National Aeronautics and Space Administration

HIGH-END COMPUTING CAPABILITY PORTFOLIO

William Thigpen
NASA Advanced Supercomputing Division

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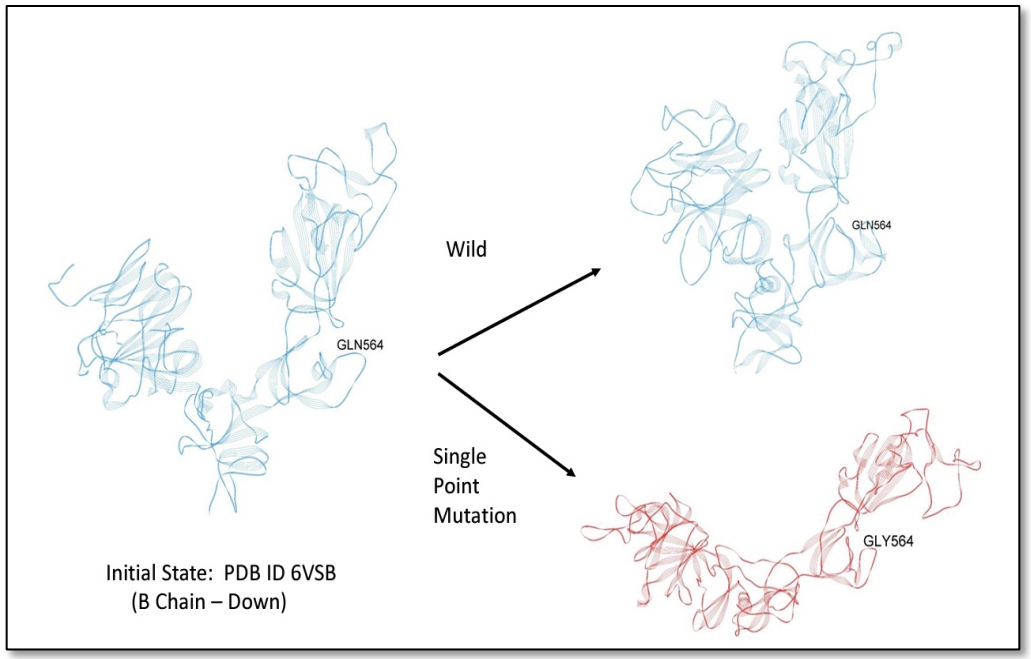
APP Team Optimizes Code Used in COVID-19 Research

- The Applications Performance and Productivity (APP) team installed, tested, and optimized NAMD, a molecular dynamics application being used on HECC resources to conduct a research project studying COVID-19 treatment, as part of the COVID-19 HPC consortium (https://covid19-hpc-consortium.org/).
- NAMD is being used to explore the dynamic and energetic underpinnings of the SARS-CoV-2 spike protein by carrying out all-atom simulations of the spike protein's fluctuations and motions. The results provide insight into how the protein behaves and can therefore steer the design of new therapeutics that might be used to treat the disease.
- APP staff carried out extensive testing of numerous compiler settings and parallel communication approaches, improving simulation performance from 17 nanoseconds (ns) per day up to 25.6–27.7 ns/day.
- The resulting setup minimizes the turnaround time for each simulation, thus facilitating multiple rounds of exploratory research in a rapid prototyping approach.

IMPACT: Faster simulations allow more molecular structures to be investigated, increasing the likelihood of identifying residue-specific drug targets for the development of effective treatments for COVID-19.

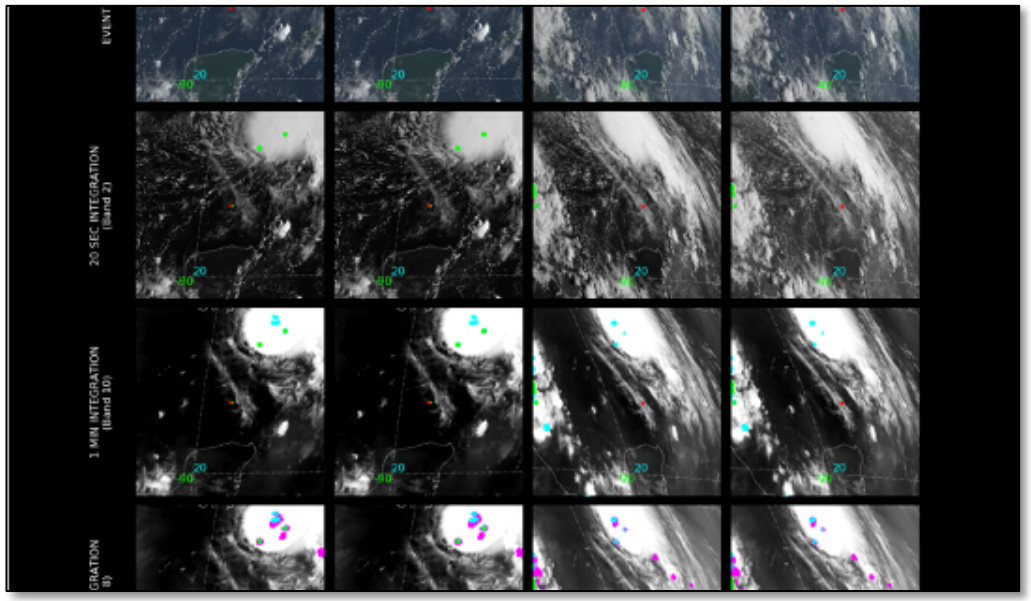


Initial dynamic test of possible latch over a period of approximately 0.1 μ sec. Blue-Wild; Red-Mutant. *Michael Peters, et al.*

Visualizing Bolide Candidates with GOES ABI and GLM Data

- HECC's Visualization and Data Analysis team is designing visualizations to support the identification and analysis of bolides.
  - The Asteroid Threat Assessment Project (ATAP) team, in collaboration with scientists and the Visualization team, developed algorithms to identify bolide candidates detected by the Geostationary Lightning Mapper (GLM) onboard the Geostationary Operational Environmental Satellite (GOES)-R Series Spacecraft.
  - Multispectral imagery from a second GOES-R instrument, the Advanced Baseline Imager (ABI), provides important geospatial and meteorological context for distinguishing bolides from lightning activity. Visually inspecting the ABI data associated with bolide candidates is an important step in the bolide candidate vetting process, previously completed manually and in a time-consuming manner.
- The Visualization team's ABI "cutouts" provide a visual snapshot of the meteorological context surrounding bolide candidates.
  - The cutouts depict local ABI data directly before and after bolide candidate events, in multiple wavebands and waveband composites, and overlaid with increasing temporal integrations of GLM data.
  - The use of ABI cutouts is greatly expediting the vetting process and is allowing for broader visual analysis of GLM data.
- This work is part of larger, ongoing efforts to visualize and analyze streaming satellite data.

IMPACT: Expediting the bolide candidate vetting process allows scientists to use their time more effectively toward analysis of these bright meteors.



ABI cutouts support NASA work to efficiently assess whether bolide candidates are isolated in space and time from lightning activity.
Nina McCurdy, NASA/Ames

HECC Completes Data Science User Survey

- The Data Science team conducted a user survey on the data science and machine learning activities offered by HECC. Over 100 users responded. Some key results include:
  - Most respondents consider themselves new to Data Science and Machine Learning.
  - Nearly two-thirds of respondents are located at a NASA center, over one-quarter are located at a university, and the rest are in industry or private, not-for-profit partners.
  - The respondents were a multidisciplinary group of researchers with over 25% working in aeronautical engineering.
  - Big data is an issue with over 2/3 of respondents reporting to have datasets larger than 1 terabyte (TB) and approximately 10% of respondents reporting to have datasets larger than 100 TB.
- Key findings:
  - There is interest among the user community to gain more knowledge and skills in data science and machine learning.
  - The Machine Learning Knowledge Base articles are kept current with example code and are a good starting point for users to learn how to do machine learning on NAS systems.
  - Tools such as Dask that address the need to process big data will become more important.
  - Model libraries, the MATLAB ML/DS environment, hyperparameter tuning and AutoML tools, and visualization tools and packages will assist our users.

IMPACT: Results from the first user survey of data science and machine learning support help HECC data science experts improve user support. Survey responses highlighted the need for additional support for user training and providing software stacks for new users.

This word cloud was generated from the text of the Wikipedia article on data science. Some of the main words are data, scientist, statistics, machine learning, analysis, software, technique, visualization, database, field, and framework. The words reflect the terms and issues that are associated with data science.

Networks Team Upgrades Switches and Routers

- The HECC Networks team upgraded and replaced NASLAN network switches and routers to remove end-of-life equipment and mitigate security vulnerabilities.
- Hardware refresh activities included:
  - Replacing network devices (occurs every 5 to 10 years, as needed) to ensure that vendor hardware and software support is maintained.
  - Replacing multiple NASLAN routers and switches with new equipment.
- Software upgrades included:
  - A new software version released by the manufacturer to fix vulnerabilities on their network devices, add new features, or patch software bugs.
  - The latest Cisco operating system and inter-network operating system on all NASLAN core switches and routers to mitigate identified security vulnerabilities.
- It is important to make sure that all network devices are always up to date with the latest and stable software to mitigate unexpected downtime or network attacks.

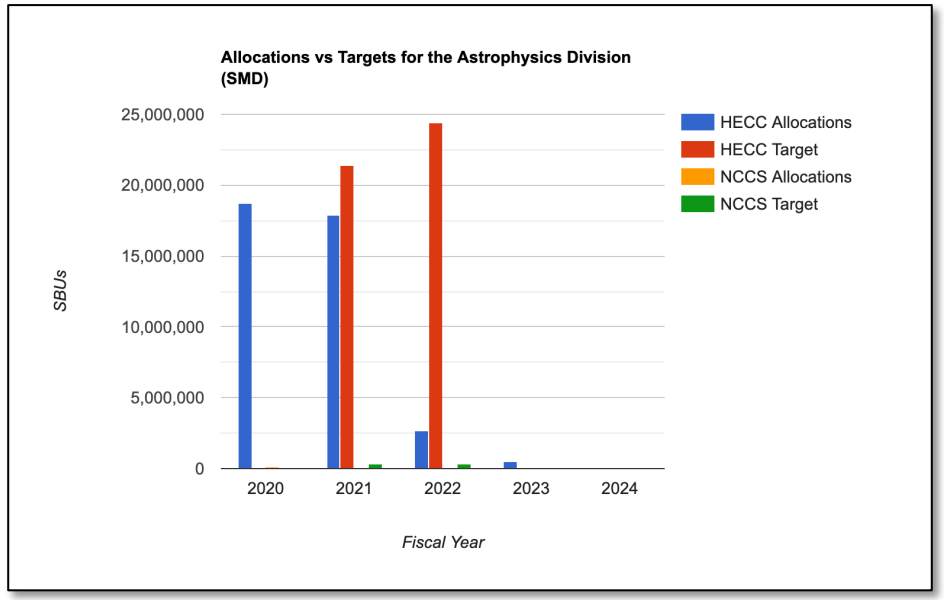
IMPACT: New equipment deployment and software upgrades enable the NAS Local Area Network (NASLAN) devices to continue to receive vendor support and protect against security vulnerabilities.

The Cisco 9300-48T is one example of the newly deployed network switches that was part of the NASLAN hardware refresh.

Resource Management System Version 1.2 Released

- HECC, in collaboration with NCCS, released version 1.2 of the Request Management System (RMS) on September 10, 2020. This tool is in development to replace REI eBooks. RMS currently only supports the Science Mission Directorate (SMD). Version 1.3 (available November 16, 2020) is a short sprint focused on reporting capabilities. The HECC Board of Advisors approved supporting the other mission directorates in version 1.4 with a targeted release date of December 31, 2020.
- This milestone concluded the second of a multi-phase deployment.
- The new RMS tool has features such as:
  - Allowing the SMD Allocation Board to set and manage allocation targets within their programs.
  - Allowing the SMD Allocation Board to allocate HECC and NCCS resources within their programs.
  - Providing the ability to search by GID, PI, and request number.
  - Capturing changes to a project's period of performance.
  - Capturing modifications to a request over the lifetime of the project.

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

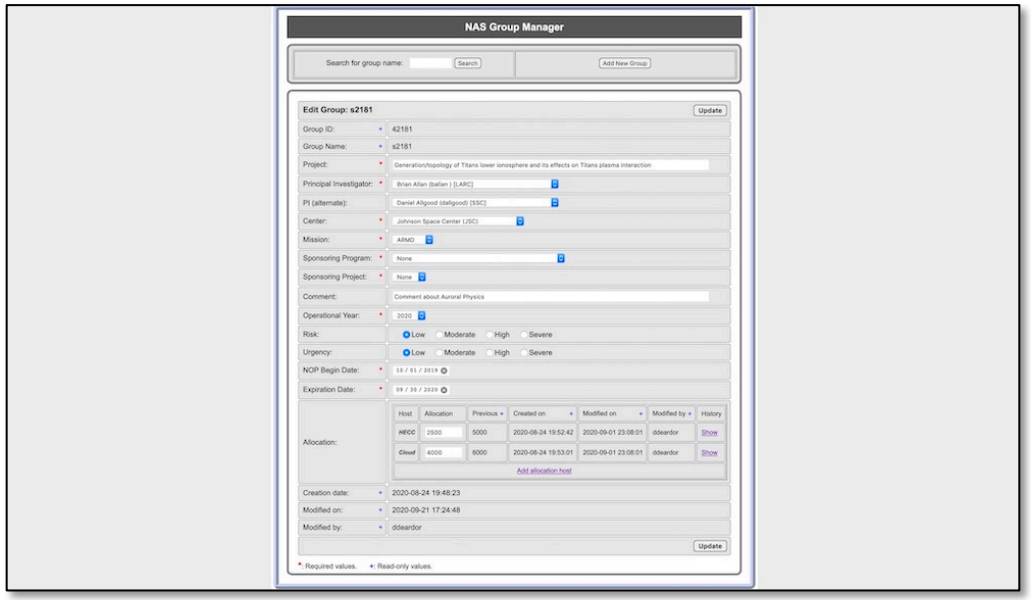


A screenshot from the new Resource Management System showing the Allocation and Targeting chart.

New HECC Project Allocation Management Tool Developed

- The HECC Tools team developed a new web application that enables efficient management of HECC user groups (projects) and their Standard Billing Unit (SBU) allocations.
- The new application, called “Group Manager,” replaces a current application based on the aging Login Account Maintenance System (LAMS) user account database and the Open-source Ticket Request System (OTRS) software.
  - The development of this application completes one of several tasks currently underway to replace LAMS as it is phased out.
- Developed using PHP, the new application will be used by the HECC User Services team to create groups and manage all group attributes, such as affiliated mission directorate, NASA center, sponsoring program and project, and allocations.
- Staff can create and manage new allocation hosts and view audit trails of all SBU allocation assignments.
- A future update will enable the Tools team to create reports for groups sorted by criteria such as Mission Directorate, principal investigator (PI), and location.

IMPACT: The Group Manager application will serve an important role in managing HECC projects and SBU allocations as a modern, more secure replacement of current capabilities that is easier to enhance and maintain.



Snapshot of the Group Manager’s group editing page, which enables HECC User Services staff to edit and manage all aspects of a user group, including description, PI, NASA center, and SBU allocations.

HECC User Communications Proposal Approved

- HECC User Services and Pubs-Media team members developed a comprehensive proposal for improving the methods HECC uses to communicate with users, with a strong emphasis on coordination and consolidation.
- Project goals include building trust between users and HECC, fostering more two-way communication, and streamlining communication procedures for support groups.
  - A recurring theme from the HECC user survey and outreach tours is that more effective communication with our user community is needed.
  - To research ways to improve communications, the project team evaluated past and current HECC communication methods and processes, along with methods used by other federal HPC centers.
  - The new plan proposes: Improving coordination of user notifications; consolidating notifications in a weekly HECC newsletter and on a new communications landing page on the HECC website; and developing an event calendar. Several options for implementation and a best estimate of the level of effort were also included. These will be carefully considered as part of Phase 2 (implementation).
  - A copy of the proposal is available upon request.
- With management approval to move forward, planning for the implementation phase is now underway.

IMPACT: A comprehensive communications plan assists the organization in coordinating and consolidating its efforts, ensuing that HECC users supporting NASA missions have all of the information they need to successfully run their projects on HECC systems.

User Communications Gap Analysis

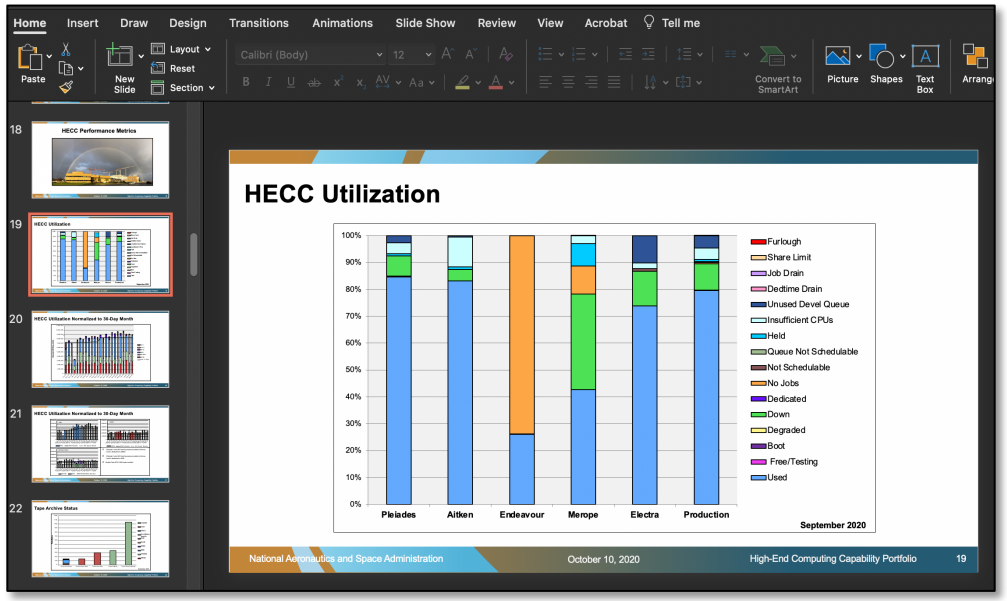
Focus Area	Desired Future State
Coordination*	A process exists for planning and communicating things like planned outages to users. Process is documented and all teams are aware. User communications occur in a consistent manner.
Informing users about types of communincations	There is a centralized place on the website to indicate what information can be found where, along with types of email communications/subscriptions, if applicable. Past issues of newsletter are also available.

The project team conducted a gap analysis to help determine where improvements can be made in the HECC user communication process. *The coordination aspect of this project overlaps with the Configuration Change Management Project.

Tools Team Continues Improvements to the HECC Performance Metric Monthly Reporting Process

- The Tools team completed Phase 2 of a three-phase project to improve the HECC monthly reporting process.
- The team completed Reports Automation Phase 2, including the following activities:
  - Leveraging from the work completed in Phase 1, created PowerPoint slides from the Excel format data for performance metrics.
  - In completing the above task, the team automated the creation of the slides and then emailing those slides to User Services staff.
- The team not only decreased the time it took to run these reports from hours to minutes, it also removed many manual activities.
- The Tools team continues to move to a more streamlined approach to produce reports. This project will reduce the complexity and substantial costs (labor and maintenance) associated with report production, as well as the project's reliance on third-party software, and lays the foundation for future reporting improvements.

IMPACT: As the complexity of the HECC computing environment increases, continuous automation of usage reporting helps staff ensure accuracy and meet aggressive reporting schedules.



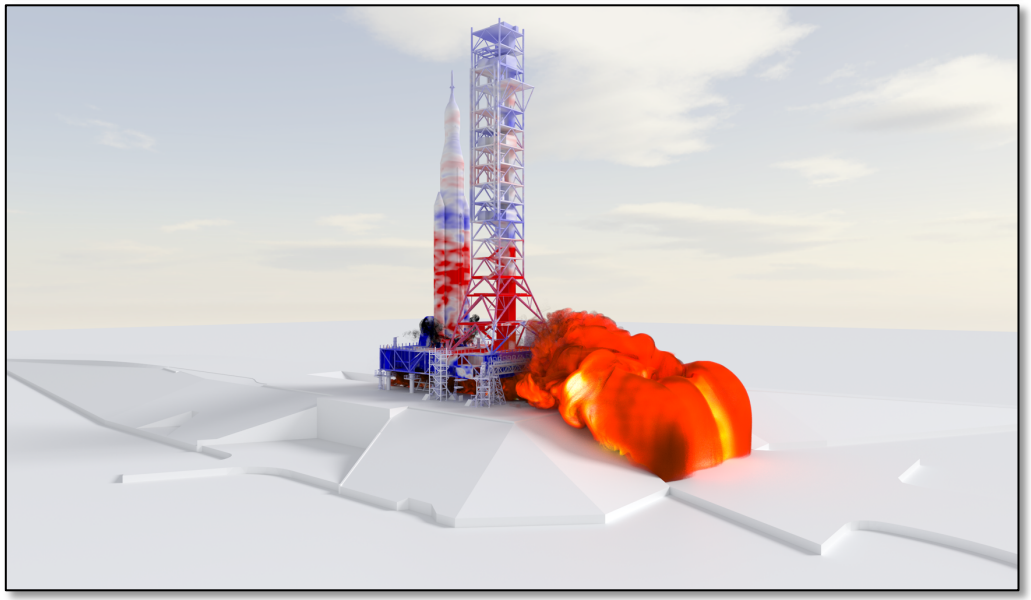
Example of the formatted reports that are automatically created on the first of every month through the HECC reports automation tools.

