HIGH-END COMPUTING CAPABILITY PORTFOLIO

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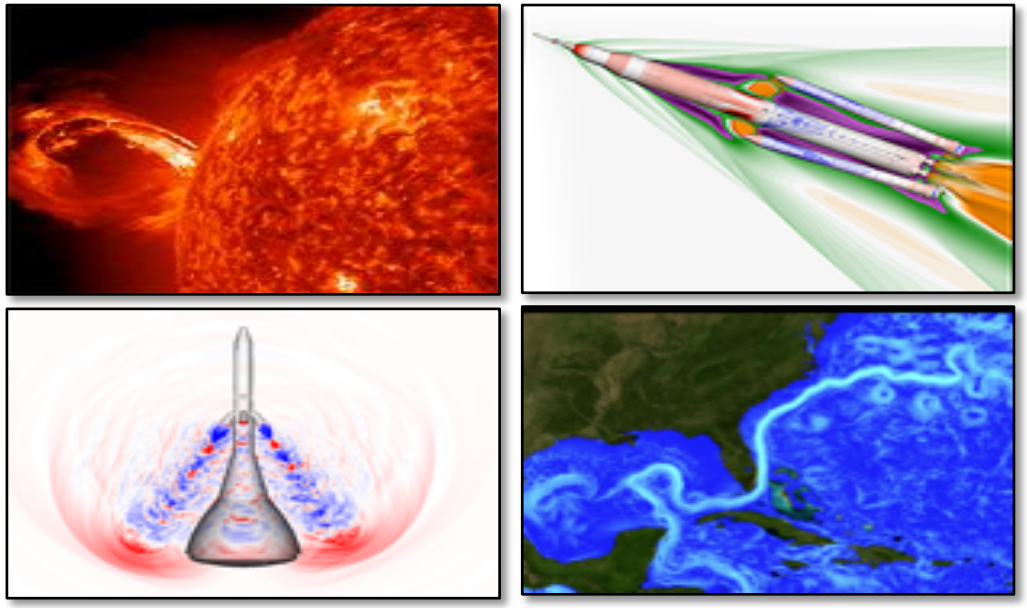
NASA Advanced Supercomputing Division

April 10, 2020

HECC Continues Vital Support During COVID-19 Pandemic

- Beginning March 8, 2020, Ames Research Center went on Mandatory Telework due to the COVID-19 virus. This status was recently extended to May 3, 2020.
- NASA/HECC joined the Department of Energy, National Science Foundation, and private industry to provide access to agency supercomputers to researchers working to fight the COVID-19 virus (see slide 4).
- All HECC remote assets remain operational and accessible to the NASA user community.
  - Control Room analysts continue to come to the center; they maintain social separation, have instituted new cleaning policies for their work areas, and continue to respond to user or system problems as they arise.
  - Systems and Network staff monitor and maintain the compute, storage, and networks from their homes. When critical components require hands-on action, the appropriate staff member is provided access to the center for the limited time needed to resolve the issue.
  - Application, Visualization, Cloud, Machine Learning, and Data Analytics Support staff provide second-level support to the user community from their homes, communicating with the users through email or by telephone, as appropriate.
- Local assets requiring onsite access to use—such as the hyperwall—are being maintained and used as they can; although bringing teams in to view results is not possible.

IMPACT: The ability to maintain the HECC environment for NASA—and now the nation—plays a vital role in the agency's ability to continue our work during the COVID-19 pandemic, and provides valuable resources to "significantly advance the pace of scientific discovery in the fight to stop the virus."

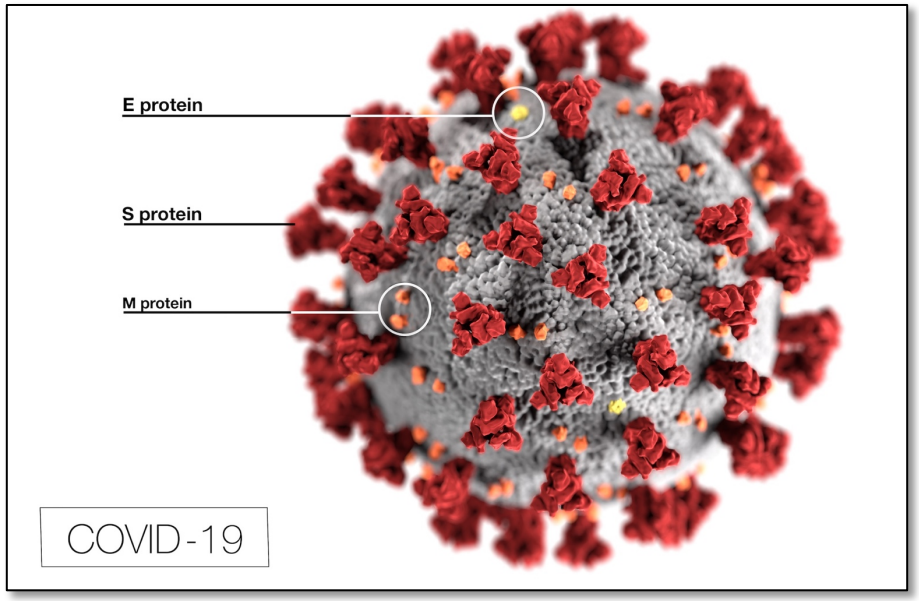


HECC provides a robust environment to tackle NASA's challenges across all mission directorates.

HECC Joins National COVID-19 HPC Consortium

- As part of the COVID-19 High-Performance Computing Consortium recently announced by the White House Office of Science & Technology Policy, NASA is providing access to HECC resources and expertise to support researchers in the fight to understand the pandemic and to develop treatments and vaccines.
- Research proposals submitted to the consortium are reviewed by a panel of experts to quickly assess potential impact, computational feasibility, overall resource requirements, and timeline.
- For proposals that are selected for allocations, HECC support teams are helping researchers create accounts, gain access to the systems, and run their applications.
- Information for researchers and the general public is provided on the HECC website http://www.nas.nasa.gov/hecc.

IMPACT: Access to HECC resources and services provides COVID-19 researchers with a crucial tool in the fight to stop the SARS-CoV-2 virus and find solutions that can help bring an end to the pandemic.

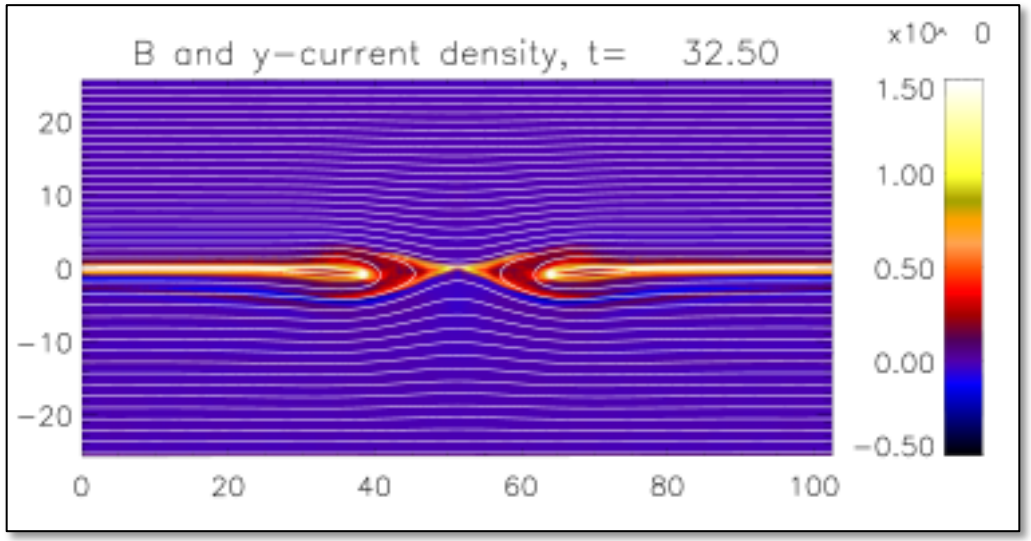


This illustration, created at the Centers for Disease Control and Prevention (CDC), reveals ultrastructural morphology exhibited by coronaviruses. A novel coronavirus, named Severe Acute Respiratory Syndrome coronavirus 2 (SARS-CoV-2), was identified as the cause of coronavirus disease 2019 (COVID-19).

Applications Experts Achieve Performance Win for NASA's Magnetospheric Multiscale Mission

- HECC's Application Performance and Productivity (APP) team identified a runtime fix that reduced the modeling time of magnetic explosions in space by 40%.
- The APP team's weekly power monitoring tool flagged the user's jobs showing potential inefficient node utilization.
  - The total number of processes and threads running on each node was correct, but the 28 threads were bunched up on 14 cores with each core doing double-duty while the remaining 14 cores on each Broadwell node were completely idle.
  - The runtime fix entailed proper placement of the threads so that the work was load balanced across the node.
  - The user was highly impressed by the depth of the team's expert analysis work and willingness to reach out and help.
- This simulation models magnetic reconnection that powers solar eruptions and energizes particles in space to dangerous energy levels.
  - The dramatically reduced execution time enabled more rapid provision of simulations tailored to specific events.
  - Modeling, even in the simplest cases, requires about 250,000 CPU hours per run.

IMPACT: Leveraging the expertise of HECC's application experts improves efficient use of computational assets, reduces users' job turnaround times, and enables additional modeling and simulation.

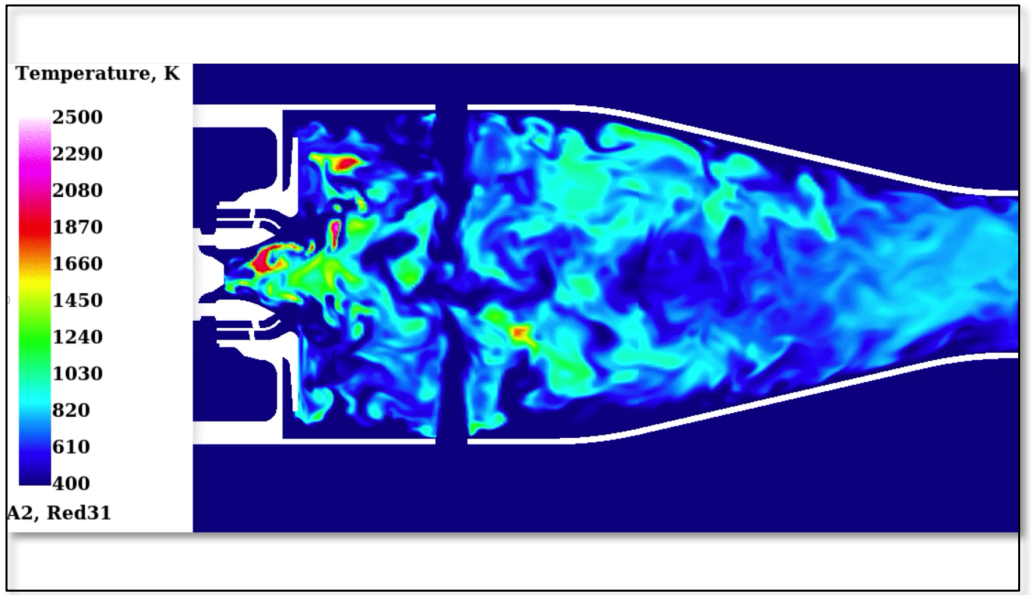


Magnetic field and current density (color) from a high-precision simulation of magnetic reconnection. *Michael Hesse, University of Bergen and Southwest Research Institute*

APP Team Optimizes Heavily Used Turbomachinery Code

- The HECC Applications Performance and Productivity (APP) team recently improved the performance of the OpenNCC code by 35%. OpenNCC is a high-fidelity, three-dimensional unsteady flow solver used at Glenn Research Center for simulations of combustors in gas-turbine engines. In 2019, the code was the 8th highest consumer of compute resources in HECC, using about 2.8% of the total SBUs.
- After porting to the latest versions of the Intel compiler and HPE-MPI library, the APP team identified several opportunities for code improvement:
  - Decreasing the use of expensive floating-point operations, such as divide and square root.
  - Sites with large function call overhead.
  - Communication using many small messages that could be aggregated into fewer, larger ones.
- The user implemented fixes based on APP suggestions and saw a 35% improvement in program performance. If future usage is similar to usage in 2019, this is the equivalent of freeing up nearly one full rack of Broadwell nodes on a continuing basis.

IMPACT: Performance improvements for heavily used codes not only improve the time-to-solution for users' workflows, but also result in system resources being available for other work.

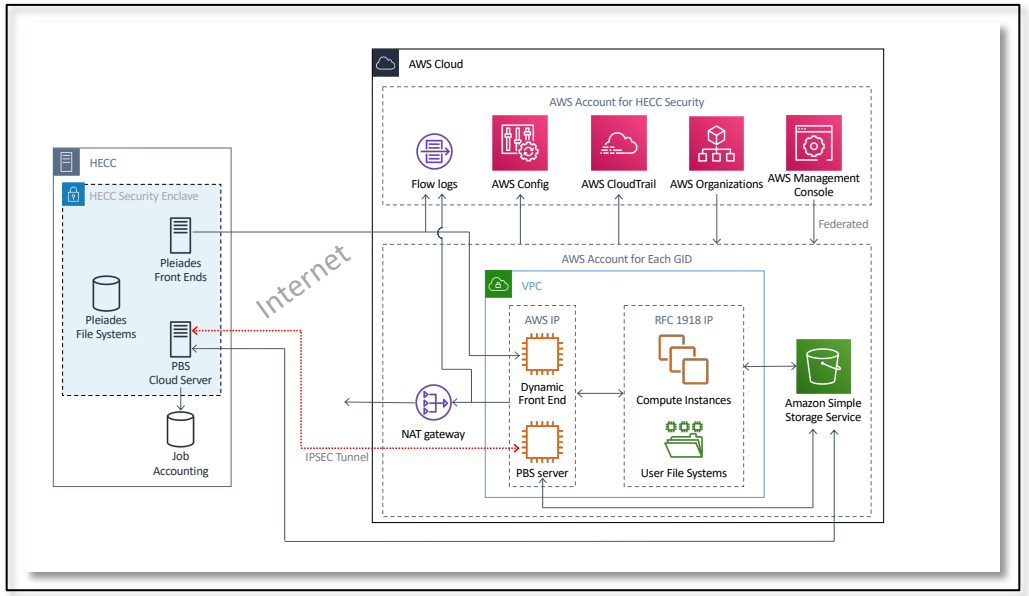


As part of the National Jet Fuel Combustion Program, OpenNCC is being used to study lean blowout, flashback, and combustion dynamics for different jet fuels. This image shows transient temperature involving lean blowout of Cat-A2 fuel. *Thomas Wey, NASA/Glenn*

HECC Cloud Team Performs Impact Analysis for Using HECC Funds on Commercial Clouds

- In order to support mission directorate (MD) leadership in choosing whether to use HECC budget funds to provide access to commercial clouds, the Cloud team recently analyzed the impact of such spending.
- Their analysis showed that funds spent on cloud resources could reasonably only come from the NAS Technology Refresh (NTR) part of HECC's budget. The impact would be a reduction in the computer resources purchased that year to augment existing HECC systems.
- MDs that chose not to spend HECC funds in the cloud would not be affected; the impact would be borne by the MD that did, as follows:
  - For every $1 million spent by an MD on cloud services, its share of the HECC resources purchased by NTR in 2020 would decrease by 1.8M SBUs/year for the lifetime of those resources—likely more than 10M SBUs in total.
  - When all likely costs are included, the $1M spent for spot-price cloud resources would yield the HECC equivalent of 0.66M SBUs of work.

IMPACT: While HECC believes that its on-premises resources are a very good value to the agency, it is also enabling the use of commercial cloud resources in cases where mission directorates determine that it is warranted.

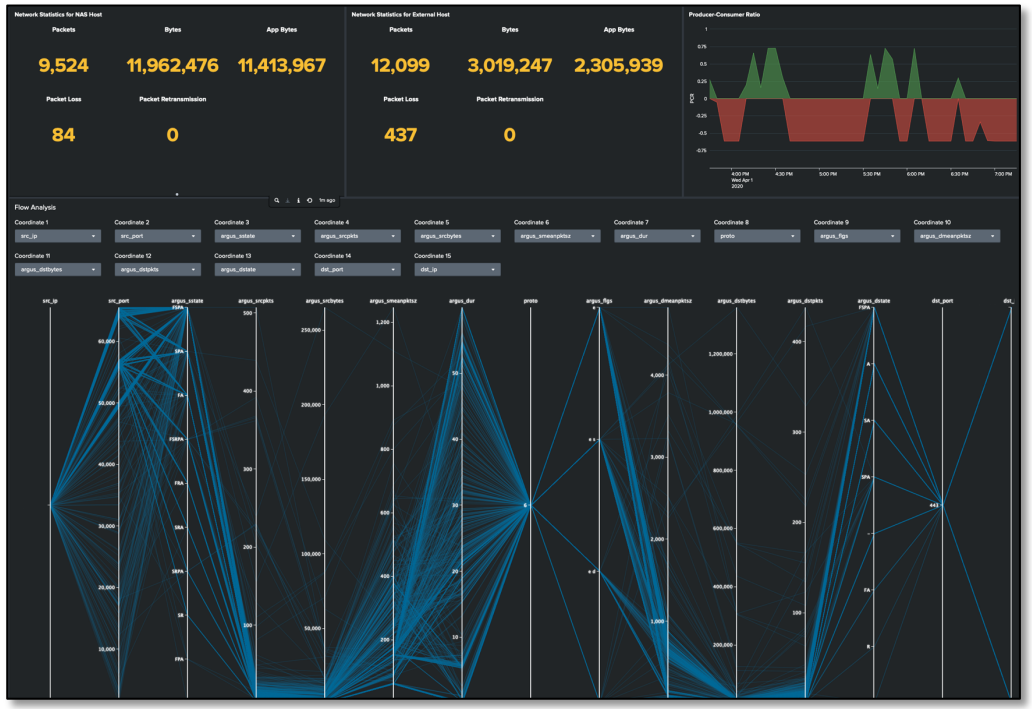


The HECC project implemented a commercial cloud capability that accepts users who bring their own funding. Recent analysis by the Cloud team describes the process by which a mission directorate could use their portion of future HECC expansions to acquire cloud resources.

New Network Flow Analysis Capabilities Improve HECC Security Monitoring System

- HECC security experts added new capabilities to the HECC security monitoring systems. Capabilities include:
  - Network flow statistics, including total packets, bytes, and application bytes sent and received; and packet loss and retransmission statistics.
  - Producer-consumer ratio for network flow activity used to identify signs of data exfiltration and other malicious activity.
  - Fully interactive parallel coordinate plot of network flow activity, allowing security analysts to visualize the relationship between the 86 flow attributes in 16 coordinates.
- These increased capabilities provide the Security team with greater insight into suspicious activity that may indicate compromise, as well as how HECC computer systems communicate with external computer systems.

IMPACT: New capabilities provide security analysts with unified tool to analyze network traffic, providing better awareness of the threats and risks to HECC resources.



Screenshot of part of the Flow Analysis Dashboard showing flow statistics, producer-consumer ratio, and parallel coordinate plot of flow activity.

Network Software Upgraded to Mitigate Security Risks

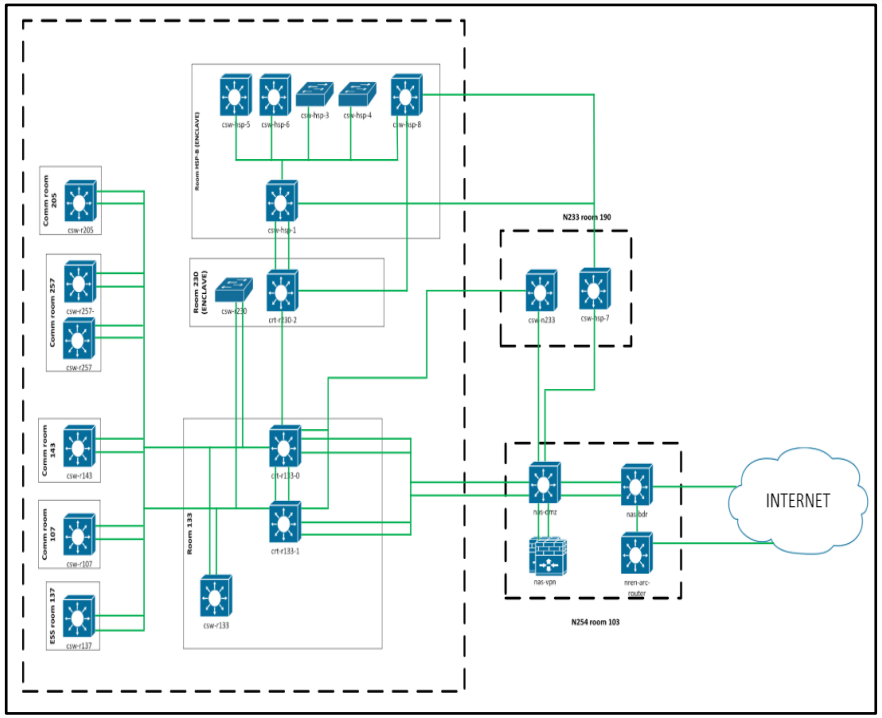
- HECC network engineers recently completed operating system software upgrades on the NAS network to mitigate risks from identified security vulnerabilities.
- The network comprises a variety of 23 routers, switches, and virtual private network appliances. The following access switches connect end users to the NAS network; these switches were upgraded first, as they had less impact on the network:

csw-r107	csw-r143
csw-r205	csw-257
csw-r257-vis	csw-r226a
csw-r137	Vpnac

- Later, the core and distribution network switches and routers that connect the NAS network with the Internet were upgraded:

nas-bdr	nas-dmz
csw-n233	csw-r133
crt-r230-2	crt-r133-0
crt-r133-1	

IMPACT: Software upgrades on agency network devices fix software bugs and security vulnerabilities, improve device functionality, and sometimes introduce new features to the operating system.

