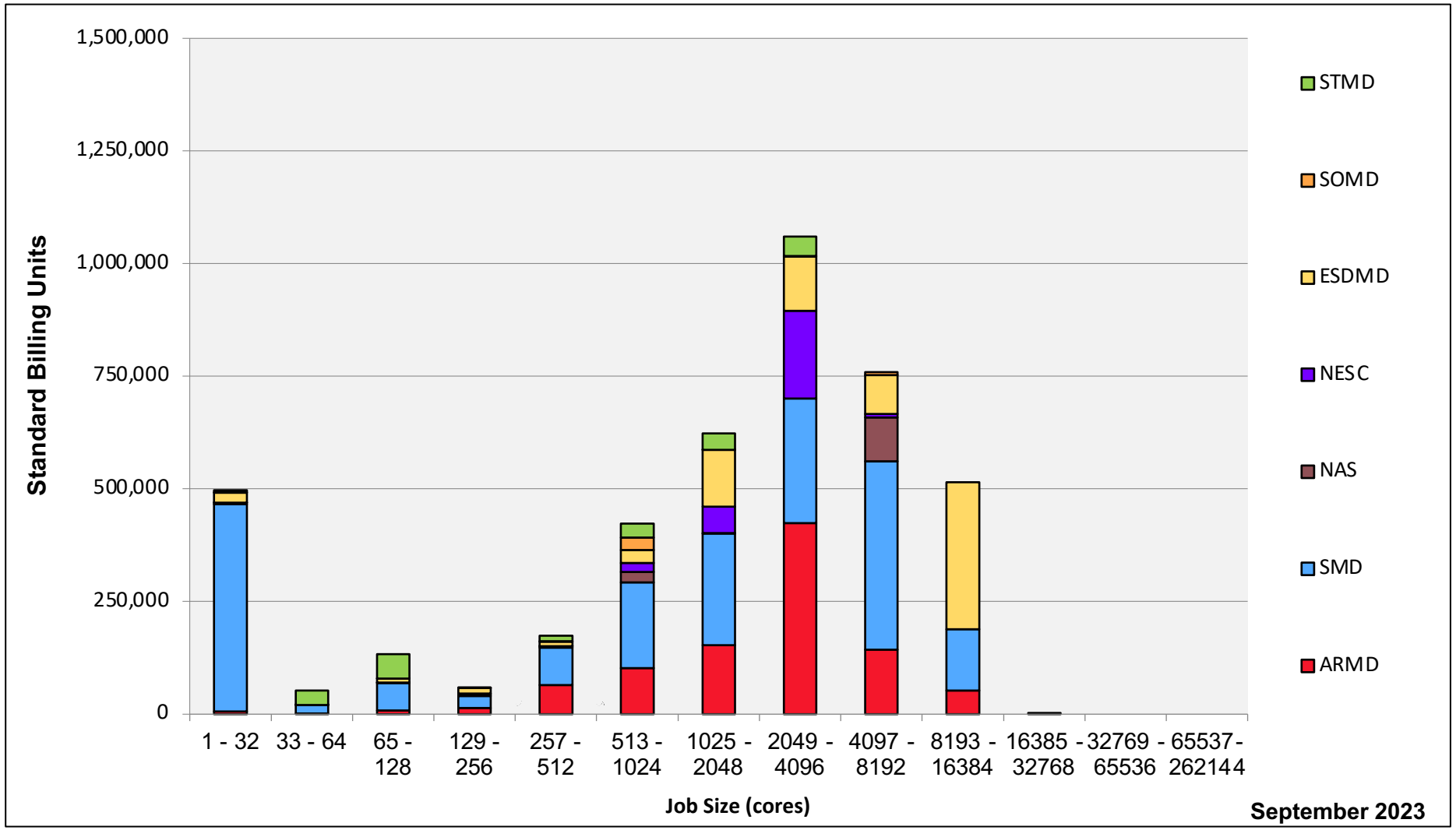
Pleiades: Devel Queue Utilization



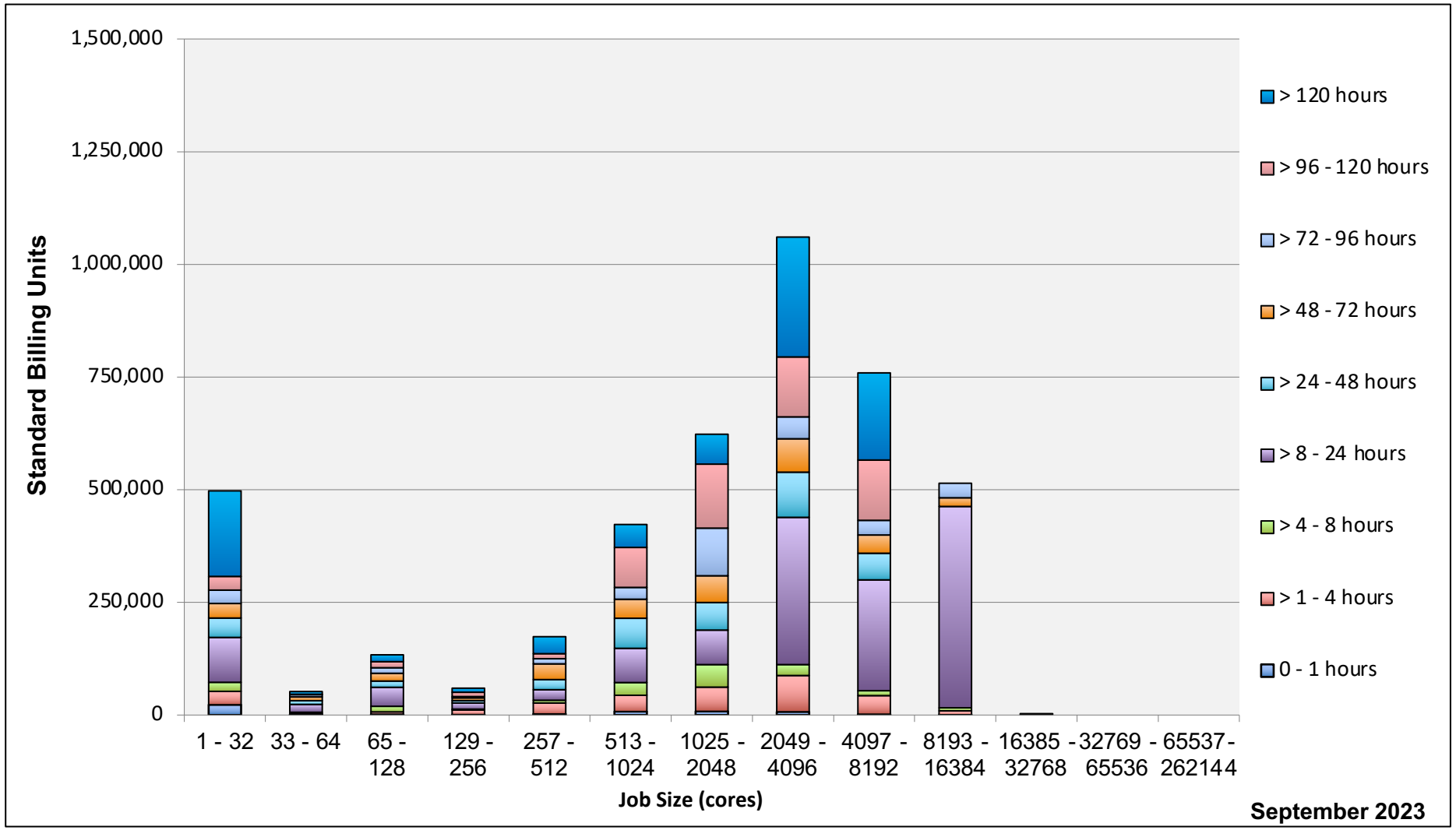
Pleiades: Monthly Utilization by Job Length



