National Aeronautics and
Space Administration

HIGH-END COMPUTING CAPABILITY PORTFOLIO

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Facility Mods for Incoming GPGPUs & hyperwall Complete

- Facility modifications were completed in Building N258 computer room in preparation for the delivery and installation of seven new general-purpose graphics processing units (GPGPUs) racks and nine new hyperwall racks.
  - Installed 32 new circuit breakers in the Power Distribution Unit (PDU) panelboards. To support higher power demands of the new GPGPU and hyperwall racks, installed new 60A 3-pole circuit breakers after removing existing 30A 2-pole breakers from the PDUs.
  - Connected 40 new electrical conduits (whips) to the PDU circuit breakers under the raised computer floor with the power receptacles placed underneath each targeted rack location. The whips are made of water-resistant, seal-tight steel conduit with four 6 American Wire Gauge (AWG) conductors terminating with a 60A IEC60309 receptacle.
- In addition, raised floor tiles were modified to accommodate the power drops from the racks, and perforated floor tiles were placed in front of each targeted rack location for cooling.
- The new GPGPU racks will provide HECC users with new technology resources to run their analyses, and the new hyperwall racks will allow for larger visualization problem sets.

IMPACT: GPGPUs are an emerging computer technology that the HECC program is making available to the user community. An updated hyperwall allows for larger, more comprehensive visualizations to improve users' ability to analyze their datasets.

Power Distribution Unit Panelboard in the NASA Advanced Supercomputing facility's main computer room, undergoing breaker and whip installation. *Chris Tanner, NASA/Ames*

APP Team Evaluates Potential Pathfinding Systems

- As part of investigations into pathfinding systems that might be suitable for future HECC procurements, the Applications Performance and Productivity (APP) team recently started evaluating the NEC SX Aurora TSUBASA, which uses a Vector Engine processor; and the Fujitsu PRIMEHPC FX700, which uses an A64FX ARM-based processor.
  - Both systems use high-bandwidth memory (called HBM2), which may address the very common memory-bandwidth performance bottlenecks seen in NASA's high-end computing applications.
  - Because work-from-home status precluded locating the test system at NASA, Supersmith, a subcontractor on the NASA Advanced Supercomputing Services contract, hosted the NEC test in their facility. The FX700 was located at Fujitsu in Sunnyvale, CA.
- The goal of the evaluations is to determine whether further testing of the systems is warranted. In both cases, the performance results are encouraging, with some benchmarks exceeding performance seen on HECC's newest Intel Xeon-based systems.
- The next step is to factor those results into HECC's FY21 plan for pathfinding activities, including potential acquisition of a small test system for each architecture to conduct in-depth analysis.

IMPACT: Identifying the most cost-effective computing resources for NASA's high-performance computing requirements ensures that HECC maximizes the science and engineering impact of its procurement budget.

Test node containing two NEC SX-Aurora TSUBASA Vector Engine cards, each capable of 2.15 $\times$ 10^{12} double-precision floating point operations per second. *Dave Barker, Supersmith*

APP Team Responds to Shelter-in-Place Restrictions

- Like most NASA staff, HECC's Application Performance and Productivity team (APP) has been subject to Shelter-in-Place (SIP) restrictions since March 9 but continue helping users who are themselves working from home.
- In many respects, work is unchanged from the period before SIP started.
  - The team has handled 366 user trouble tickets since SIP started, compared to 300 in the same period during 2019. User requests for help and APP responses currently all happen via email. Previously, a small number of users also got help by calling in or visiting a staff member.
  - The team continues to proactively identify users with performance issues and contact them with offers to help. For example, since SIP started there have been three cases where the team helped users improve resource utilization after being identified in the weekly load imbalance report.
  - The team also continues its longer-term performance analysis and optimization efforts. One current project is for the Geostationary Carbon Observatory (GeoCarb) mission to map key carbon gases from geostationary orbit.
- In new work, the team supports three projects using HECC resources for COVID-19 HPC Consortium research—for example, in porting and tuning their codes.
- The most noticeable change since SIP started is an increase in requests for help with Virtual Network Computing (VNC), which provides a low-latency way for users to run sessions on HECC front-end machines from remote computers. VNC help requests now average about 17 per month, up from 1–2 per month before SIP.

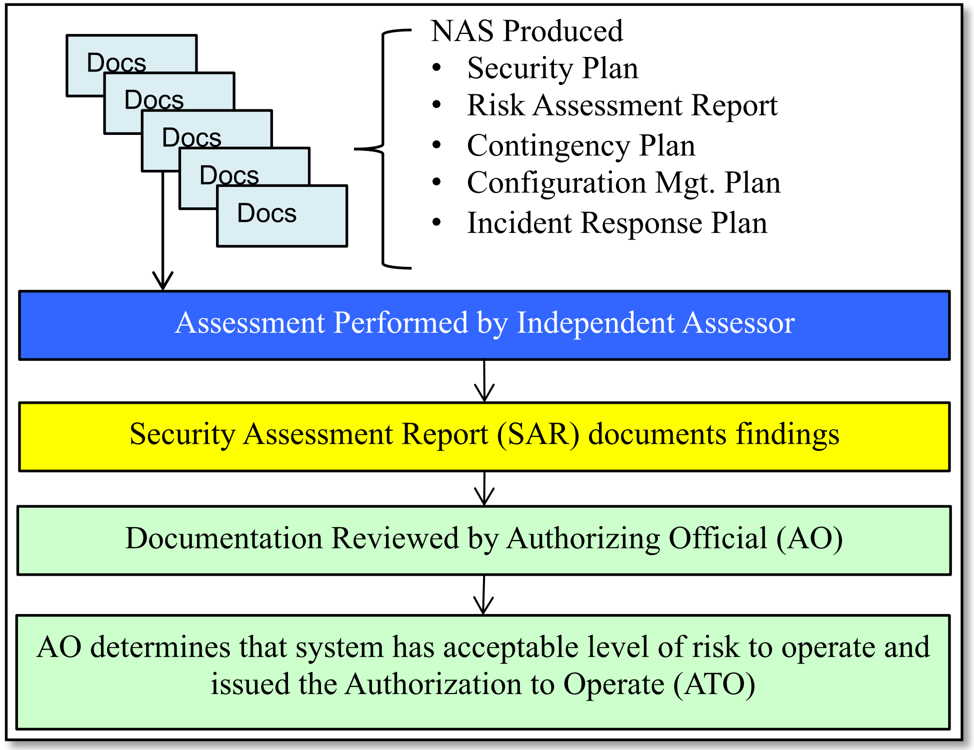
IMPACT: HECC's application services experts enable researchers to better utilize NASA's supercomputing resources for their modeling and simulation projects, supporting the agency's mission goals.

HECC's Application Performance and Productivity team provides a variety of services aimed at maximizing users' allocations on the supercomputing resources. Services include helping with application issues, code optimization, system benchmarking, and tool development.

Authorization to Operate Approved

- The HECC Security team successfully submitted NAS's security plan for 2020 to the NASA Ames Deputy Center Director, who is the authorizing official (AO) for the security plan that includes the HECC systems. The AO indicated that the security plan is acceptable, and the Authorization to Operate (ATO) for all NAS facility systems was awarded on July 7, 2020.
- The approved ATO is the final step in the annual security assessment required of all NASA systems.
- The annual assessment must be conducted by an independent assessor who evaluates the compliance of the facilities, systems, and operations under the NAS security plan that covers the NAS Division systems, including HECC systems.
- The ATO ensures the continued operation of HECC systems, in compliance with NASA security requirements.

IMPACT: The Authorization to Operate allows HECC supercomputers and support systems to continue to provide supercomputing resource to NASA missions, programs, and projects.

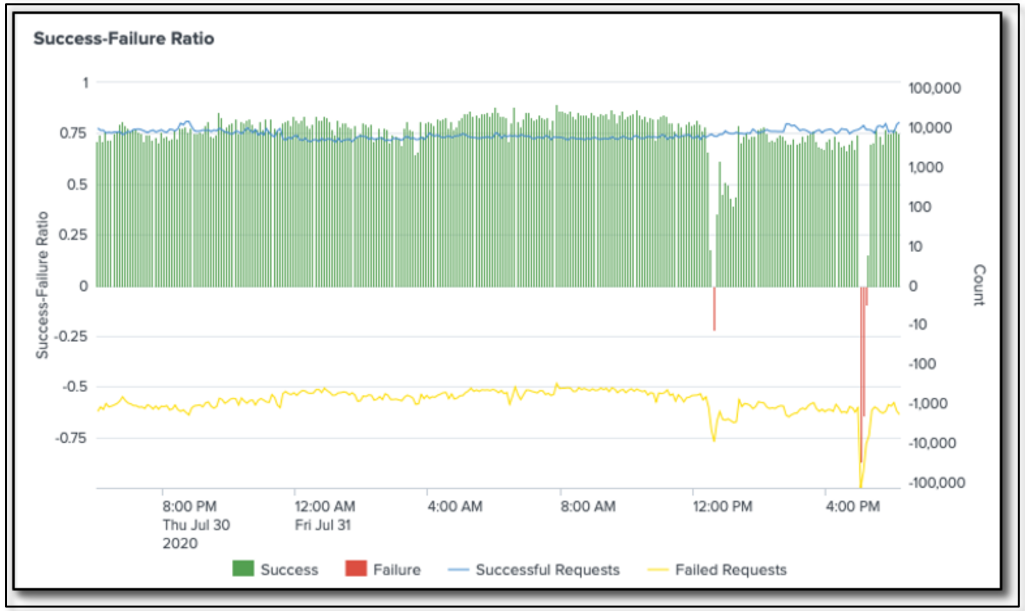


Flow chart outlining the evaluation and approval process leading to receiving an Authorization to Operate (ATO).

New Web Server Activity Analysis Capability Improves HECC Security Monitoring System

- HECC security experts added a new Success-Failure Ratio (SFR) to the HECC security monitoring systems to monitor and analyze web server activity.
- SFR analysis helps to identify suspicious connections to web servers, as well as potential server issues. The SFR value is calculated using the following formula:
  - $\mathrm{SFR} = \frac{\mathrm{Success} - \mathrm{Failure}}{\mathrm{Success} + \mathrm{Failure}}$
  - Success is the number of successful client requests.
  - Failure is the number of failed client requests.
- A positive SFR value from 0 to 1 indicates more requests to the web server are succeeding than failing.
  - The higher the value, the more requests succeeding.
- A negative SFR value from 0 to -1 indicates more requests to the web server are failing than succeeding.
  - A web server with an SFR value closer to -1 may indicate a web server is under attack or the web server is experiencing a problem.

IMPACT: Using the success-failure ratio, HECC security experts can quickly identify potential problems with a web servers that may indicate an attack and take proactive steps to stop the attack.

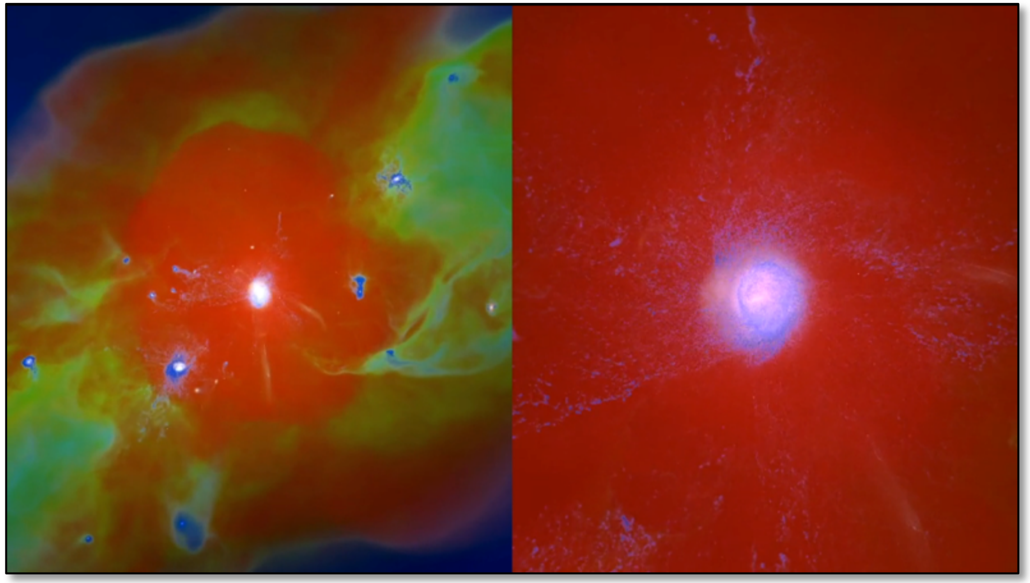


Success-Failure Ratio (SFR) time series chart from HECC Security Monitoring System. The red dip indicated the web server was not able to successfully fulfill a high number of client requests indicating either a server error or possible attack. **Count of successful (positive) and failed (negative) requests sampled in 5-minute increments.*

Simulating the Milky Way and Ultra-Faint Dwarf Galaxies*

- Researchers at the University of Oklahoma are running their fully cosmological, hydrodynamic code ChaNGa (Charm N-body GrAvity solver) on Pleiades to simulate Milky Way-like galaxies and the nearby faint dwarf and ultra-faint dwarf (UFD) galaxies that surround them.
  - Although data from observatories such as NASA's Hubble Space Telescope greatly increase our knowledge of dwarf and UFD galaxies, many uncertainties remain—including galaxy star formation histories, chemical compositions, kinematics, and distributions around the Milky Way.
  - ChaNGa contains the physics to model supernova feedback, star formation, and gas outflows in order to create realistic simulated galaxies easily comparable to observations from modern telescopes.
- The simulations are the first ever developed that can be resolved down to the ultra-faint regime—a requirement for interpreting current and future observations of dwarf and UFD galaxies.
- The researchers were able to reproduce a variety of observations across many orders of magnitude in luminosity and over a wide range of galaxy shapes, star formation histories, and gas contents.
- In one notable result, the simulations showed that several UFD and faint dwarf galaxies have appreciable gas mass despite not being star-forming. This prediction comes as a surprise to observers hunting for these objects.

IMPACT: This large sample of simulated galaxies will provide an ideal tool for analyzing and understanding upcoming observations by NASA's Nancy Grace Roman Space Telescope, James Web Space Telescope, and other observatories.



Evolution of a simulated Milky Way-like galaxy from the Big Bang to present day. Red represents very hot gas; blue is cold. Fine details are visible in the zoomed-in view at right. *Ferah Munshi, University of Oklahoma; Alyson Brooks, Rutgers University*

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

Microscale Analysis to Improve Heat Shield Materials*

- Scientists at NASA Ames have developed codes to compute ablative heat shield material properties and simulate ablation at the microscale using HECC resources. Evaluating these materials is difficult, requiring precise knowledge of their properties.
- The Porous Microstructure Analysis (PuMA) software imports sets of grayscale images representing a material’s microstructure to create a geometrically accurate computational domain.
  - The team uses finite volume and particle-based methods to compute properties for the material, such as thermal conductivity and porosity.
  - They also use Direct Simulation Monte Carlo (DSMC) methods to analyze heat shield microstructures. DSMC allows for more complex environments with many chemical reactions.
  - These capabilities have been extensively tested and verified using numerous test cases obtained from literature or developed in house. Findings show the computed material properties are accurate for many materials with known properties.
- NASA is currently investigating woven carbon fiber composites for use as heat shields due in part to their customizability and desirable thermal properties.

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

IMPACT: Simulations run on HECC supercomputers are leading to a better understanding of current heat shields, which could in turn lead to improved materials that would allow spacecraft to survive higher temperatures and allow for greater flexibility in future missions.

Video showing microscale ablation of a heat shield due to oxidation. Particles enter from the top; as the simulation progresses, the surface material is eaten away. The material represented here is the carbon fiber precursor to the Phenolic Impregnated Carbon Ablator (PICA). *Timothy Sandstrom, NASA/Ames*

Papers

- “**A Remnant Planetary Core in the Hot-Neptune Desert**,” D. Armstrong, et al., Nature, vol. 583, July 1, 2020. *
https://www.nature.com/articles/s41586-020-2421-7
- “**The K2 & TESS Synergy I: Updated Ephemerides and Parameters for K2-114, K2-167, K2-237, & K2-261**,” M. Ikwut-Ukwa, et al., arXiv:2007.00678 [astro-ph.EP], July 1, 2020. *
https://arxiv.org/abs/2007.00678
- “**Two Intermediate-Mass Transiting Brown Dwarfs from the TESS Mission**,” T. Carmichael, et al., The Astronomical Journal, vol. 160, no. 1, July 2, 2020. *
https://iopscience.iop.org/article/10.3847/1538-3881/ab9b84/meta
- “**Carbon Monitoring System Flux Net Biosphere Exchange 2020 (CMS-Flux NBE 2020)**,” J. Liu, et al., Earth System Science Data, published online July 7, 2020. *
https://essd.copernicus.org/preprints/essd-2020-123/
- “**The Role of Stellar Feedback in the Chemical Evolution of a Low Mass Dwarf Galaxy**,” A. Emerick, G. Bryan, M.-M. Mac Low, arXiv:2007.03702 [astro-ph.GA], July 7, 2020. *
https://arxiv.org/abs/2007.03702
- “**GW190814: Spin and Equation of State of a Neutron Star Companion**,” A. Tsokaros, M. Ruiz, S. Shapiro, arXiv:2007.05526 [astro-ph.HE], July 10, 2020. *
https://arxiv.org/abs/2007.05526

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

Papers (cont.)

- "**The Formation of Ultra-Diffuse Galaxies in the RomulusC Galaxy Cluster Simulation**," > Tremmel, et al., Monthly Notices of the Royal Astronomical Society, published online July 13, 2020. *
  https://academic.oup.com/mnras/article-abstract/doi/10.1093/mnras/staa2015/5870683
- "**Hydrodynamic Winds from Twin-Star Binaries**," M. MacLeod, A. Loeb, arXiv:2007.07252 [astro-ph.SR], July 14, 2020. *
  https://arxiv.org/abs/2007.07252
- "**Sampling Error in Aircraft Flux Measurements Based on a High-Resolution Large Eddy Simulations of the Marine Boundary Layer**," G. Petty, Atmospheric and Oceanic Sciences, published online July 21, 2020. *
  https://amt.copernicus.org/preprints/amt-2020-235/
- "**Cloud Properties and Correlations with Star Formation in Self-Consistent Simulations of the Multiphase ISM**," S. A. Mao, E. Ostriker, C.-G. Kim, The Astrophysical Journal, vol. 898, no. 1, July 22, 2020.
  https://iopscience.iop.org/article/10.3847/1538-4357/ab989c/meta
- "**TIC 278956474: Two Close Binaries in One Young Quadruple System Identified by TESS**," P. Rowden, et al., The Astronomical Journal, vol. 160, no. 2, July 23, 2020 *
  https://iopscience.iop.org/article/10.3847/1538-3881/ab9d20/meta
- "**Black Hole – Galaxy Co-Evolution in FIRE: The Importance of Black Hole Location and Mergers**," O. Çatmabacak, et al., arXiv:2007.12185 [astro-ph.GA], July 23, 2020. *
  https://arxiv.org/abs/2007.12185

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Papers (cont.)