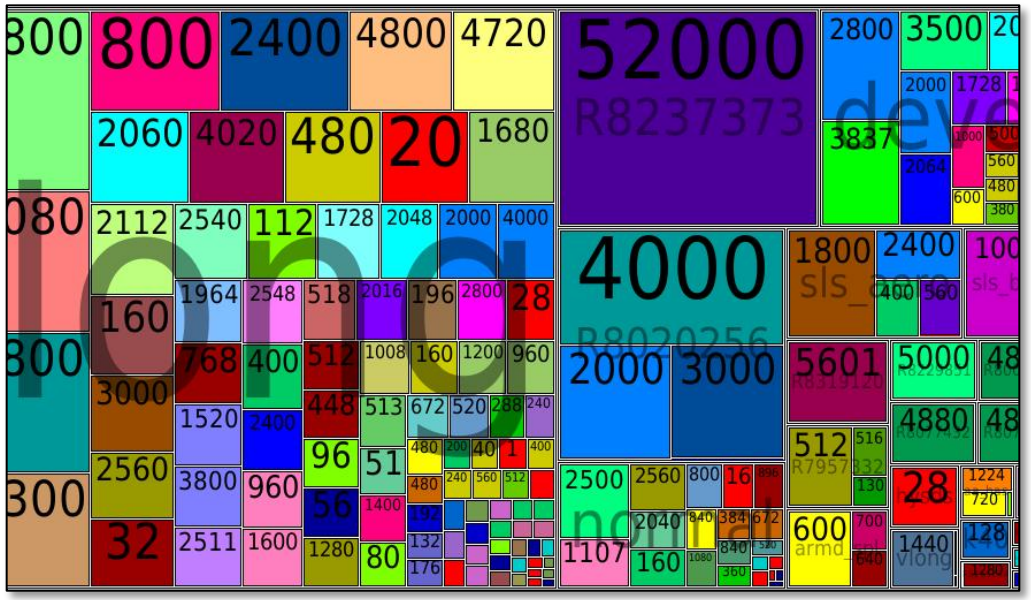


NAS network topology diagram showing all network switches and routers on the network.

Systems Team Upgrades Supercomputing Job Software

- HECC engineers recently completed the deployment of the PBS Professional (PBSPro) batch scheduler software to version 19 on Pleiades, Electra, Aitken and Merope.
- In order to migrate to PBSPro 19, several person-months of HECC staff developer time was needed to port, test and verify the NASA specific modifications with PBSPro 19 as there was significant changes from the previous version.
- With the new version of PBSPro, several features were added that will be beneficial to HECC users and include the ability to alter reservation start time and/or duration, sending job output directly to the user's directory, support for multiple schedulers and support for better limits on memory usage of jobs.
- The roll out was staggered with the first system being Merope so that issues could be identified and resolved prior to deploying more broadly. Once we were confident in the software, PBSPro 19 was installed on Pleiades, Electra, and Aitken.

IMPACT: Users will benefit from new features developed by the vendor specifically for the HECC environment. Several of these features improve reliability for large jobs.



Snapshot of running jobs, showing core counts for each job, grouped by PBS queue.

Urban Air Mobility and Quadcopter Simulations Take Flight at GoFly Event

- On leap day (February 29), Moffett Airfield at NASA Ames hosted the GoFly Prize Final Fly-Off contest.
  - GoFly is a unique event where participants from around the world compete by building personal flying devices that must be safe, quiet, ultra-compact, and near-VTOL—and, capable of carrying a single person for a distance of 20 miles without refueling or recharging.
  - The event had a capacity of 800 attendees, and staff in the Ames booth greeted approximately 700 who were eager to speak with experts showing visualizations on urban air mobility and predicting quadcopter drone noise using the Lattice Boltzmann Method, as well describing how simulations are made and the role of distributed computing.
- The exhibit had several high-profile visitors, including ARMD Associate Administrator Robert Pearce and Ames Center Director Eugene Tu. While aerodynamics simulations were the main focus, most attendees were equally interested in the example of distributed computing by the Raspberry Pi cluster demo and the simulation process.

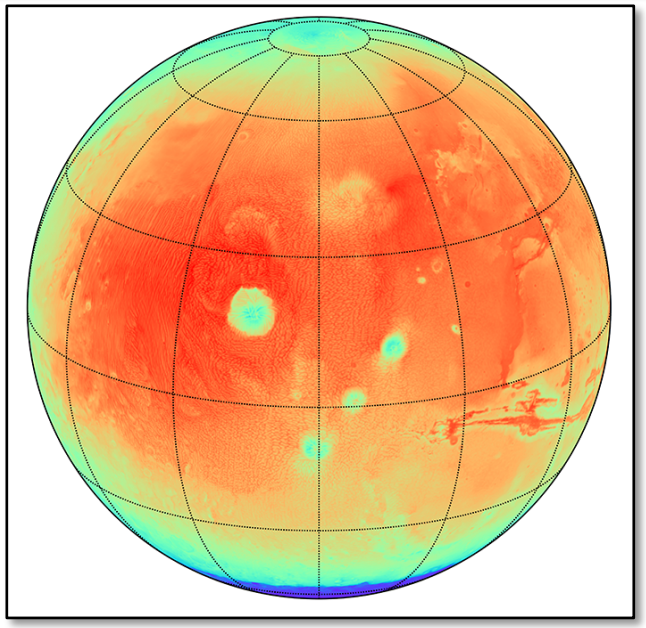
Impact: NASA's exhibit at GoFly provided an excellent public outreach opportunity to highlight the critical role of HECC resources in aerodynamic engineering.

NAS Division scientist Patricia Ventura Diaz demonstrates her work on urban air mobility to ARMD Associate Administrator Robert Pearce (at left).

Numerically Modeling the Weather and Climate of Mars*

- Planetary scientists at Aeolis Research ran numerical atmospheric and climate models on the Pleiades supercomputer to improve both the understanding of the basic physics of Martian meteorology and the forecasting of conditions for design and operation of NASA spacecraft.
- Better study of Mars—in many ways analogous to the Earth's climate system—allows better understanding of fundamental planetary climate system behaviors, and testing terrestrial meteorological and climate models in novel regimes.
- The scientists developed Martian adaptations of the National Center for Atmospheric Research (NCAR) Weather Research and Forecasting (WRF) and Model for Prediction Across Scales (MPAS) terrestrial models at the micro-, meso-, and global scales.
- Results enabled a range of observations to be conceptually understood; for example, Curiosity rover observations of surface pressure are now widely understood in terms of a locally induced hydrostatic rebalancing of air over the varying local topographic relief, in addition to the more commonly understood large-scale thermal tides.

Impact: The wide variety of studies supported by this modeling helps NASA achieve its goal of understanding how planetary systems work and assists the agency in designing and operating spacecraft.



Daytime near-surface (8 meters) air temperature simulated by the Mars Weather Research and Forecasting (MarsWRF) model projected on a globe. Deep blue is 150 Kelvin (K); deep red is 230 K. Major Martian volcanoes appear as roughly oval shapes. *Mark Richardson, Aeolis Research*

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

HECC Facility Tours in March 2020

- HECC hosted two tour groups in March; guests learned about the agency-wide missions being supported by HECC assets, and also viewed the D-Wave 2000Q quantum system. Visitors this month included:
  - A technical group from the Federal Aviation Administration (FAA).
  - A group of interns from the NASA Academic Mission Services (*NAMS*) Student Research & Development (*R&D*) Program who are working with Universities Space Research Association at Ames.

Darrel Robertson (right), a research engineer in the NASA Advanced Supercomputing (NAS) Division, briefs guests from Federal Aviation Administration, showing them the D-Wave Quantum 2000Q system. *Gina Morello, NASA/Ames*

Papers

- "**Pre-Common-Envelope Mass Loss from Coalescing Binary Systems**," M. MacLeod, A. Loeb, arXiv:2003.01123 [astro-ph.SR], March 2, 2020. *
  https://arxiv.org/abs/2003.01123
- "**The CARMENES Search for Exoplanets Around M Dwarfs. Two Planets on the Opposite Sides of the Radius Gap Transiting the Nearby M Dwarf LP 729-54**," G. Nowak, et al., arXiv:2003.01140 [astro-ph.EP], March 2, 2020. *
  https://arxiv.org/abs/2003.01140
- "**A Pair of TESS Planets Spanning the Radius Valley Around the Nearby Mid-M Dwarf LTT 3780**," R. Cloutier, et al., arXiv:2003.01136 [astro-ph.EP], March 2, 2020. *
  https://arxiv.org/abs/2003.01136
- "**Energetic Submesoscale Dynamics in the Ocean Interior**," L. Siegelman, Journal of Physical Oceanography, March 3, 2020. *
  https://journals.ametsoc.org/doi/10.1175/JPO-D-19-0253.1?mobileUi=0
- "**Characterizing the Radio Quiet Region Behind the Lunar Farside for Low Radio Frequency Experiments**," N. Bassett, et al., arXiv:2003.03468 [astro-ph.IM], March 6, 2020. *
  https://arxiv.org/abs/2003.03468
- "**A Link Between Ram Pressure Stripping and Active Galactic Nuclei**," A. Ricarte, et al., arXiv:2003.05950 [astro-ph.GA], March 12, 2020. *
  https://arxiv.org/abs/2003.05950

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

Papers (cont.)

- "**Three Short Period Jupiters from TESS**," L. D. Nielsen, et al., arXiv:2003.05932 [astro-ph.EP], March 12, 2020. * https://arxiv.org/abs/2003.05932
- "**Systematic Phase Curve Study of Known Transiting Systems from Year 1 of the TESS Mission**," I. Wong, et al., arXiv:2003.06407 [astro-ph.EP], March 13, 2020. * https://arxiv.org/abs/2003.06407
- "**A Small and Round Heliosphere Suggested by Magnetohydrodynamic Modelling of Pick-Up Ions**," M. Opher, A. Loeb, J. Drake, G. Toth, Nature Astronomy, published online March 16, 2020. * https://www.nature.com/articles/s41550-020-1036-0
- "**Effects of Atmospheric Turbulence Unsteadiness on Ship Airwakes and Helicopter Dynamics**," R. Thedin, S. Murman, J. Horn, S. Schmitz, Journal of Aircraft, published online March 17, 2020. * https://arc.aiaa.org/doi/full/10.2514/1.C035643
- "**impact of Current-Wind Interaction on Vertical Processes in the Southern Ocean**," H. Song, et al., Journal of Geophysical Research: Oceans, vol.125, issue 4, March 17, 2020. * https://agupubs.onlinelibrary.wiley.com/doi/abs/10.1029/2020JC016046
- "**LHS 1815b: The First Thick-Disk Planet Detected by TESS**," T. Gan, A. Shporer, J. Livingston, et al., The Astronomical Journal, vol. 159, no. 4, March 18, 2020. * https://iopscience.iop.org/article/10.3847/1538-3881/ab775a/meta

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

Papers (cont.)

- "**TESS Spots a Hot Jupiter with an Inner Transiting Neptune**," C. Huang, S. Quinn, A. Vanderburg, et al., The Astrophysical Journal Letters, vol. 892, no. 1, March 19, 2020. *
  https://iopscience.iop.org/article/10.3847/2041-8213/ab7302/meta
- "**Origin of Star-Forming Rings around Massive Centres in Massive Galaxies at $z<4$**," A. Dekel, et al., arXiv:2003.08984 [astro-ph.GA], March 19, 2020. *
  https://arxiv.org/abs/2003.08984
- "**The TESS-Keck Survey I: A Warm Sub-Saturn-Mass Planet and Caution about Stray Light in TESS Cameras**," P. Dalba, et al., arXiv:2003.10451 [astro-ph.EP], March 23, 2020. *
  https://arxiv.org/abs/2003.10451
- "**A Remnant Planetary Core in the Hot Neptunian Desert**," D. Armstrong, T. Lopez, V. Adibekyan, et al., arXiv:2003.10314 [astro-ph.EP], March 23, 2020. *
  https://arxiv.org/abs/2003.10314
- "**Cropland Carbon Uptake Delayed and Reduced by 2019 Midwest Floods**," Y. Yin, et al., American Geophysical Union Advances, vol.1, issue 1, March 25, 2020. *
  https://agupubs.onlinelibrary.wiley.com/doi/full/10.1029/2019AV000140

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

Presentations

- “**NASA Advanced Supercomputing Division at GoFly**,” J. Boustani, presented at the GoFly Event, Moffett Field, California, February 29, 2020. https://ntrs.nasa.gov/archive/nasa/casi.ntrs.nasa.gov/20200001464.pdf (10.7 MB)
- **"NASA’s High-End Computing Capability Project: Analysis and Visualization of Scientific Data"** P. Mehrotra, presented at the National Academy of Sciences' Space Science Week, March 31, 2020.

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

News & Events

- **We All Live in a Croissant-Shaped Giant Bubble, Say Astronomers**, *Forbes*, March 22, 2020—Physicists using the Pleiades supercomputer at the NASA Advanced Supercomputing Facility have revealed a refined new model of the heliosphere–the vast region around the Sun extending more than twice as far as Pluto. https://www.forbes.com/sites/jamiecartereurope/2020/03/22/we-all-live-in-a-croissant-shaped-giant-bubble-say-astronomers/#65ef2b401642
- **White House Announces New Partnership to Unleash U.S. Supercomputing Resources to Fight COVID-19**, *White House Statement*, March 23, 2020—The White House announced the launch of the COVID-19 High Performance Computing Consortium to provide COVID-19 researchers worldwide with access to the world's most powerful high performance computing resources that can significantly advance the pace of scientific discovery in the fight to stop the virus. This unique public-private consortium, spearheaded by The White House, the U.S. Department of Energy, and IBM, includes government, industry, and academic leaders who have volunteered free compute time and resources on their machines, including the NASA Advanced Supercomputing Facility. https://www.whitehouse.gov/briefings-statements/white-house-announces-new-partnership-unleash-u-s-supercomputing-resources-fight-covid-19/
- **NASA Supercomputers Join Fight Against Coronavirus**, *Space.com*, March 23, 2020—As the U.S. scrambles to respond to the spreading COVID-19 pandemic, NASA supercomputers are joining the effort to look for potential treatment and vaccine candidates. https://www.space.com/nasa-supercomputers-join-fight-against-coronavirus.html

News & Events (cont.)

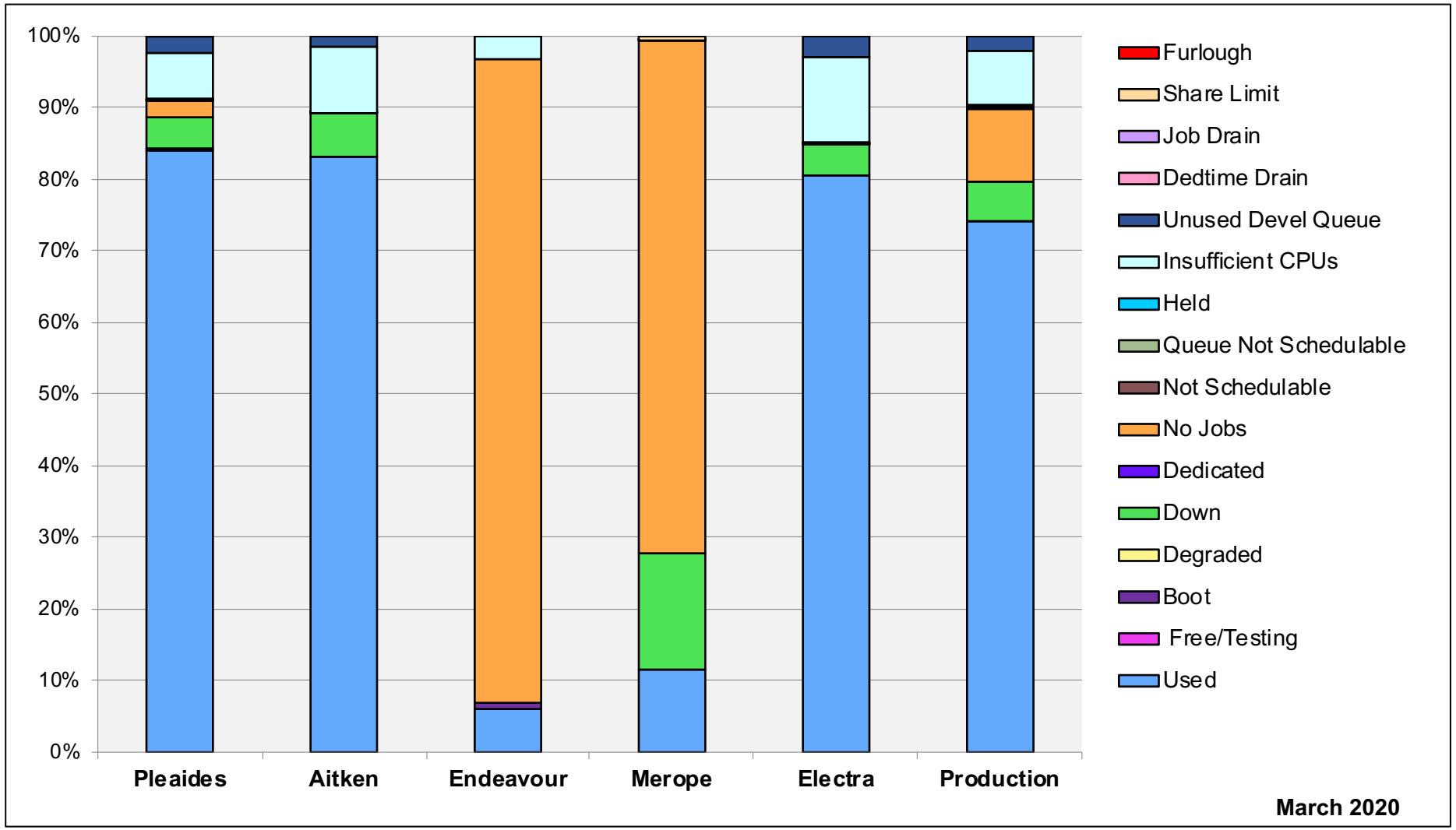
- **Can Enough Federal Petaflops Whack the Virus?**, *Federal Drive with Tom Temin*, March 30, 2020—Thanks to a collaboration led by NASA and the National Science Foundation, much of the U.S. supercomputing capacity will become available to researchers looking for answers about coronavirus. The COVID-19 High Performance Computing Consortium, is already receiving proposals to use the offered supercomputers, according to Piyush Mehrotra, NASA Advanced Supercomputing Division Chief. https://federalnewsnetwork.com/tom-temin-commentary/2020/03/can-enough-federal-petaflops-whack-the-virus/

  - **Tackling the Coronavirus with Supercomputers**, *Federal News Network,* March 31, 2020—In the search to understand the coronavirus and its implications, the government is marshaling much of its supercomputer capacity. That includes NASA and its high-performance computing complex. In this podcast, *Federal Drive with Tom Temin* turned to NASA Advanced Supercomputing Division Chief, Piyush Mehrotra. https://federalnewsnetwork.com/technology-main/2020/03/tackling-the-coronavirus-with-supercomputers/

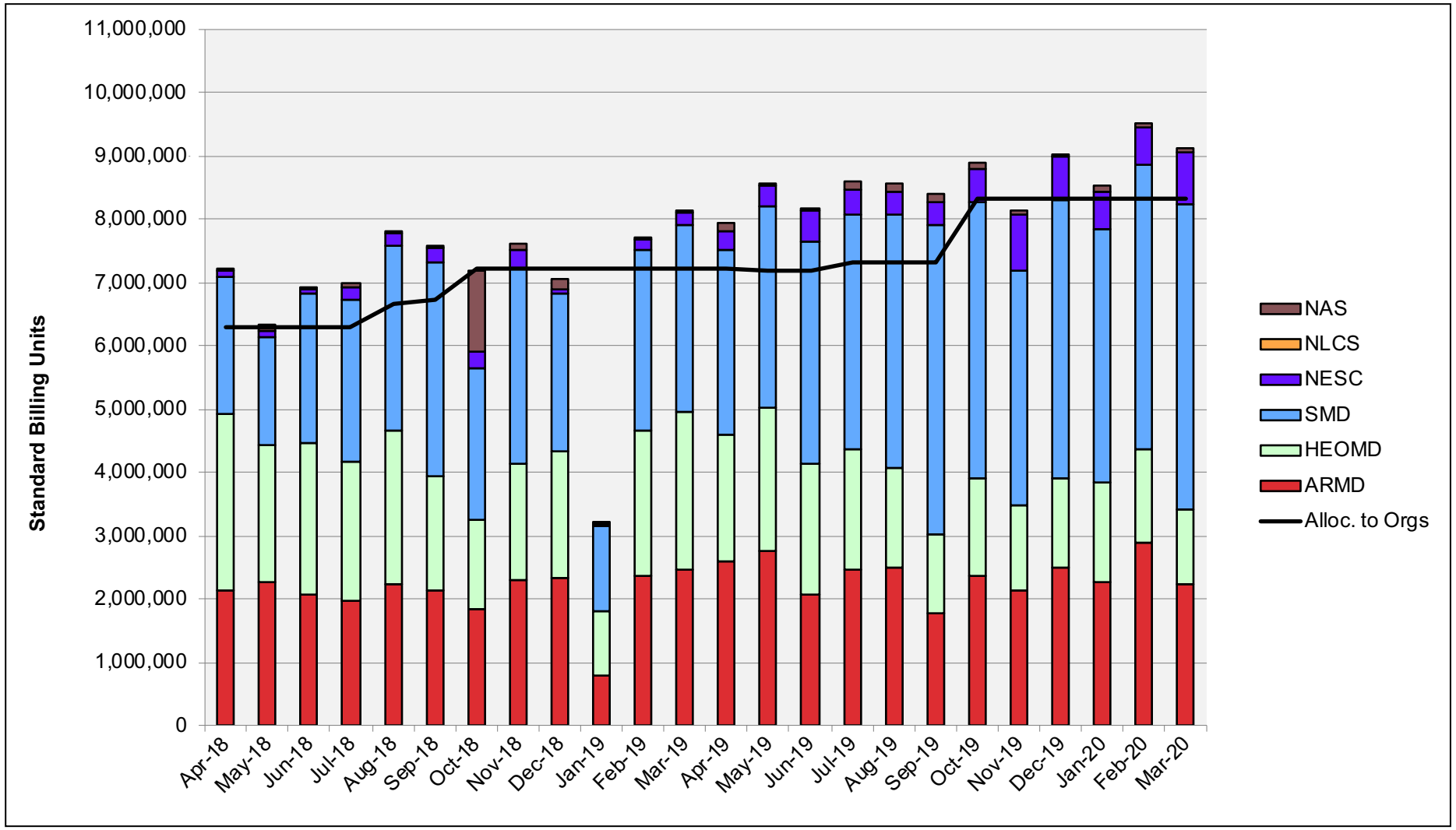
Social Media

- **Coverage of NAS Stories**
  - Announcement of NASA participation in COVID-19 HPC Consortium:
    - Administrator Jim Bridenstine: Twitter (313 retweets, 1.7k likes)
    - Deputy Administrator Jim Morhard: Twitter (242 retweets, 1.3k likes)
    - NASA Supercomputing: Twitter (1 retweet, 10 likes); Facebook (15k users reached, 1.4k engagements, 70 likes, 85 shares)
    - NAS Division: Twitter (24 retweets, 100 likes)
  - White Dwarf Accretion Disk Formation (throwback):
    - NASA Supercomputing: Facebook (253 users reached, 30 engagements, 9 likes, 3 shares)
    - NAS Division: Twitter (3 retweets, 6 likes)

