



Project Status Report

High End Computing Capability Strategic Capabilities Assets Program

February 10, 2013

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New SGI Testbed System Installed to Evaluate Next-Generation Capability



- The HECC Supercomputing Systems team installed a new SGI system with Intel Xeon Phi coprocessors, in order to evaluate its performance capability for the next-generation HECC supercomputer.
- The new system, named Maia, has 128 nodes, each with 2 Intel Xeon Sandy Bridge processors, 2 Intel Xeon Phi coprocessors, and 32 gigabytes of memory.
- With a theoretical peak performance of 301.4 teraflops (TF), the system ranked #117 on the Nov. 2012 Top500 list at 212.9 TF for the LINPACK benchmark run at SGI's manufacturing facility.
- The system is being evaluated within the HECC environment, as part of the NAS Technology Refresh (NTR) process (see slide 5), and the results will be used to determine if this new processor type will be included in the competitive acquisition of the full system later this year.

Mission Impact: Evaluating leading-edge technologies reduces risks and increases the probability of selecting cost-effective systems that provide the best solution to meet the Agency's supercomputing requirements.



The new SGI testbed system with Intel Xeon Phi-based coprocessors is named after Maia, one of the stars in the Pleiades open star cluster.

POCs: Bob Ciotti, bob.ciotti@nasa.gov, (650) 604-4408, NASA Advanced Supercomputing Division; Davin Chan, davin.chan@nasa.gov, (650) 604-3613, NASA Advanced Supercomputing Division, Computer Science Corp.

Successful Workshop on Performance Optimization for New SGI Testbed System



•HECC, SGI, and Intel systems experts led a three-day workshop at the NASA Advanced Supercomputing (NAS) facility to help users take advantage of, and identify potential applications for, the new testbed system, Maia (see slide 3). The workshop included:

- 12 informative presentations by vendors;
- Interactive sessions on compiler and tools;
- Productive hands-on sessions for selected NASA applications.

•Attendees gave very positive feedback:

- “Gained much more insight into architecture and performance on Xeon and Xeon Phi processors”;
- “Valuable interactions with Intel experts”;
- “Demonstrated performance improvement in some cases from just one day of work.”

•This valuable workshop has paved the way for further performance optimization efforts.

Mission Impact: HECC users benefit from workshops that help them optimize their applications on current and future computing architectures, improving turnaround times for simulation and design processes.

Using the whole node in a cluster

	Symmetric MPI (native)	Offload
Analysis effort	Parallel fraction, relative perf overall, load balancing, MPI communication	Granularity analysis, relative perf @ function, functional vs. data //ism, dependence analysis
Porting effort	Load balancing	Adding pragmas
Tuning	Exposing parallelism, parallel performance, load balancing	Exposing parallelism, parallel performance,
Scalar-sequential perf	10x slower than Xeon	
Available MPI bandwidth, latency hiding	Subject to long scalar-sequential path lengths	Host-card bandwidth currently higher for offload

Representative presentation slide given at the performance optimization workshop, showing use of an entire computing node. The workshop was held January 14–17, 2013 at NASA Ames Research Center.

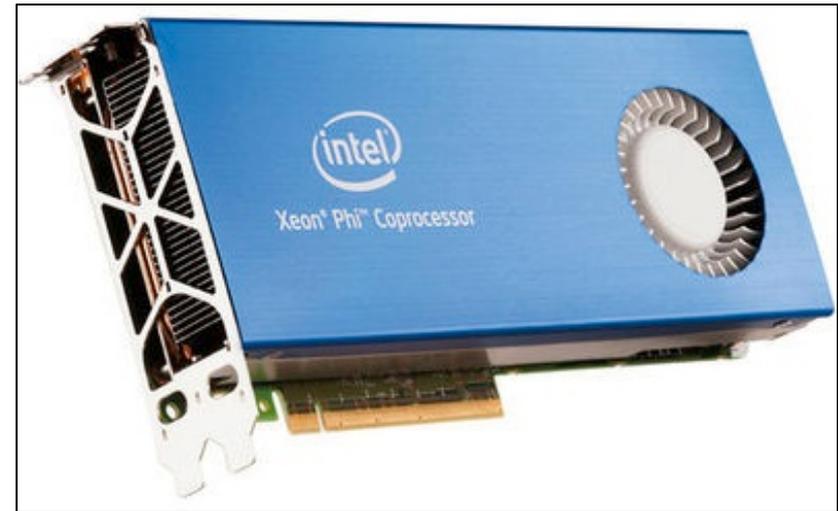
POCs: Henry Jin, haoqiang.jin@nasa.gov, (650) 604-0165; Piyush Mehrotra, piyush.mehrotra@nasa.gov, (650) 604-5126; NASA Advanced Supercomputing Division.