Multiphysics Prediction for the KSC Launch Environment*

- When engineers at NASA's Kennedy Space Center (KSC) redesigned and rebuilt the main flame deflector at Launch Complex 39B, computational fluid dynamics (CFD) experts at the NASA Advanced Supercomputing (NAS) facility were called in to help identify thermal, pressure, and flow environments on and around the geometrically complex structure.
- The Launch Ascent and Vehicle Analysis (LAVA) team investigated both ignition overpressure waves and thermal conjugate heat transfer around the flame deflector, mobile launcher, tower, and other key components of the launch pad.
- The results of these simulations were used to evaluate the ability of the launch facility's Ignition Overpressure Protection and Sound Suppression system to prevent violent acoustic waves that could damage the launch structure or vehicle.
- These highly-detailed simulations, run with CFD flow solvers within the LAVA framework, are some of the largest ever conducted on HECC systems; each contains over 555 million cells and over 500,000 timesteps, and utilizes more than 4,000 Intel Skylake cores on the Electra supercomputer.

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

IMPACT: The results of this work provided a more complete picture of the extreme conditions around the launch system and helped engineers redesign the launch environment at NASA Kennedy, reducing the risk to future agency missions.



Snapshot from a simulation of launch ignition for NASA's next-generation Space Launch System. Surfaces are colored by pressure (red is high; blue is low), while particles are colored by temperature (orange is hot; black is cooler). *Michael F. Barad, Timothy Sandstrom, NASA/Ames*

Papers

- "**An Unusually Low Density Ultra-Short Period Super-Earth and Three Mini-Neptunes around the Old Star TOI-561**," G. Lacedelli, et al., arXiv:2009.02332 [astro-ph.EP], September 4, 2020. * https://arxiv.org/abs/2009.02332
- "**The TESS-Keck Survey II: Masses of Three Sub-Neptunes Transiting the Galactic Thick-Disk Star TOI-561**," L. Weiss, et al., arXiv:2009.03071 [astro-ph.EP], September 7, 2020. * https://arxiv.org/abs/2009.03071
- "**As a Matter of Tension – Kinetic Energy Spectra in MHD Turbulence**," P. Grete, B. O'Shea, K. Beckworth, arXiv:2009.03342 [physics.plasm-ph], September 7, 2020. * https://arxiv.org/abs/2009.03342
- "**A Super-Earth and a Sub-Neptune Orbiting the Bright, Quiet M3 Dwarf TOI-1266**," B.-O. Demory, et al., arXiv:2009.04317 [astro-ph.EP], September 9, 2020. * https://arxiv.org/abs/2009.04317
- "**Particle Acceleration in Relativistic Electron-Positron Jets with Helical Magnetic Fields**," A. Meli, et al., arXiv:2009.04158 [astro-ph.HE], September 9, 2020. * https://arxiv.org/abs/2009.04158

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

Papers (cont.)

- "**Particle-in-Cell Simulations of Secondary Magnetic Islands: Ion-Scale Flux Ropes and Plasmoids**," S. Lu, et al., The Astrophysical Journal, vol. 900, no. 2, September 10, 2020. * https://iopscience.iop.org/article/10.3847/1538-4357/abaa44/meta
- "**Measuring Transit Signal Recovery in the Kepler Pipeline. IV. Completeness of the DR25 Planet Candidate Catalog**," J. Christiansen, et al., The Astronomical Journal, vol. 160, no. 4, September 10, 2020. * https://iopscience.iop.org/article/10.3847/1538-3881/abab0b/meta
- "**One-Two Quench: A Double Minor Merger Scenario**," N. N. Sanchez, et al., arXiv:2009.05581 [astro-ph.GA], September 11, 2020. * https://arxiv.org/abs/2009.05581
- "**Antarctic Ice Sheet Response to Sudden and Sustained Ice-Shelf Collapse (ABUMIP)**," S. Sun, et al., Journal of Glaciology, Cambridge University Press, September 14, 2020. * https://www.cambridge.org/core/journals/journal-of-glaciology/article/antarctic-ice-sheet-response-to-sudden-and-sustained-iceshelf-collapse-abumip/C08970BDF95EA737AD941D3690EBB3C5/core-reader
- "**Growth of Jupiter: Formation in Disks of Gas and Solids and Evolution to the Present Epoch**," G. D'Angelo, et al., Icarus, published online September 14, 2020. * https://www.sciencedirect.com/science/article/abs/pii/S0019103520304358

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

Papers (cont.)

- "**How Dense of a Circumstellar Medium is Sufficient to Choke a Jet?**" P. Duffell, A. Ho, The Astrophysical Journal, vol. 900, no. 2, September 15, 2020. *
  https://iopscience.iop.org/article/10.3847/1538-4357/aba90a/meta
- "**An Earth-like Stellar Wind Environment for Proxima Centauri C**," J. Alvarado-Gomez, et al., arXiv:2009.07266 [astro-ph.SR], September 15, 2020. *
  https://arxiv.org/abs/2009.07266
- "**Cluster Difference Imaging Photometric Survey. II. TOI 837: A Young Validated Planet in IC 2602**," L. Bouma, et al., arXiv:2009.07845 [astro-ph.EP], September 16, 2020. *
  https://arxiv.org/abs/2009.07845
- "**A Planetary System with Two Transiting Mini-Neptunes Near the Radius Valley Transition around the Bright M Dwarf TOI-776**," R. Luque, et al., arXiv:2009.08338 [astro-ph.EP], September 17, 2020. *
  https://arxiv.org/abs/2009.08338
- "**Magnetic Reconnection and Kinetic Waves Generated in the Earth's Quasi-Parallel Bow Shock**," N. Bessho, et al., Physics of Plasmas, vol. 27, issue 9, September 18, 2020. *
  https://aip.scitation.org/doi/full/10.1063/5.0012443

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

Papers (cont.)

- "**Magnetic Ergostars, Jet Formation and Gamma-Ray Bursts: Ergoregions Versus Horizons**," M. Ruiz, et al., arXiv:2009.08982 [astro-ph.HE], September 18, 2020. * https://arxiv.org/abs/2009.08982
- "**An Ultrahot Neptune in the Neptune Desert**," J. Jenkins, et al., Nature Astronomy: Letters, September 21, 2020. * https://www.nature.com/articles/s41550-020-1142-z
- "**Far-Ultraviolet Aurora Identified at Comet 67P/Churyumov-Gerasimenko**," M. Galand, et al., Nature Astronomy, September 21, 2020. * https://www.nature.com/articles/s41550-020-1171-7

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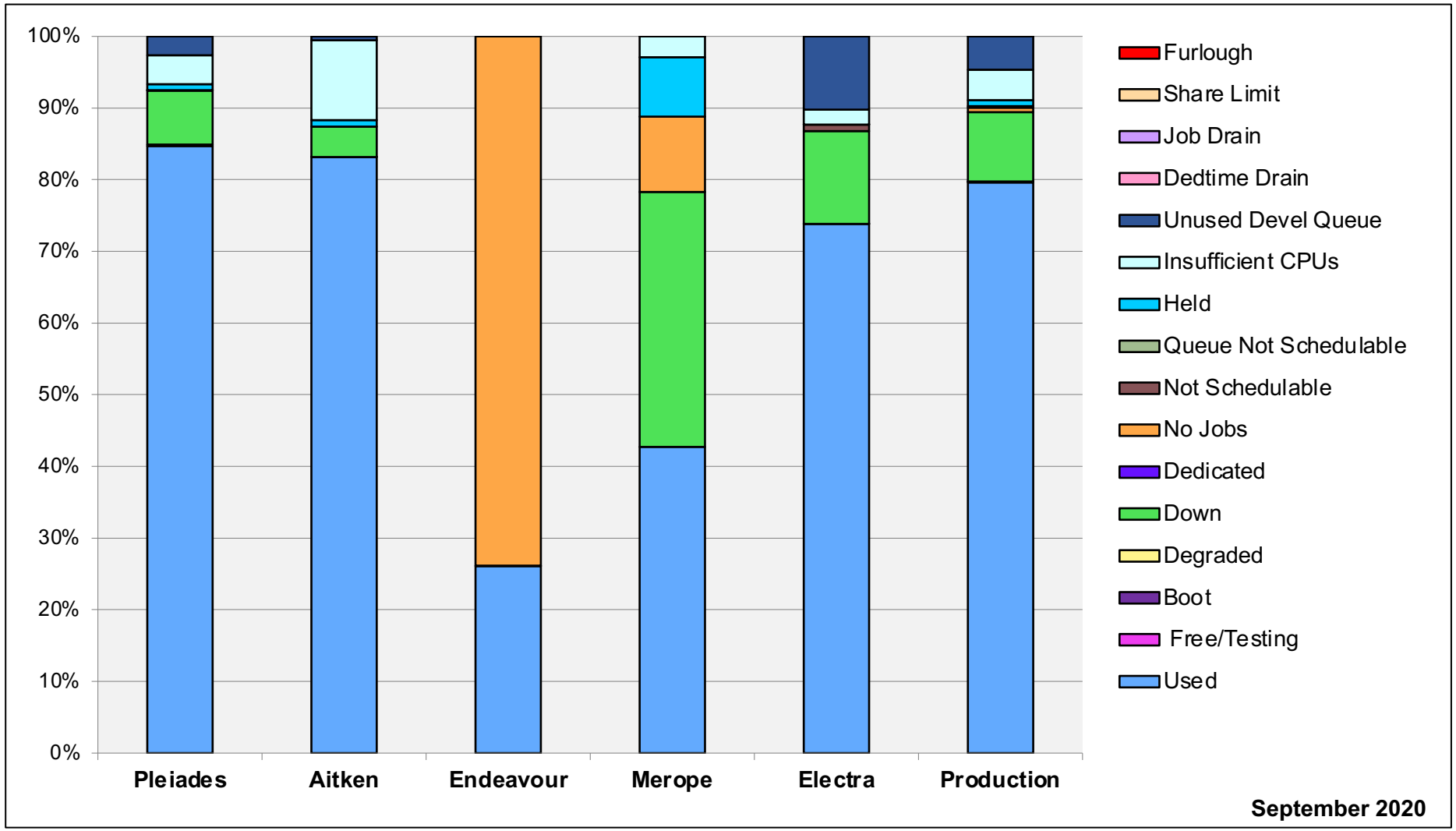
News and Events

- **NASA Missions Spy First Possible ‘Survivor’ Planet Hugging White Dwarf Star**, *NASA Press Release*, September 16, 2020–An international team of astronomers using NASA's Transiting Exoplanet Survey Satellite (TESS) and retired Spitzer Space Telescope reported what may be the first intact planet found closely orbiting a white dwarf star. The NASA Advanced Supercomputing Division processed the TESS data products employed in the study, published in *Nature*. https://www.nasa.gov/press-release/nasa-missions-spy-first-possible-survivor-planet-hugging-white-dwarf-star

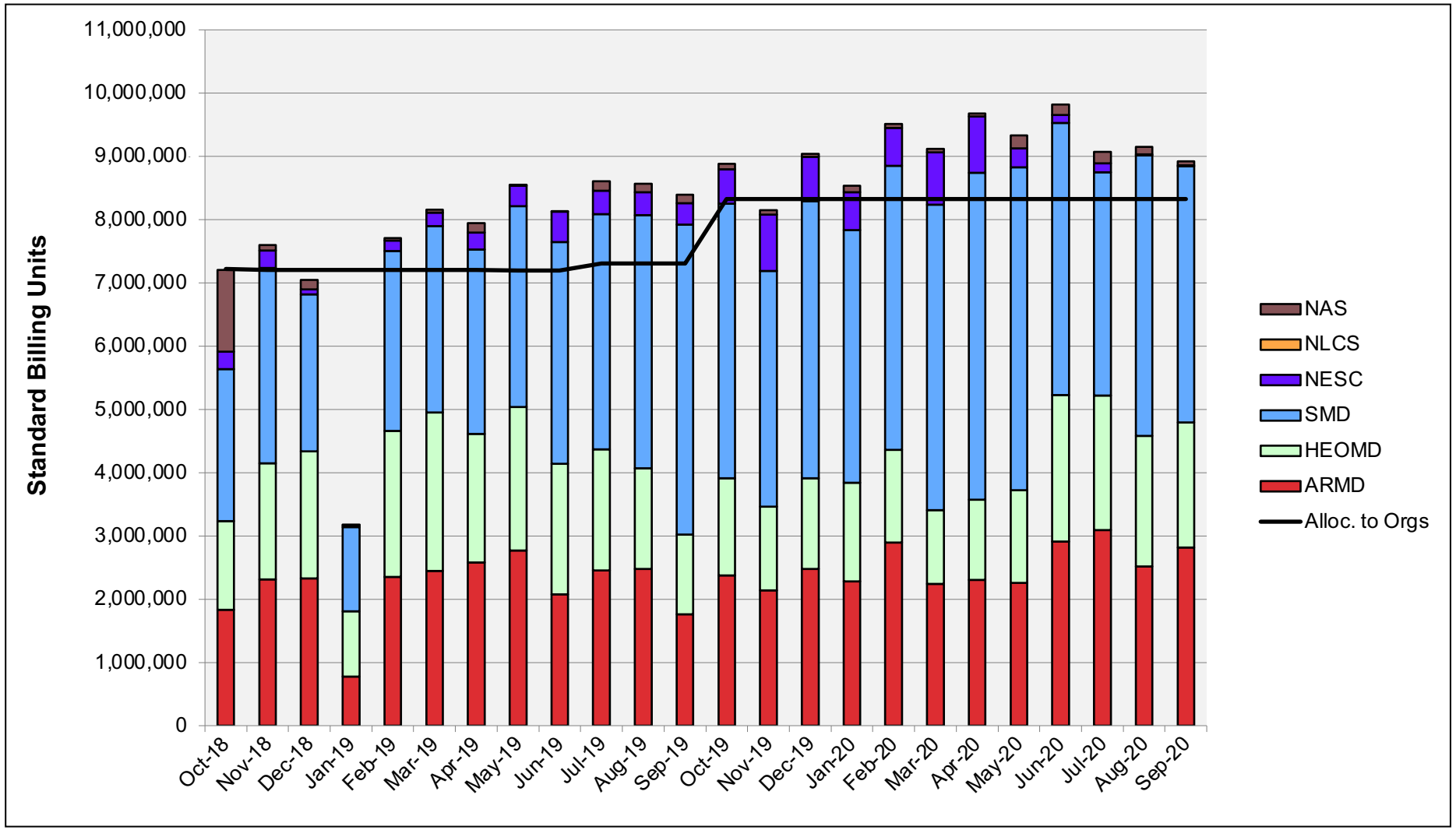
News and Events: Social Media

- **Coverage of NAS Stories**
  - Northrop Grumman names next Cygnus spacecraft after Kalpana Chawla, astronaut and former researcher at NAS:
    - NASA: Twitter (does not mention NAS) 2.4k retweets, 257 quote tweets, 12.2 likes
    - NAS: Twitter 6 retweets, 12 favorites
  - NASA and NOAA announce new solar cycle predictions, with help from HECC supercomputers:
    - NAS: Twitter 15 retweets, 9 likes; Facebook 597 users reached, 34 engagements, 12 likes, 6 share.

HECC Utilization



HECC Utilization Normalized to 30-Day Month



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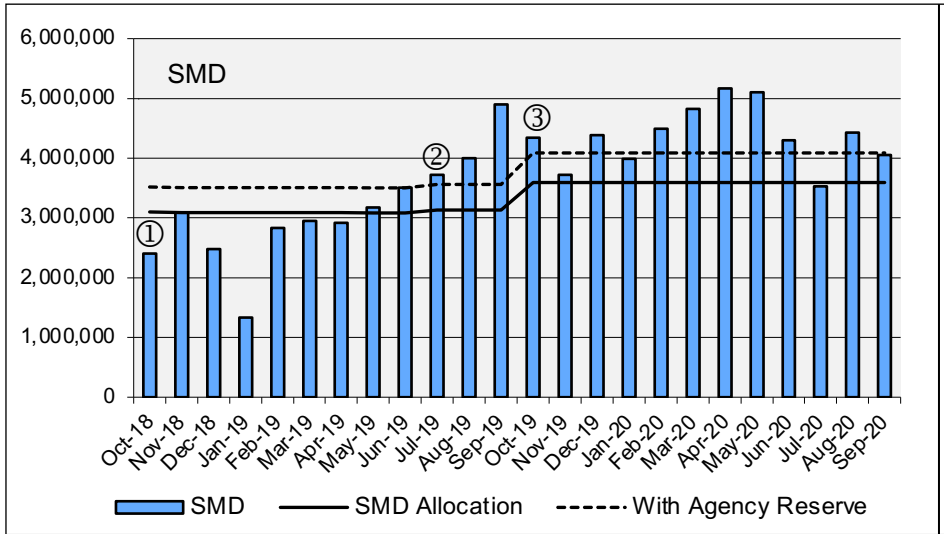
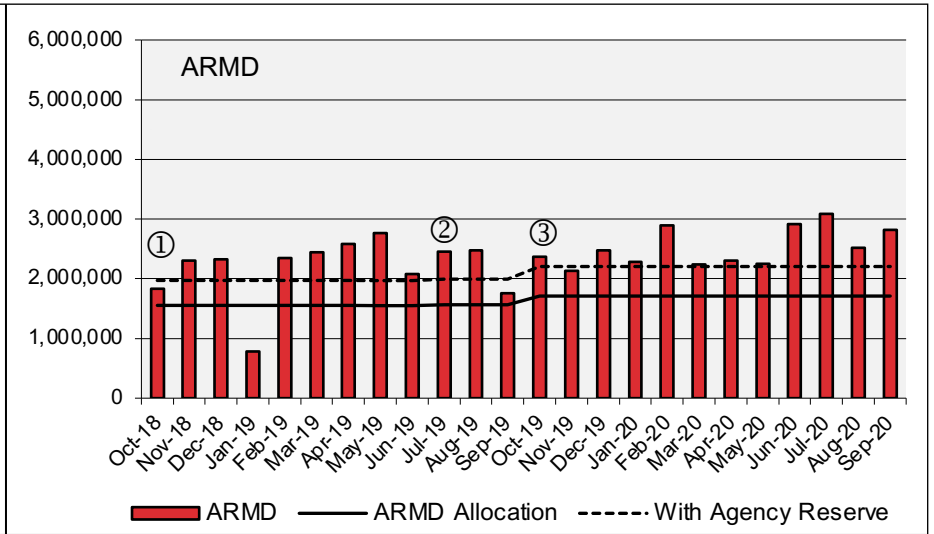
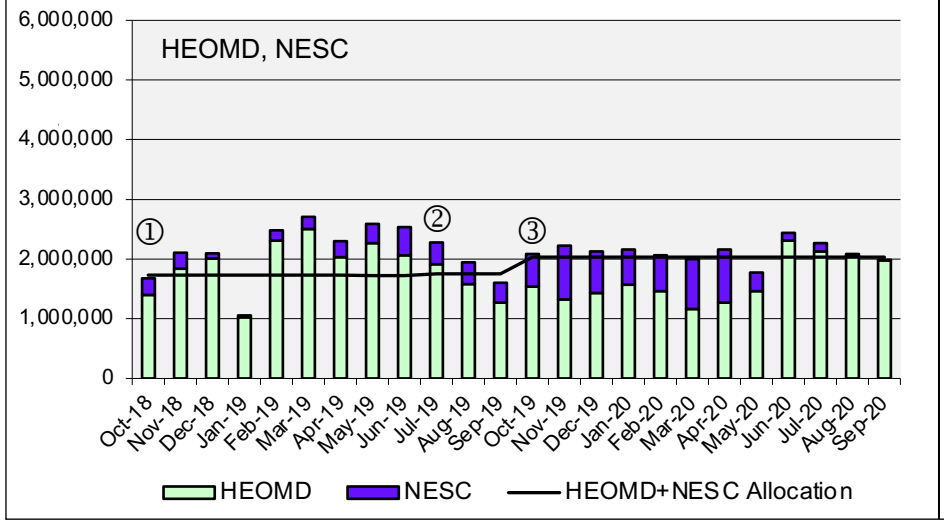