HECC Utilization



HECC Utilization Normalized to 30-Day Month



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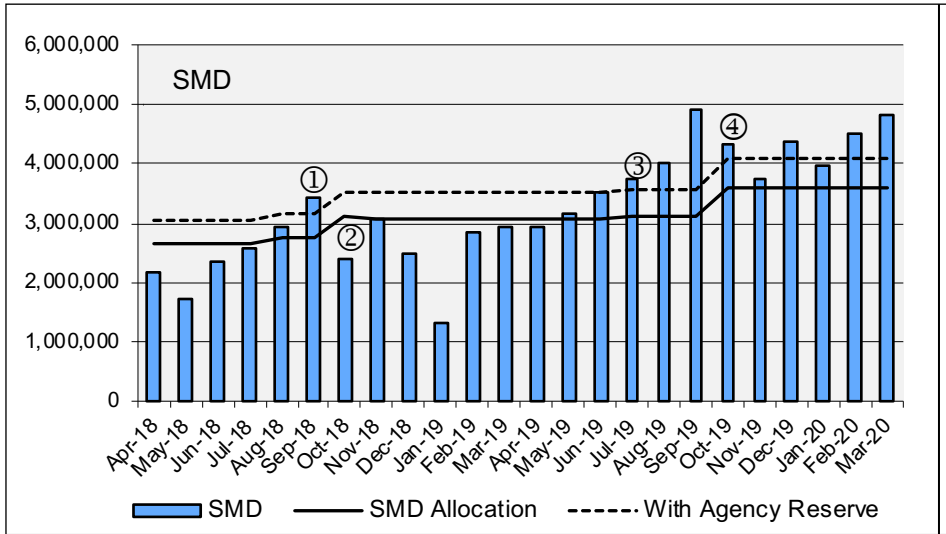
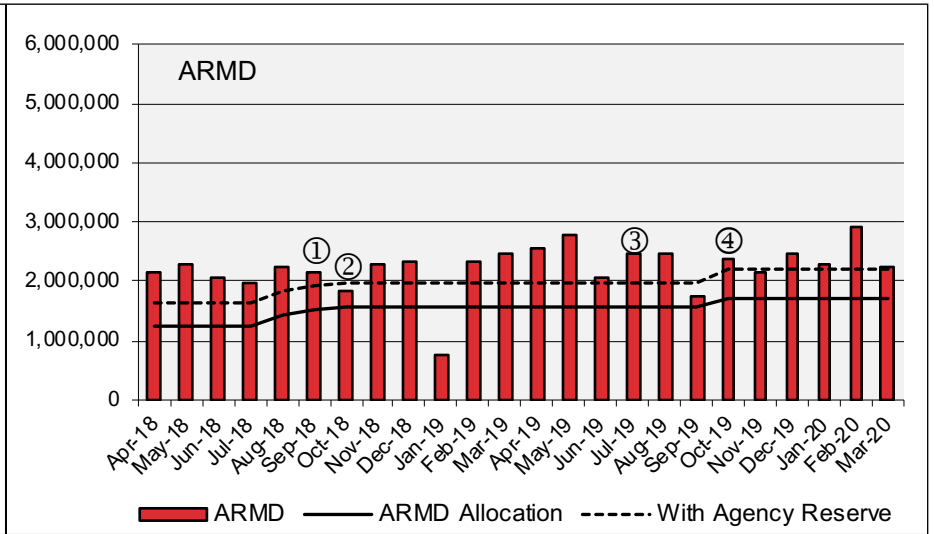
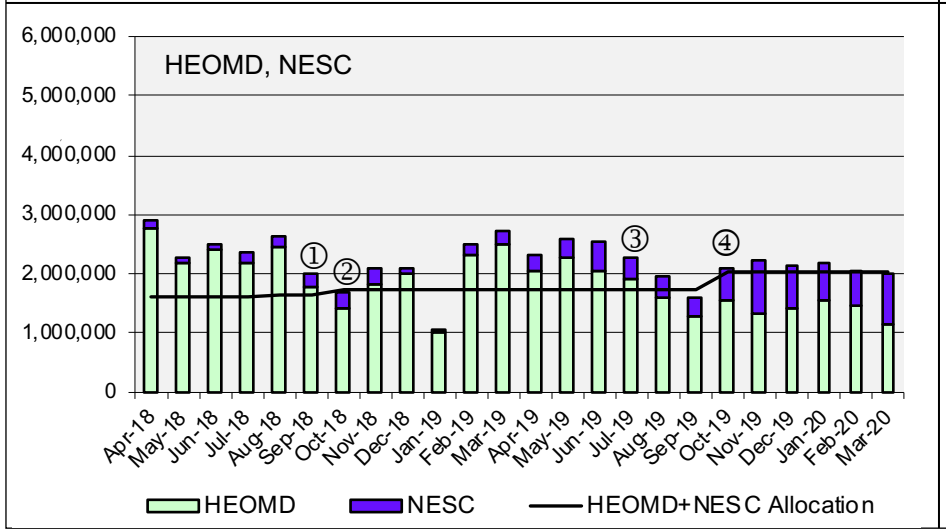






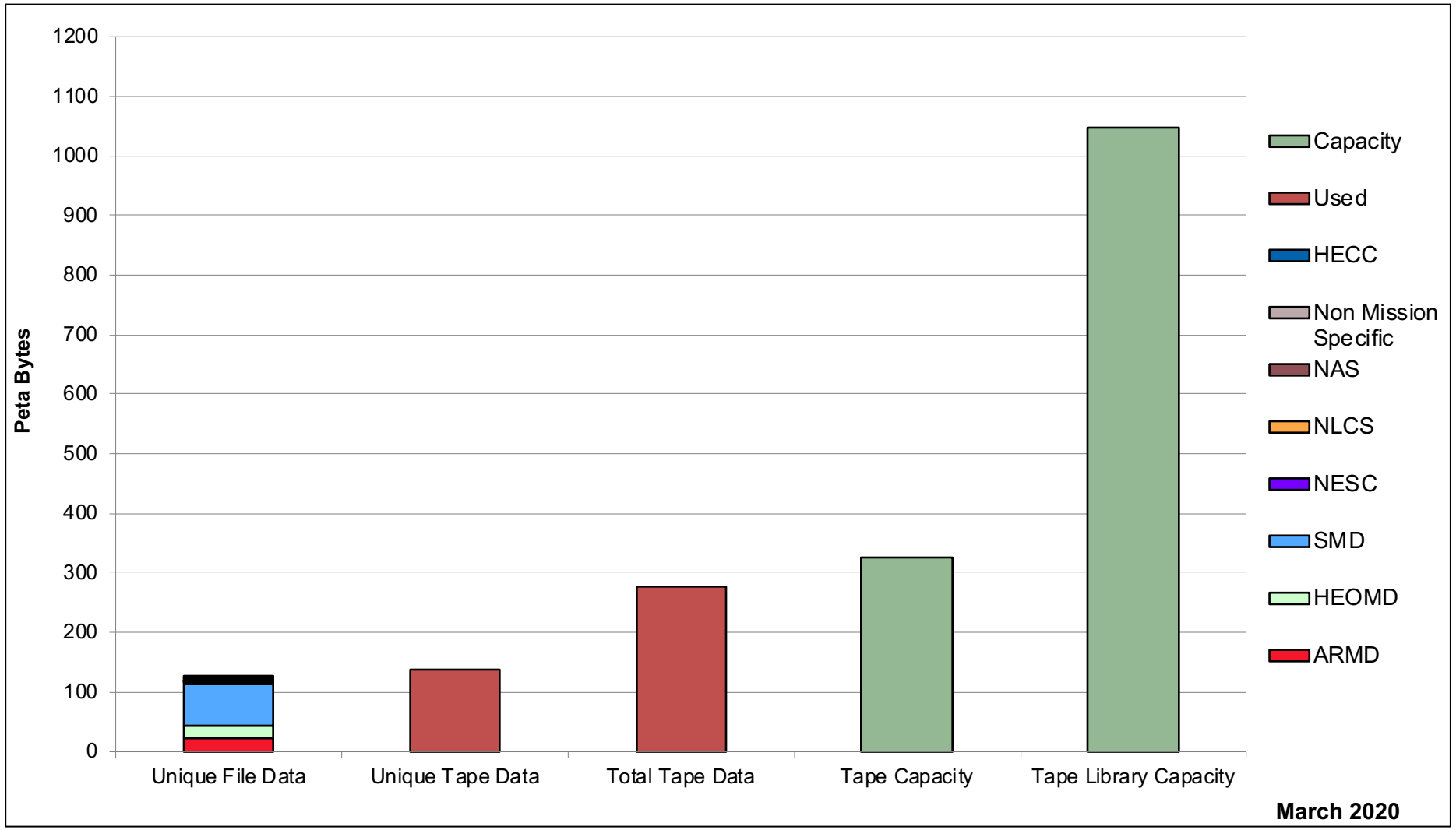
① 4 Skylake E cells (16 D Rack Equivalence) added to Electra

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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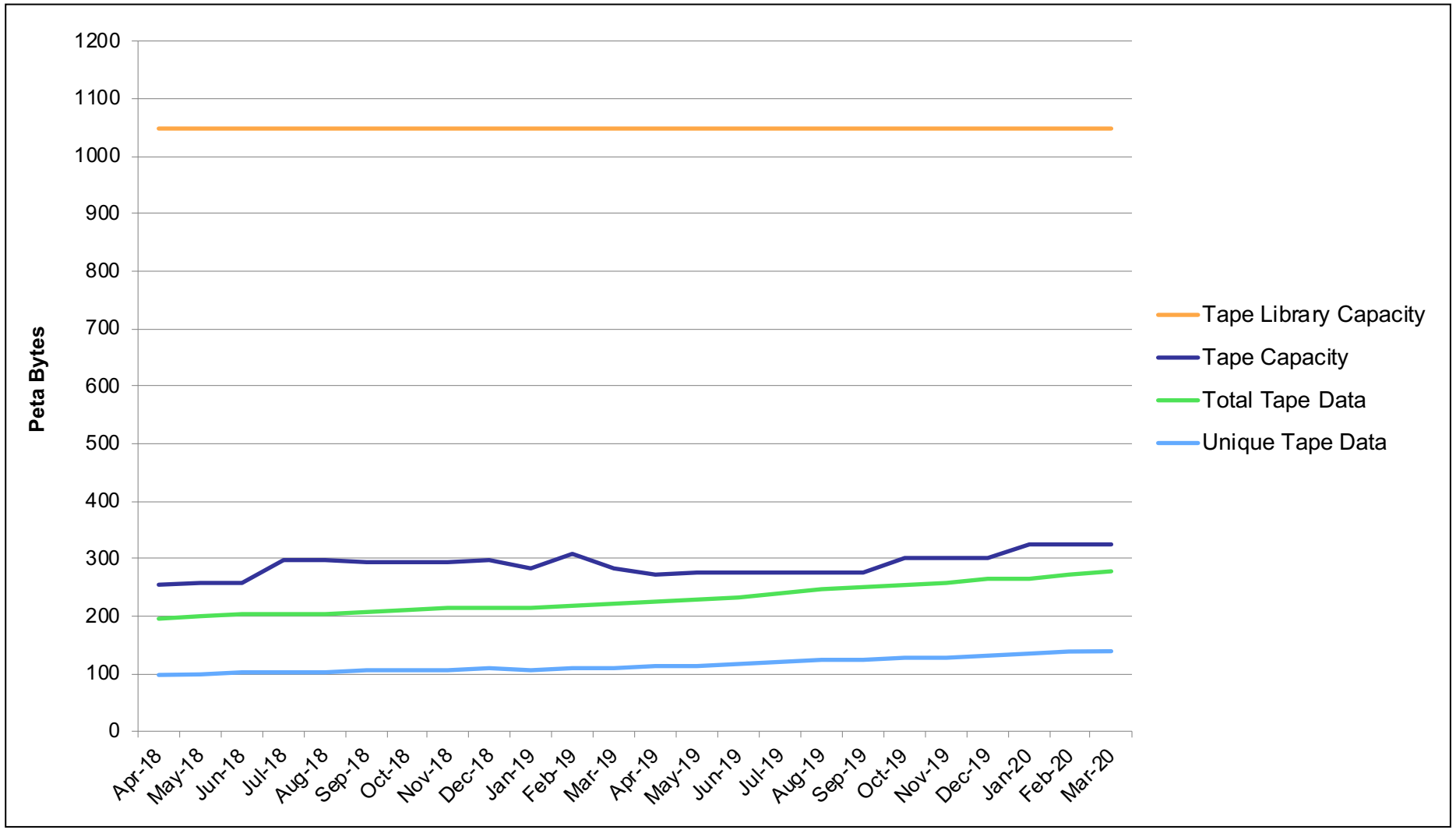
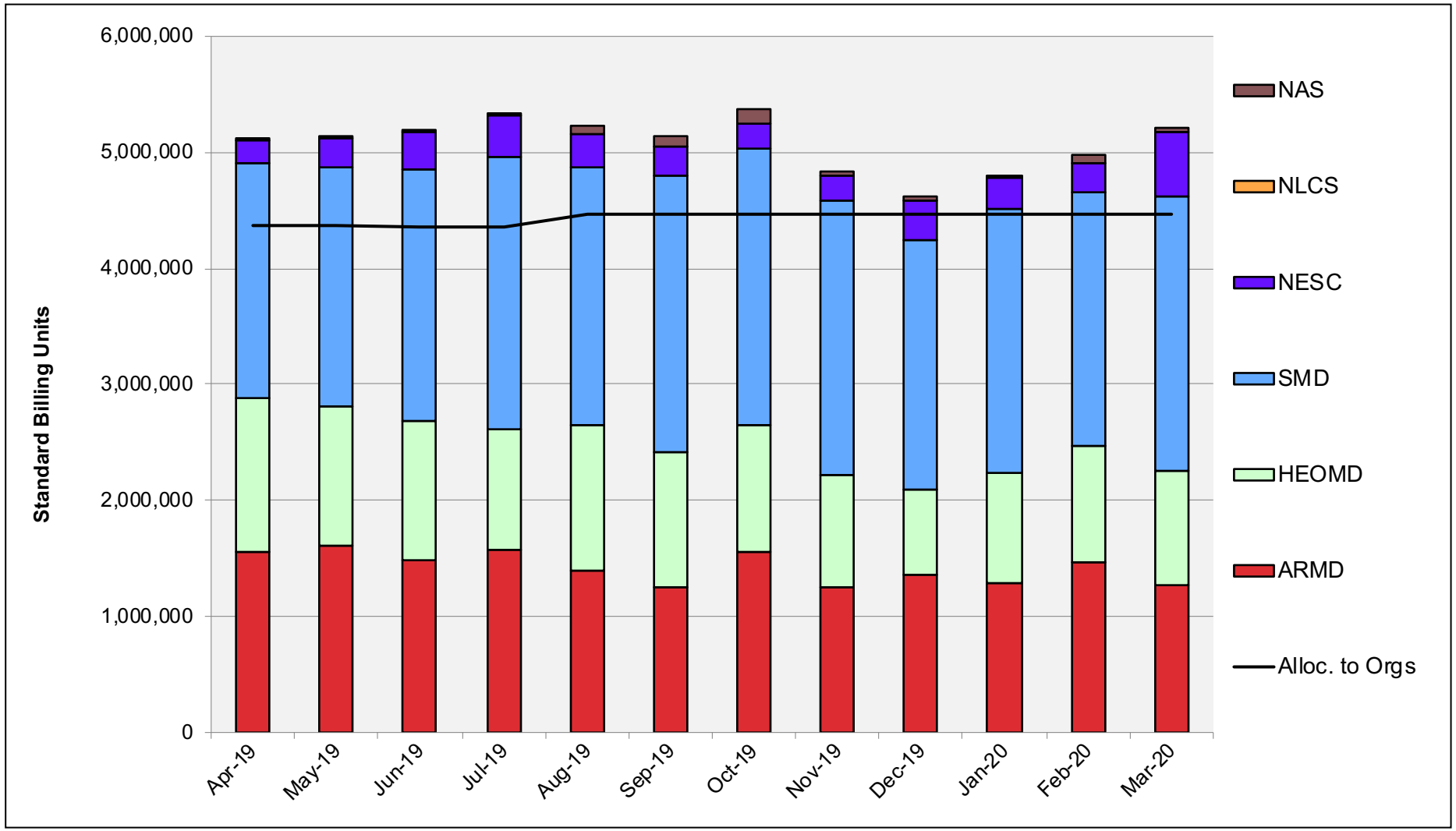
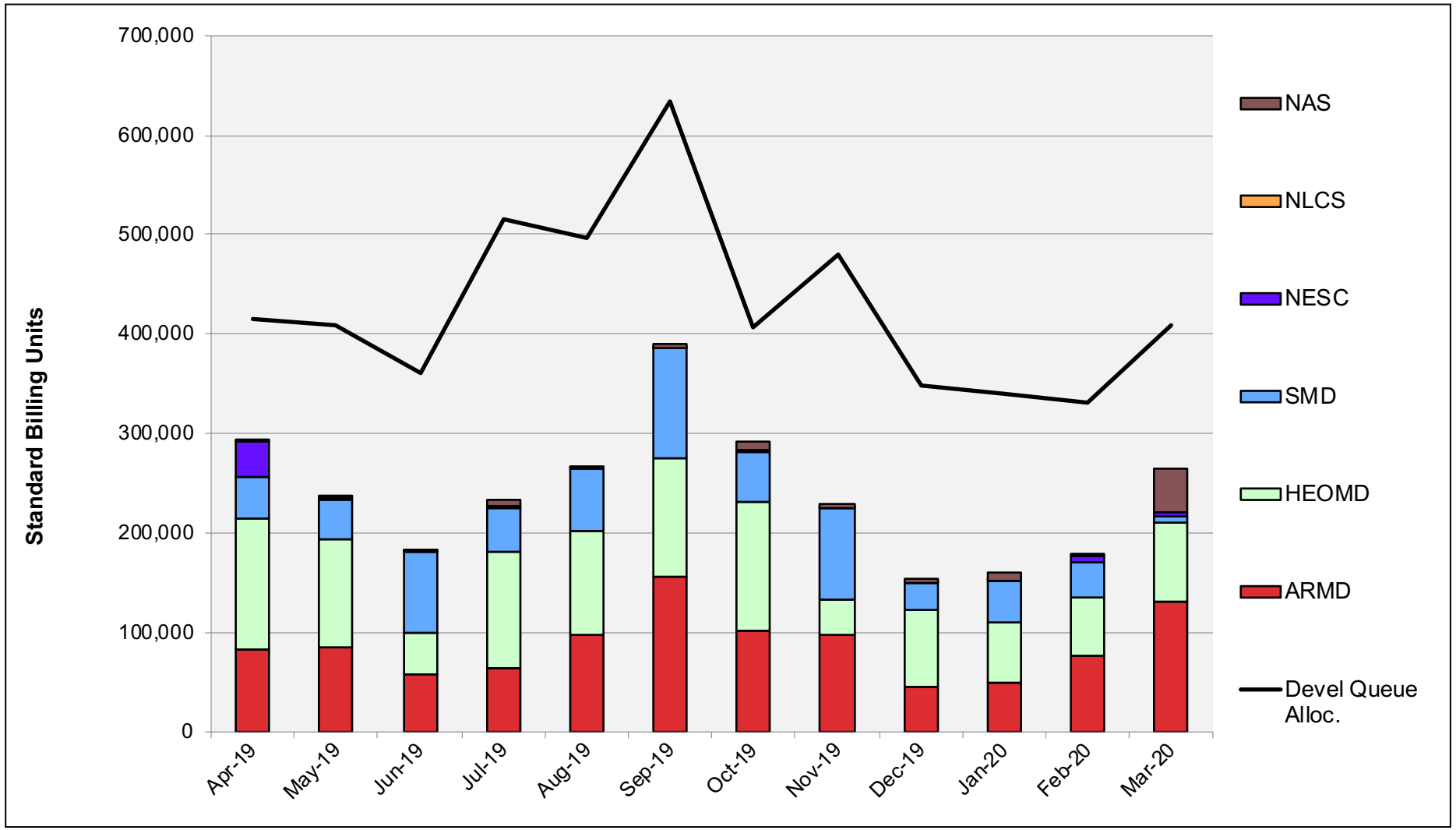


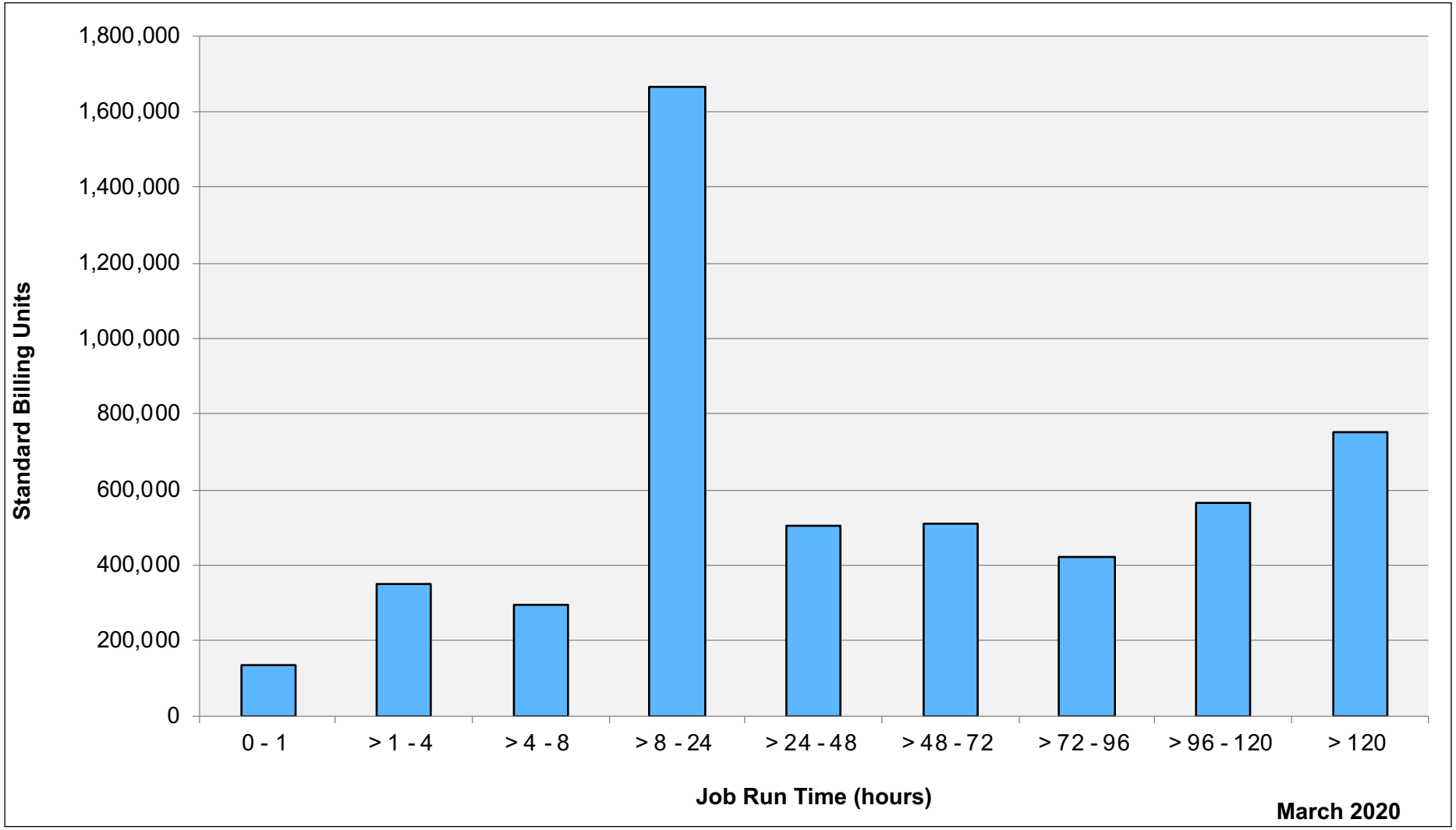
Pleiades: SBUs Reported, Normalized to 30-Day Month



