National Aeronautics and Space Administration

HIGH-END COMPUTING CAPABILITY PORTFOLIO

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NASA Advanced Supercomputing Division

January 10, 2020

New hyperwall Capability Significantly Increased

- HECC system integrators installed a nine-rack replacement of the compute portion of the hyperwall system, providing a significant performance boost from the current hyperwall installed in 2014.
  - The new hyperwall comprises 128 nodes, each with two 24-core Intel Xeon Cascade Lake processors and 192 gigabytes of memory, for a total of 6,144 CPU cores and 512 teraflops peak processing power.
  - Additionally, each node is also paired with 128 NVIDIA Quadro RTX 6000 graphics processing units, 2.1 petaflops peak processing power, and a 1.8 petabytes BeeGFS filesystem built on SSDs.
  - Like the current hyperwall, it is connected to the HECC Lustre filesystems via InfiniBand, allowing visualization experts to read data directly for pre- and post-processing on the hyperwall, saving many hours of time copying very large data files.
- The hyperwall was released to the Visualization team in early December for transitioning their workflow from the previous hyperwall.
- The new hyperwall increased compute performance by 900%, GPU performance by 480%, and SSD storage capacity by 900% over the previous generation hyperwall.

IMPACT: The new hyperwall compute capability will allow visualization experts to develop significantly more complex models and produce visualization products in a much shorter timeframe.

The new hyperwall compute racks during the early installation phase. *Matt Lepp, HPE*

RHEL 7 Upgrade Complies with NASA Security Mandates

- The HECC Engineering Servers and Services (ESS) team completed the deployment of Red Hat Enterprise Linux (RHEL) 7 to all ESS-supported Linux systems at the NASA Advanced Supercomputing facility on December 17.
  - 253 Linux servers.
  - 123 workstations.
- The RHEL 7 open-source operating system supports:
  - 64-bit AMD and Intel architectures.
  - The highly scalable high-performance XFS filesystem.
  - The systemd daemon to easily supervise and control processes.
  - Enhanced multi-thread Linux Unified Key Setup (LUKS) disk encryption.
- This upgrade complies with agency security-driven mandates.
- Testing has begun on the RHEL 8 operating system, with approval and deployment expected by early 2021.

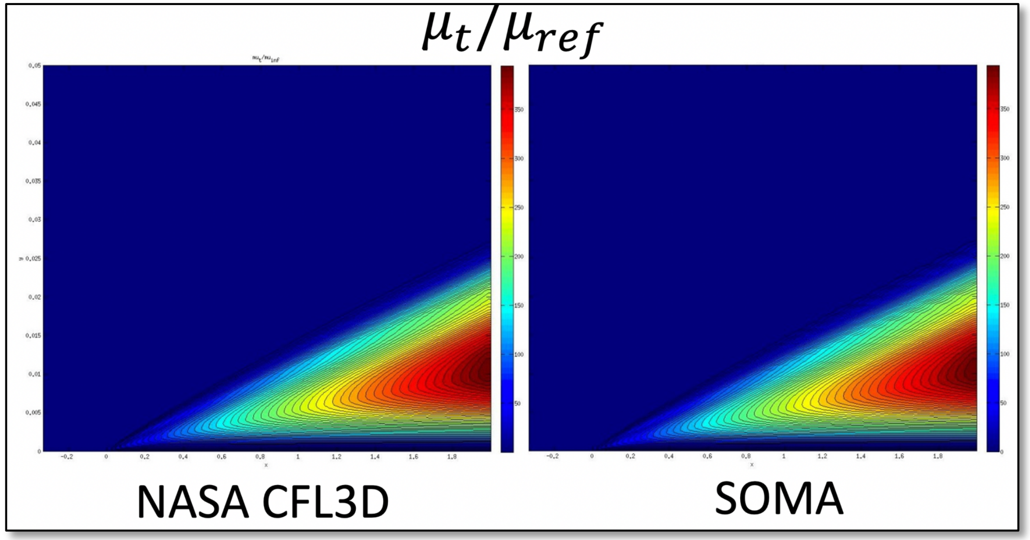
IMPACT: The RHEL 7 upgrade enables new capabilities such as: large filesystems up to 16 exabytes, parallelized job execution, and detailed logging for system/startup error messages while complying with NASA security mandates.

The NVIDIA V100 General-Purpose Graphics Processing Units (GPGPUs) racks are among the 253 Linux servers at the NAS facility that were upgraded to RHEL 7 in December 2020.

APP Team Parallelizes SOMA Code, Achieves 20x Speedup

- The HECC Applications Performance and Productivity (APP) team parallelized the Sequentially Optimized Meshfree Approximation (SOMA) application, which is used by NASA Ames researchers to improve the performance and usability of large-scale and production geometries.
  - The SOMA code is a mesh-free solver for differential equations that uses artificial neural networks (ANN) with Gaussian Radial Basis functions as the neurons. The code provides high accuracy for the adaptive, mesh- and matrix-free solution of aerodynamic problems.
- As a preliminary step to parallelization, the APP team added profiling routines to better understand where time was being spent; they found that most of the time is spent in the ANN algorithm.
- After profiling, the team used OpenMP threads to parallelize the code, and switched to a native random number generator to ensure fast performance. The resulting code runs 20 times faster on a 28-core Broadwell node compared to single-thread performance.
- Future projects may include a hybrid (MPI and OpenMP) parallelization regime and production-type multi-grid geometries.

IMPACT: Parallelization of the SOMA code allows researchers supporting NASA missions to solve large-scale flow problems on HECC systems in hours instead of weeks, improving their ability to meet project milestones.



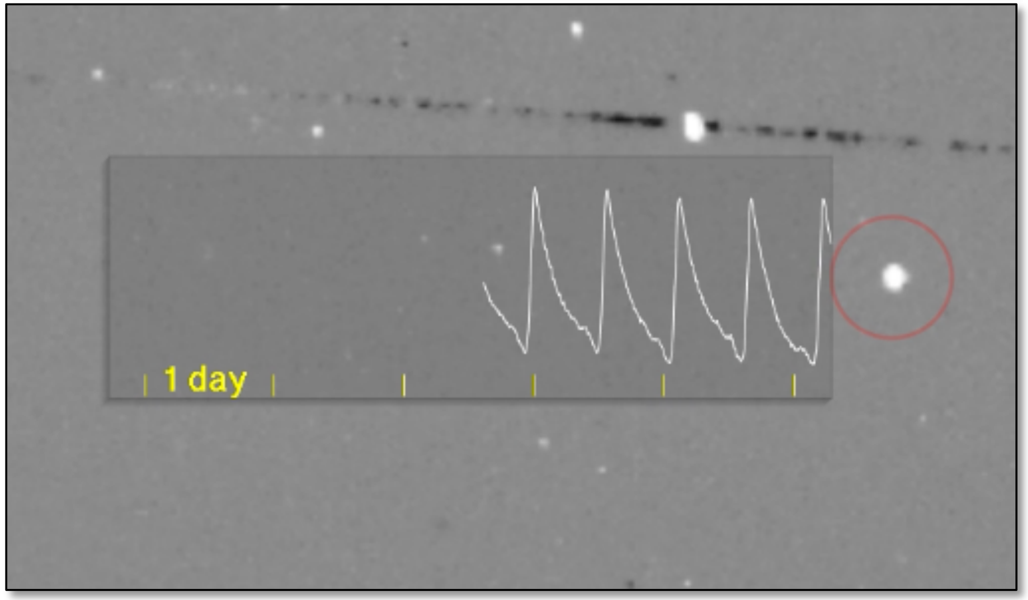
Comparison of the viscosity parameter (ratio of dimensional turbulent viscosity and reference Newtonian viscosity) from two codes, CFL3D and SOMA, on compressible flow past a flat plate. The CFL3D code was chosen for comparison because it used the same turbulence model—the Menter SST two-equation model—as SOMA. *Andrew Meade, NASA Ames*

HECC Resources, Services Enable TESS's All-Sky Survey*

- During its two-year primary mission, NASA's Transiting Exoplanet Survey Satellite (TESS) mapped approximately 75% of the sky, generating enormous amounts of data that were processed on Pleiades by the Science Processing Operations Center (SPOC). The SPOC is currently processing data produced by TESS during its extended mission.
  - Each month during its primary mission, TESS observed a 24-by-96-degree swath of sky, taking a 64-gigabyte Full Frame Image (FFI) every half hour and 20,000 images of select target stars every two minutes. In its extended mission, TESS now collects FFIs every 10 minutes and up to 1,000 target images every 20 seconds.
  - TESS has discovered 91 exoplanets to date, 54 of which are smaller than Neptune, and over 2,000 planet candidates.
- Pleiades is used to calibrate the digital images, measure the brightness of each target star over time, correct instrumental effects, and search for the tell-tale "dips" in the light curve that occur when an exoplanet crosses the face of its star. The SPOC's dedicated computer hardware is co-located with Pleiades in HECC's secure enclave to minimize data transfer time.
- Five levels of data products are produced from uncalibrated pixel flight data. The data products are exported to the Mikulski Archive for Space Telescopes (MAST) for teams at NASA, university partners, and for citizen scientists around the world to analyze.

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

IMPACT: HECC resources are a key enabling technology for TESS. The Science Processing Operations Center is a critical part of NASA's TESS mission, turning data into astronomical results and datasets that anyone can use to discover and analyze exoplanets.

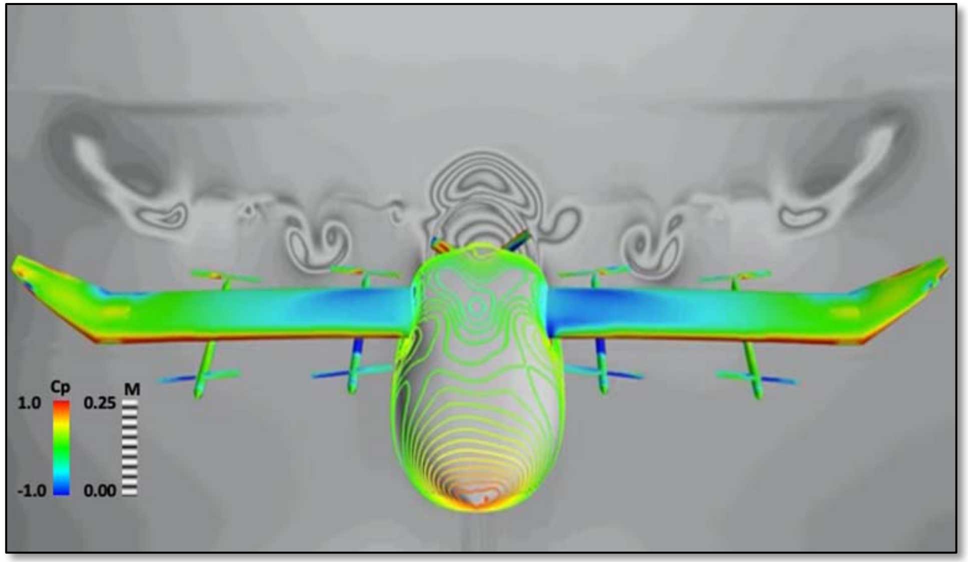


Video showing difference imaging of the 10-minute TESS FFI data. Pixels of constant brightness are colored 50% gray; pixels growing in brightness are lighter; and pixels decreasing in brightness are darker. Most of the objects seen here are variable stars. The bright moving objects are asteroids. *Chris Henze, NASA Ames*

Simulating Aeroelasticity of eVTOL Air Taxis*

- Researchers at NASA Ames successfully simulated an electric vertical take-off and landing vehicle (eVTOL) configuration with eight lifting propellers and one pushing propeller, for an advanced air mobility project.
  - Flexible eVTOL wings reduce vehicle weight but are susceptible to aeroelastic oscillation that can be triggered from sudden wind gusts, leading to instability.
  - The researchers added a new aeroelastic module to NASA's OVERFLOW software, in order to model wing structures using finite-element-based modal equations.
- Simulations were made using Navier-Stokes (NS)-based CFD coupled with structural equations of motion; and an in-house RUNDUA protocol (dual-level parallel) that facilitates automatic running of multiple cases.
  - The NS equations are essential to obtain accurate simulations. Prior to this work, all aeroelastic simulations generated generated elsewhere for eVTOL by using NS equations are limited to quasi-steady loose coupling methods.
  - Flight conditions often involve time-dependent transient cases, which require time-accurate simulation.
  - With the RUNDUA protocol, about 250 simulations can be completed in approximately 100 hours of wall-clock time, using 5,000 cores on Pleiades.
- The next step will be to extend the prediction capability to include trajectory equations, with a goal to automatically produce 1,000 simulations in 100 hours of wall-clock time.

IMPACT: The accurate prediction of aeroelastic oscillations of wing and lifting propellers due to sudden wind gusts demonstrates the usefulness of new computational capabilities for NASA's Advanced Air Mobility projects.



Animation showing the aeroelastic response of an air taxi during a sudden gust of wind. Contours of surface pressure are shown (red is positive pressure; blue is suction pressure) and field Mach numbers (black and white ranging from 0 to 0.25 in zebra scaling). Insufficient structural damping could lead to adverse instability in flight.
Guru Guruswamy, NASA/Ames

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Papers

- "**Two Planetary Systems and Field Stars with Ages Between 20 and 320 Myr from TESS**," G. Zhou, et al., The Astronomical Journal, vol. 161, no. 1, December 2, 2020. *
https://iopscience.iop.org/article/10.3847/1538-3881/abba22/meta
- "**Analysis of Time-Distance Helioseismology for Detection of Emerging Active Regions**," J. Stefan, A. Kosovichev, A. Stejko, arXiv:2012.01367 [astro-ph.SR], December 2, 2020. *
https://arxiv.org/abs/2012.01367
- "**The Role of Early Giant Planet Instability in the Terrestrial Planet Formation**," D. Nesvorny, F. Roig, R. Deienno, arXiv:2012.02323 [astro-ph.EP], December 3, 2020. *
https://arxiv.org/abs/2012.02323
- "**TOI 122b and TOI 237b: Two Small Warm Planets Orbiting Inactive M Dwarfs Found by TESS**," W. Waalkes, et al., The Astrophysical Journal, vol. 161, no. 1, December 7, 2020. *
https://iopscience.iop.org/article/10.3847/1538-3881/abc3b9/meta
- "**Spectral Modeling Using Radiative Transfer Theory with Packing Density Correction: Demonstration for Saturnian Icy Satellites**," L. Kolokolova, et al., The Planetary Science Journal, vol. 1, no. 3, December 8, 2020. *
https://iopscience.iop.org/article/10.3847/PSJ/abb5b3/meta
- "**Thermal Instability and Multiphase Gas in the Simulated Interstellar Medium with Conduction, Viscosity and Magnetic Fields**," R. M. Jennings, Y. Li, arXiv:2012.05252 [astro-ph.GA], December 9, 2020. *
https://arxiv.org/abs/2012.05252

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Papers (cont.)

- “**Unravelling the Physics of Multiphase AGN Winds Through Emission Line Tracers**,” A. Richings, C.-A. Faucher-Giguere, J. Stern, arXiv:2012.06592 [astro-ph.GA], December 11, 2020. *
https://arxiv.org/abs/2012.06592
- “**Vetting of 384 TESS Objects of Interest with TRICERATOPS and Statistical Validation of 12 Planet Candidates**,” S. Giacalone, et al., The Astronomical Journal, vol. 161, no. 1, December 11, 2020. *
https://iopscience.iop.org/article/10.3847/1538-3881/abc6af/meta
- “**Compounding Factors for Extreme Flooding Around Galveston Bay During Hurricane Harvey**,” W. Huang, et al., Ocean Modeling (Elsevier), vol. 158, published online December 13, 2020. *
https://www.sciencedirect.com/science/article/abs/pii/S1463500320302377
- “**Molecular Machine Learning with Conformer Ensembles**,” S. Axelrod, R. Gomez-Bombarelli, arXiv:2012.08452 [cs.LG] December 15, 2020. *
https://arxiv.org/abs/2012.08452
- “**Revisiting the HD 21749 Planetary System with Stellar Activity Modeling**,” T. Gan, et al., Monthly Notices of the Royal Astronomical Society, published online December 24, 2020. *
https://academic.oup.com/mnras/advance-article-abstract/doi/10.1093/mnras/staa3886/6047182

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

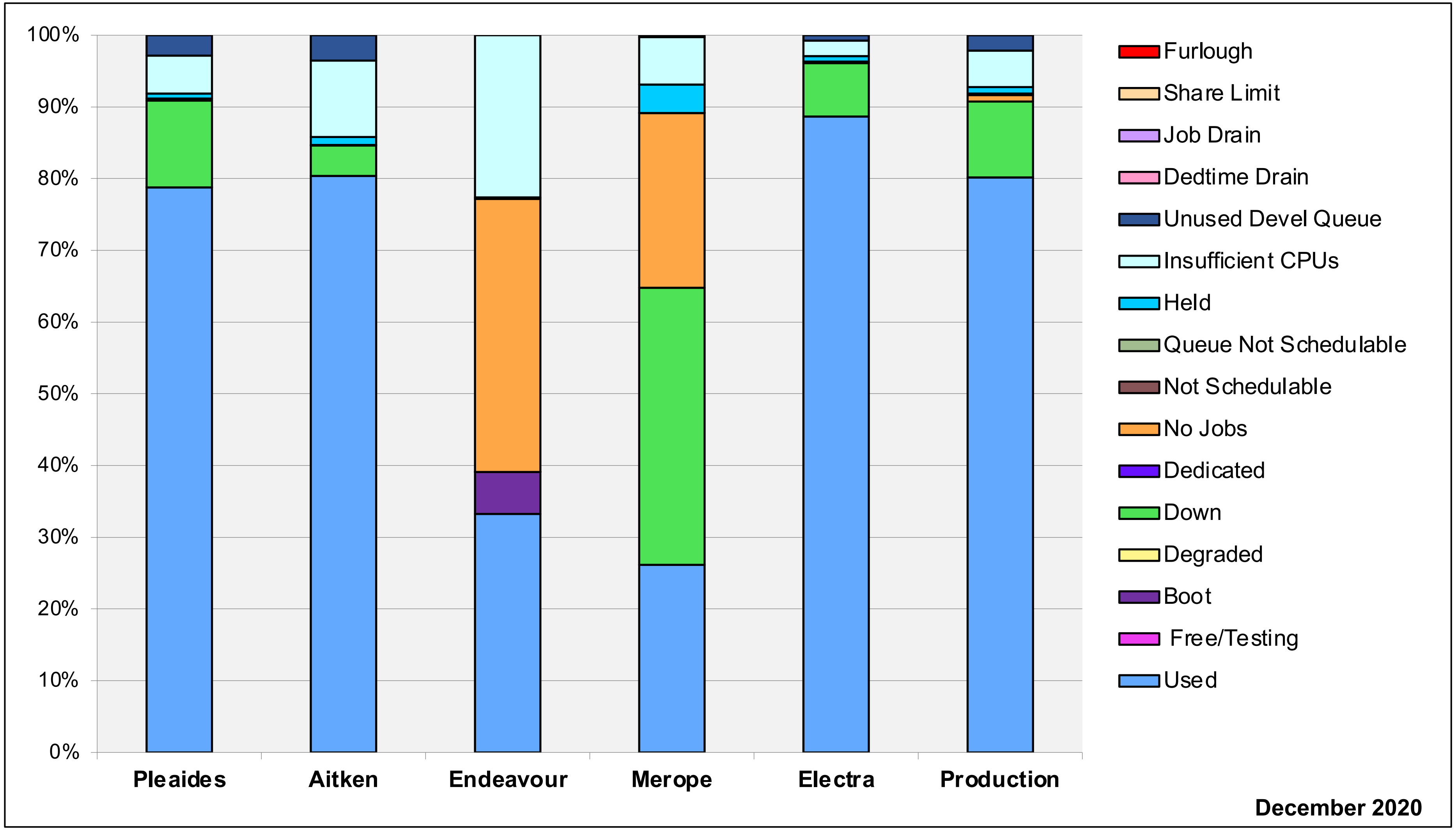
News and Events

- **Aeronautical Artwork, Computing Simulation, or Both?** *NASA Aeronautics Feature,* December 1, 2020—Utilizing the powerful supercomputers at the NAS facility, aeronautics researchers created complex simulations of supersonic shockwaves around the X-59 Quiet SuperSonic Technology aircraft currently under construction in Palmdale, California. https://www.nasa.gov/aeroresearch/aeronautical-artwork-computer-simulation-or-both
- **Visualizing the Future of Advanced Air Mobility**, *NASA Aeronautics Feature*, December 10, 2020—The Pleiades and Electra supercomputers at the NAS facility processed hundreds of millions of data points in a simulation of the airflow among four rotors in a concept for a six-passenger quadcopter. https://www.nasa.gov/aeroresearch/visualizing-the-future-of-advanced-air-mobility/
- **Scientists Use NASA Data to Predict Appearance of Dec. 14 Eclipse**, *NASA Goddard Feature*, December 16, 2020—Predictive Science Inc. used data from NASA's Solar Dynamics Observatory (SDO) to develop a prediction of the total solar eclipse, which was visible in Chile and Argentina. NAS Division supercomputers supported the computations. https://www.nasa.gov/feature/goddard/2020/scientists-use-nasa-data-predict-appearance-corona-dec-14-total-solar-eclipse
  - **Coronal Prediction for the December 14, 2020 Total Solar Eclipse**, *Predictive Science Inc.,* December 2020. http://www.predsci.com/corona/dec2020eclipse/home.php

