Project Status Report

High End Computing Capability

Strategic Capabilities Assets Program

June 10, 2018

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Progress Continues on NAS Facility Expansion Construction

- The HECC Facilities team, in collaboration with NASA Ames Code JCE and vendors Jacobs, Tri-Technic, HPE, and Schneider Electric, continued work toward the November 2018 date for completing the NAS Facility Expansion (NFE) site construction.
- Activities in May included:
  - The aggregate base for the concrete pad was brought up to within 8 inches of its final height.
  - Module designers HPE & Schneider completed their 60% design package.
  - Duct-bank construction and manhole installation under the streets began and is ahead of schedule.

Mission Impact: The NFE design builds on the enormous success of HECC’s prototype Modular Supercomputing Facility, which proved to be a much more cost-effective and energy-efficient way to operate and manage a supercomputing environment.

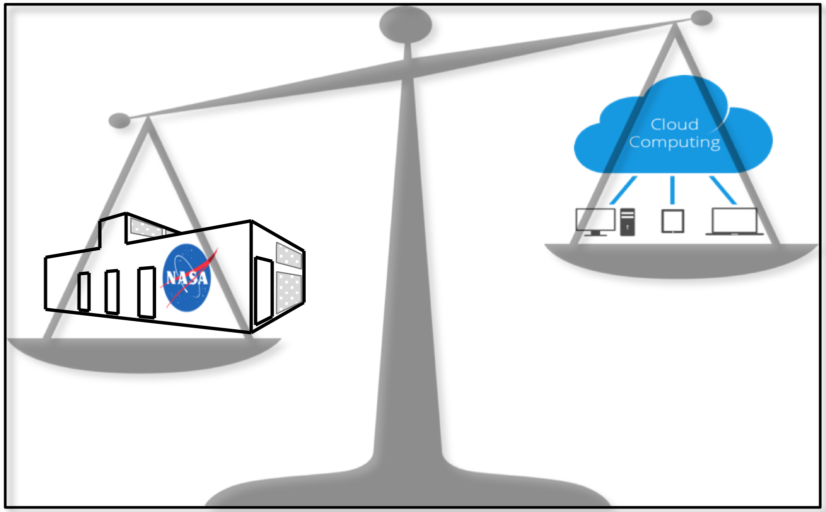
The communications duct bank being installed under the road between the NAS Facility Expansion site and the main NASA Advanced Supercomputing facility. Single-module fiber will be installed in the conduits.

POCs: William Thigpen, william.w.thigpen@nasa.gov, (650) 604-1061, NASA Advanced Supercomputing (NAS) Division; Christopher Tanner, christopher.l.tanner@nasa.gov, (650) 604-6754, NAS Division, CSRA LLC

HECC Applications Team Completes Report on Cloud Trade Study

- HECC's Application Performance and Productivity (APP) team recently completed a report on its Cloud Trade Study, which compared the performance and cost of running NASA HPC applications on HECC in-house resources versus the commercial cloud.
- APP used the NAS Parallel Benchmarks and a set of full applications representing the current HECC workload. Tests were conducted on the Pleiades and Electra systems and on similarly configured cloud resources at Amazon and Penguin.
- The team's primary finding was that HECC in-house resources were significantly cheaper than cloud resources for running the NASA workload. The study further found that:
  - Applications with tightly coupled communication requirements run better on HECC resources.
  - Cloud resources cost more than HECC resources, per core-hour, even when using the most optimistic estimate of cloud costs and the most pessimistic one for HECC's.
- The report found that there may be some situations where cloud use would be cost effective, and the team began follow-on work to prepare for a broadening of HECC services to include running jobs in the cloud.

Mission Impact: While confirming that the bulk of NASA's modeling and simulation workload is run most cost effectively on in-house resources, the report recommends studying some cases that might result in improved efficiency or cost to HECC if run in the cloud.



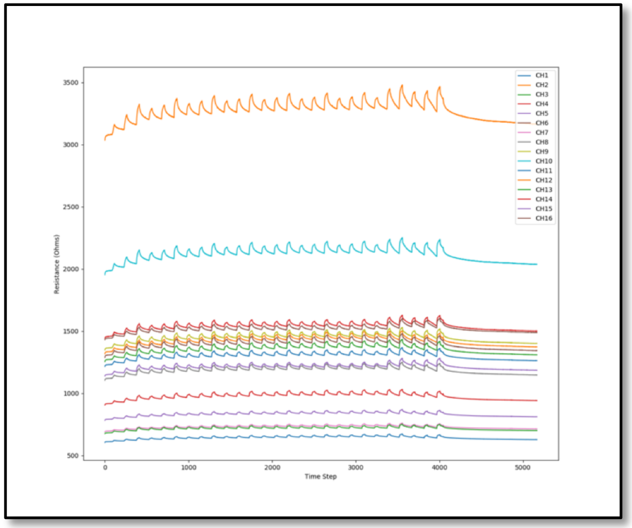
HECC's Application Performance and Productivity Team conducted a Cloud Trade Study and found that the using on-premises HECC resources for NASA's workload was significantly more cost effective than running in the cloud.

POCs: Henry Jin, haoqiang.jin@nasa.gov, (650) 604-0165, NASA Advanced Supercomputing (NAS) Division; Robert Hood, robert.hood@nasa.gov, (650) 604-0740, NAS Division, CSRA LLC

Machine Learning For Carbon Nanotube Chemical Sensor Arrays

- A team of HECC experts worked with the Carbon Nanotube Chemical Sensor (CNTCS) team, on the initial Data Analytics project, and provided significant preliminary results that allowed CNTCS to move forward.
  - The goal of CNTCS project is to produce a low cost, lightweight sensor to detect and quantify concentrations of gases.
- CNTCS provided three ammonia (NH_3) datasets. Each data point comprised the resistance change over 16 sensor channels in response to NH_3 exposures at varying concentration and humidity.
- A Support Vector Machine was fit with 80% of the data chosen at random, and tested on the remaining 20%. The prediction accuracy was better than 94%.
- The Data Analytics team will continue to work with CNTCS staff after they collect more data (thousands of exposures) with different gases (CO, CO_2, CH_2O). With this larger dataset, the team will apply neural net techniques for machine learning.

Mission Impact: HECC's new capability will support infusion of machine learning technology into NASA research efforts in order to successfully demonstrate scientific results with faster time to discovery.



Plot of resistance versus time for sixteen channel CNT sensor array when exposed to NH_3 at 15ppm, 20ppm and 35ppm at 46% humidity. Each resistance jump is due to a gas exposure (higher concentration causes larger change). This data was used to train (fit) a Support Vector Machine.

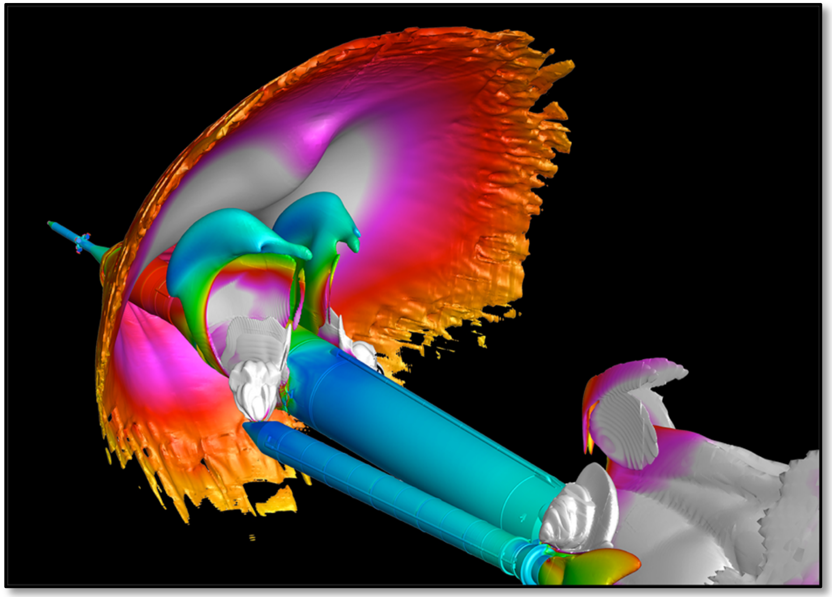
POCs: Shubha Ranjan, shubha.ranjan@nasa.gov, (650) 604-1918, NASA Advanced Supercomputing (NAS) Division; Jeff Becker, jeffrey.c.becker@nasa.gov, (650) 604-4645, NAS Division, CSRA LLC

HECC Supercomputer Usage in May 2018 Sets New Record

- In May, the combined usage on HECC supercomputers set a new record of 32,778,836 Standard Billing Units (SBUs*).
- The usage by 372 of NASA's science and engineering groups exceeded the previous record of 28,161,309 SBUs set in December of 2017 by 4,617,527 SBUs.
- The record was achieved in great part by dedicated resources for the Space Launch System using computational fluid dynamics (CFD) simulations focused on the prediction of the launch-induced environment.
- Usage of Pleaides, Electra, Merope, and Endeavour contributed to this record.
- The top 10 projects used between 545,207 and 8,627,753 SBUs, and together accounted for over 52% of the total usage.
- The HECC Project continues to evaluate and plan resources to address the future requirements of NASA's users.

* 1 SBU (Standard Billing Unit) represents the work that can be performed on a dual-socket Westmere node in one hour.

Mission Impact: The increased capacity of HECC systems and working with users to optimize their job runs provides mission directorates with more resources to accomplish their goals and objectives.



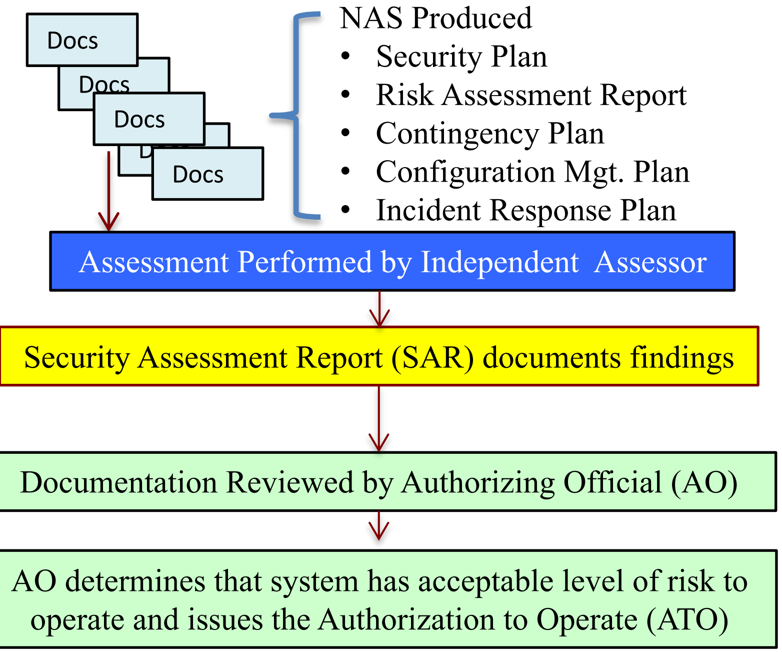
Example of work done on HECC systems: Space Launch System booster separation flow field: isosurfaces of density (colored by pressure) illustrate a shock wave on the front of the vehicle; isosurfaces of plume-gas species (colored by Mach number) show the booster separation-motor plumes. Vehicle surface is colored by pressure. *Stuart Rogers, Derek Dalle, NASA/Ames*

POC: Blaise Hartman, blaise.hartman@nasa.gov, (650)-604-2539, NASA Advanced Supercomputing Division, CSRA LLC

Authorization to Operate Renewed Following Annual Independent Security Assessment

- The Ames Research Center CIO, the Authorizing Official for the NAS security plan that includes HECC systems, approved a renewed Authorization to Operate (ATO) dated February 10, 2018.
- The approved ATO is the final step in the annual security assessment required of all NASA systems.
- This annual security assessment validates that the facilities, systems, and operations comply with the NAS Supercomputing Storage and Support Systems (NS4), CD-9999-M-ARC-3232 security plan, and with NASA regulations.
- The ATO ensures the continued operation of HECC Systems is in compliance with NASA security requirements.
- The new authorization expires in one year on March 11, 2019—the normal period for NASA ATOs.

Mission Impact: The Authorization to Operate allows HECC supercomputers and support systems to continue to operate, and the independent assessment provides an important confirmation regarding the security compliance of HECC systems.



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

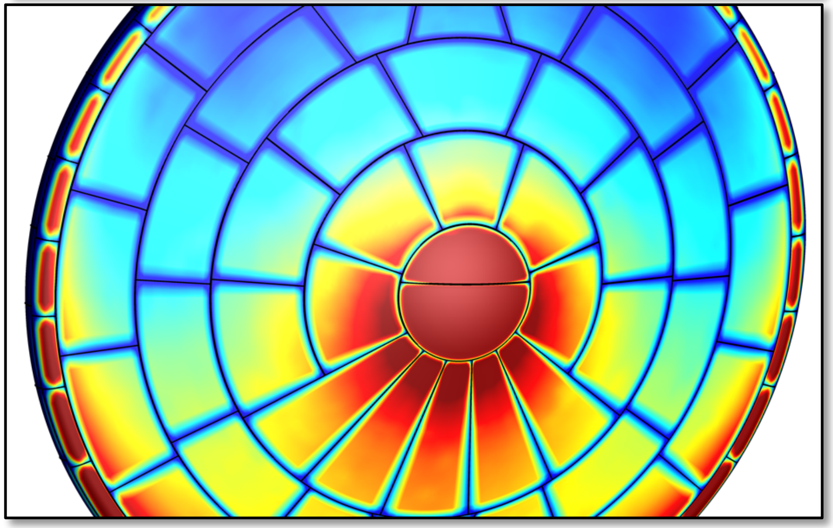
POC: Thomas Hinke, thomas.h.hinke@nasa.gov, (650) 279-4053, NASA Advanced Supercomputing Division

Simulating Heat Shields in 3D to Improve TPS Materials for Future Space Vehicles

- NASA Ames aerospace engineers are producing unique 3D simulations of the Mars Science Laboratory (MSL) heat shield on Pleiades.
- The simulations will help engineers improve thermal protection system (TPS) materials for future space exploration missions.
  - The team used the MSL's 4.5-meter diameter heat shield as a test case to successfully show that their Porous-material Analysis Toolbox based on OpenFOAM (PATO) software can perform massively parallel simulations of material thermal response and recession rates—providing a better understanding of these key design features to ensure an optimum trade-off between vehicle mass and safety.
  - Results showed that the differential recession between the tiles and the gap filler promotes the formation of a "fence," which poses design challenges as it may promote transition to turbulence—an important factor in prediction and control of heat transfer during atmospheric entry.
- The project goal is to develop a material design framework to enable rapid development of mission-tailored TPS materials for large-payload missions to Mars, Venus, Jupiter, and Saturn.

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

Mission Impact: HECC resources help NASA engineers develop modeling and simulation tools that enable analysis of heat shield thermal material response in order to reduce the need for extensive testing and to accelerate the design cycle process.



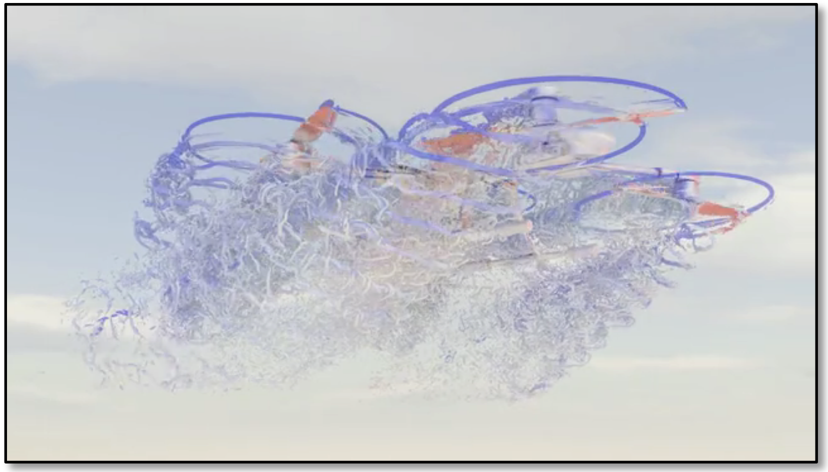
3D view of the estimated recession at the MSL's heat shield front surface, 70 seconds after Mars entry during peak heating, from a simulation produced with the PATO software. This image shows the tiles' influence on heat shield recession, which is a potential promoter of transition from laminar to turbulent flow. *Jeremie B. E. Meurisse, NASA/Ames*

POCs: Jeremie B.E. Meurisse, jeremie.b.meurisse@nasa.gov, (650) 604-1658, NASA Advanced Supercomputing (NAS) Division, Science & Technology Corp.;
Nagi N. Mansour, nagi.n.mansour@nasa.gov, (650) 604-6420, NAS Division

Complex Rotorcraft Simulations Move Researchers Toward Urban Air Mobility

- As part of NASA's commitment to leading the Urban Air Mobility (UAM) community to identify key challenges, researchers at NASA Ames ran high-fidelity CFD simulations on Pleiades and Electra to study the performances of three multirotor UAV designs, with variations of each.
- Researchers modeled the surface grids of the DJI Phantom 3 and Straight Up Imaging (SUI) Endurance quadcopters, and the Elytron 4S UAV concept UAM. Among their discoveries and innovations:
  - Interactions between rotor wakes in the standard SUI configuration reduced rear rotor performance in forward flight.
  - Using two undermount front rotors and two overmount rear rotors reduced the influence of front rotor wakes on back rotors and front arms.
  - The resulting increase in forward thrust allows the quadcopter to fly longer on the same battery charge, greatly improved range, autonomy, and efficiency, without increasing the vehicle weight.
- HECC experts produced customized visualizations that were critical to understanding the multirotor UAMs' complex, unsteady, turbulent flow interactions.