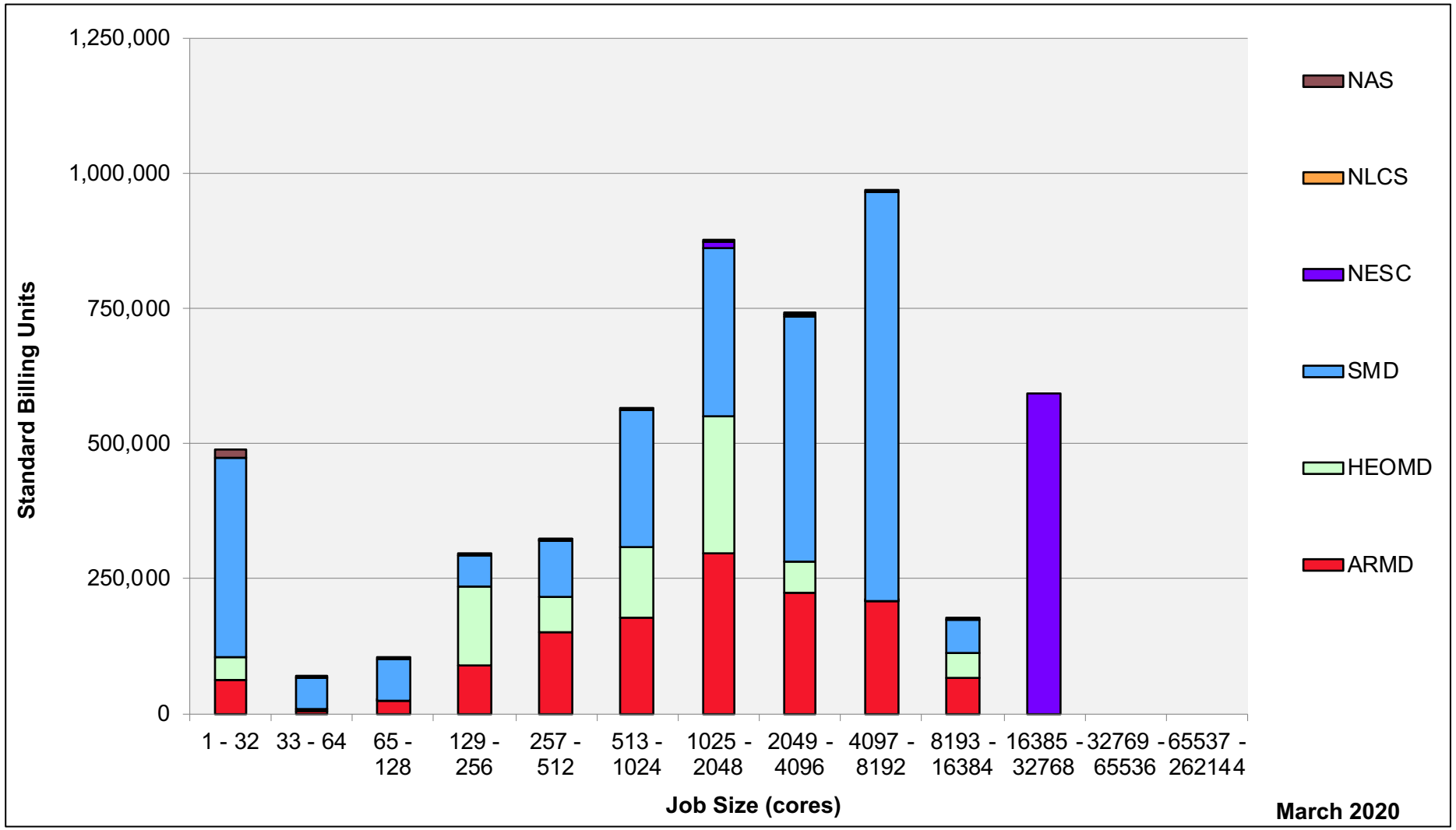
Pleiades: Devel Queue Utilization



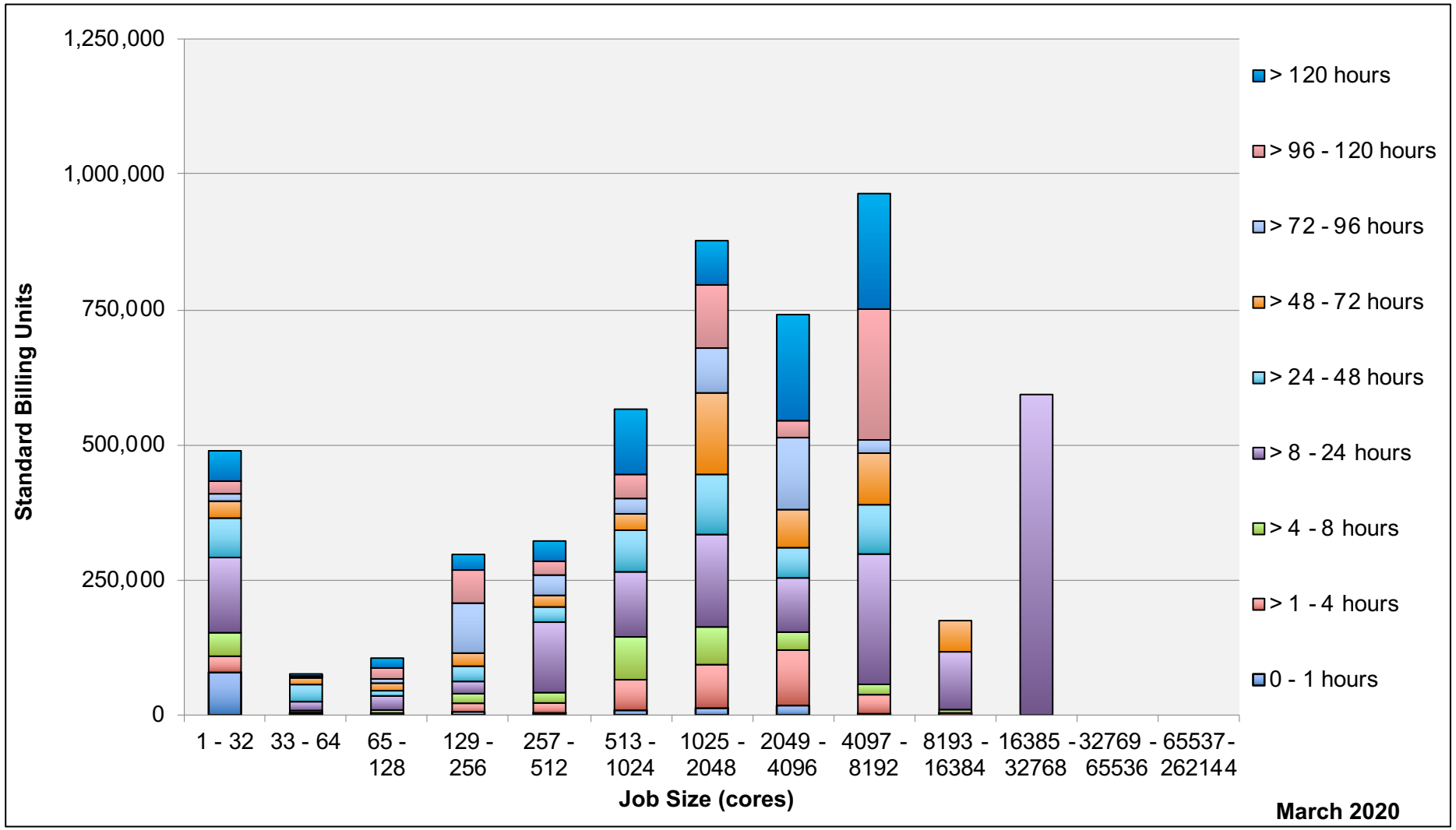
Pleiades: Monthly Utilization by Job Length



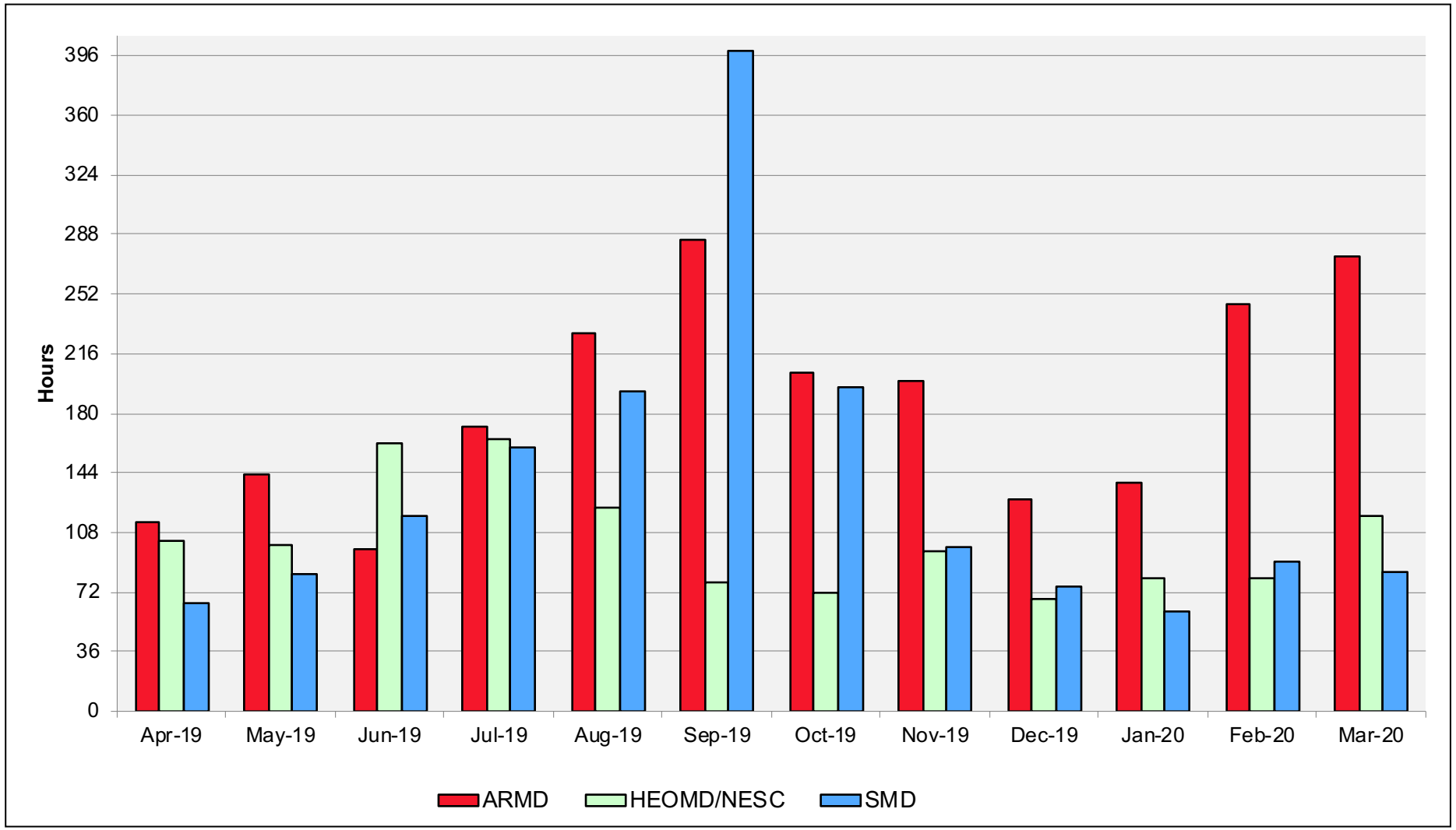
Pleiades: Monthly Utilization by Job Length



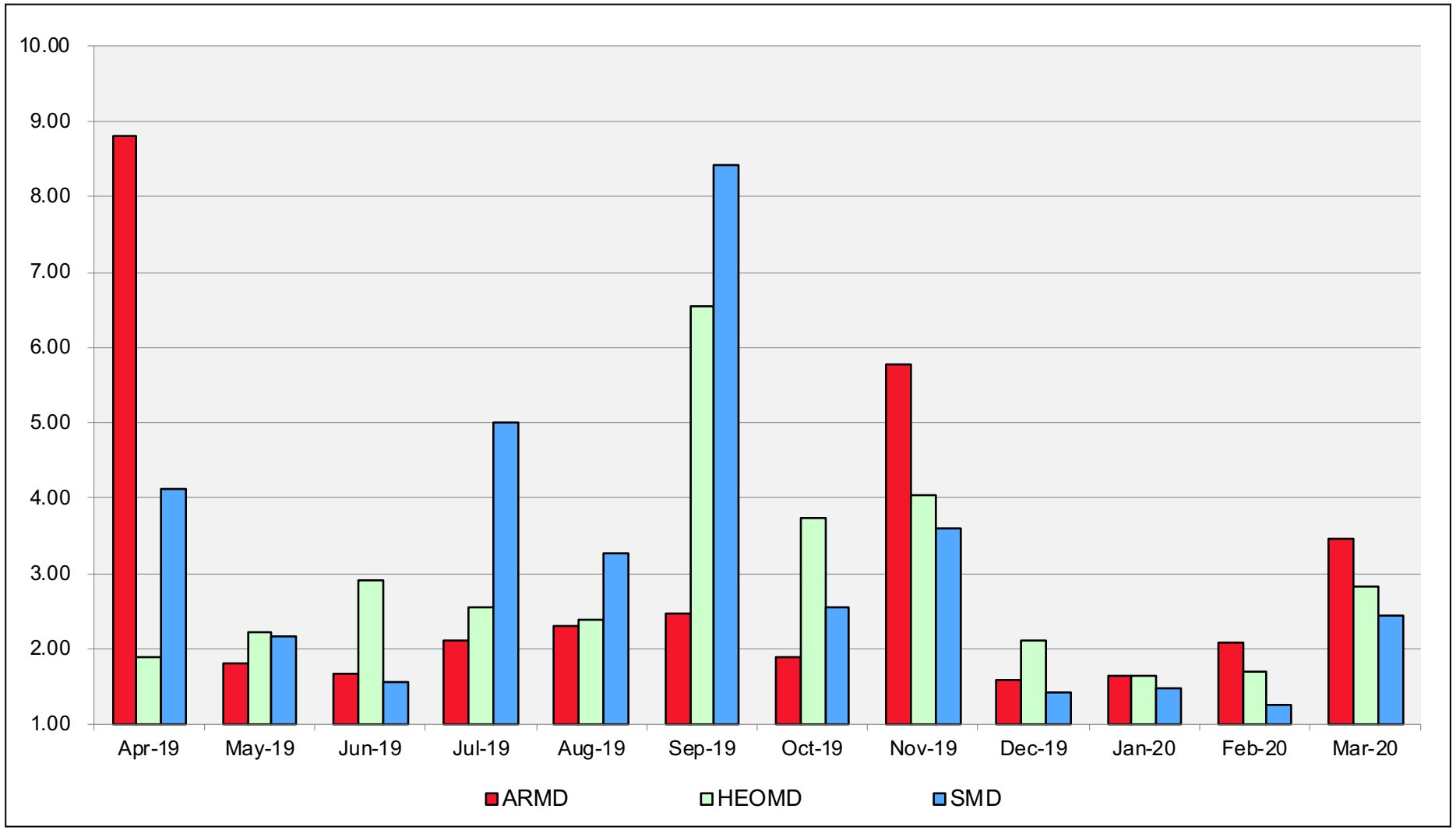
Pleiades: Monthly Utilization by Size and Length



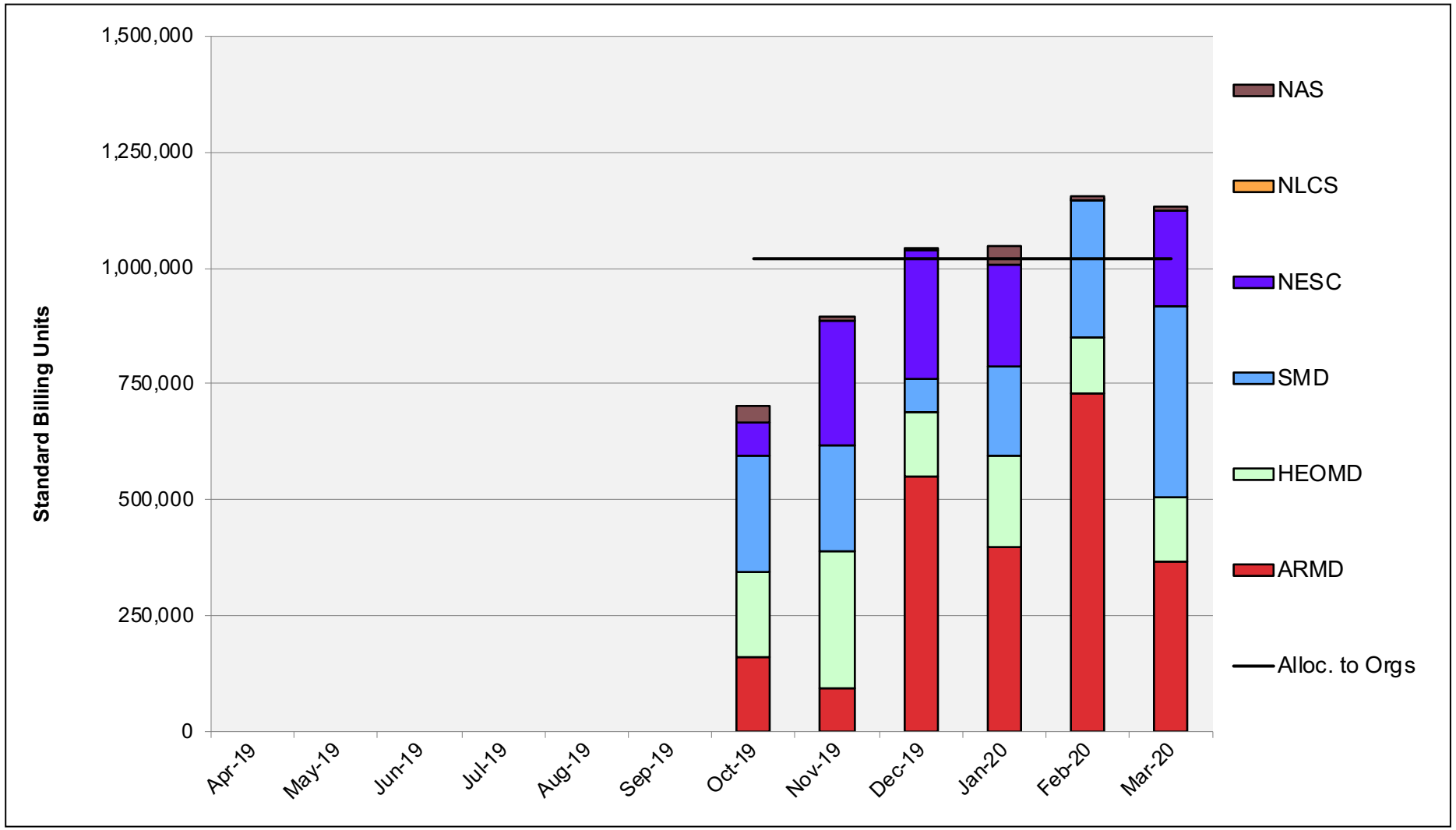
Pleiades: Average Time to Clear All Jobs