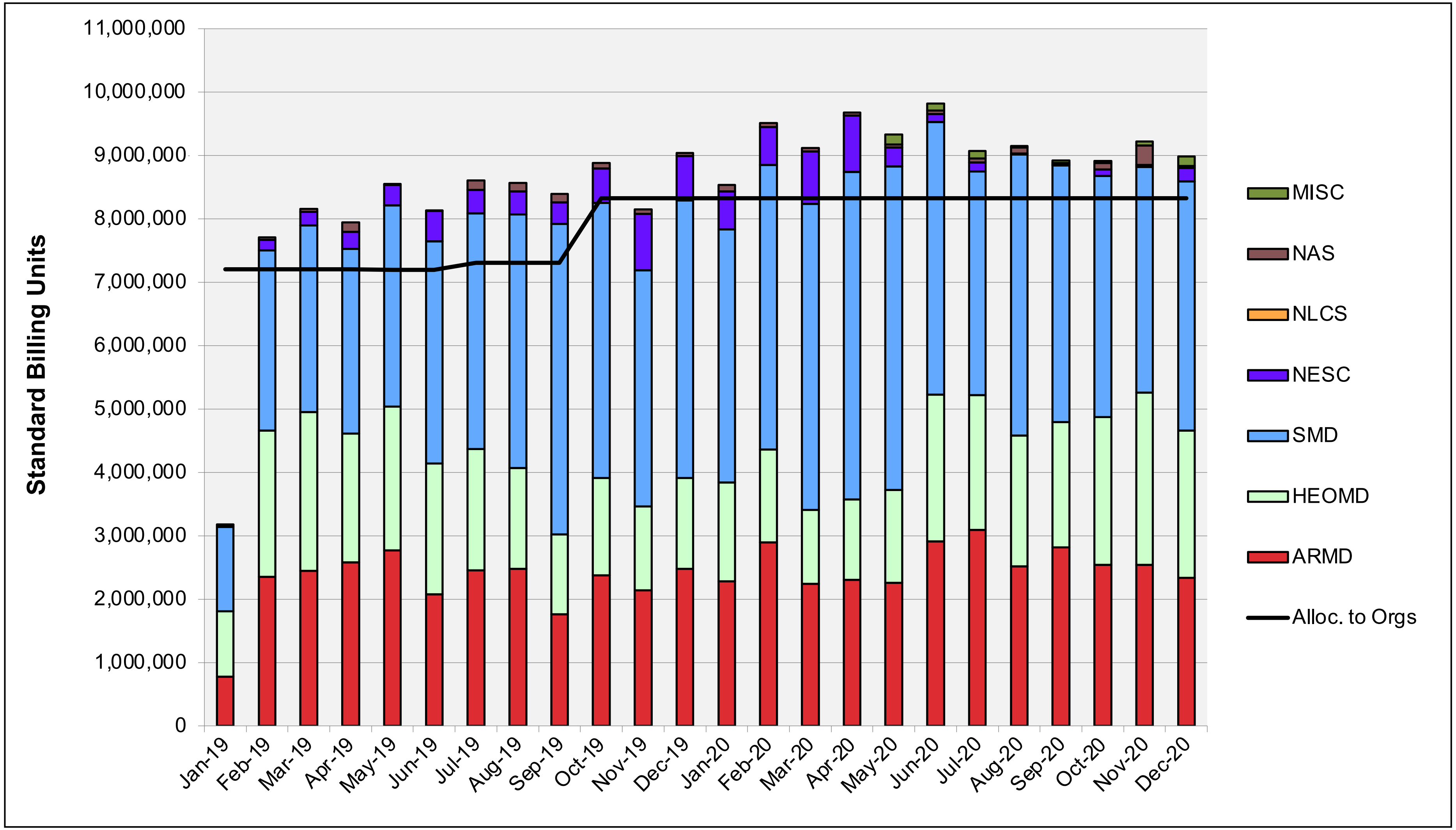
News and Events: Social Media

- **Coverage of NAS Stories**
  - X-59 Low Boom Visualization:
    - NASA Aero: Twitter 13 retweets, 89 favorites; Facebook 47 likes, 6 shares.
  - Visualizing Advanced Air Mobility:
    - NASA Aero: Twitter 8 retweets, 28 favorites, Facebook 19 likes, 3 shares.
  - 2020 Visualization Wrap-up:
    - NAS: Twitter 4 retweets, 5 likes; Facebook 679 users reached, 67 engagements, 24 likes, and 6 shares.
    - NASA Aero: Facebook 35 likes, 3 shares.
  - Aeronautics Visualizations (from SC20):
    - NASA Video: YouTube 2,646 views, 280 likes.
    - NASA Aero: Twitter (10 tweet thread) 59 retweets, 480 likes; Facebook 28 likes, 7 shares.

HECC Utilization



HECC Utilization Normalized to 30-Day Month



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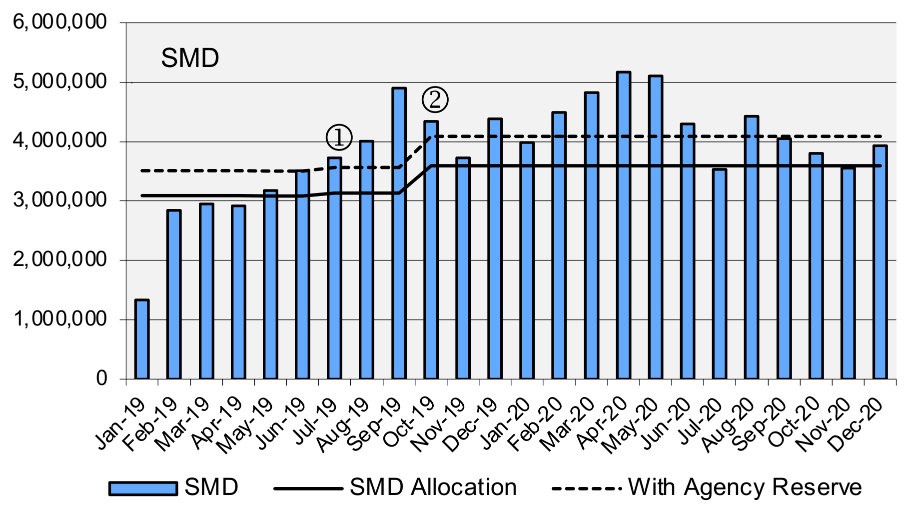
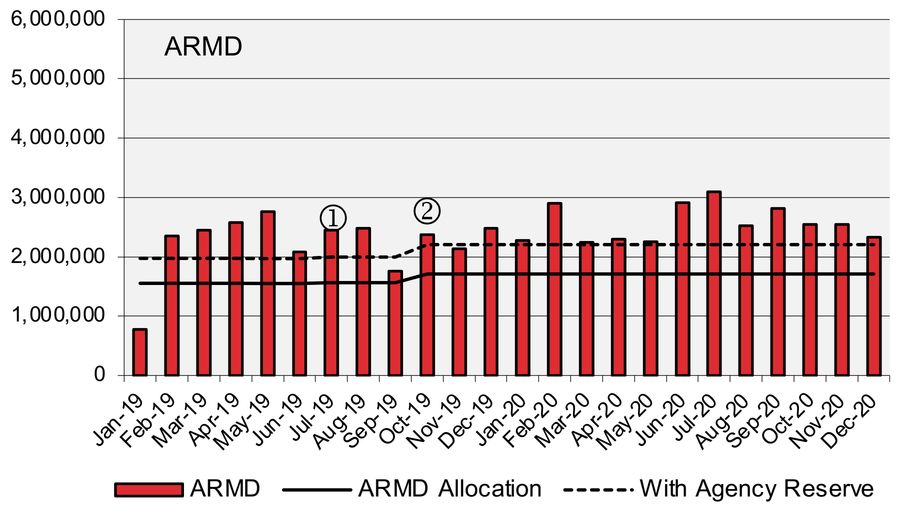
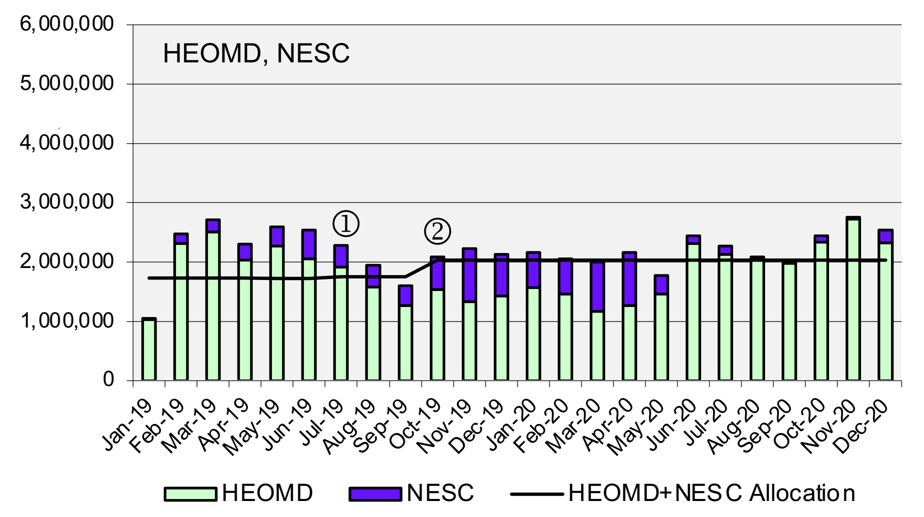