HECC Selects Additional Intel Xeon Phi-based Testbed System for Evaluation



- In addition to the Maia testbed, HECC selected a second Intel Xeon Phi-based testbed system to evaluate supercomputing resources needed to meet the Agency's increasing high-performance computing (HPC) requirements.
- As part of the annual NAS Technology Refresh (NTR) process, five proposals were evaluated using several factors, including proposed technology, system performance, total cost of ownership, and strategic concerns such as the vendors' HPC experience and support models.
- Based on the evaluation, HECC selected a system manufactured by Appro International (since acquired by Cray Inc.), comprising 64 nodes, each with 2 Intel Xeon Sandy Bridge processors, 2 Intel Xeon Phi coprocessors, and 32 gigabytes of memory.
- Over the coming months, HECC experts will evaluate this new system from the perspectives of performance, maintenance, and integration with the HECC environment to determine if it is suitable to meet the Agency's HPC needs.
- This is the second Intel Xeon Phi-based testbed procured by HECC (see slide 3), which provides another platform to evaluate the suitability of Intel Xeon Phi architecture for NASA's HPC workload and provides a second procurement source if found viable.

Mission Impact: Utilizing the process of in-house testing of small testbeds before procuring a full system allows HECC to evaluate new resources before deployment and reduces the risk to both the Agency and users.



Intel's latest coprocessor, the Xeon Phi, is based on the company's Many Integrated Core (MIC) architecture. Each coprocessor has 60 cache-coherent cores, 512-bit vector processing unit registers, and 8 gigabytes of Graphics Double Data Rate, version 5 (GDDR5) memory.

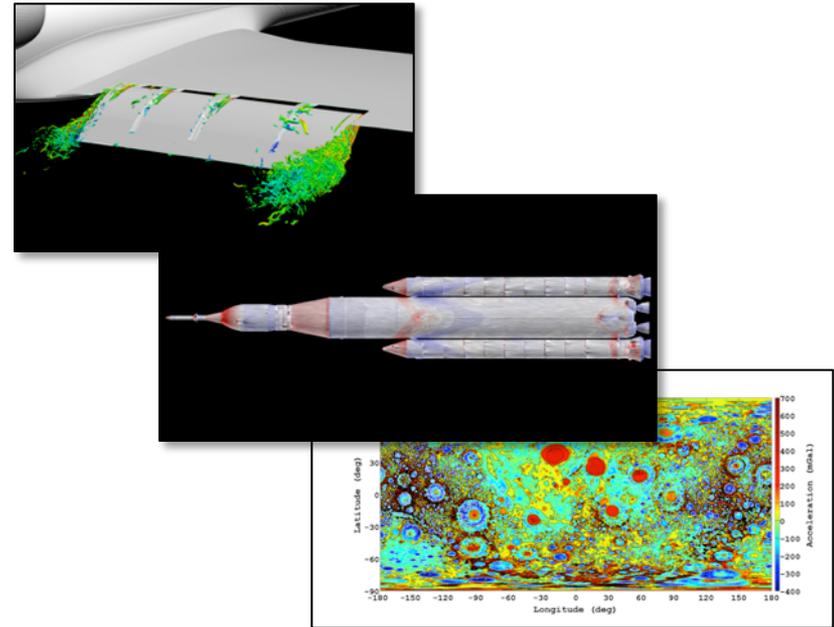
POC: Piyush Mehrotra, piyush.mehrotra@nasa.gov, (650) 604-5126;
NASA Advanced Supercomputing Division

Record-High Usage on Pleiades Provides Maximum Resources for NASA Missions



- January showed record-high usage of HECC's Pleiades supercomputer, with nearly 6.9 million Standard Billing Units (SBUs) used by NASA's Mission Directorates and mission support organizations—exceeding the previous record of 6.5 million SBUs by over 4%.
- This increase was enabled by the addition of 144 Pleiades nodes and through efficient operations that delivered better than 99% availability and more than 88% system utilization (75% utilization is target).
- Eight projects (2 from ARMD, 2 from HEOMD, and 4 from SMD) each used over 200,000 SBUs and together accounted for 29% of the usage.
- The next eight projects (with the same distribution between Mission Directorates) each used 150,000 to 200,000 SBUs and accounted for another 21% of the usage.

Mission Impact: Increasing Pleiades' system capacity provides Mission Directorates with more resources for the accomplishment of their goals and objectives.



Images representing projects that used the most time in their respective mission directorates. From top to bottom: Evaluation of Noise Reduction Concepts for Flap, ARMD, M. Khorrami; CFD Support for SLS Ascent Aerodatabase, HEOMD, C. Kiris; GRAIL Lunar Gravity, SMD, A. Konopliv.