Mission Impact: Simulations carried out using HECC resources led to development of a new hybrid quadcopter that will fly faster, quieter, and longer. Results will have far-reaching impacts for future multirotor Unmanned Aerial Vehicles and Urban Air Mobility vehicle design and manufacturing.



Video from a simulation of the Straight Up Imaging Endurance quadcopter hybrid design in forward flight, showing NASA's novel hybrid design modification, where front rotors are undermounted and back rotors are kept overmounted. *Timothy Sandstrom, NASA/Ames*

POCs: Patricia Ventura Diaz, patricia.venturadiaz@nasa.gov, (650) 604-0075, NASA Advanced Supercomputing (NAS) Division, Science and Technology Corp.; Seokkwan Yoon, s.yoon@nasa.gov, (650) 604-4482, NAS Division

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

HECC Facility Hosts Several Visitors and Tours in May 2018

- HECC hosted 9 tour groups in May; guests learned about the agency-wide missions being supported by HECC assets, and some groups also viewed the D-Wave 2X quantum computer system. Visitors this month included:
  - James Reuter, Acting Associate Administrator, Space Technology Mission Directorate.
  - Deron Bilious and Jason Kripps, Minister and Deputy Minister of Economic Development & Trade, Province of Alberta.
  - Fifty attendees from the NASA Ames-hosted 2018 Global Learning and Observation to Benefit the Environment (GLOBE) Conference, including teachers, award-winning students, and college professors.
  - Several guests from the United States Geological Survey (USGS) and Geosciences Australia.
  - 20 German researchers who were at Ames for meetings with onsite military partners from the U.S. Army and Air Force.
  - Attendees of the Electric Vertical Take-Off and Landing workshop.
  - 20 students from the Aalto University located in Greater Helsinki, Finland, who visited Ames as part of their summer technology tour.

Piyush Mehrotra, Chief, NASA Advanced Supercomputing Division, gives a tour of the Pleiades supercomputer floor to German researchers and active U.S. military guests.

POC: Gina Morello, gina.f.morello@nasa.gov, (650) 604-4462, NASA Advanced Supercomputing Division

Papers

- "**Reconnection in the Martian Magnetotail: Hall-MHD with Embedded Particle-in-Cell Simulations**," Y. Ma, et al., Journal of Geophysical Research: Space Physics, April 30, 2018. *
  https://agupubs.onlinelibrary.wiley.com/doi/abs/10.1029/2017JA024729
- "**Quasi-Periodic Counter-Propagating Fast Magnetosonic Wave Trains from Neighboring Flares: SDO/AIA Observations and 3D MHD Modeling**," L. Ofman, W. Liu, arXiv:1805.00365 [astro-ph.SR], May 1, 2018. *
  https://arxiv.org/abs/1805.00365
- "**The Importance of Vertical Resolution in the Free Troposphere for Modeling Intercontinental Plumes**," J. Zhuang, D. Jacob, S. Eastham, Atmospheric Chemistry and Physics, vol. 18, May 2, 2018. *
  https://www.atmos-chem-phys.net/18/6039/2018/
- "**Kinetic Dissipation Around a Dipolarization Front**," M. Sitnov, V. Merkin, V. Roytershteyn, M. Swisdak, Geophysical Research Letters, May 4, 2018. *
  https://agupubs.onlinelibrary.wiley.com/doi/abs/10.1029/2018GL077874
- "**Subresolution Activity in Solar and Stellar Coronae from Magnetic Field Line Tangling**," A. Rappazzo, R. Dahlburg, G. Einaudi, M. Velli, Monthly Notices of the Royal Astronomical Society, May 11, 2018. *
  https://academic.oup.com/mnras/advance-article/doi/10.1093/mnras/sty1132/4995224

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

Papers (cont.)

- "**Dark Matter Halo Properties vs. Local Density and Cosmic Web Location**," T. Goh, et al., arXiv:1805.04943 [astro-ph.GA], May 13, 2018. *
https://arxiv.org/abs/1805.04943
- "**Evaluating Uncertainties in Coronal Electron Temperature and Radial Speed Measurements Using Simulation of the Bastille Day Eruption**," N. Reginald, O. St. Cyr, J. Davila, L. Rastaetter, T. Török, *Solar Physics*, published online May 15, 2018. *
https://link.springer.com/article/10.1007/s11207-018-1301-x
- "**Program Power Profiling Based on Phase Behaviors**," X. Ma, Z. Du, J. Liu, Sustainable Computing: Informatics and Systems, May 17, 2018. *
https://www.sciencedirect.com/science/article/pii/S2210537917302007
- "**Numerical Study of Turbulent Separation Bubbles with Varying Pressure Gradient and Reynolds Number**," G. Coleman, C. Rumsey, P. Spalart, Journal of Fluid Dynamics, vol. 847, published online May 17, 2018. *
https://doi.org/10.1017/jfm.2018.257
- "**Orientation and Stability of Asymmetric Magnetic Reconnection X-Line**," Y.-H. Liu, M. Hesse, T. Li, M. Kuznetsova, A. Le, arXiv:1805.07774 [physics.space-ph], May 20, 2018 *
https://arxiv.org/abs/1805.07774

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

Papers (cont.)

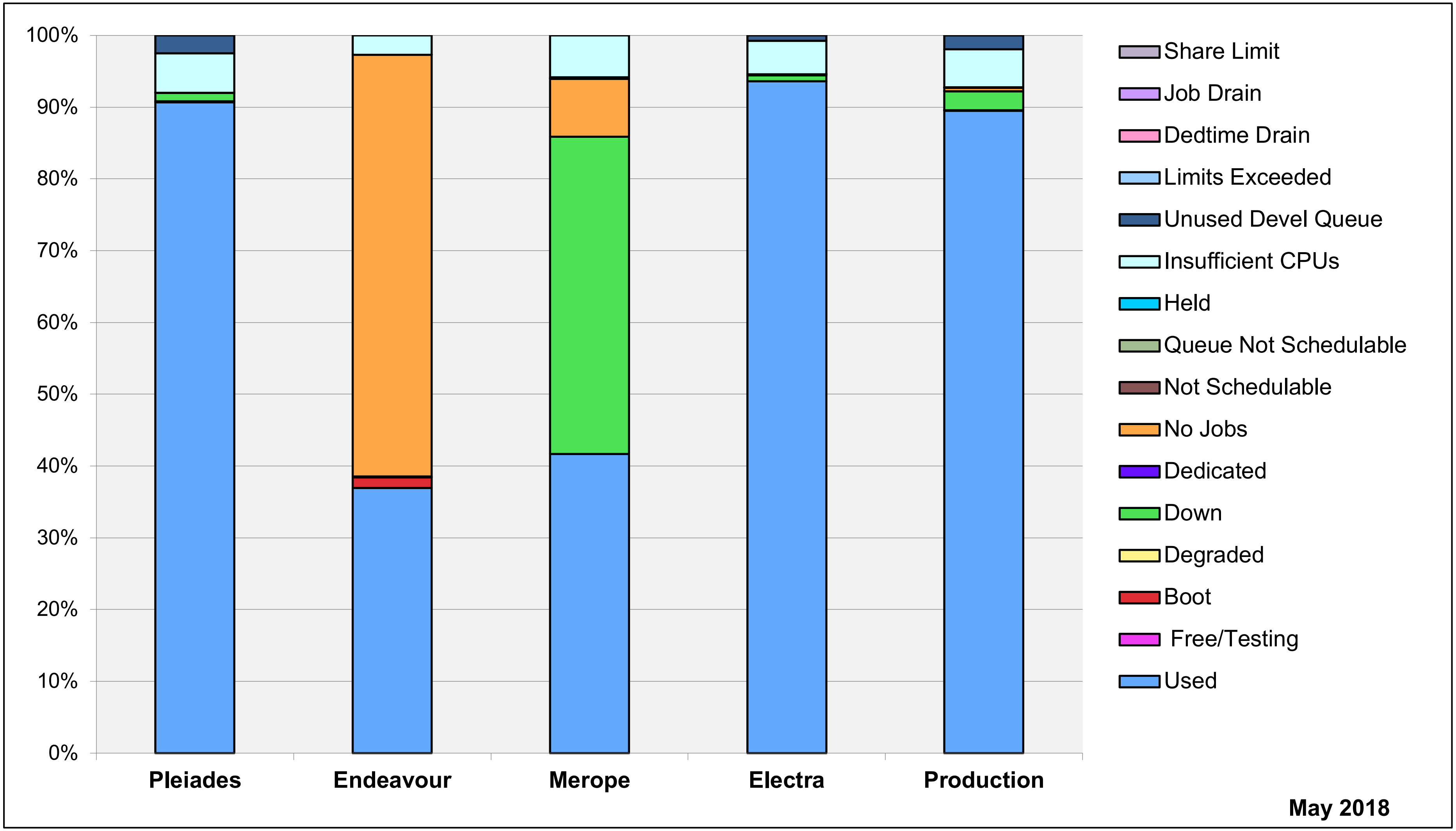
- **"Modeling Martian Atmospheric Losses Over Time: Implications for Exoplanetary Climate Evolution and Habitability**," C. Dong, et al., The Astrophysical Journal Letters, vol. 859, no. 1, May 23, 2018. *
  http://iopscience.iop.org/article/10.3847/2041-8213/aac489/meta
- "**Interaction Energy for Fullerene Encapsulated in Carbon Nanotorus**," P. Sarapat, D. Baowan, J. Hill, Zeitschrift für angewandte Mathematik und Physik, May 24, 2018. *
  https://link.springer.com/article/10.1007/s00033-018-0972-3
- "**DirtyGrid I: 3D Dust Radiative Transfer Modeling of Spectral Energy Distributions of Dusty Stellar Populations**," K.-H. Law, K. Gordon, K. Misselt, The Astrophysical Journal Supplement Series, vol. 236, no. 2, May 25, 2018. *
  http://iopscience.iop.org/article/10.3847/1538-4365/aabf41
- **"Evaluating the Suitability of Commercial Clouds for NASA's High Performance Computing Applications: A Trade Study**," S. Chang, R. Hood, H. Jin, S. Heistand, J. Chang, S. Cheung, J. Djomehri, G. Jost, D. Kokron, NAS Technical Report NAS-2018-01, May 31, 2018. *https://www.nas.nasa.gov/assets/pdf/papers/NAS_Technical_Report_NAS-2018-01.pdf*

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

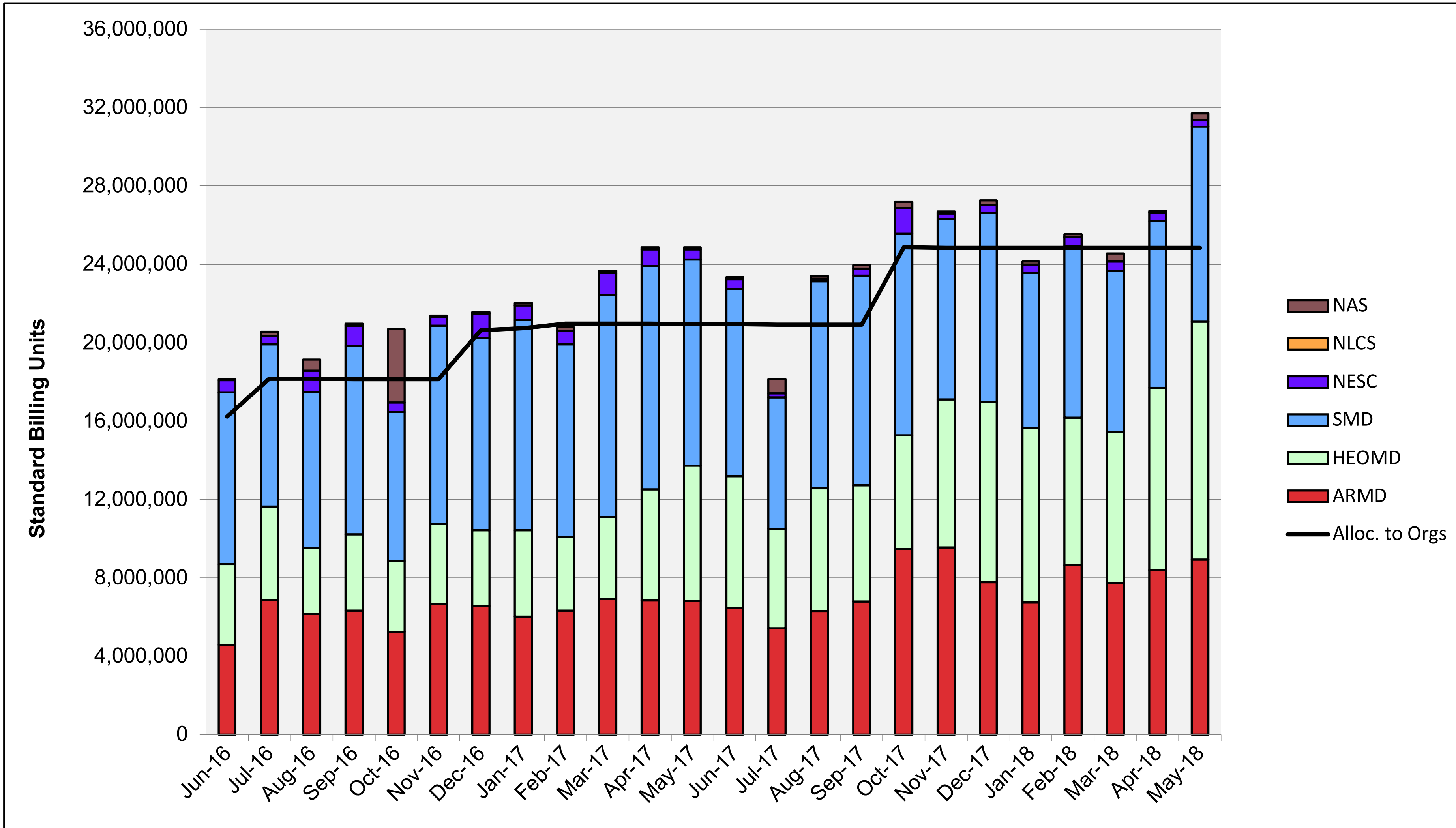
News & Events

- **AA-2 – NASA's JSC Getting Orion Simulator Ready for Key Test**, *Spaceflight.com,* April 30, 2018—An image from a HECC video feature of an Orion abort simulation was featured as part of this article about the crew module simulator work at NASA Johnson. *https://www.nasaspaceflight.com/2018/04/nasas-jsc-getting-orion-simulator-key-test/*
- **Swirl Features Reproduced by Modeling Solar Wind Standoff**, *NASA Science: Earth's Moon*, May 7, 2018—A team of researchers at the Institute for Modeling Plasma, Atmospheres and Cosmic Dust (IMPACT) at the University of Colorado Boulder, have developed the first 3D simulations to disentangle the movement of ions and electrons as the solar wind interacts with lunar magnetic anomalies. The researchers used the Pleiades supercomputer, combined with lunar satellite observations, to show that solar wind standoff can reproduce lunar swirl features. *https://moon.nasa.gov/news/48/lunar-swirl-features-reproduced-by-modeling-solar-wind-standoff/*
- **NASA Awards Contract for Advanced Computing Services**, *NASA Ames Press Release*, May 17, 2018—NASA has selected InuTeq LLC of Beltsville, Maryland, to provide high-performance computing to all NASA missions in support of mission-driven science and engineering. InuTeq will provide direct support to the NASA Advanced Supercomputing division at NASA's Ames Research Center and the NASA Center for Climate Simulation at NASA's Goddard Space Flight Center, and provide advanced computing services to other NASA centers. *https://www.nasa.gov/press-release/nasa-awards-contract-for-advanced-computing-services*
  - **NASA Awards Contract for Advanced Computing Services**, *HPCwire*, May 18, 2018. *https://www.hpcwire.com/off-the-wire/nasa-awards-contract-for-advanced-computing-services/*