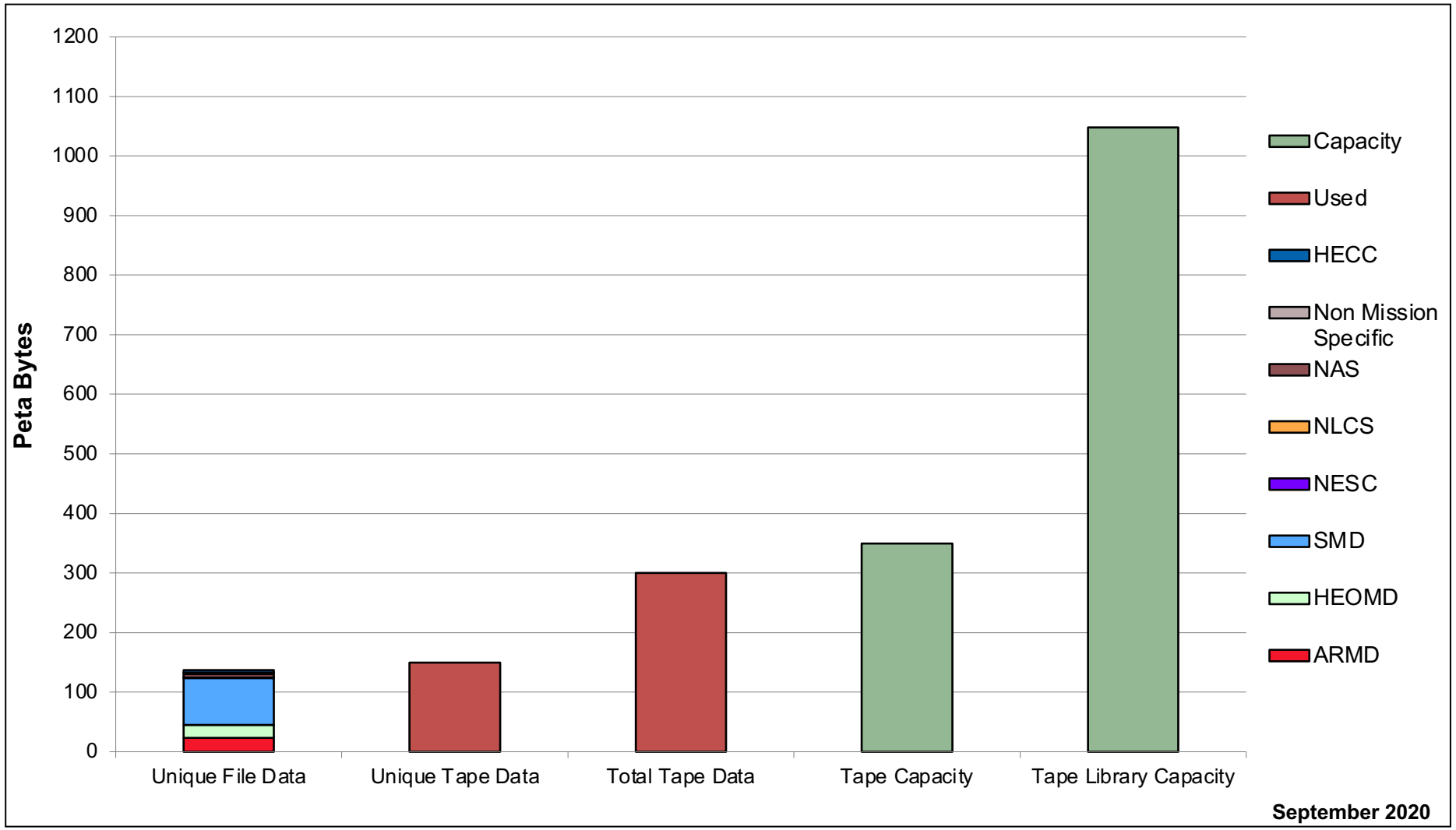


① 2 Skylake E cells (8 D Rack Equivalence) added to Electra;
1 rack is dedicated to ARMD

② 2 Skylake E cells (8 D Rack Equivalence) added to Electra;
1 rack is dedicated to SMD

③ Skylake Tesla GPU V100 Nodes installed

Tape Archive Status



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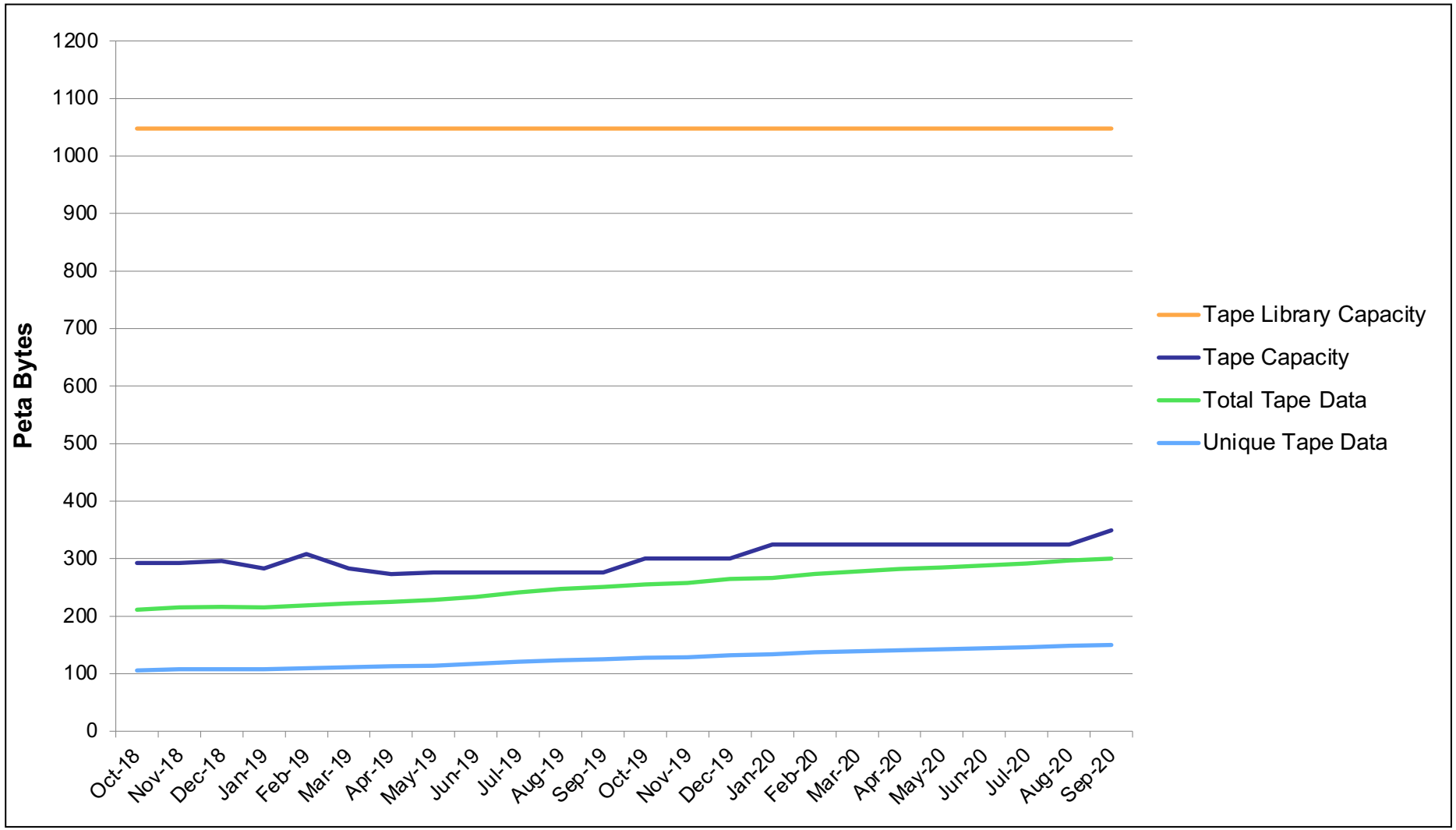
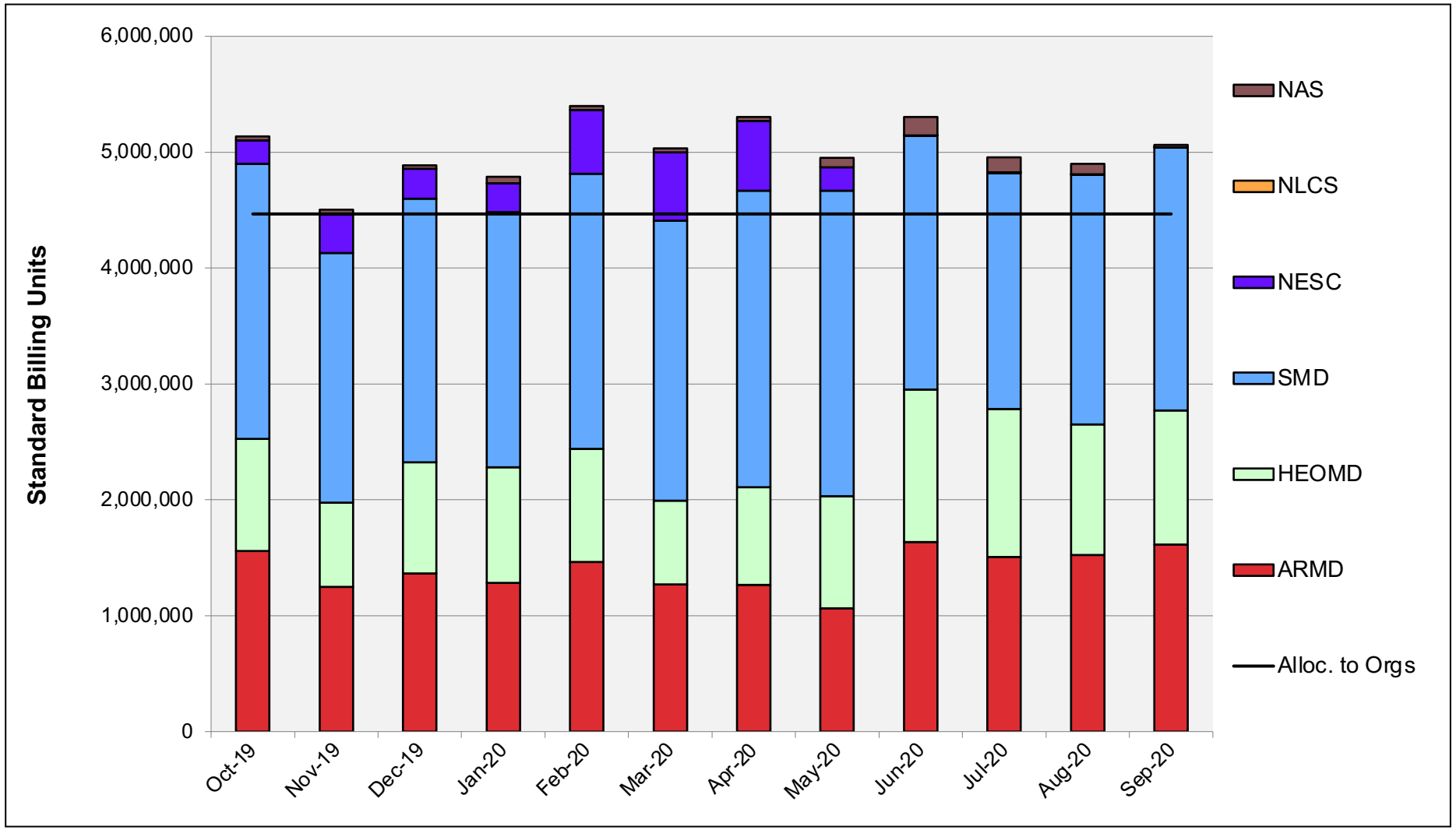
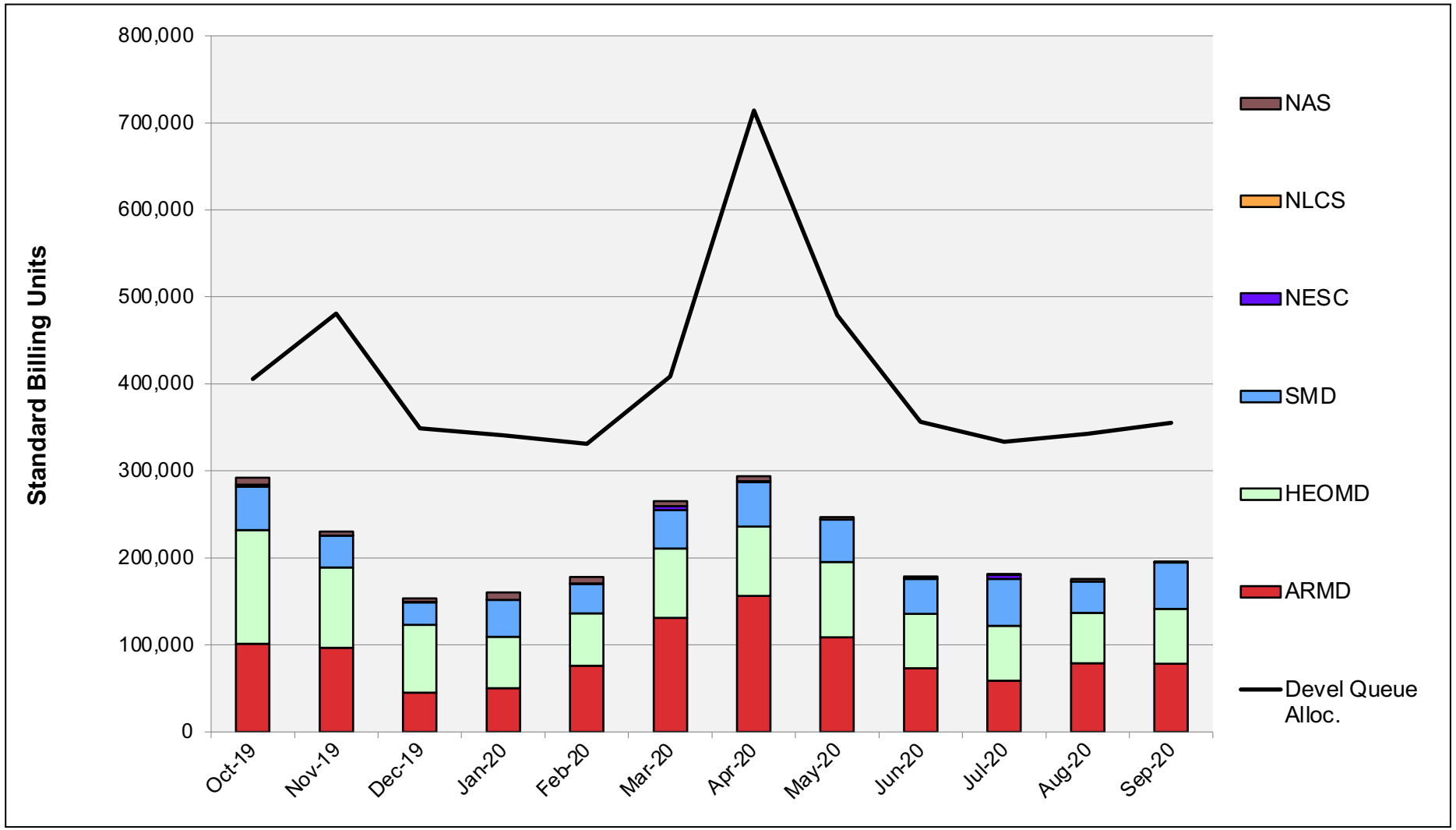


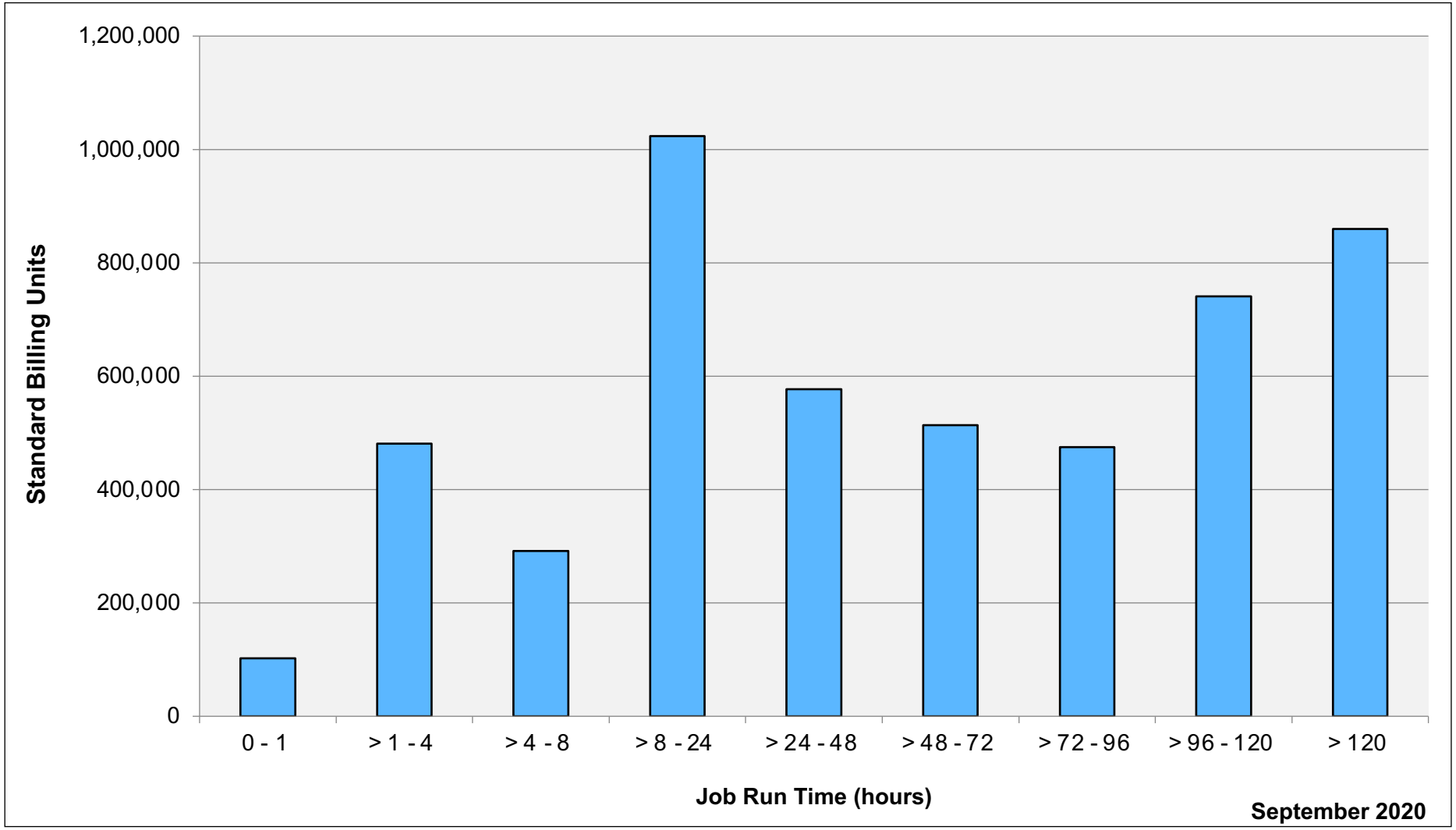
Pleiades: SBUs Reported, Normalized to 30-Day Month