- “**A Fast-Growing Tilt Instability of Detached Circumplanetary Disks**,” R. Martin, et al., The Astrophysical Journal: Letters, vol. 898, no. 1, July 24, 2020. *
  https://iopscience.iop.org/article/10.3847/2041-8213/aba3c1/meta
- “**Atmospheric Simulations of Total Column CO_2 Mole Fractions from Global Mesoscale within the Carbon Monitoring System Flux Inversion Framework**,” M. Butler, et al., Atmosphere, vol. 11, issue 8, July 26, 2020. *
  https://www.mdpi.com/2073-4433/11/8/787
- “**PTFO 8-8695: Two Stars, Two Signals, No Planet**,” L. Bouma, et al., The Astronomical Journal, vol. 160, no. 2, July 30, 2020. *
  https://iopscience.iop.org/article/10.3847/1538-3881/ab9e73
- “**Exploring the Atmospheric Dynamics of the Extreme Ultrahot Jupiter KELT-9b Using TESS Photometry**,” I. Wong, et al., The Astronomical Journal, vol. 160, no. 2, July 30, 2020. *
  https://iopscience.iop.org/article/10.3847/1538-3881/aba2cb

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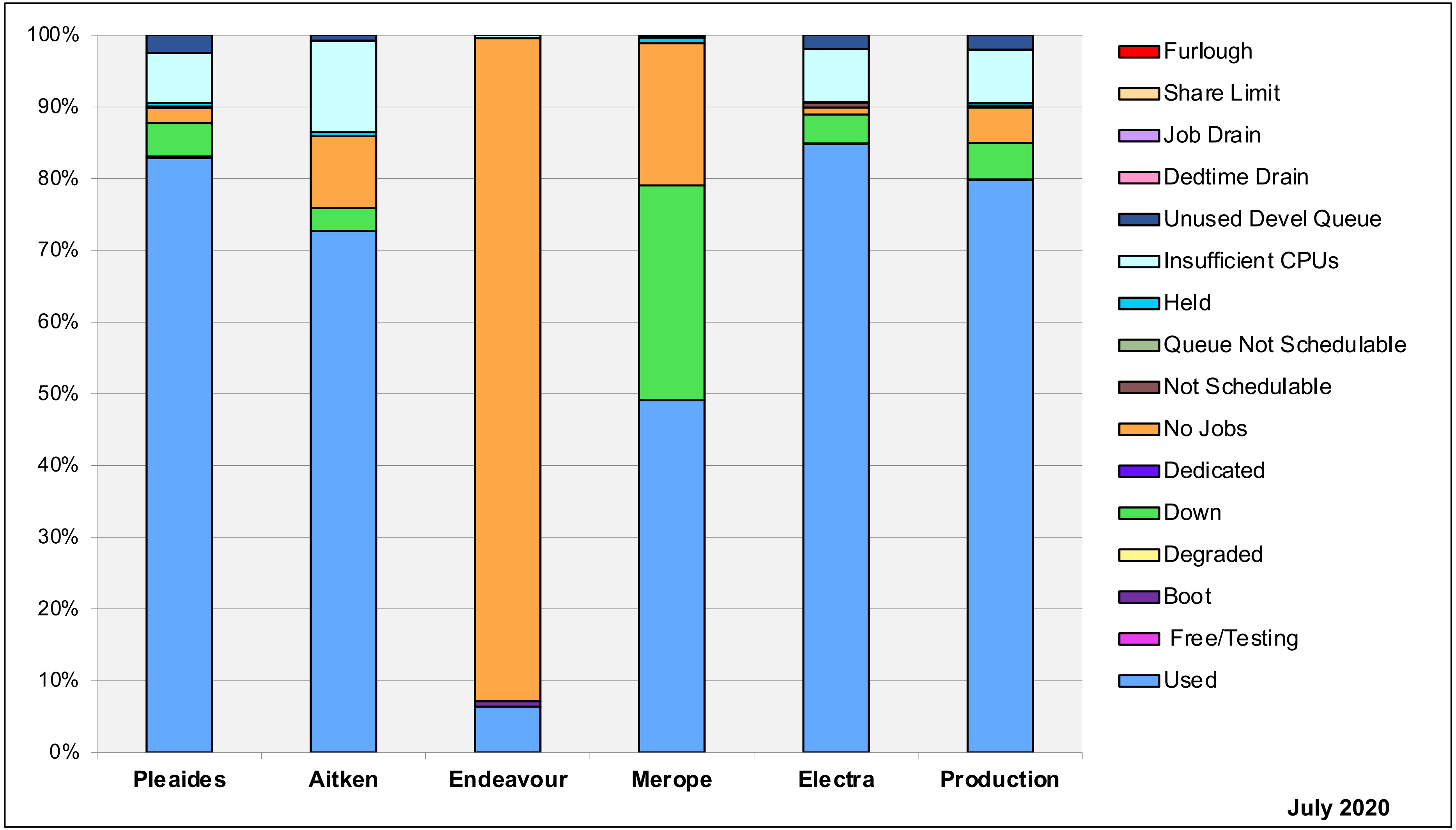
News and Events

- **Inside the U.S.-Led COVID-19 High Performance Computing Consortium**, *Nextgov*, July 8, 2020—As part of this report from Nextgov.com, two NASA Ames researchers describe how they use NAS resources to conduct genome sequencing and bioinformatics analysis to make correlations between COVID-19 severity and genetic features of individuals. NASA has been involved in the initiative from the very beginning, explained NAS Division Chief Piyush Mehrotra. https://www.nextgov.com/emerging-tech/2020/07/inside-us-led-covid-19-high-performance-computing-consortium/166734/

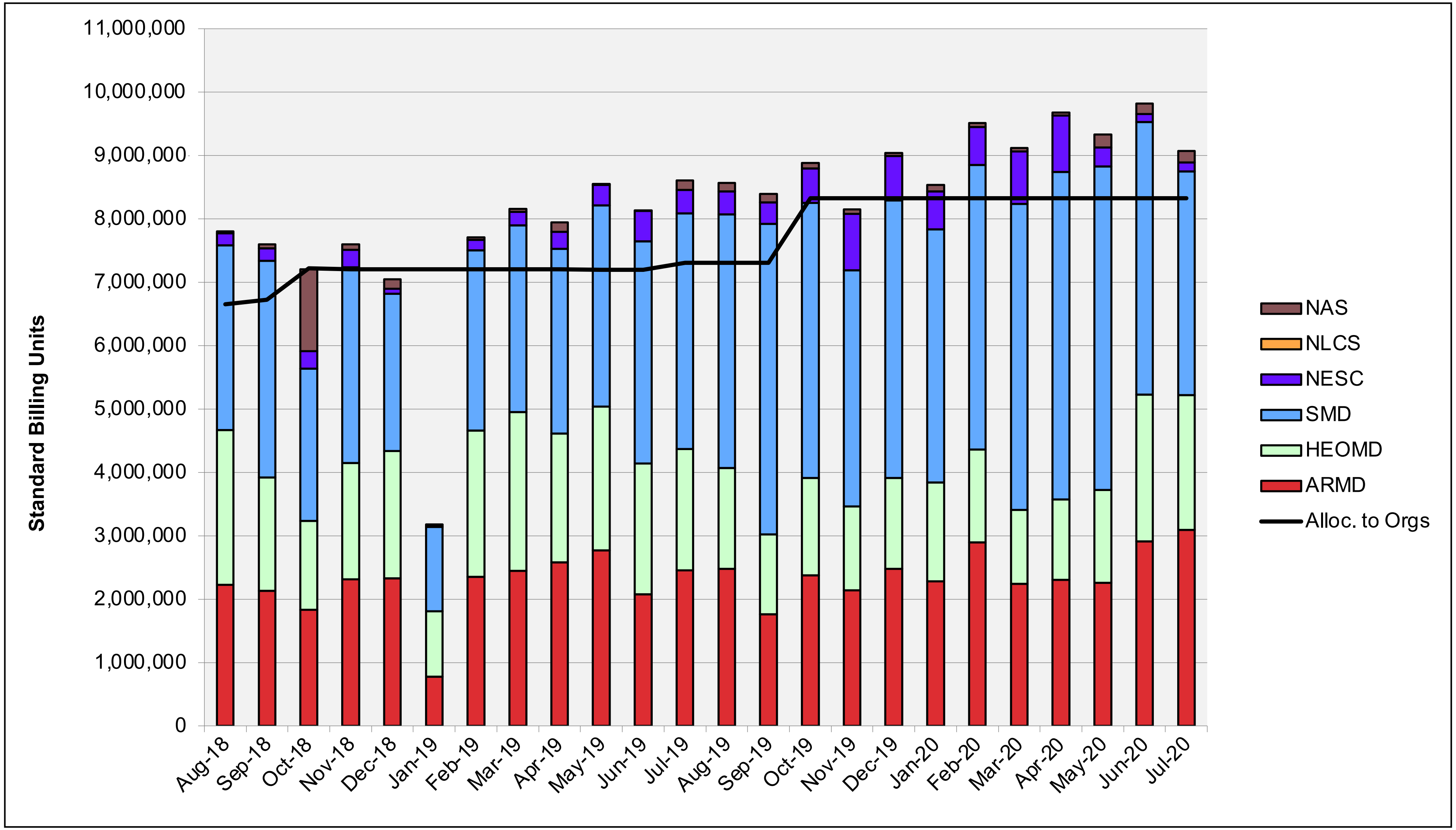
News and Events: Social Media

- **Coverage of NAS Stories**
  - Topic: Hot Jupiter from NASA TESS data (NAS part of data pipeline)
    - NAS: Twitter 6 retweets, 42 likes.
    - NASA Supercomputing: Facebook 258 users reached, 11 engagements, 6 likes, 1 share.

HECC Utilization



HECC Utilization Normalized to 30-Day Month



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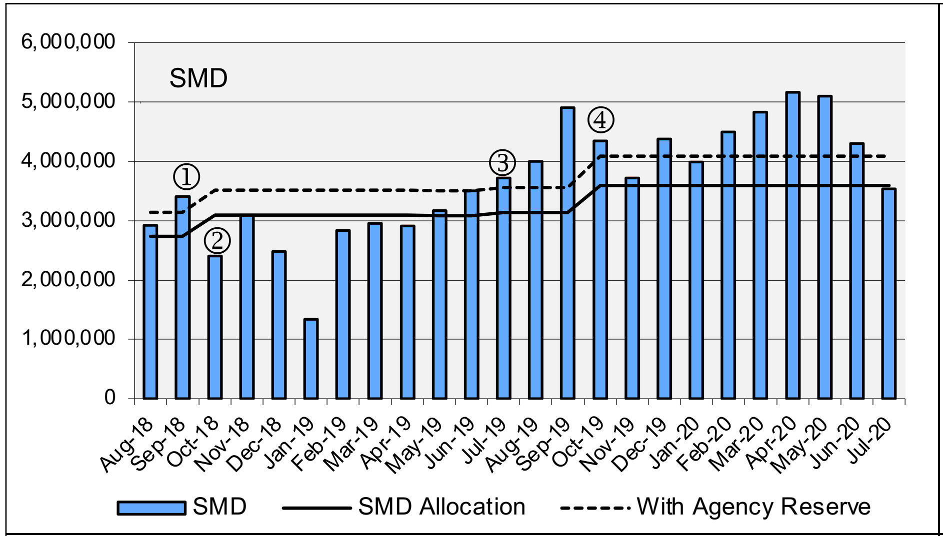
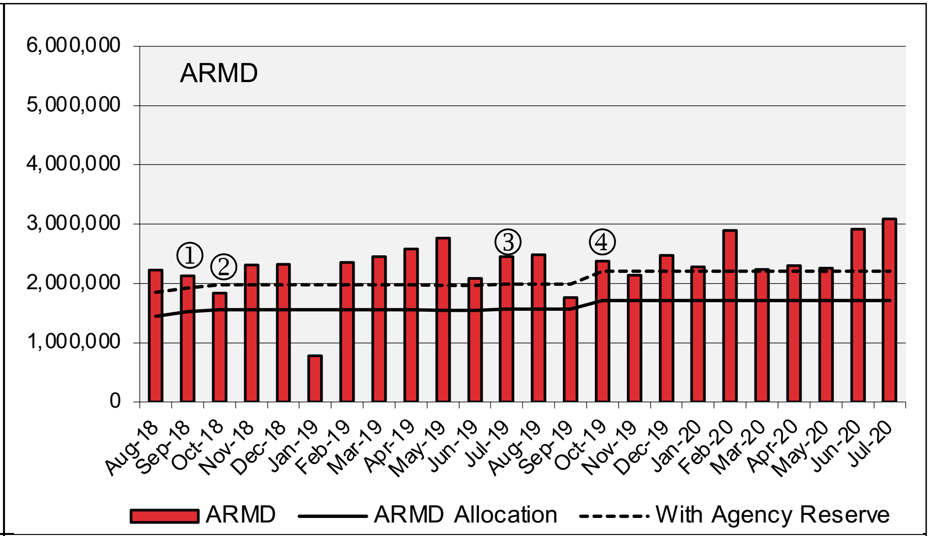
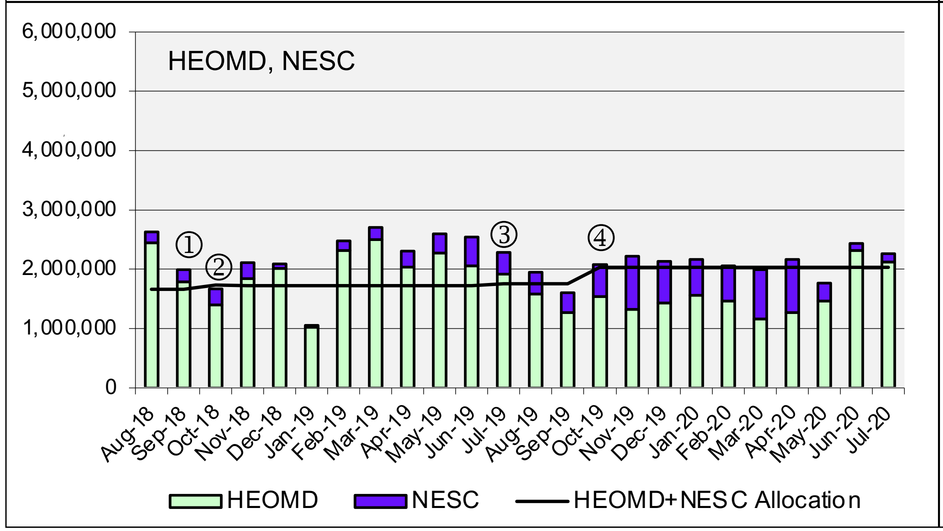






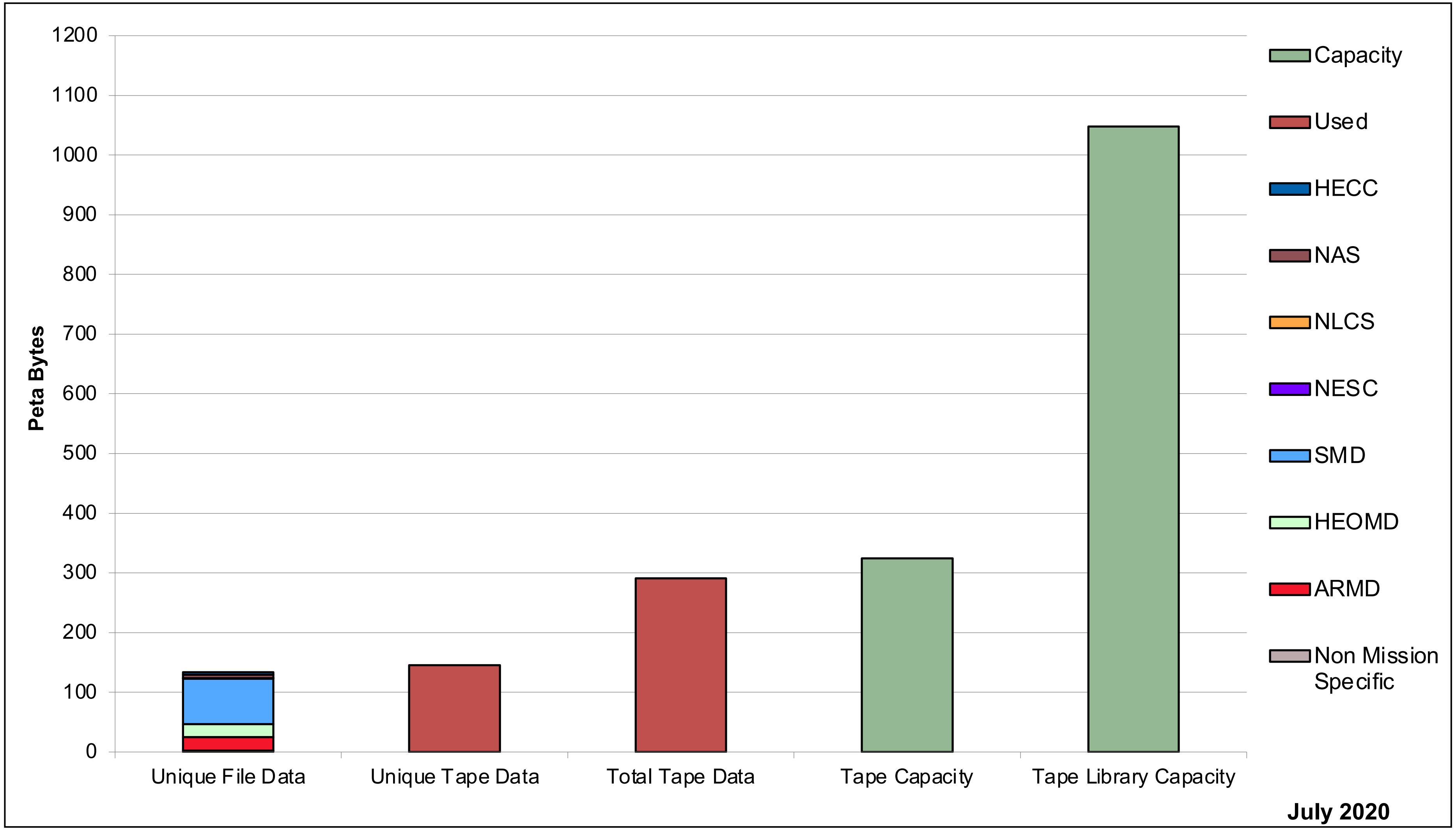
① 4 Skylake E cells (16 D Rack Equivalence) added to Electra