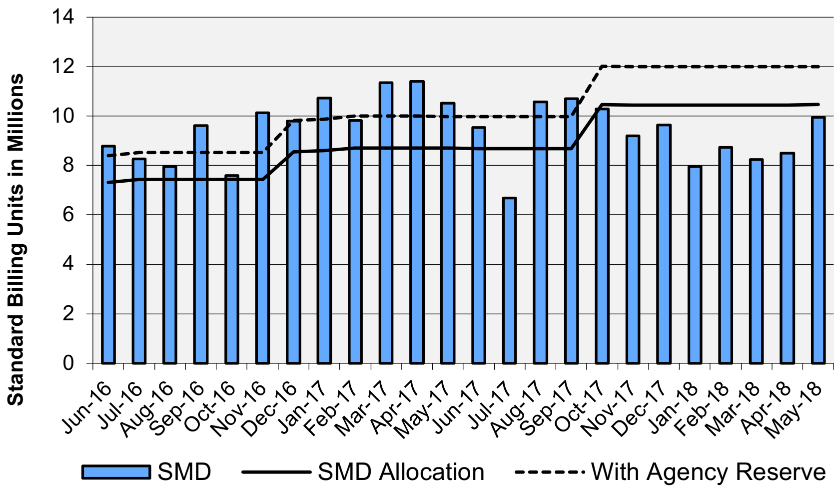
HECC Utilization

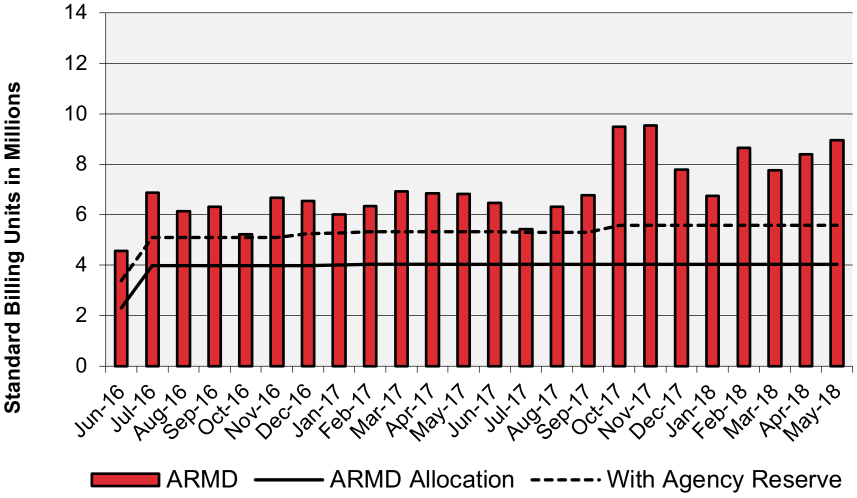


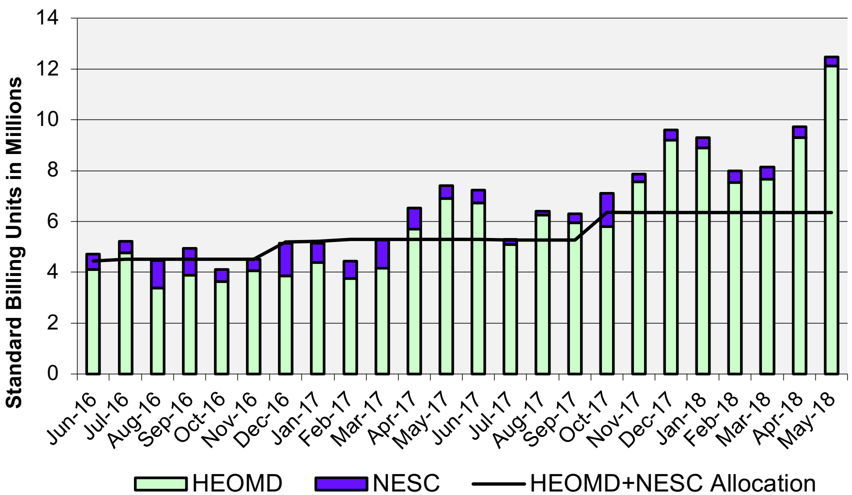
HECC Utilization Normalized to 30-Day Month



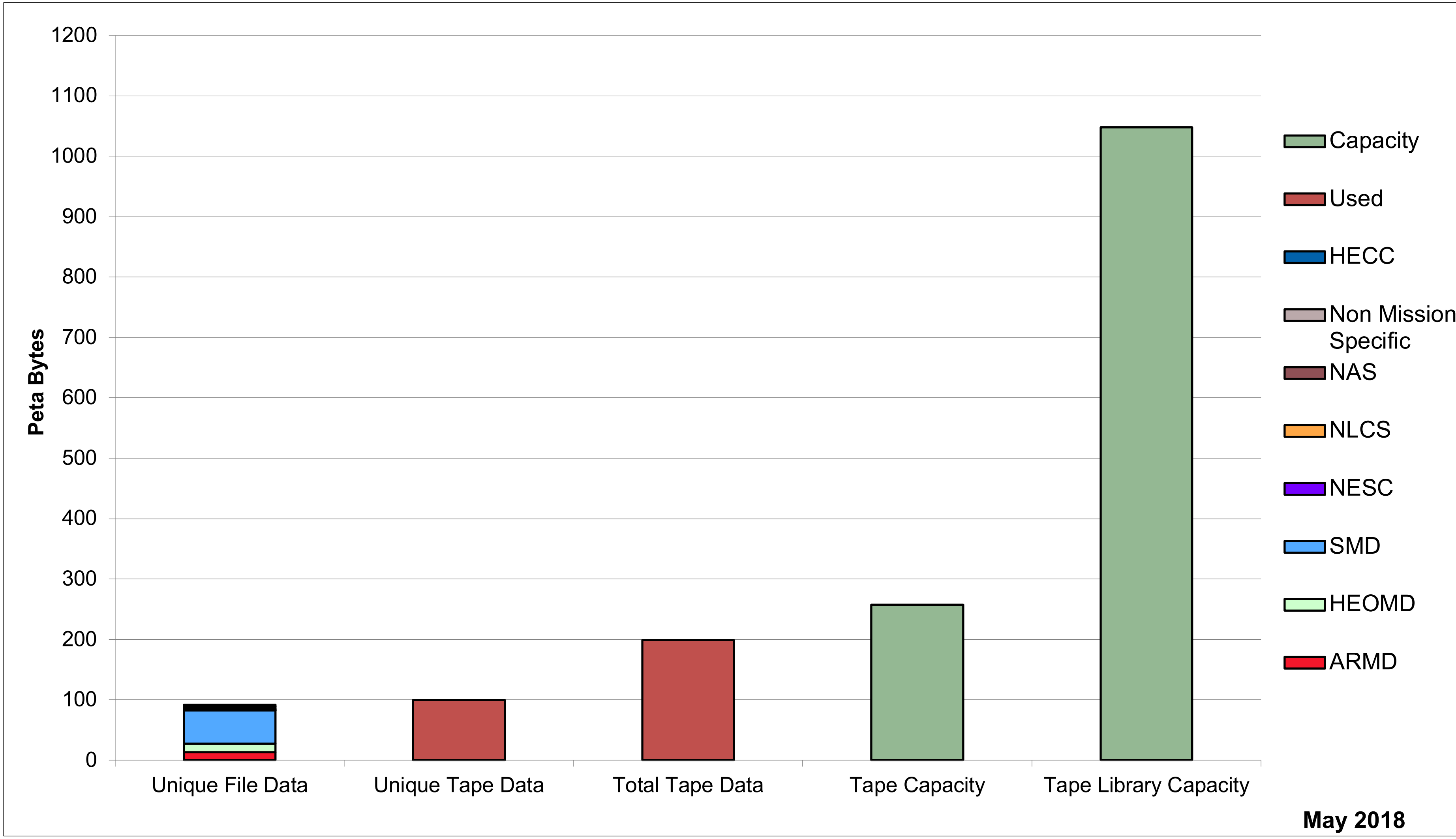
HECC Utilization Normalized to 30-Day Month







Tape Archive Status



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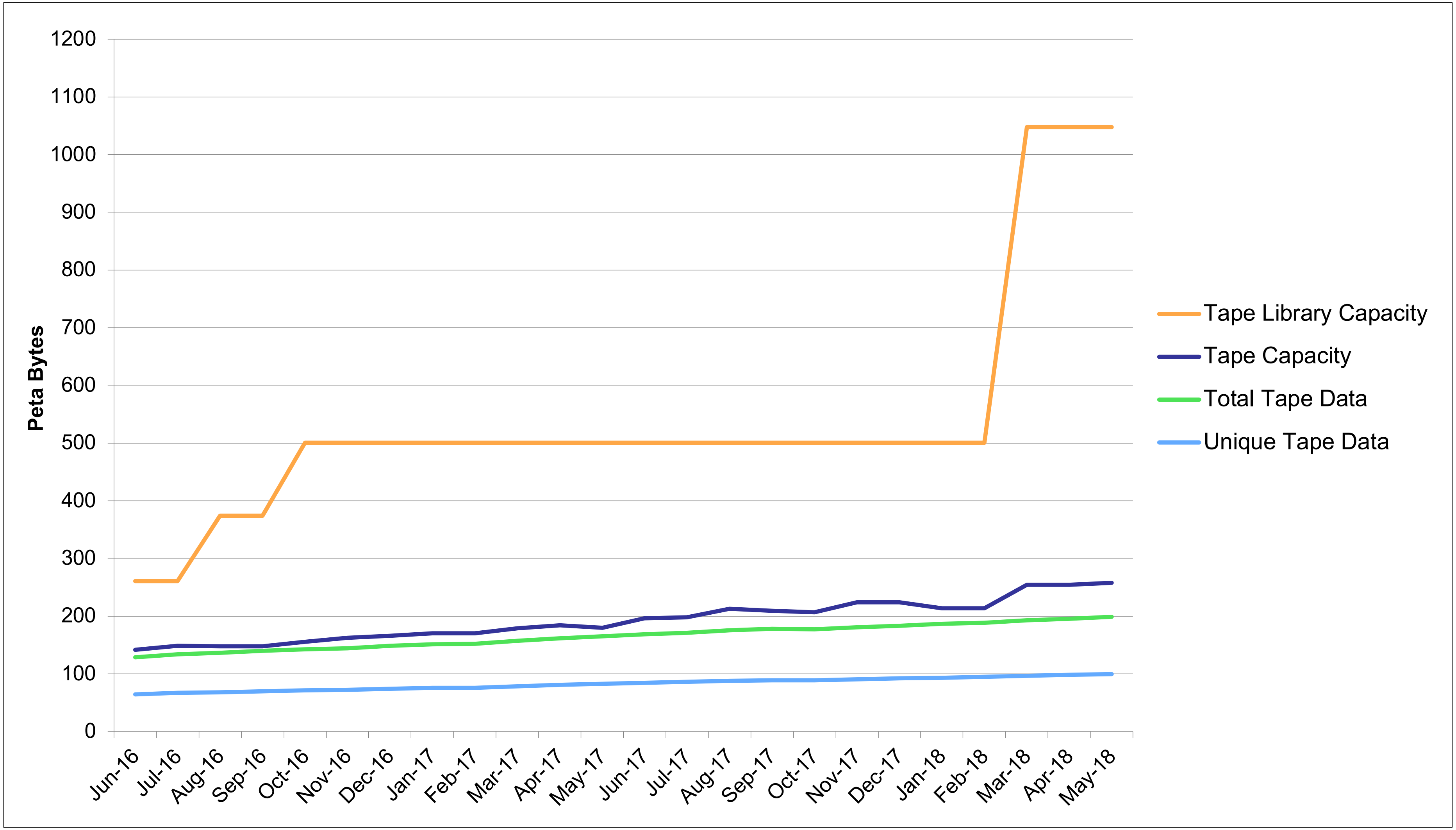
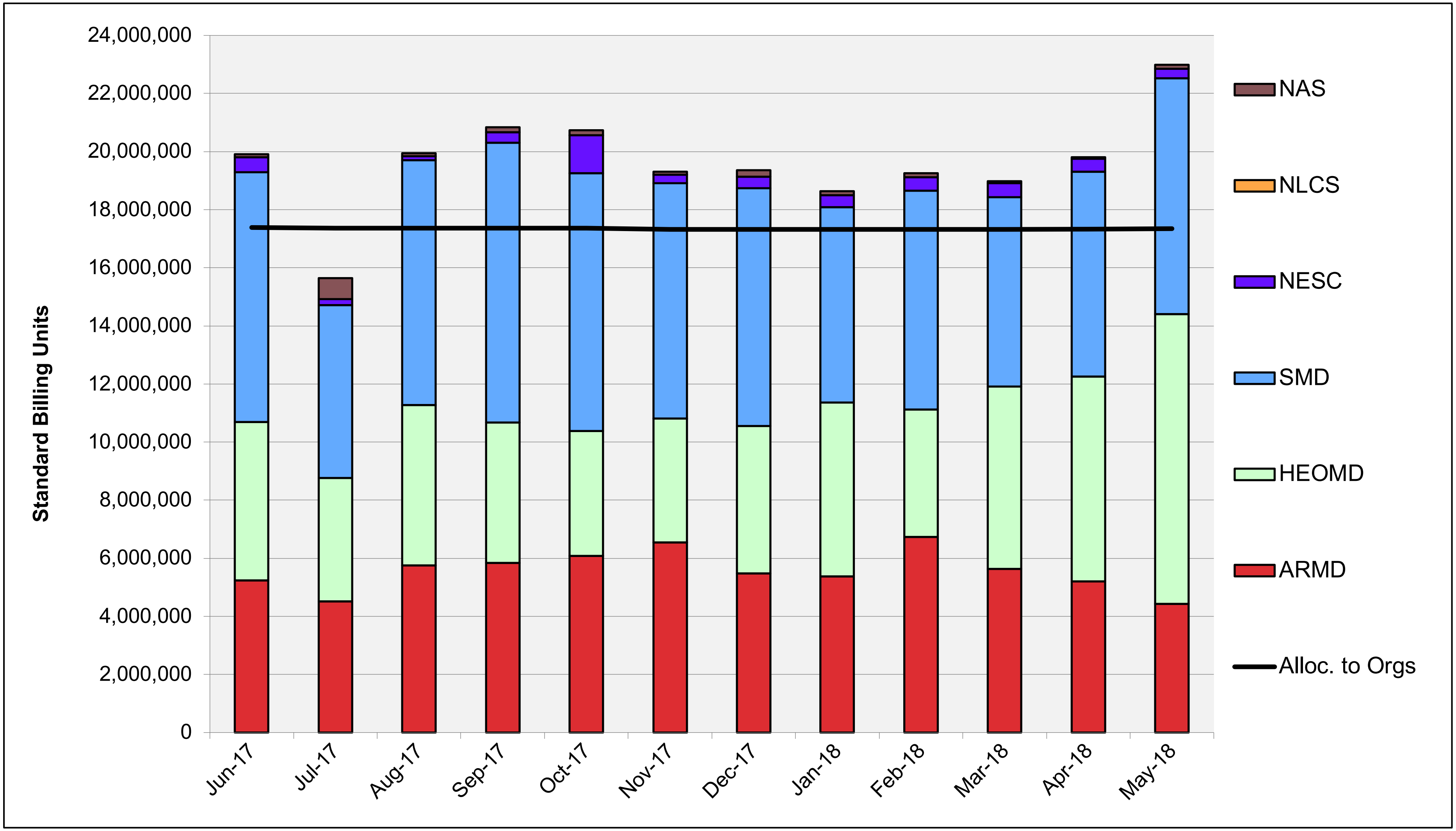
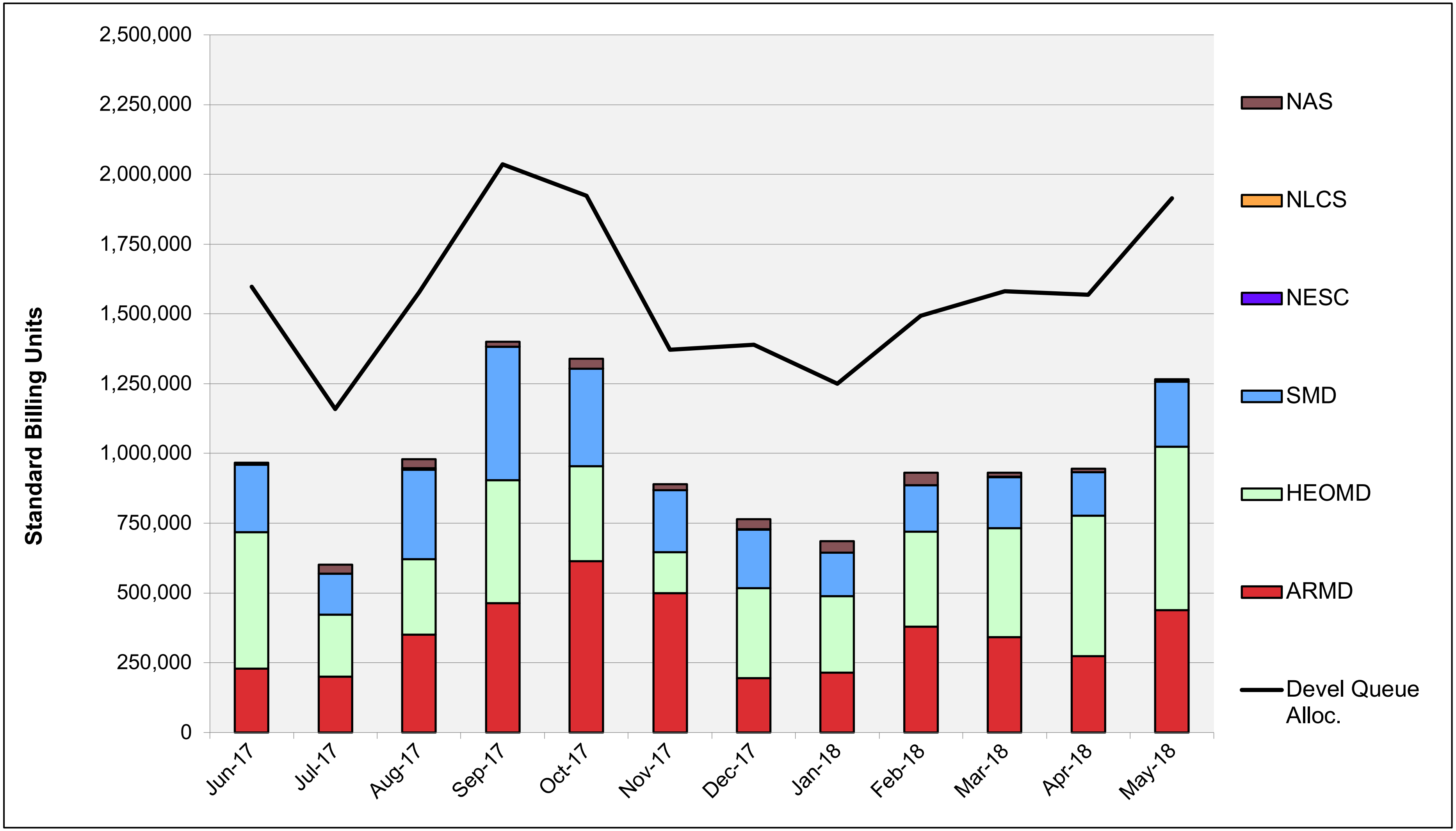