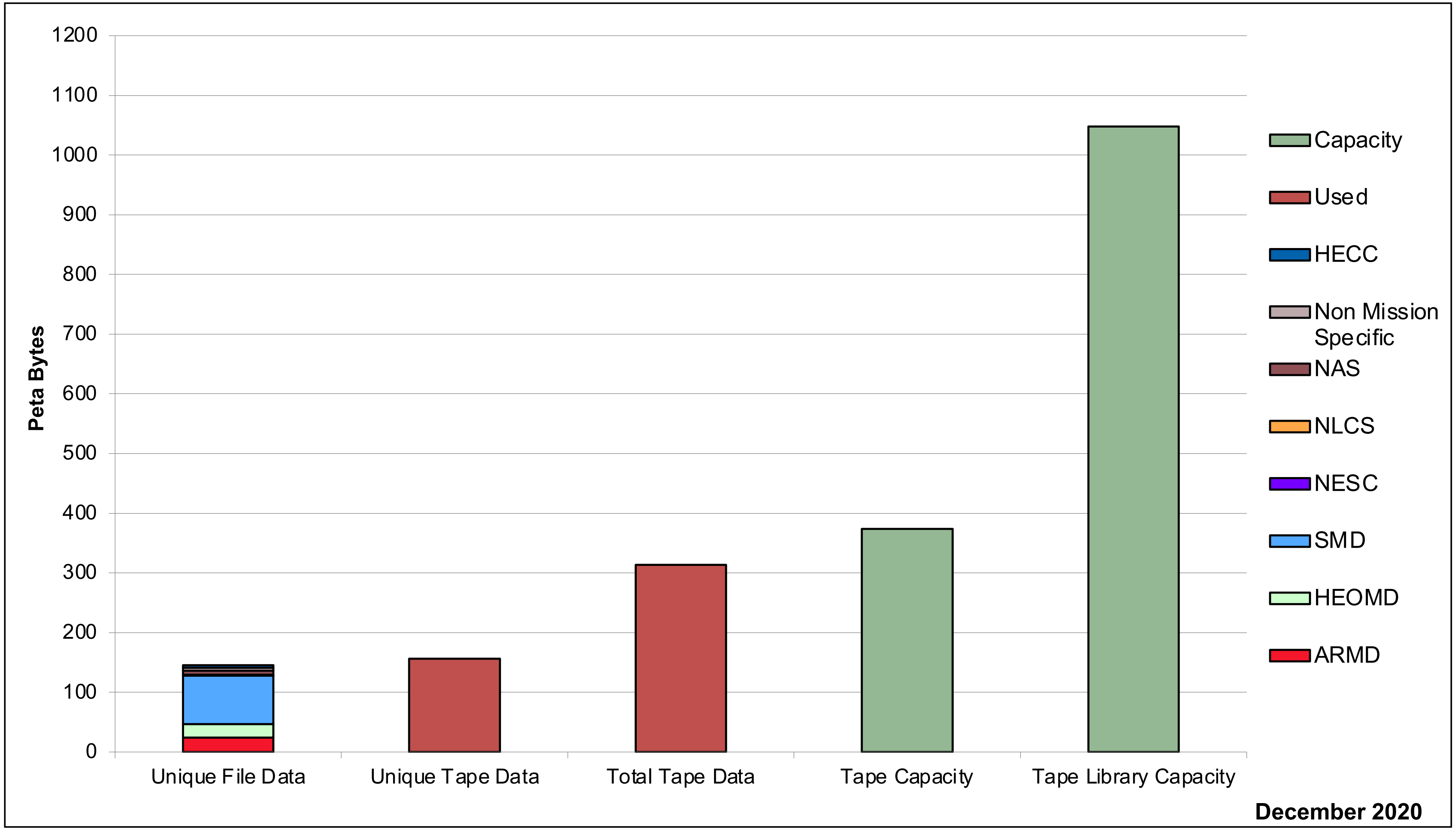




① Skylake Tesla GPU V100 Nodes installed

② 4 Cascade Lake E cells introduced into Aitken

Tape Archive Status



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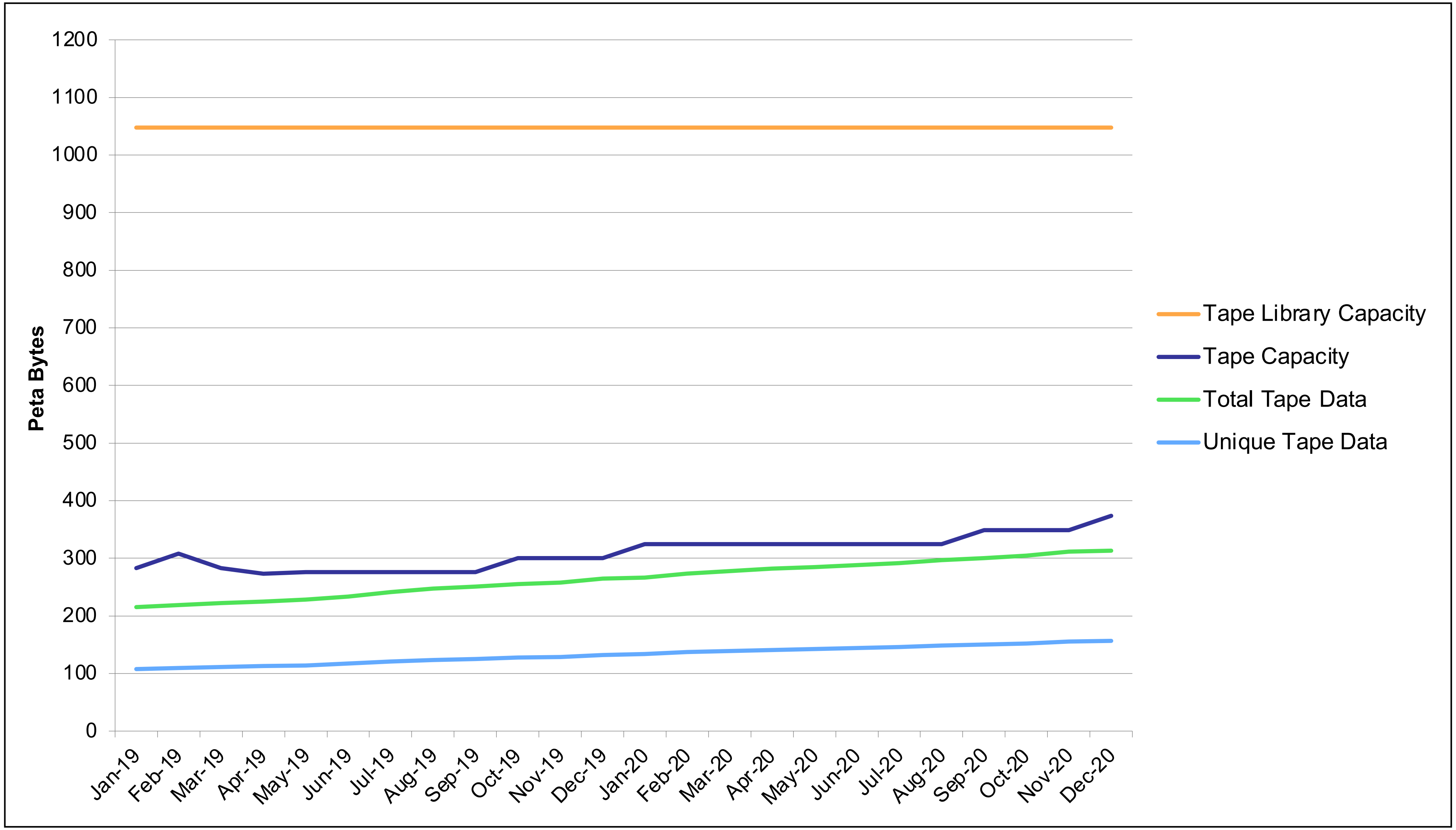
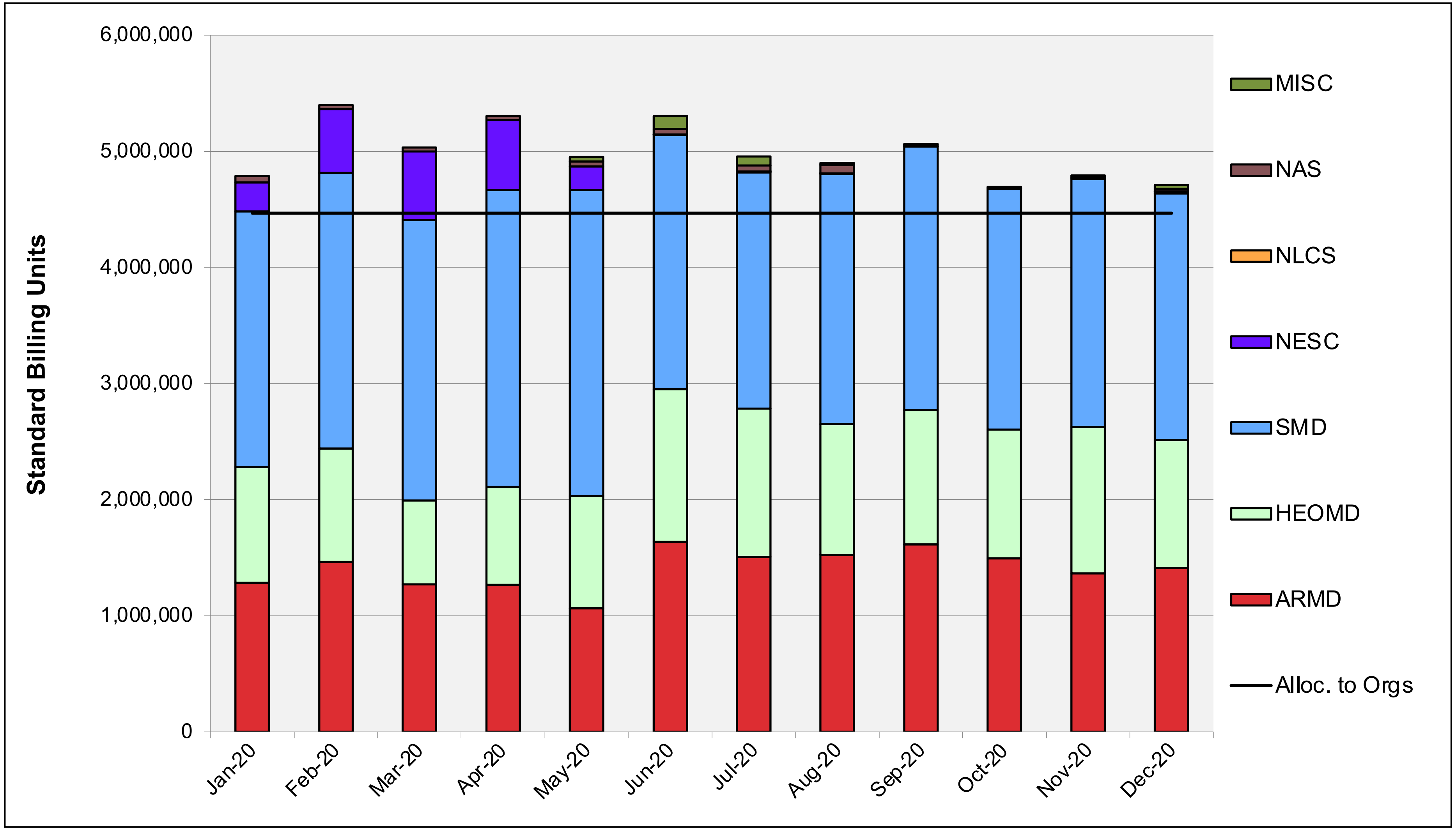
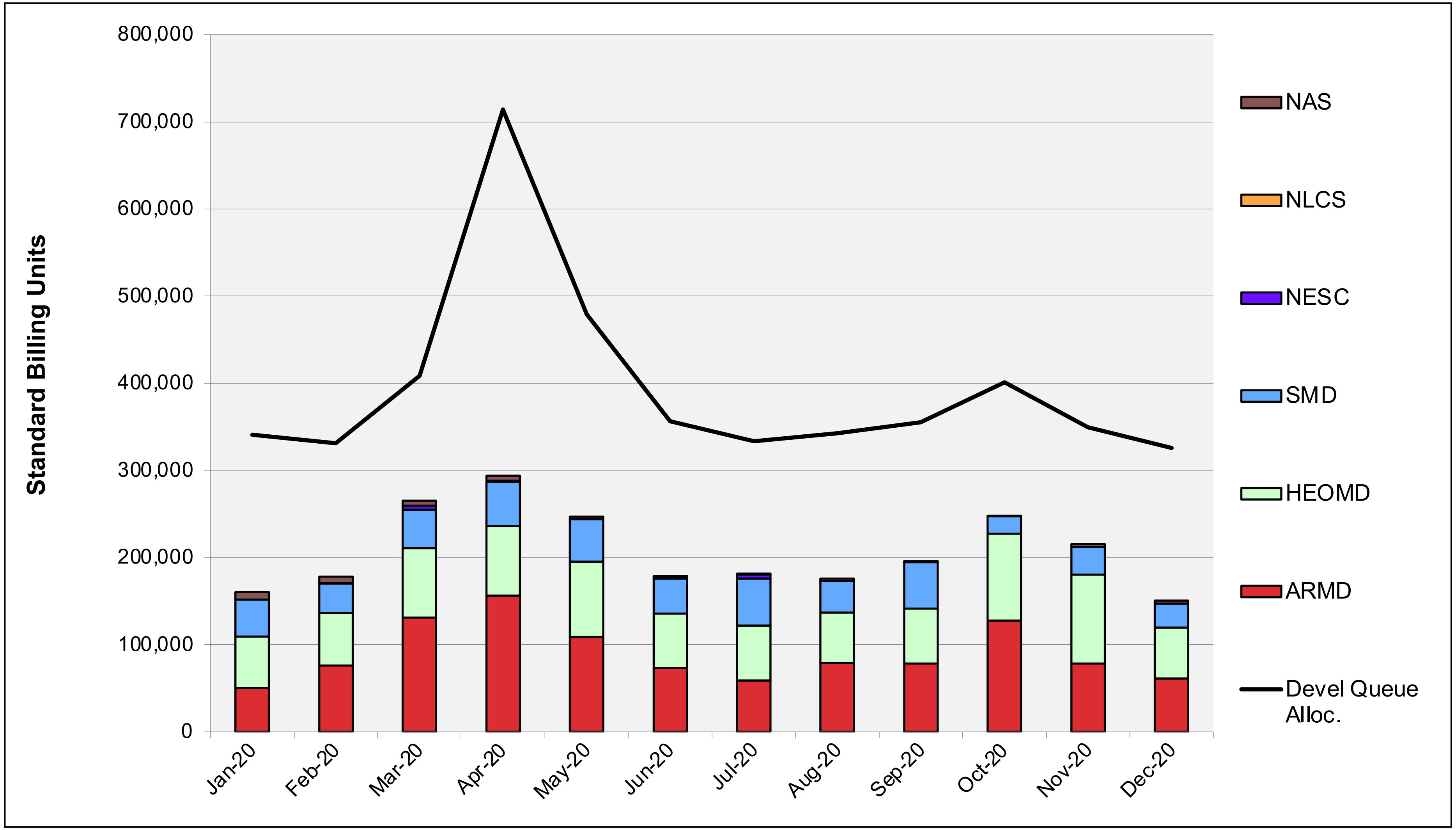


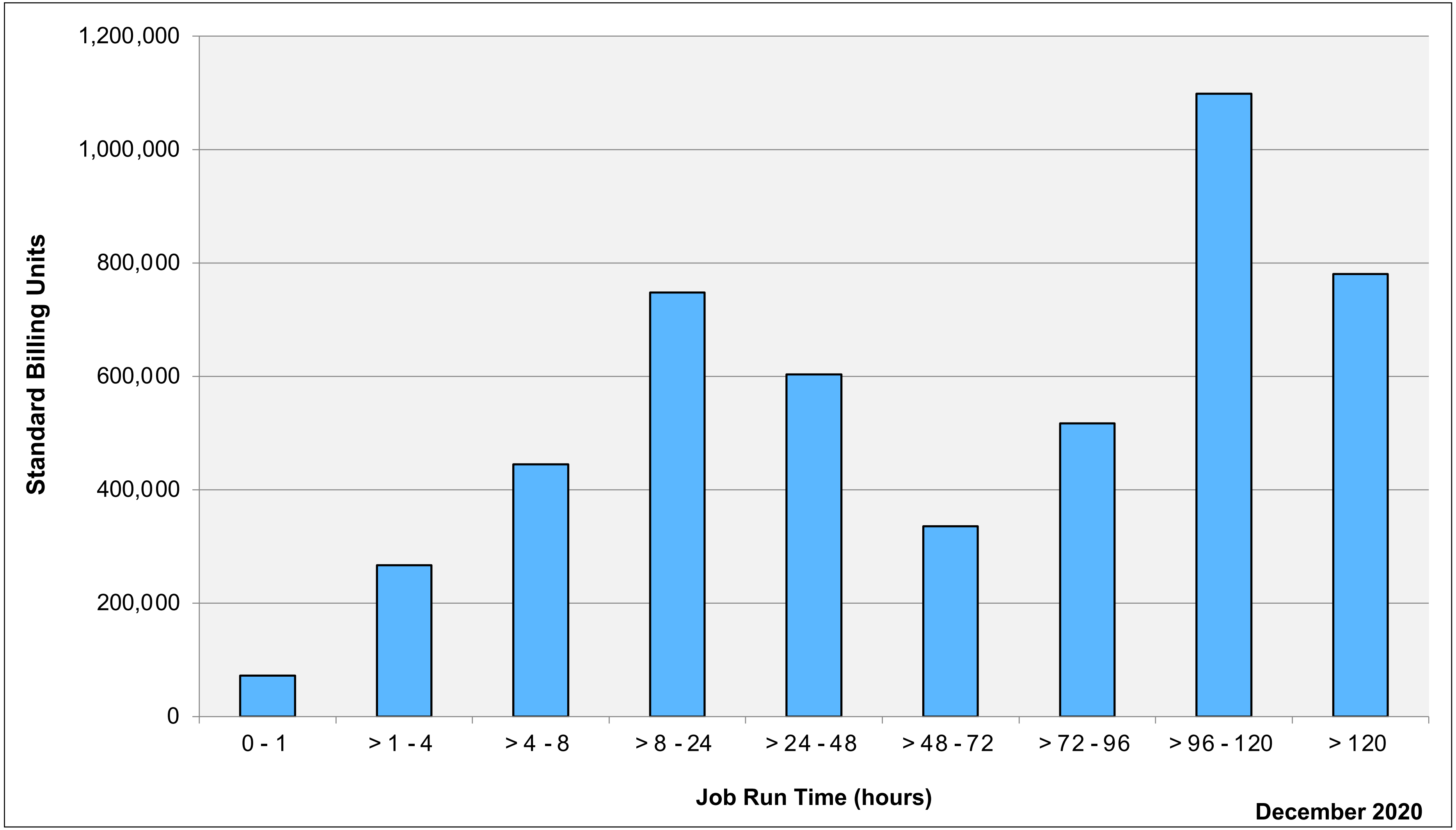
Pleiades: SBUs Reported, Normalized to 30-Day Month



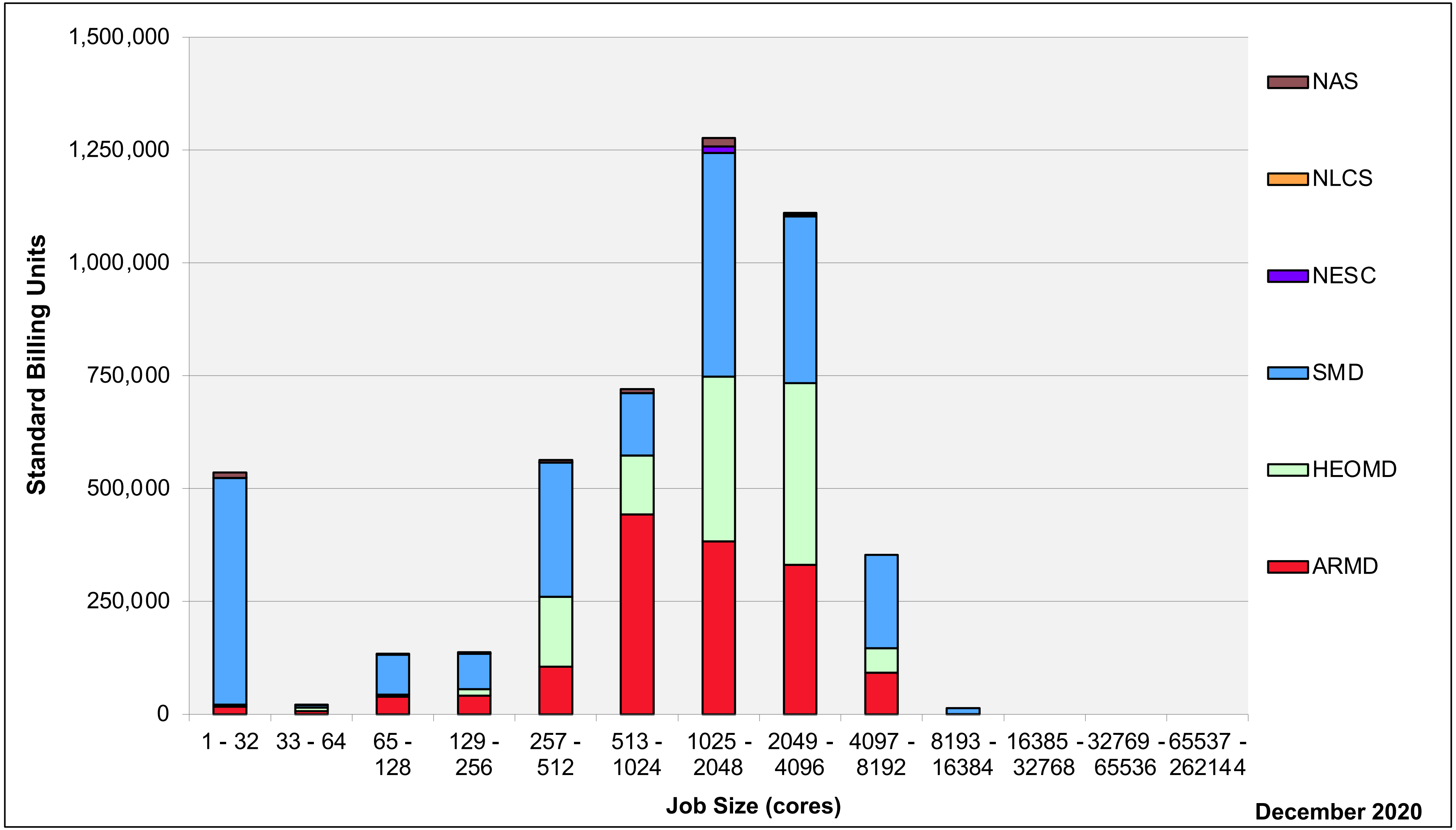
Pleiades: Devel Queue Utilization



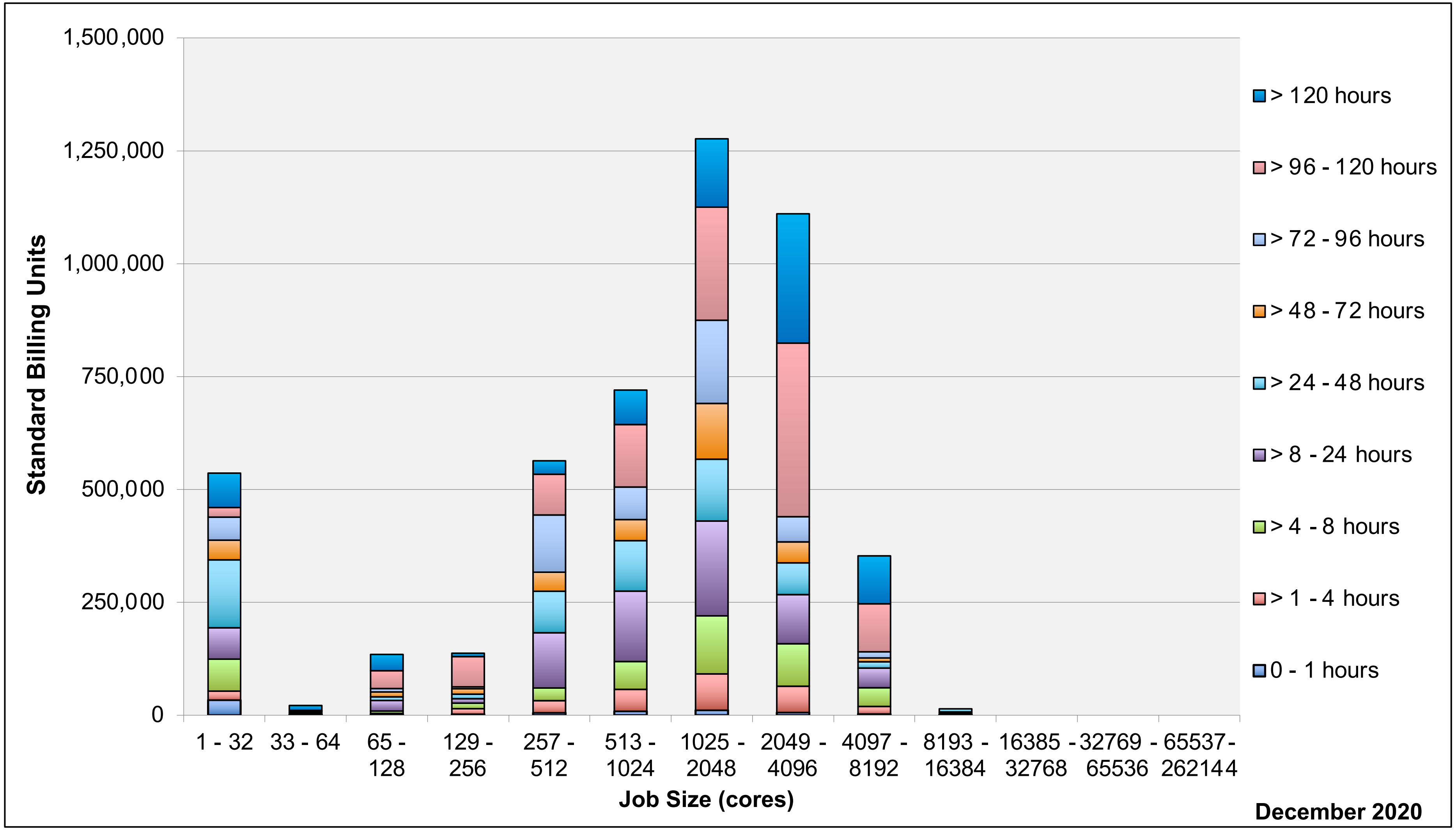
Pleiades: Monthly Utilization by Job Length



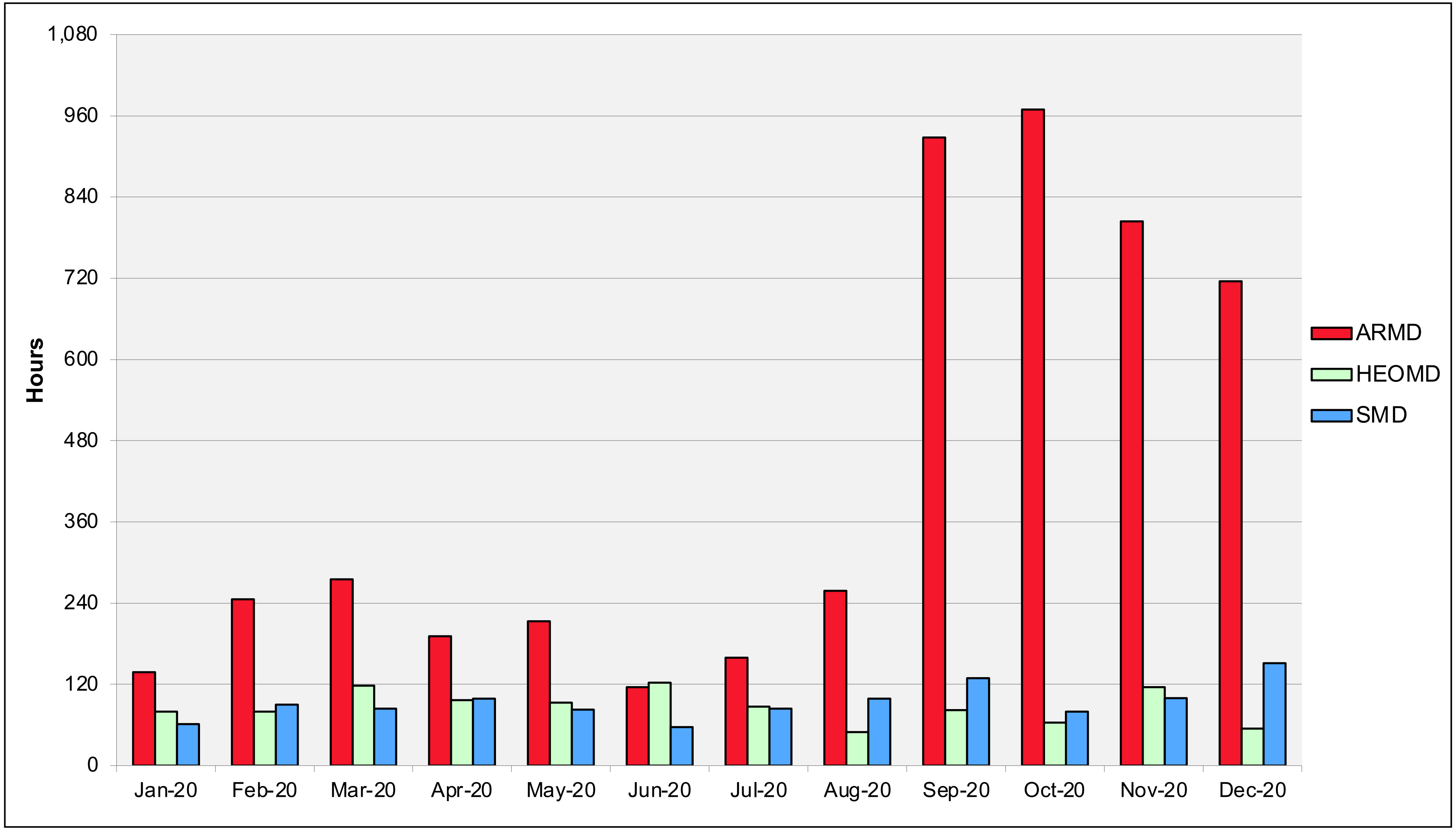
Pleiades: Monthly Utilization by Job Size