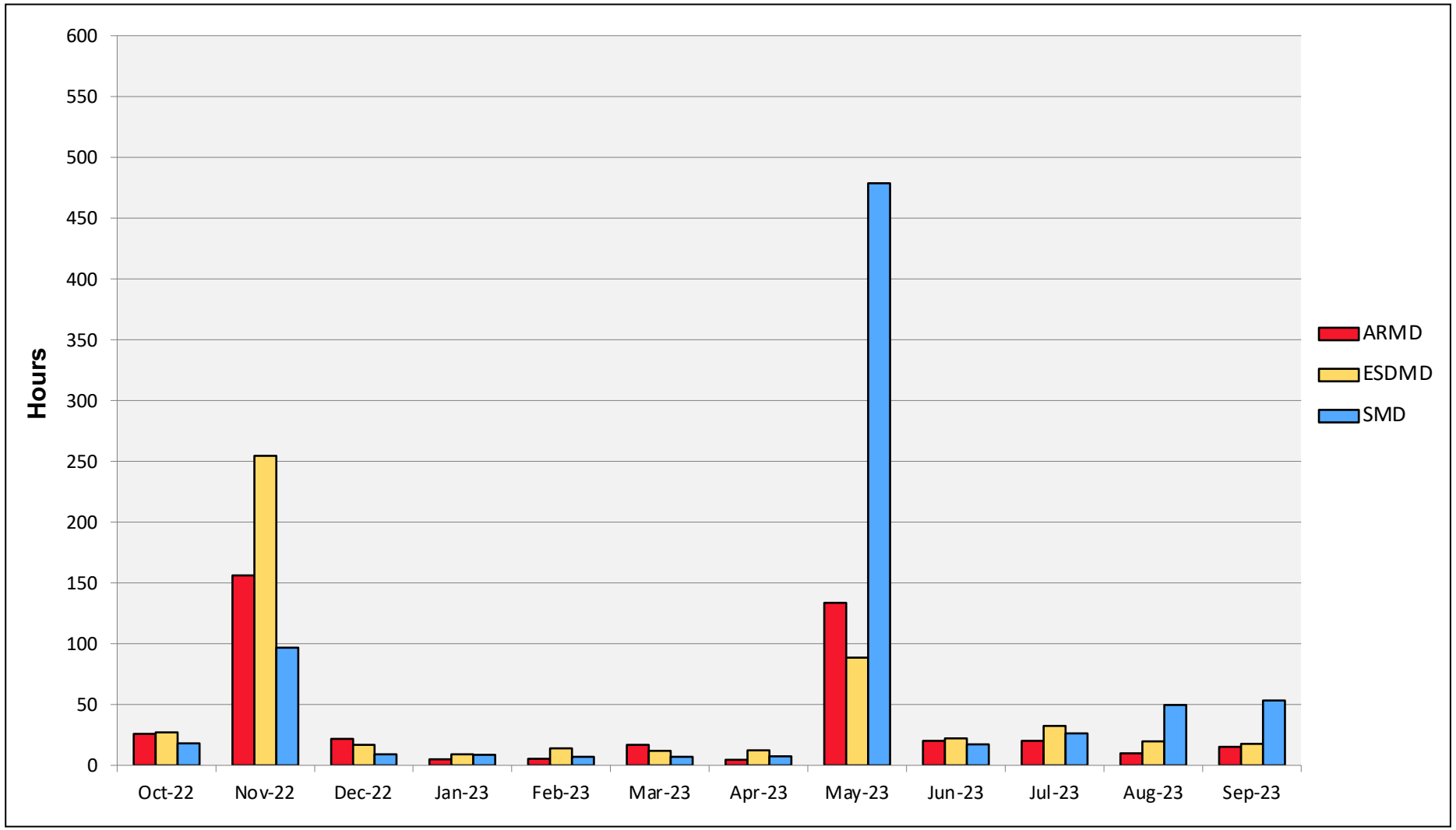
Pleiades: Monthly Utilization by Job Size



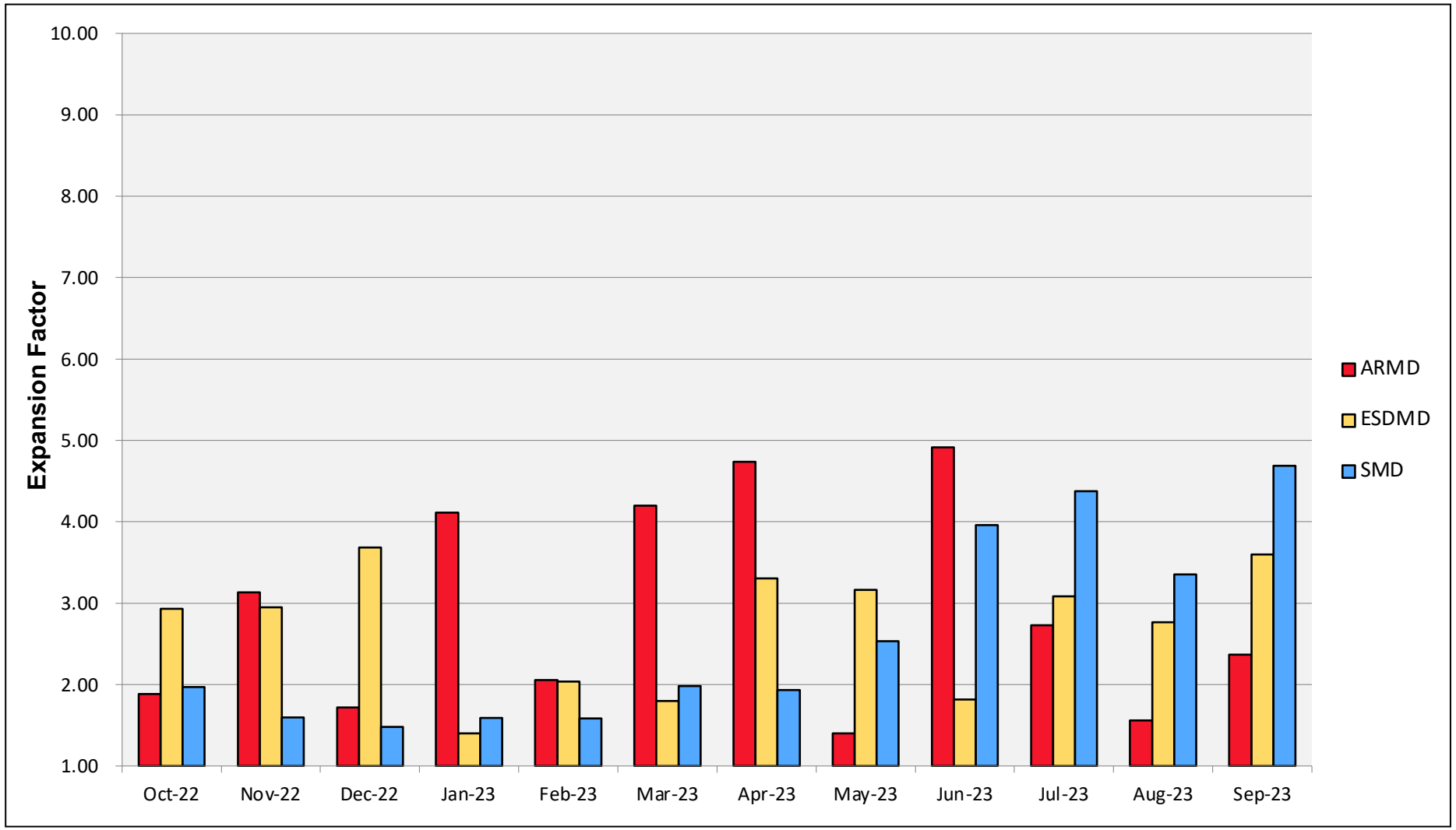
Pleiades: Monthly Utilization by Size and Length