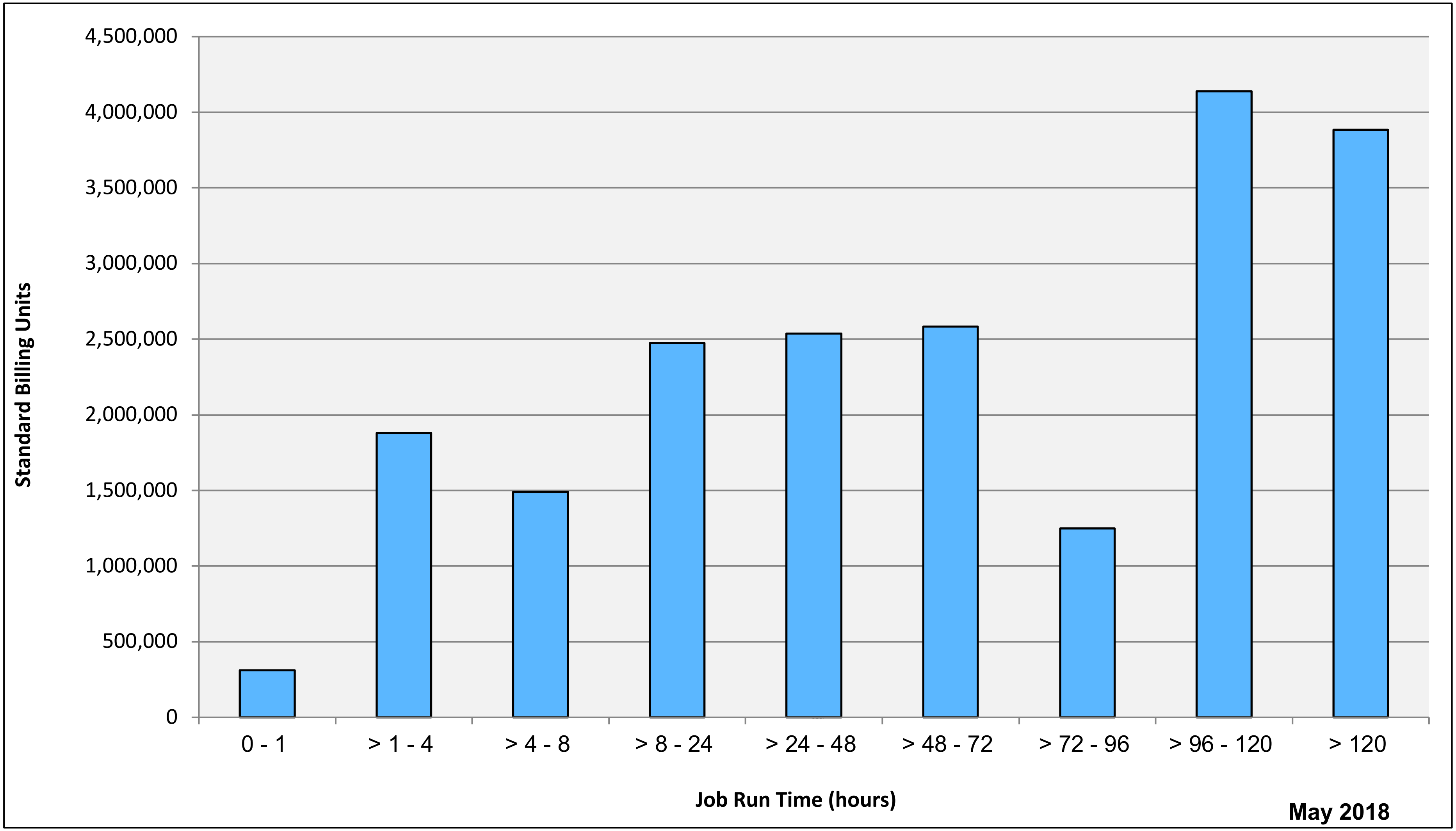
Pleiades: SBUs Reported, Normalized to 30-Day Month



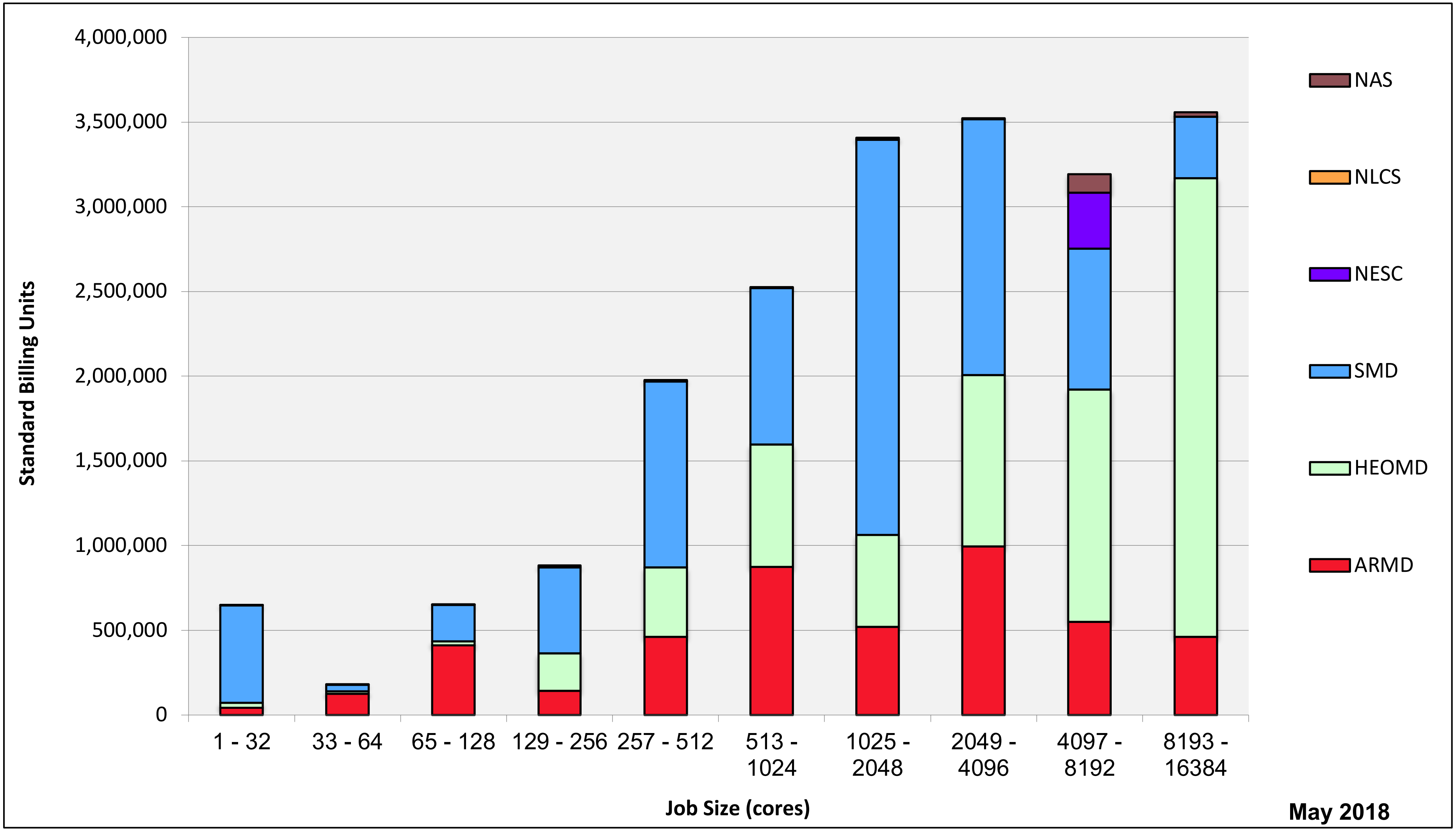
Pleiades: Devel Queue Utilization



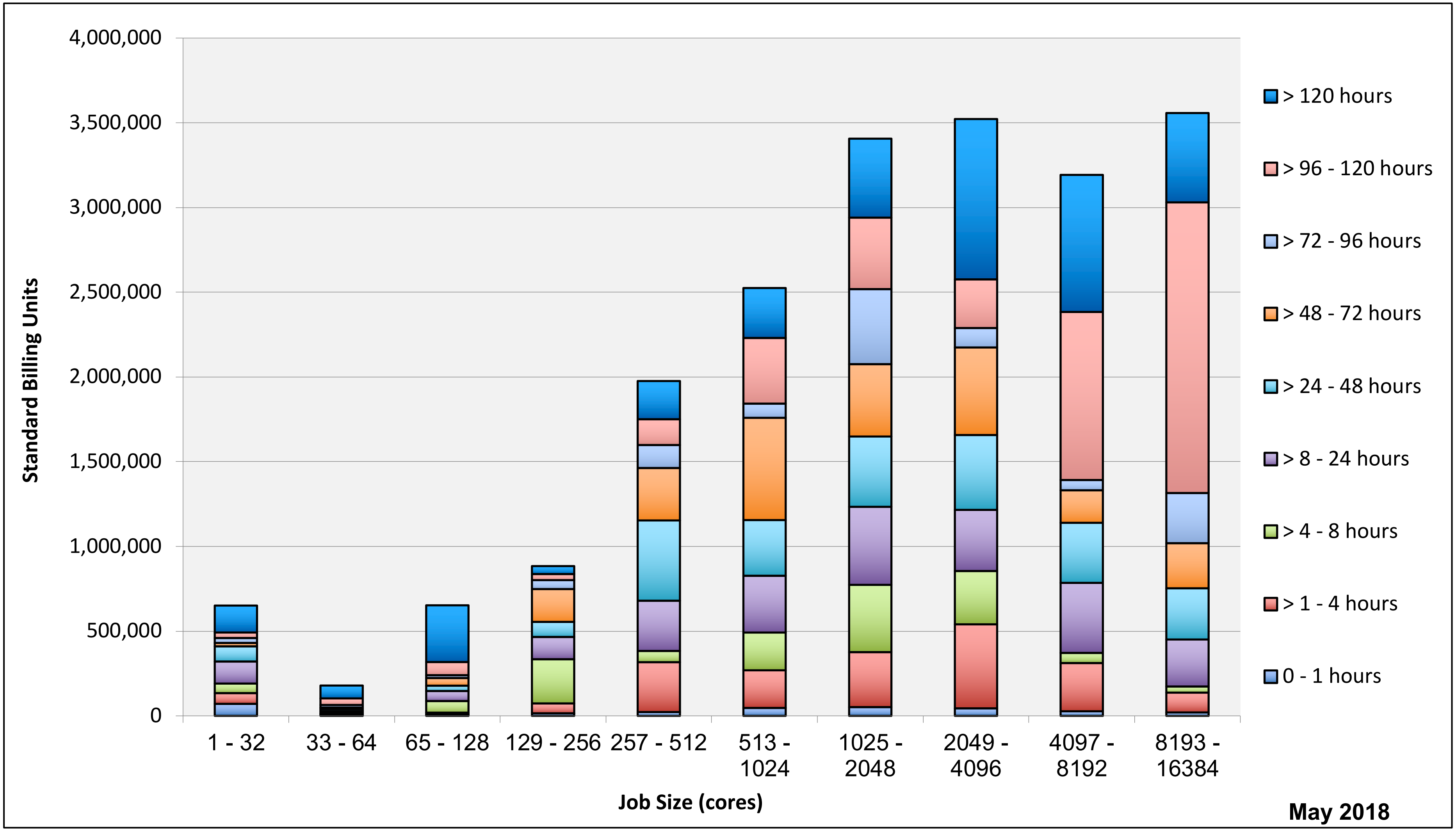
Pleiades: Monthly Utilization by Job Length



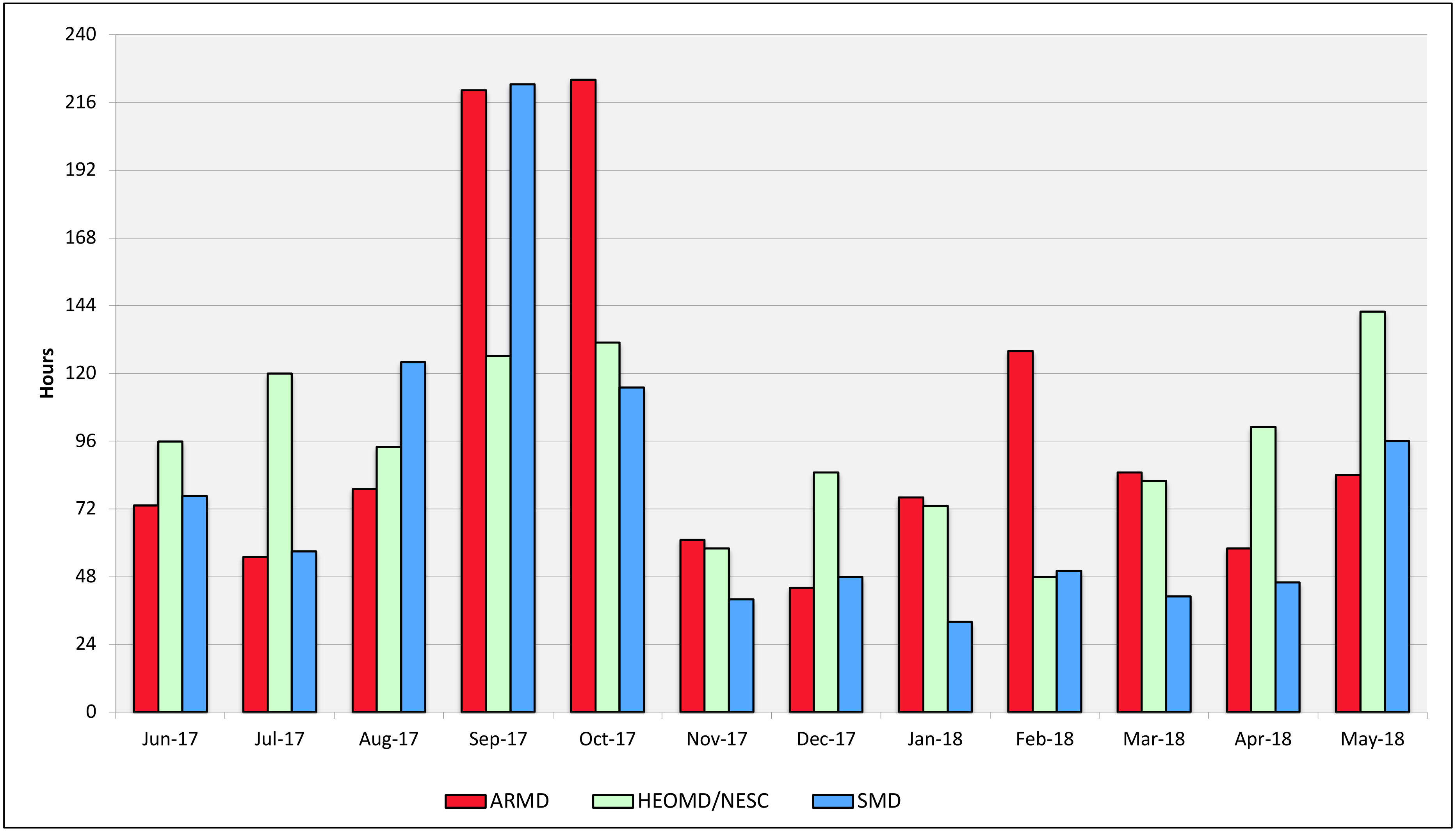
Pleiades:
Monthly Utilization by Size and Mission



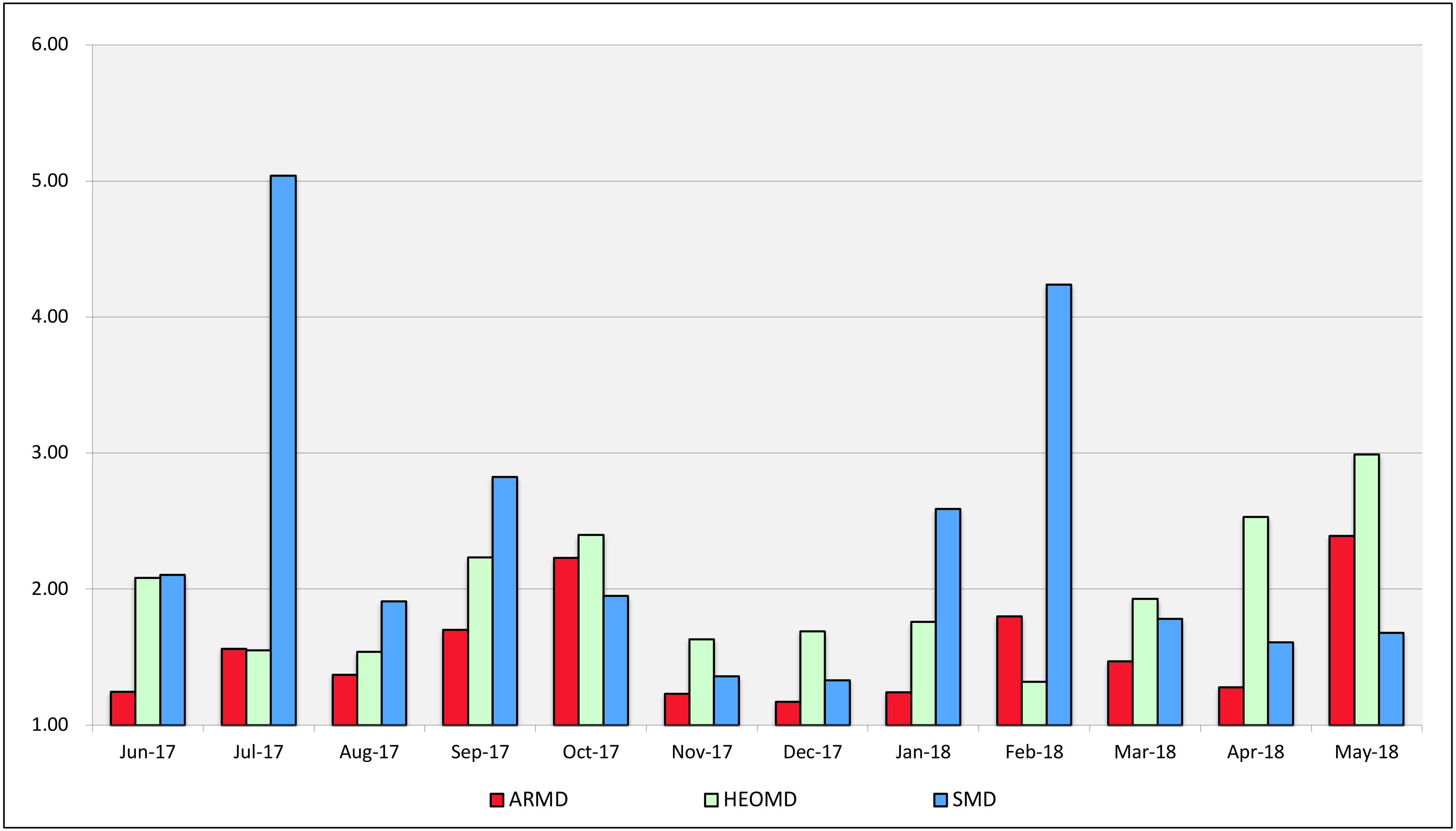
Pleiades:
Monthly Utilization by Size and Length