Pleiades: Devel Queue Utilization



Pleiades: Monthly Utilization by Job Length



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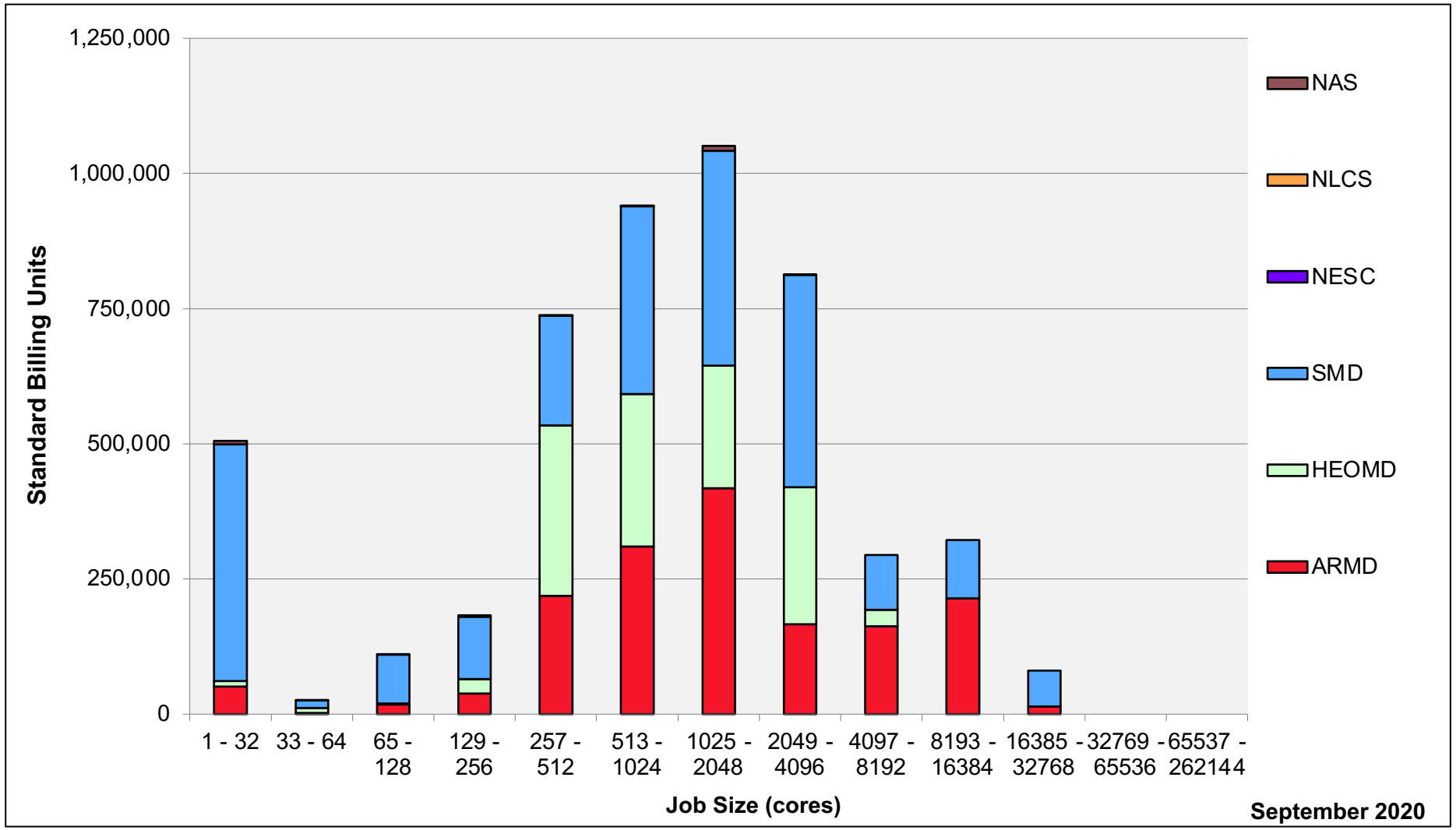
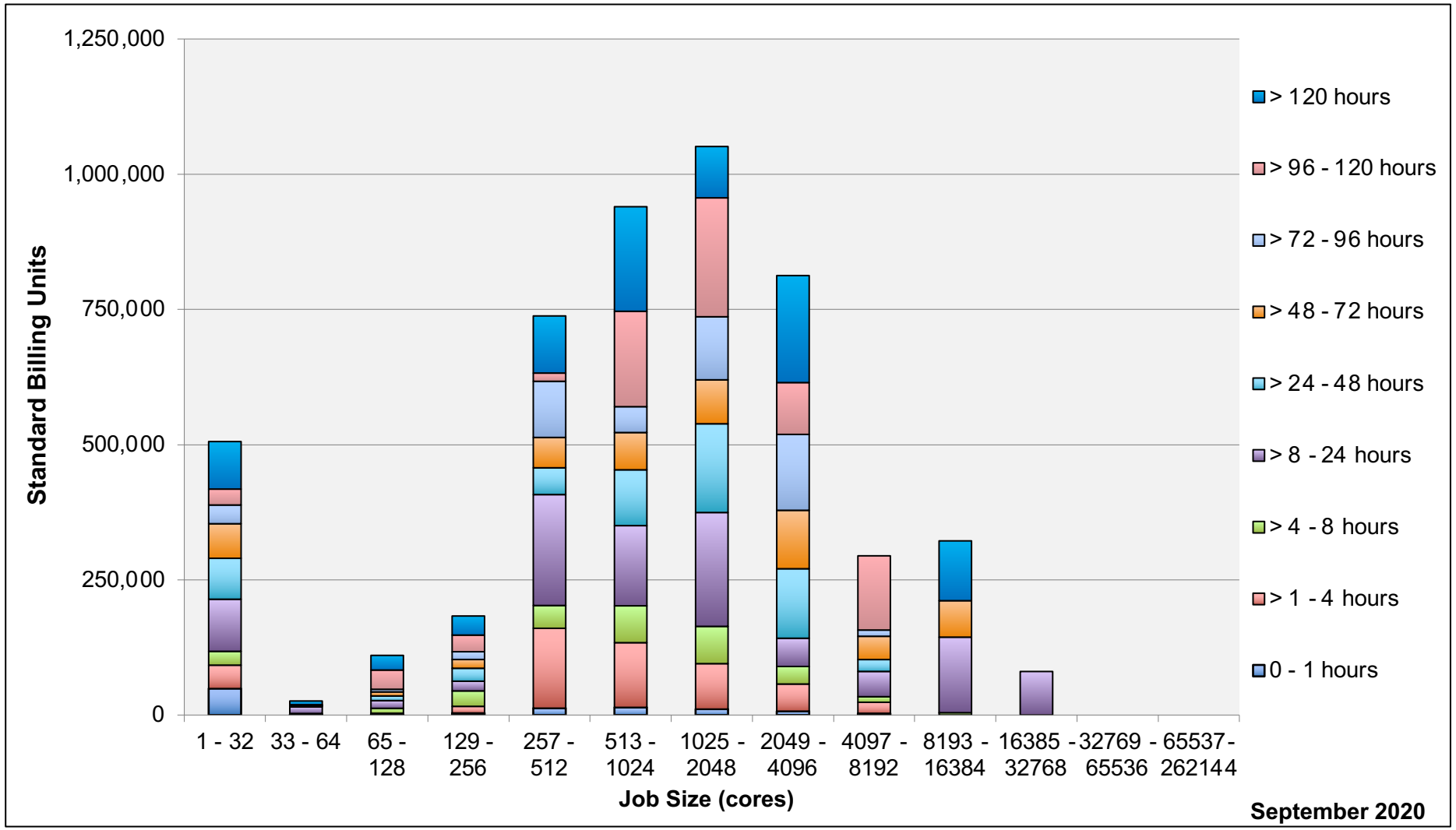
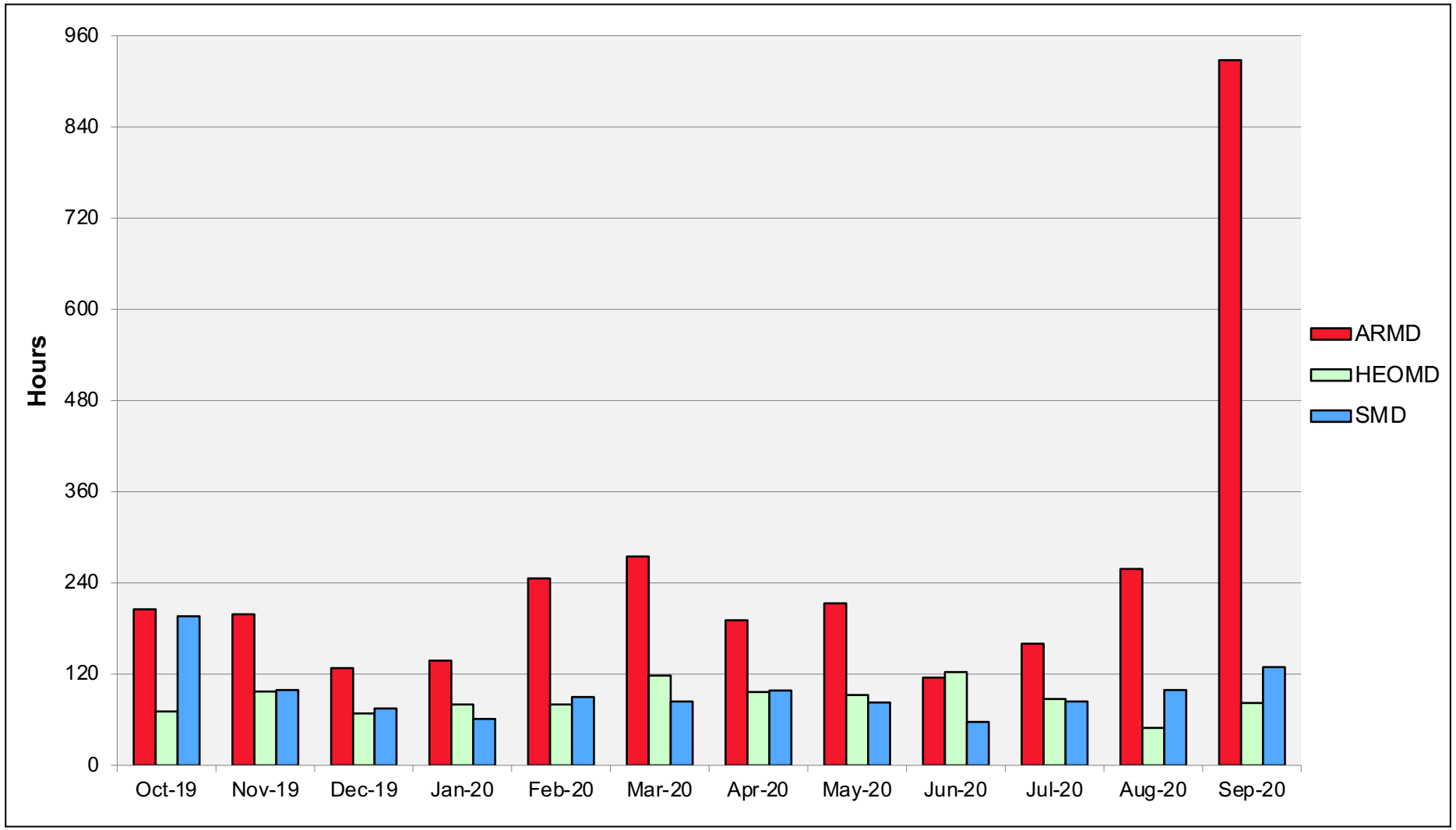


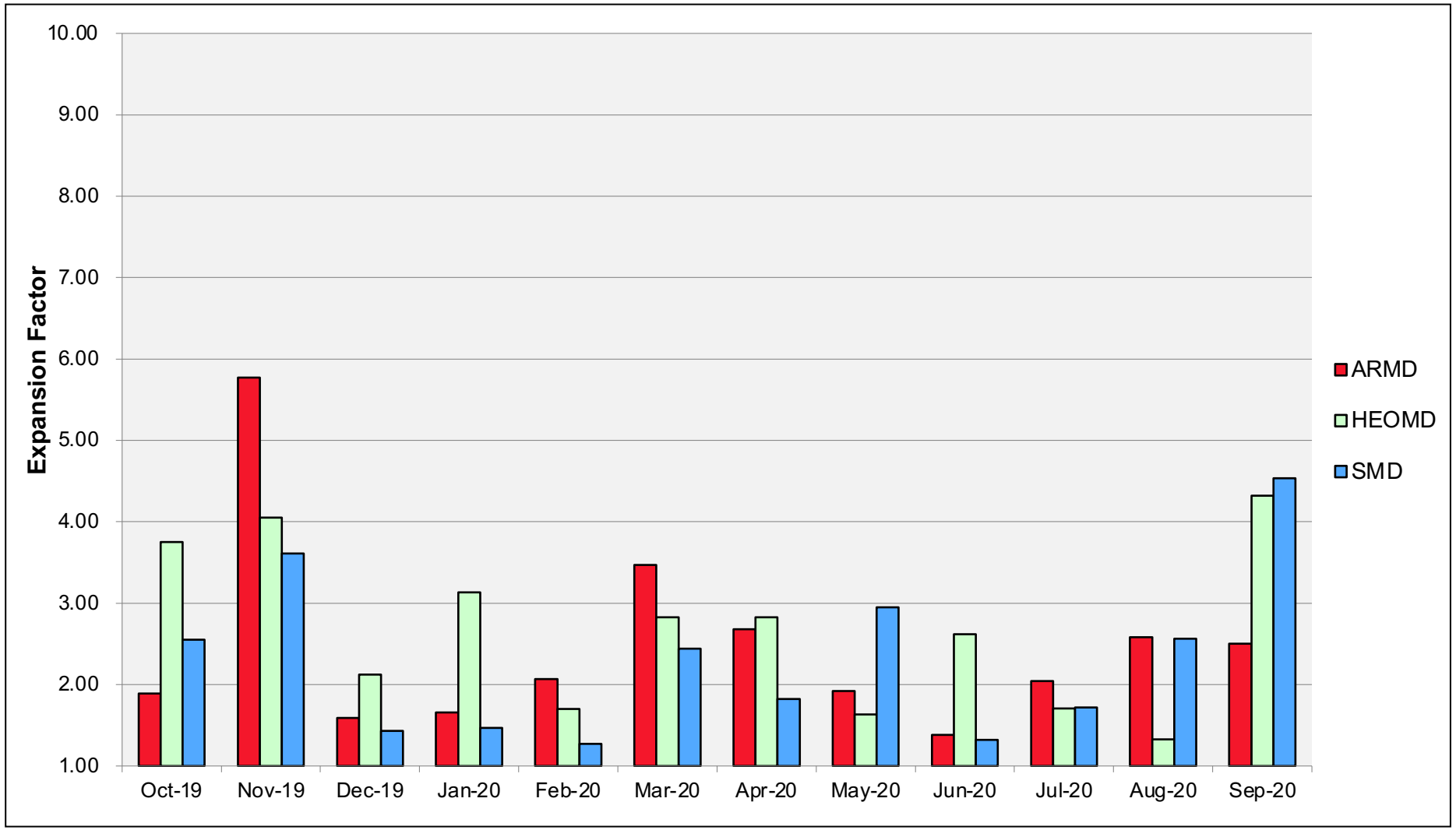
Pleiades: Monthly Utilization by Size and Length



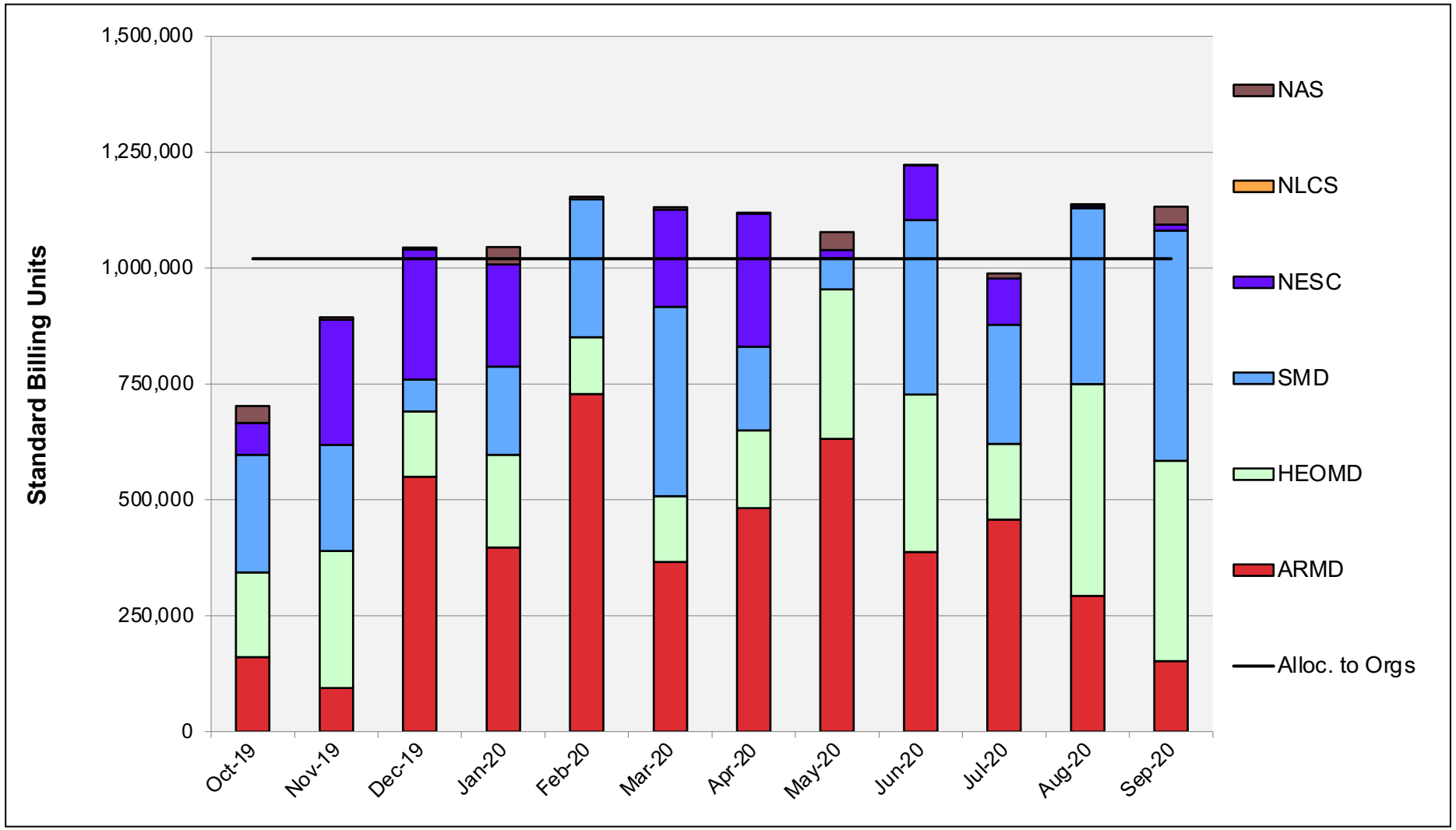
Pleiades: Average Time to Clear All Jobs



Pleiades: Average Expansion Factor



Aitken: SBUs Reported, Normalized to 30-Day Month



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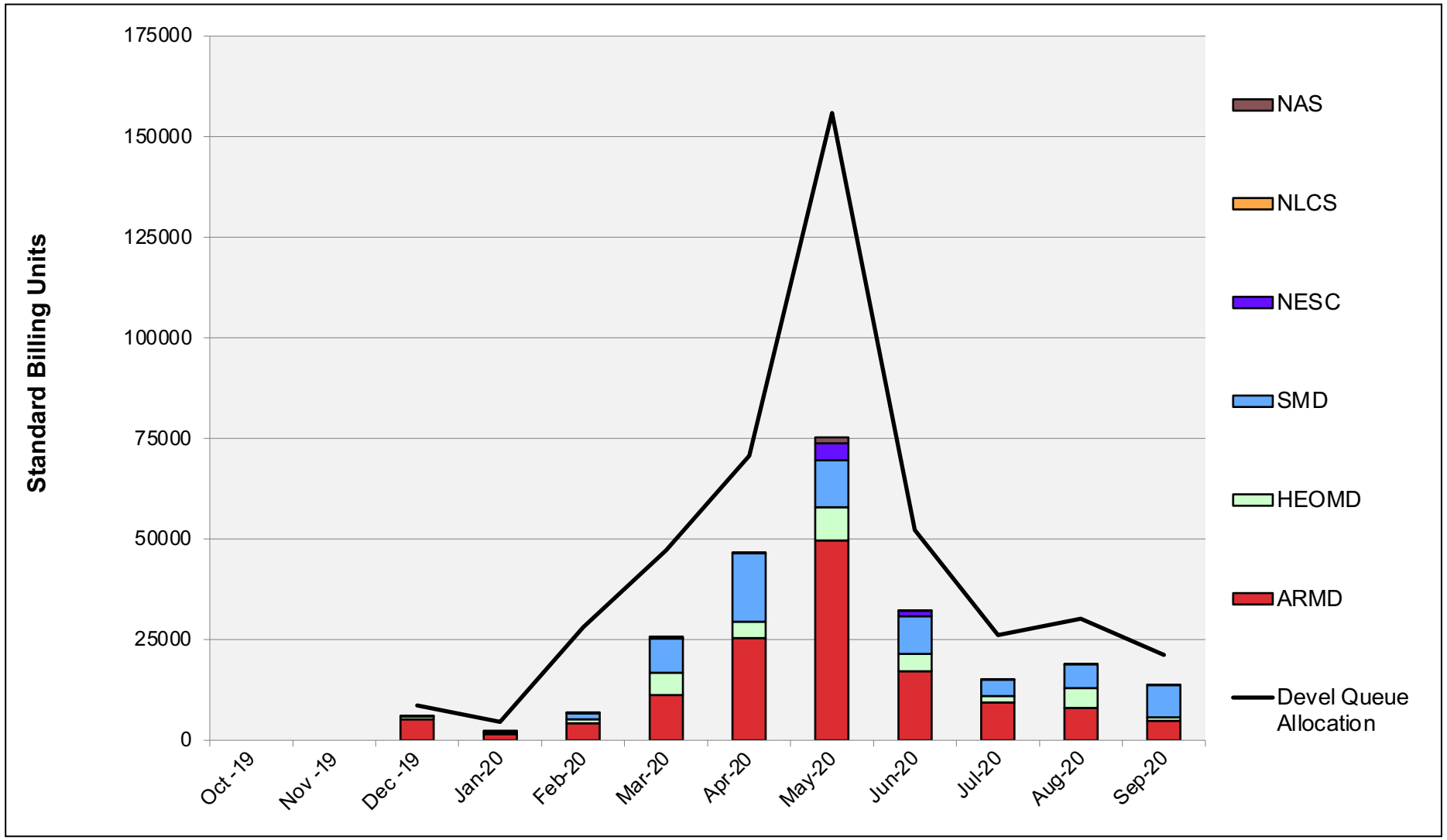