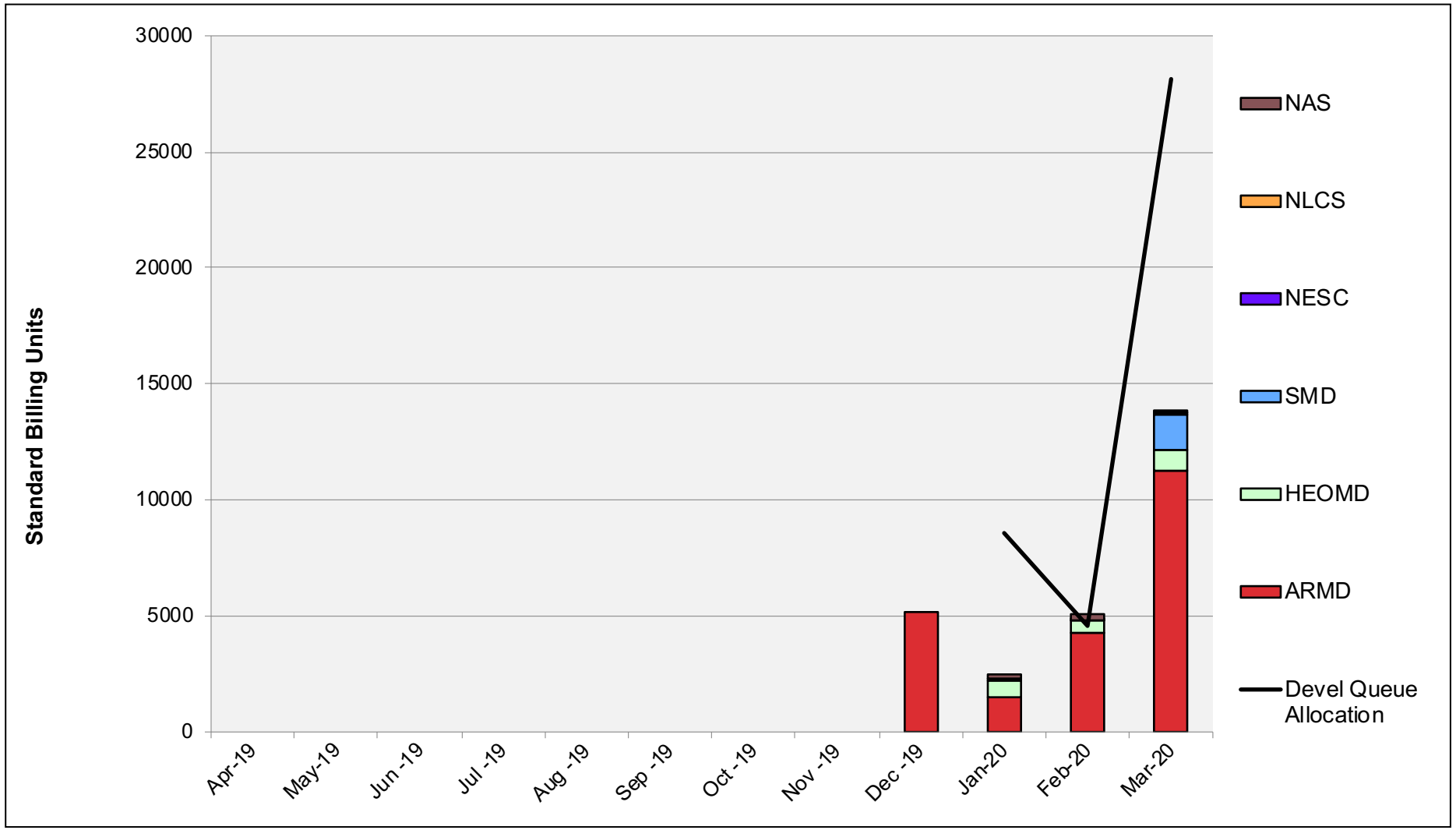
Pleiades: Average Expansion Factor



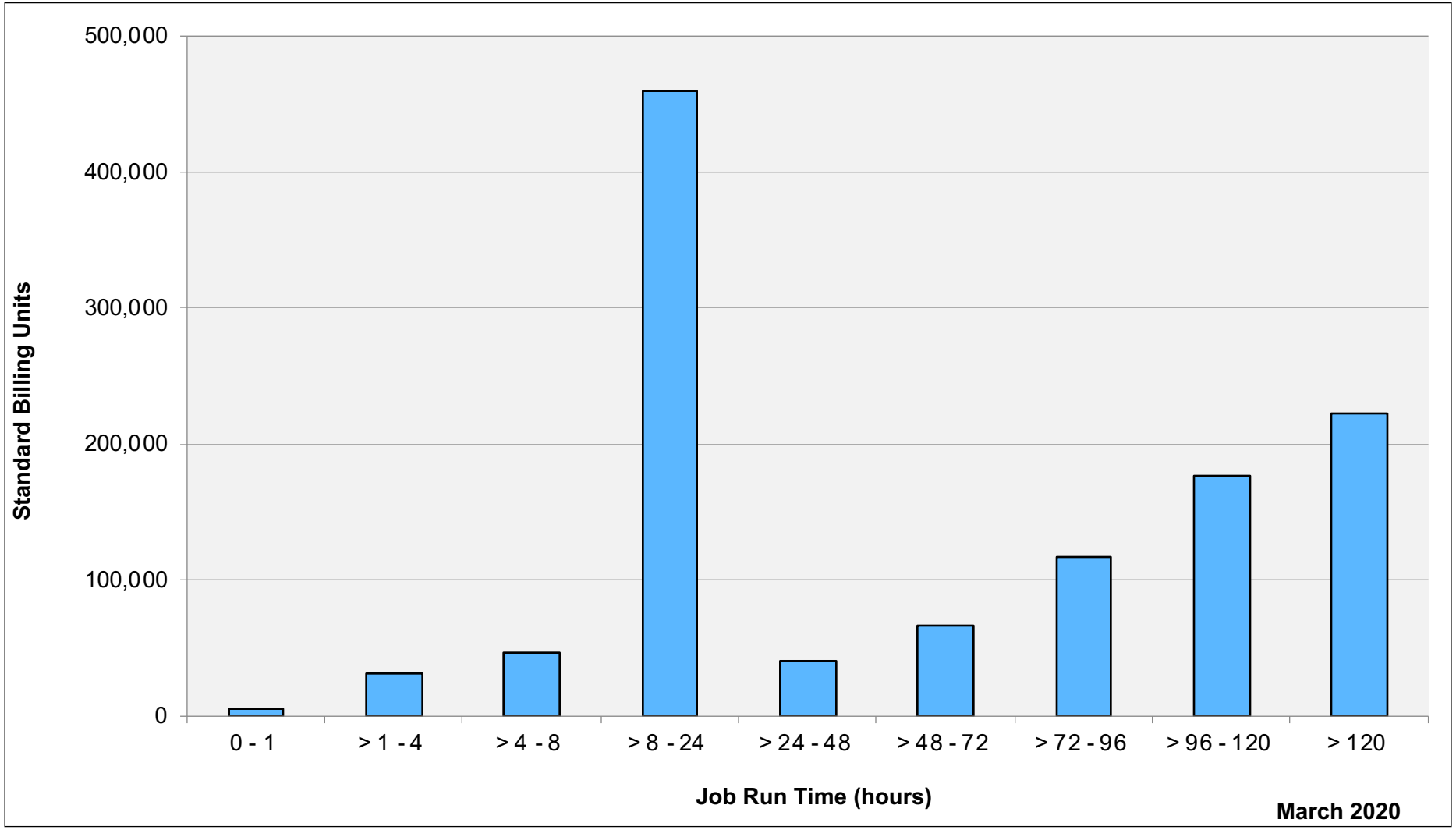
Aitken: SBUs Reported, Normalized to 30-Day Month



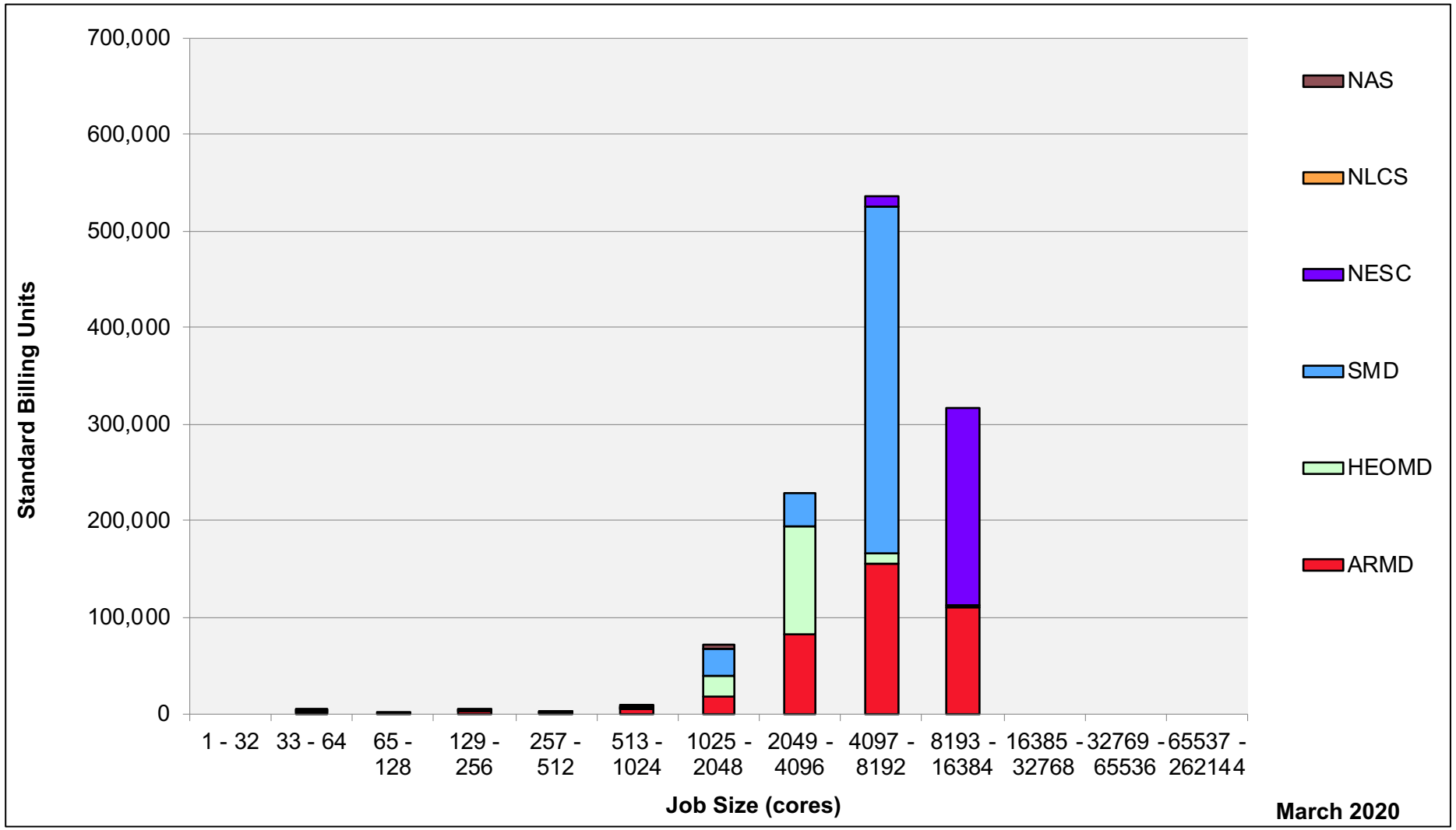
Aitken: Devel Queue Utilization



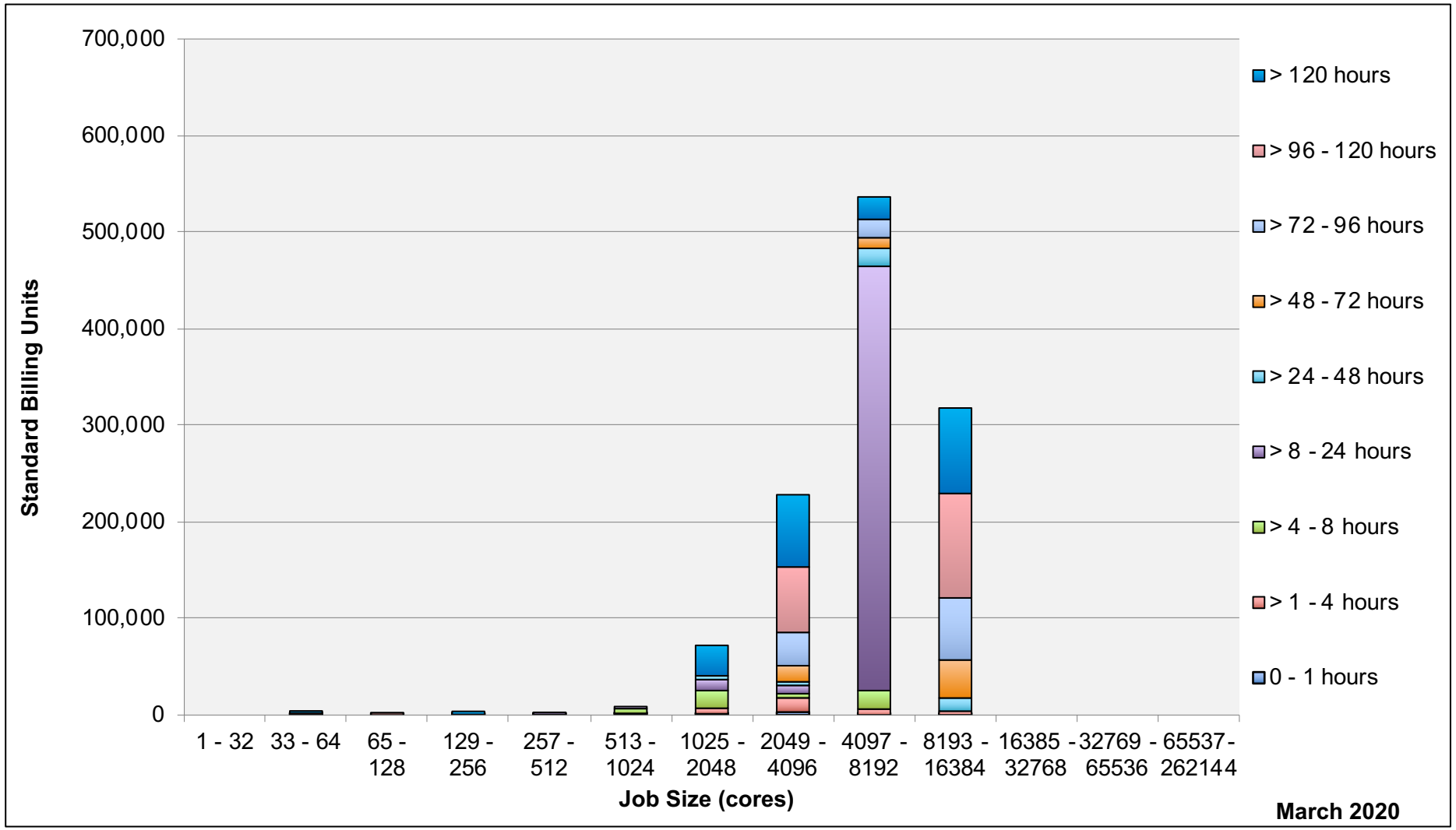
Aitken: Monthly Utilization by Job Length



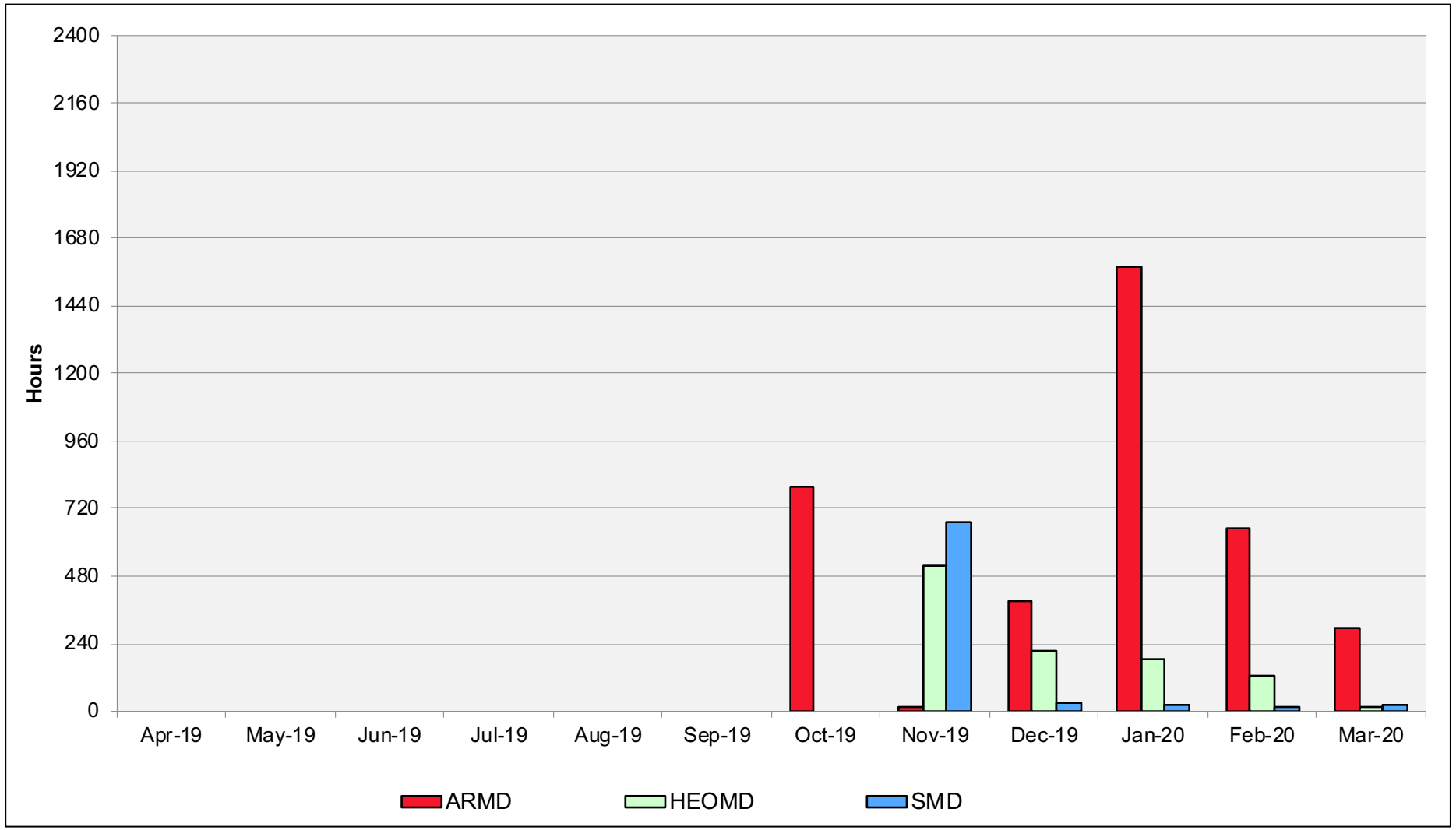
Aitken: Monthly Utilization by Job Length



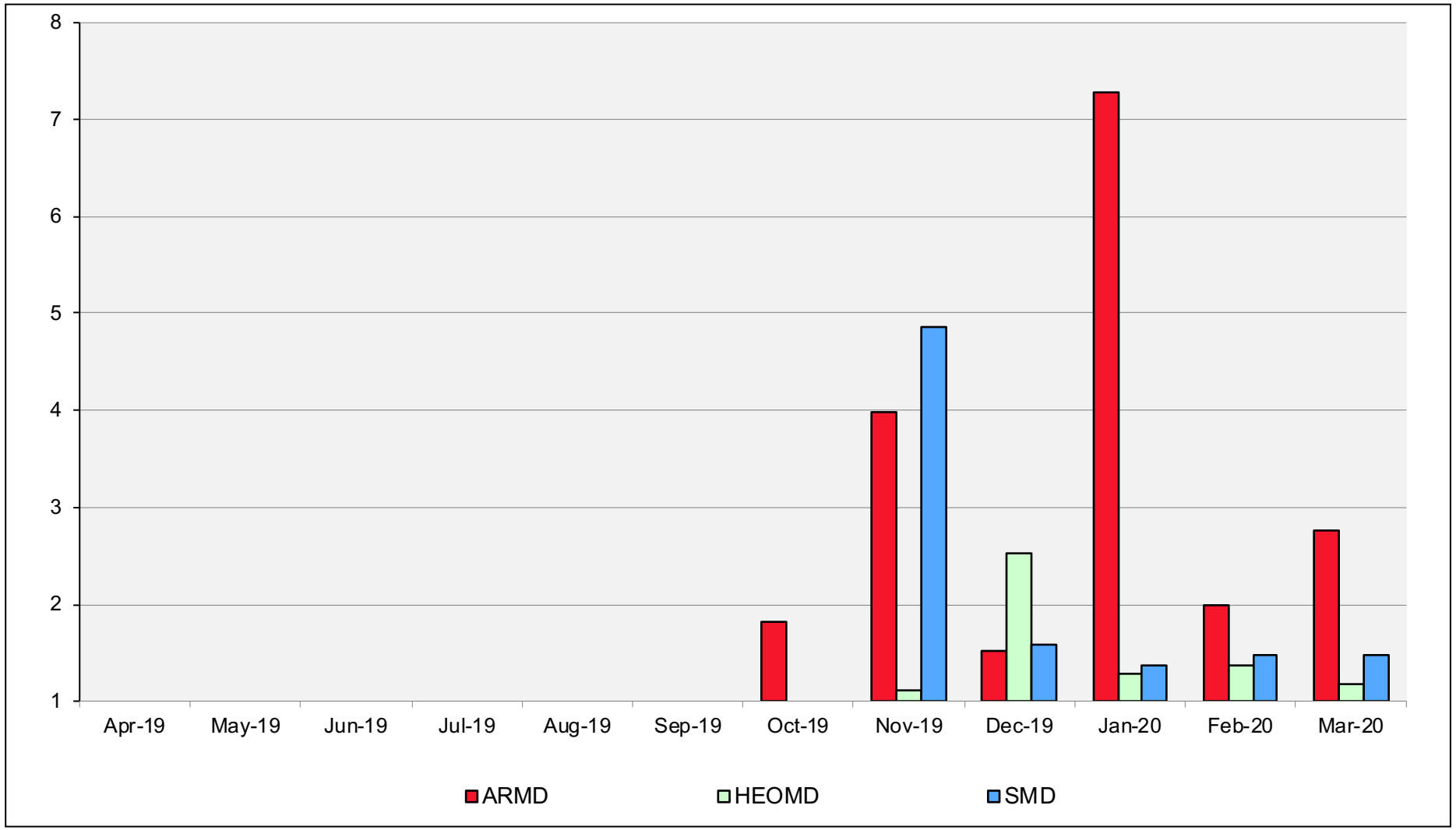
Aitken: Monthly Utilization by Size and Length