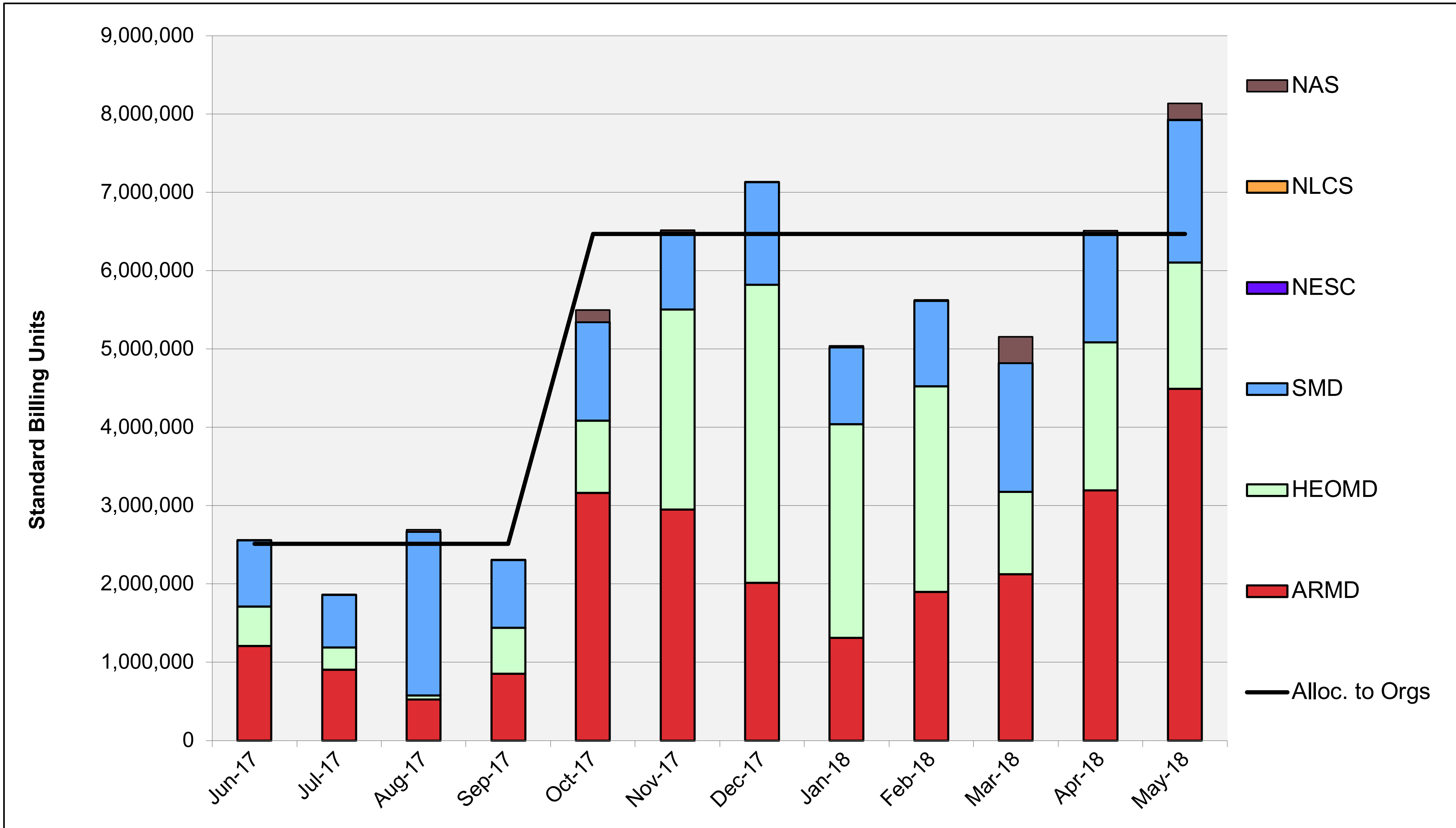
Pleiades: Average Time to Clear All Jobs



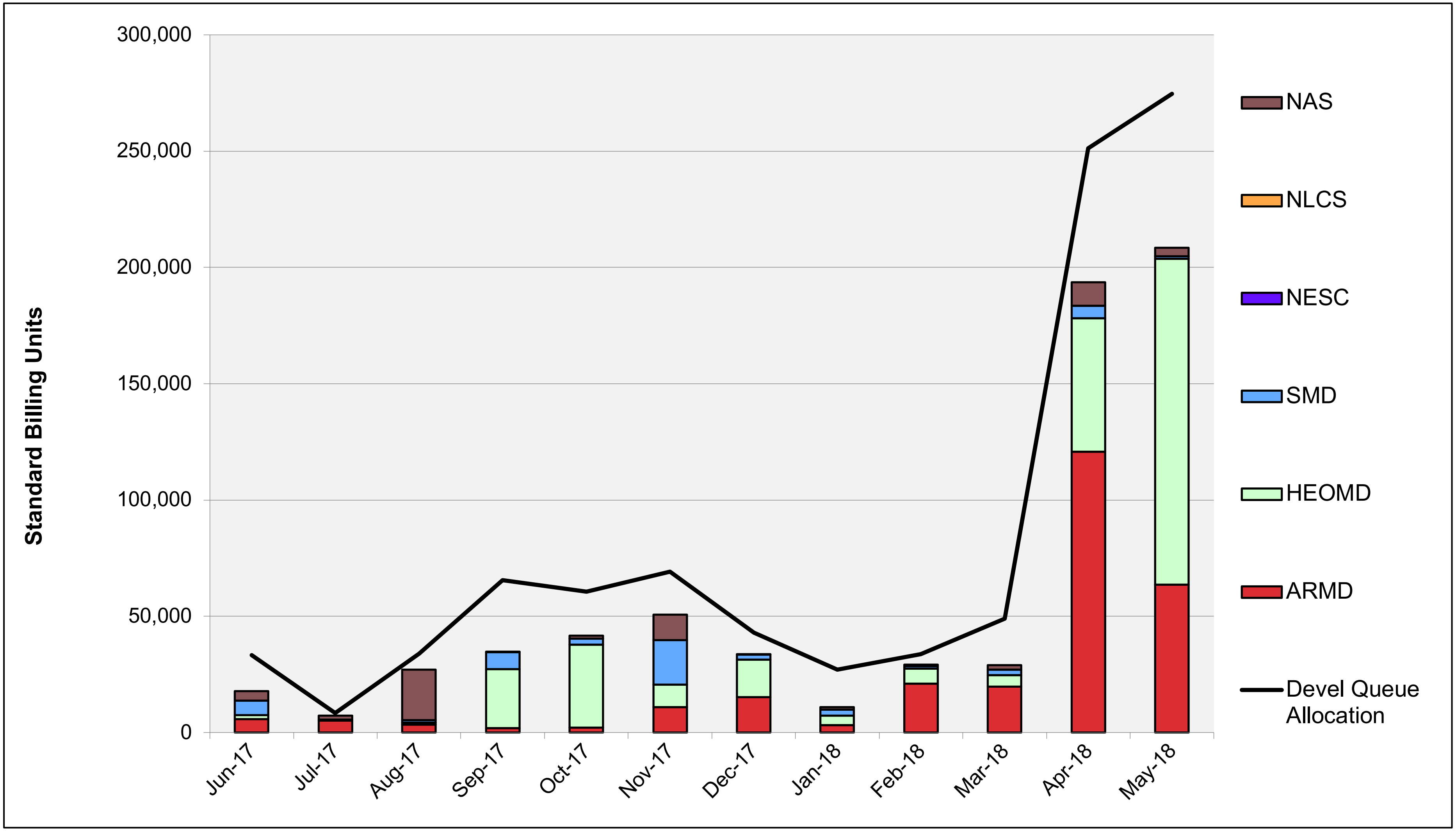
Pleiades:
Average Expansion Factor



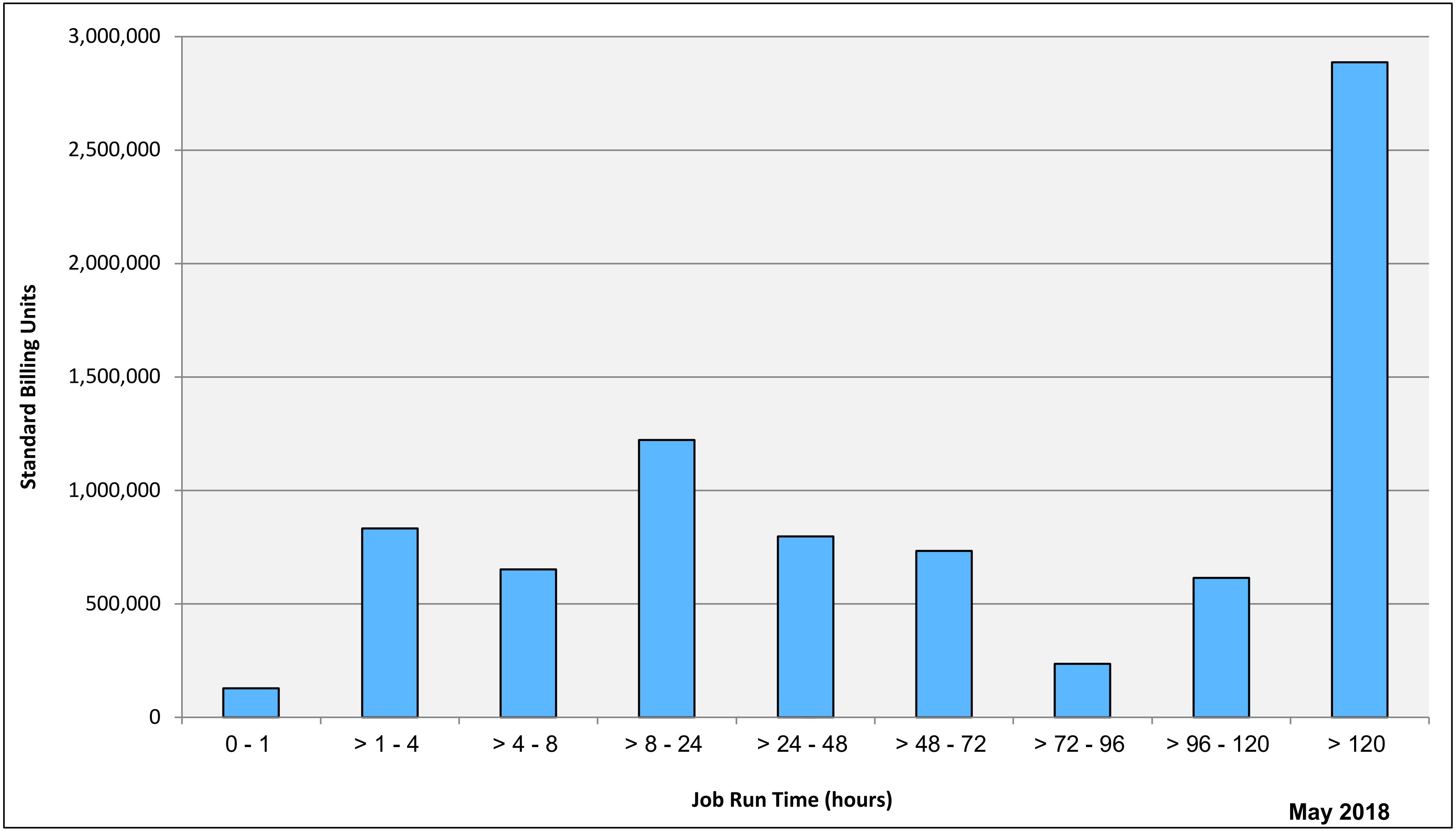
Electra: SBUs Reported, Normalized to 30-Day Month