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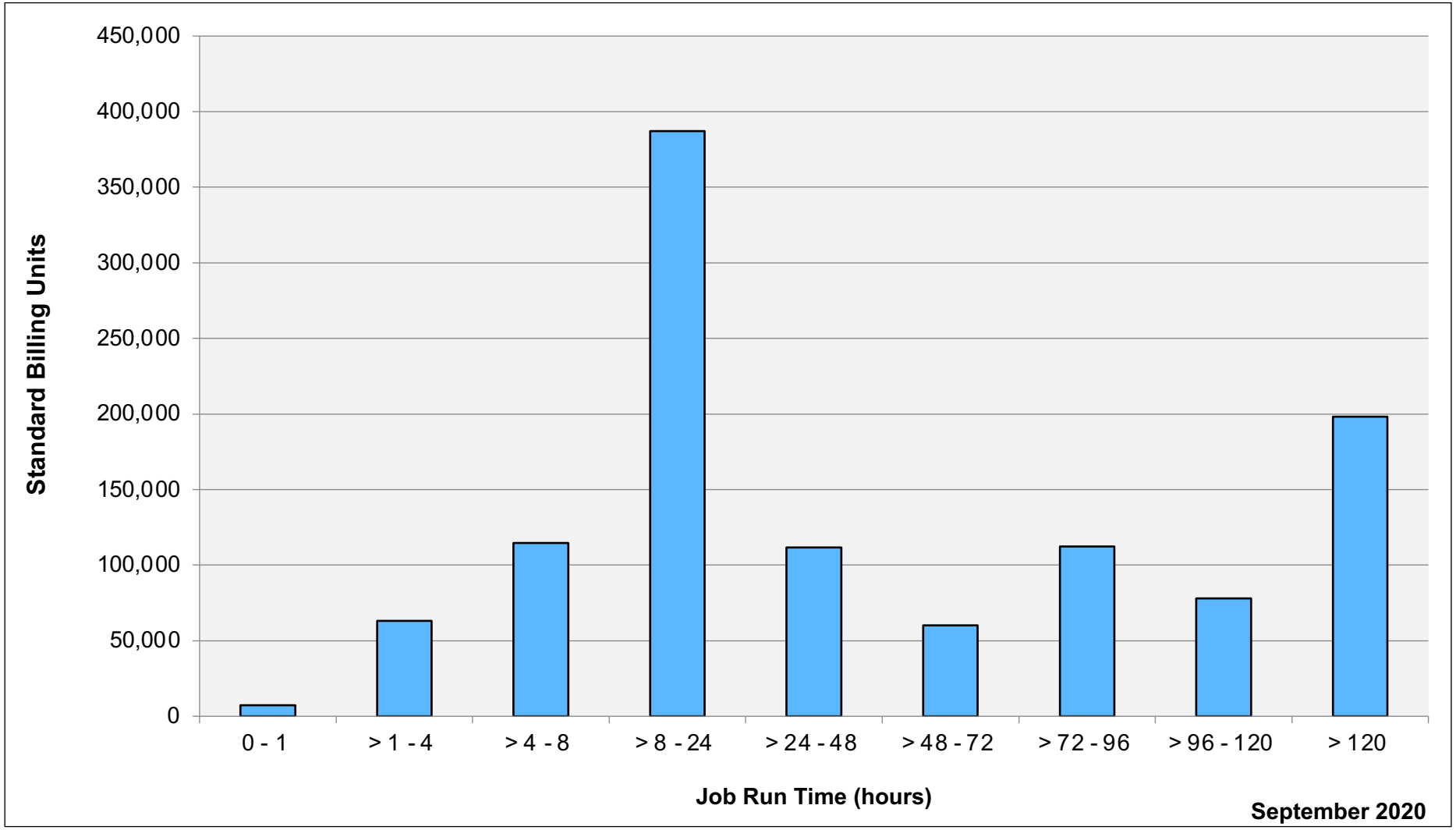
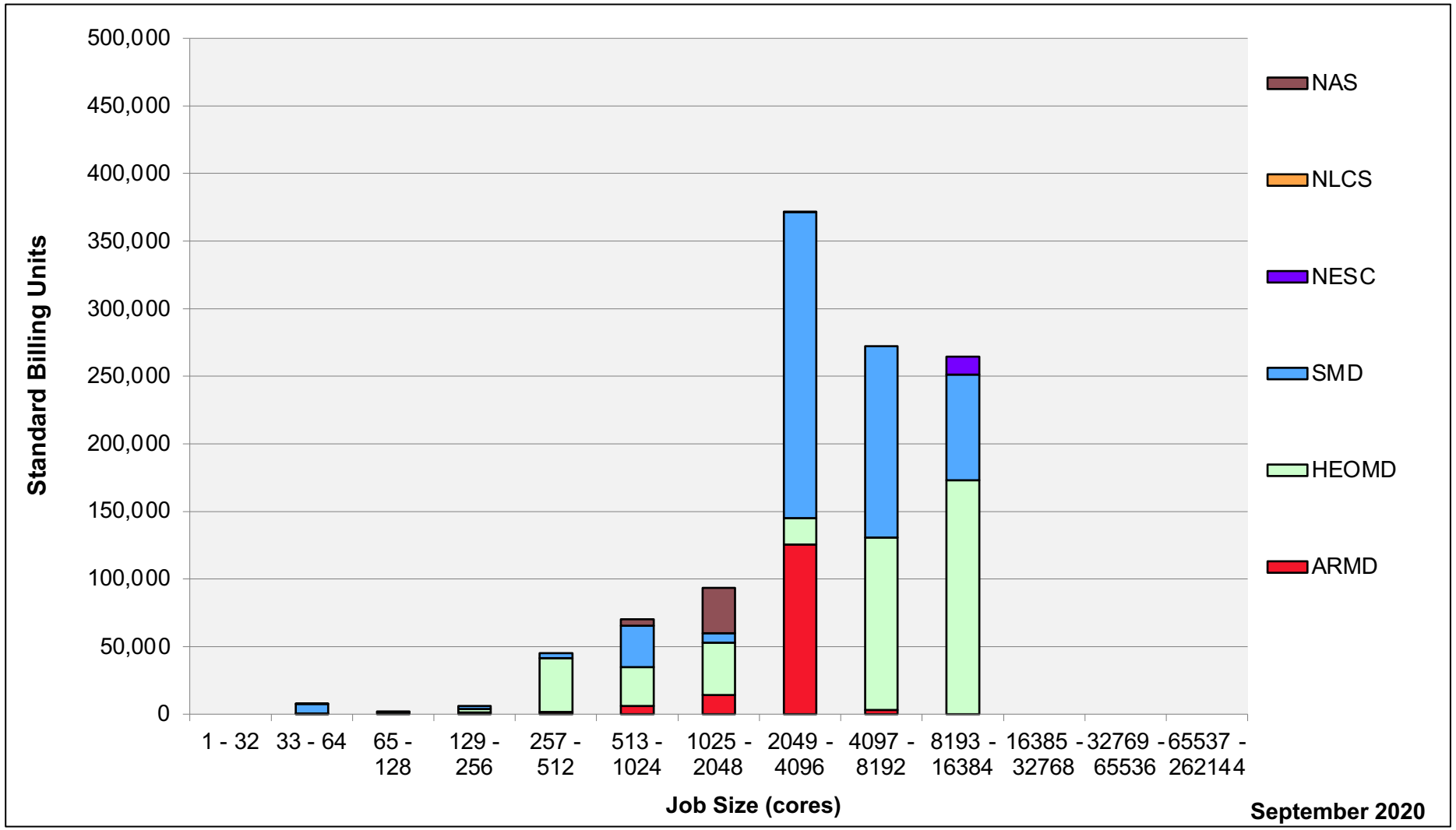
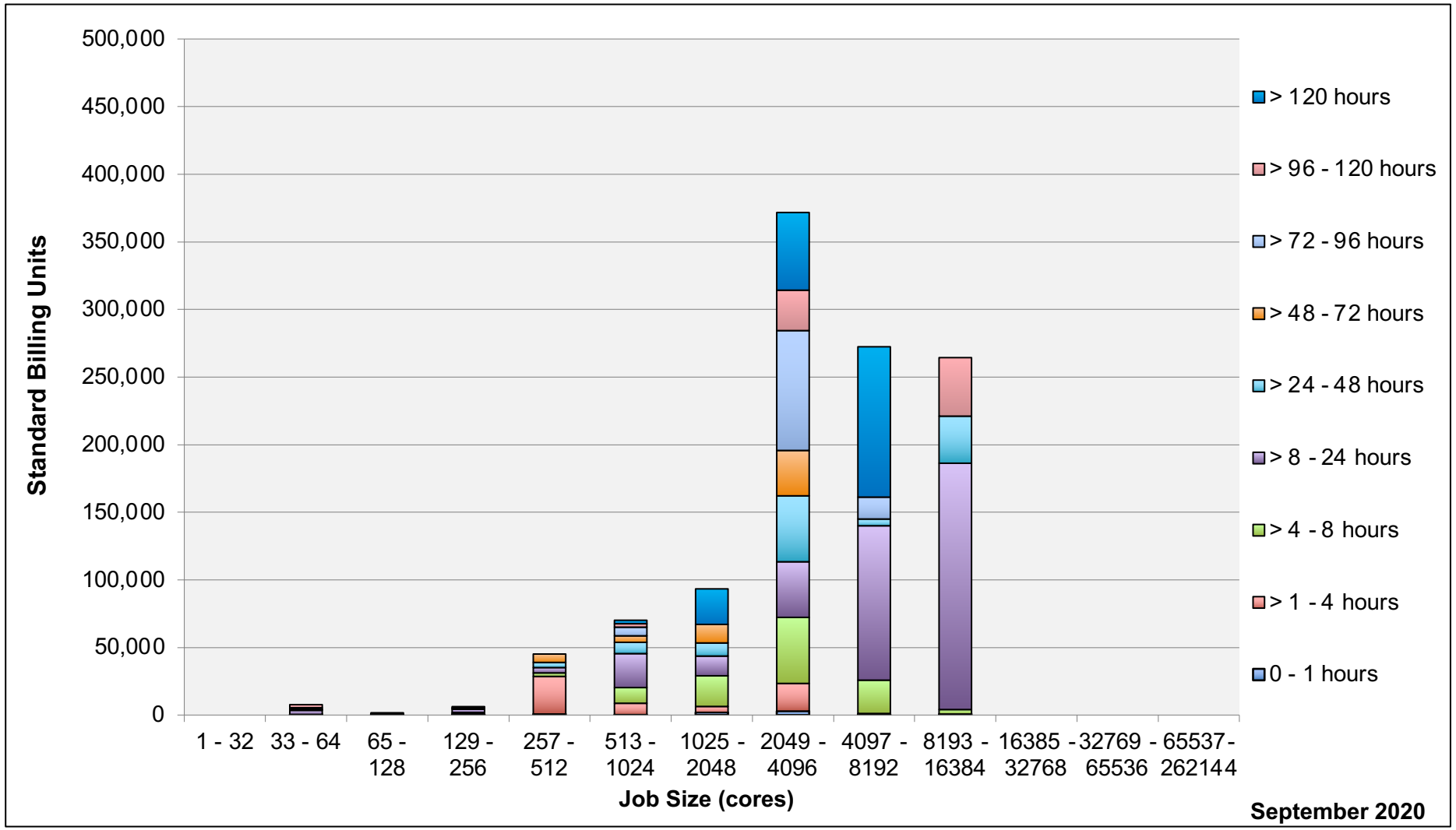


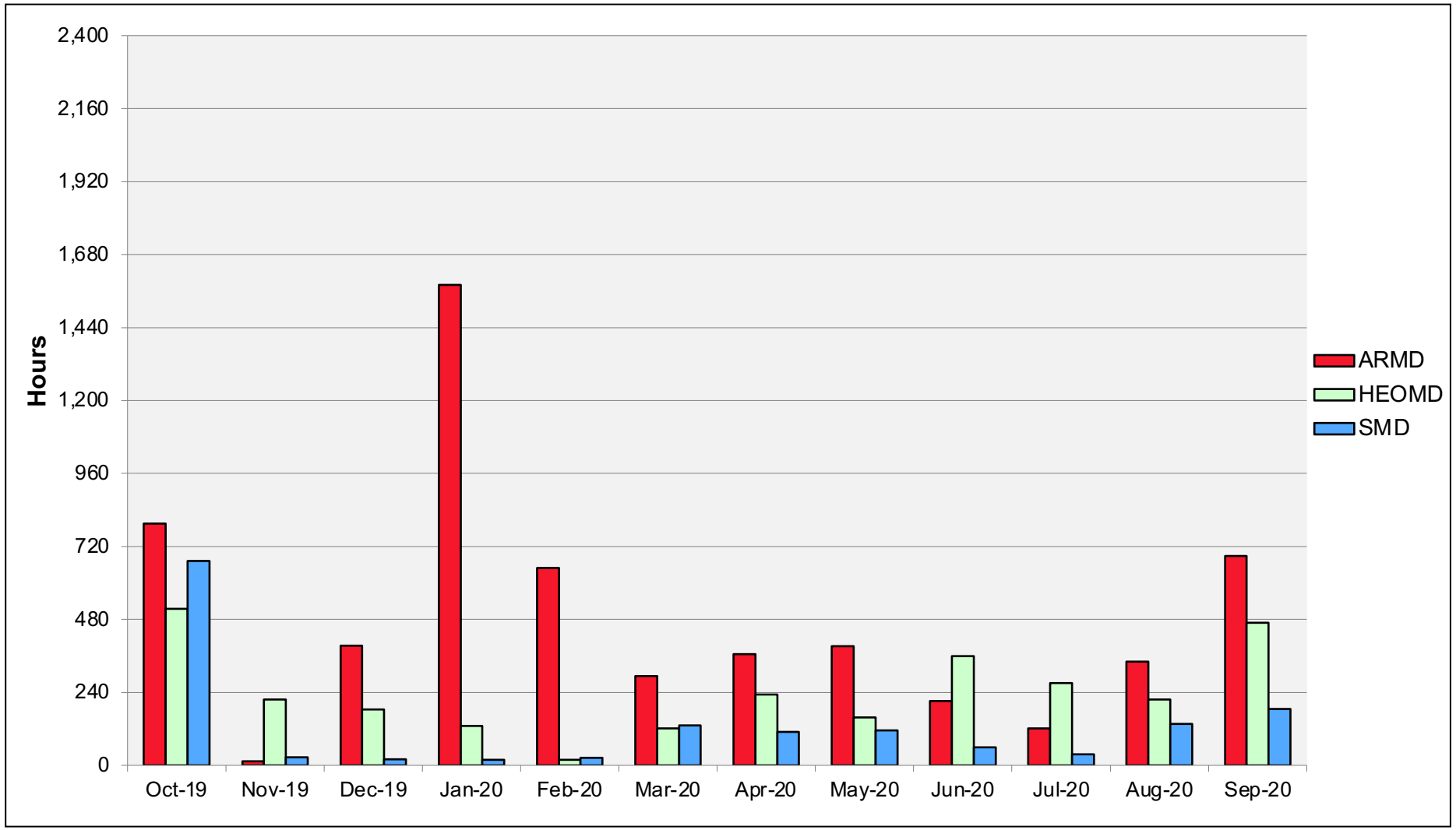
Aitken: Monthly Utilization by Job Length



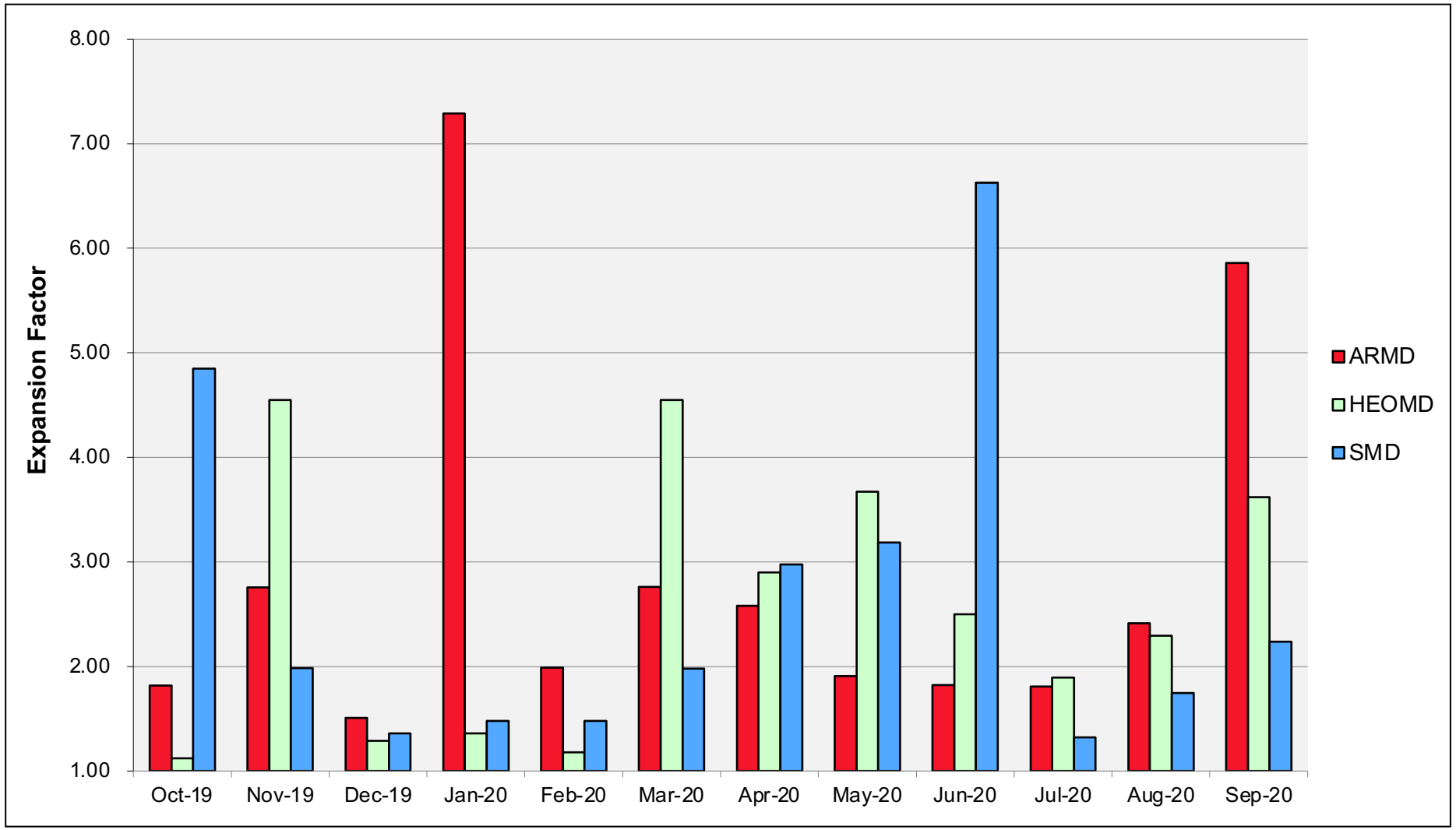
Aitken: Monthly Utilization by Size and Length