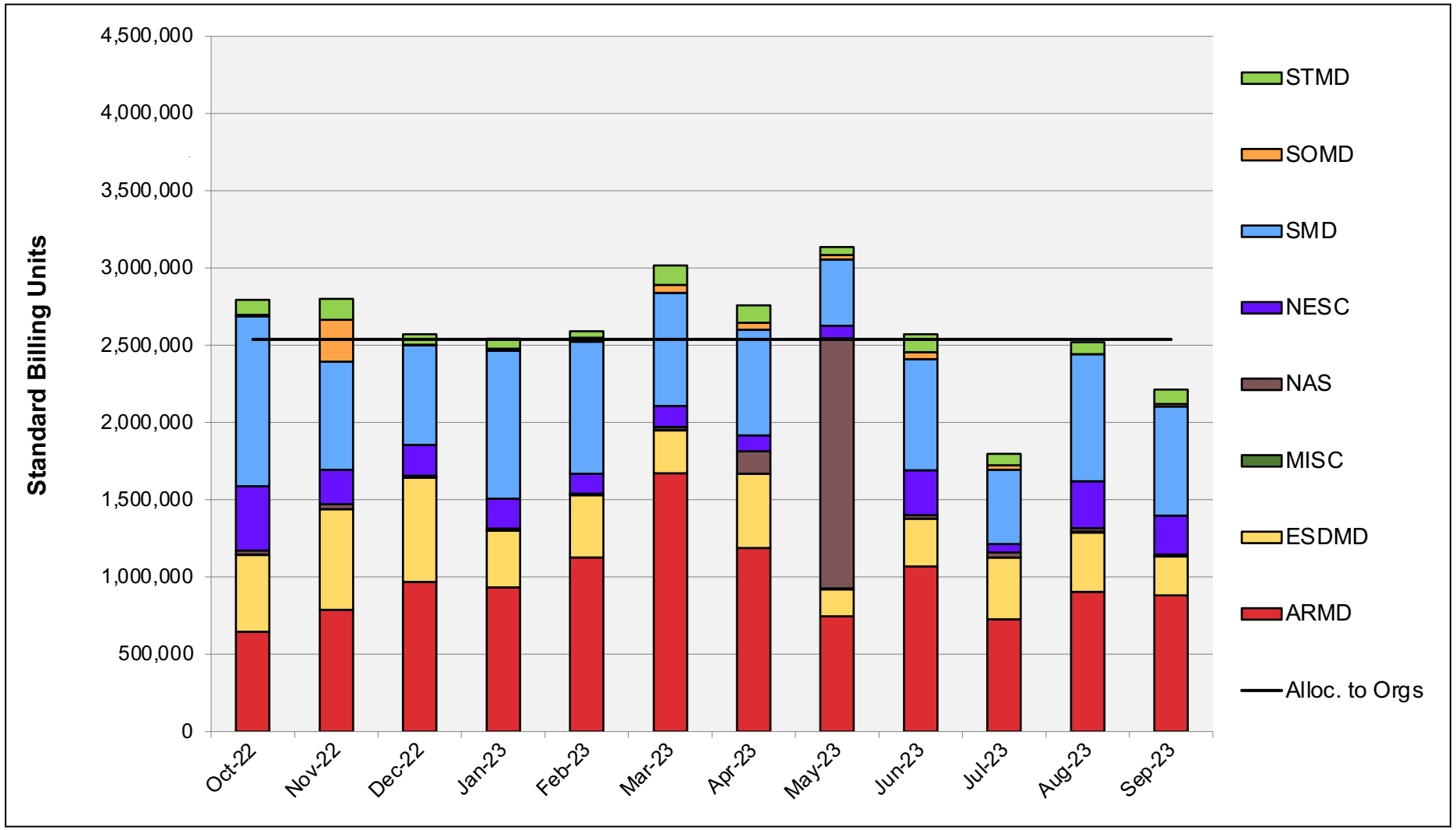
Pleiades: Average Time to Clear All Jobs