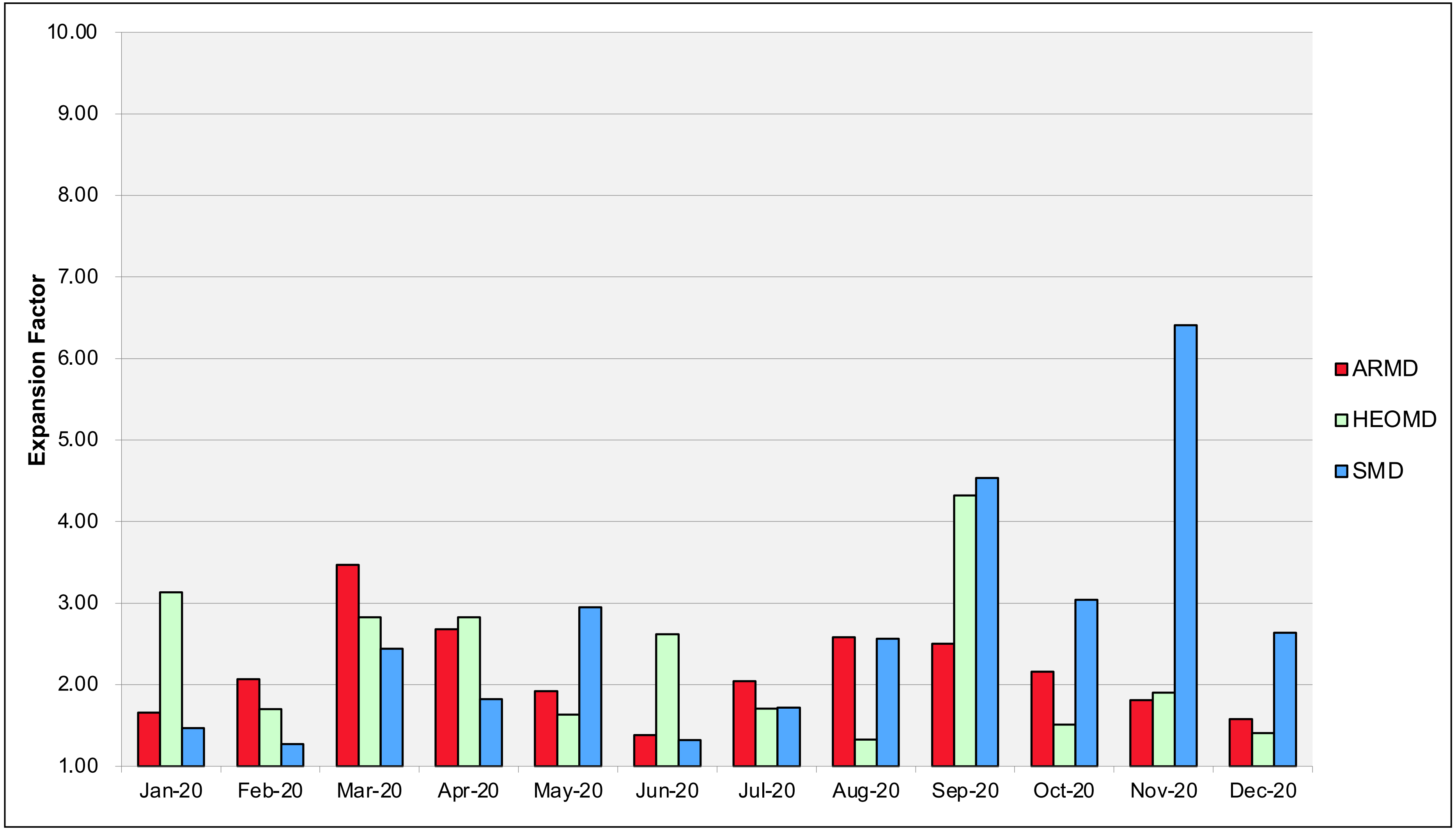
Pleiades: Monthly Utilization by Size and Length



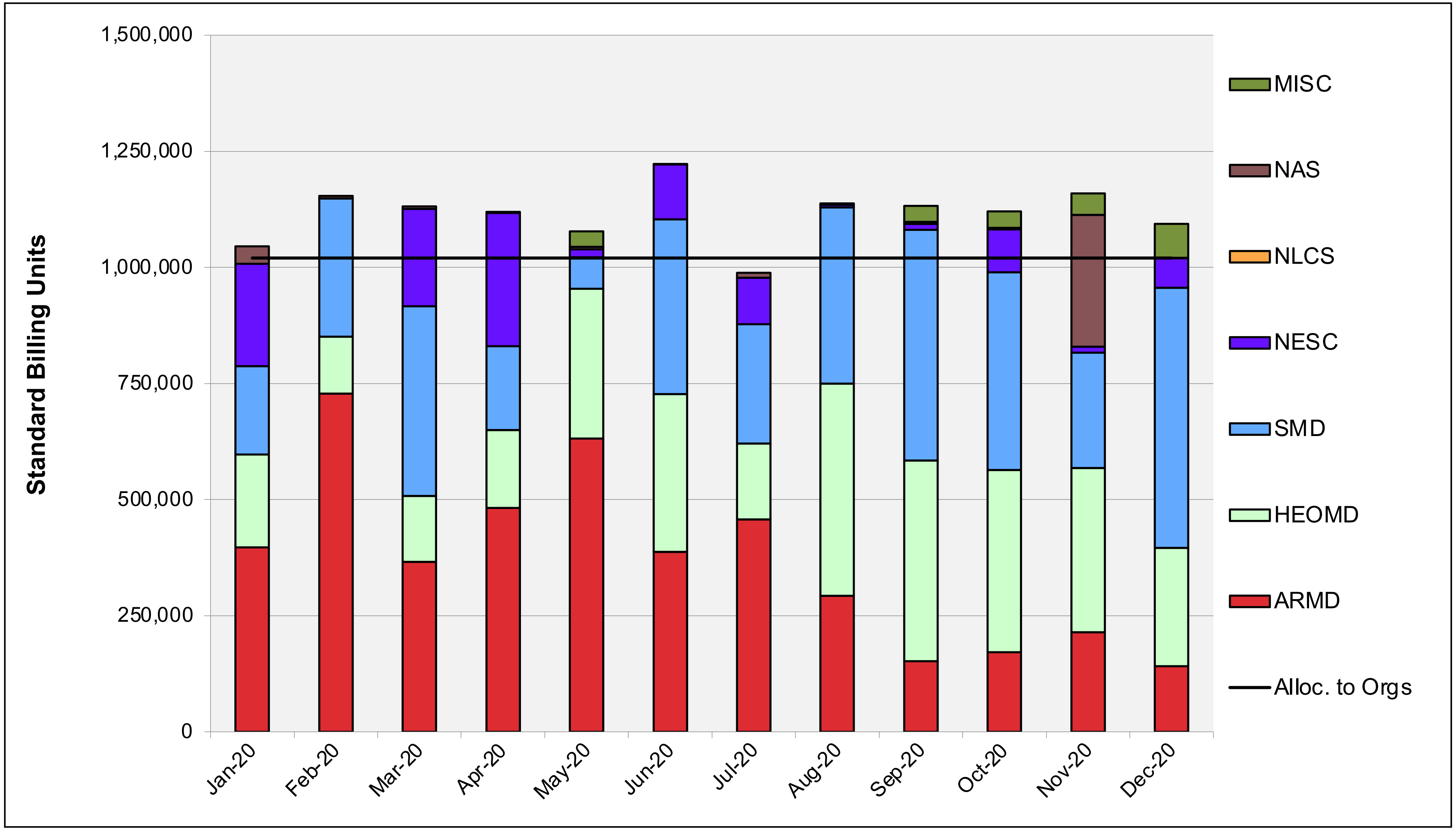
Pleiades: Average Time to Clear All Jobs



Pleiades: Average Expansion Factor



Aitken: SBUs Reported, Normalized to 30-Day Month



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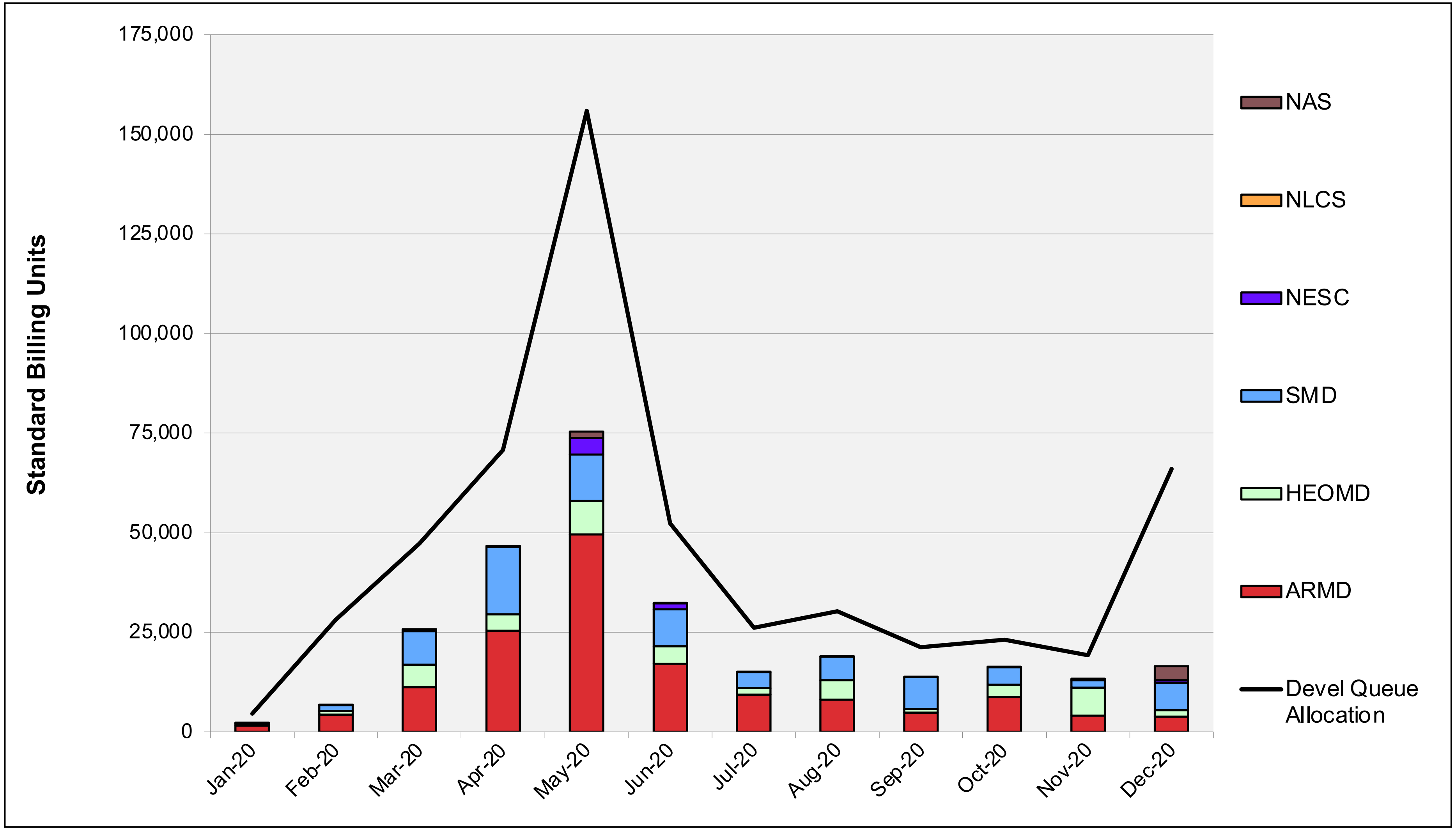
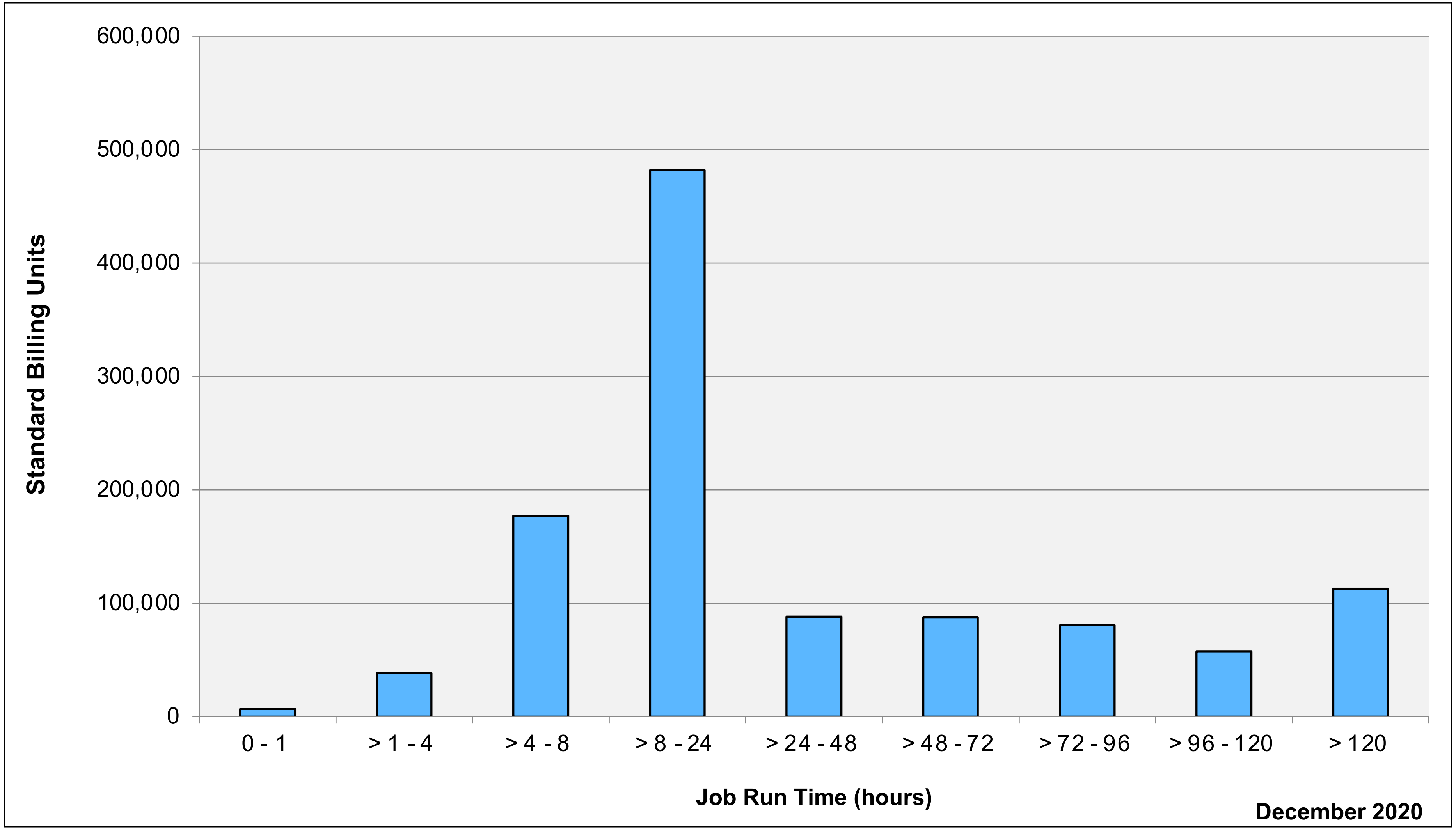