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

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

④ Skylake Tesla GPU V100 Nodes installed

Tape Archive Status



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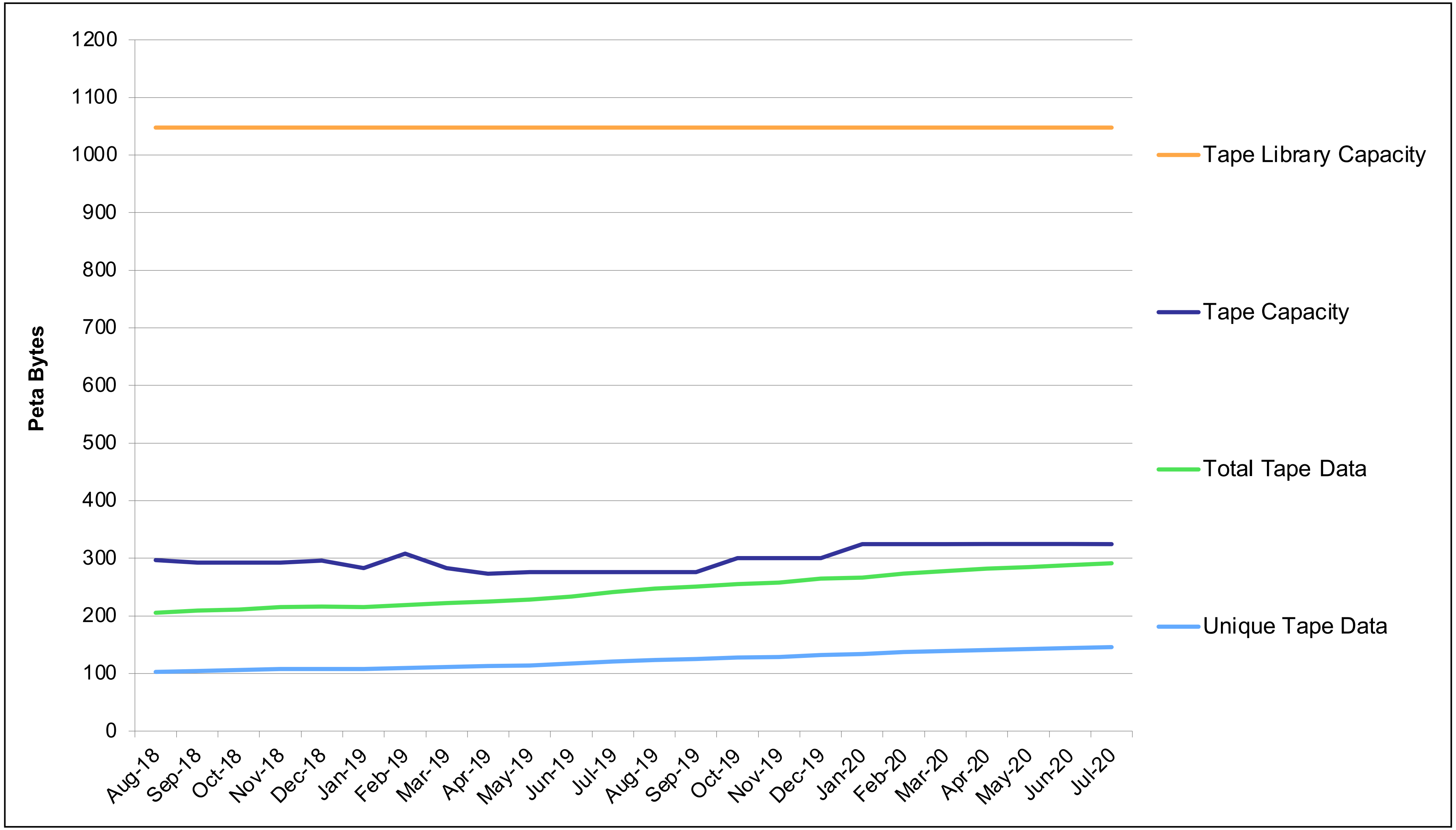
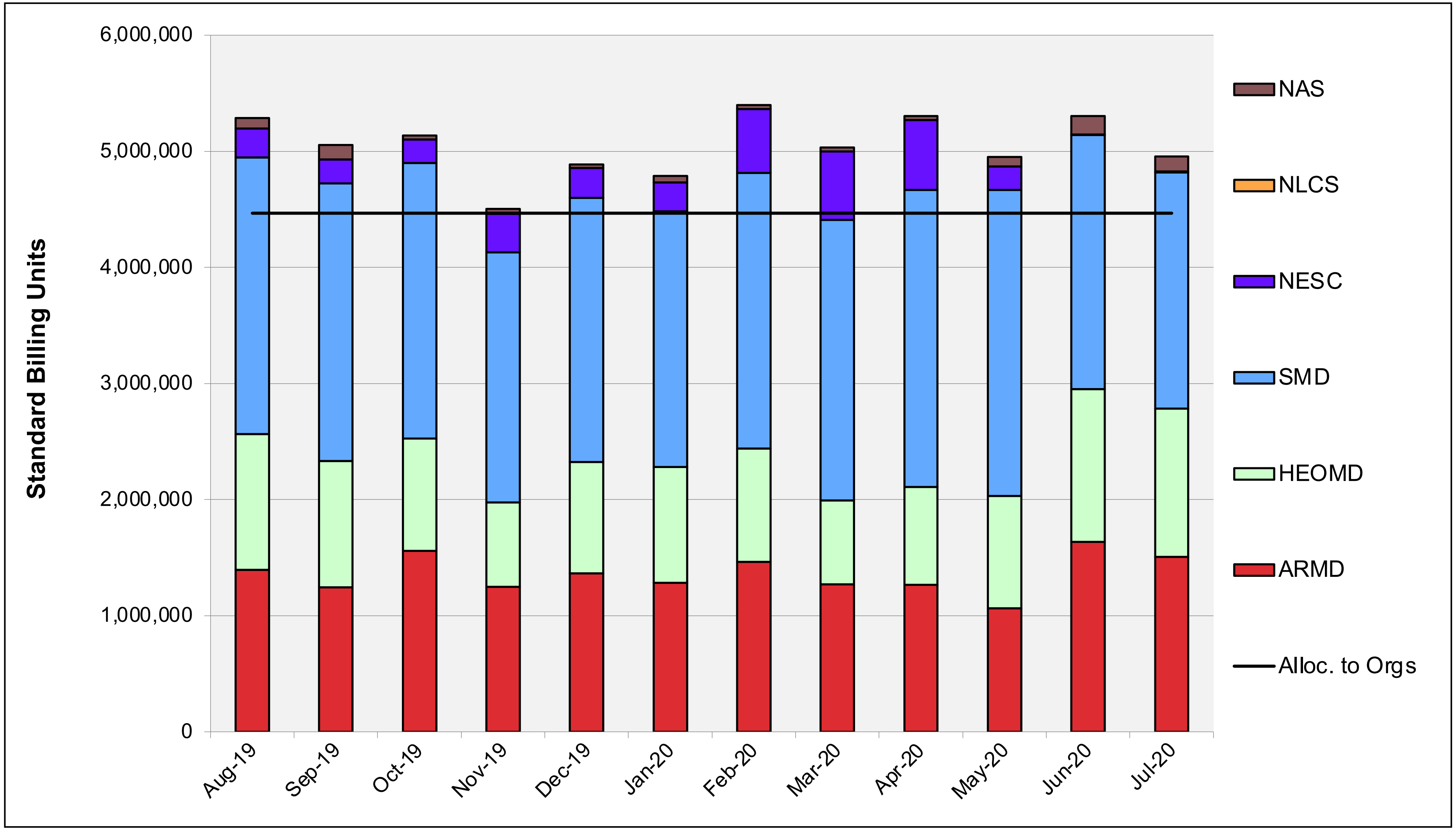
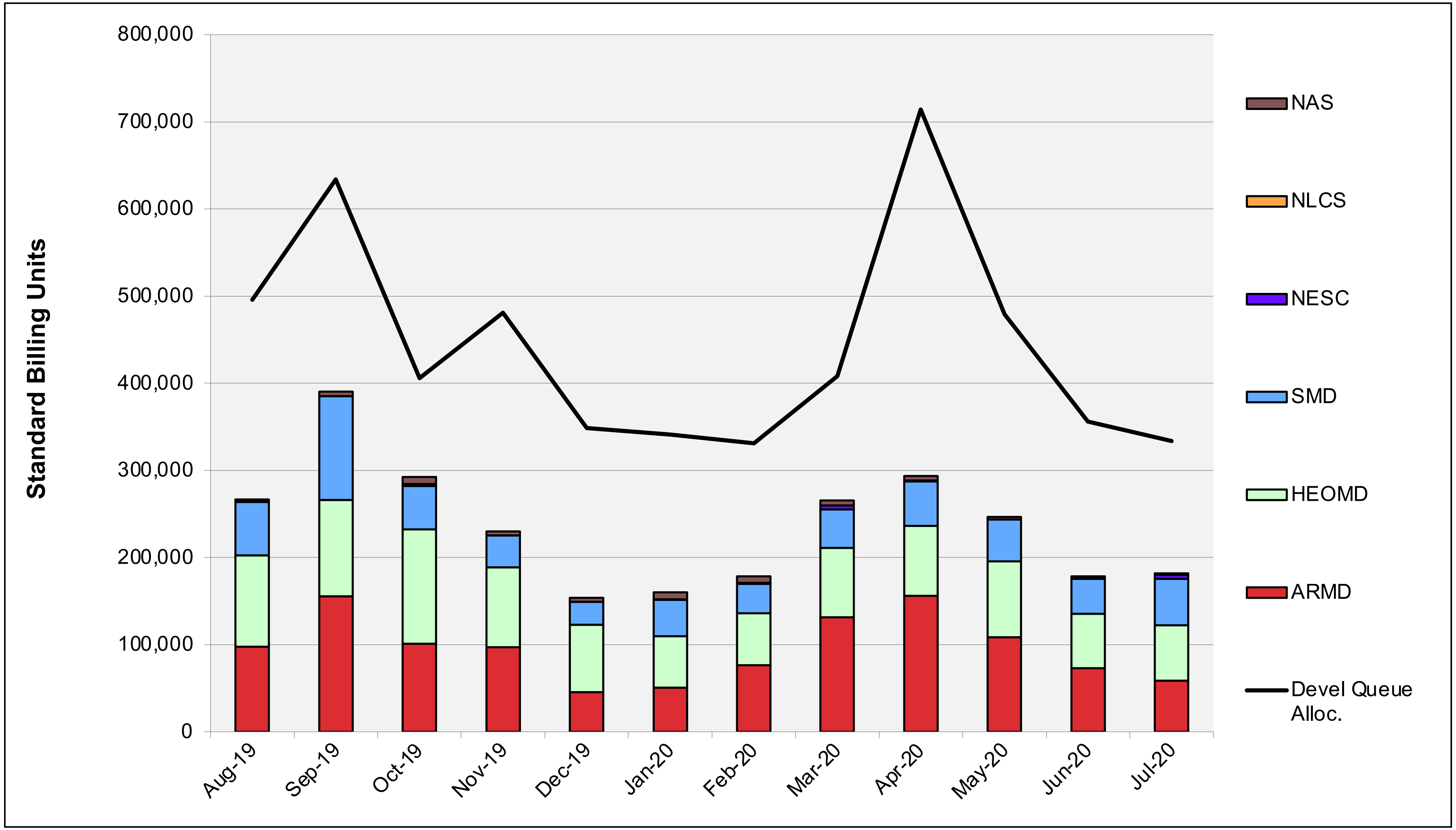


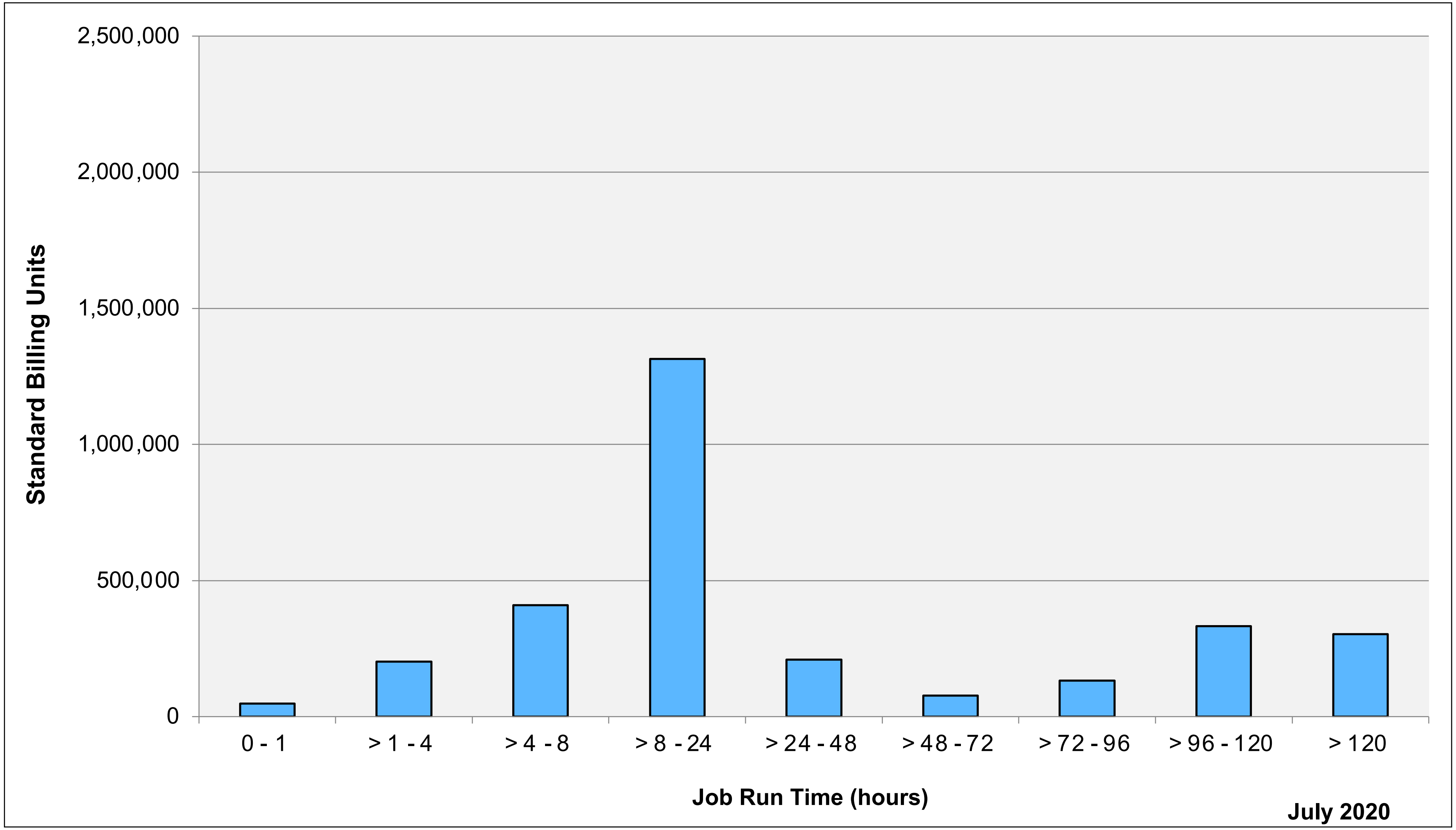
Pleiades: SBUs Reported, Normalized to 30-Day Month



Pleiades: Devel Queue Utilization



Pleiades: Monthly Utilization by Job Length



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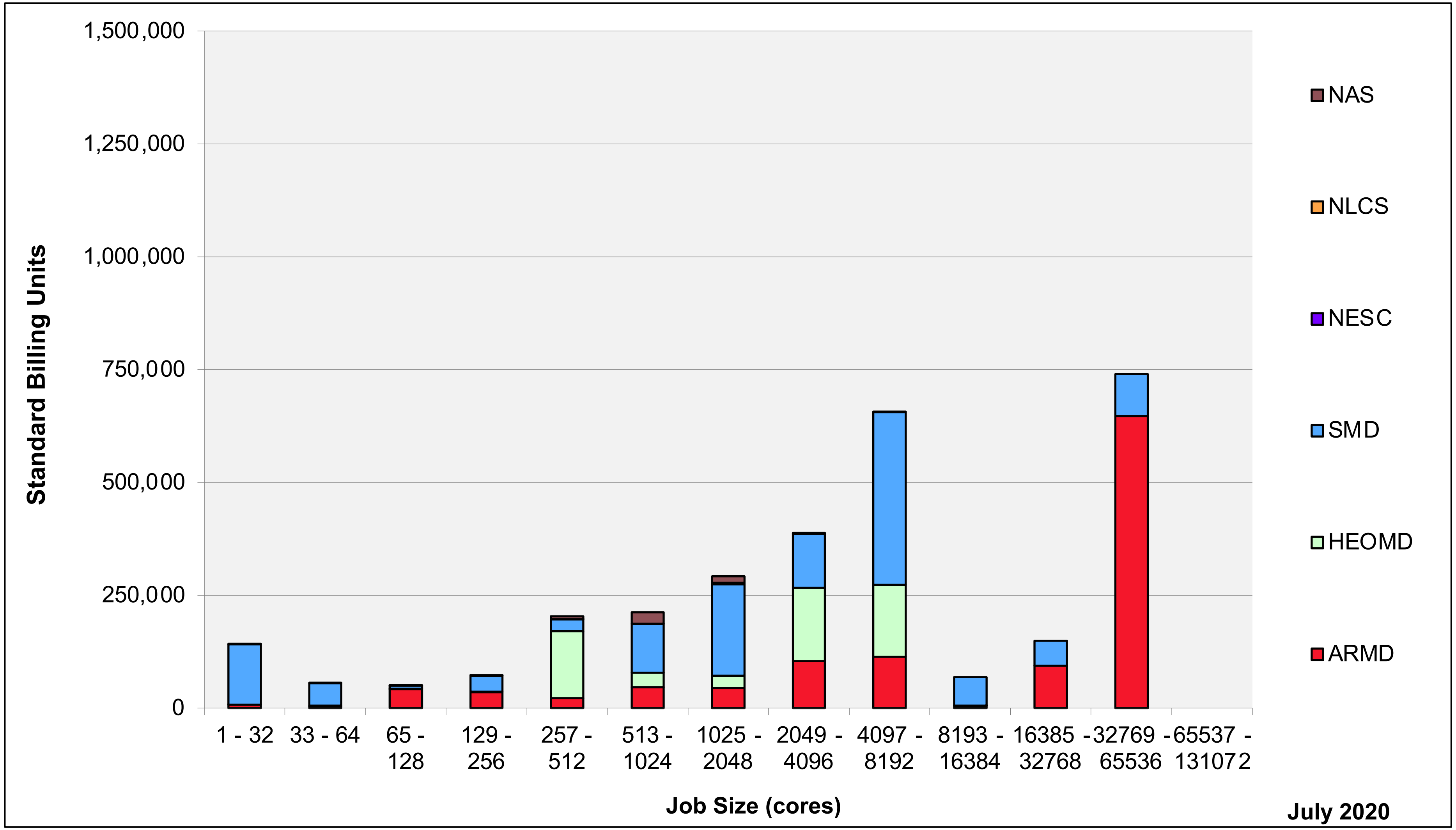
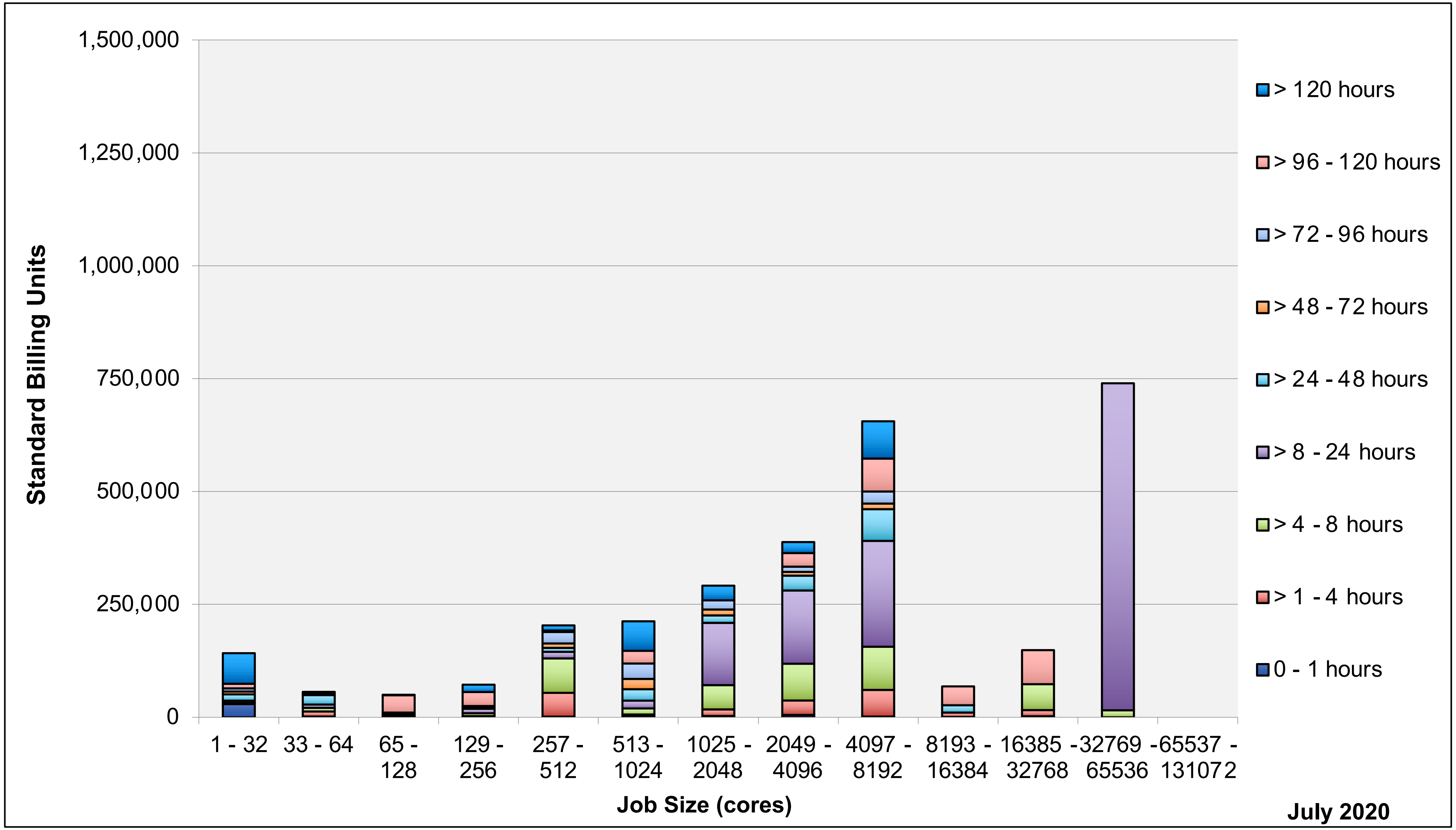
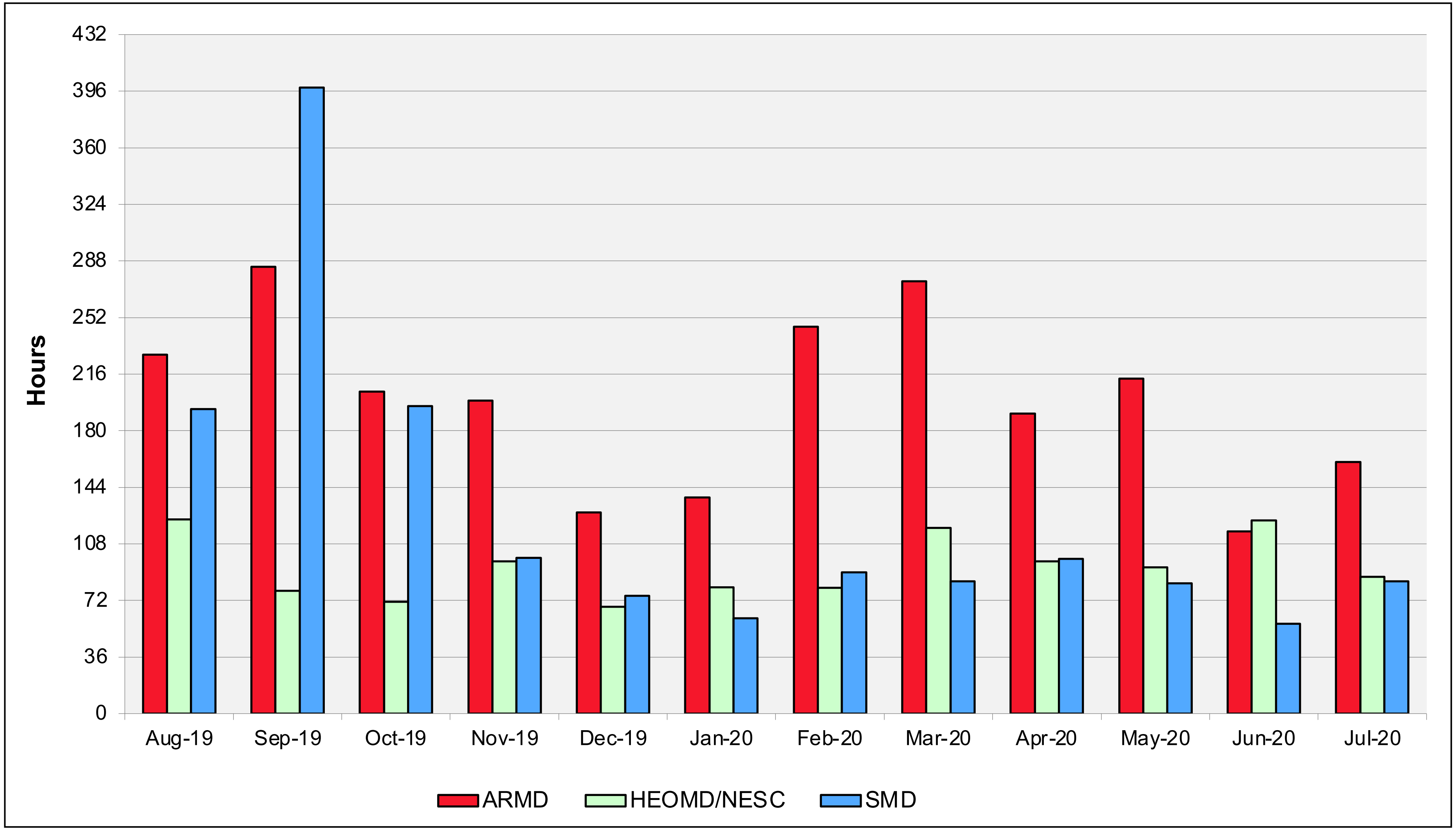