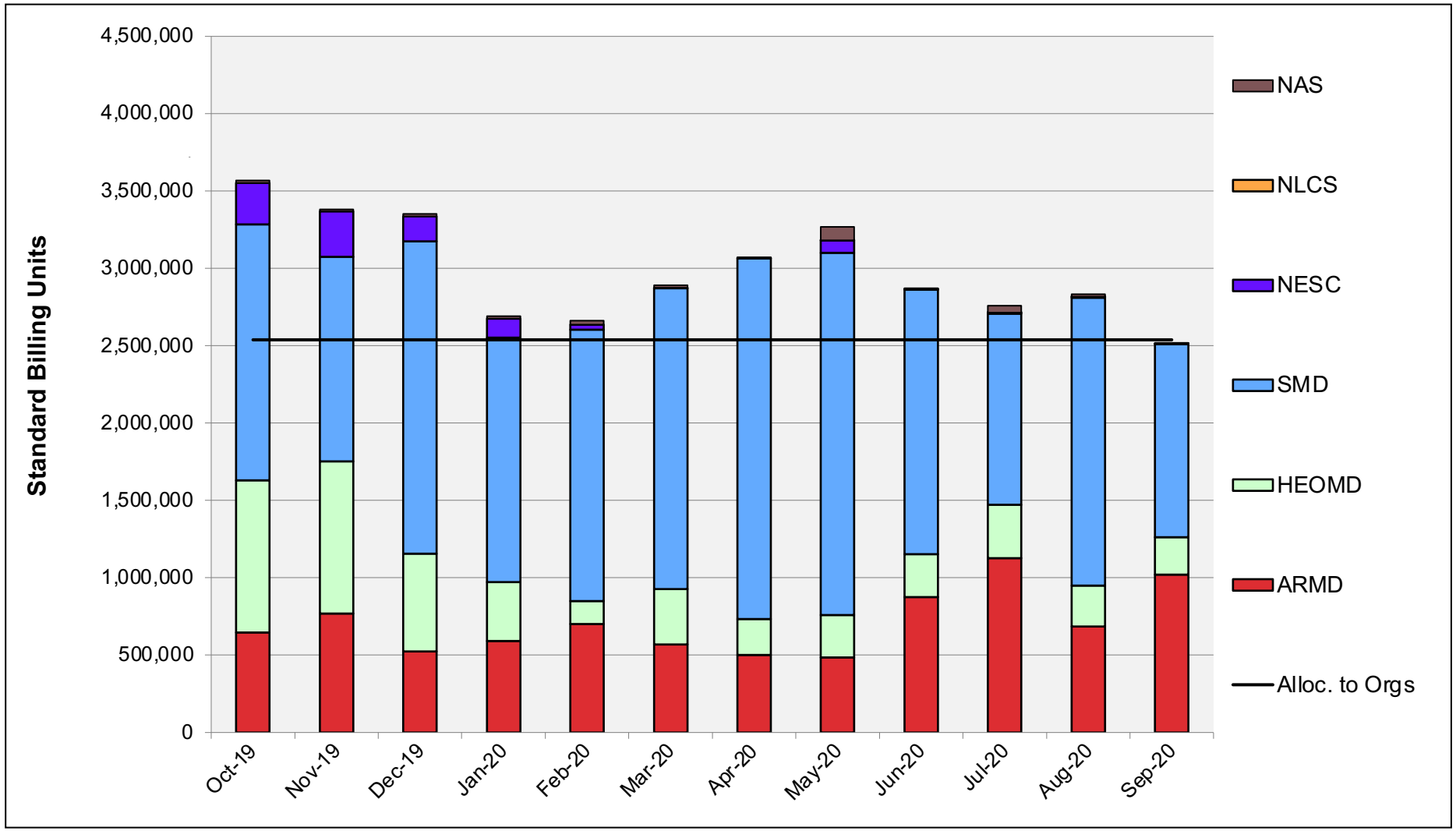
Aitken: Average Time to Clear All Jobs



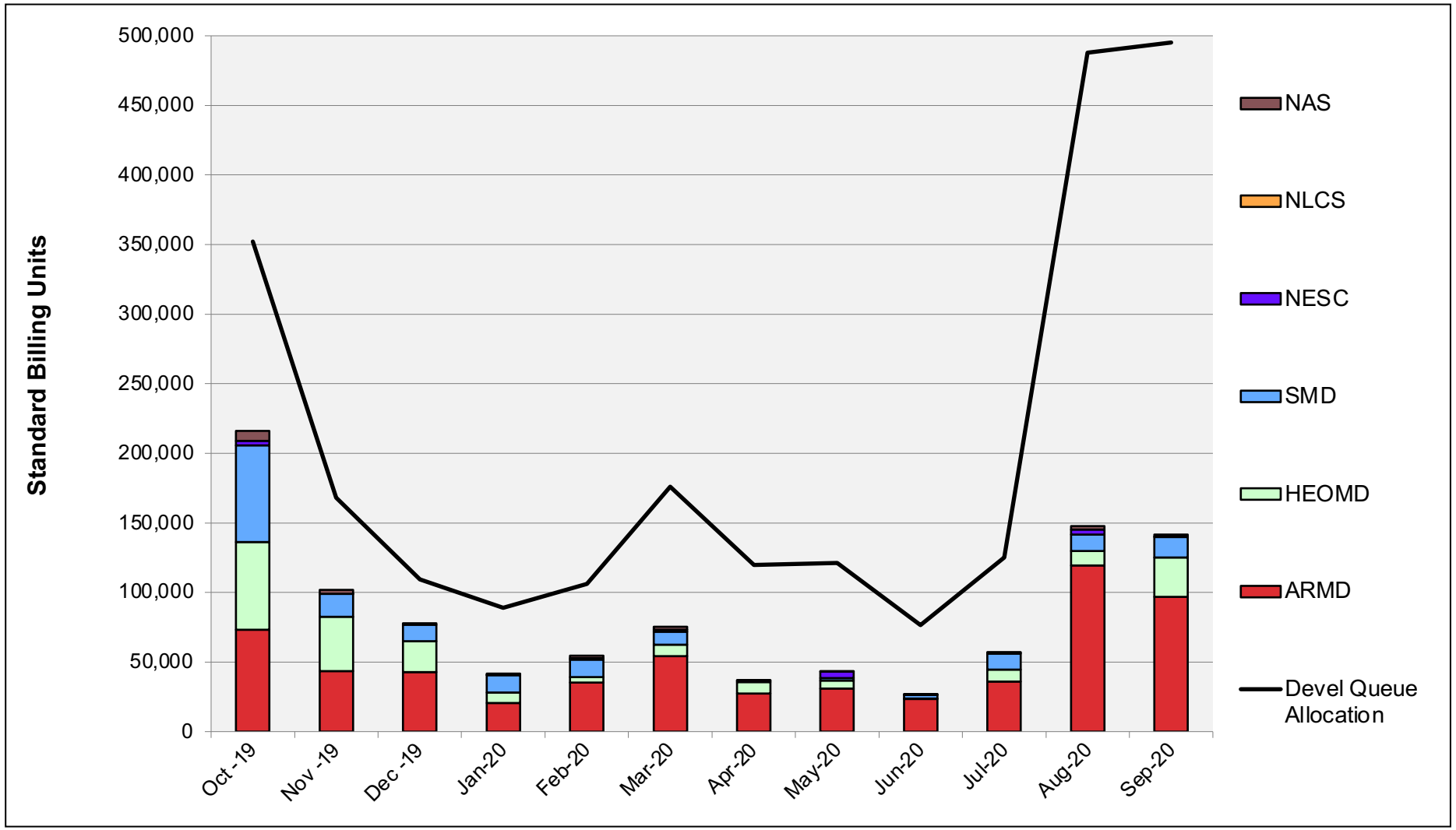
Aitken: Average Expansion Factor



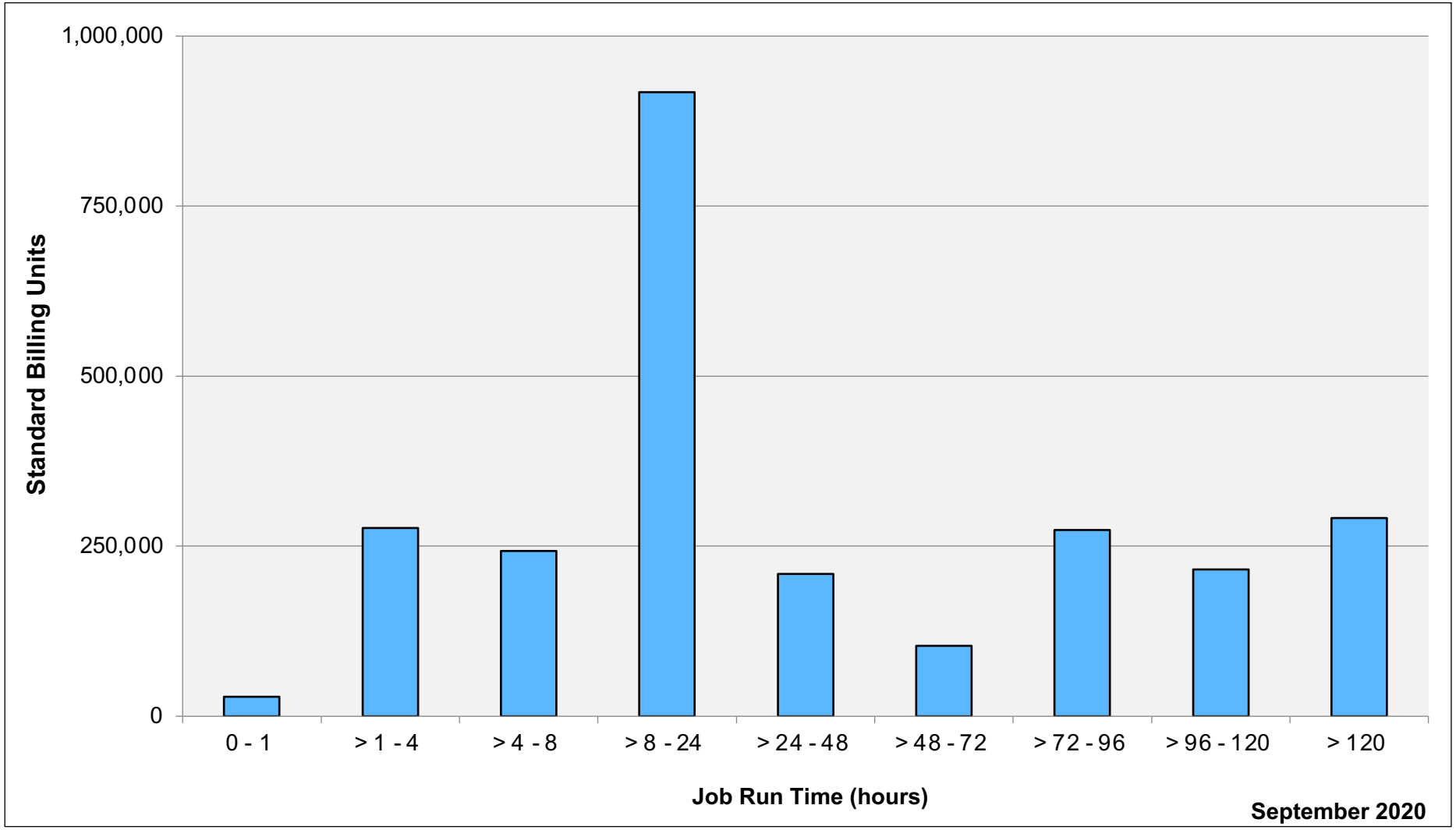
Electra: SBUs Reported, Normalized to 30-Day Month



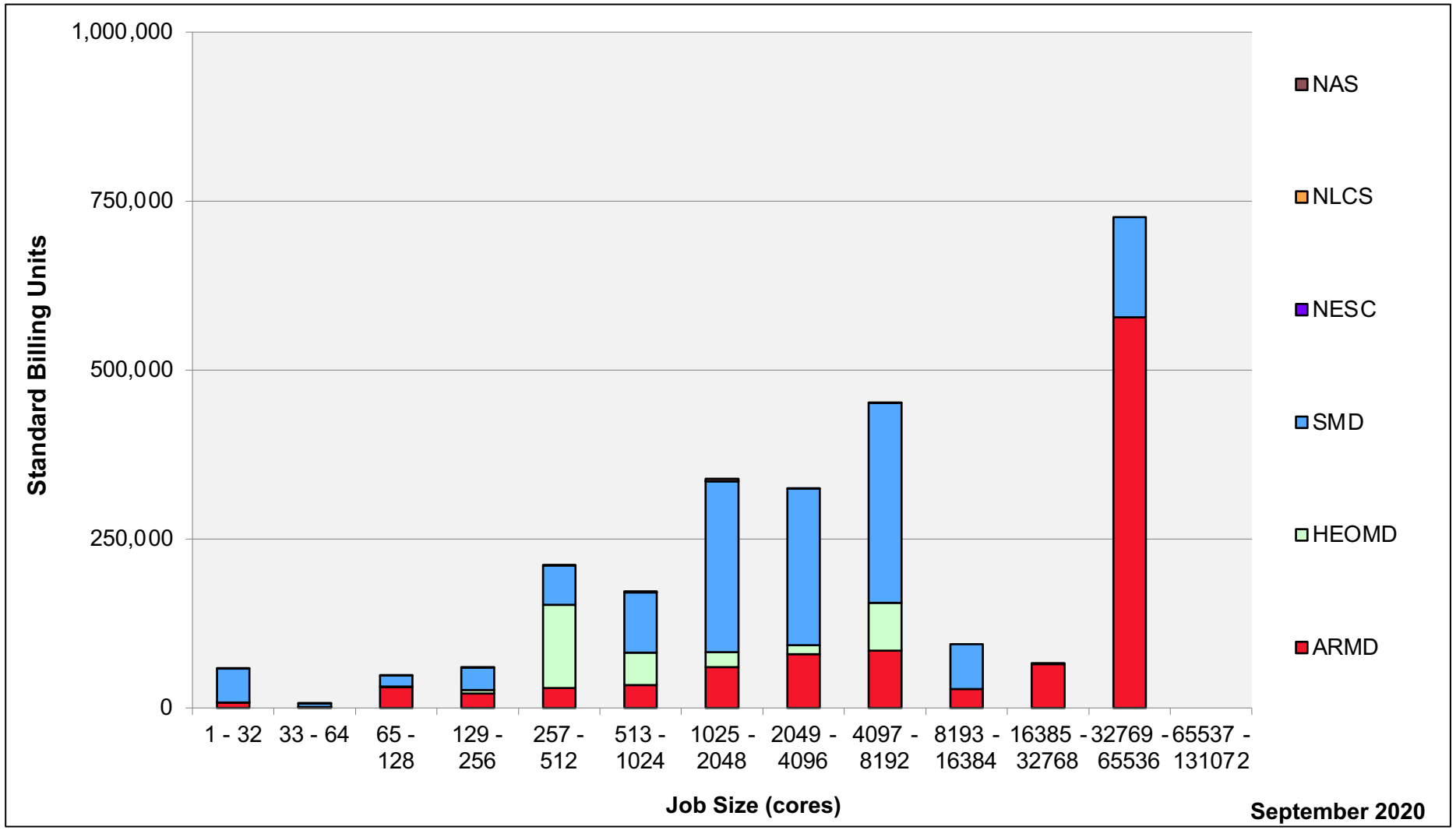
Electra: Devel Queue Utilization



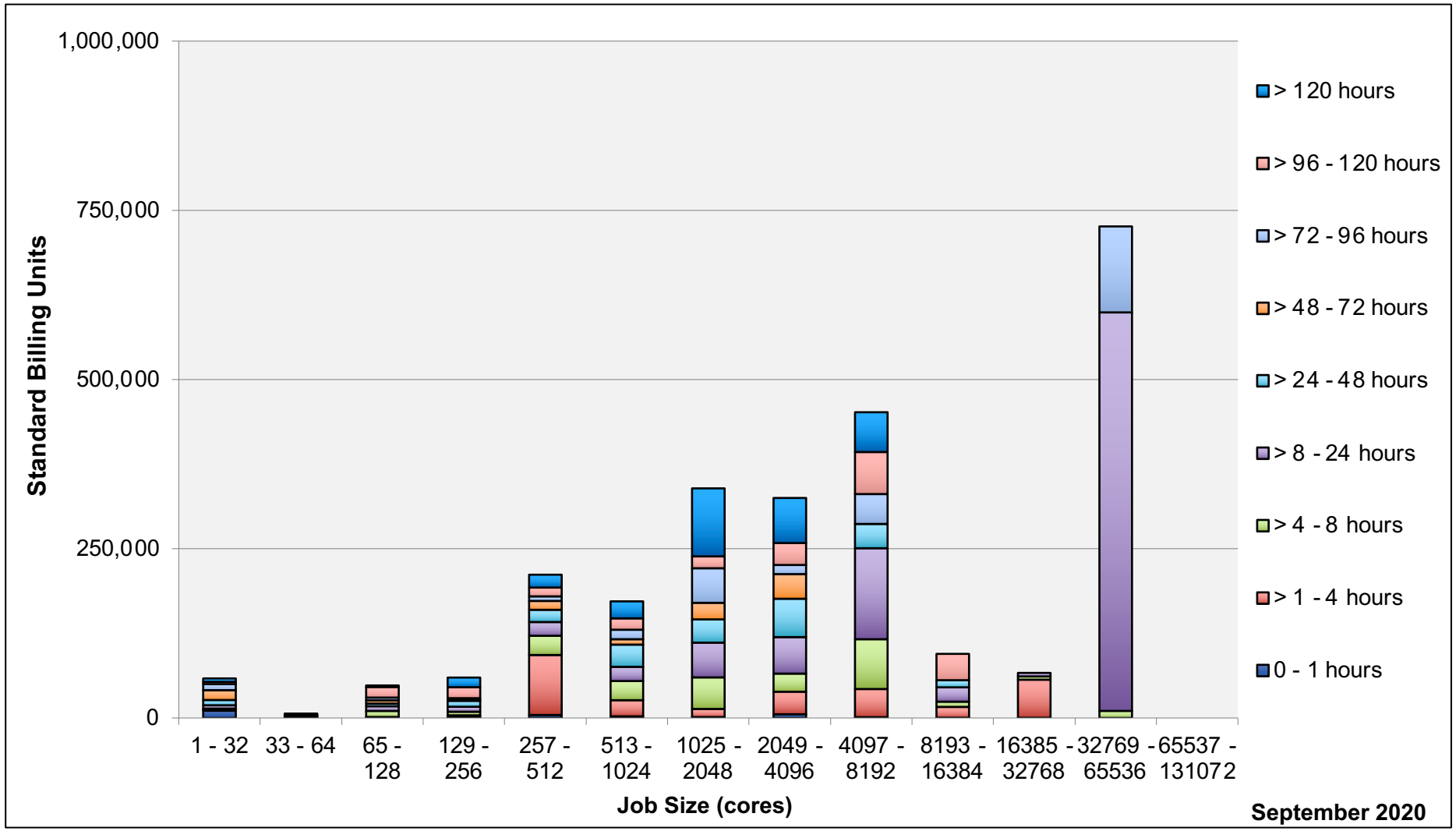
Electra: Monthly Utilization by Job Length



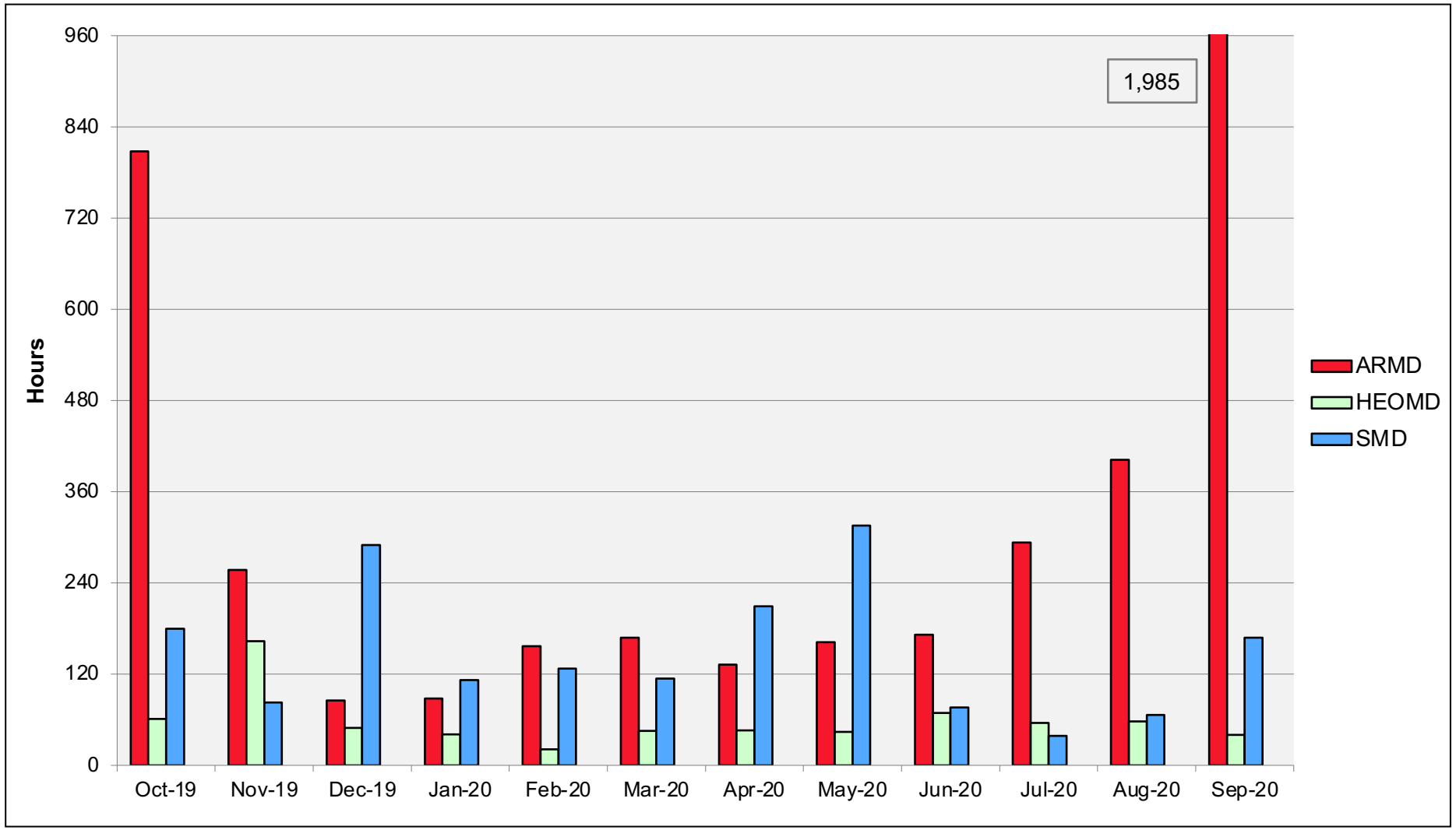
Electra: Monthly Utilization by Job Length



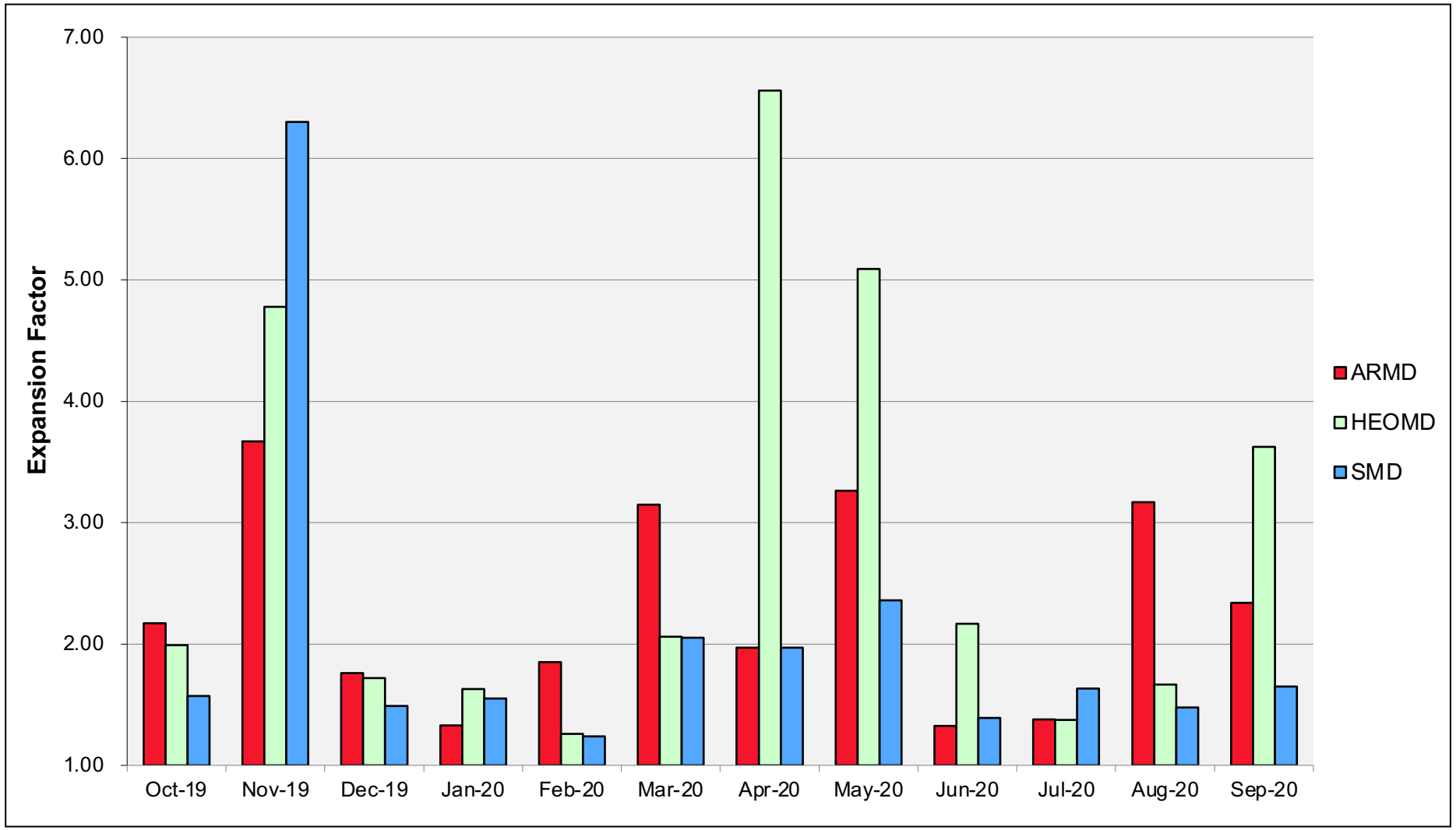
Electra: Monthly Utilization by Size and Length