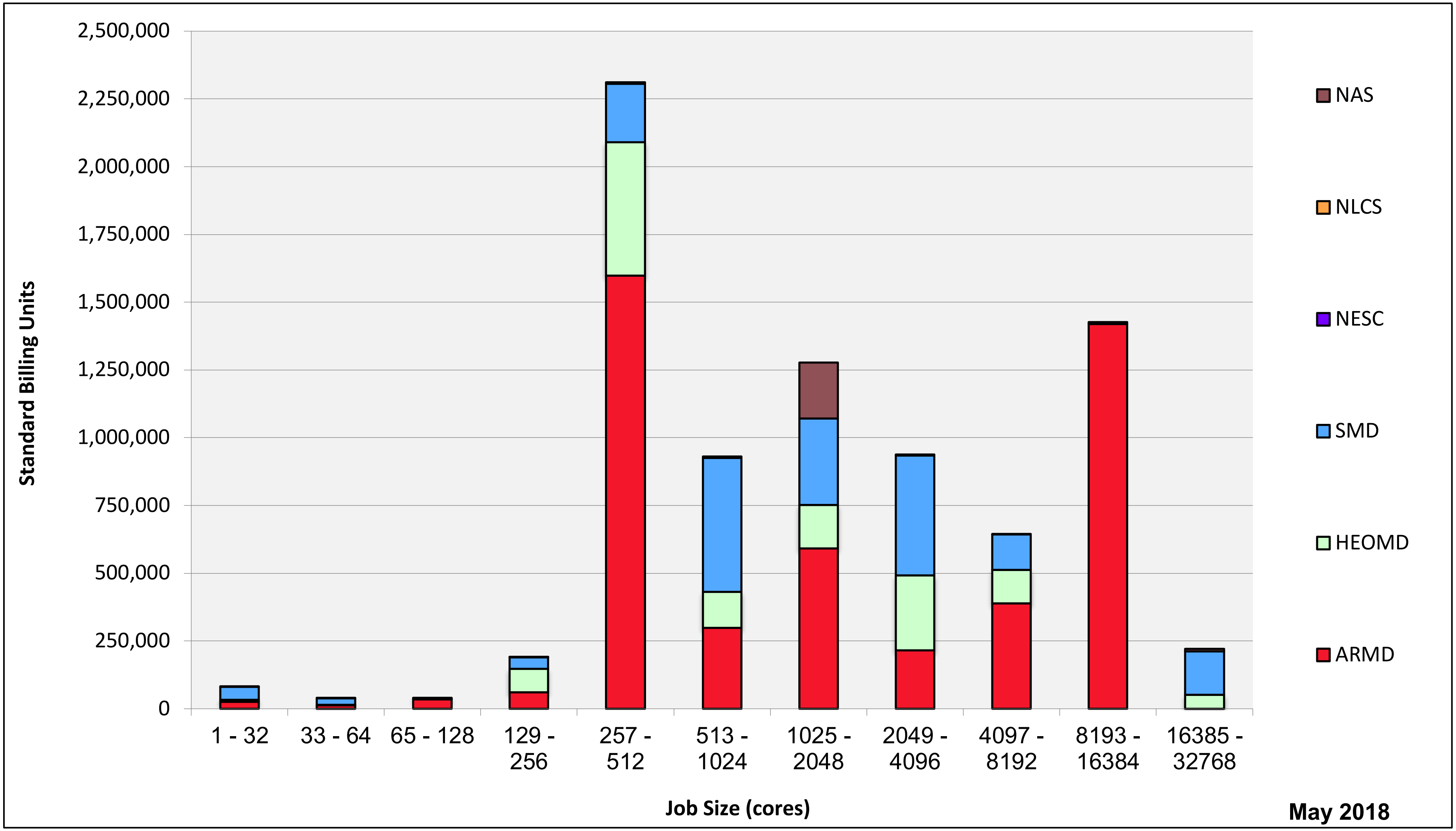
Electra: Devel Queue Utilization



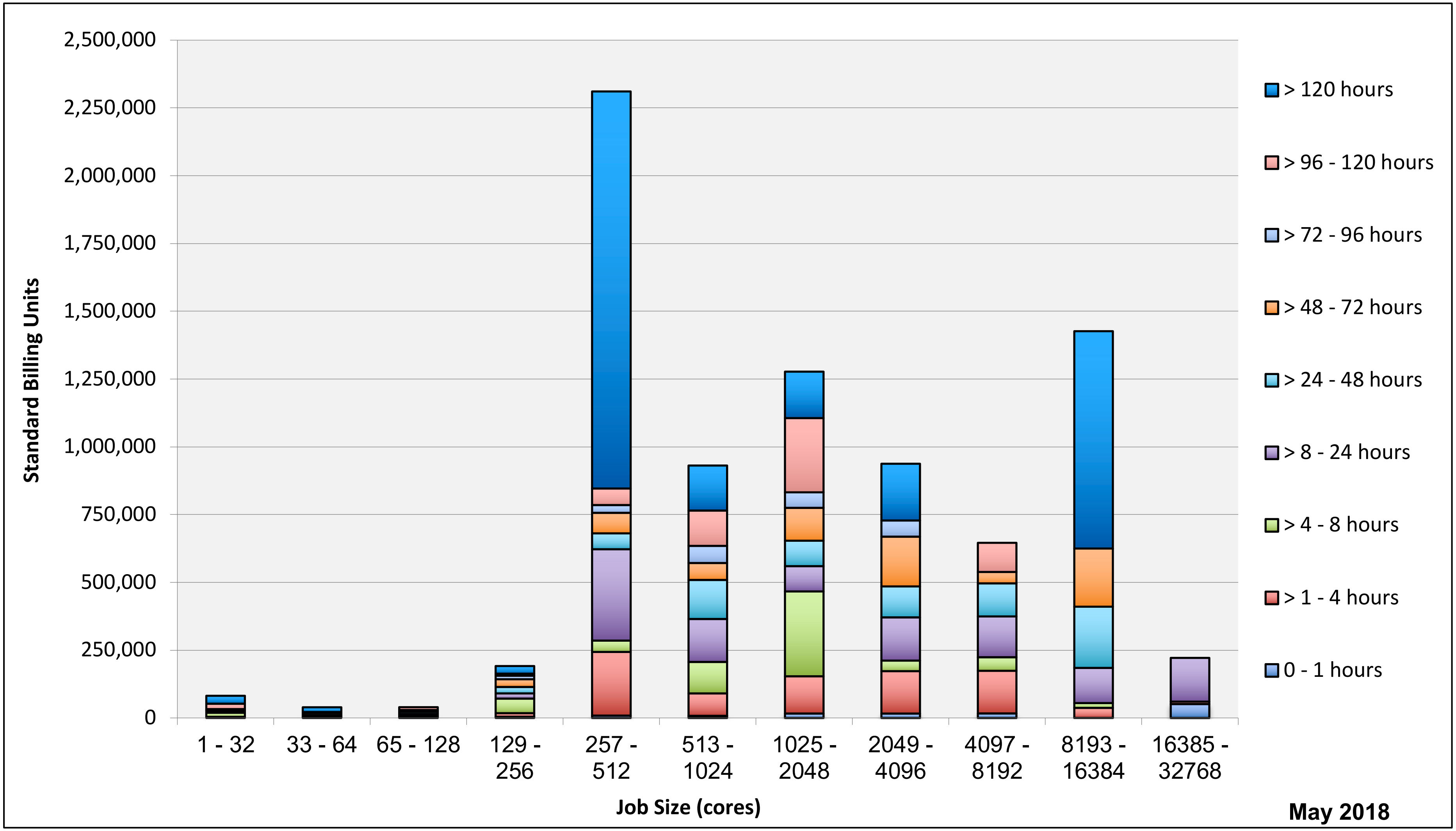
Electra: Monthly Utilization by Job Length



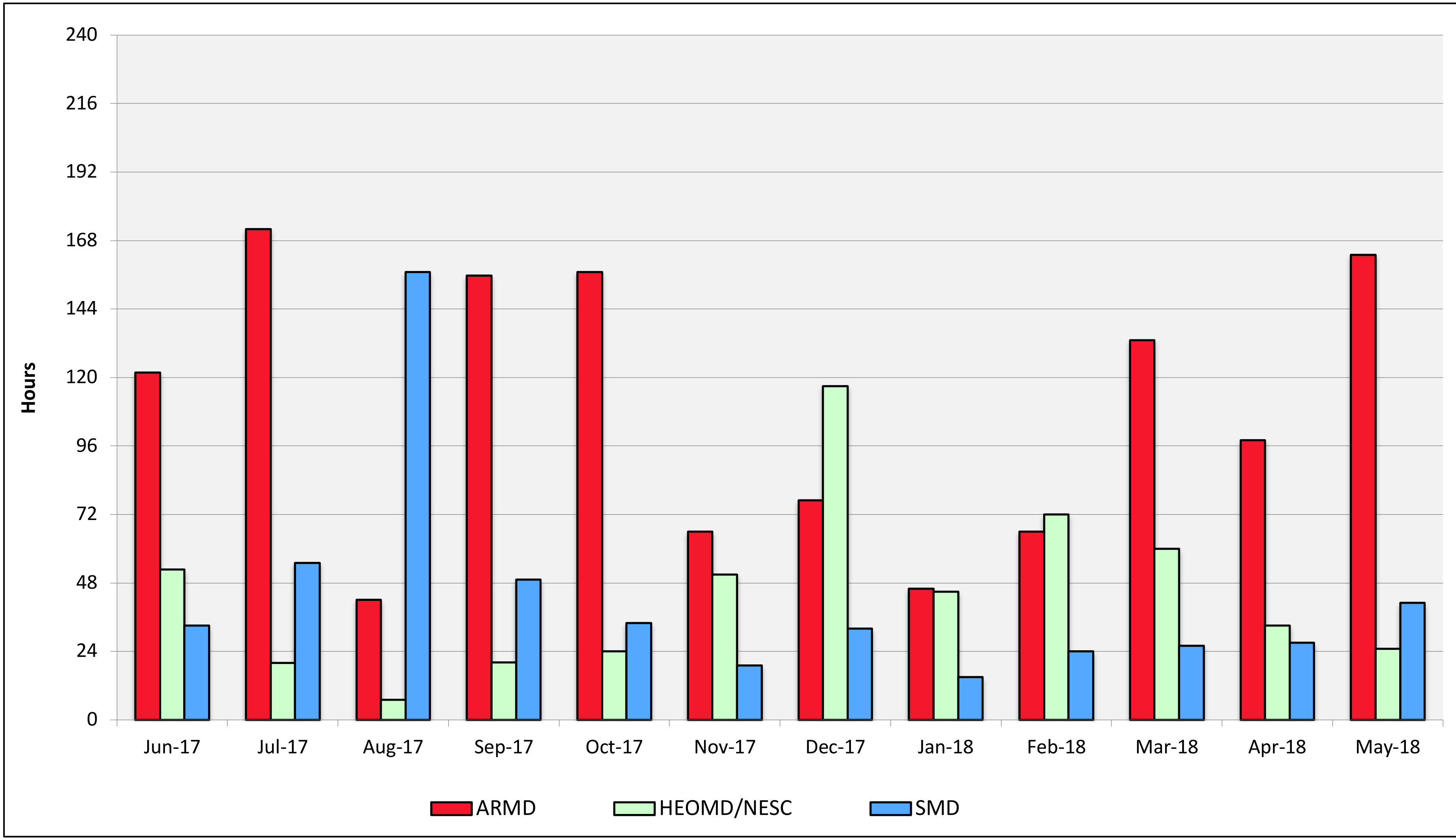
Electra: Monthly Utilization by Size and Mission



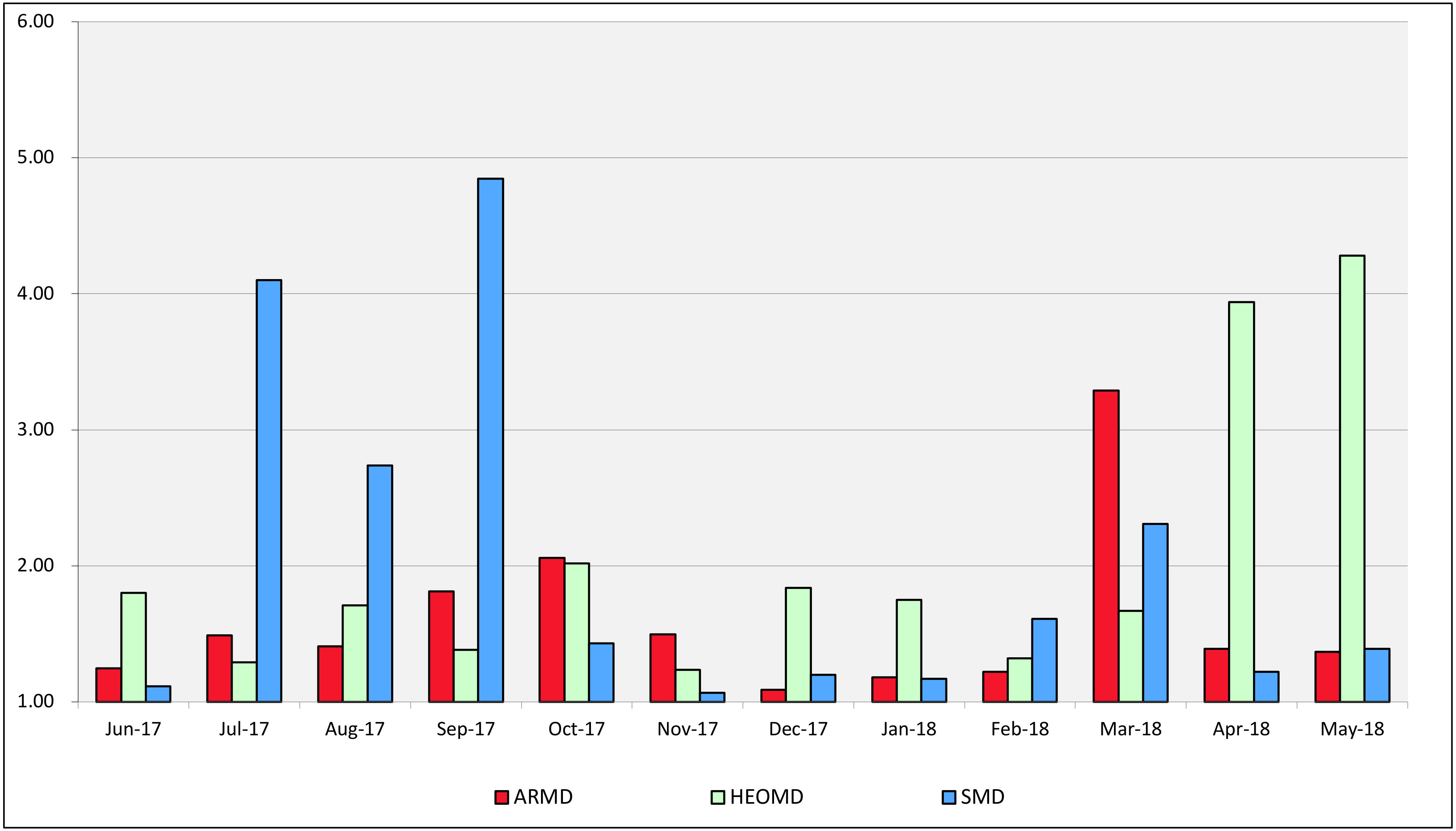
Electra:
Monthly Utilization by Size and Length