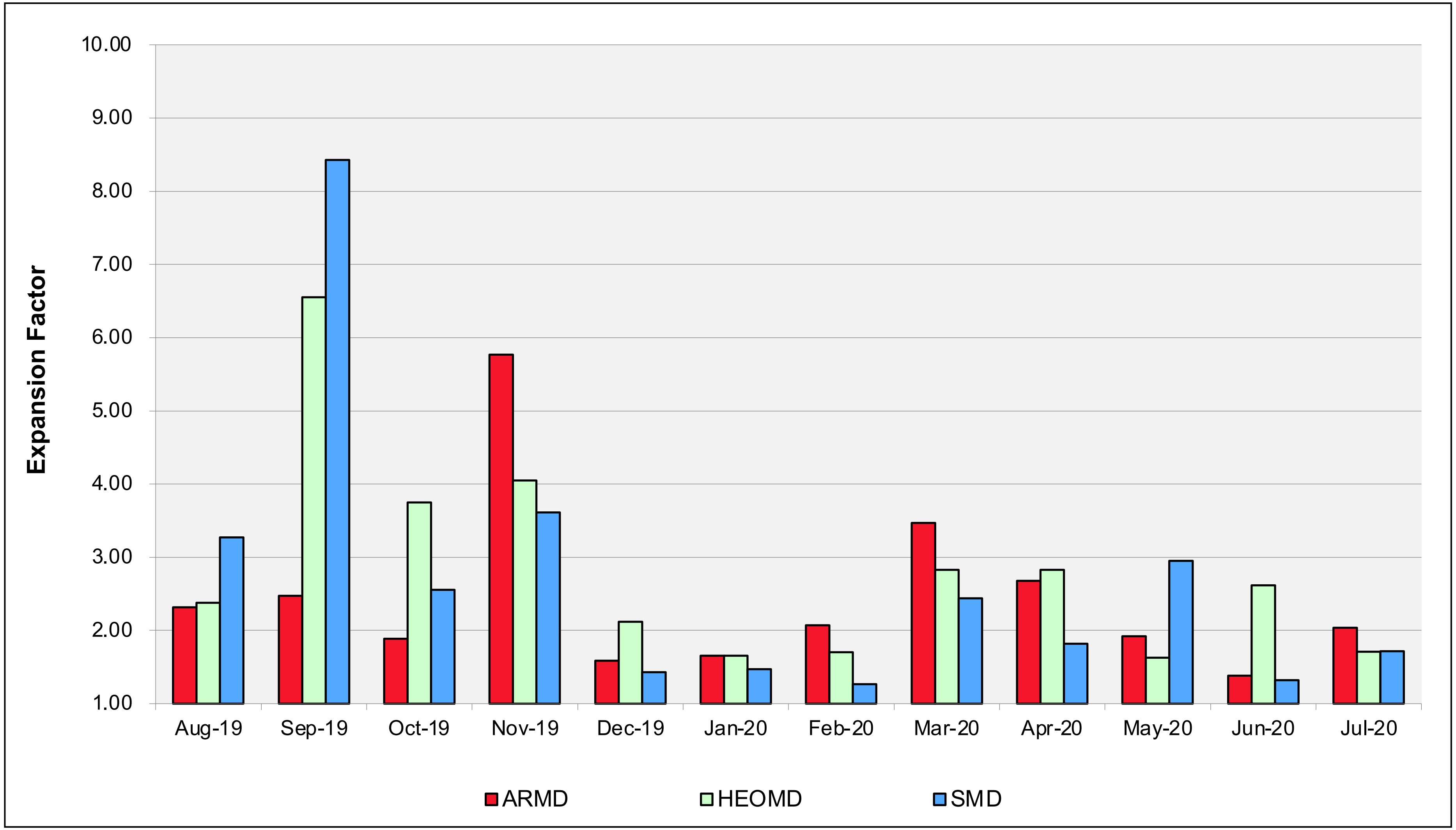
Pleiades: Monthly Utilization by Size and Length



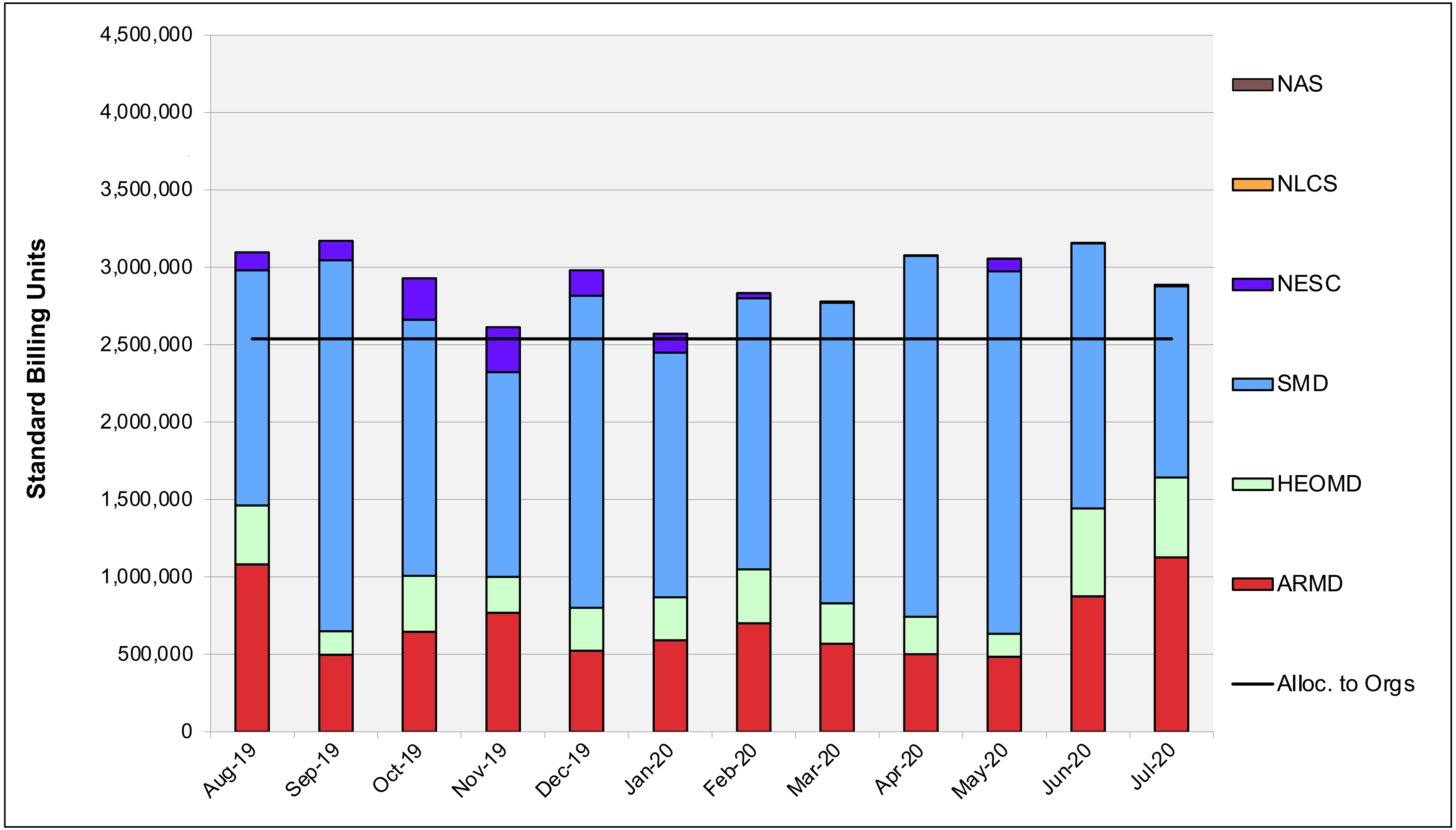
Pleiades: Average Time to Clear All Jobs



Pleiades: Average Expansion Factor



Aitken: SBUs Reported, Normalized to 30-Day Month



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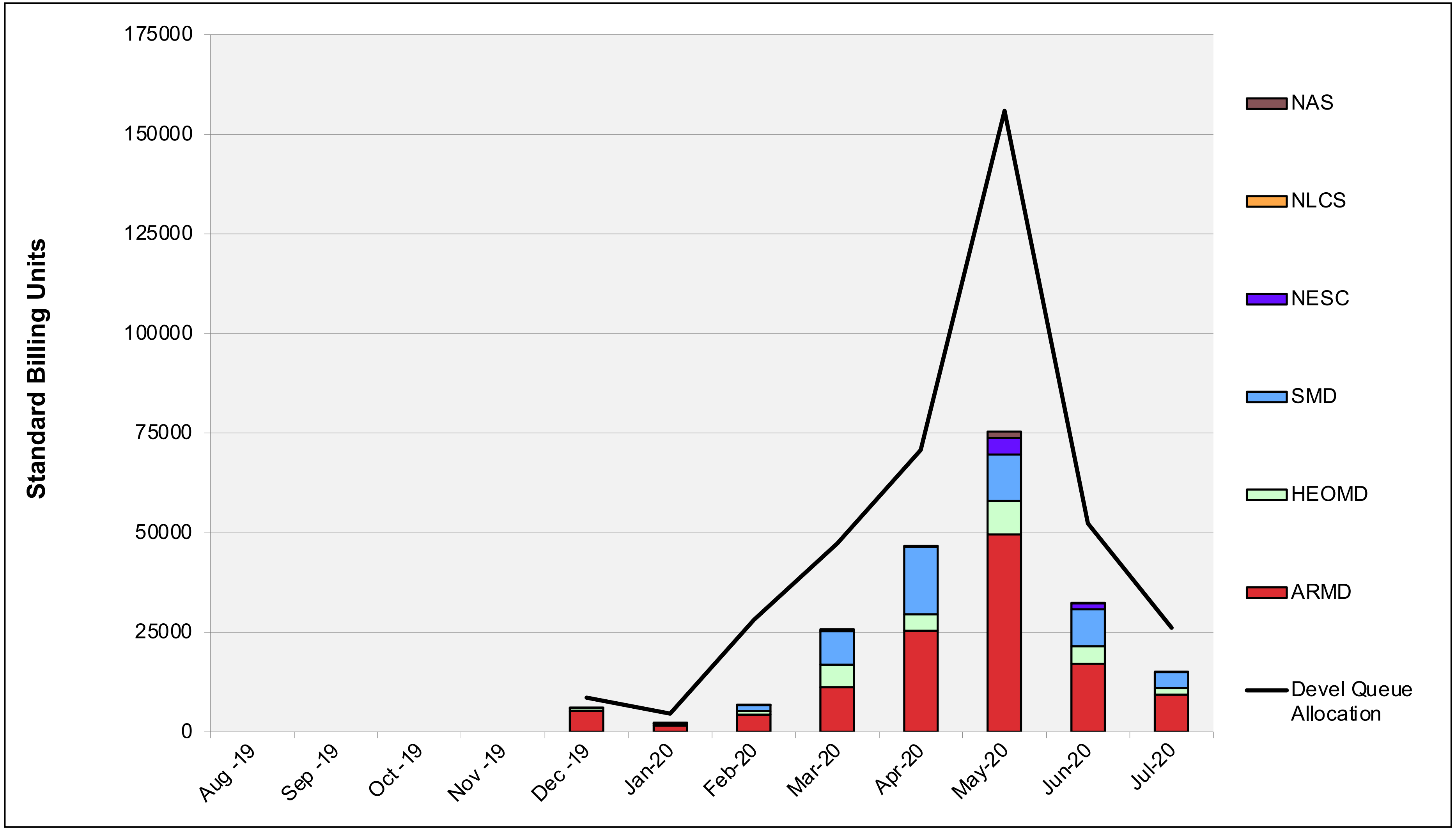
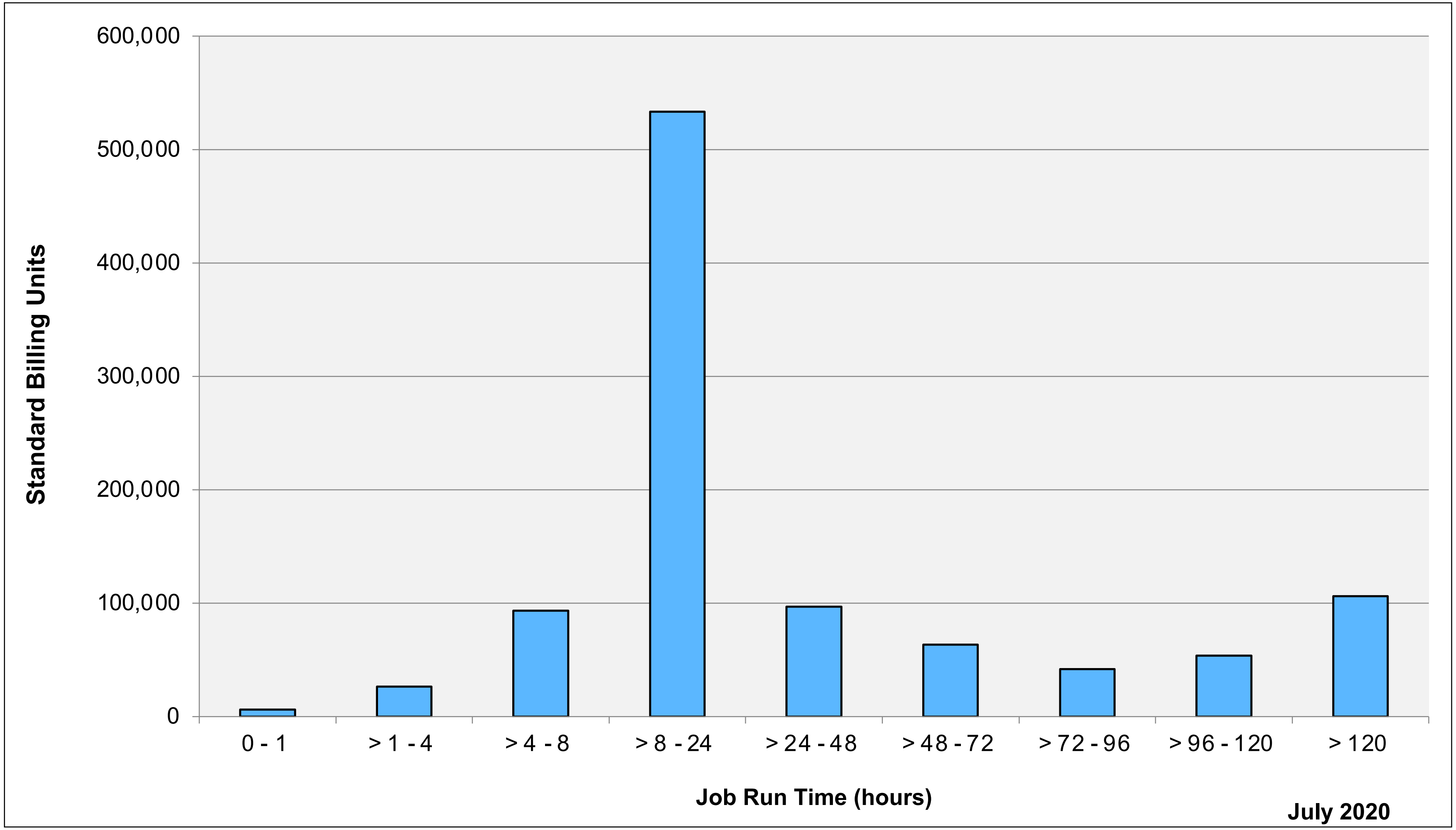


Aitken: Monthly Utilization by Job Length



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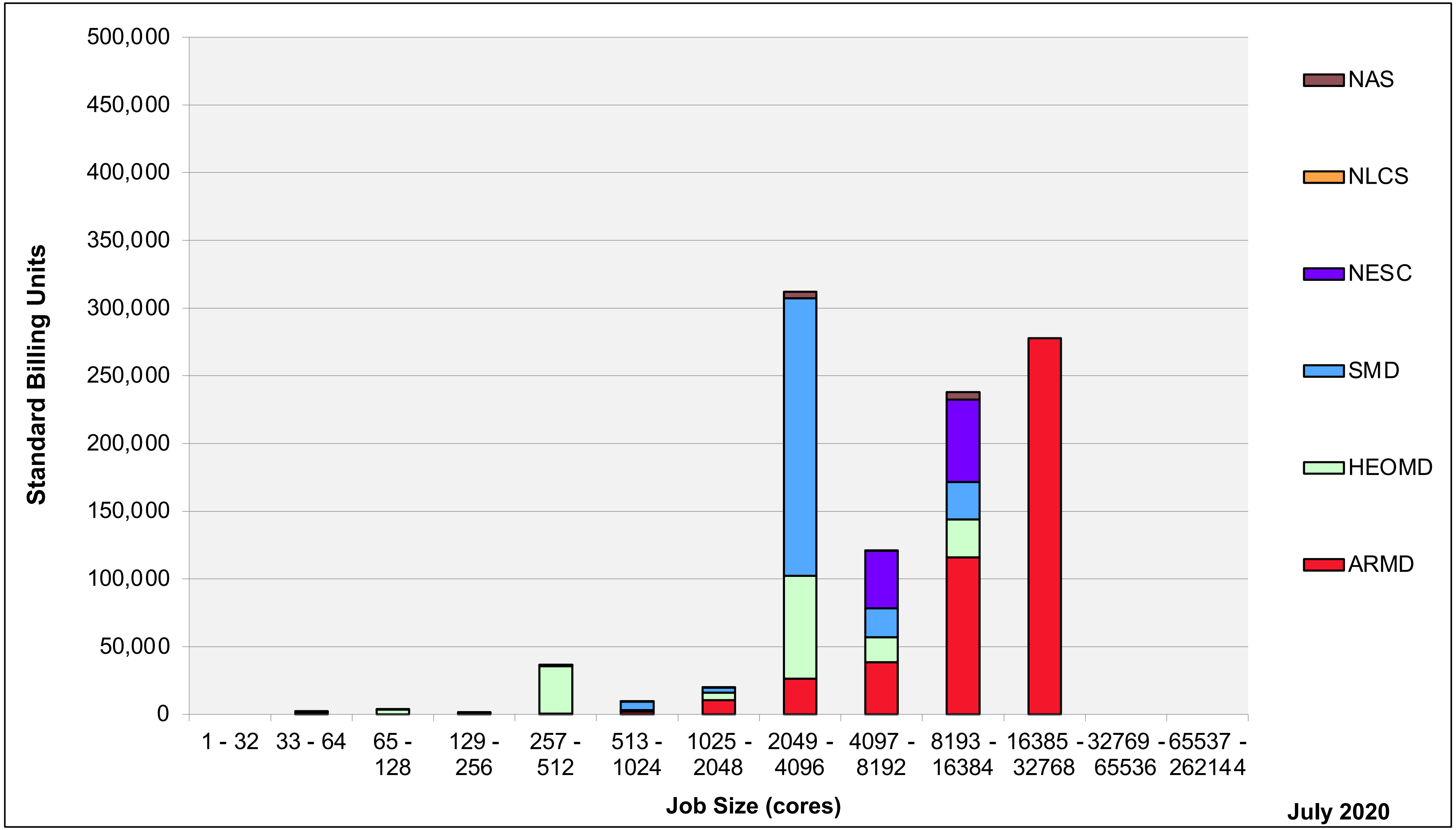