Aitken: Monthly Utilization by Job Length



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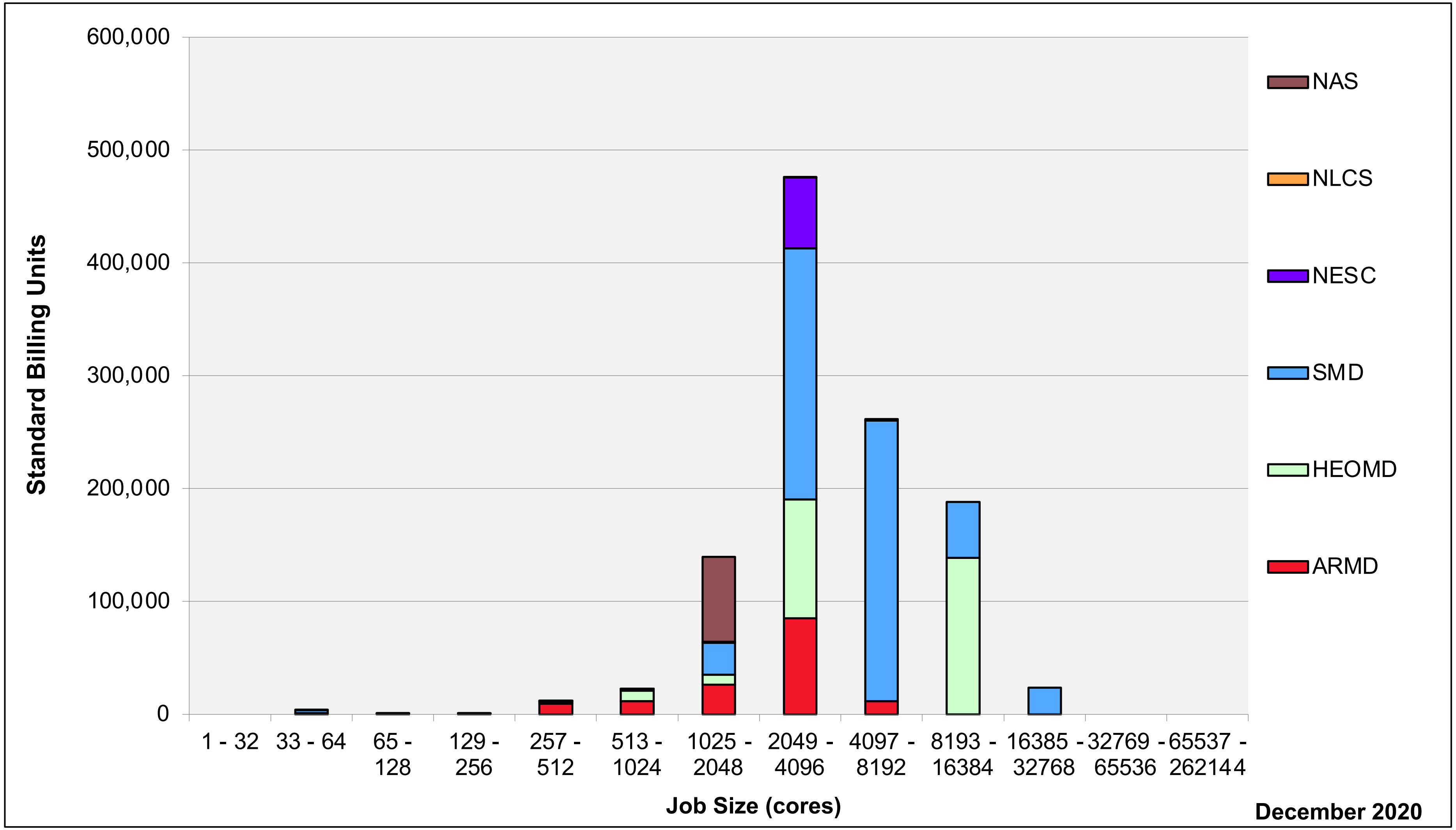
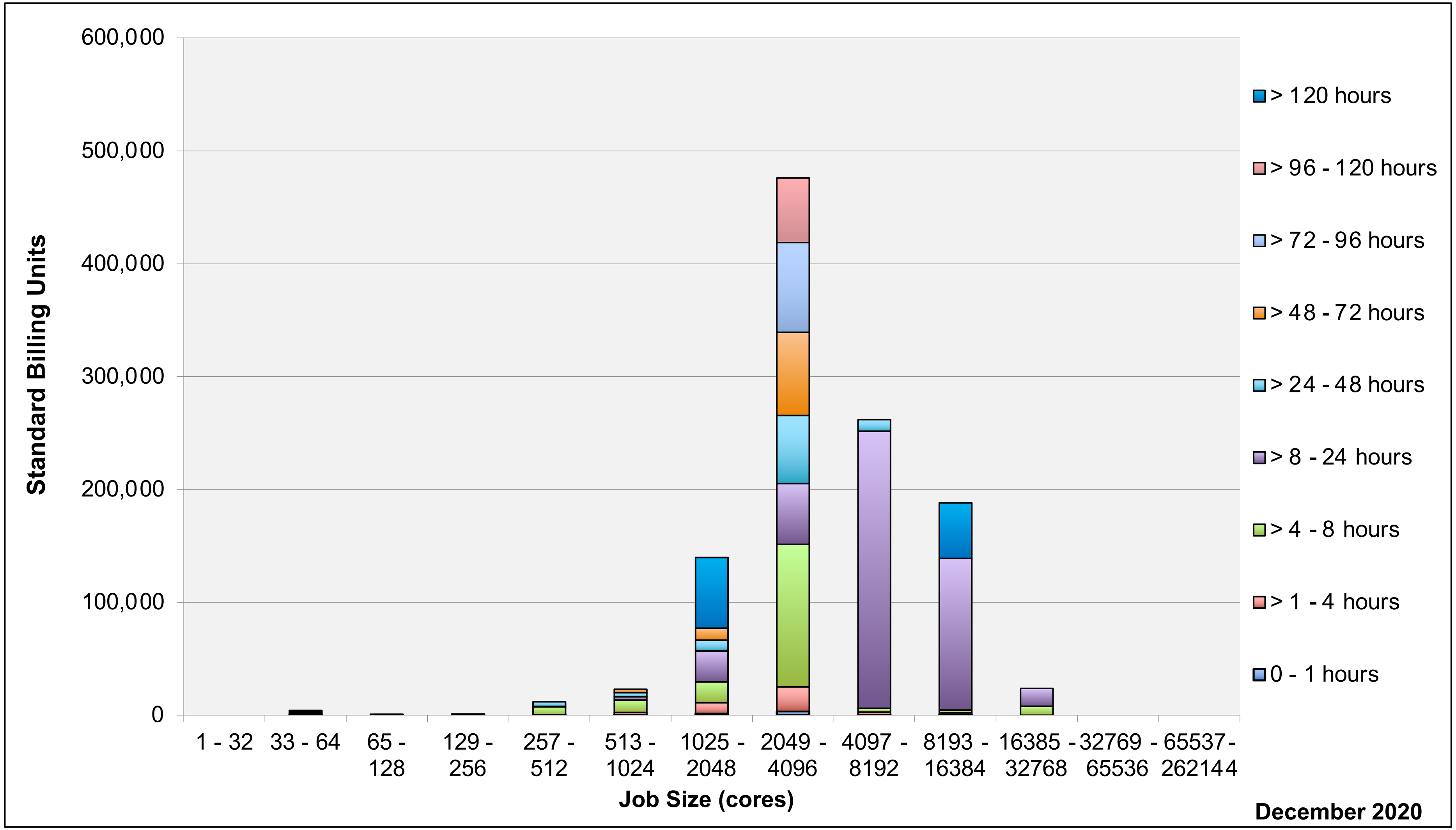
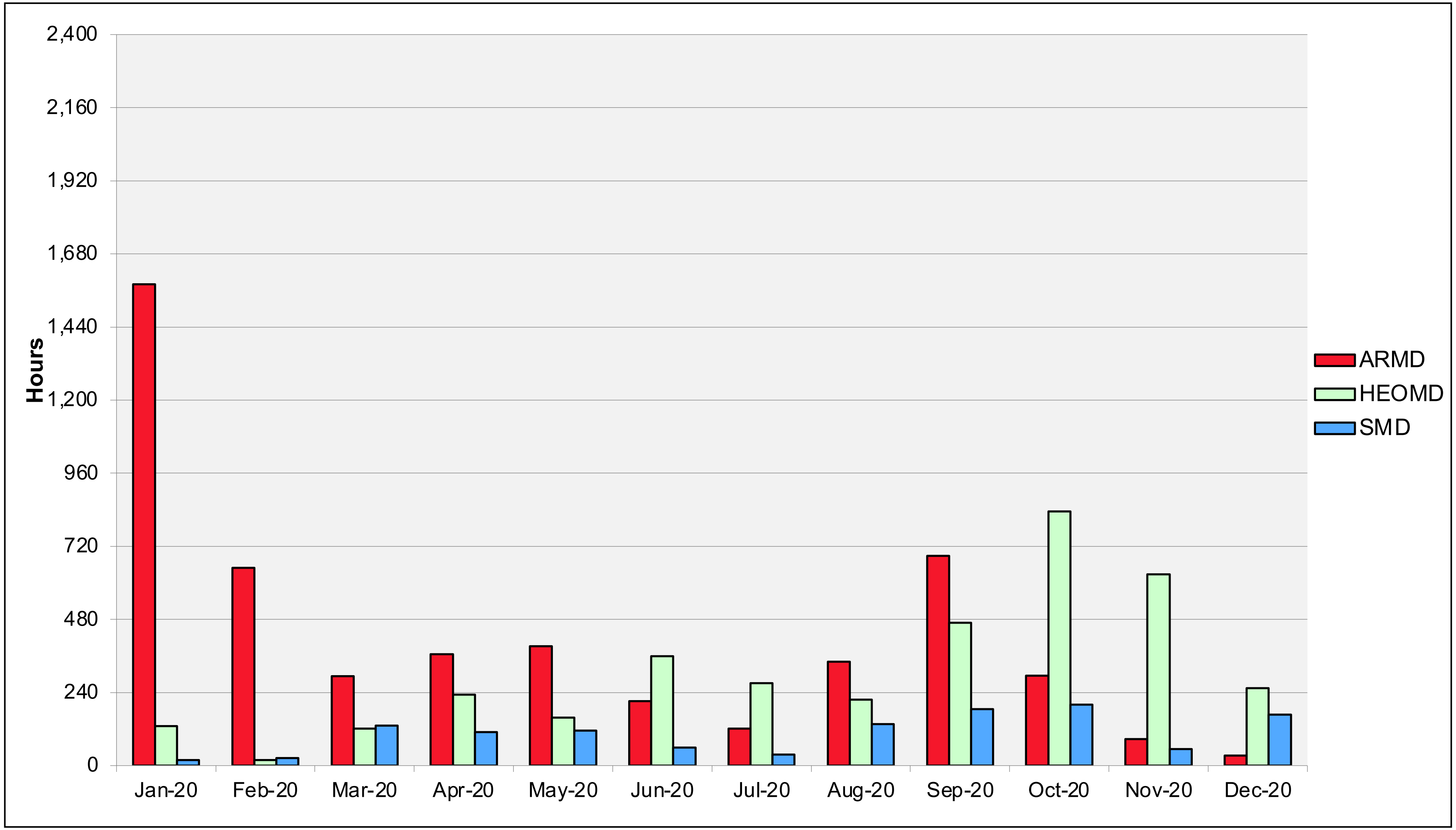


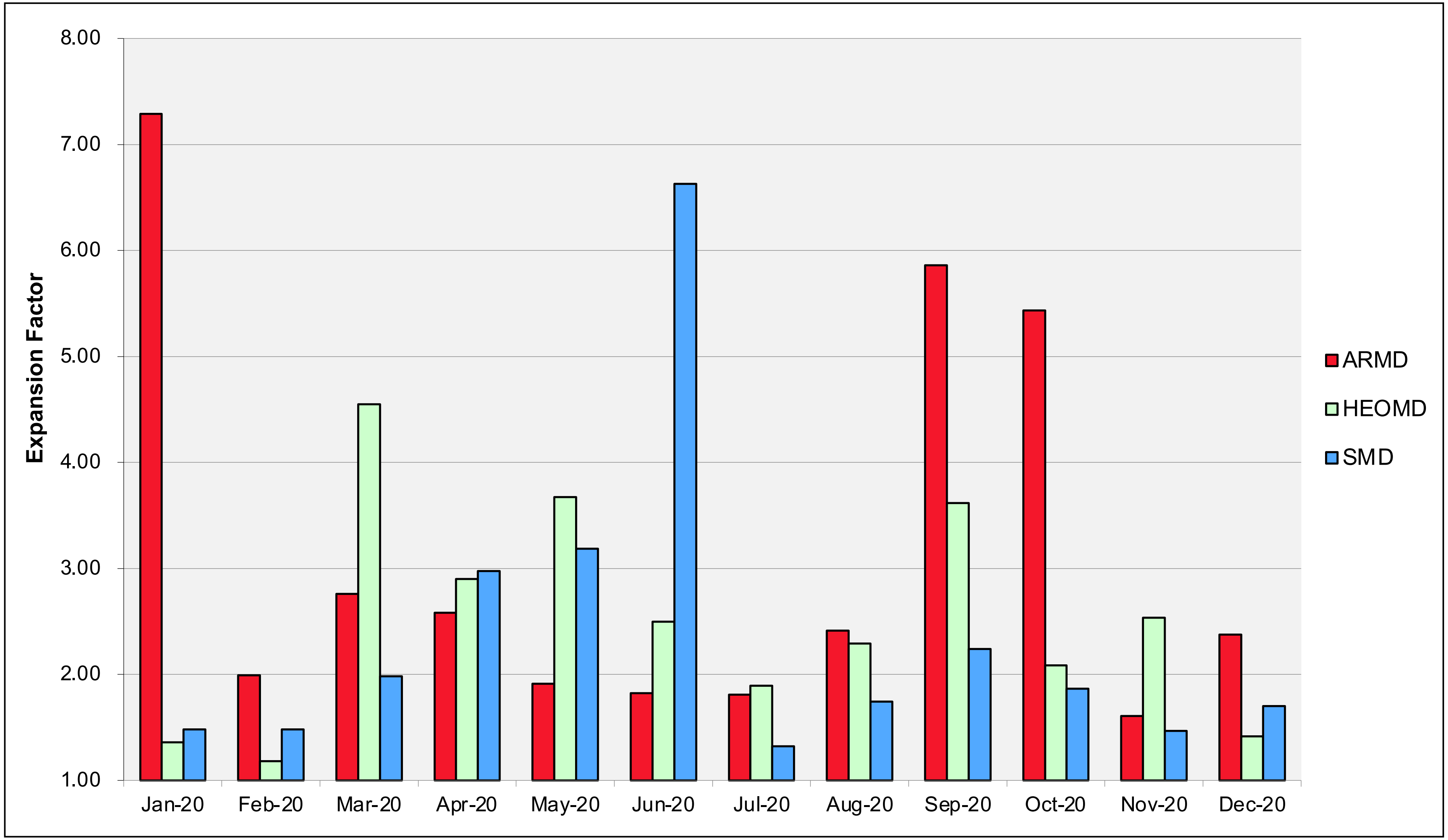
Aitken: Monthly Utilization by Size and Length



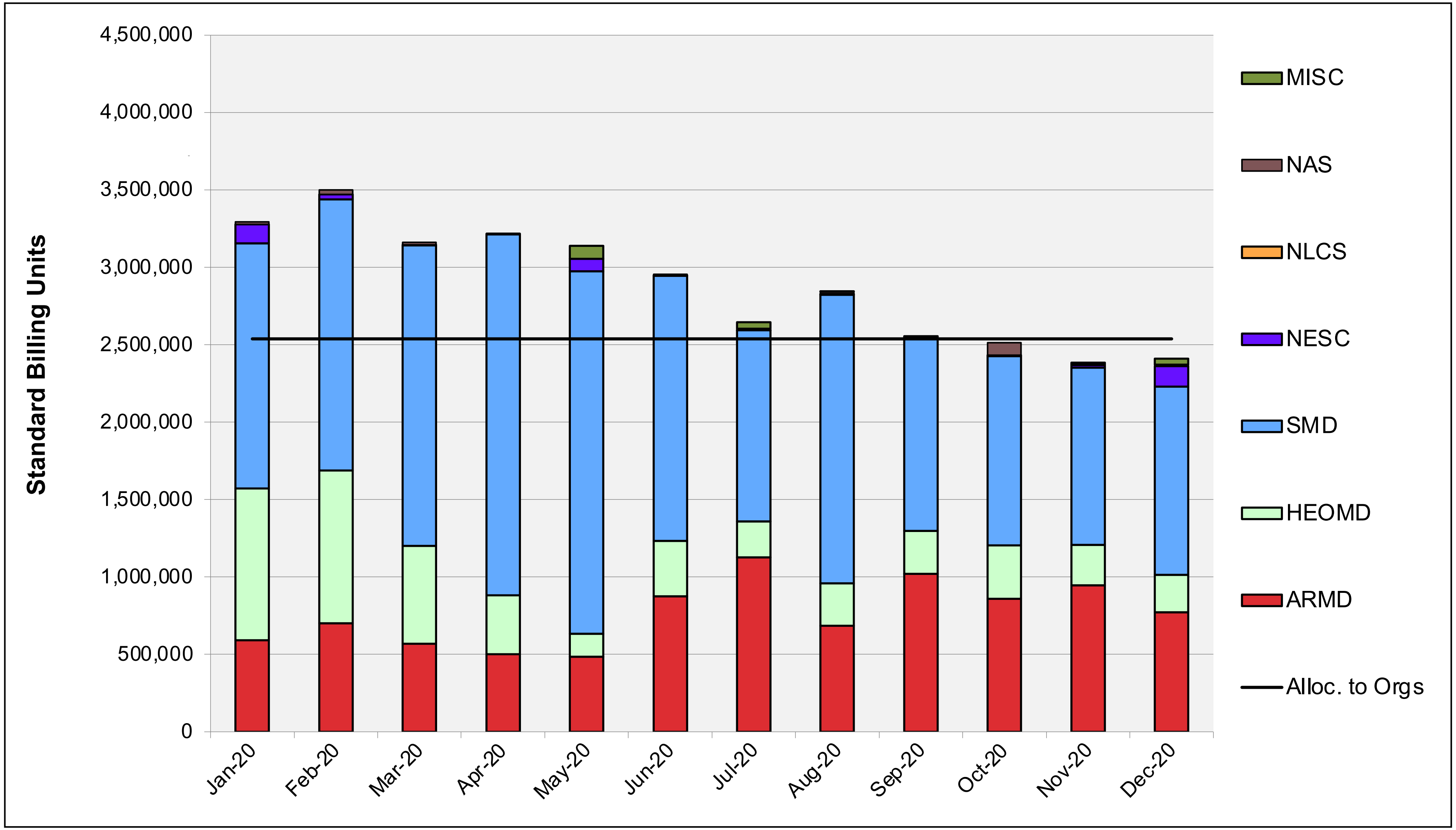
Aitken: Average Time to Clear All Jobs



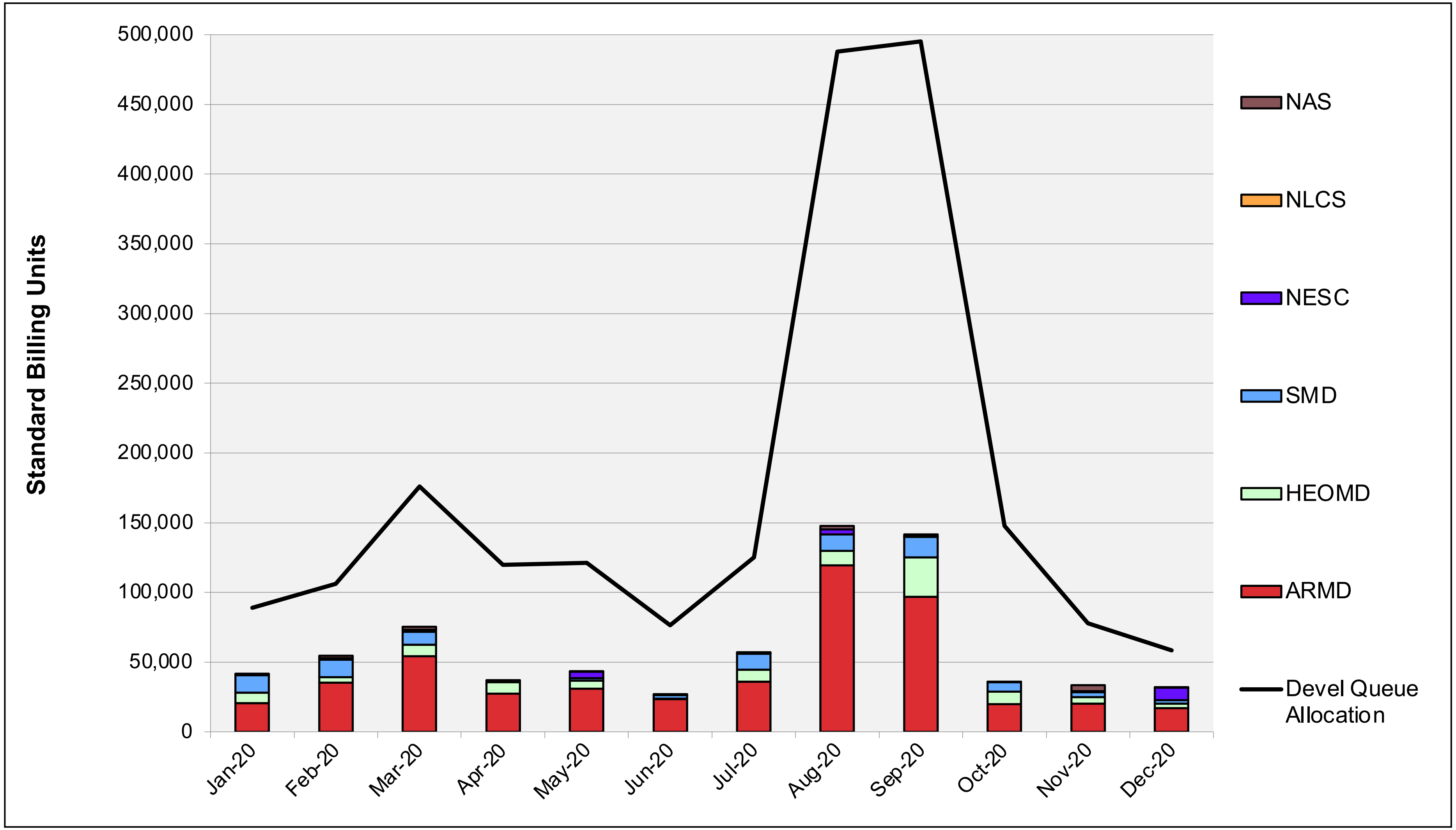
Aitken: Average Expansion Factor



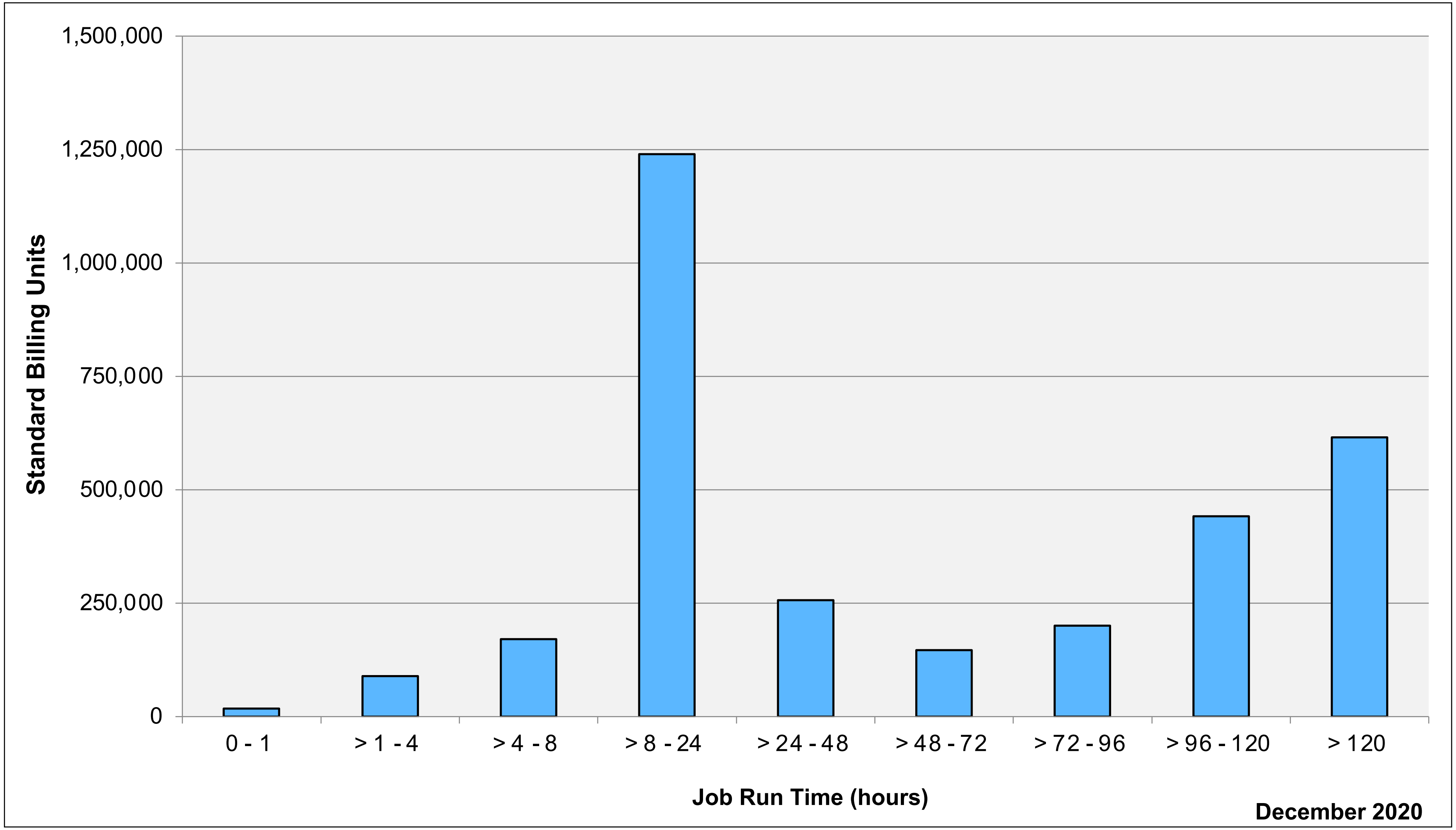
Electra: SBUs Reported, Normalized to 30-Day Month