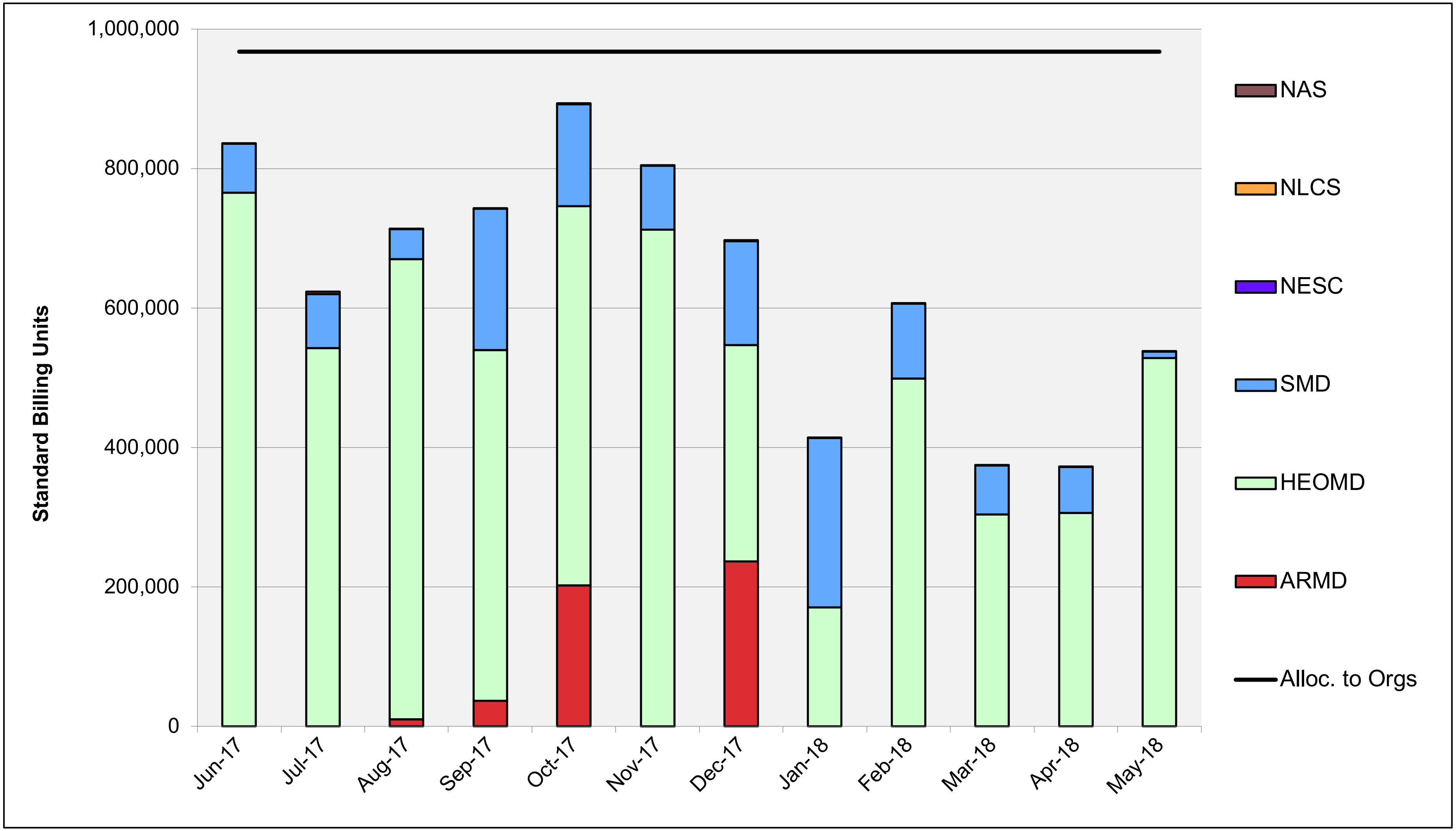
Electra: Average Time to Clear All Jobs



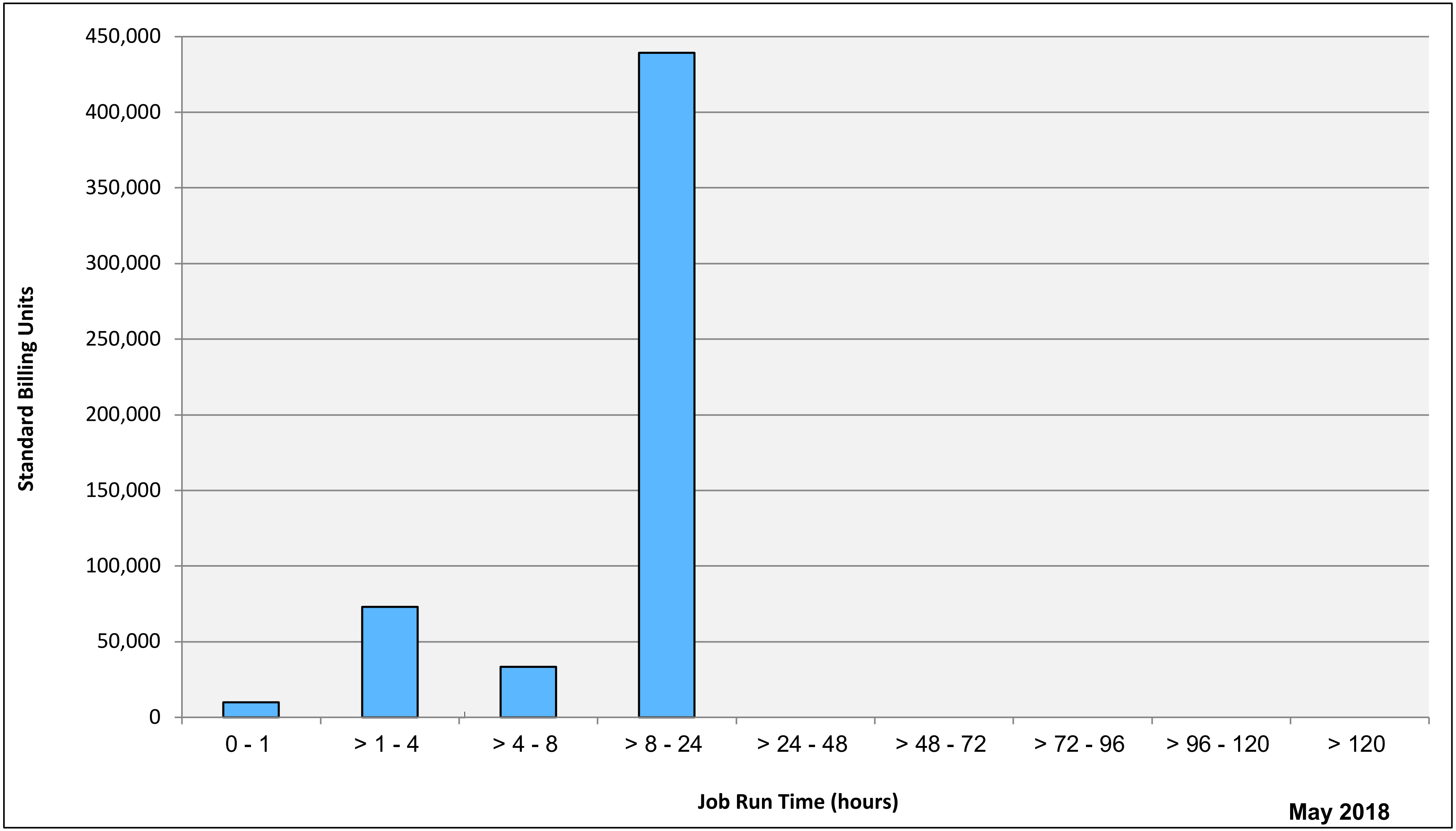
Electra:
Average Expansion Factor



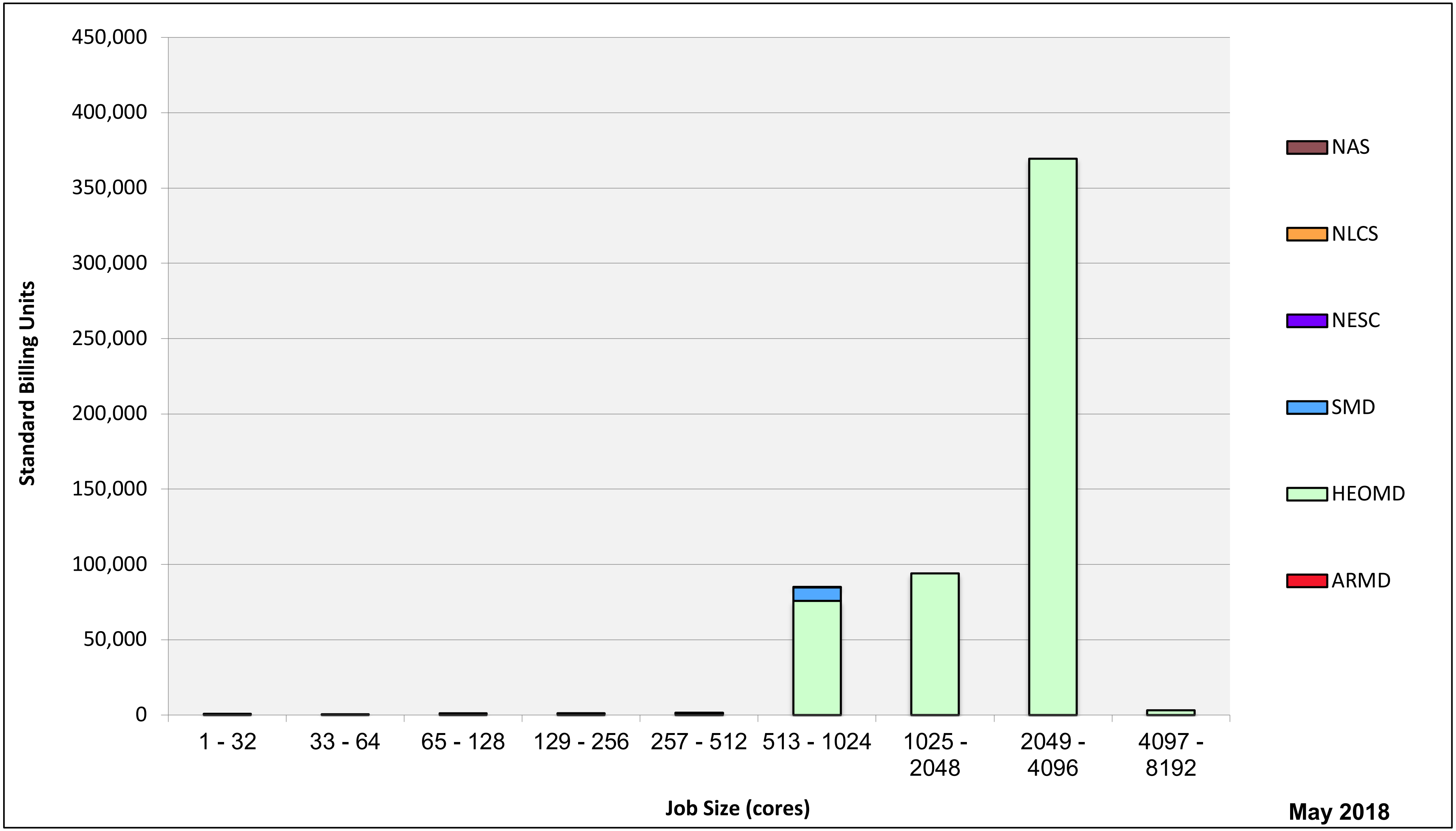
Merope:
SBUs Reported, Normalized to 30-Day Month



Merope: Monthly Utilization by Job Length



Merope: Monthly Utilization by Size and Mission



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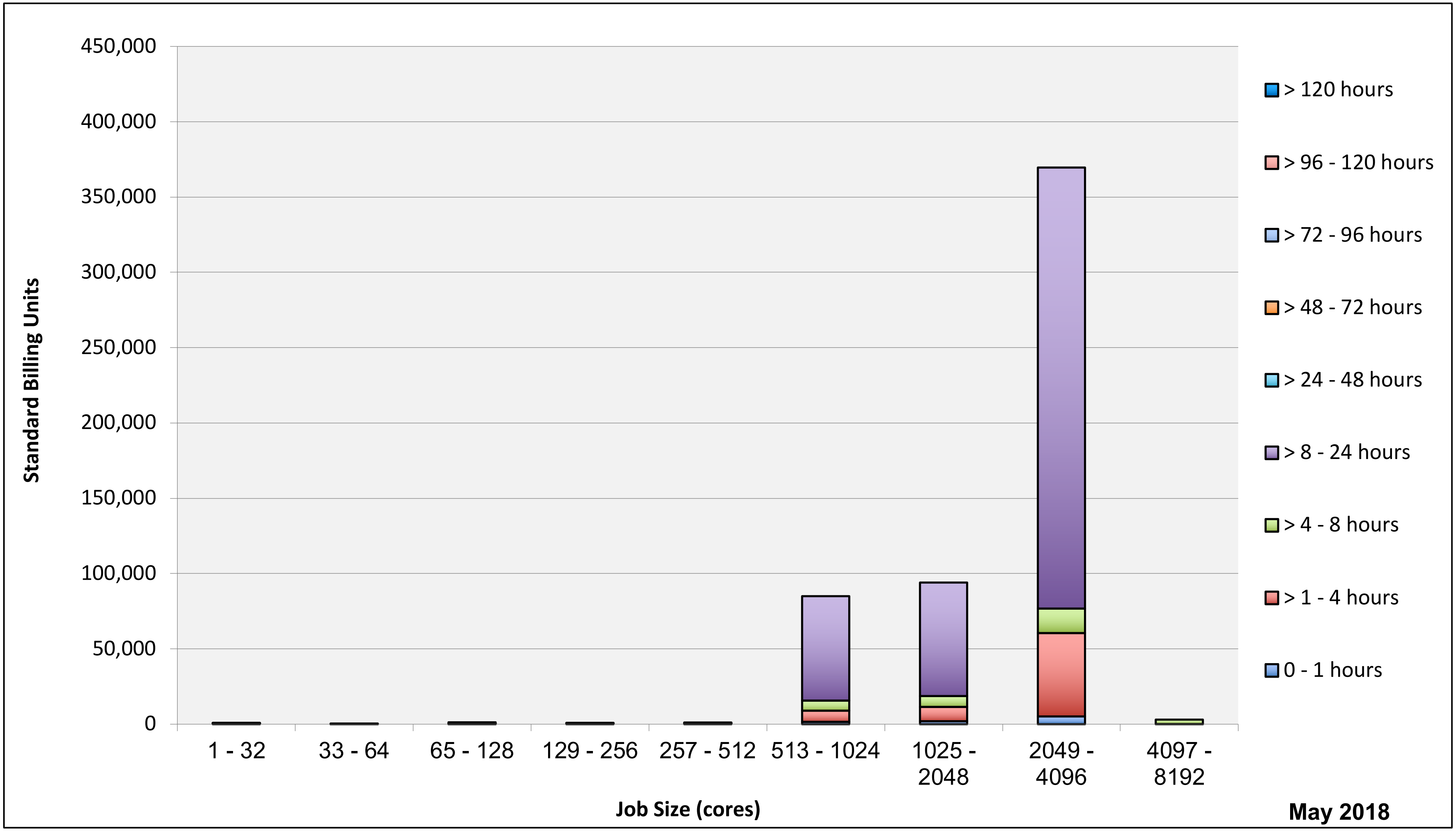
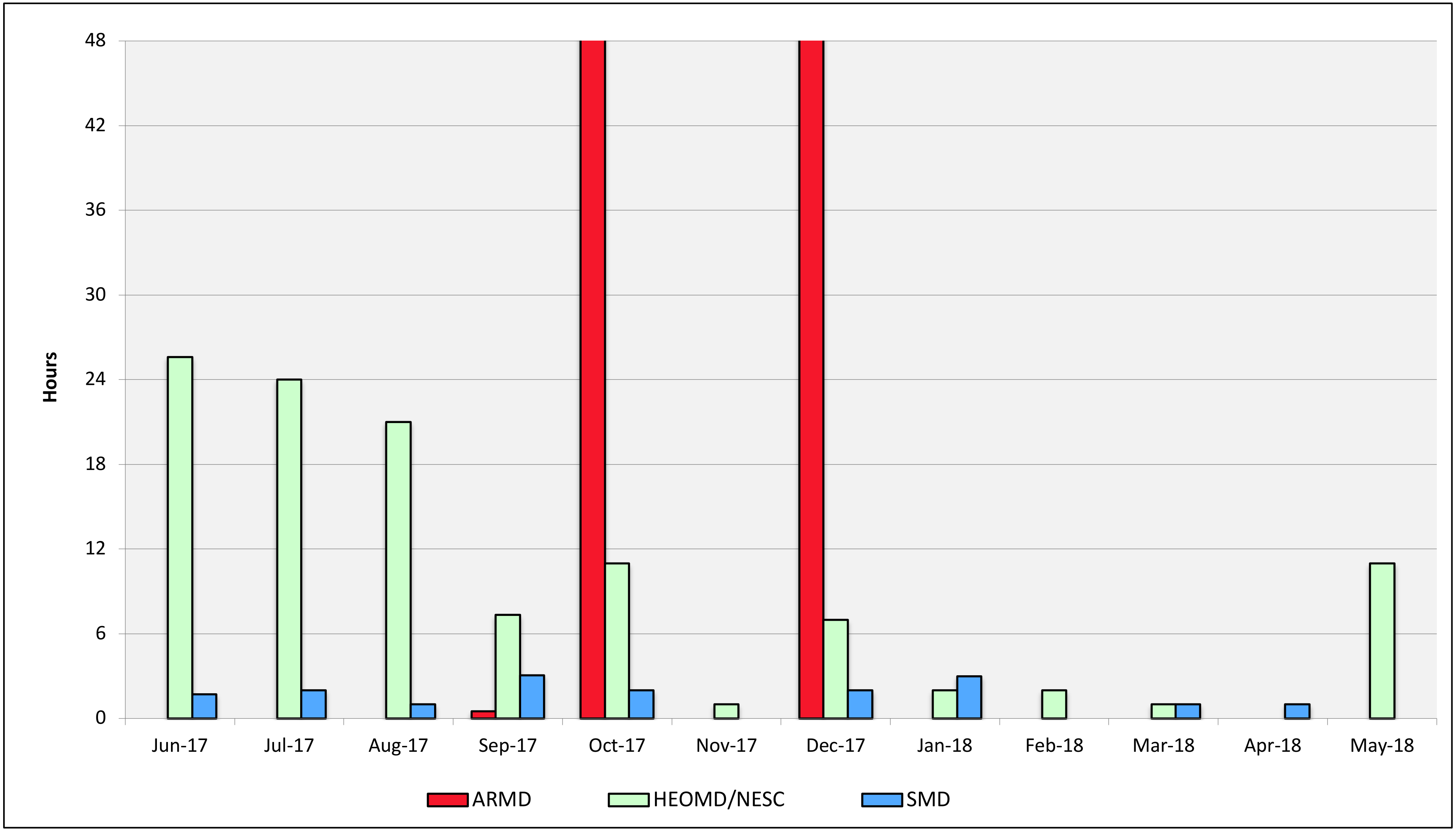
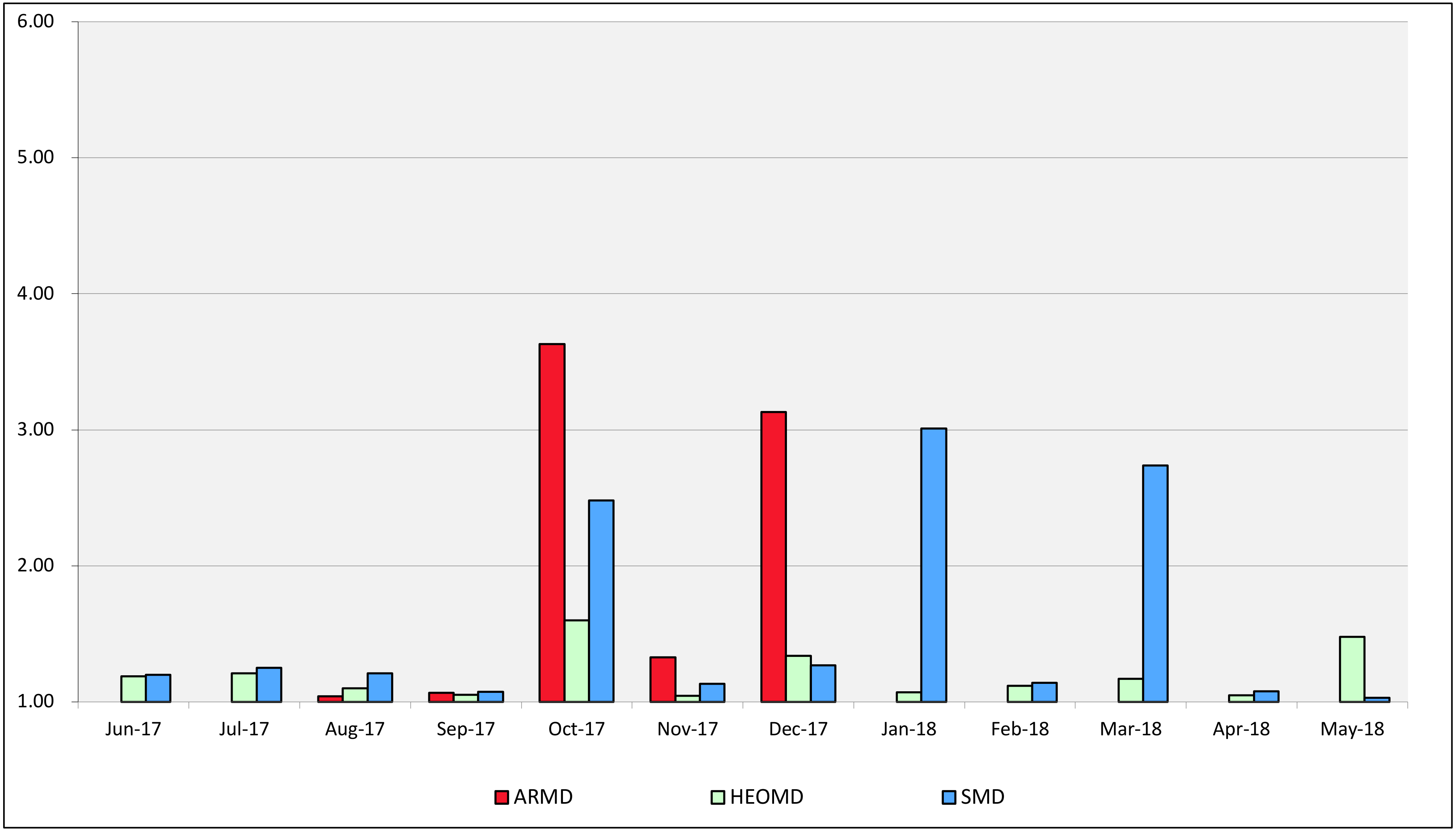