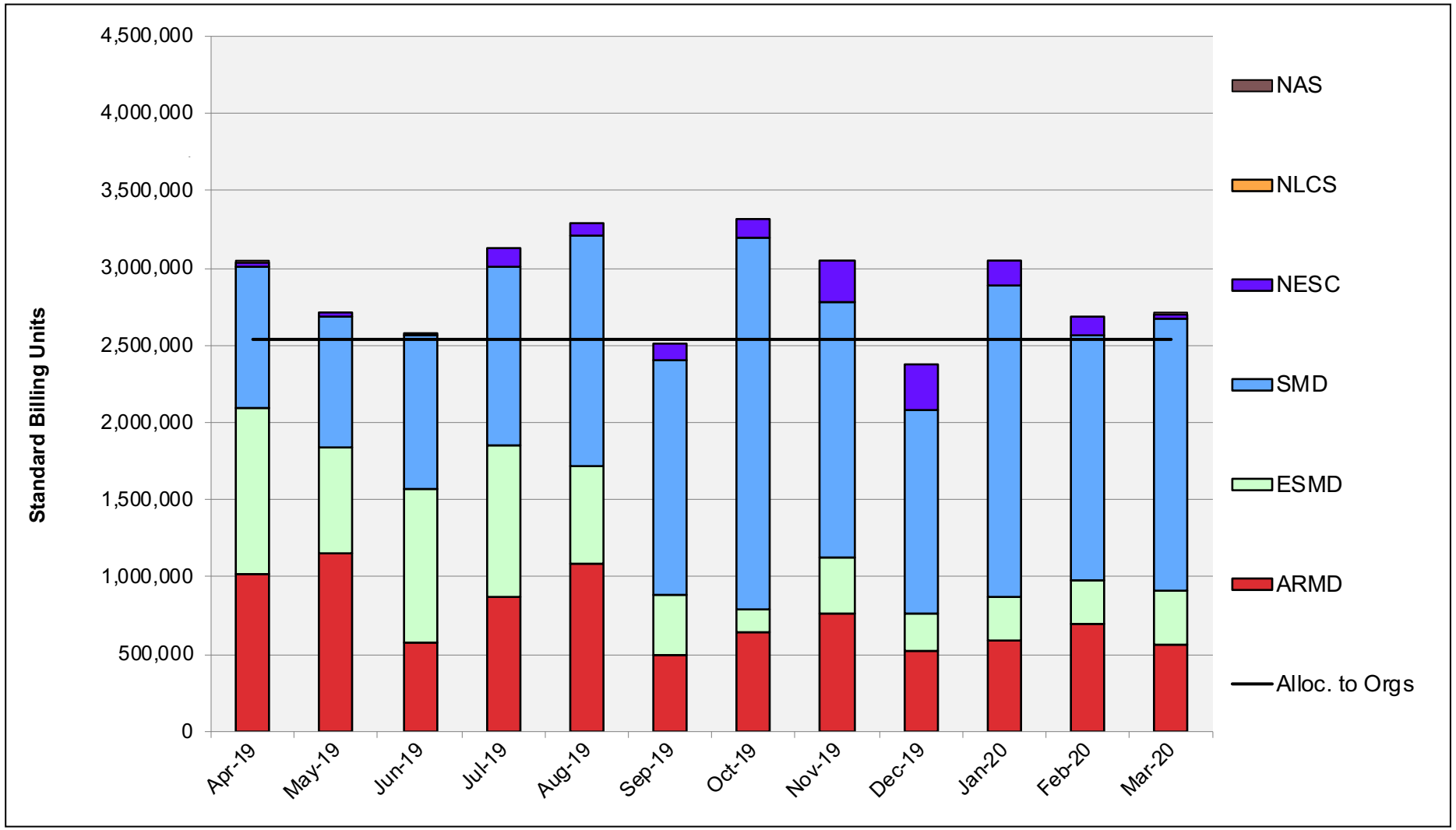
Aitken: Average Time to Clear All Jobs



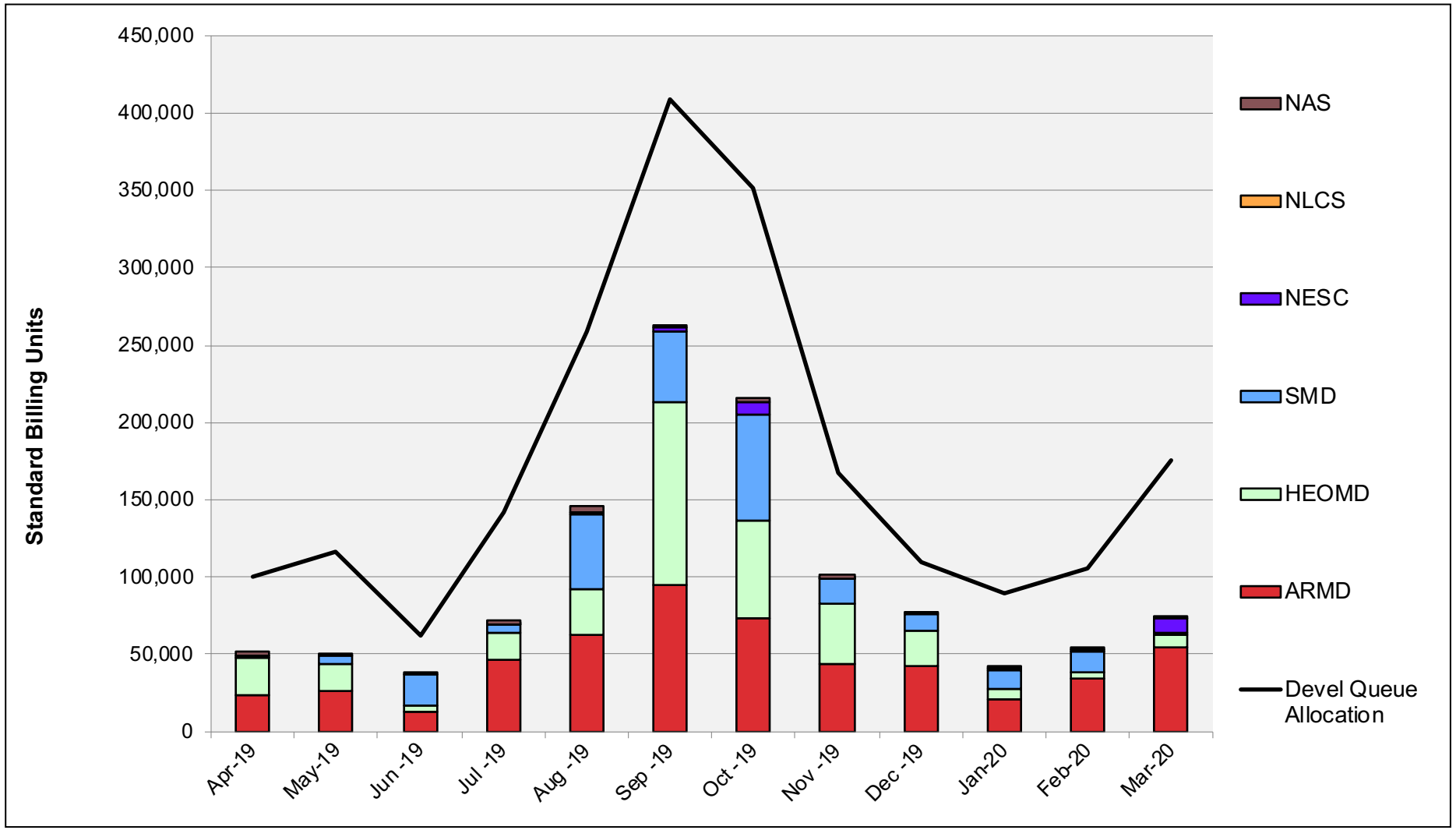
Aitken: Average Expansion Factor



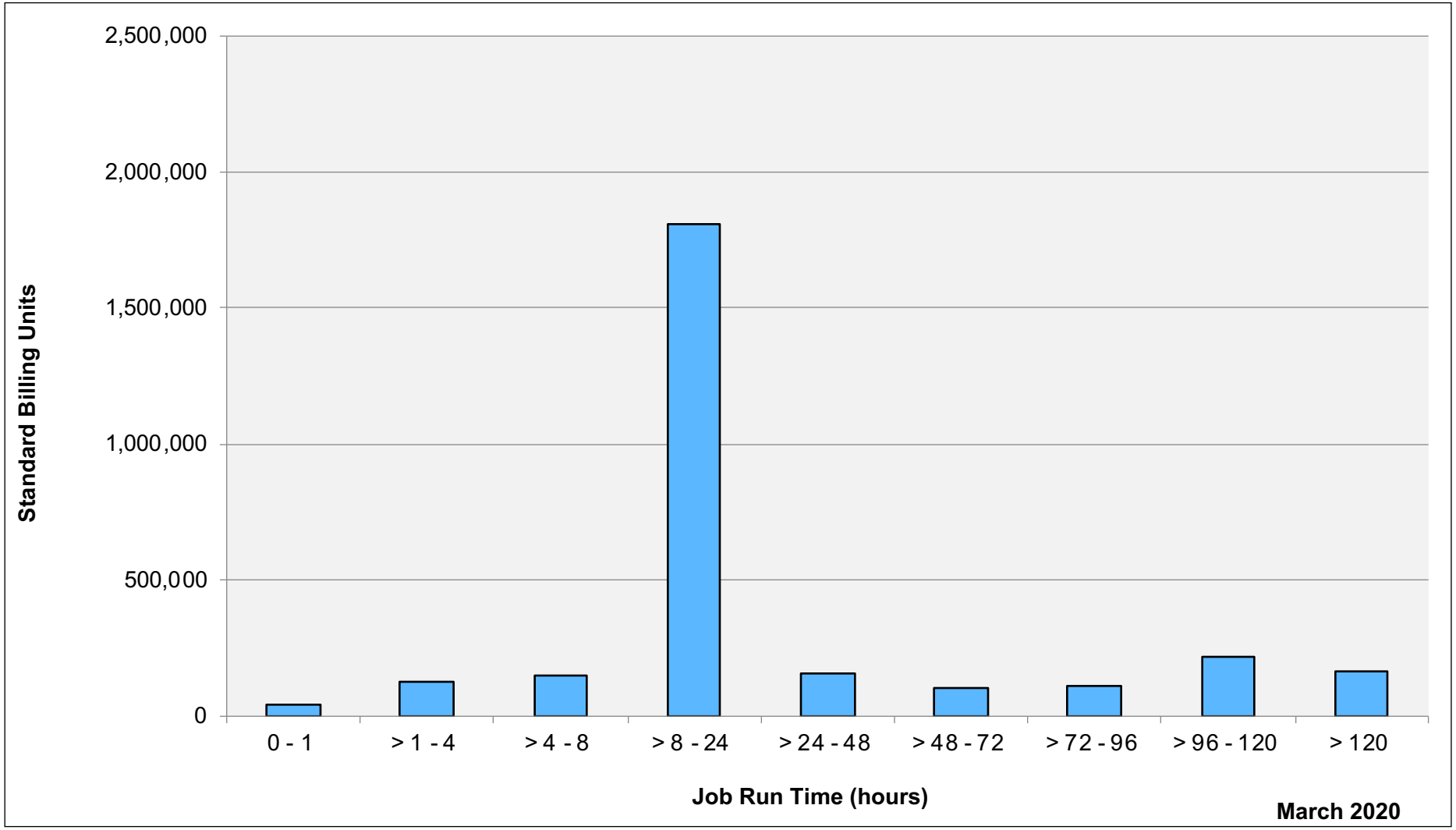
Electra: SBUs Reported, Normalized to 30-Day Month



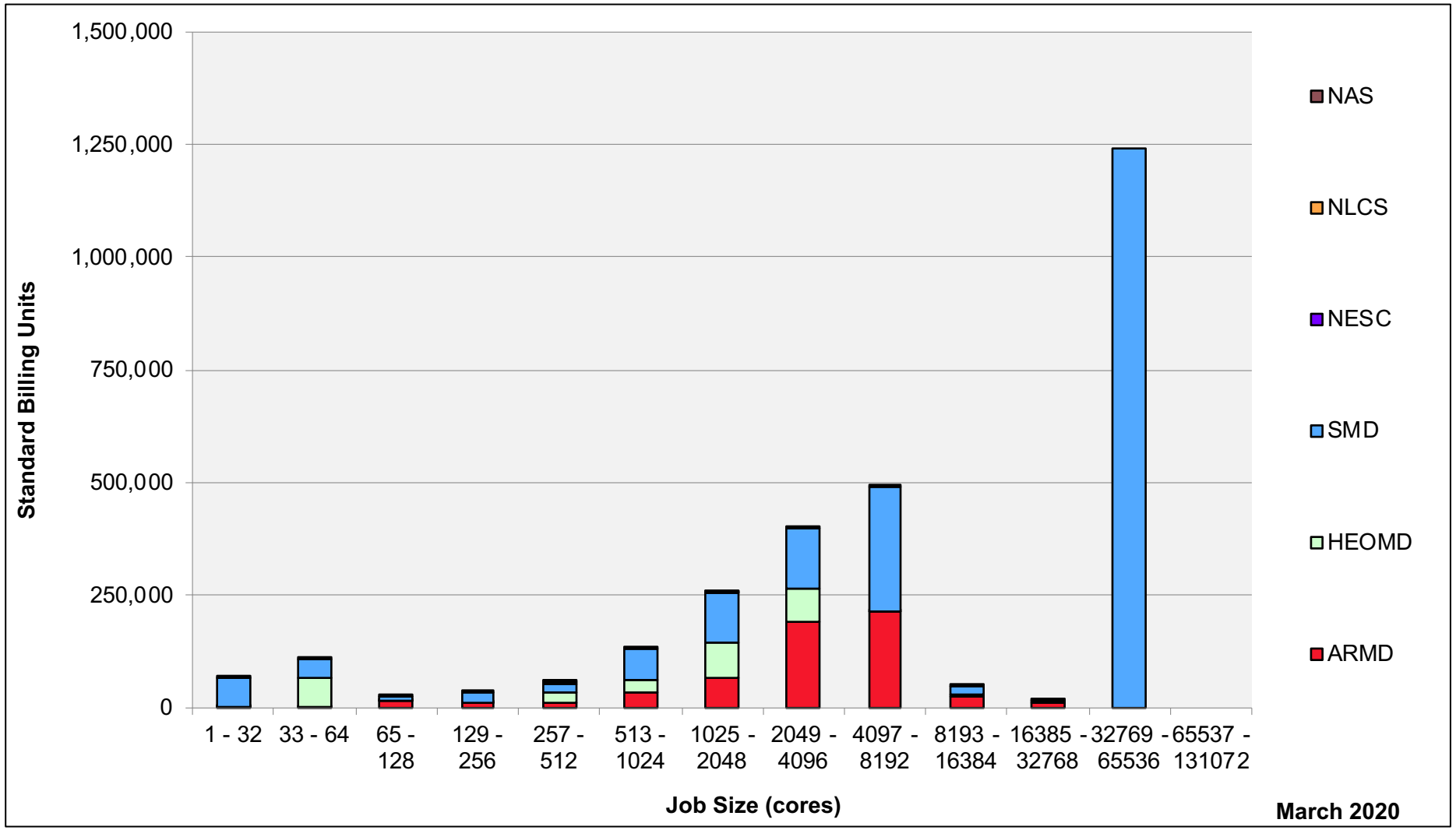
Electra: Devel Queue Utilization



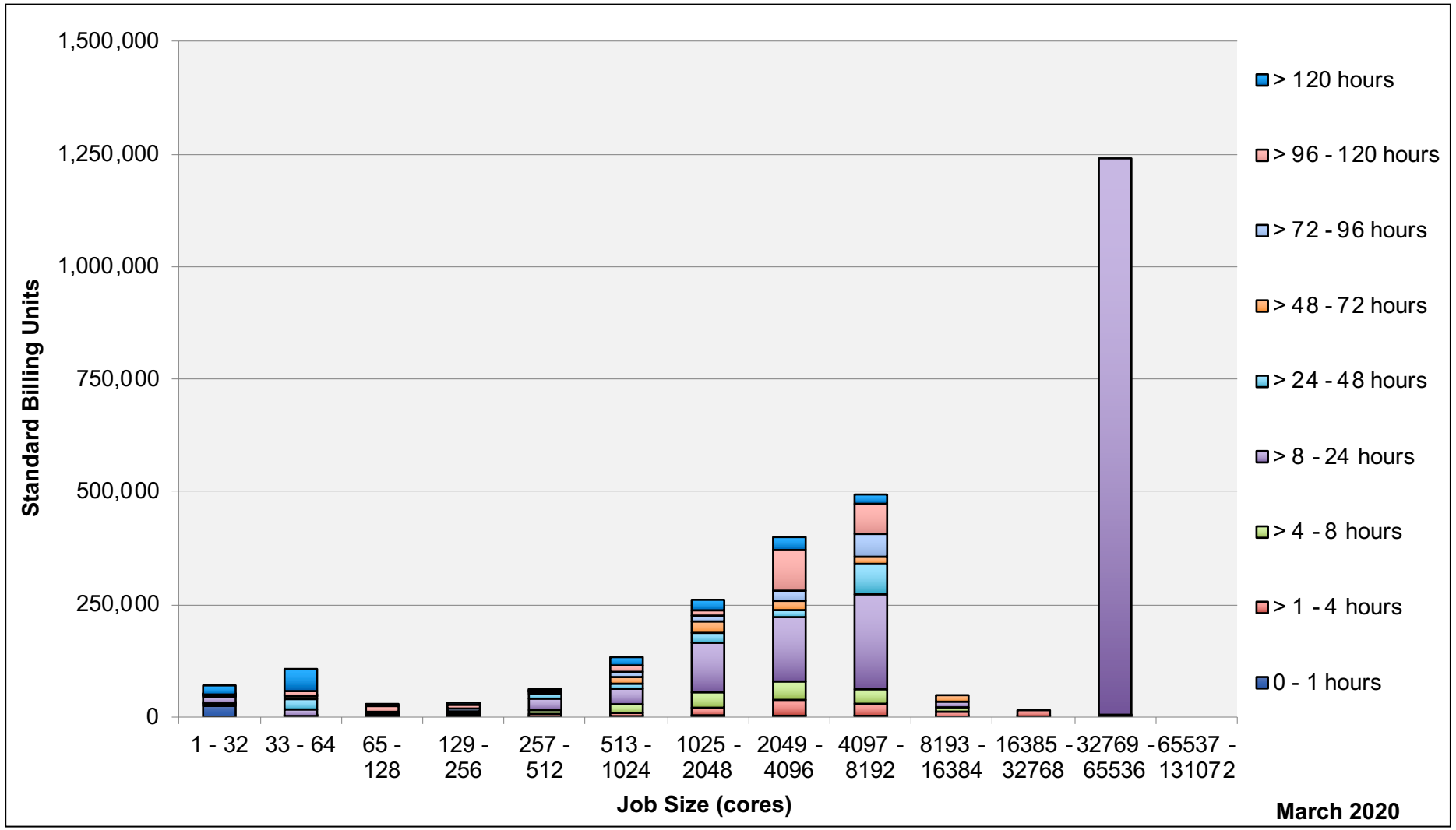
Electra: Monthly Utilization by Job Length



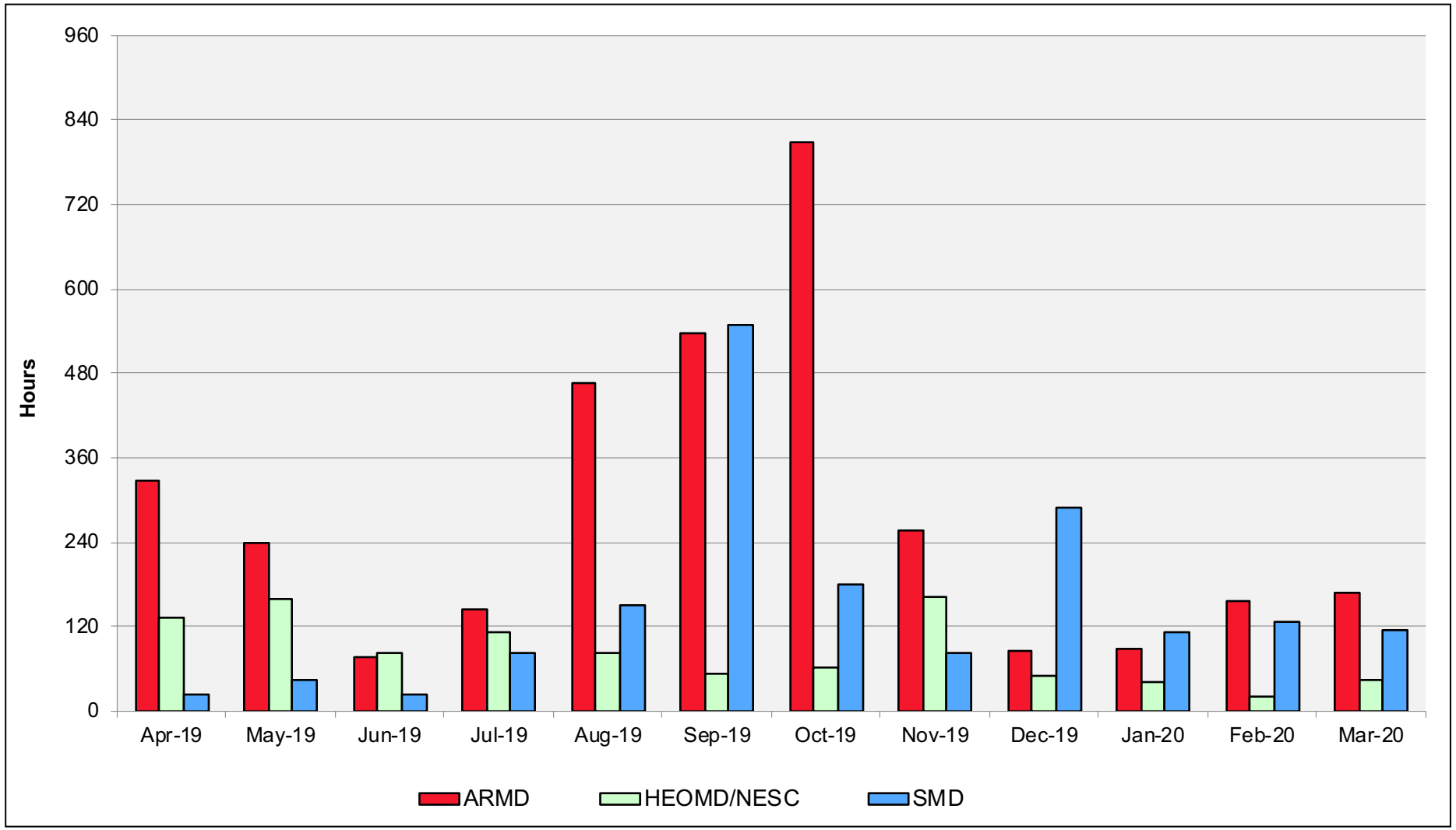
Electra: Monthly Utilization by Job Length