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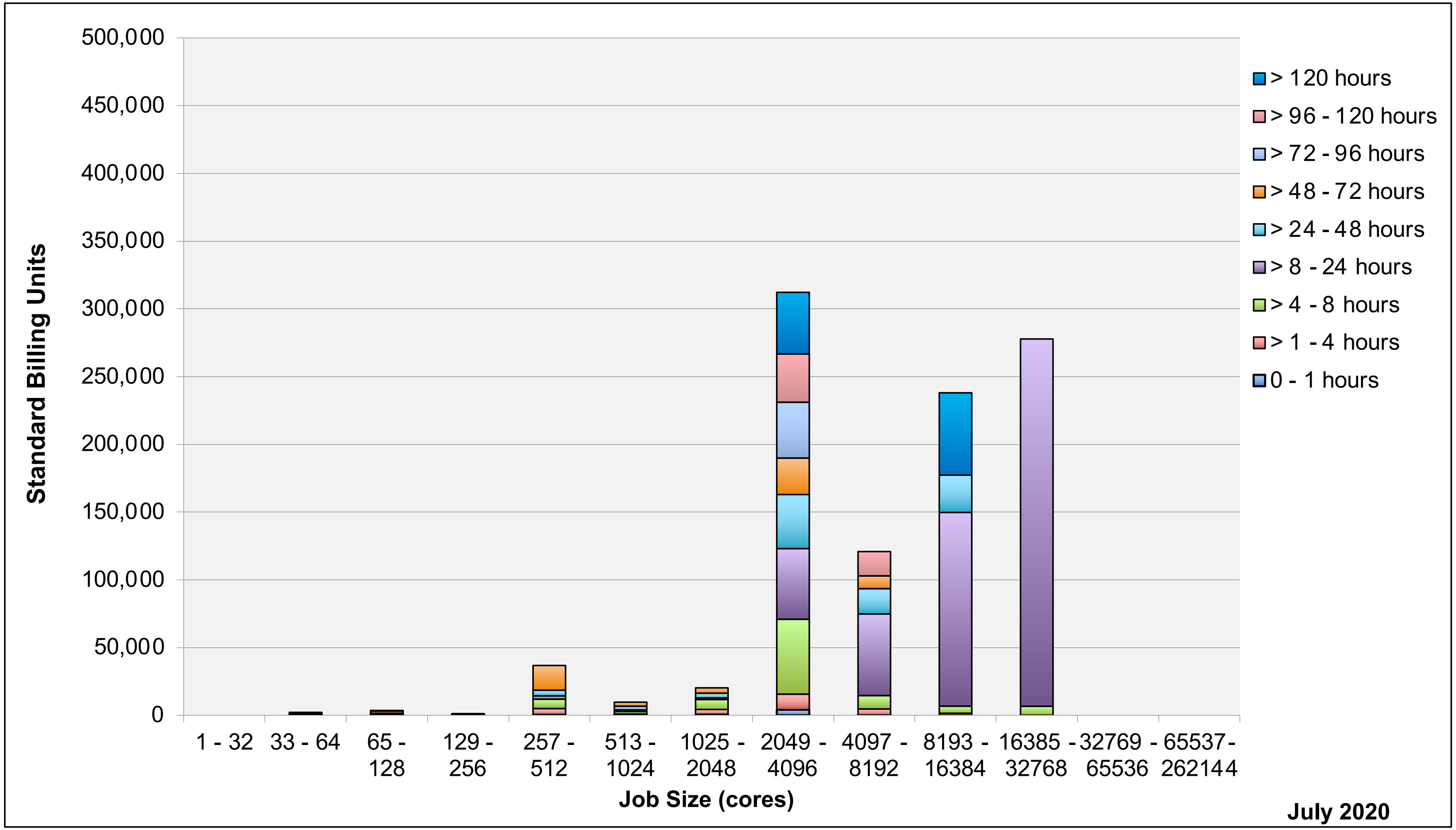

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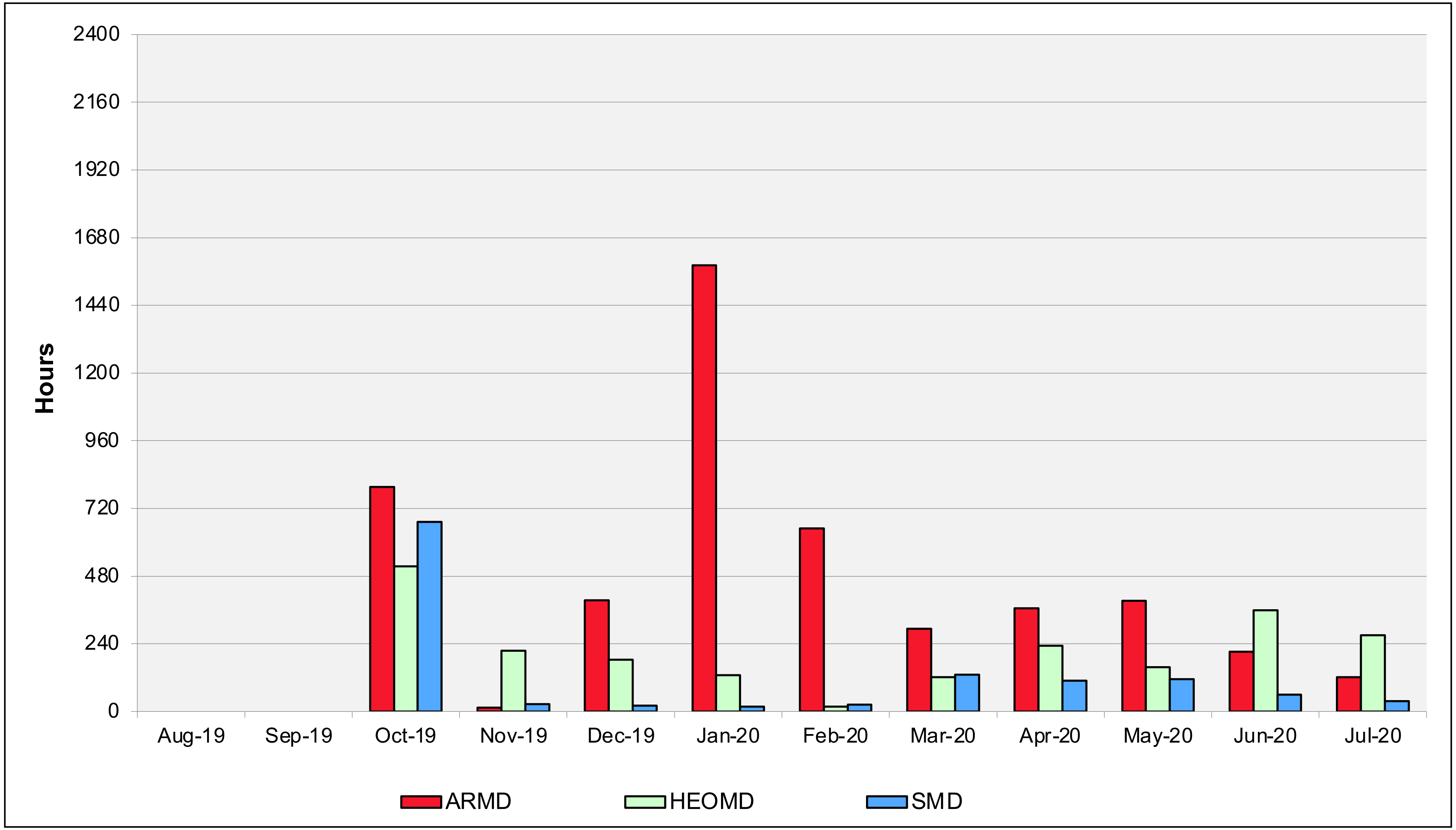
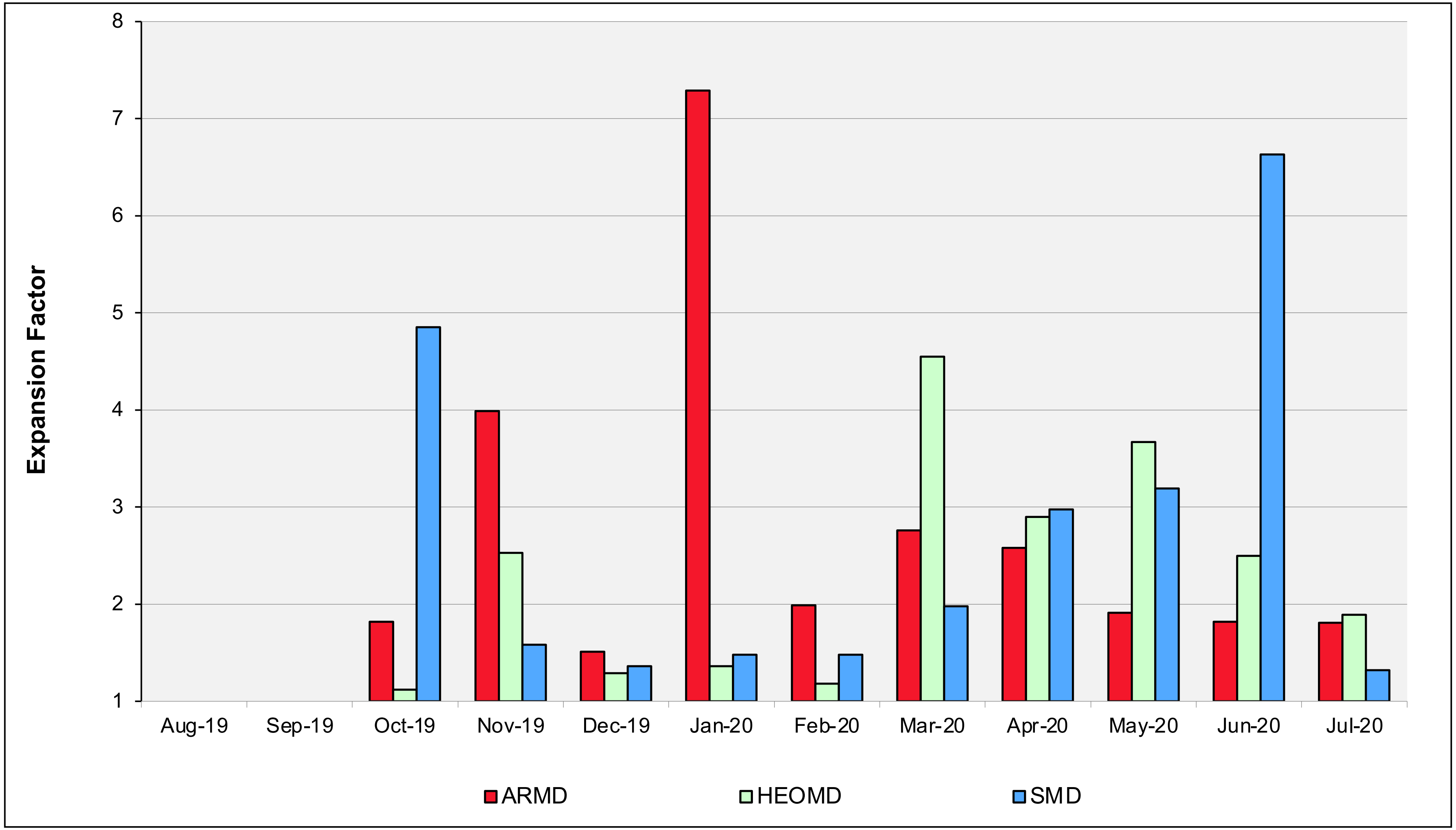
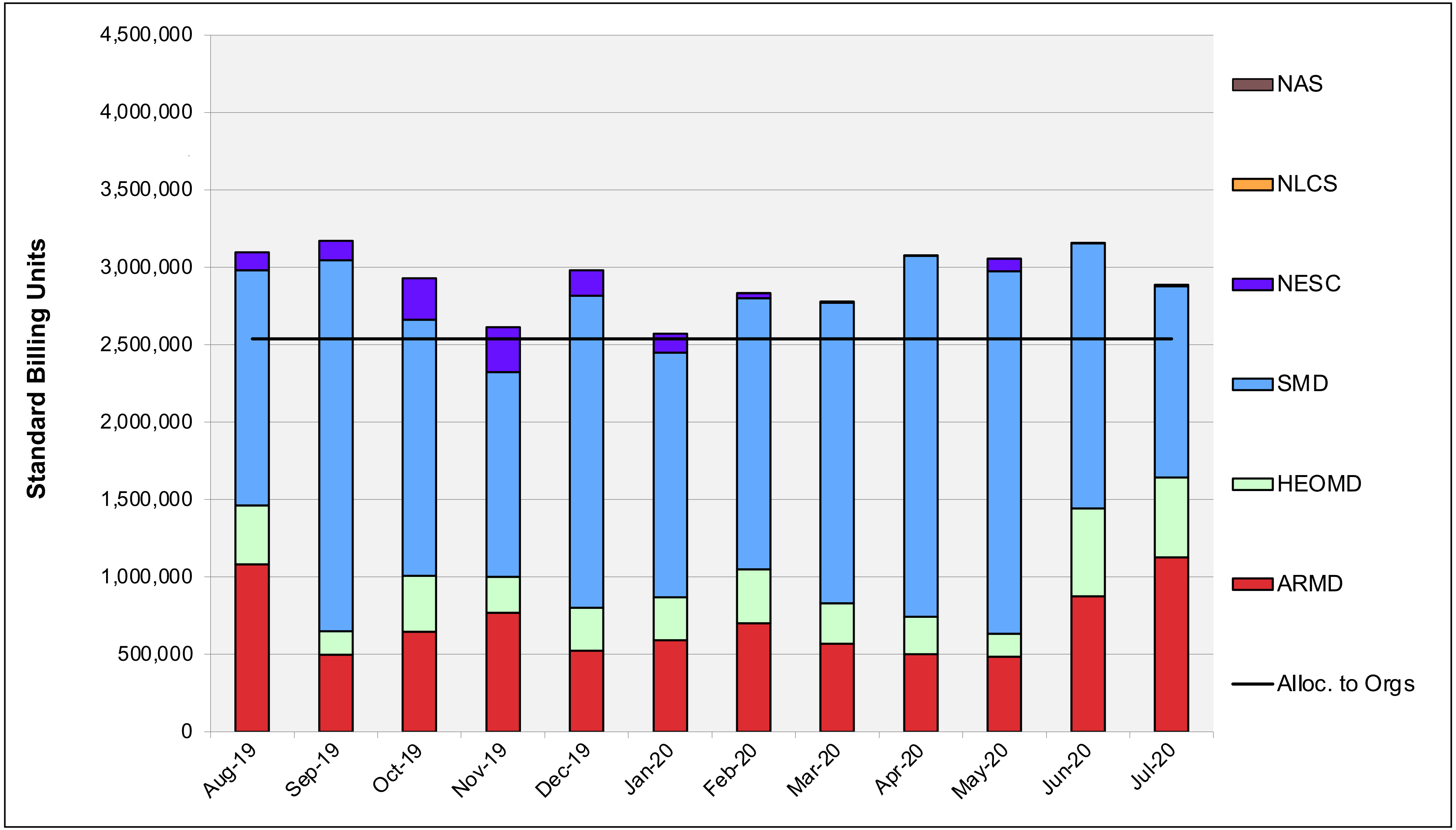