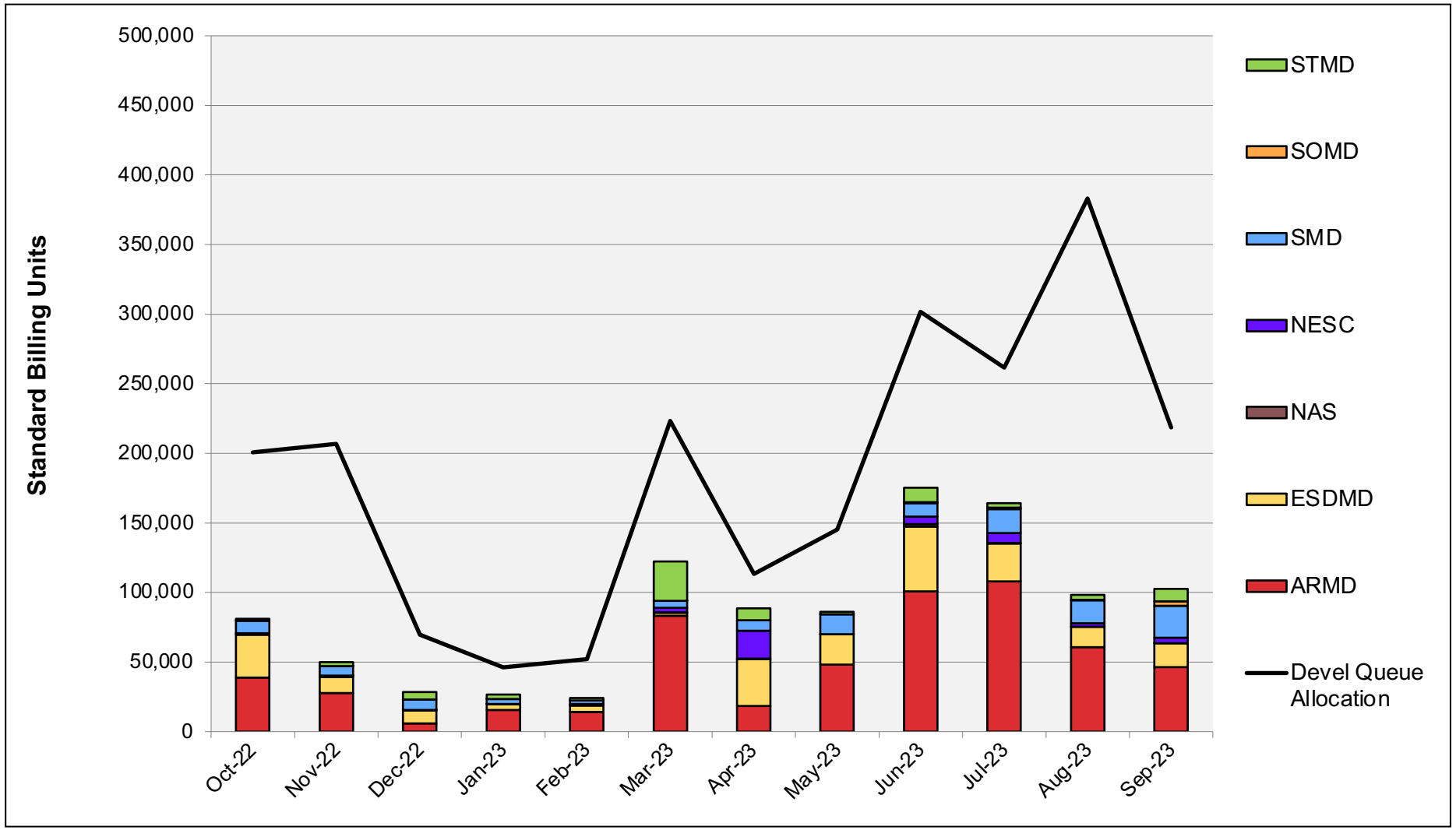
Pleiades: Average Expansion Factor



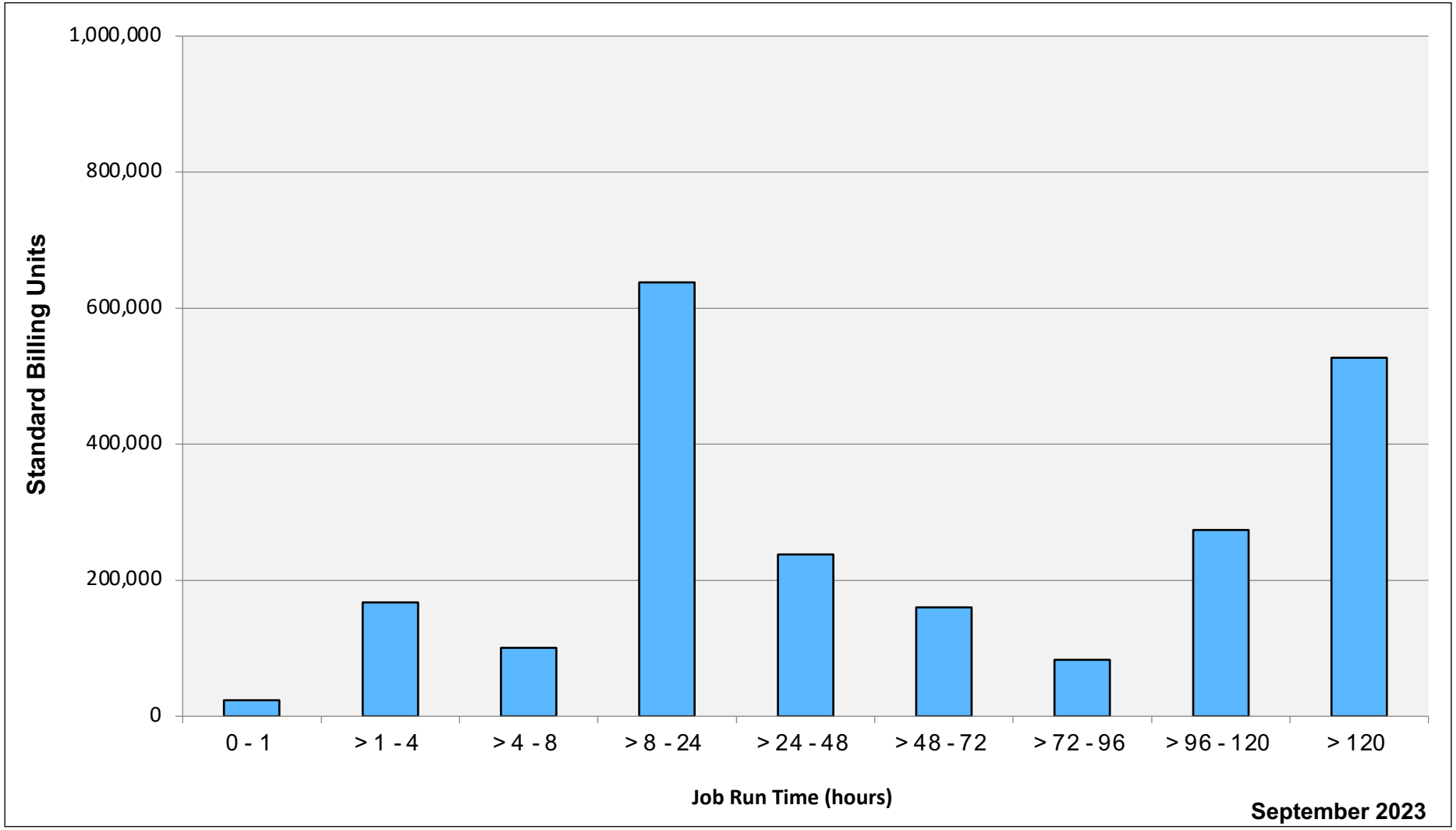
Electra: SBUs Reported, Normalized to 30-Day Month