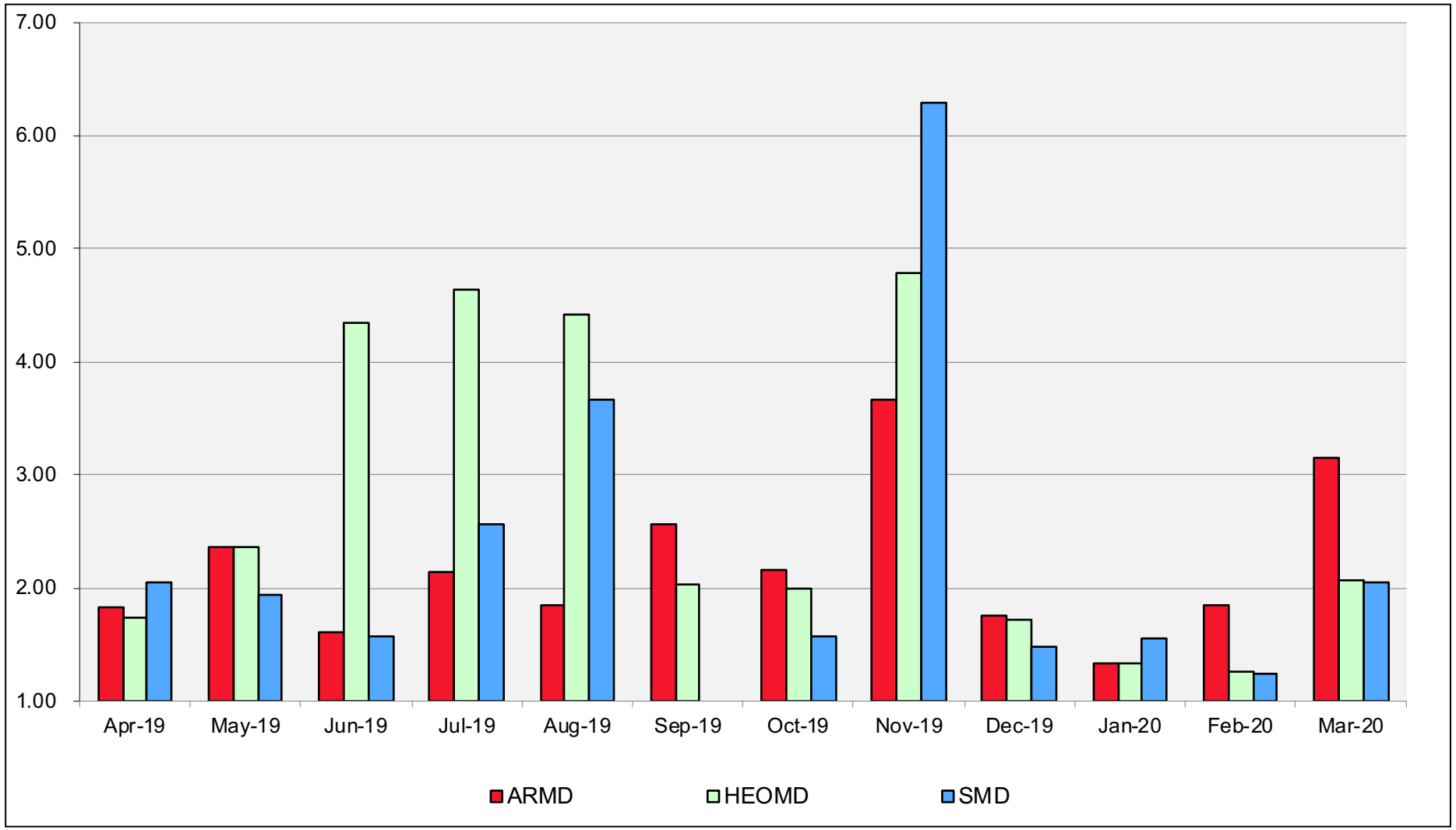
Electra: Monthly Utilization by Size and Length



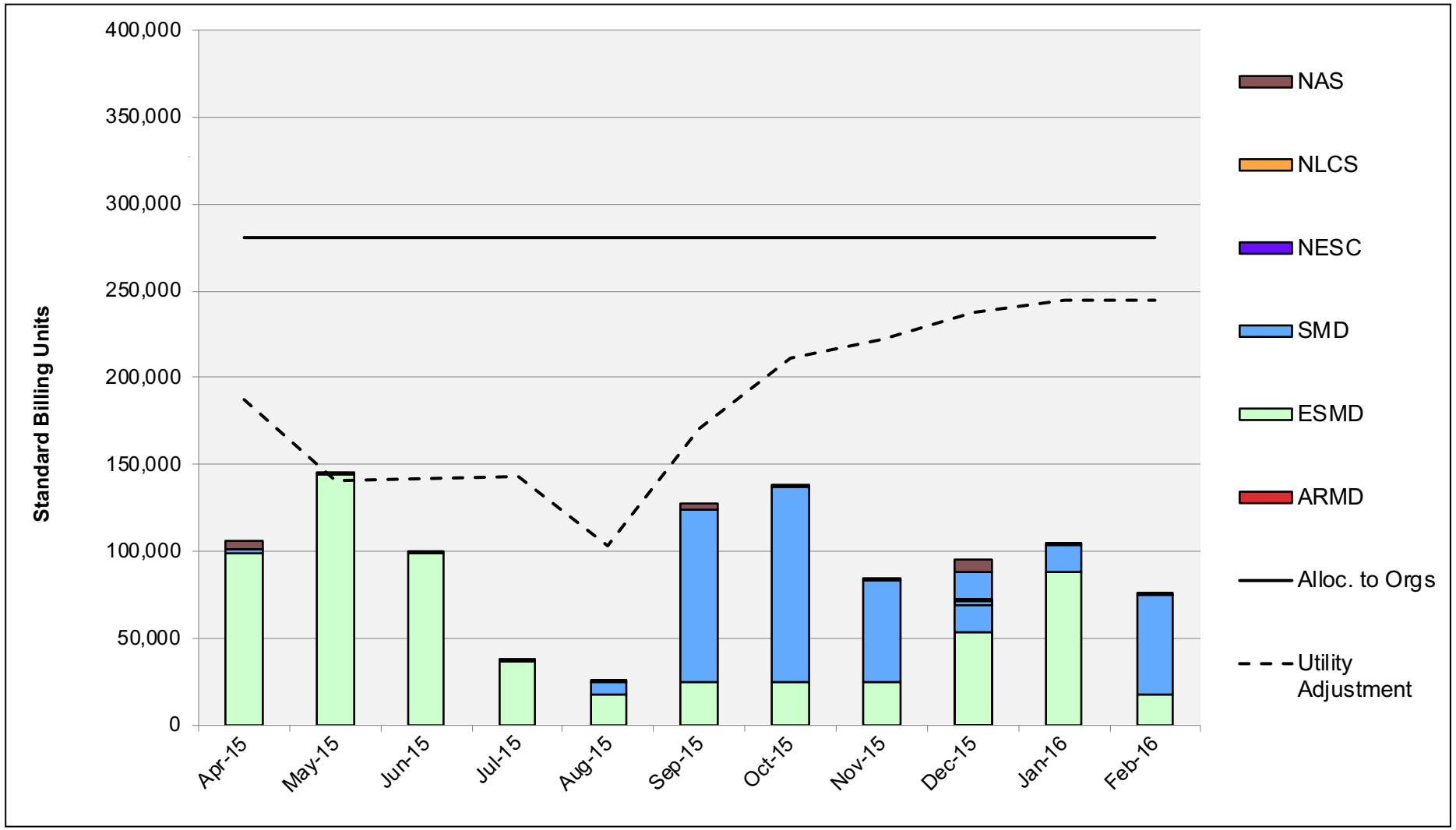
Electra: Average Time to Clear All Jobs



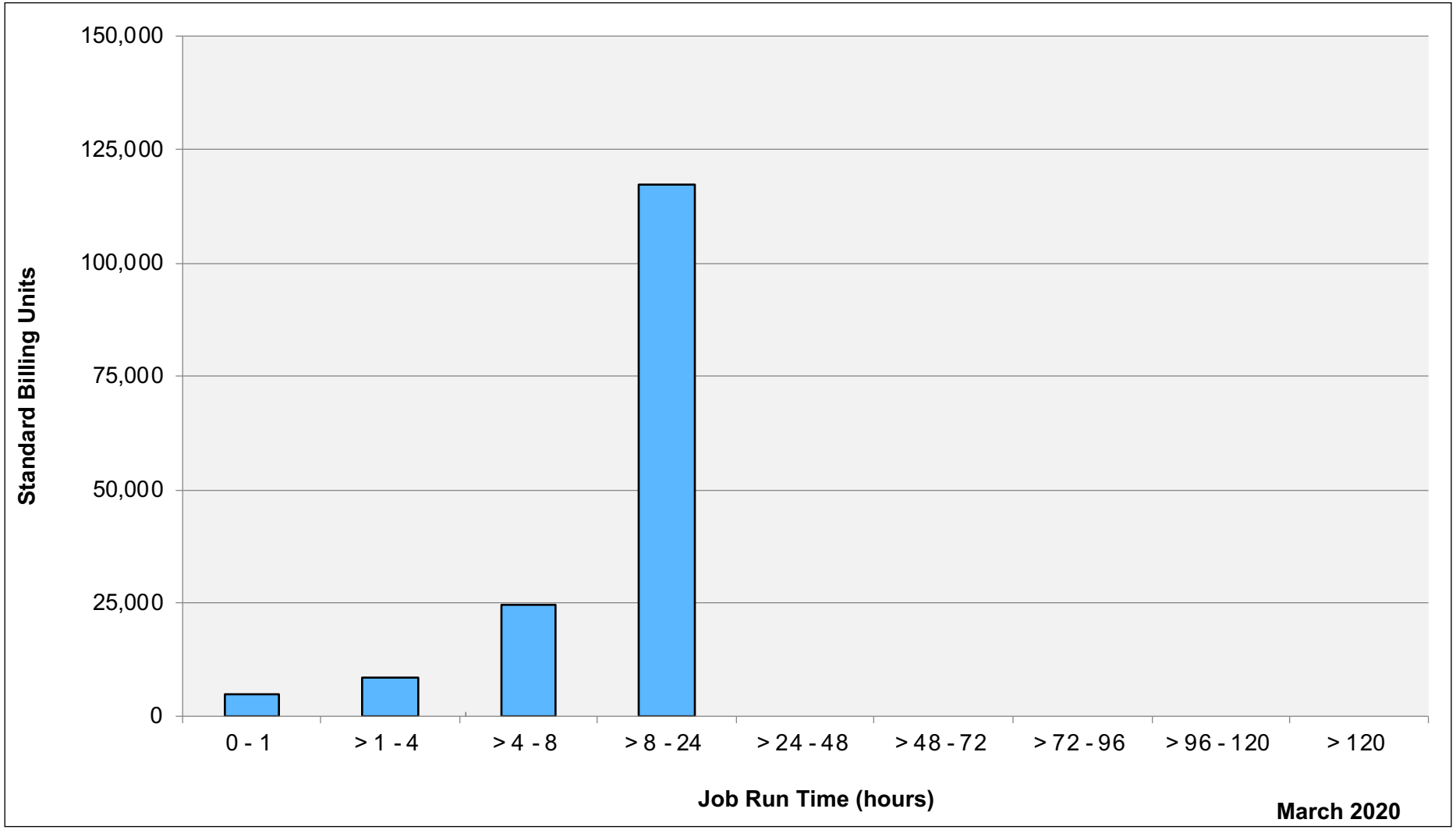
Electra: Average Expansion Factor



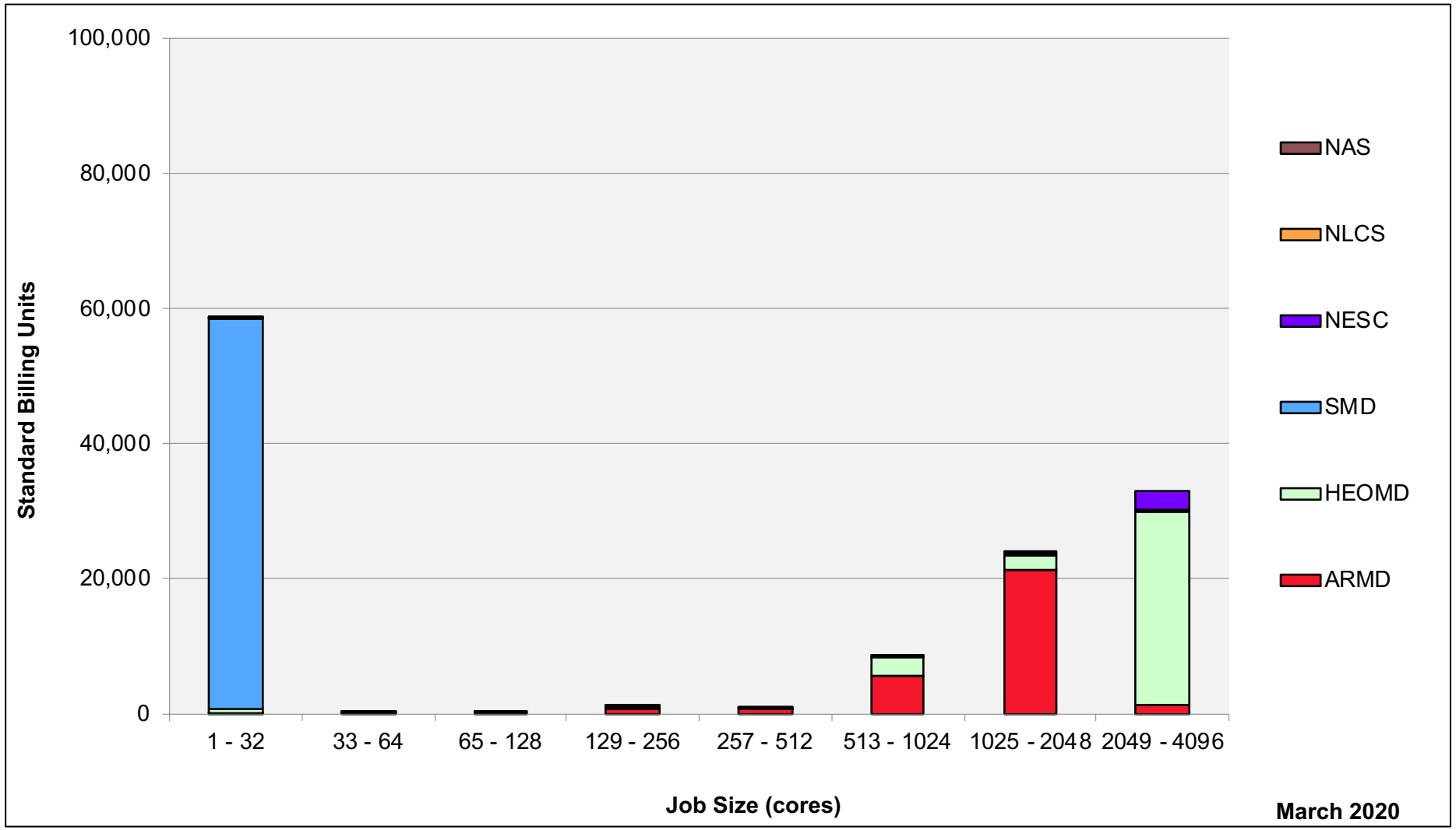
Merope: SBUs Reported, Normalized to 30-Day Month



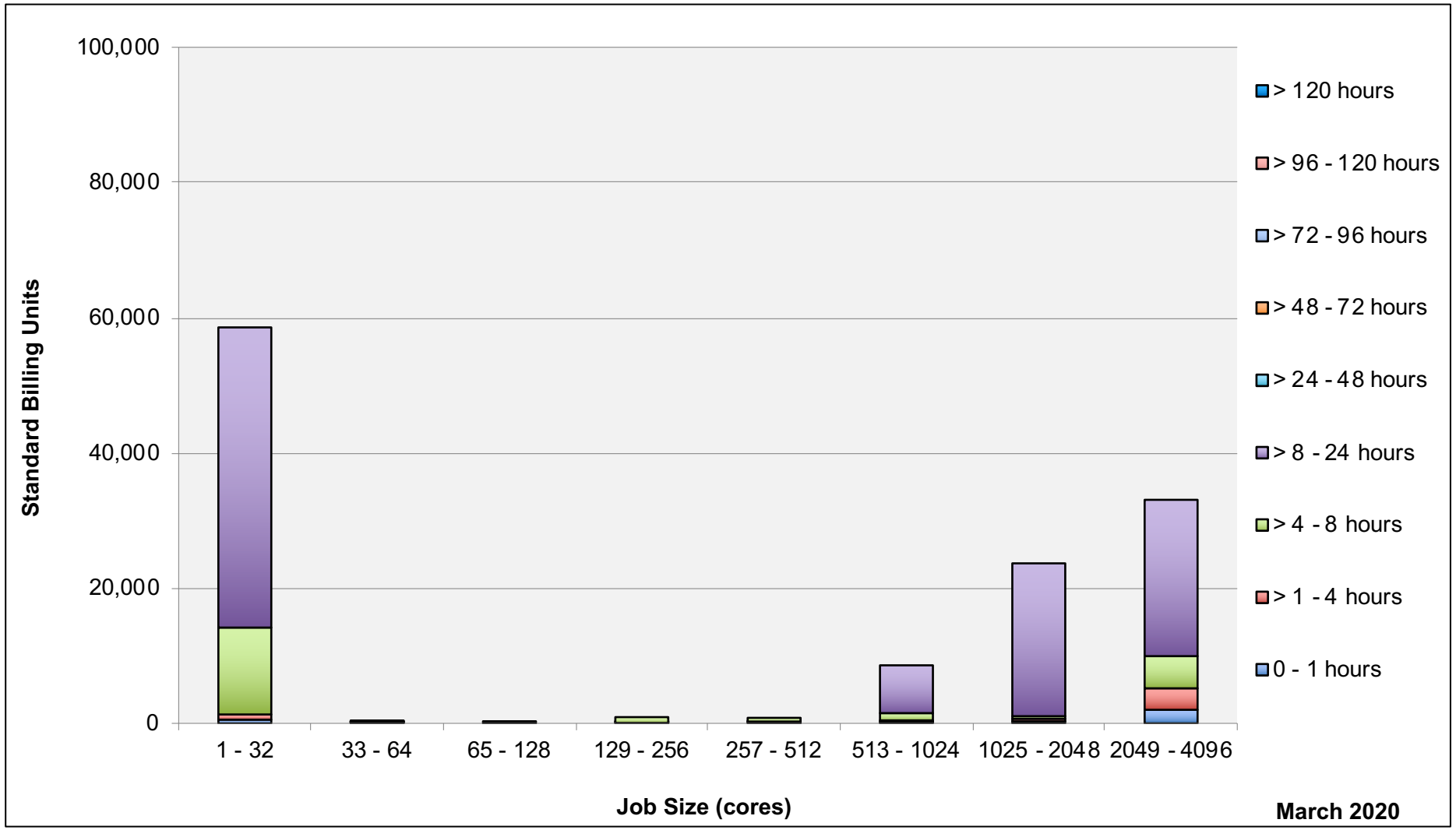
Merope: Monthly Utilization by Job Length



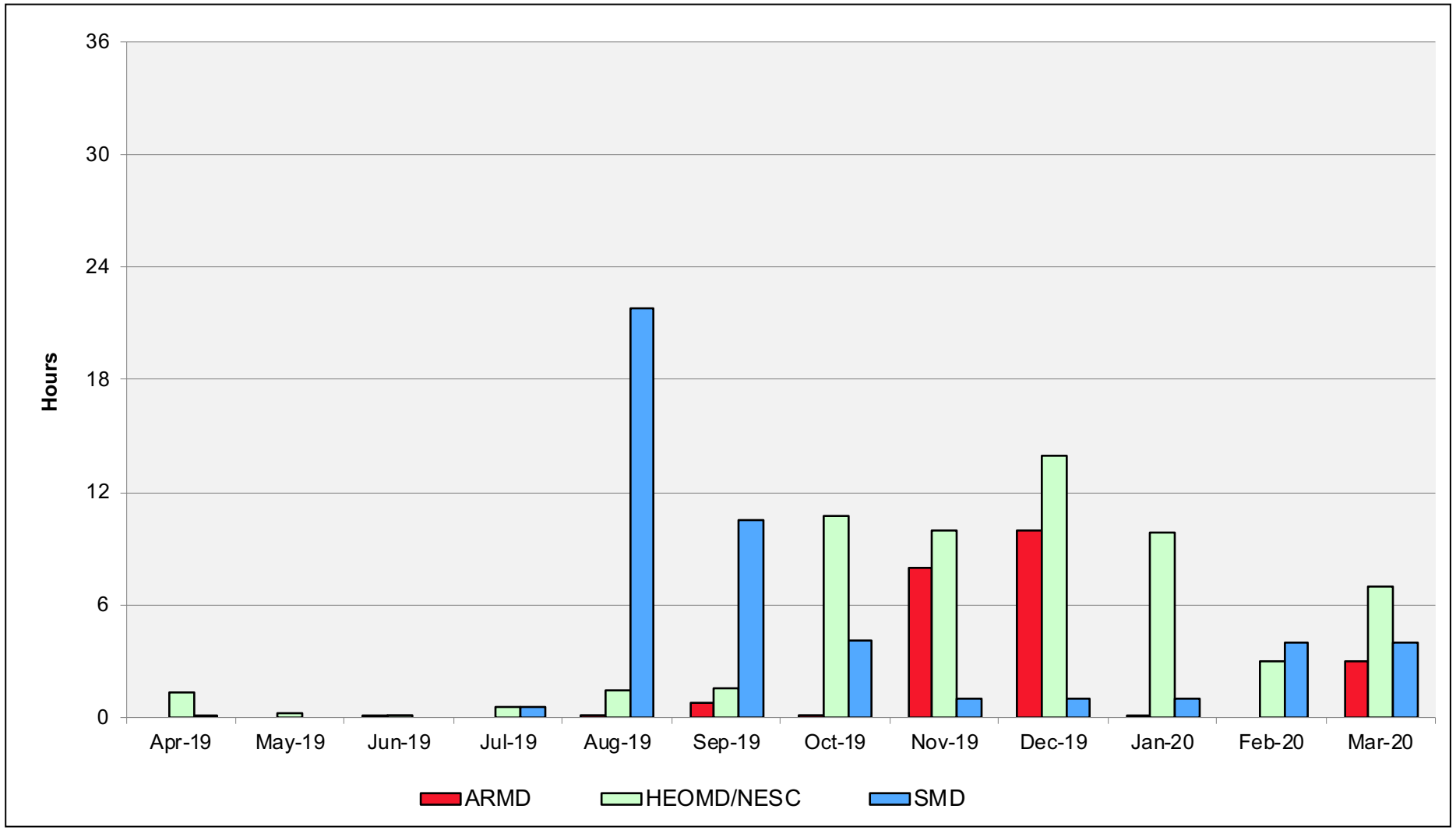
Merope: Monthly Utilization by Job Length