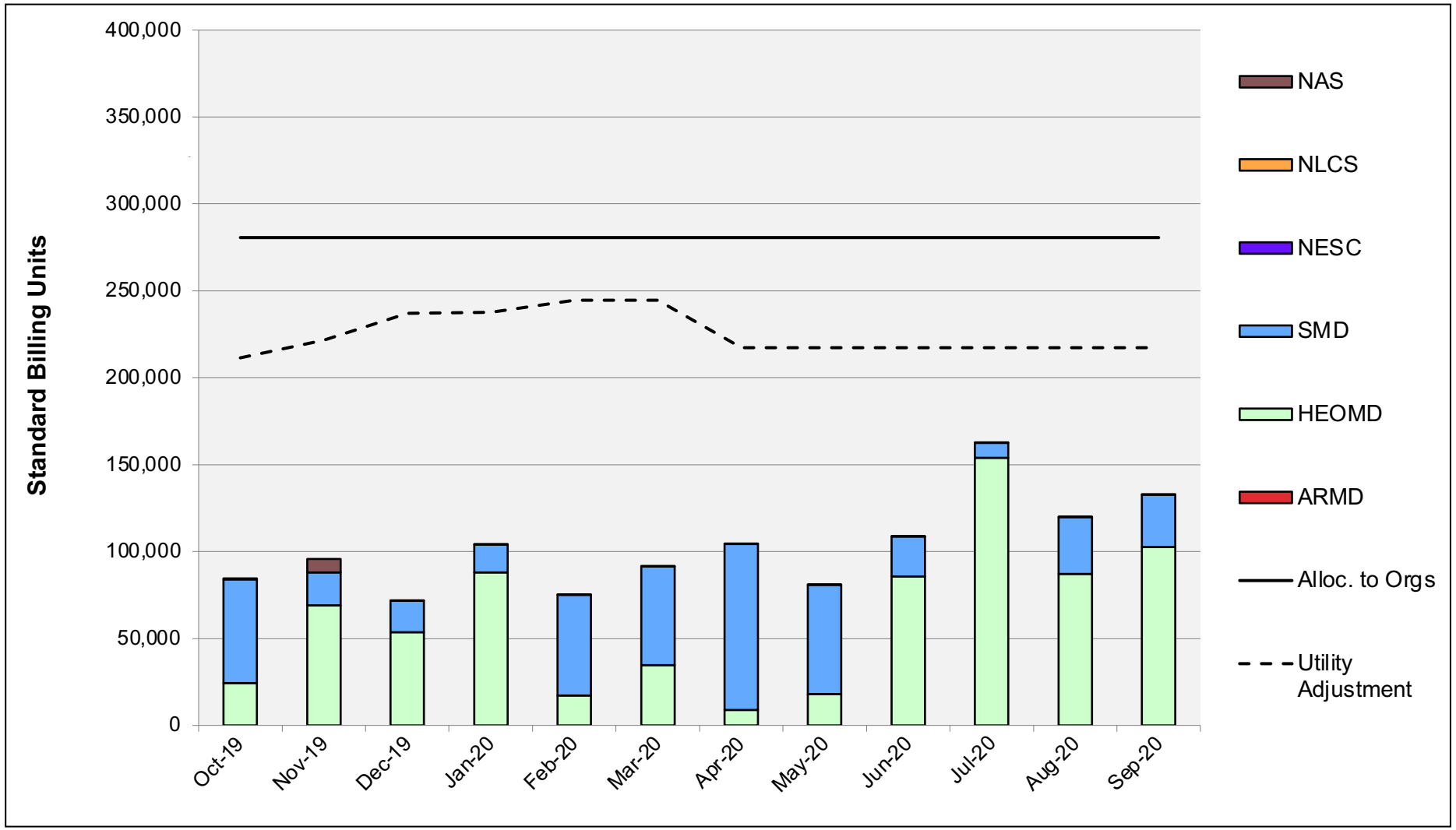
Electra: Average Time to Clear All Jobs



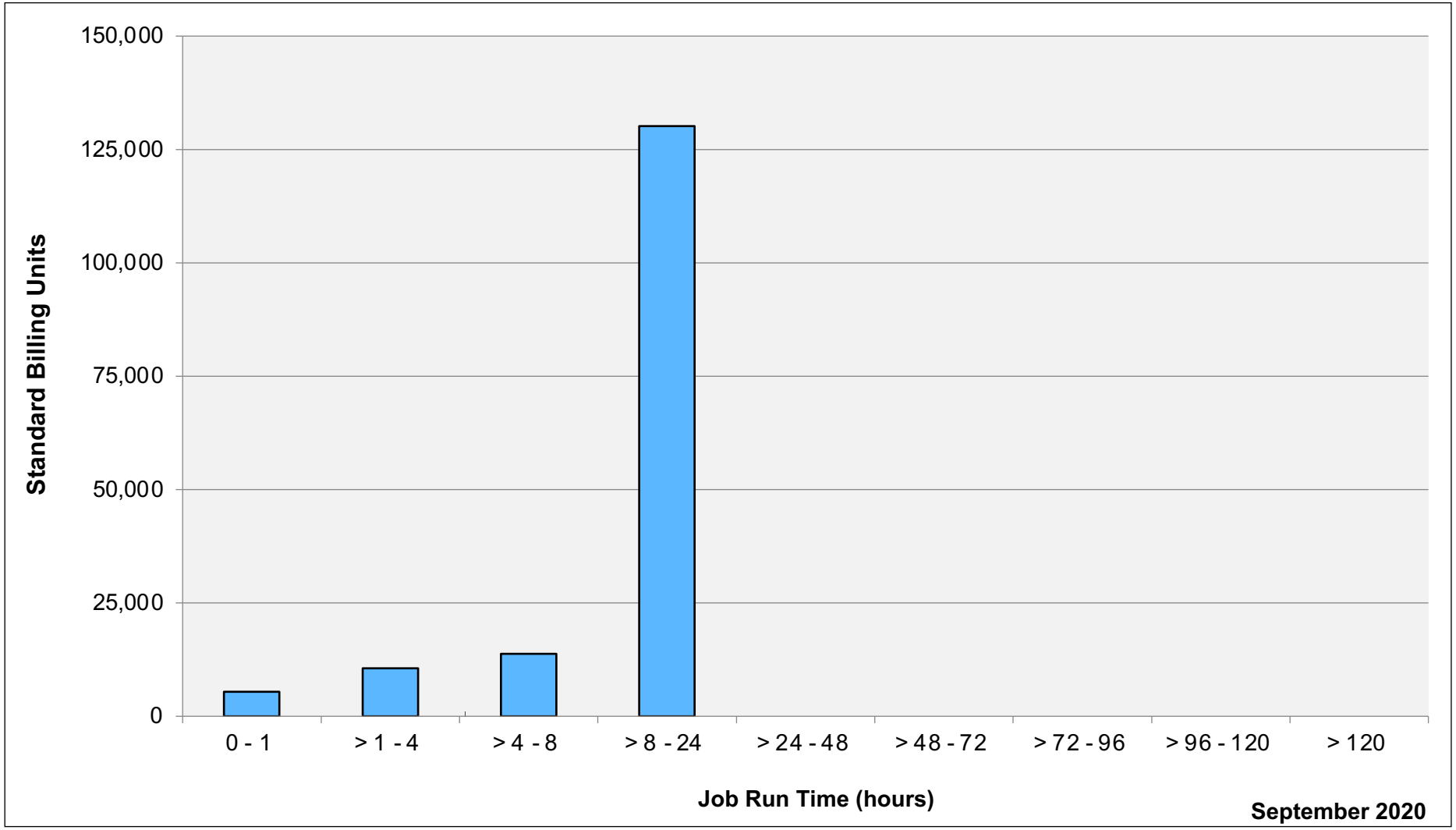
Electra: Average Expansion Factor



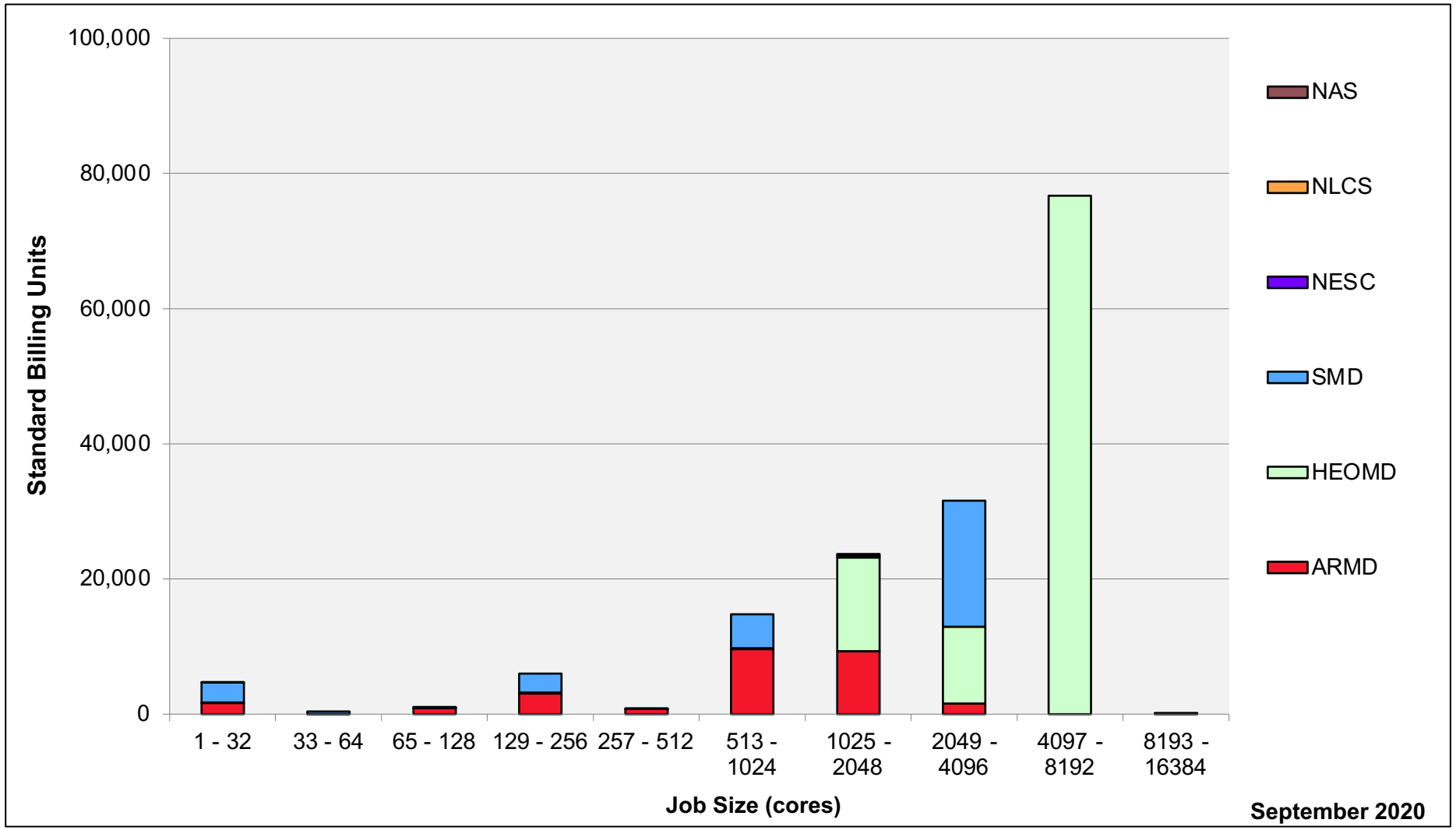
Merope: SBUs Reported, Normalized to 30-Day Month



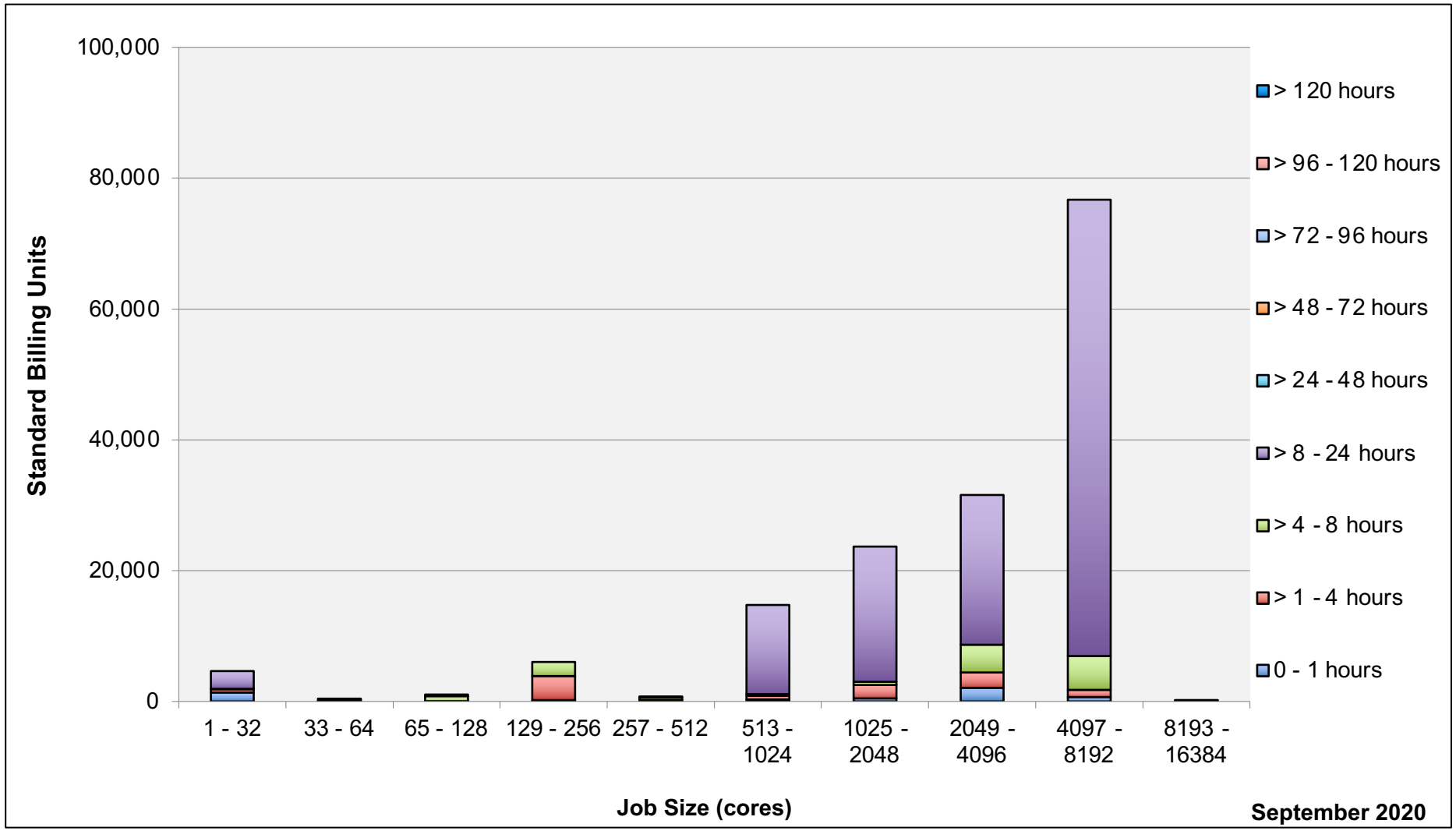
Merope: Monthly Utilization by Job Length



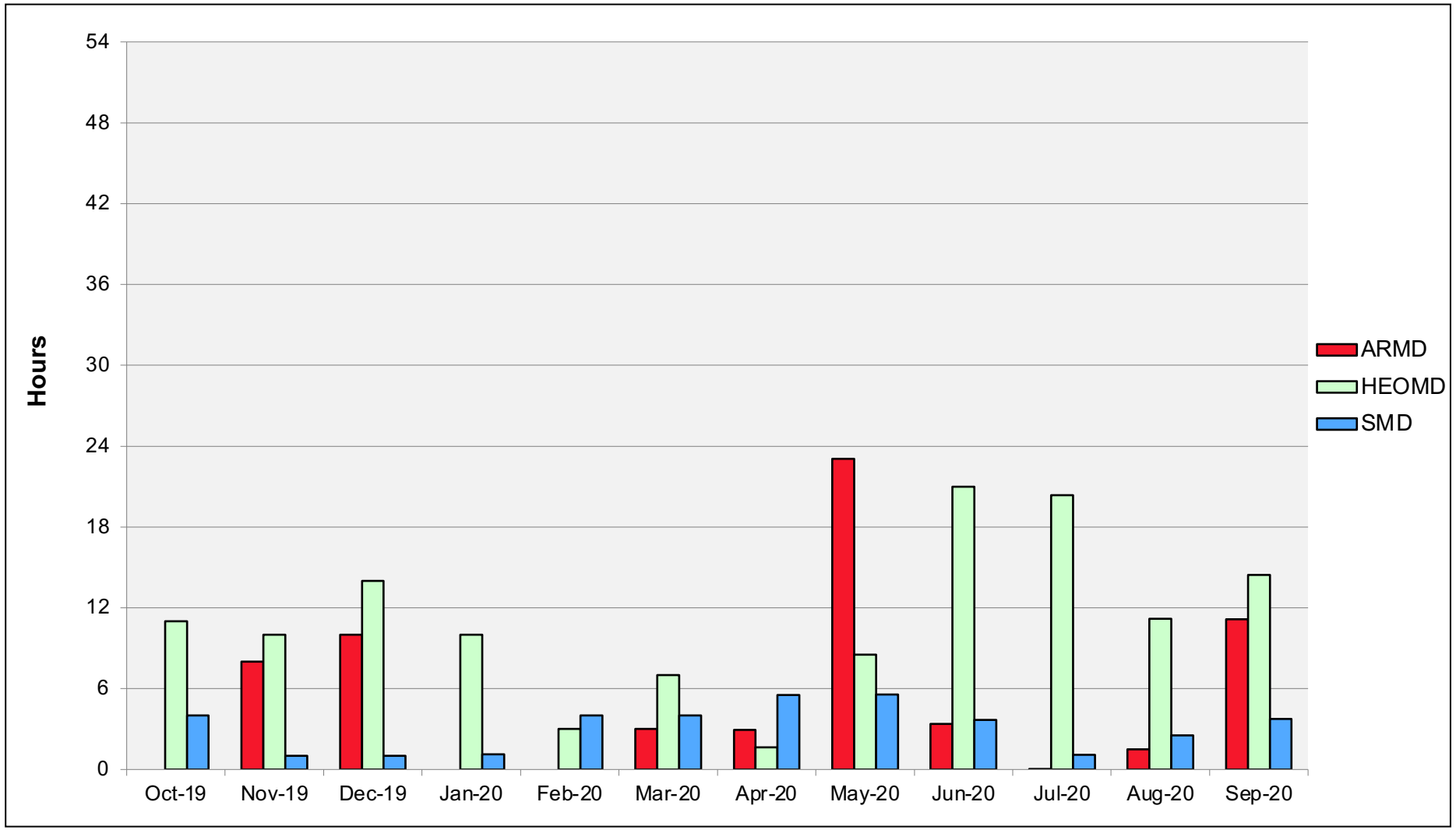
Merope: Monthly Utilization by Job Length