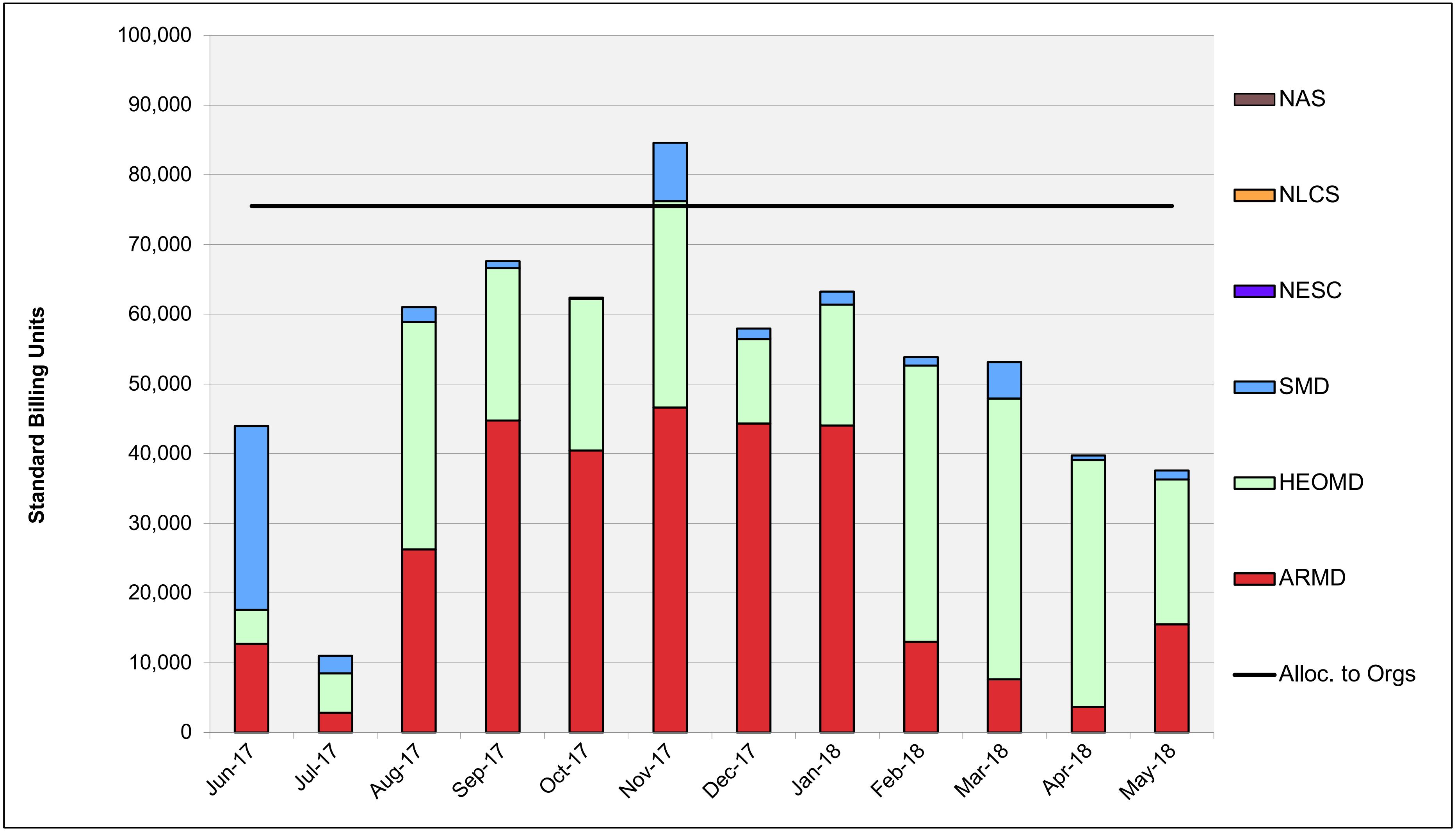
Merope:
Average Time to Clear All Jobs



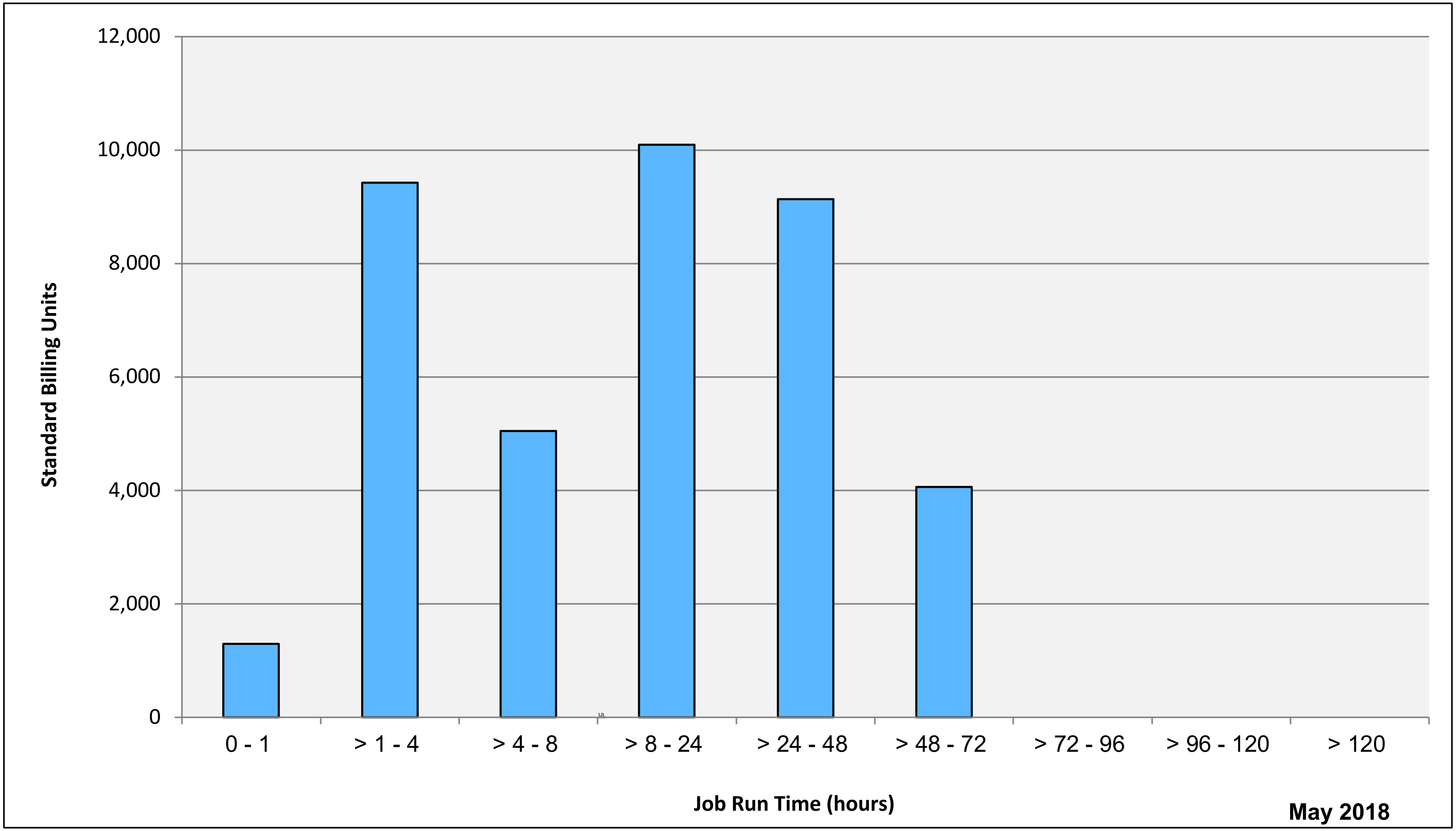
Merope:
Average Expansion Factor



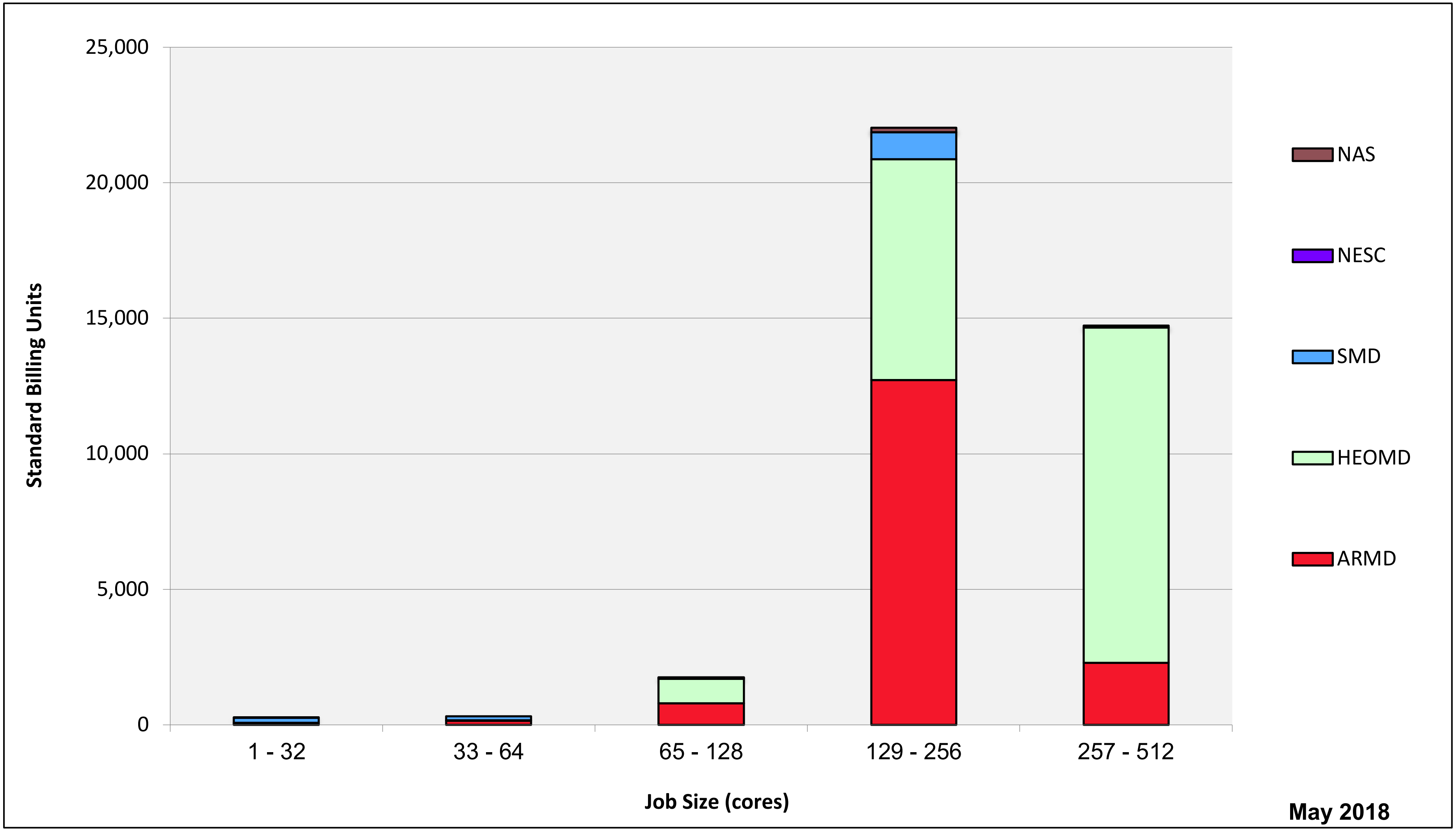
Endeavour: SBUs Reported, Normalized to 30-Day Month



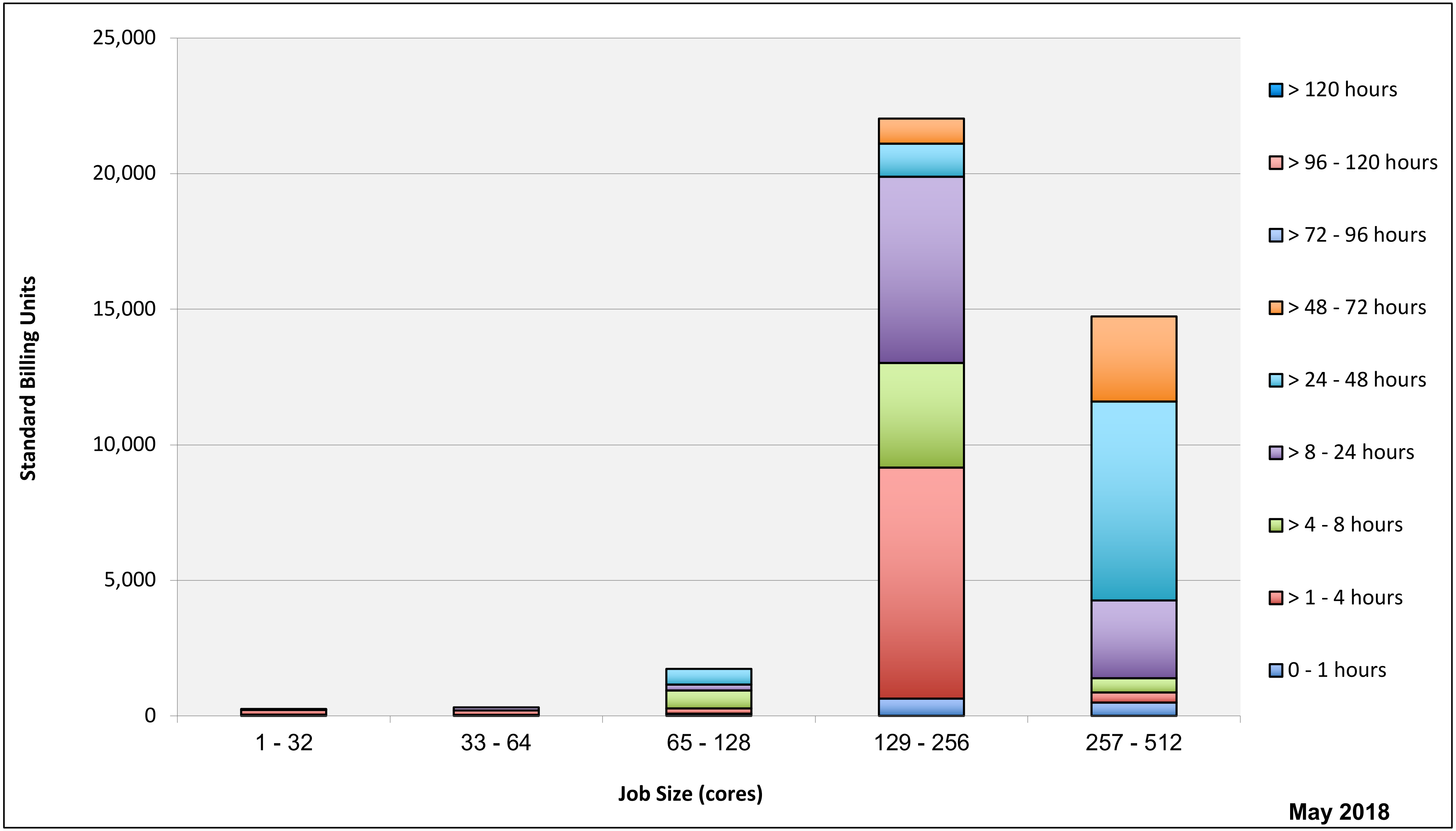
Endeavour: Monthly Utilization by Job Length



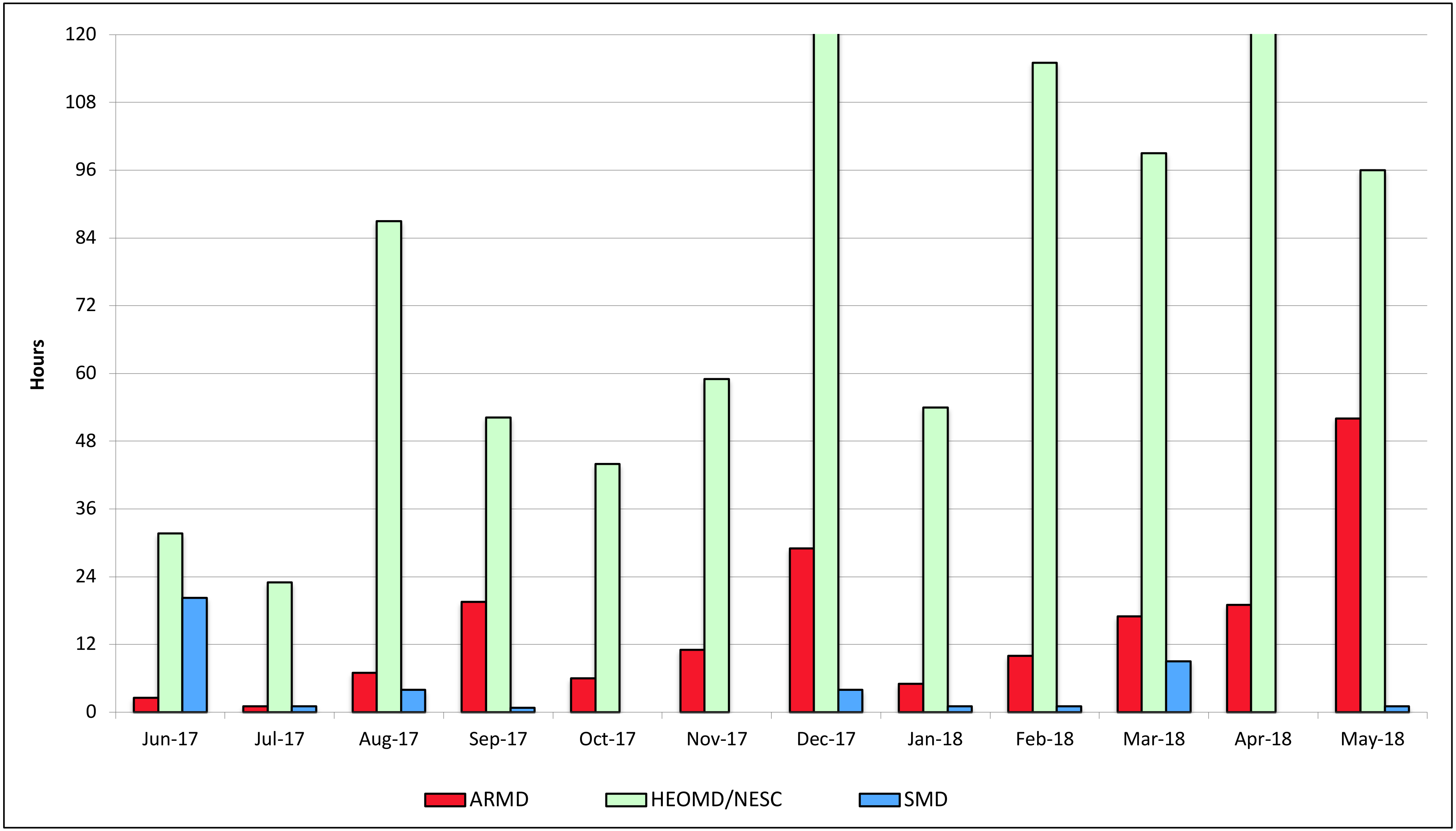
Endeavour: Monthly Utilization by Size and Mission



Endeavour: Monthly Utilization by Size and Length



Endeavour:
Average Time to Clear All Jobs



Endeavour: Average Expansion Factor