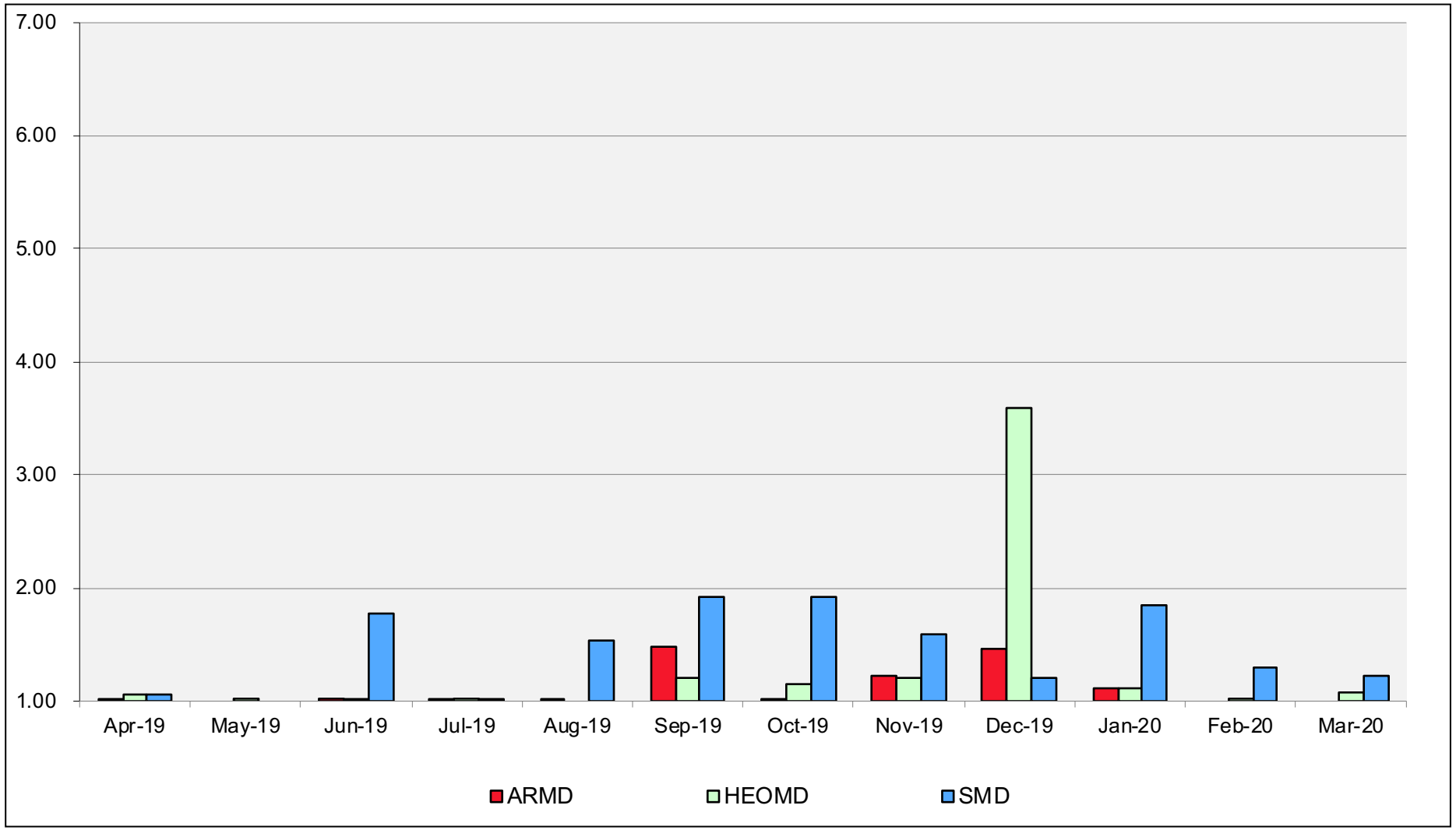
Merope: Monthly Utilization by Size and Length



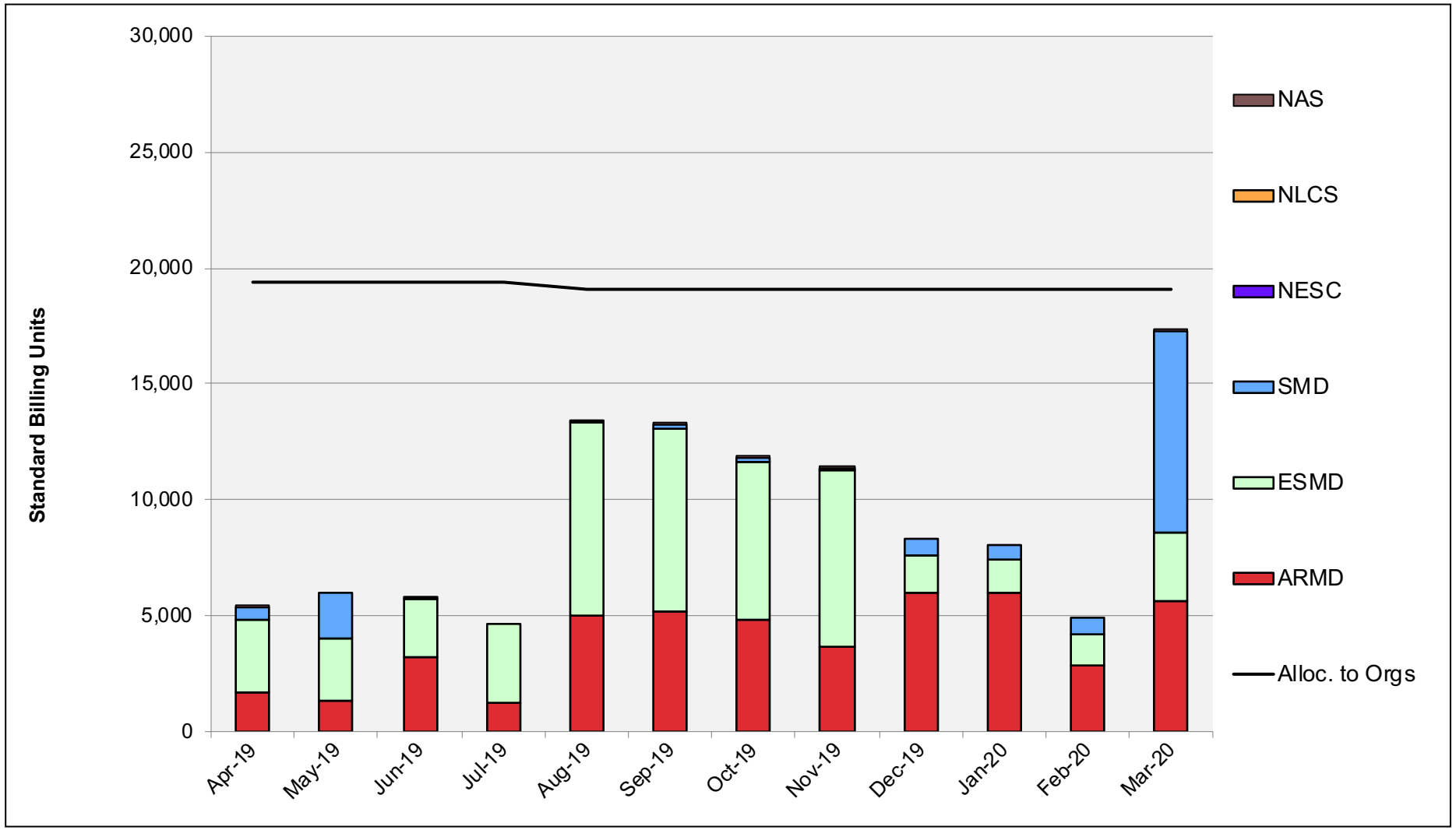
Merope: Average Time to Clear All Jobs



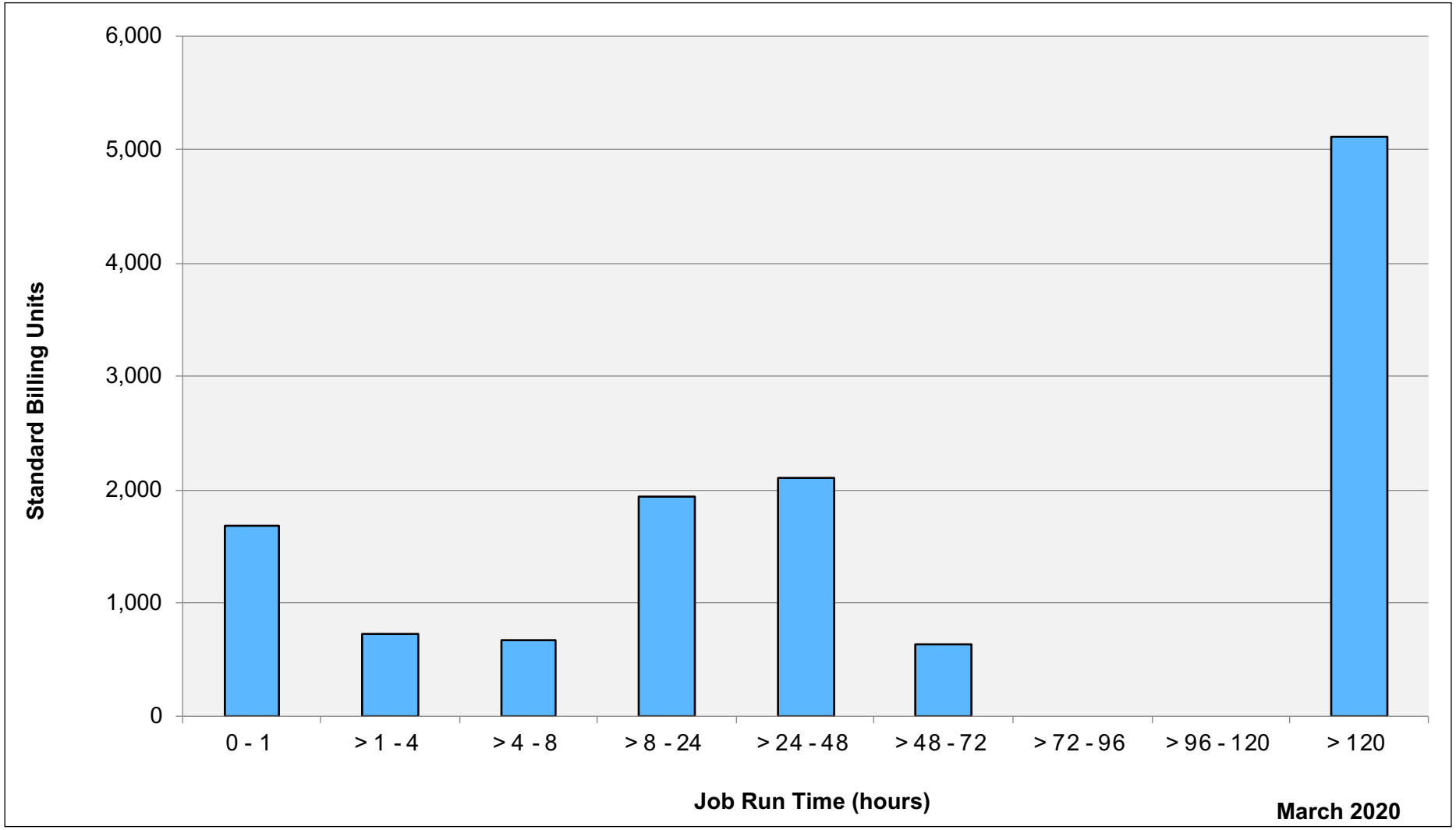
Merope: Average Expansion Factor



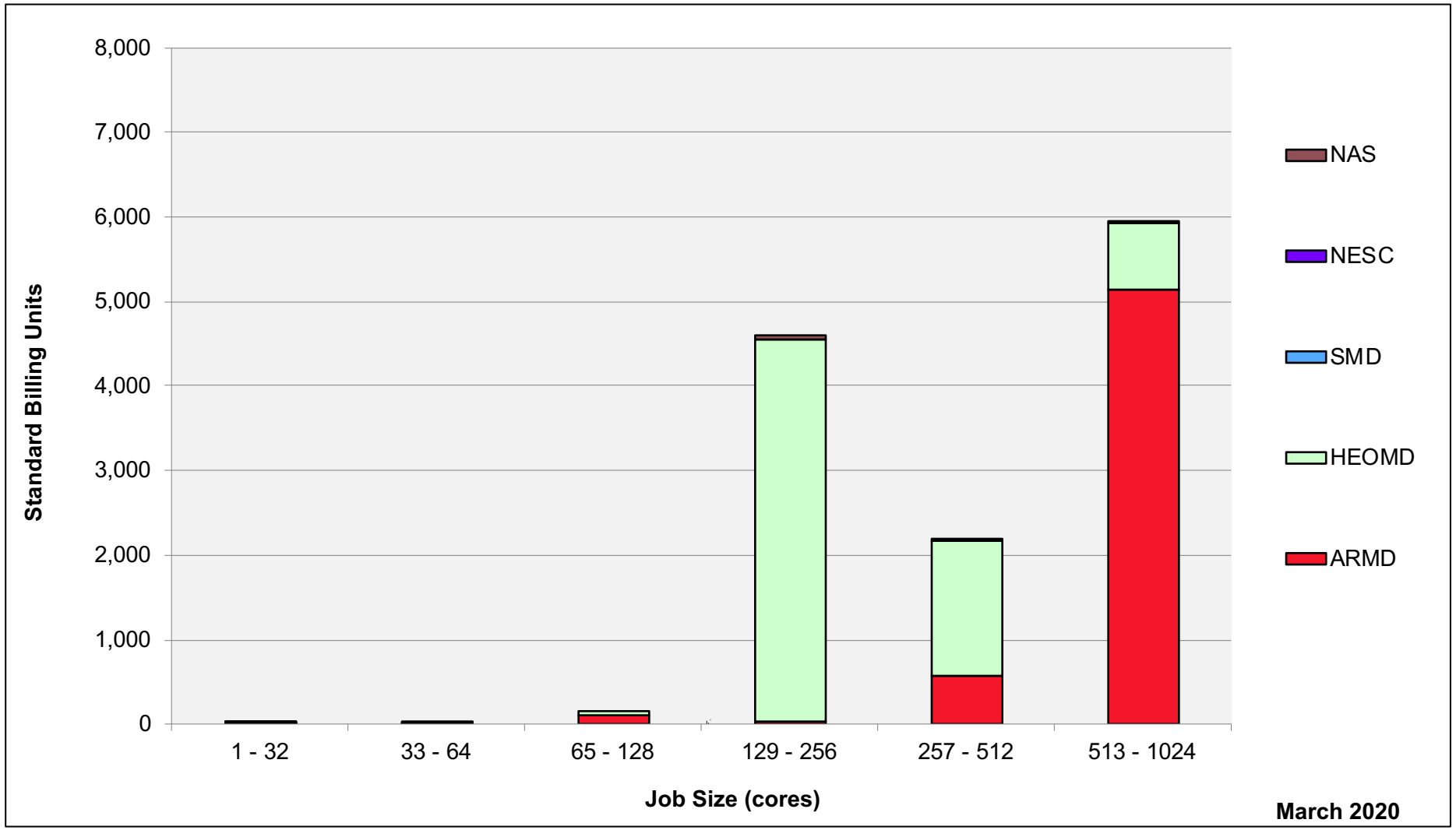
Endeavour: SBUs Reported, Normalized to 30-Day Month



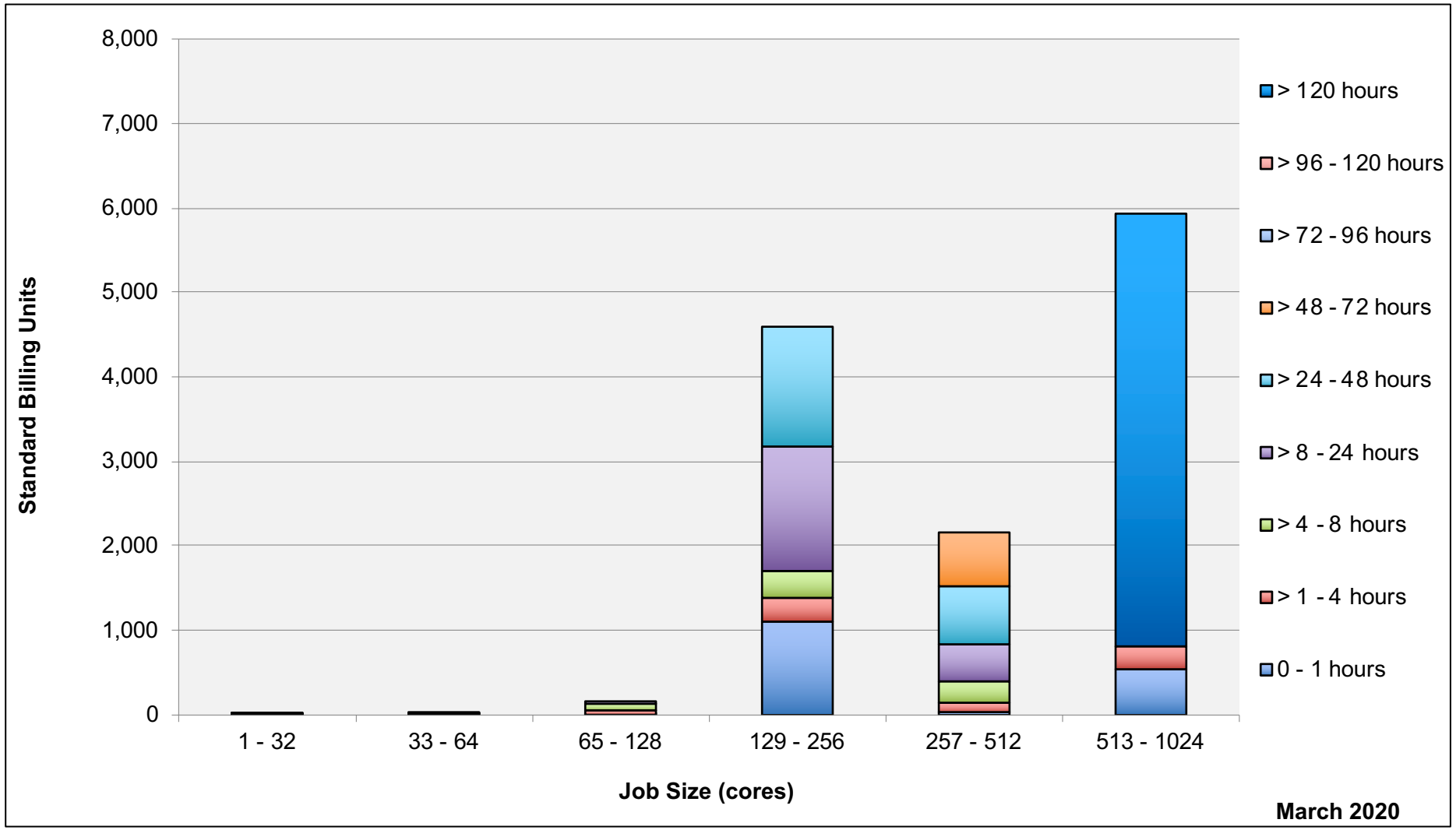
Endeavour: Monthly Utilization by Job Length



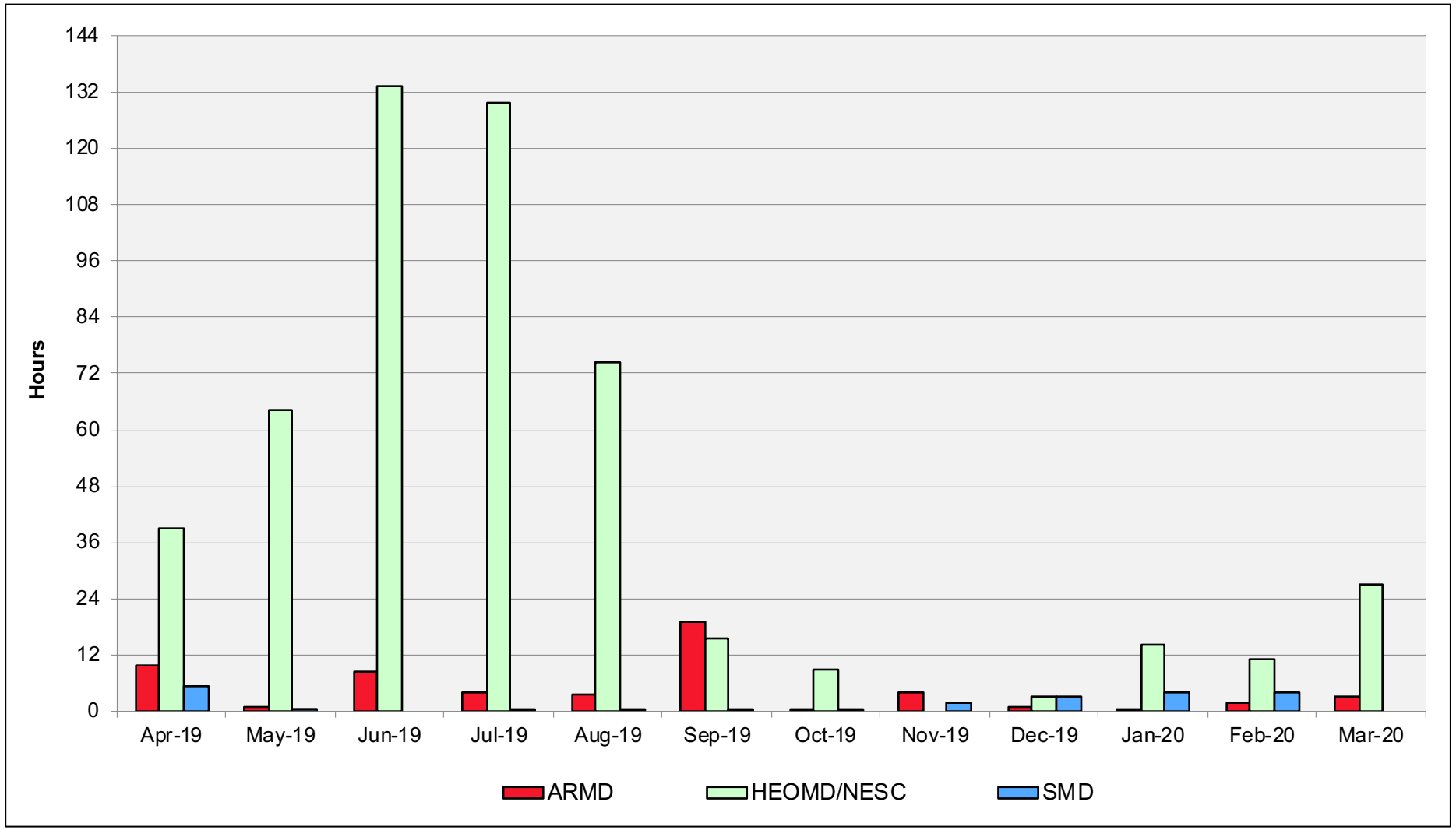
Endeavour: Monthly Utilization by Job Length



Endeavour: Monthly Utilization by Size and Length



Endeavour: Average Time to Clear All Jobs



Endeavour: Average Expansion Factor