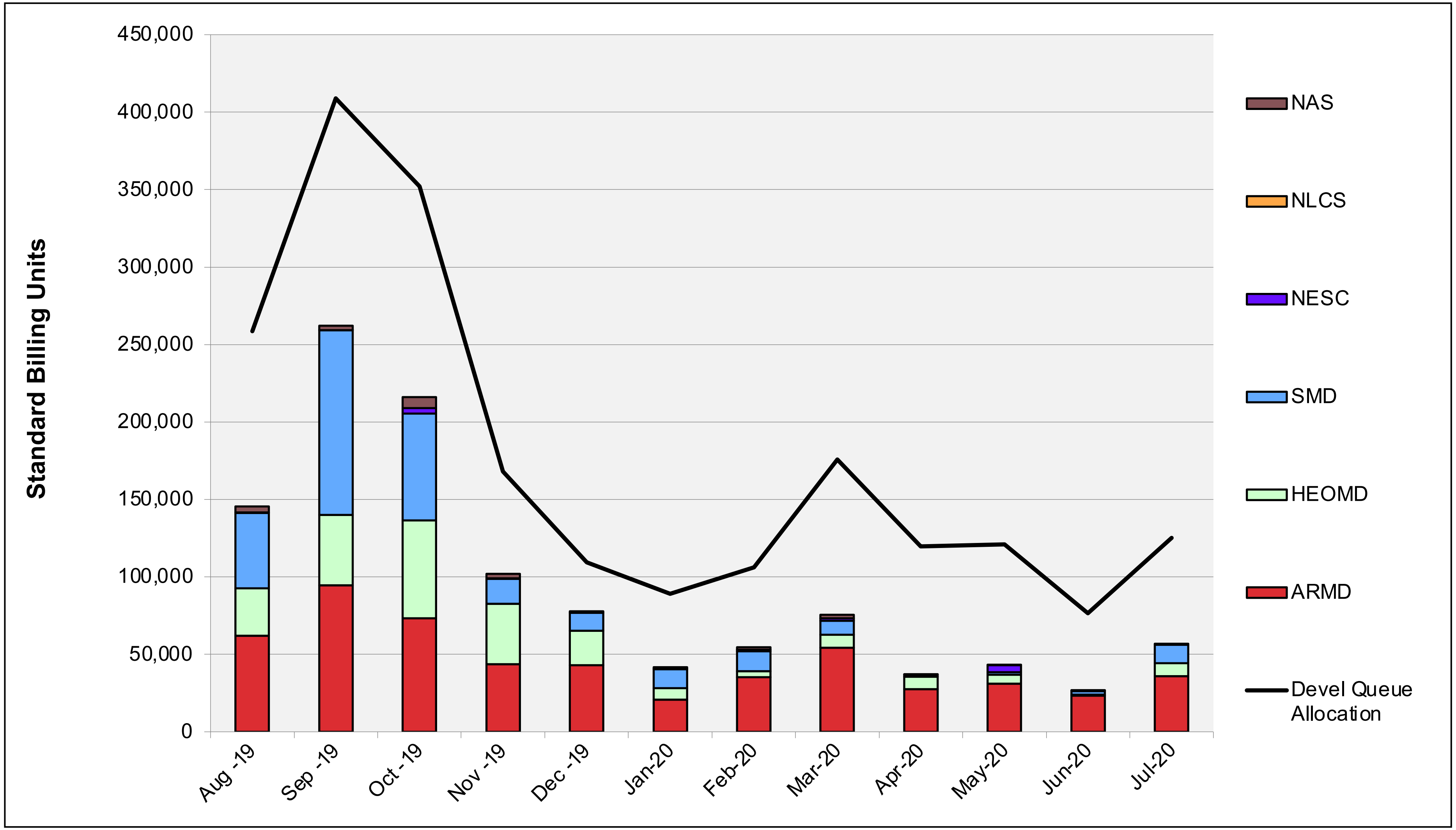
Aitken: Average Expansion Factor



Electra: SBUs Reported, Normalized to 30-Day Month



Electra: Devel Queue Utilization



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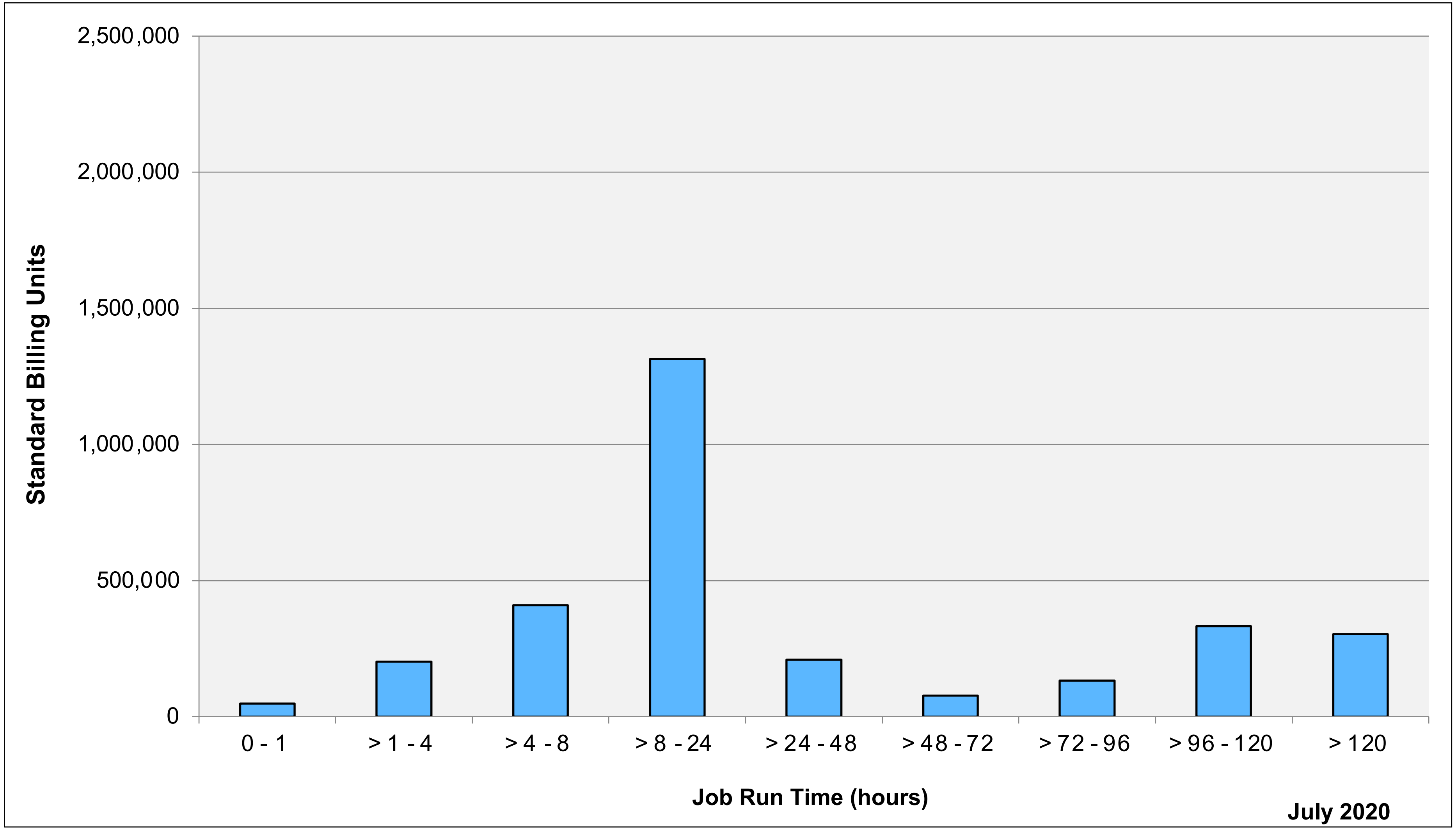

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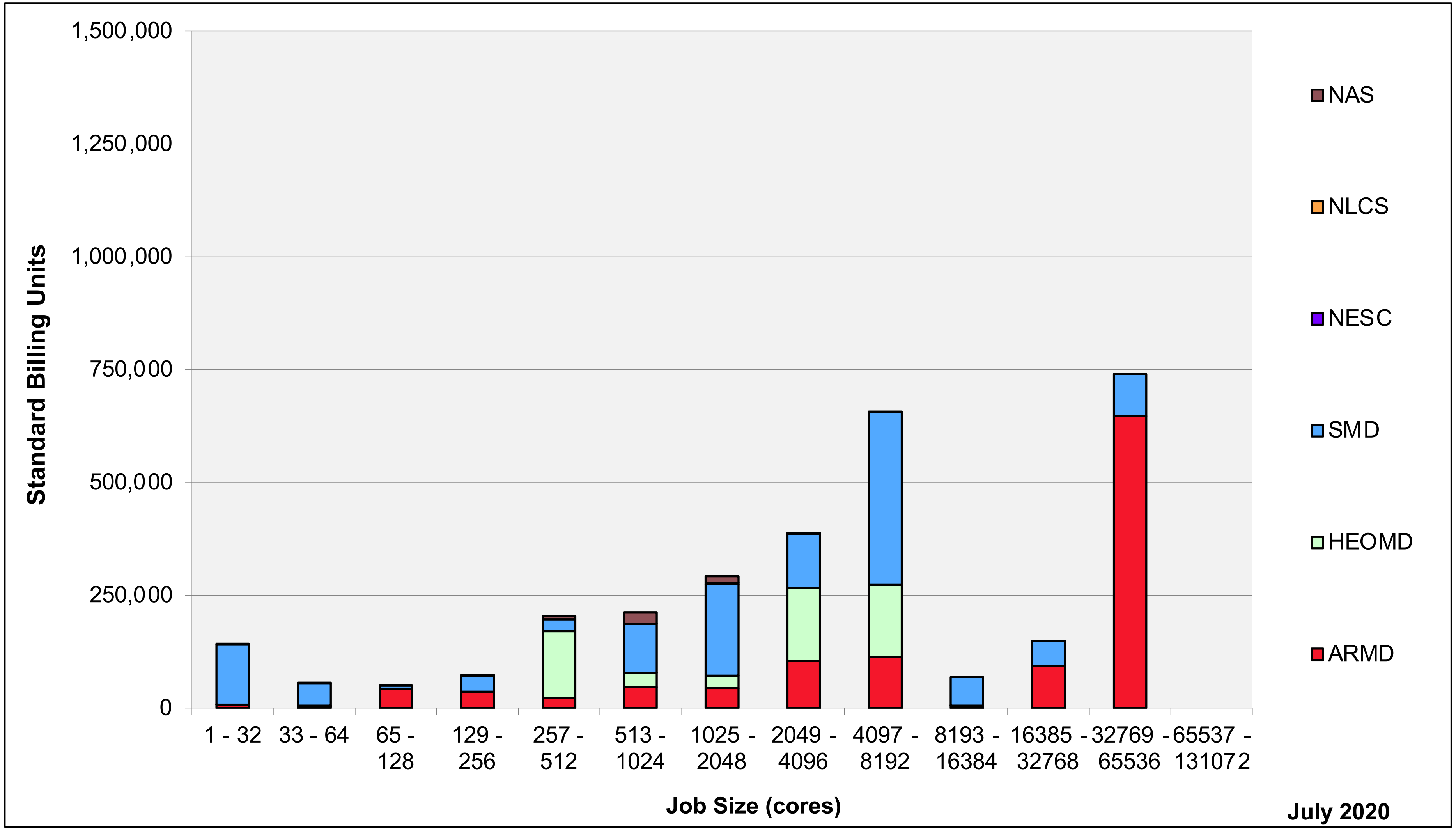

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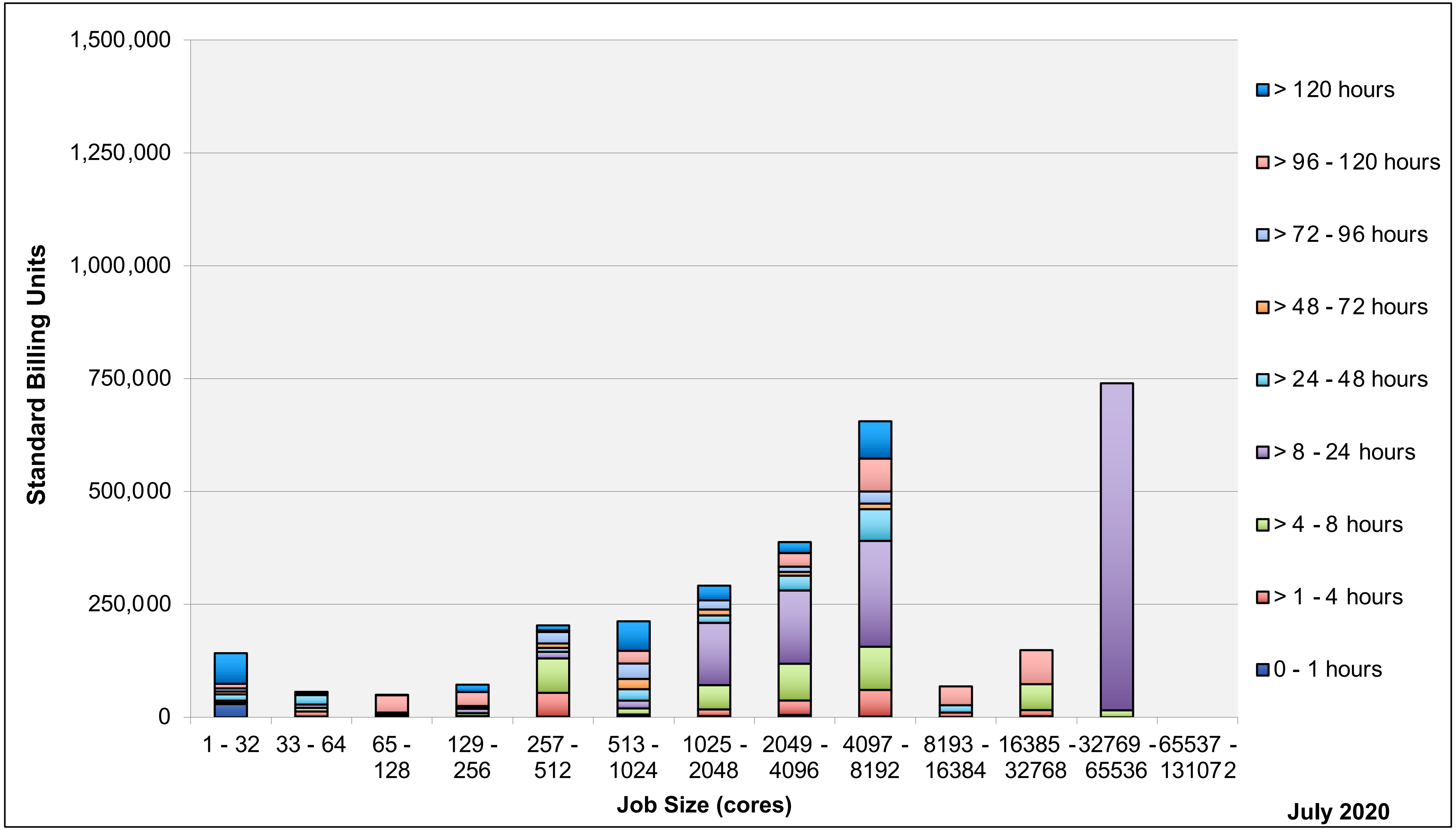

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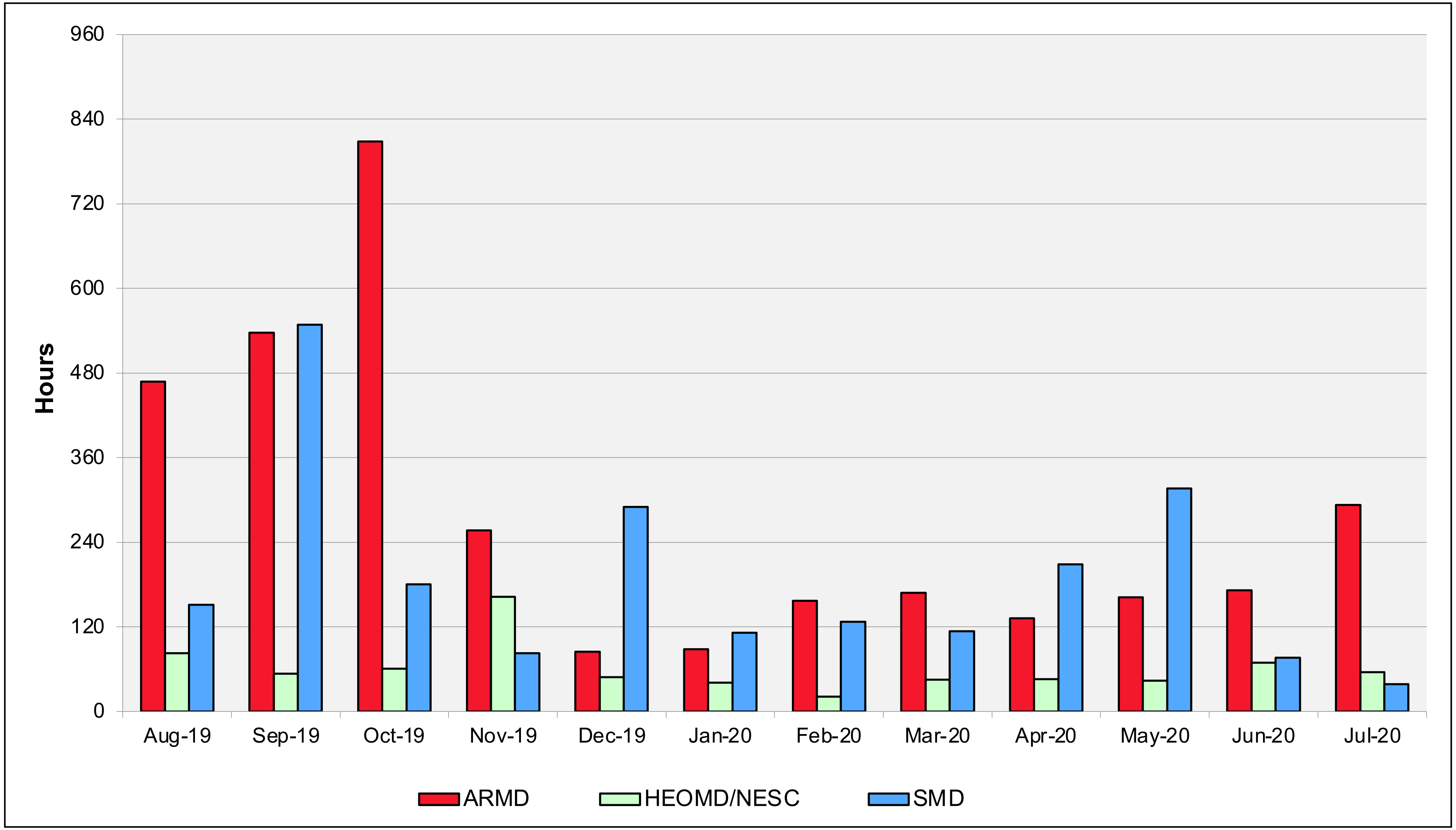

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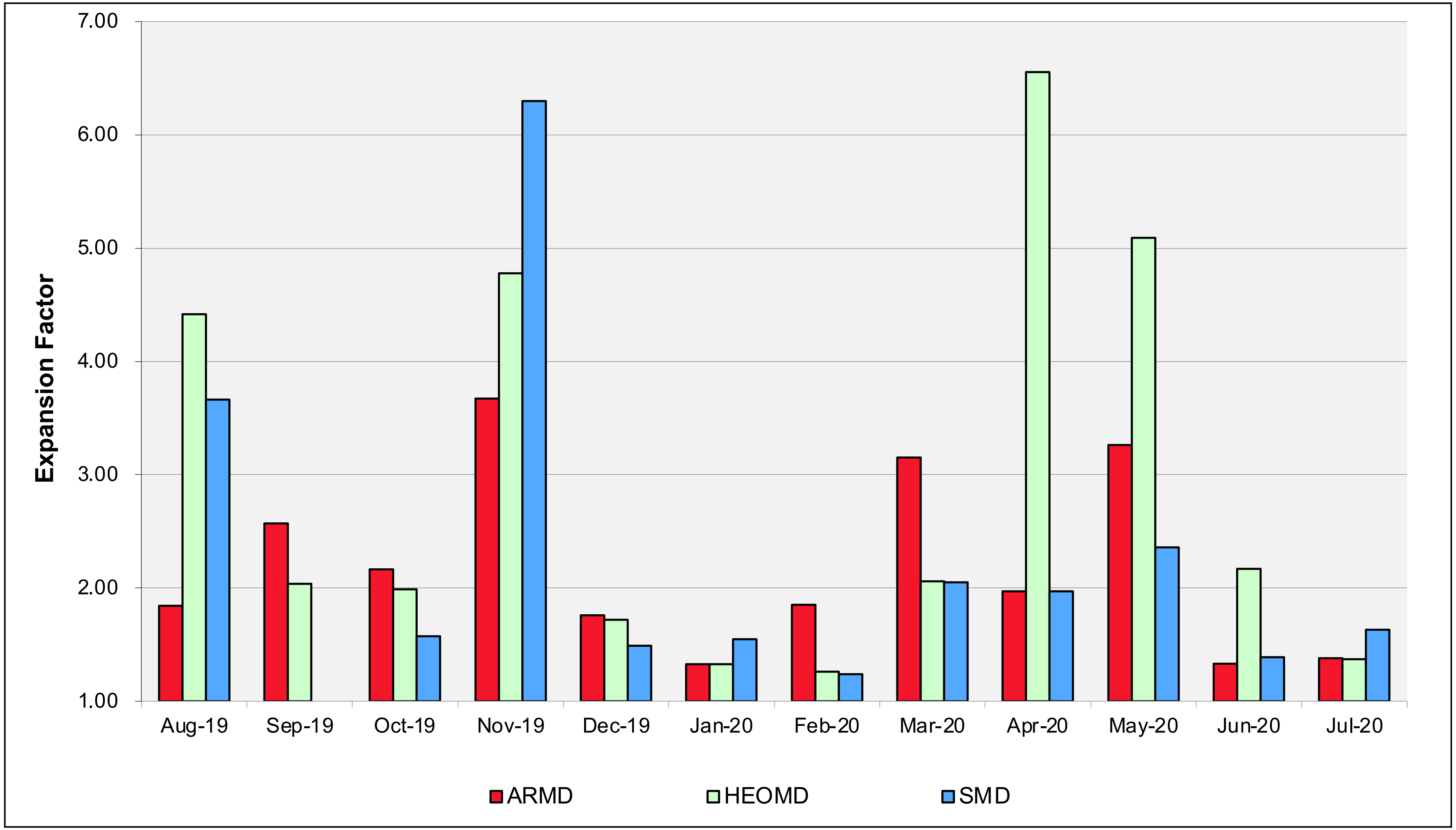
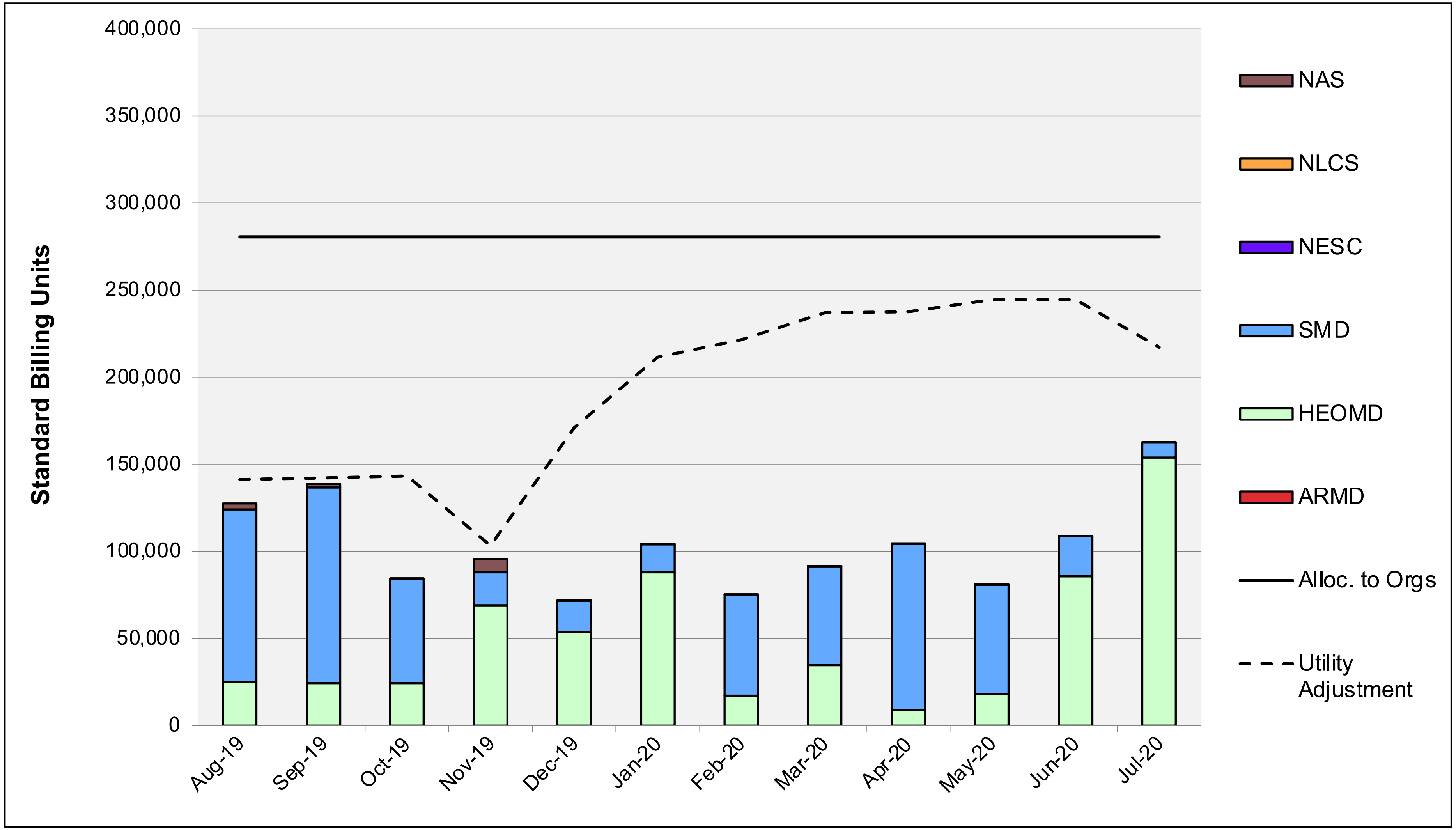