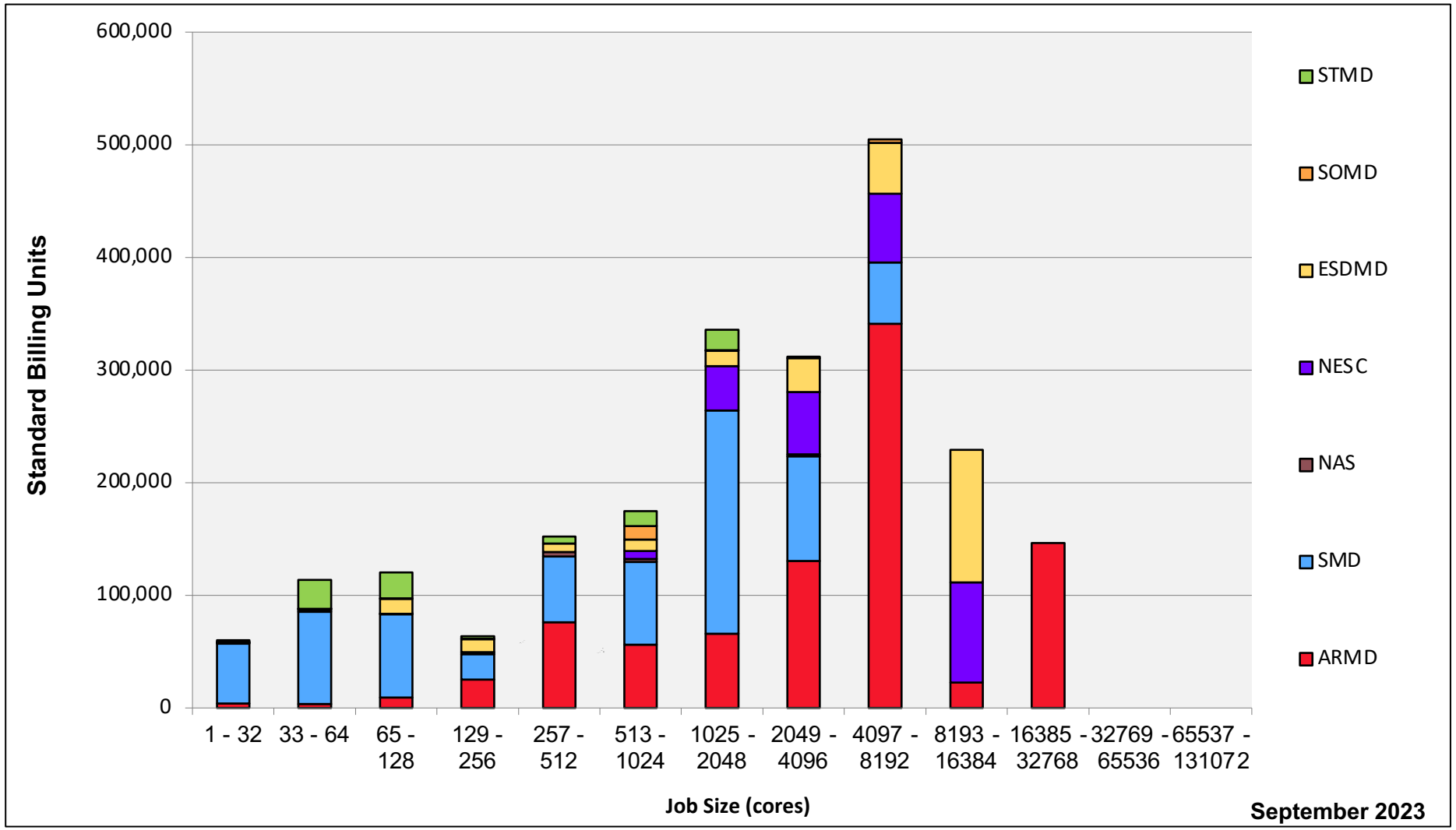
Electra: Devel Queue Utilization



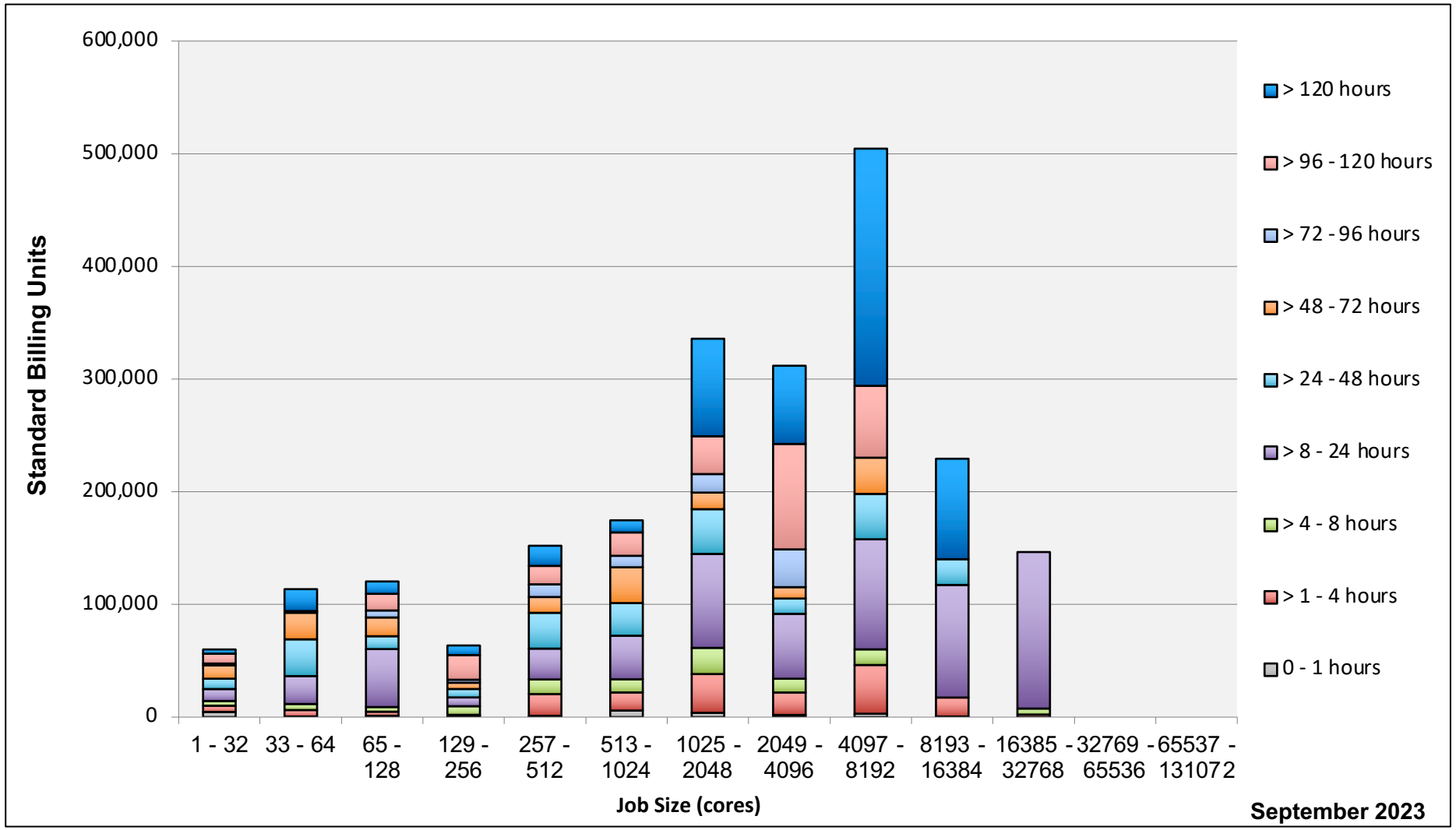
Electra: Monthly Utilization by Job Length