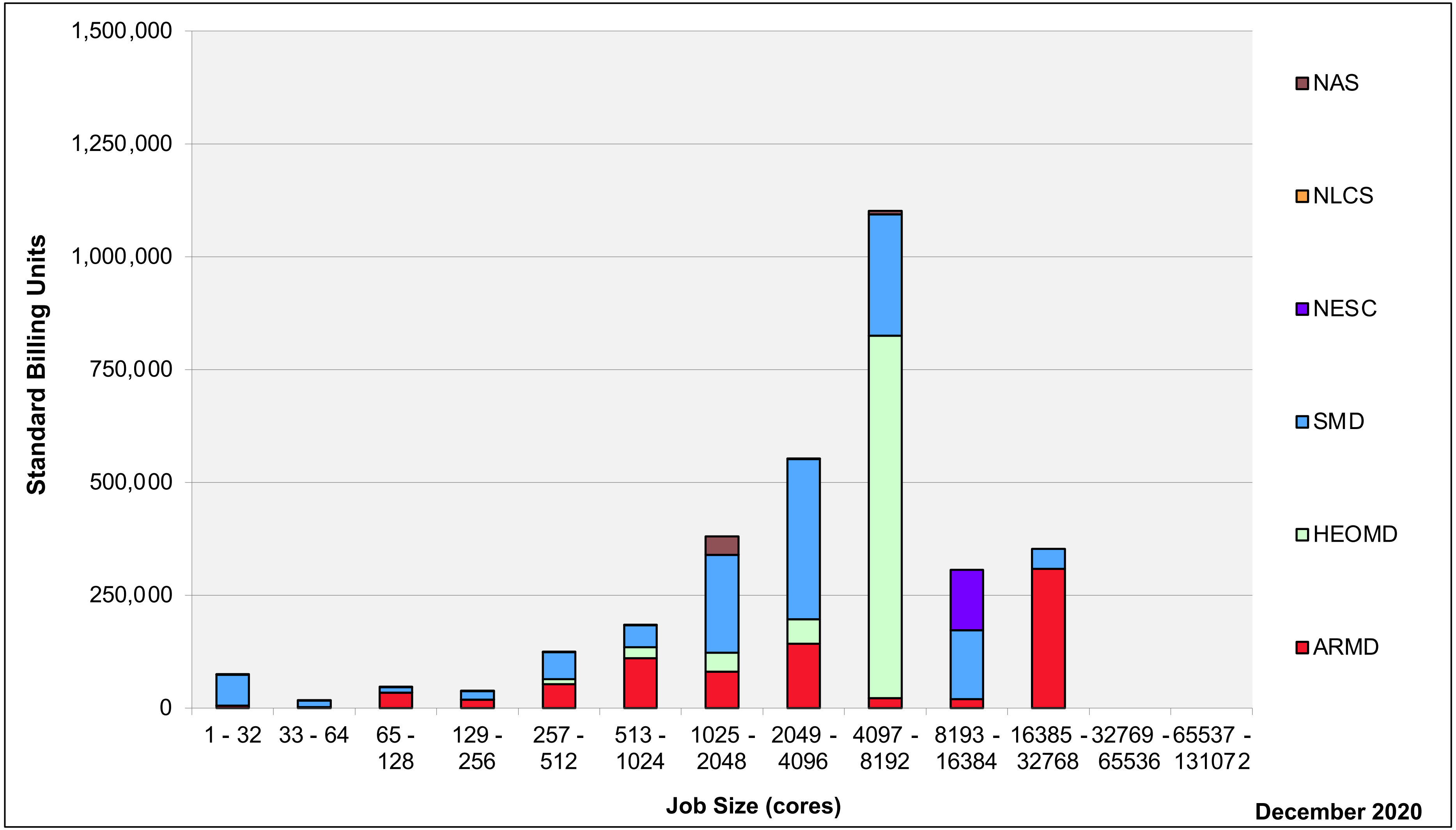
Electra: Devel Queue Utilization



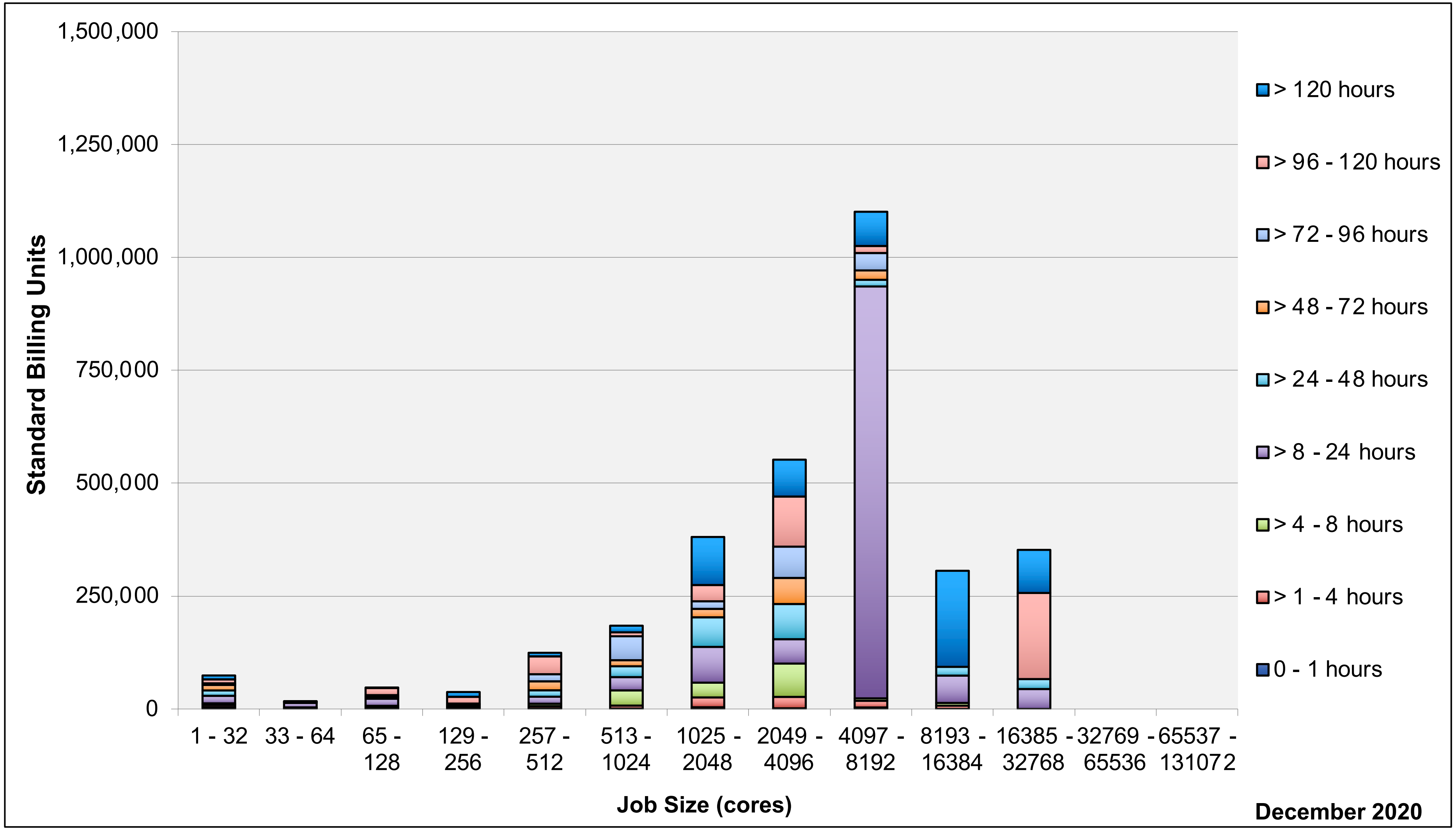
Electra: Monthly Utilization by Job Length



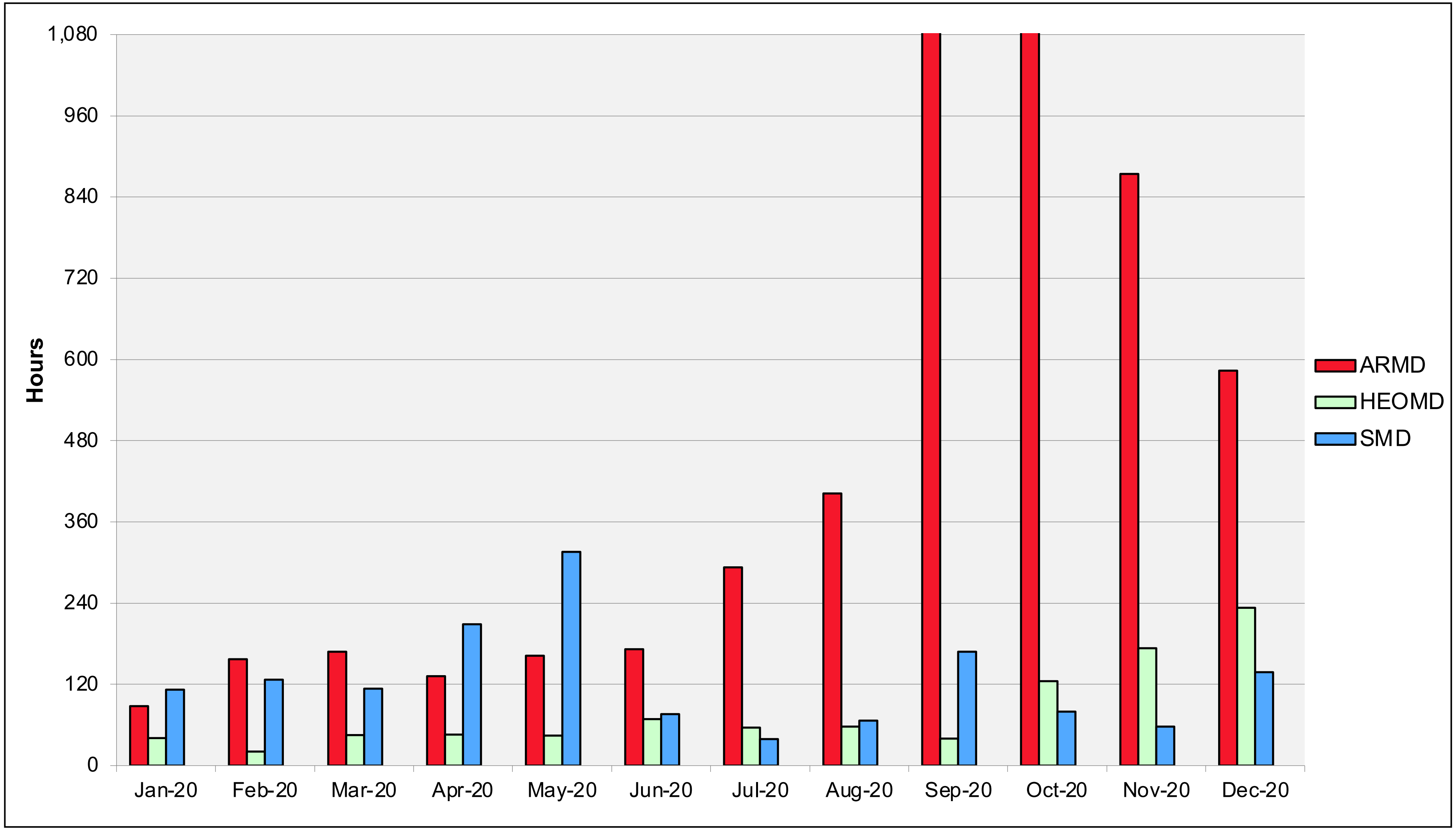
Electra: Monthly Utilization by Job Size



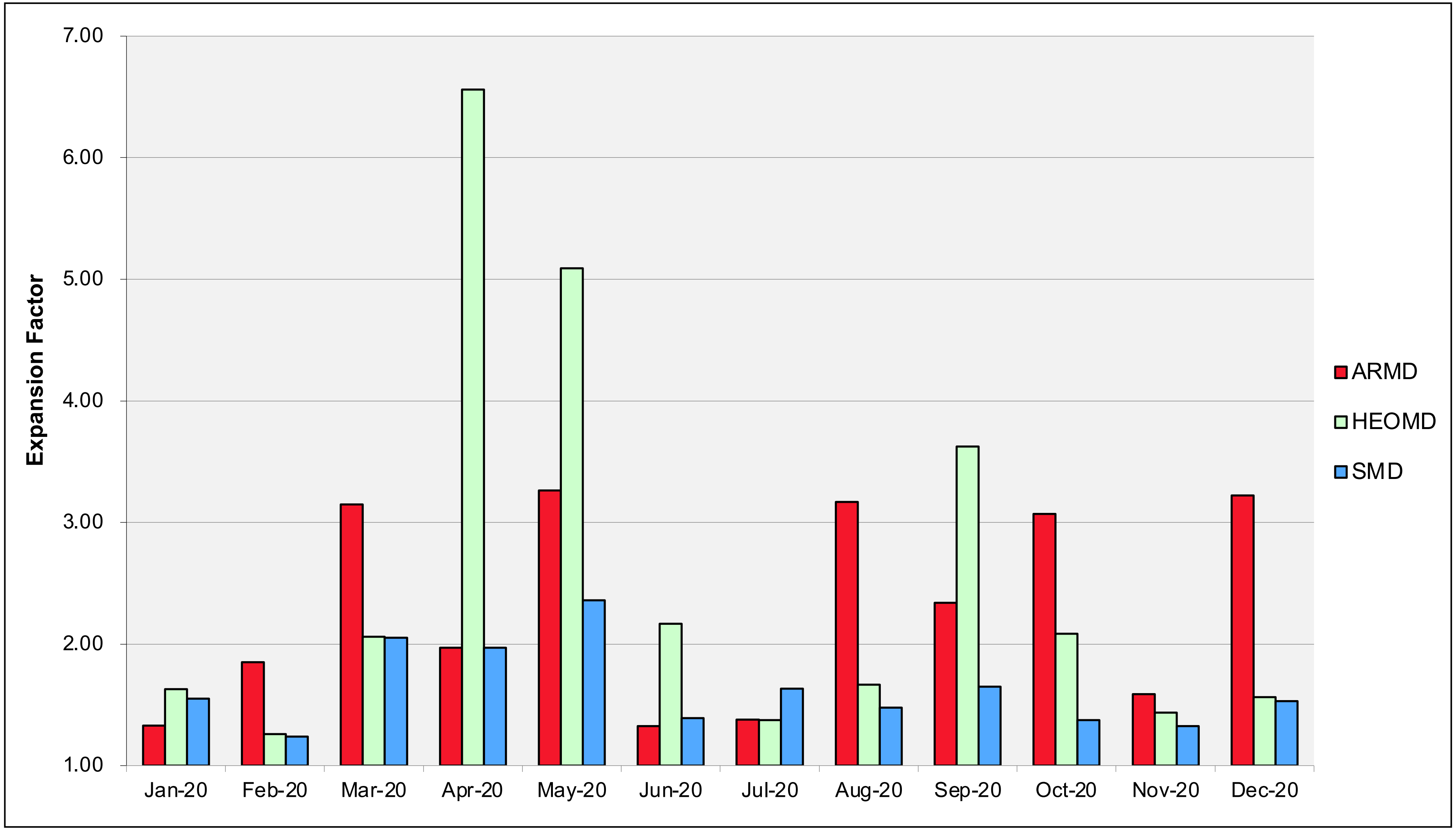
Electra: Monthly Utilization by Size and Length