Merope: SBUs Reported, Normalized to 30-Day Month



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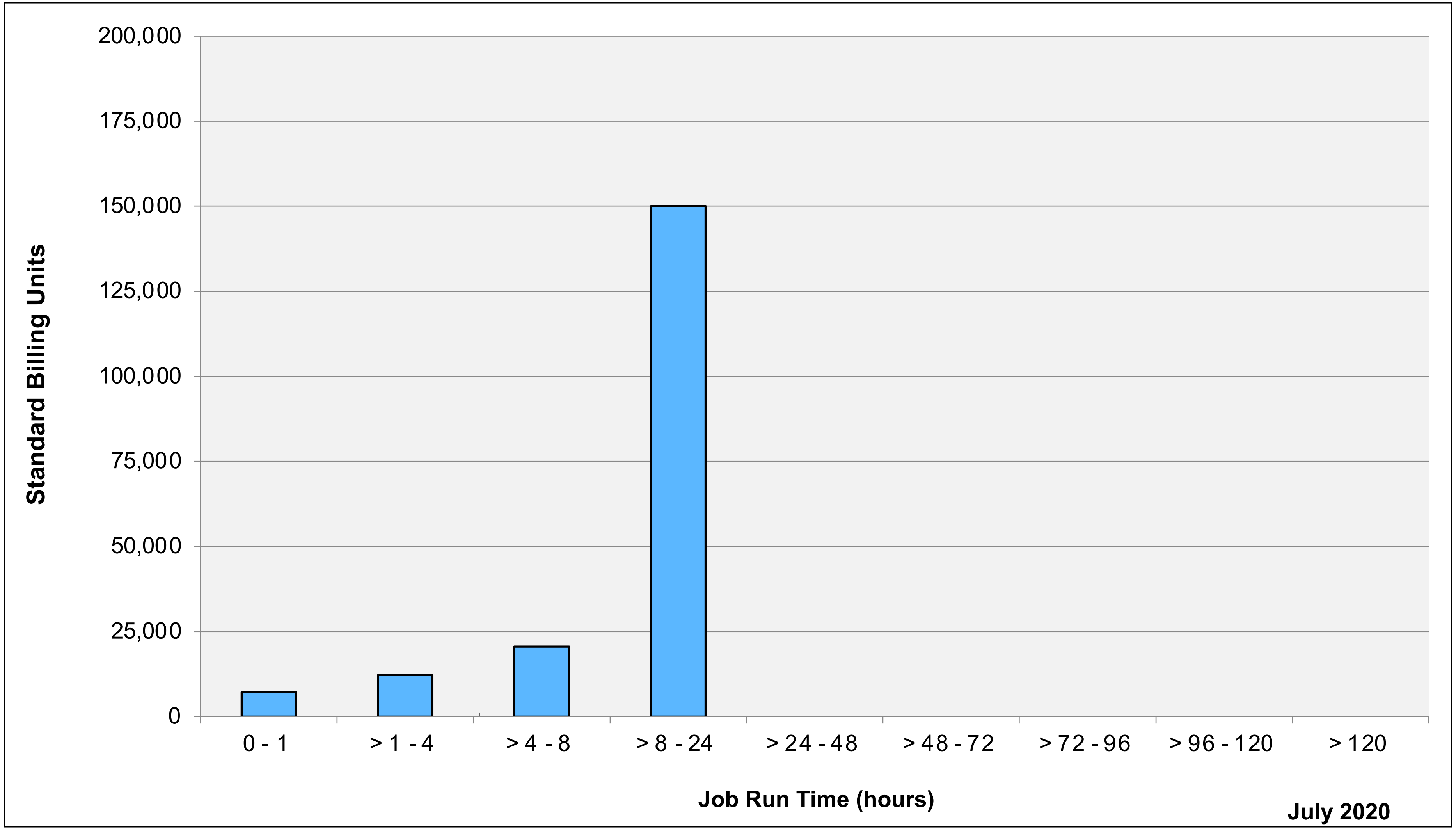

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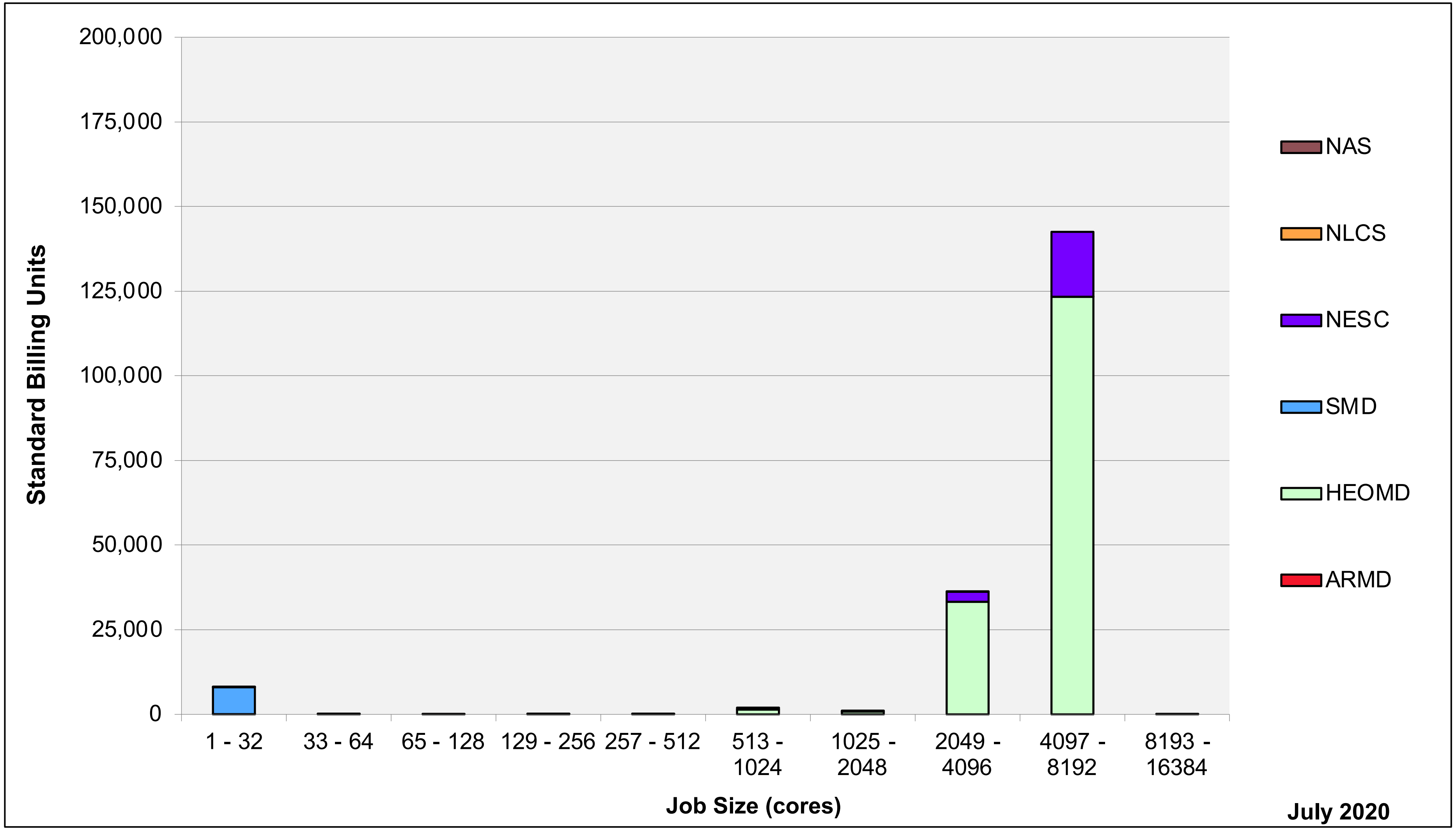
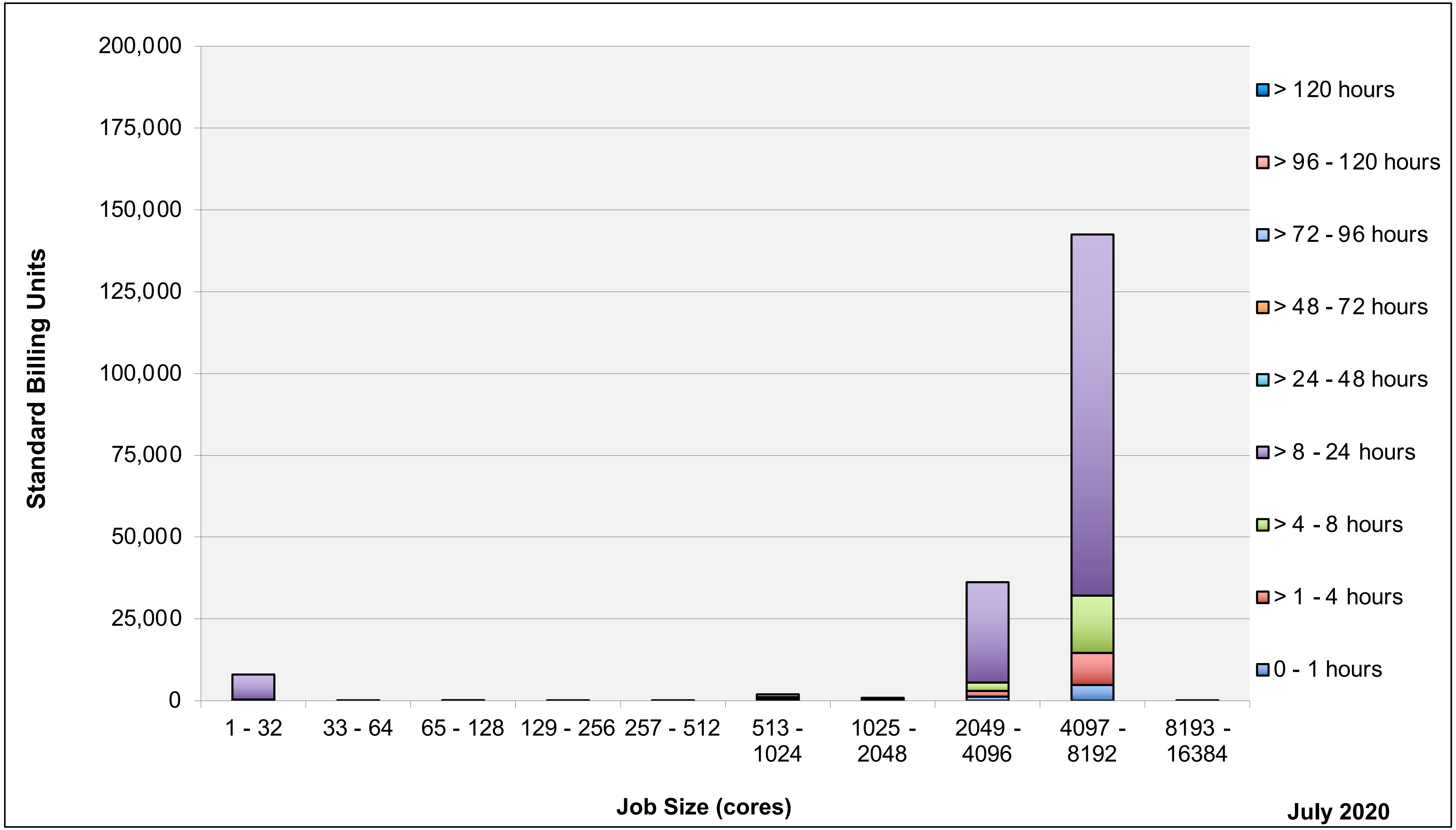
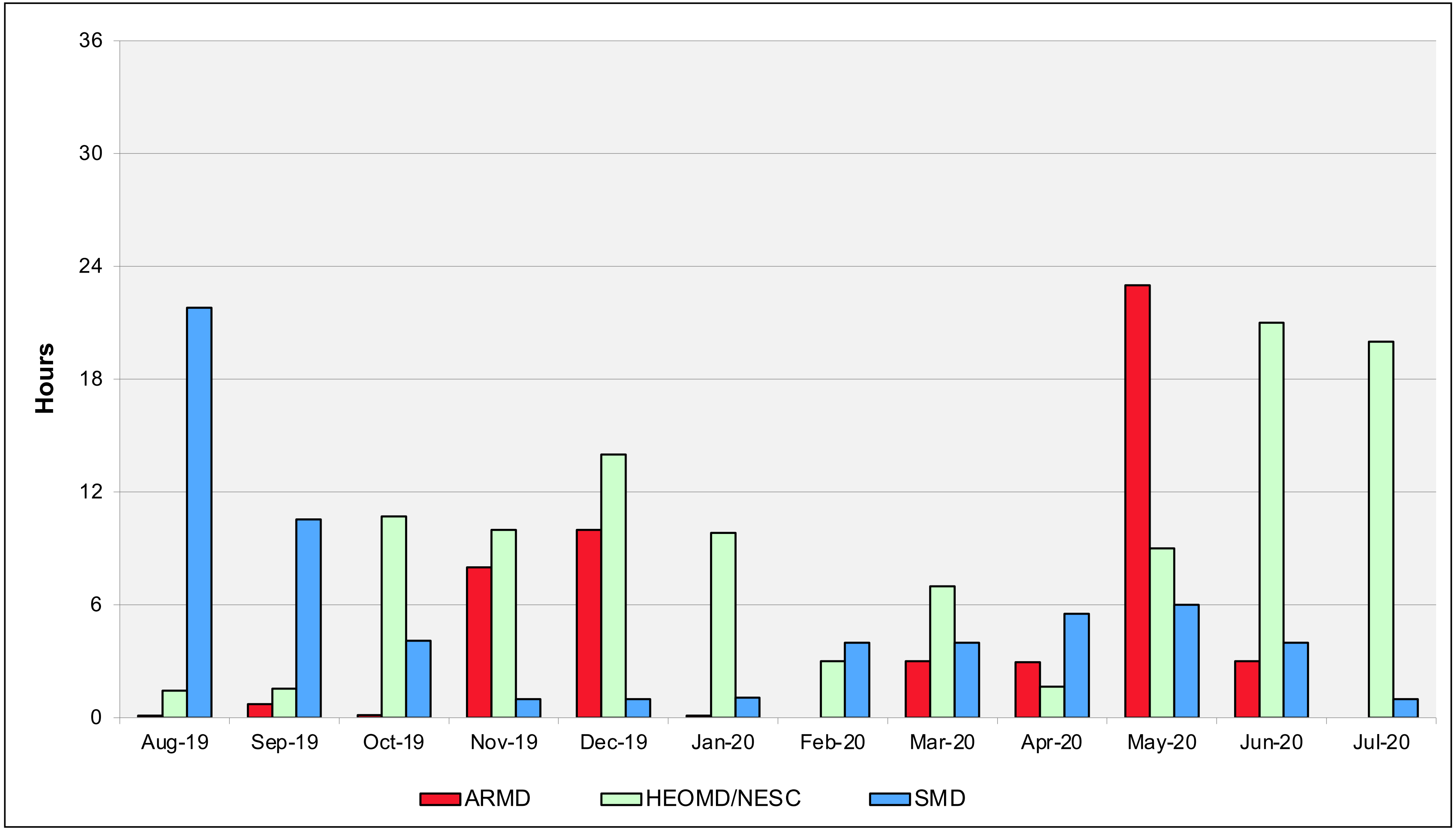


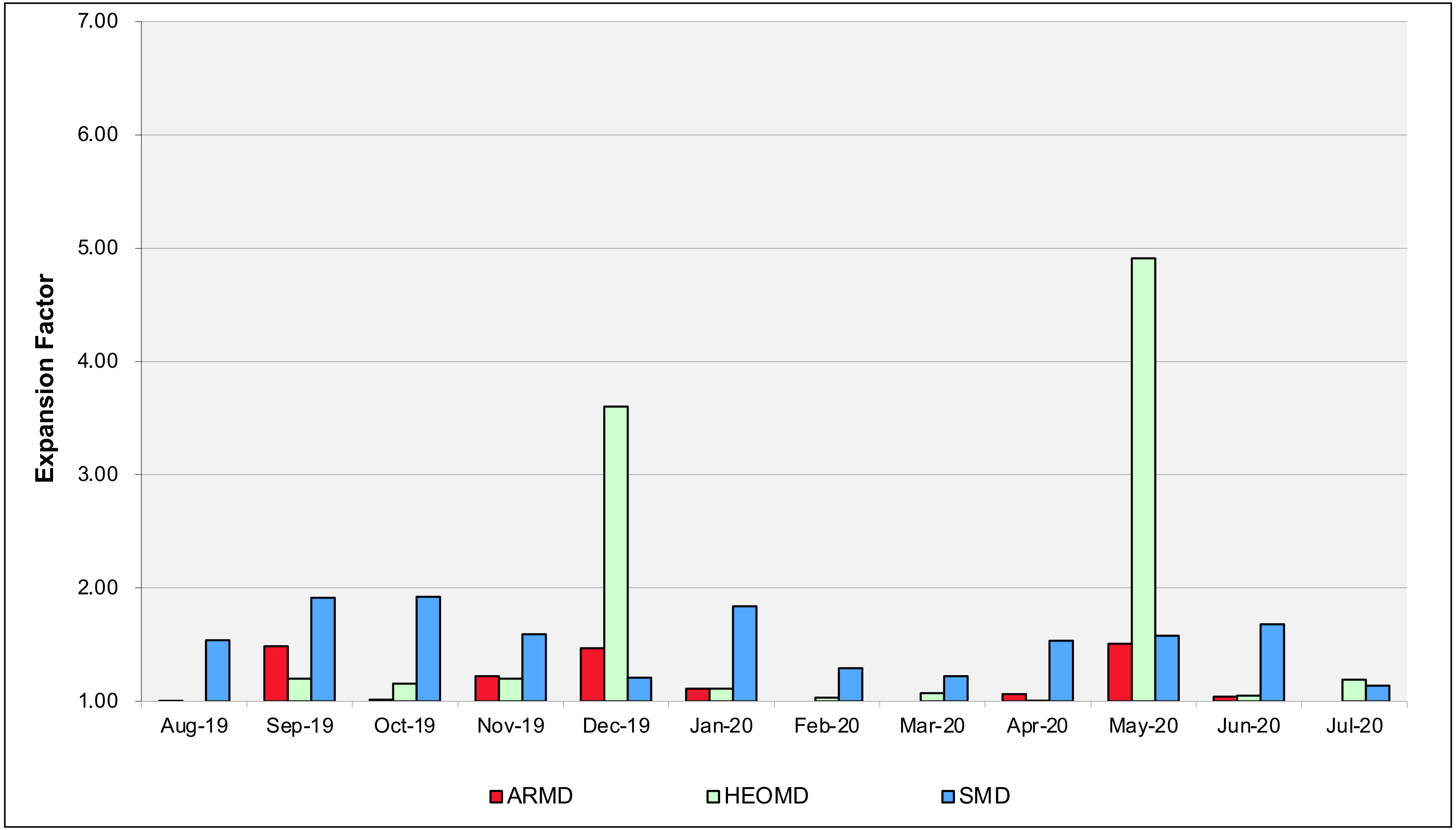
Merope: Monthly Utilization by Size and Length