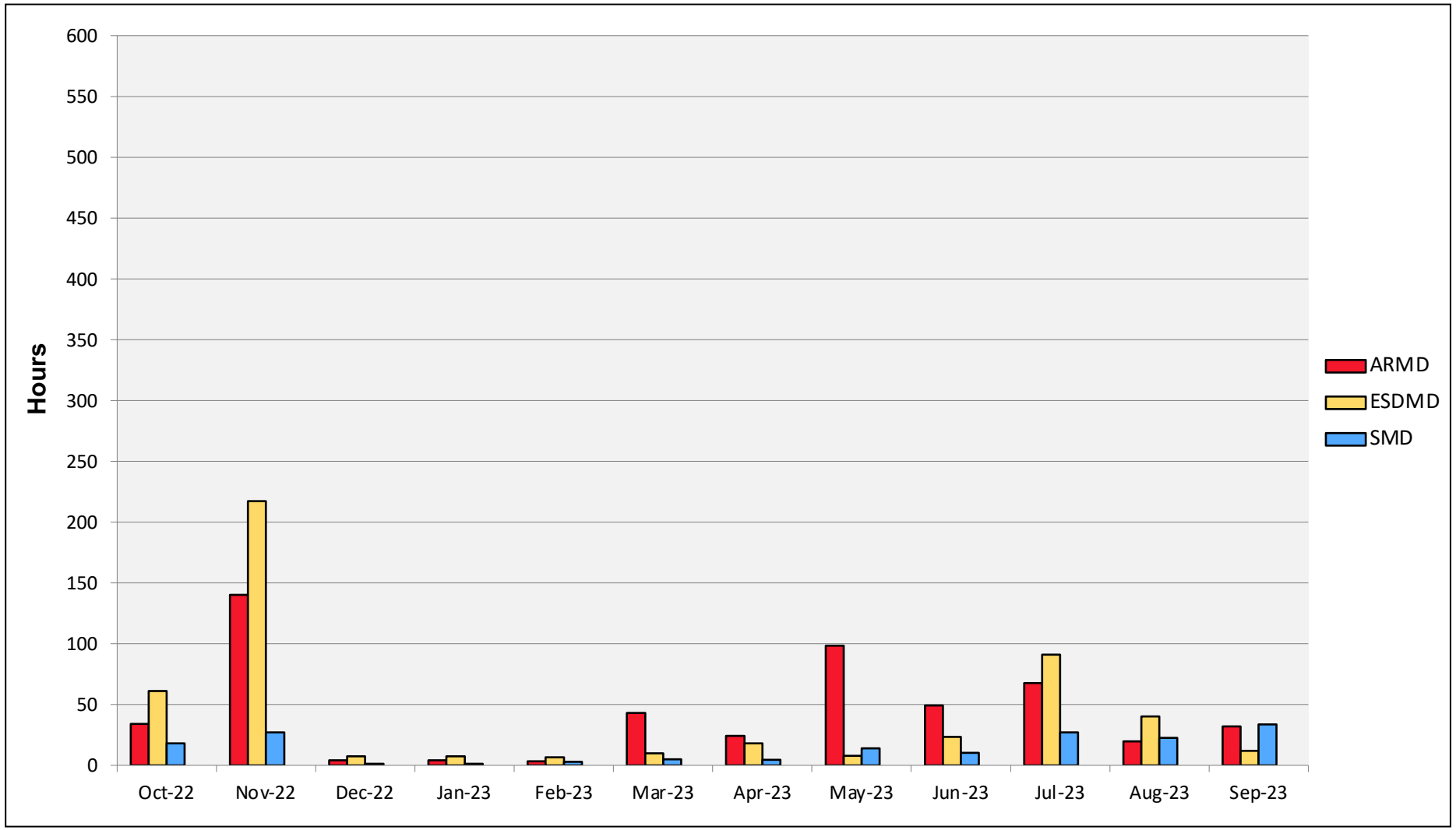
Electra: Monthly Utilization by Job Size



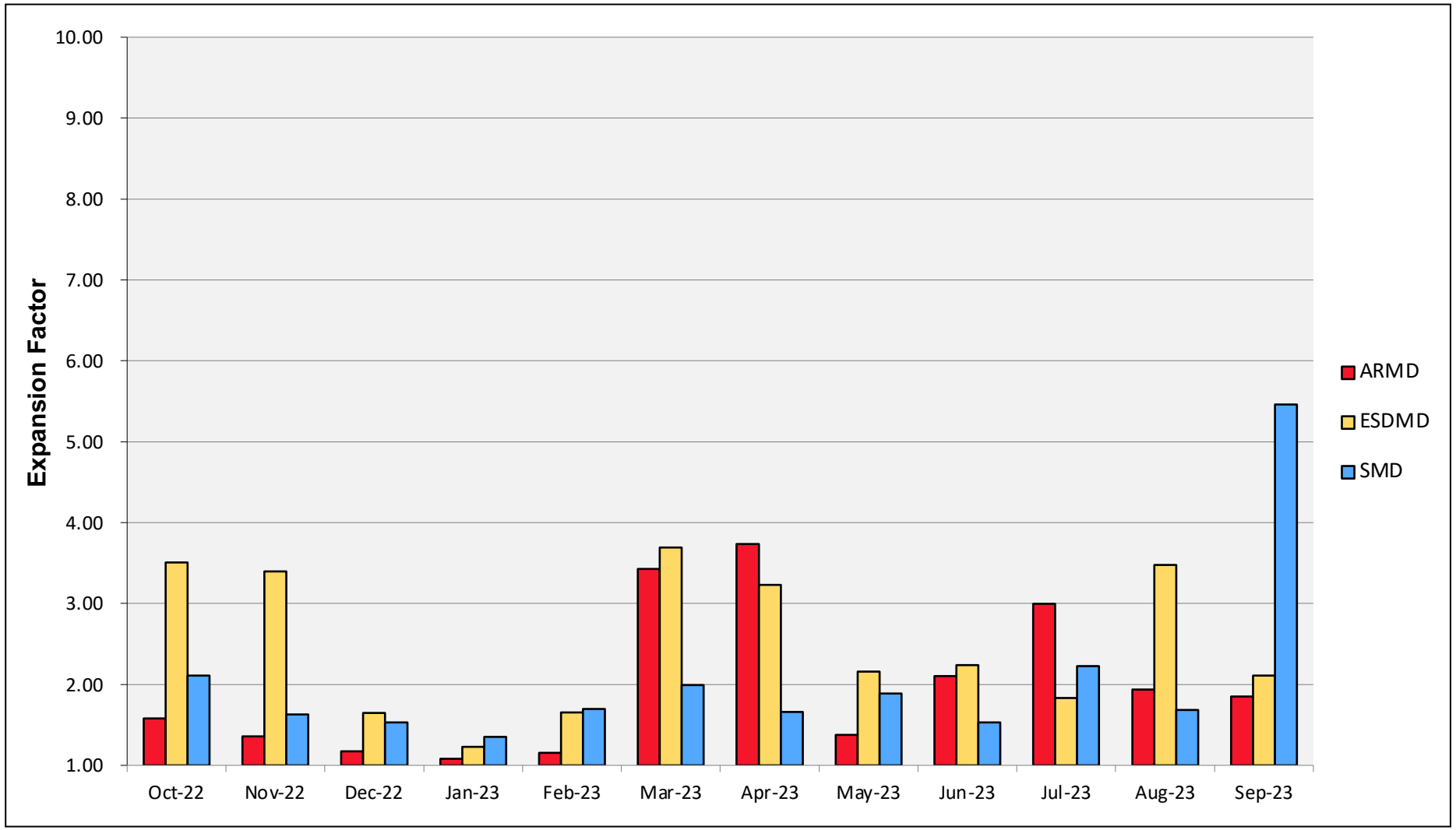
Electra: Monthly Utilization by Size and Length