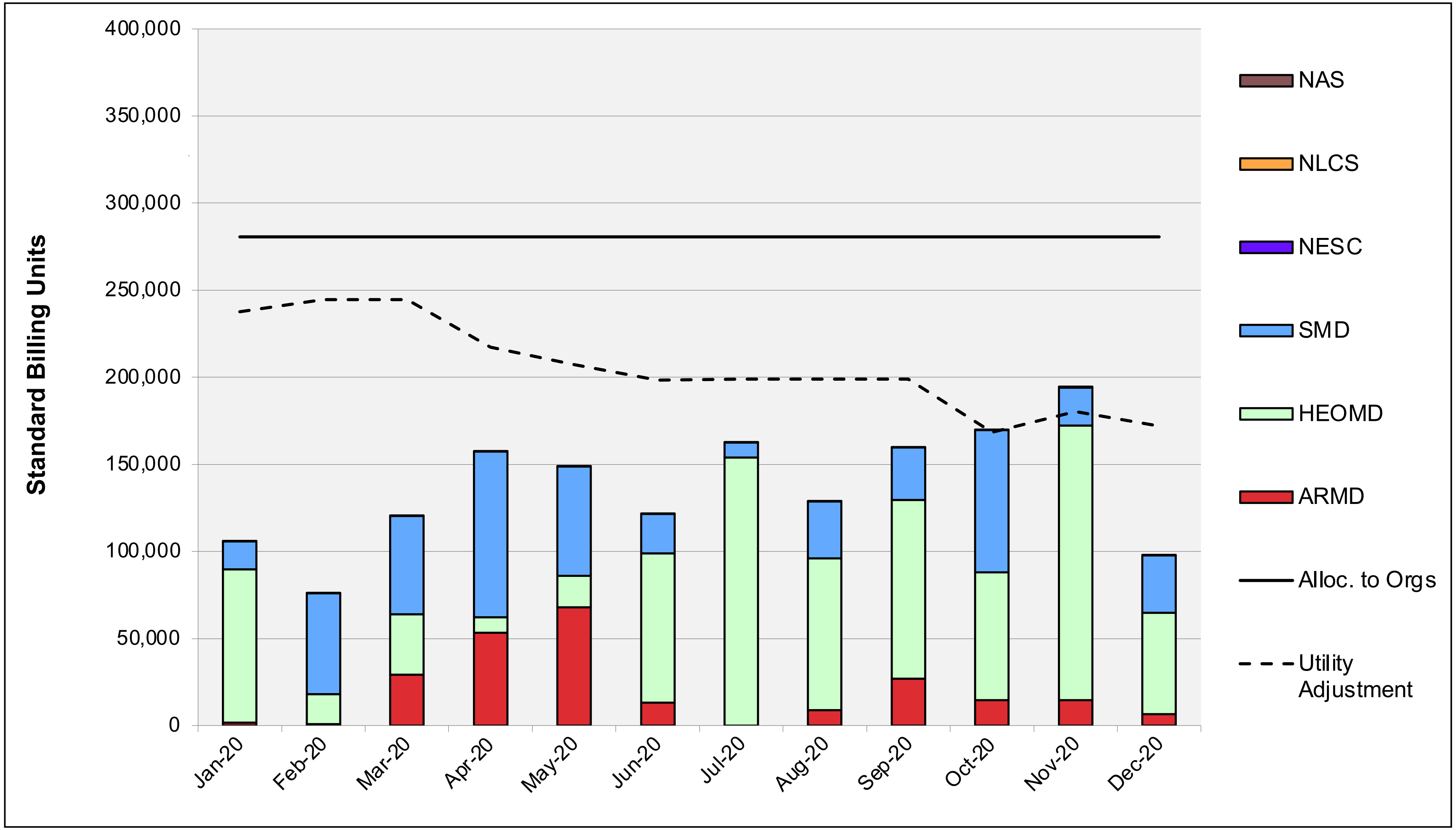
Electra: Average Time to Clear All Jobs



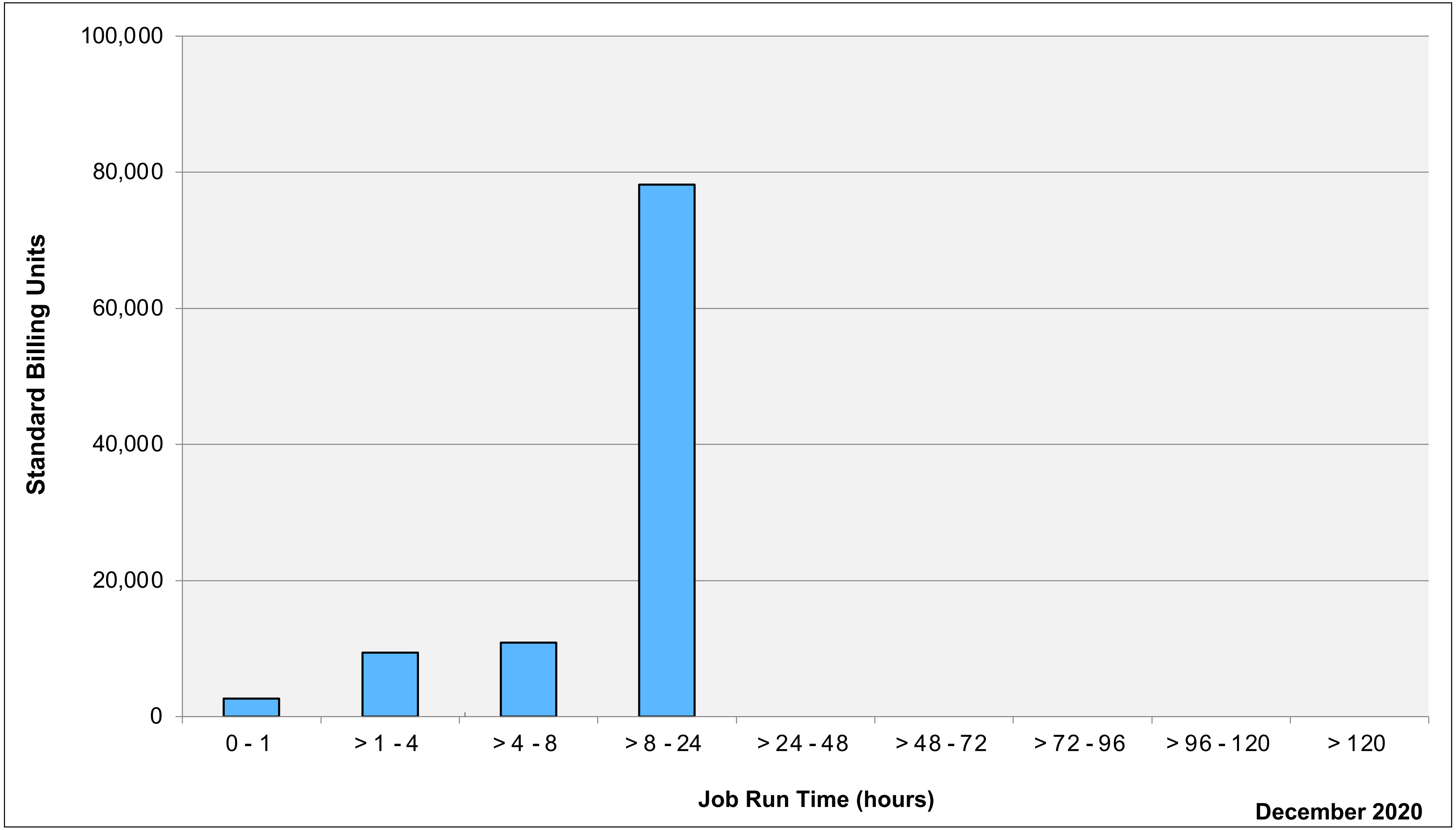
Electra: Average Expansion Factor



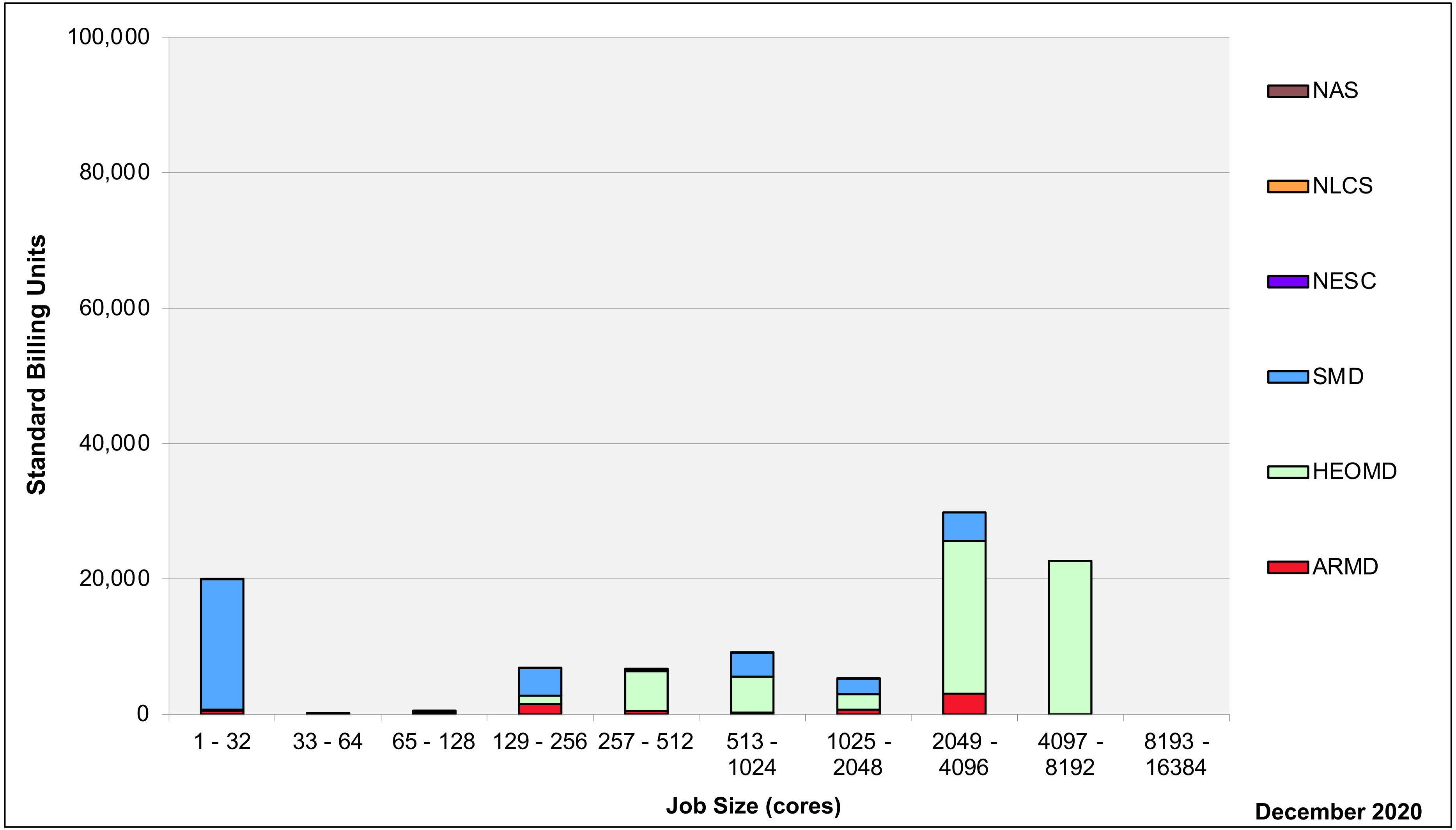
Merope: SBUs Reported, Normalized to 30-Day Month



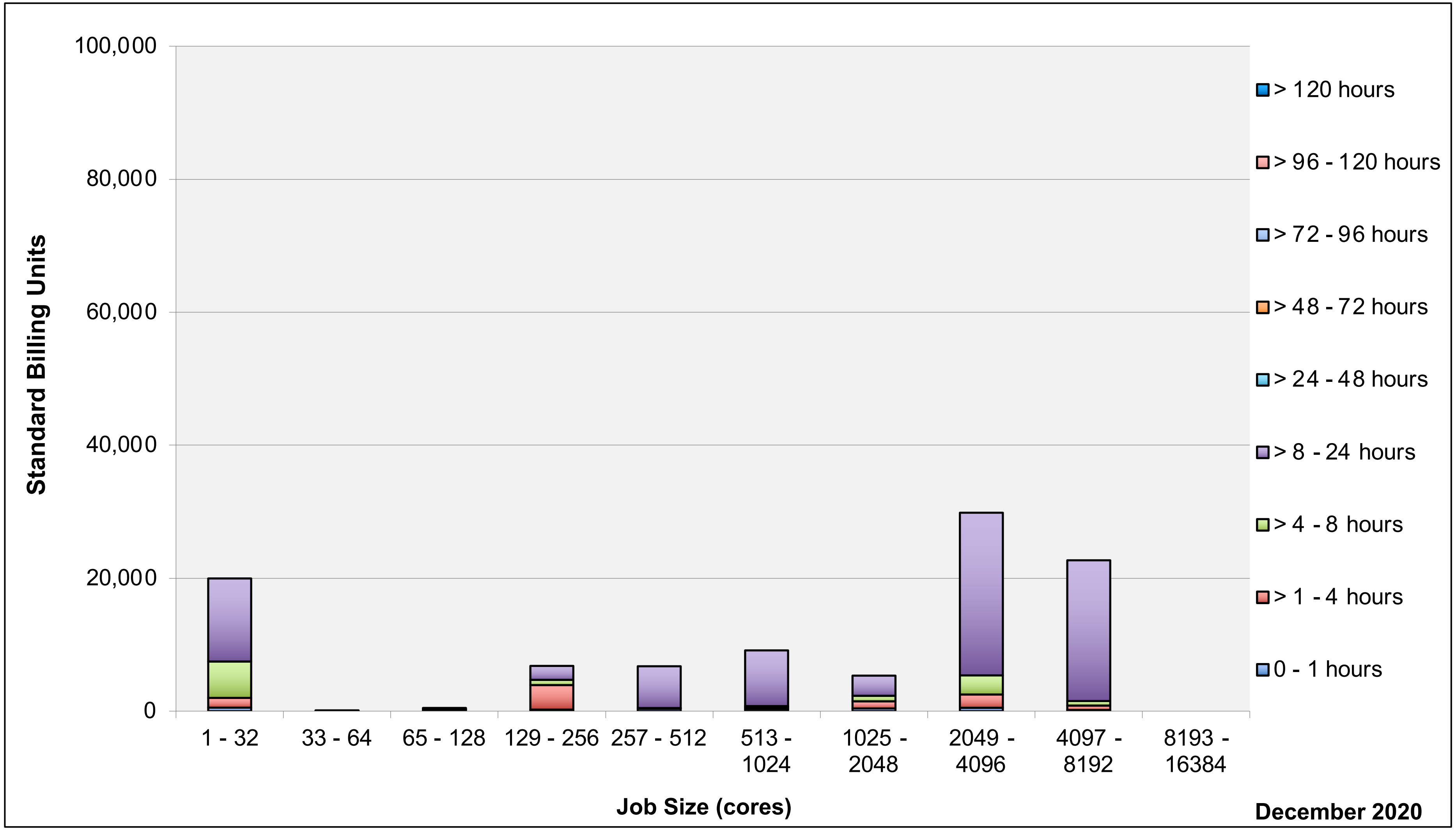
Merope: Monthly Utilization by Job Length



Merope: Monthly Utilization by Job Size



Merope: Monthly Utilization by Size and Length



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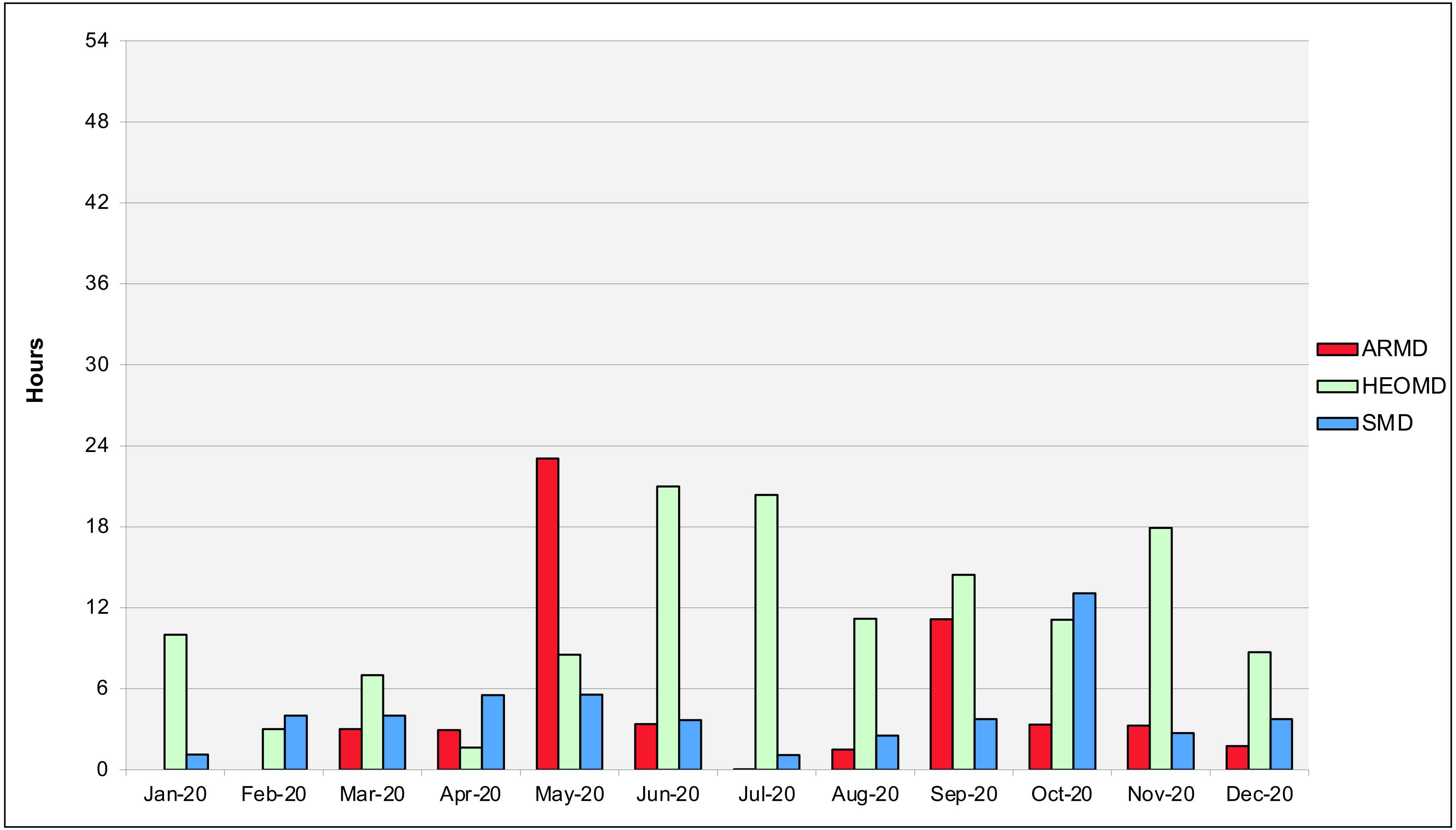