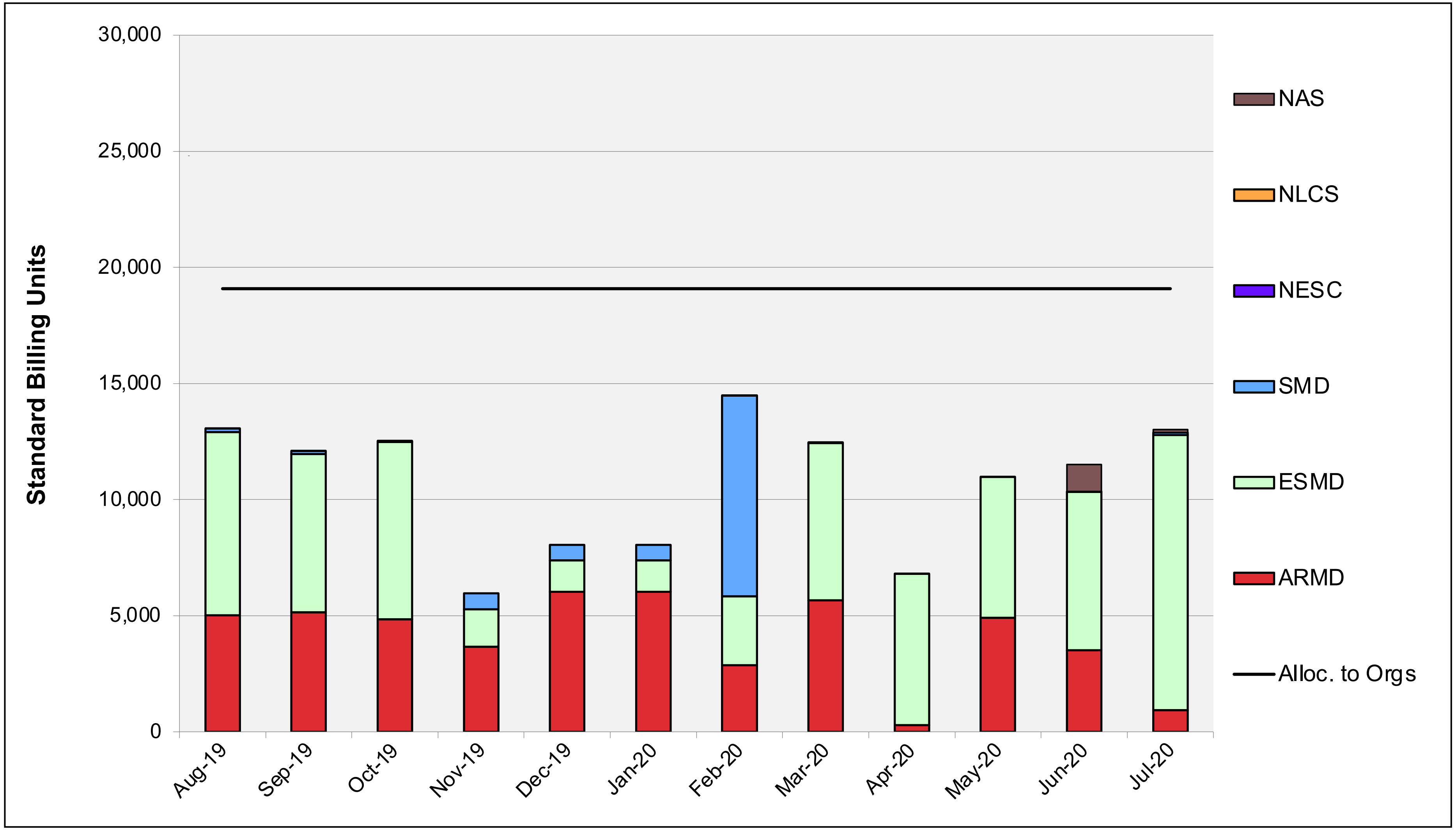
Merope: Average Time to Clear All Jobs



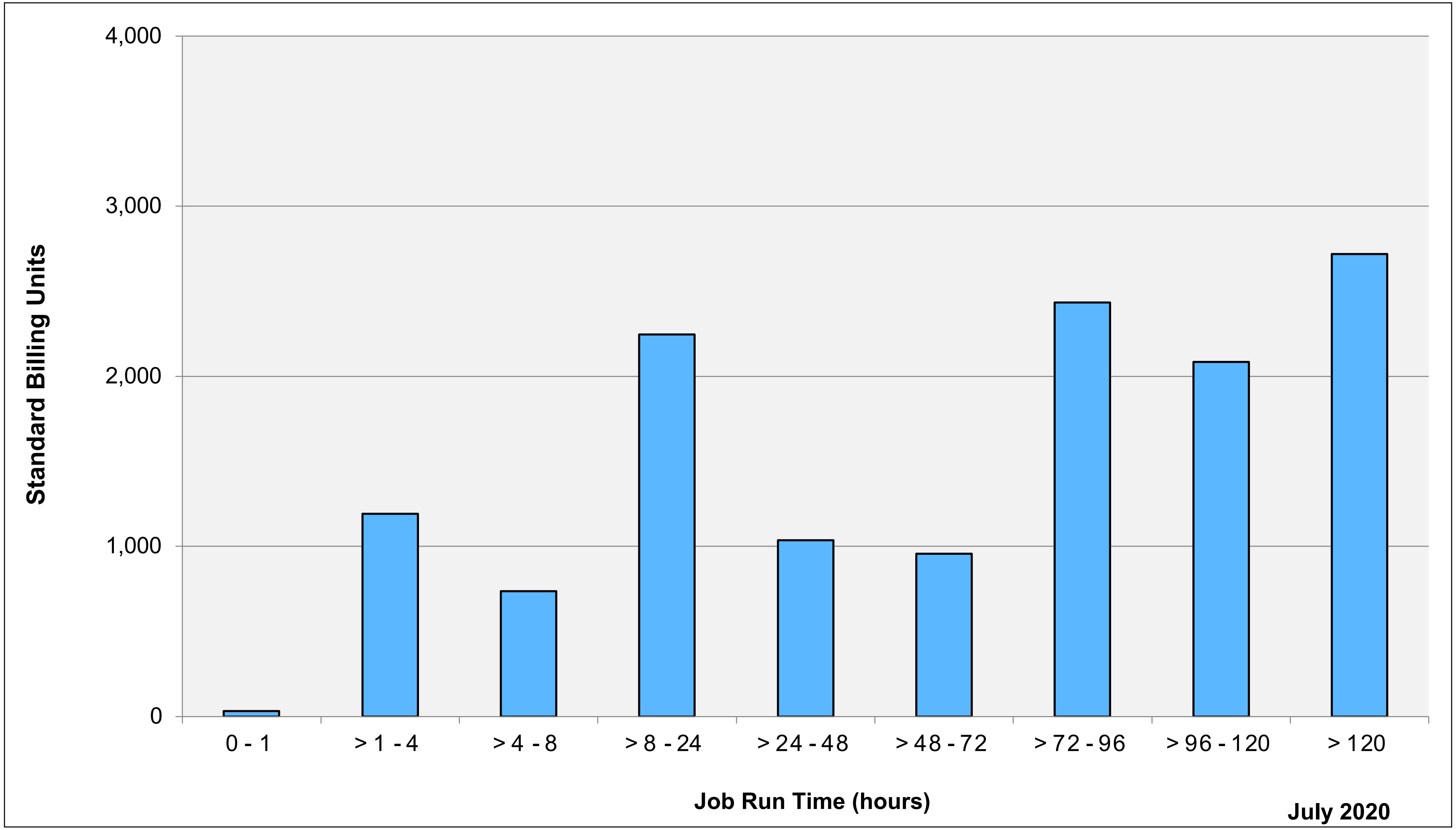
Merope: Average Expansion Factor



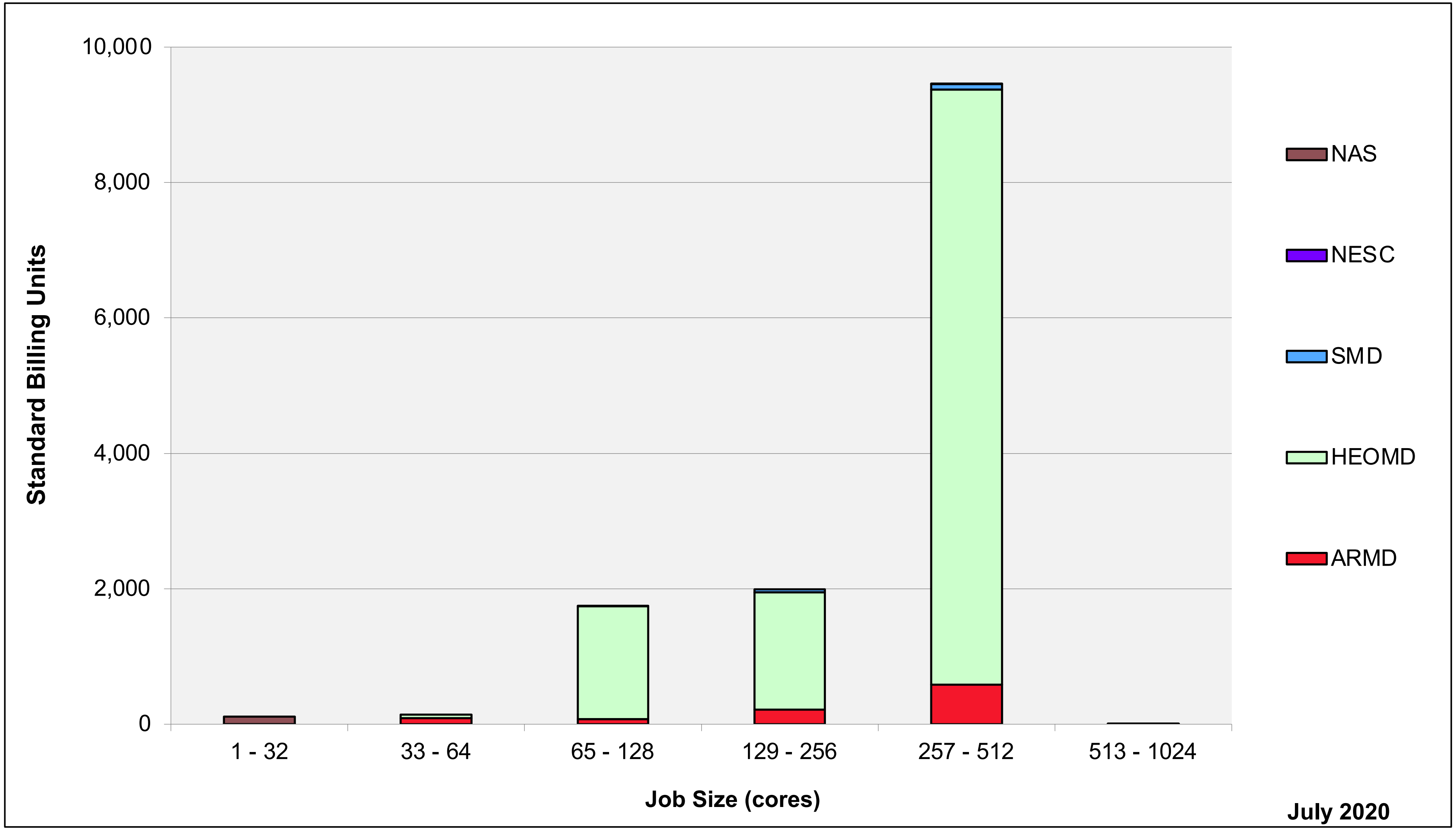
Endeavour: SBUs Reported, Normalized to 30-Day Month



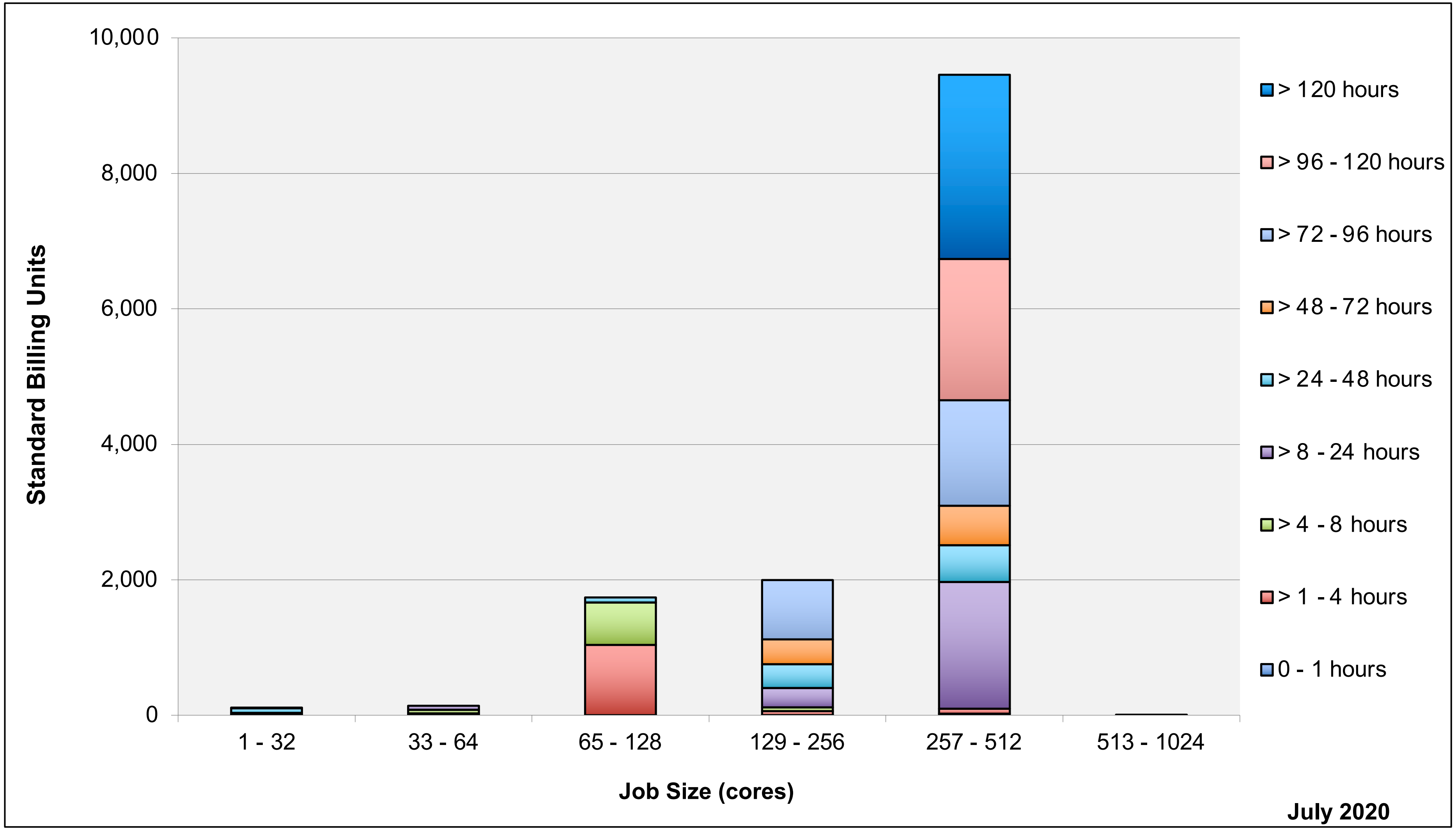
Endeavour: Monthly Utilization by Job Length



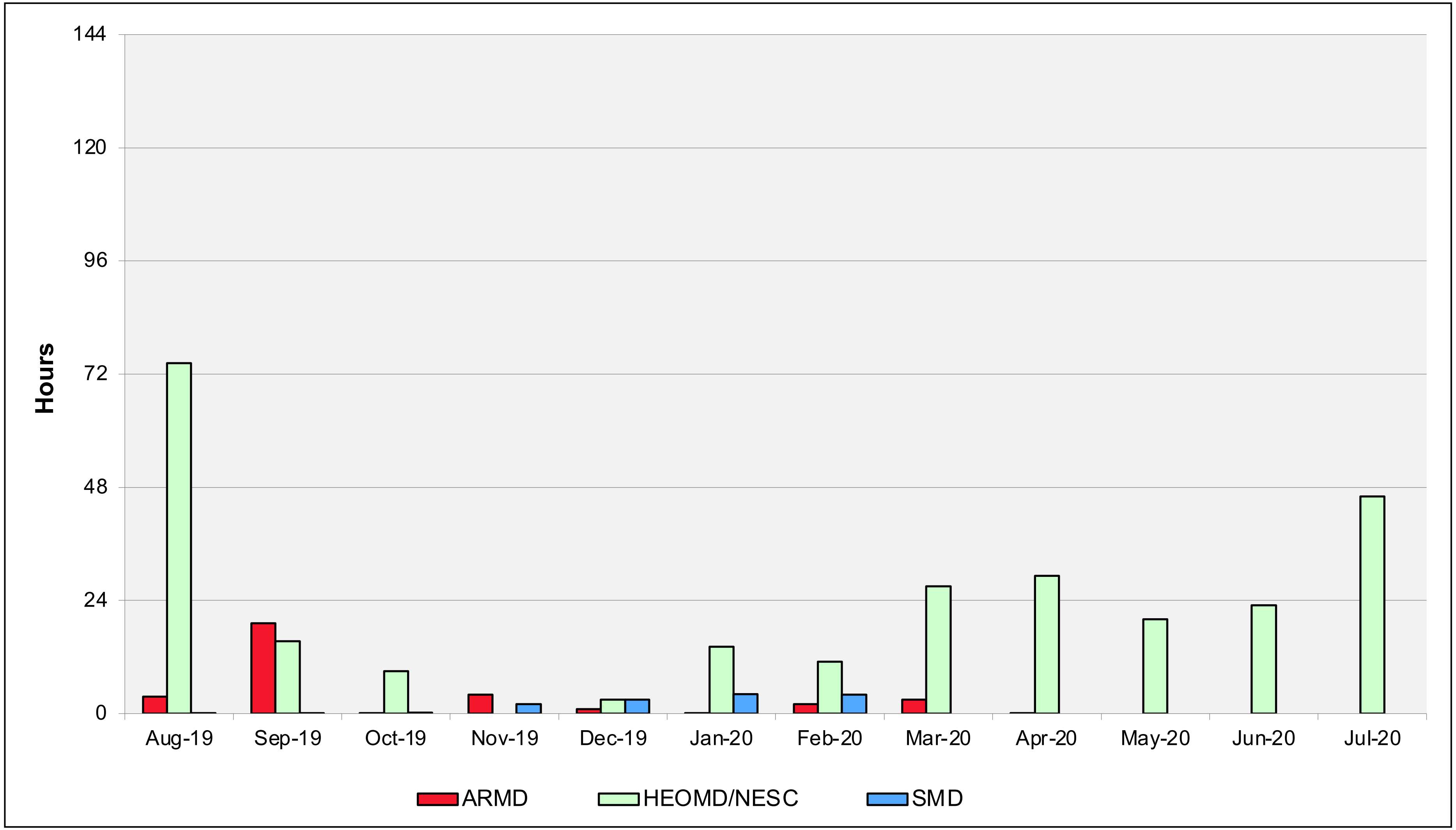
Endeavour: Monthly Utilization by Job Length



Endeavour: Monthly Utilization by Size and Length



Endeavour: Average Time to Clear All Jobs



Endeavour: Average Expansion Factor