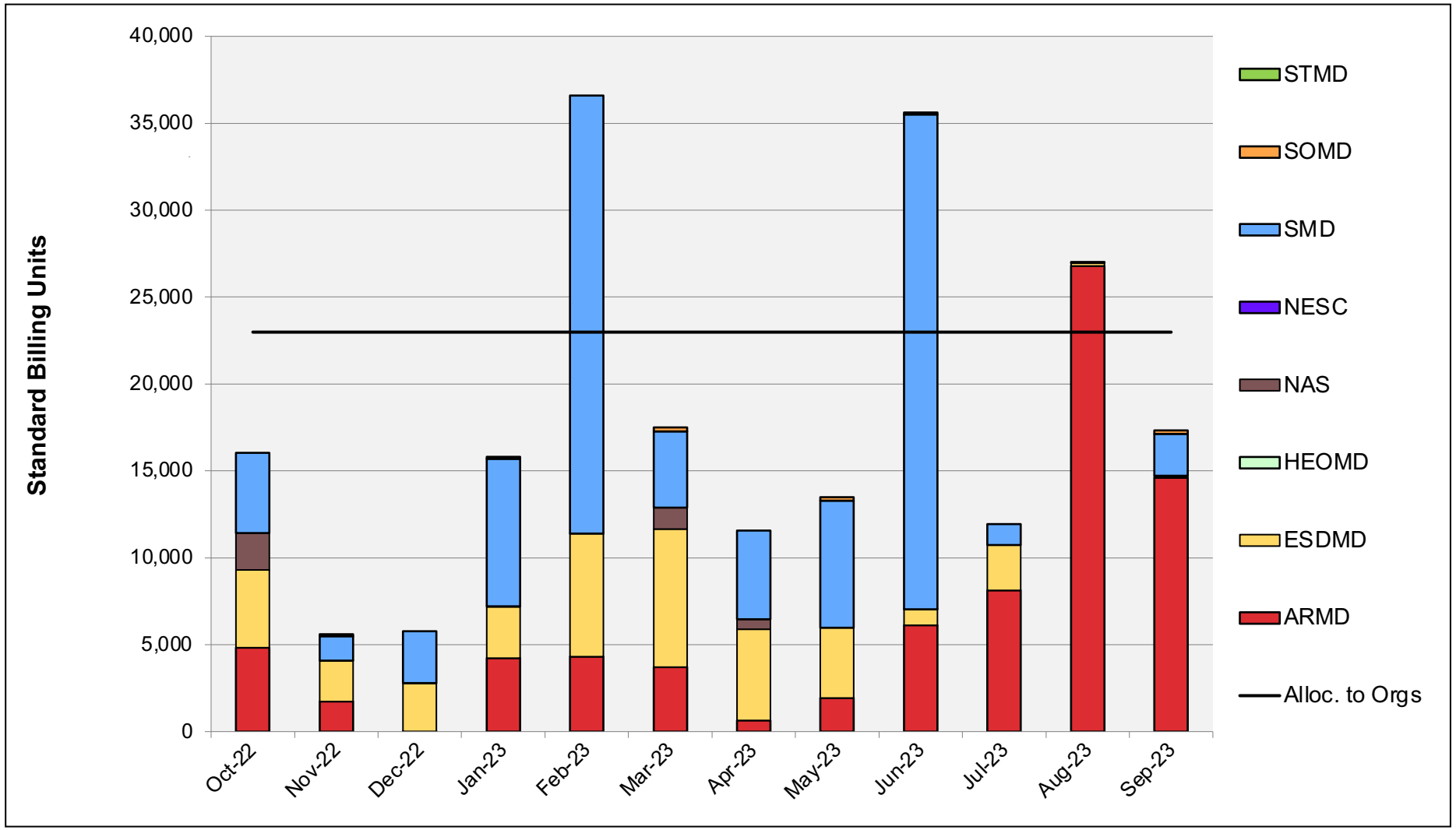
Electra: Average Time to Clear All Jobs



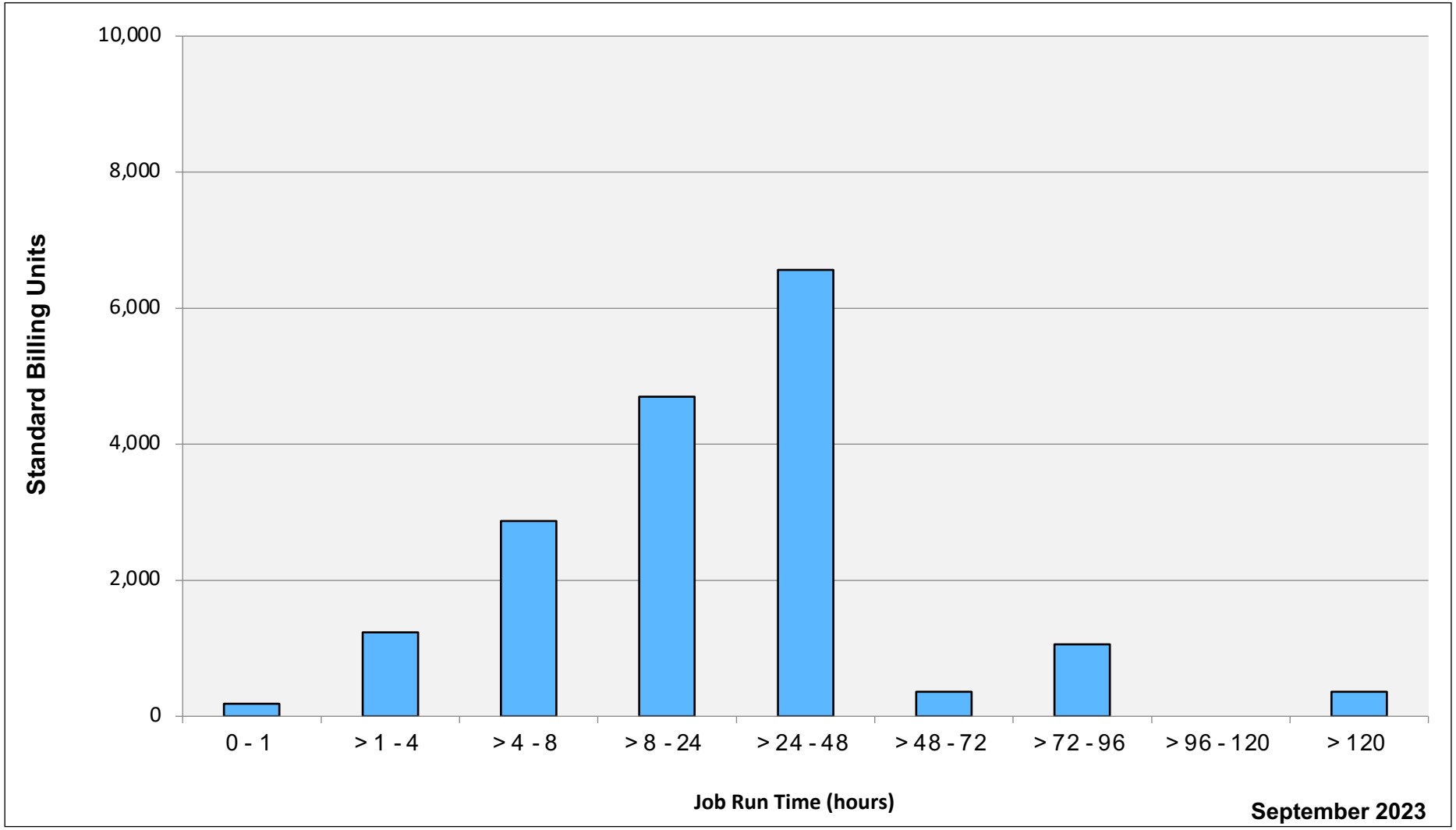
Electra: Average Expansion Factor



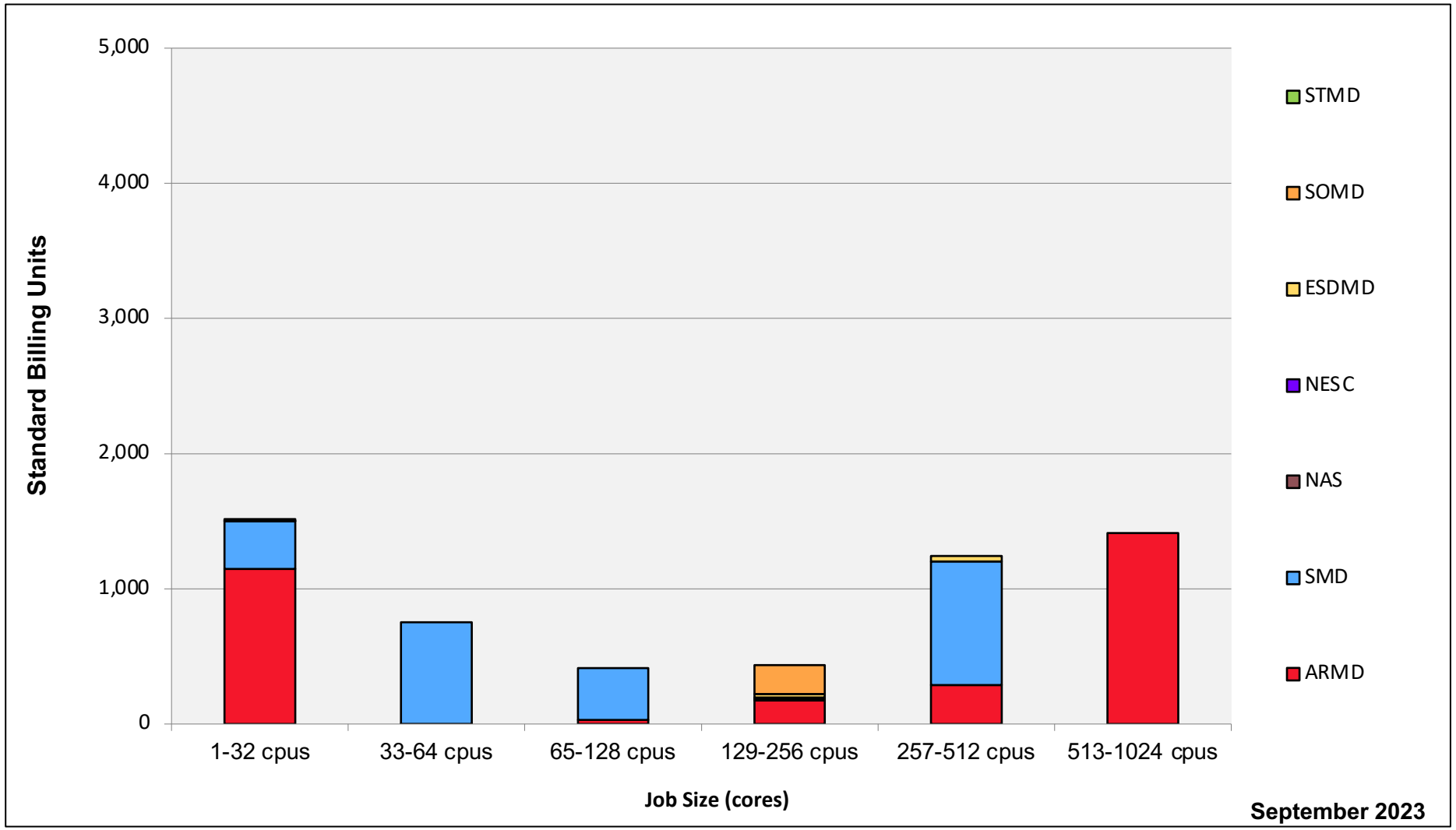
Endeavour: SBUs Reported, Normalized to 30-Day Month