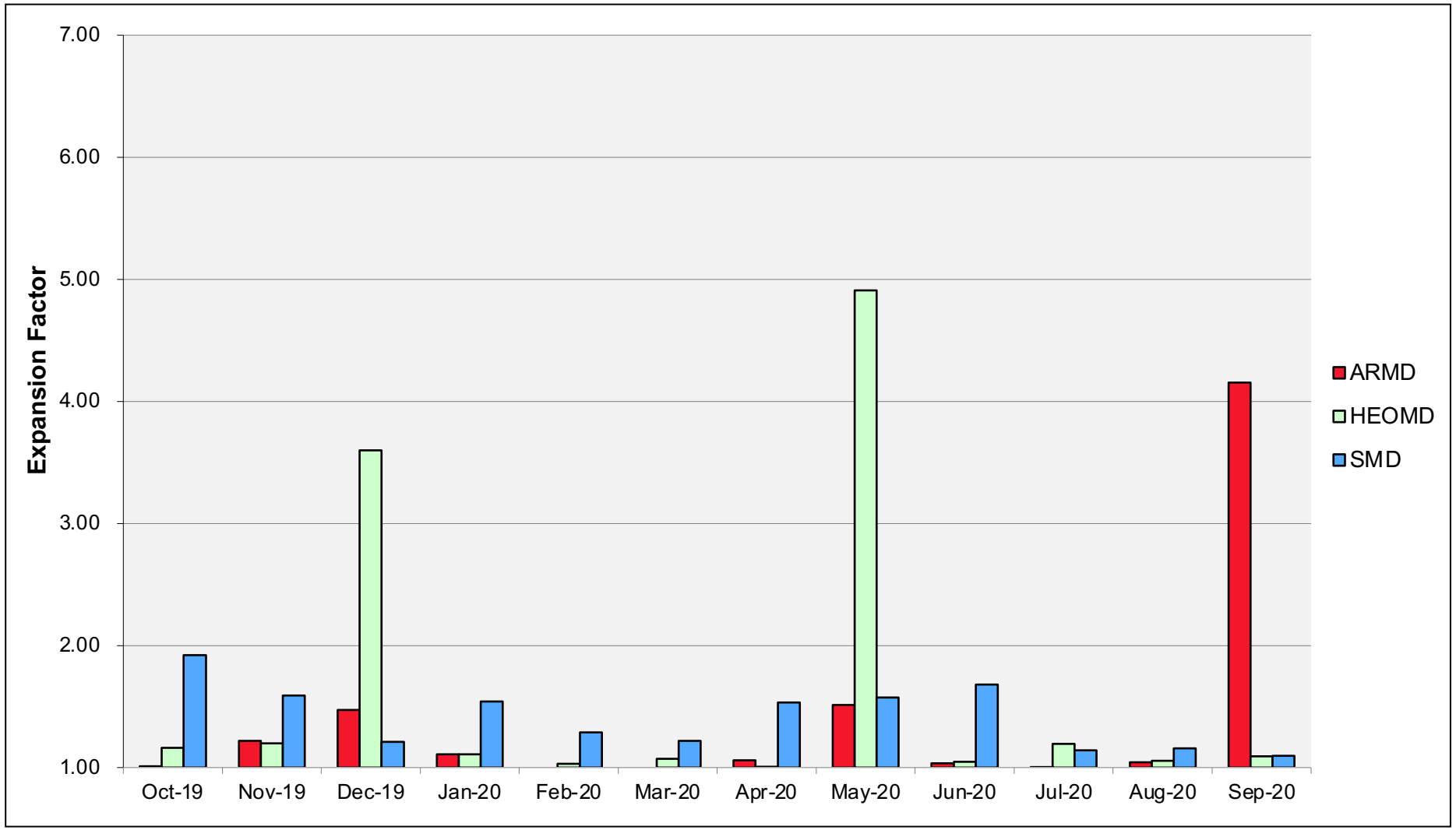
Merope: Monthly Utilization by Size and Length



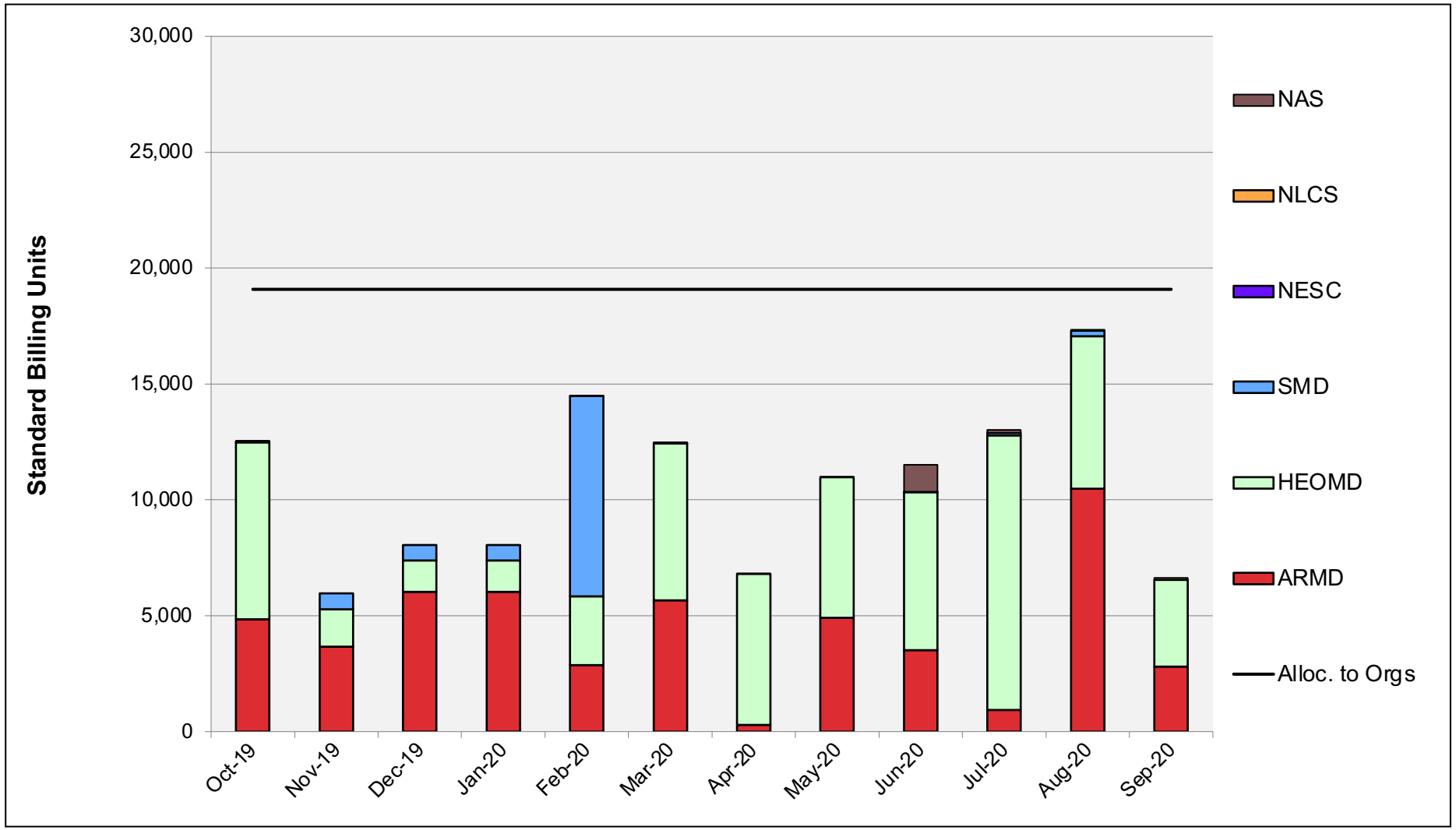
Merope: Average Time to Clear All Jobs



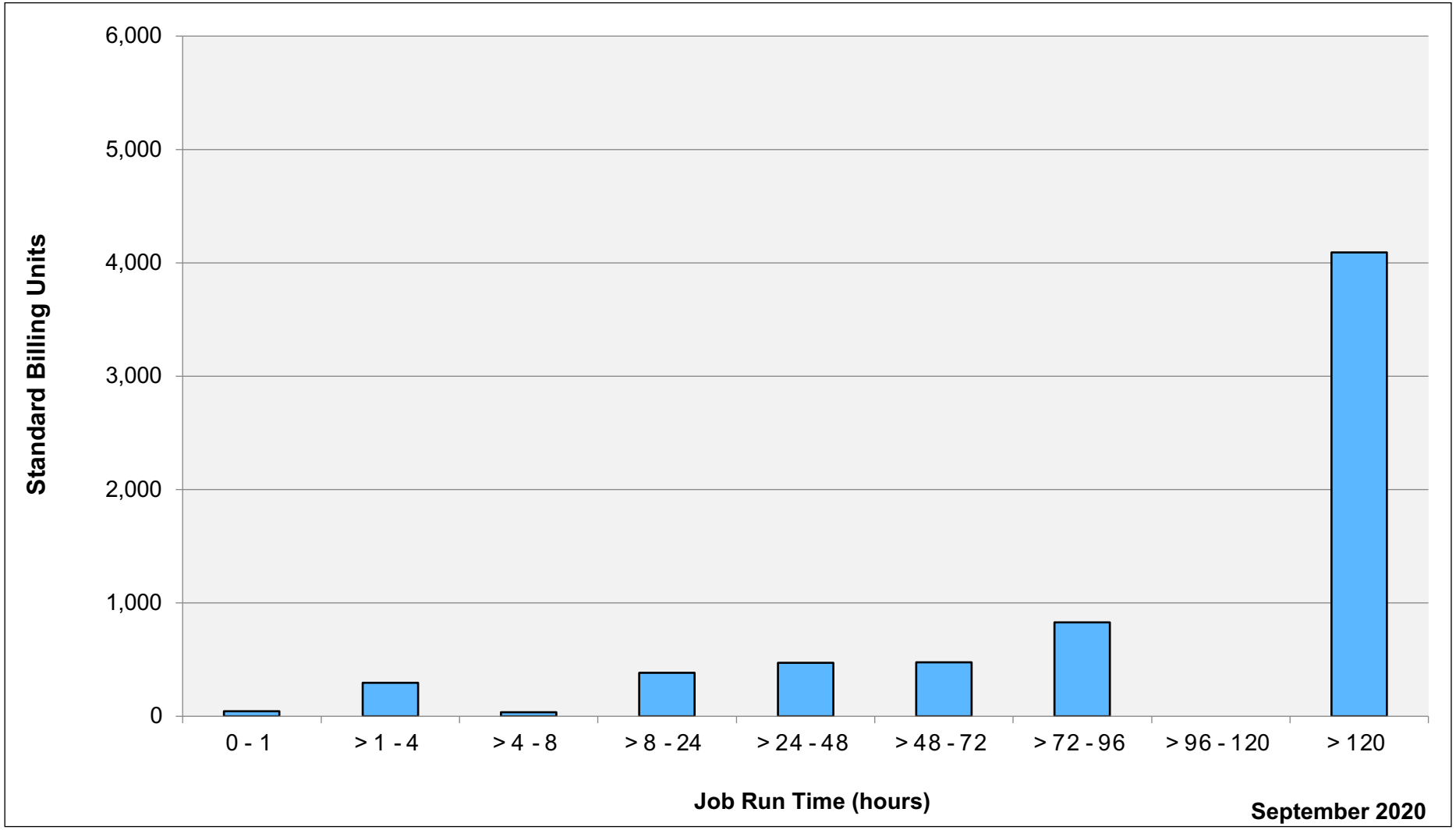
Merope: Average Expansion Factor



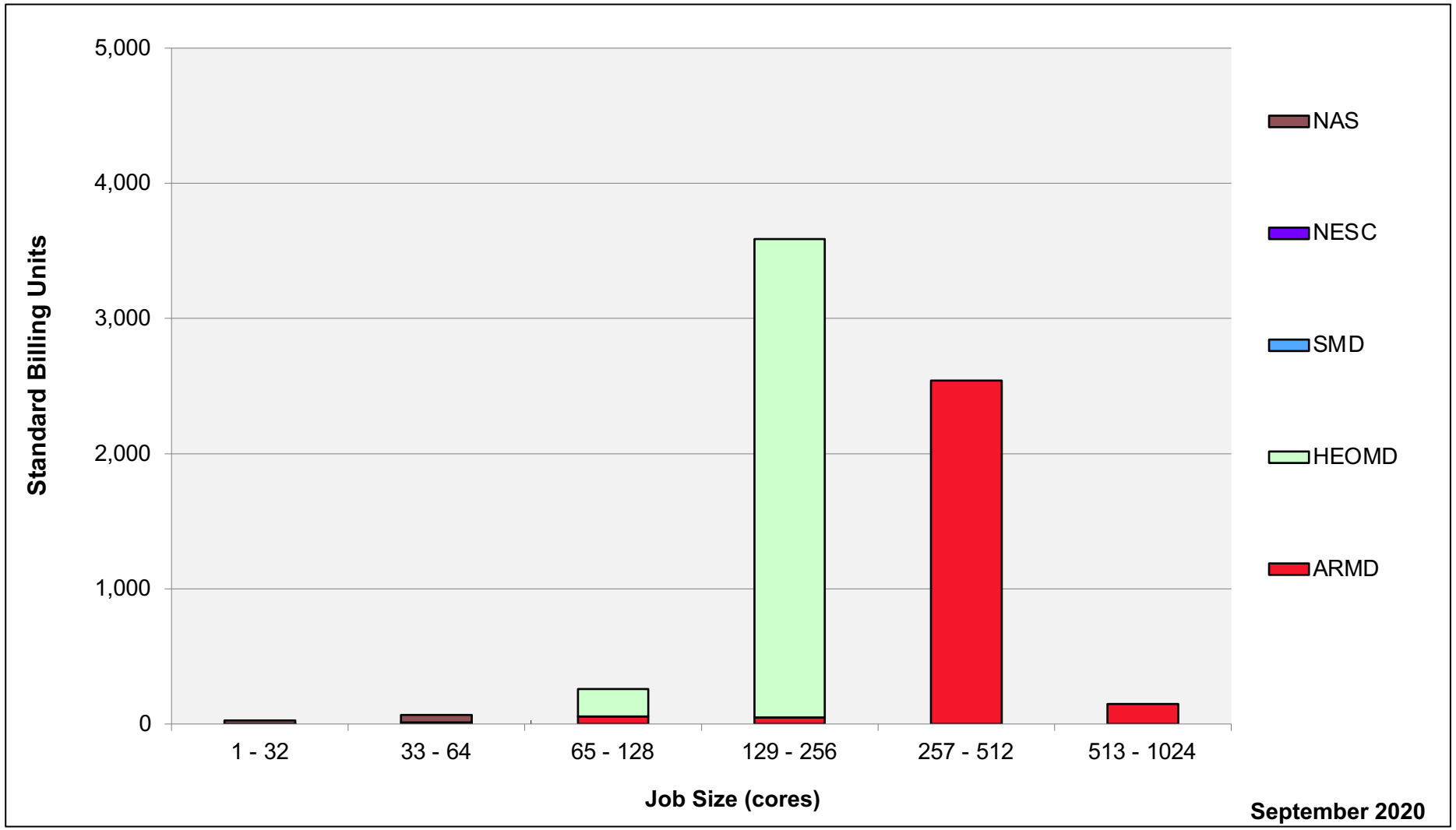
Endeavour: SBUs Reported, Normalized to 30-Day Month



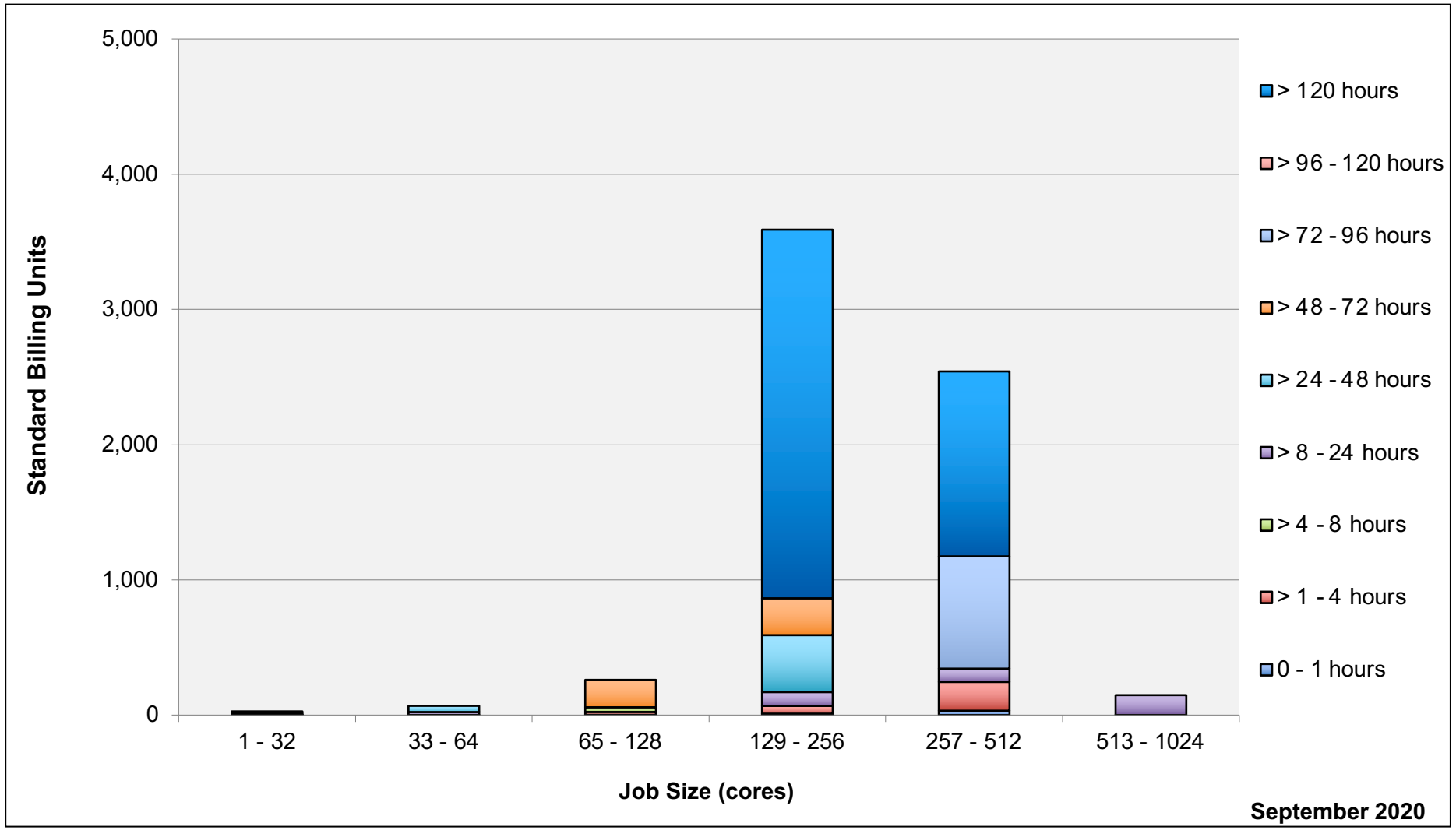
Endeavour: Monthly Utilization by Job Length



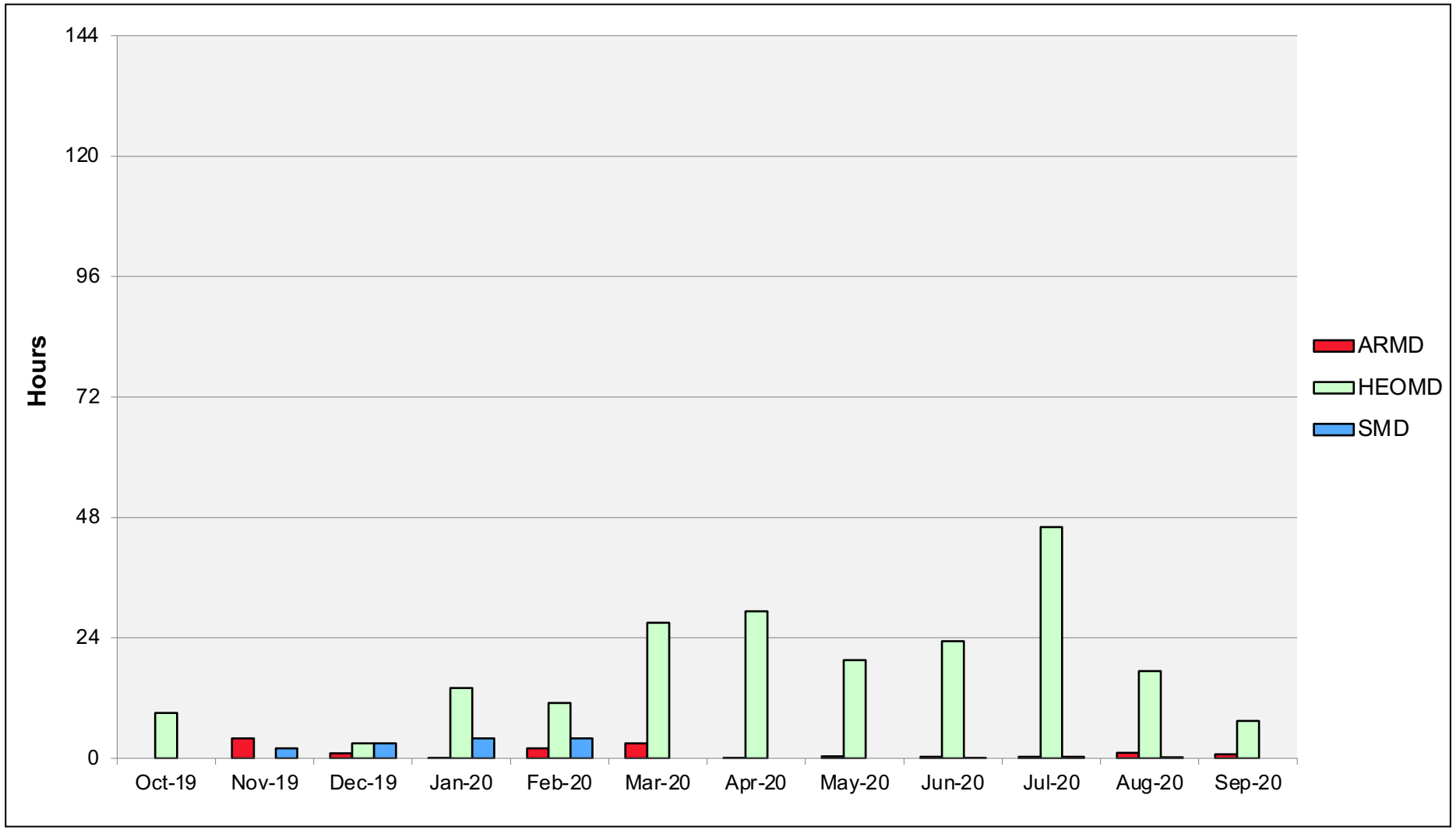
Endeavour: Monthly Utilization by Job Length



Endeavour: Monthly Utilization by Size and Length



Endeavour: Average Time to Clear All Jobs



Endeavour: Average Expansion Factor