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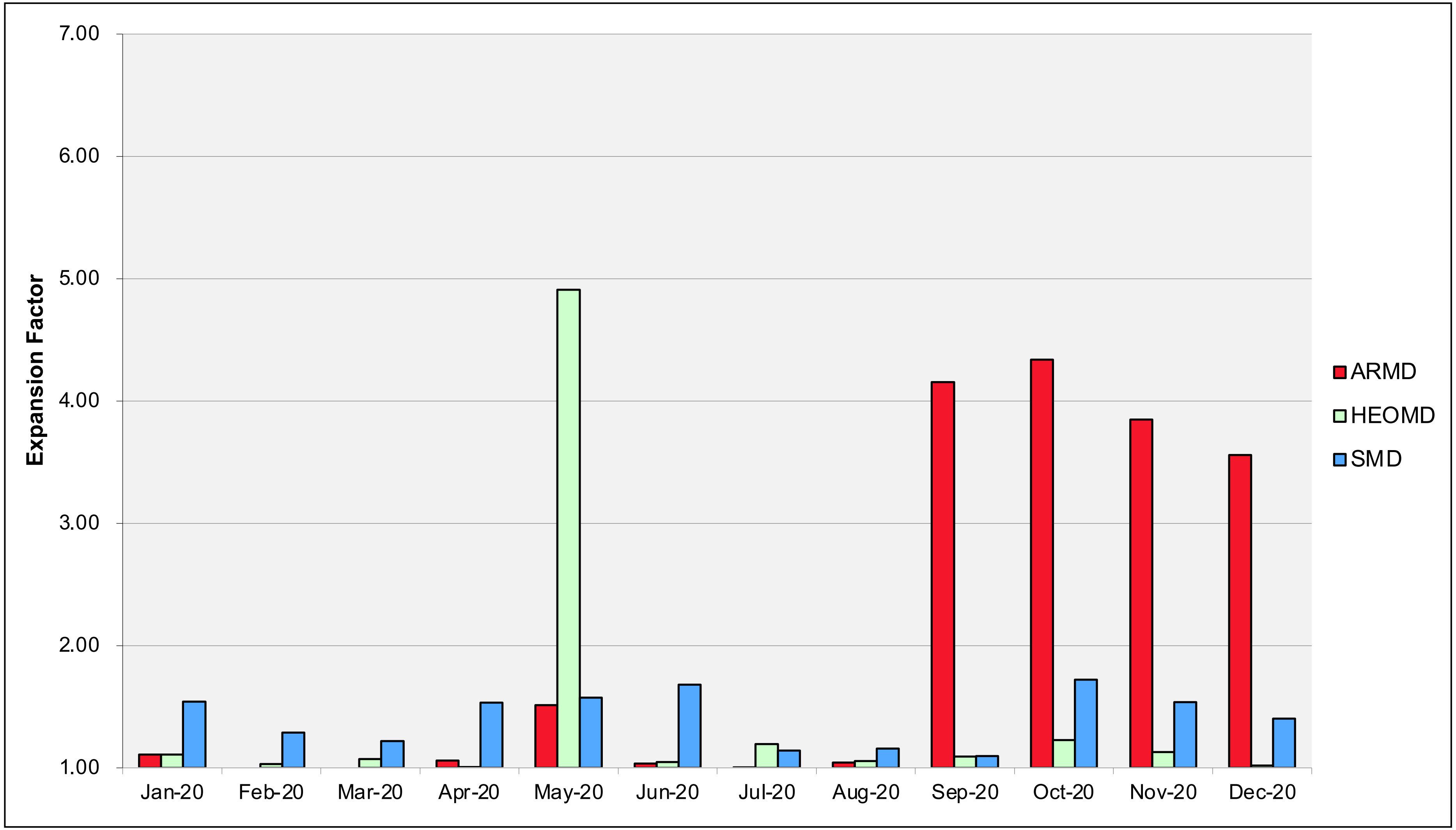
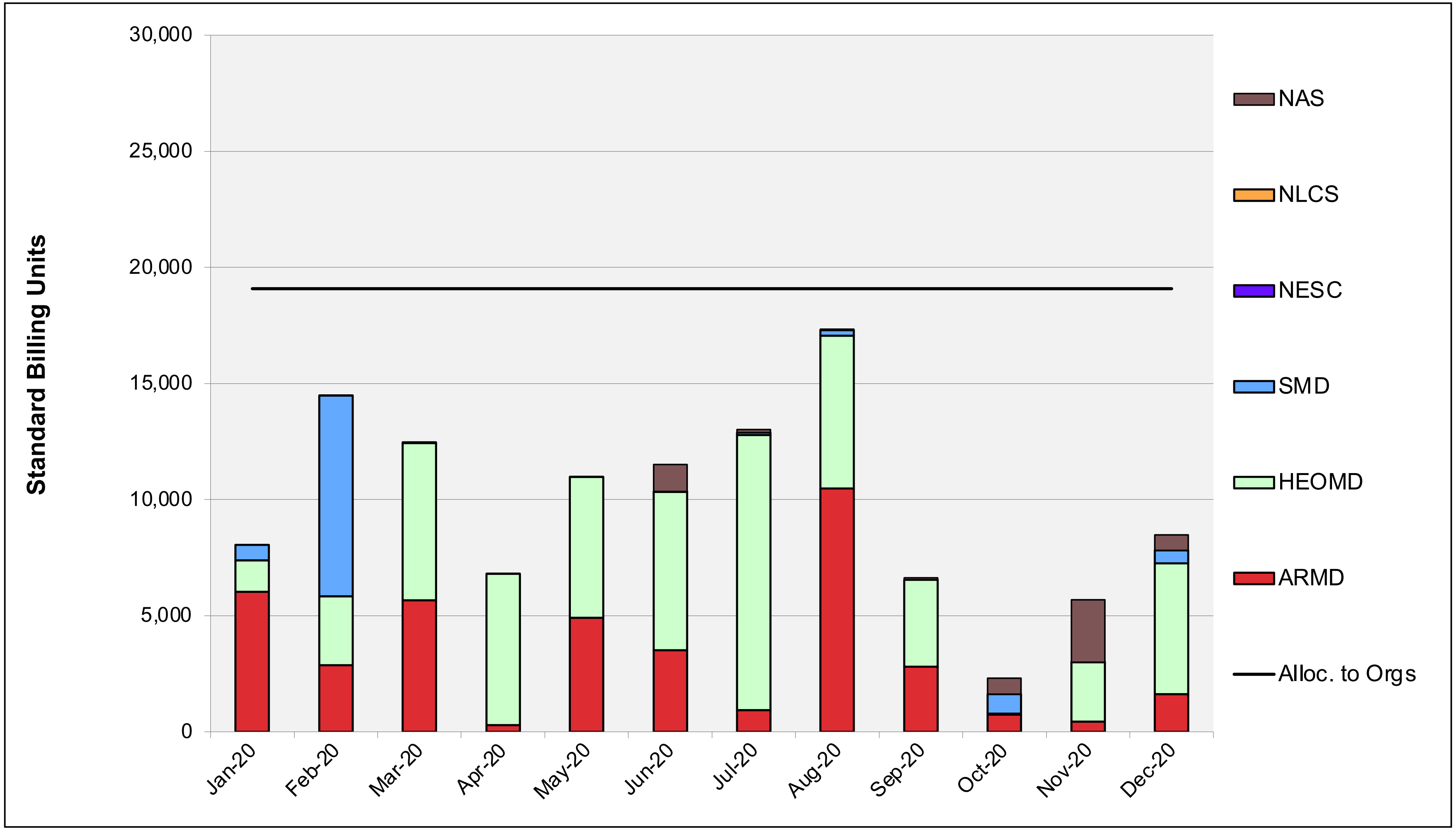
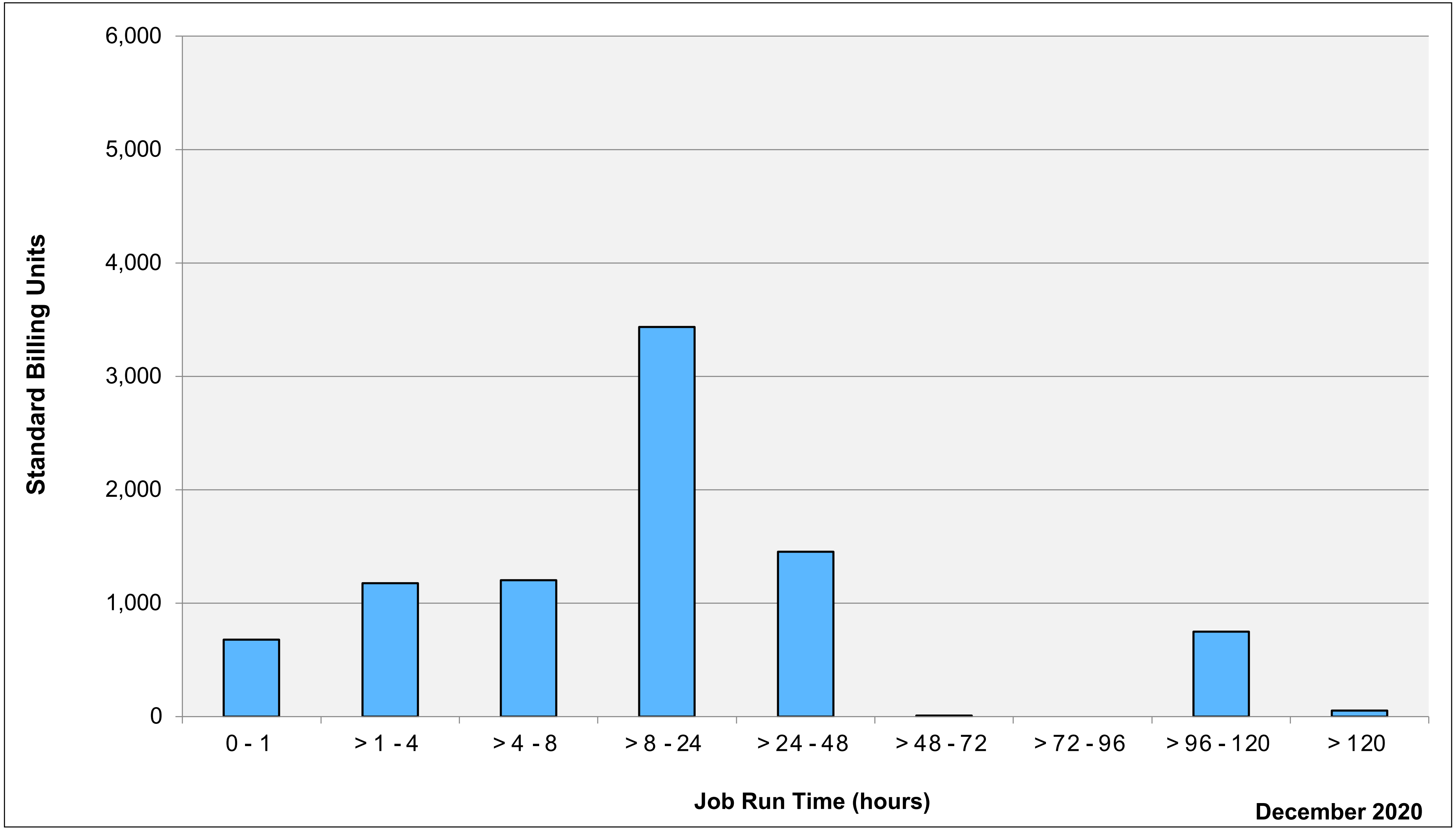


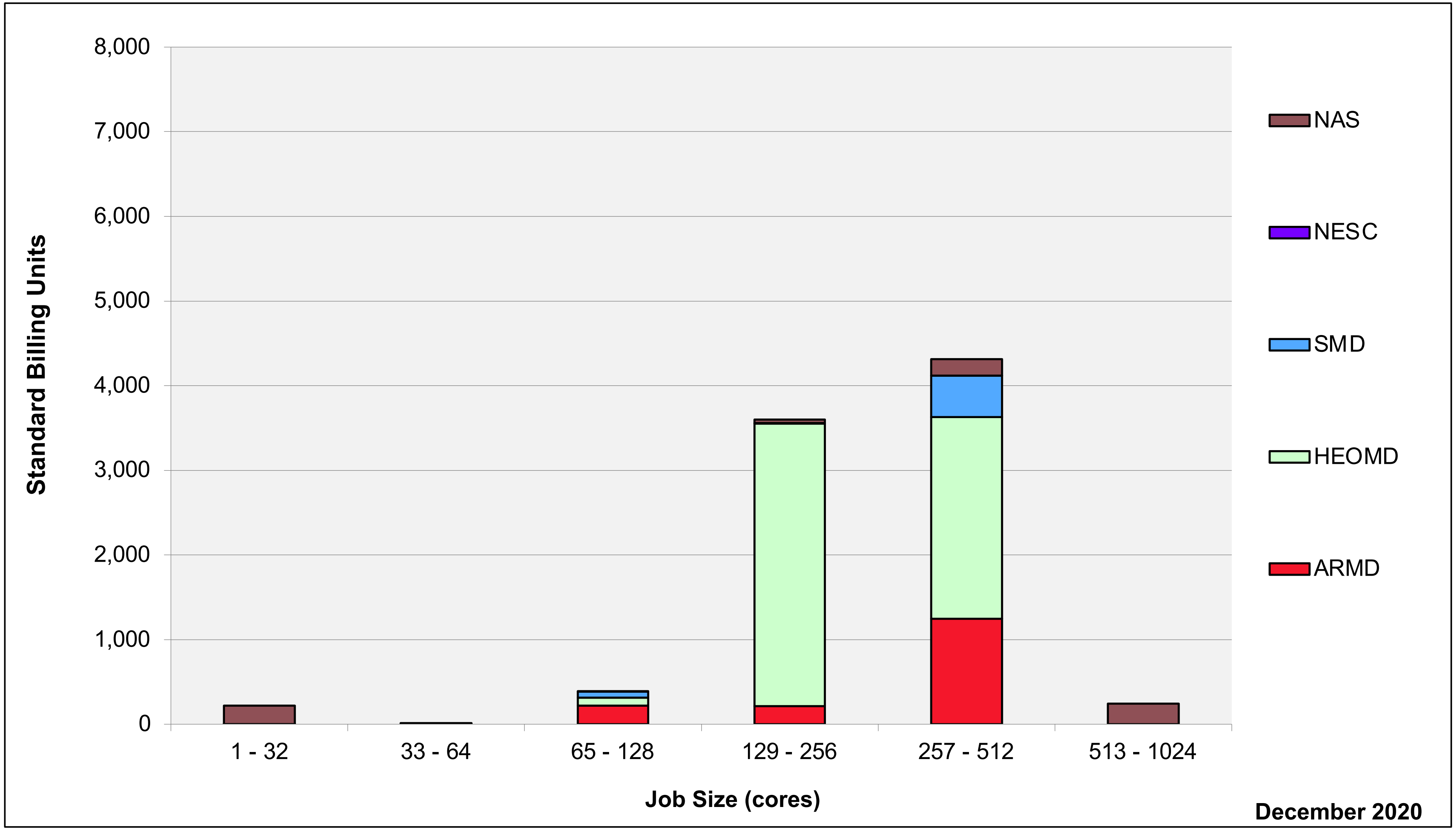
Endeavour: SBUs Reported, Normalized to 30-Day Month



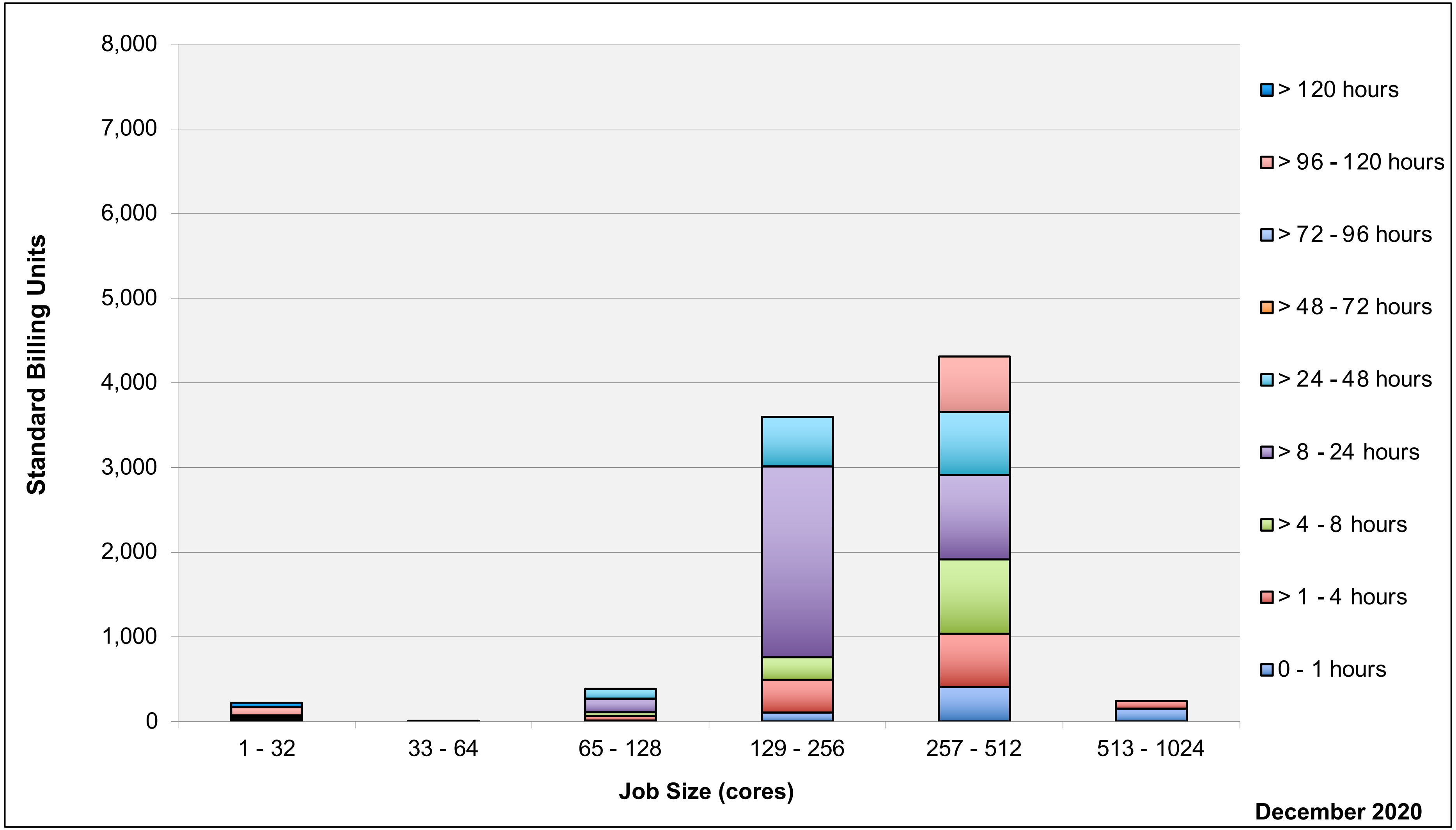
Endeavour: Monthly Utilization by Job Length



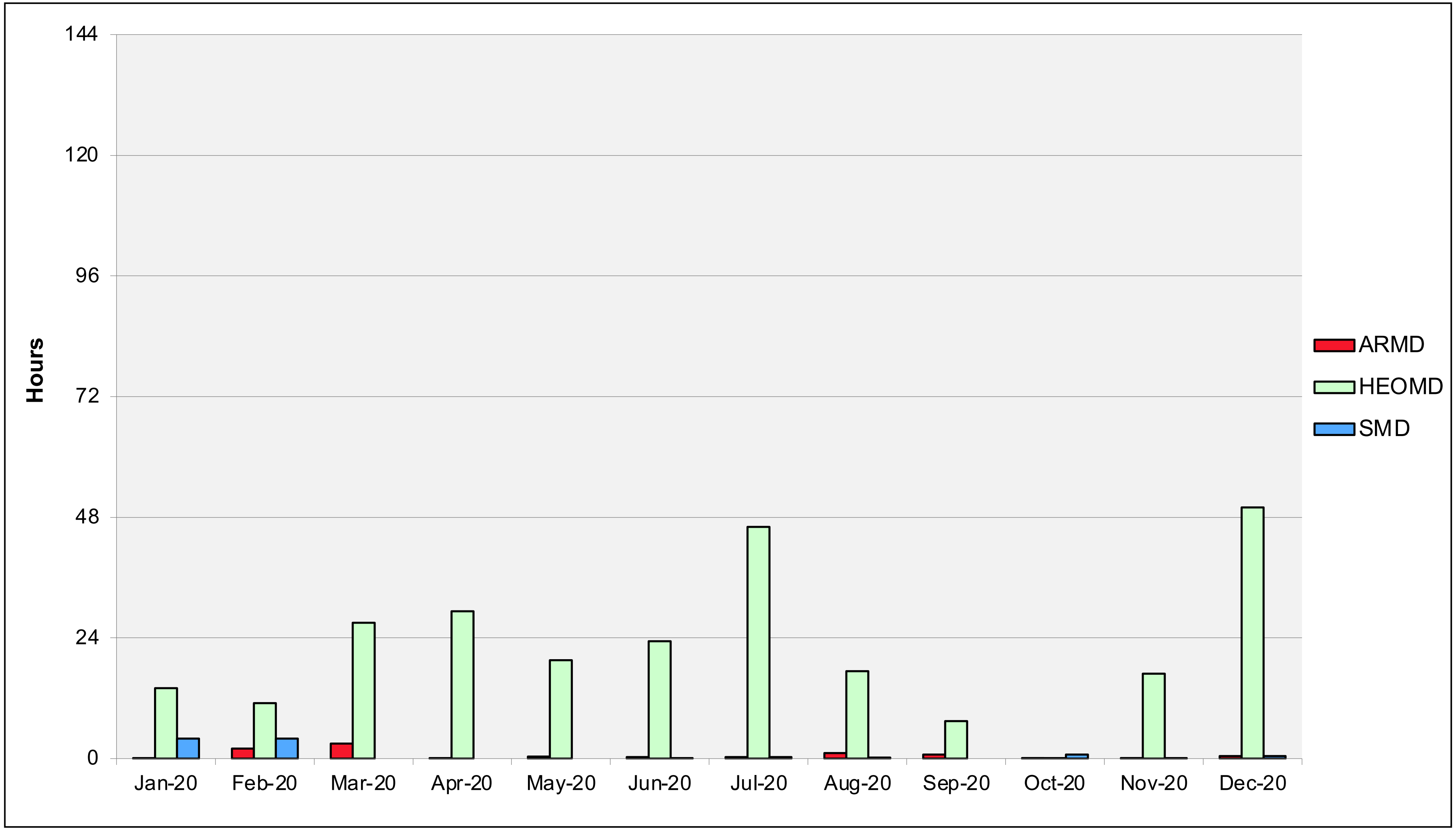
Endeavour: Monthly Utilization by Job Size



Endeavour: Monthly Utilization by Size and Length



Endeavour: Average Time to Clear All Jobs



Endeavour: Average Expansion Factor