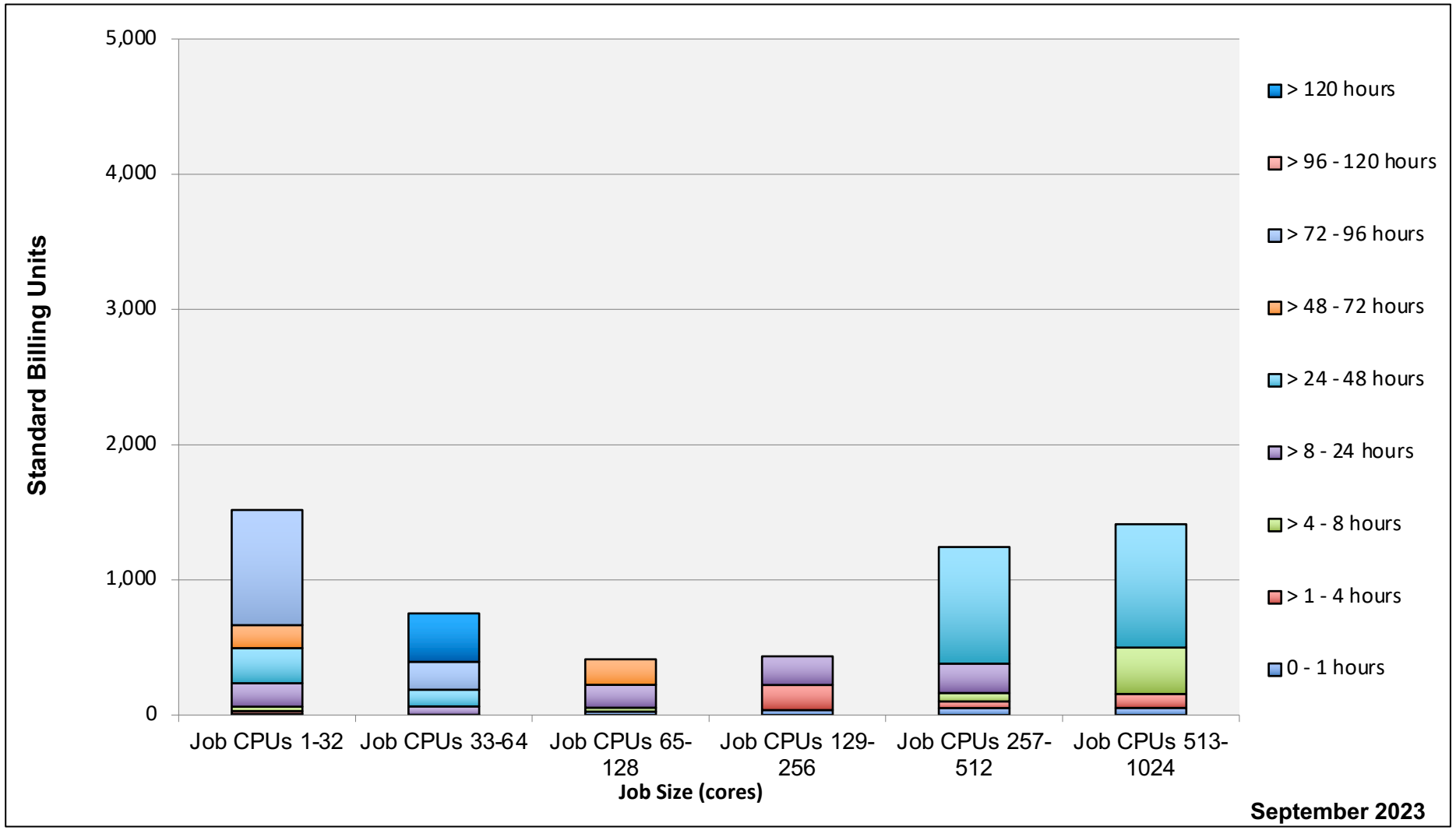
Endeavour: Monthly Utilization by Job Length



Endeavour: Monthly Utilization by Job Size



Endeavour: Monthly Utilization by Size and Length



Endeavour: Average Expansion Factor