POC: Catherine Schulbach, catherine.h.schulbach@nasa.gov,
(650) 604-3180, NASA Advanced Supercomputing Division

HECC Resources, Services are Critical to Kepler's Search for Habitable Earth-Sized Planets



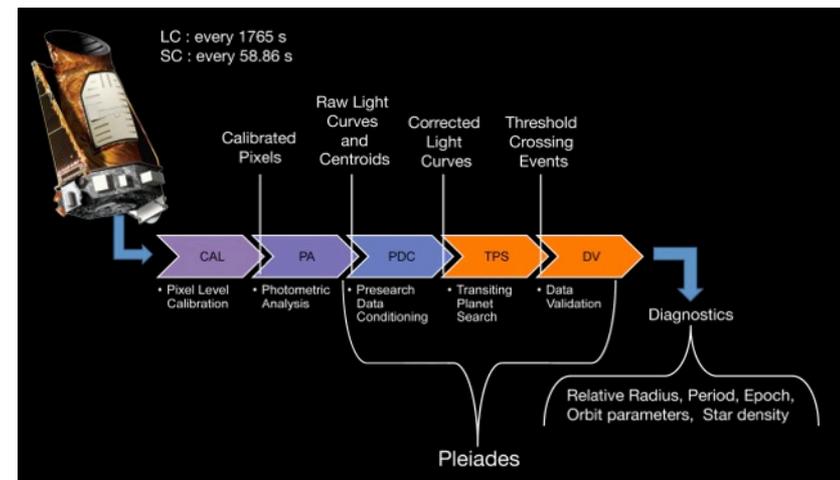
- Pleiades continues to be a critical resource to run the most computationally intensive portions of the Kepler Science Operation Center (SOC) data processing pipeline: the pre-search data conditioning, transiting planet search, and data validation modules.

- In addition, HECC computer scientists have significantly improved the accuracy and effectiveness of the pipeline software and completed all the computational runs on Pleiades over the last year.

- Processing light curves on Pleiades typically utilizes about 3,000 nodes for 20 hours, versus more than a month on SOC computers.

- With this speed-up, the SOC team can take advantage of algorithm improvements much more quickly and uncover more of the transit signals buried in the data.

Mission Impact: Use of Pleiades resources, along with HECC code optimization services, enable rapid turnaround of both the computationally intensive Kepler planetary transit searches and analyses of planet candidates.



The Kepler Science Operations Center data processing pipeline is divided into modules, each performing a specific task. As data collection increases, more of the pipeline software will need to be migrated to the Pleiades supercomputer to support both code development and data processing to meet NASA science goals.

POCs: Shawn Seader, shawn.seader@nasa.gov, (650) 604-4241, SETI Institute; Todd Klaus, todd.klaus@nasa.gov, (650) 604-2576, Lockheed Martin, NASA Ames Research Center

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

HECC Resources Enable Fast-Turnaround CFD Simulations of SLS SRB Separation



•NAS Division modeling and simulation experts used Pleiades to complete extensive computational fluid dynamics (CFD) simulations of solid rocket booster (SRB) separation for the Space Launch System (SLS), including:

- Used the efficient Cart3D code to simulate SLS core stage and SRBs with all protuberance details and plume effects from booster separation motors;
- Simulated 638 different SRB separation conditions as the boosters move away from the core stage;
- Computed aerodynamic forces, moments, surface pressures, and line loads on the SRBs and core stage for each case.

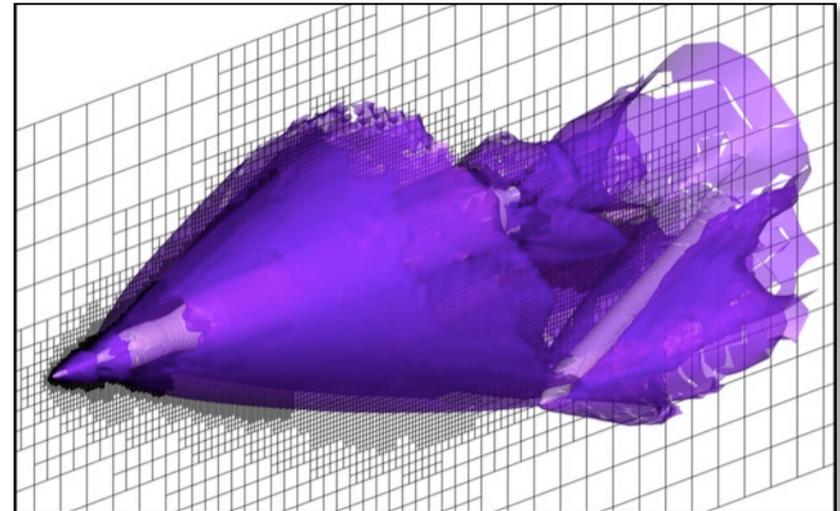
•HECC resources enabled fast-turnaround and on-time delivery of results:

- These analyses required over 200,000 processor-hours on Pleiades.
- Availability of HECC resources enabled these analyses to be completed within just two weeks and delivered on time after run matrix inputs were delayed.

•Results will be used by the SLS Guidance Navigation & Control group to plan separation trajectories and assess risk of recontact between SRBs and the core stage.

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

Mission Impact: CFD analyses of SRB separation provide critical aerodynamic data needed to design safe, effective separation systems and assess potential risks of recontact with the core stage.



Flow visualization of a Mach 4.1 iso-contour superimposed on the computational fluid dynamics grid, showing how the bow shock generated by the Multi-Purpose Crew Vehicle travels downstream and interacts with the solid rocket booster nose cone during separation. (Jeff Housman, NASA/Ames)

POC: Cetin Kiris, cetin.c.kiris@nasa.gov, (650) 604-4485, NASA Advanced Supercomputing Division

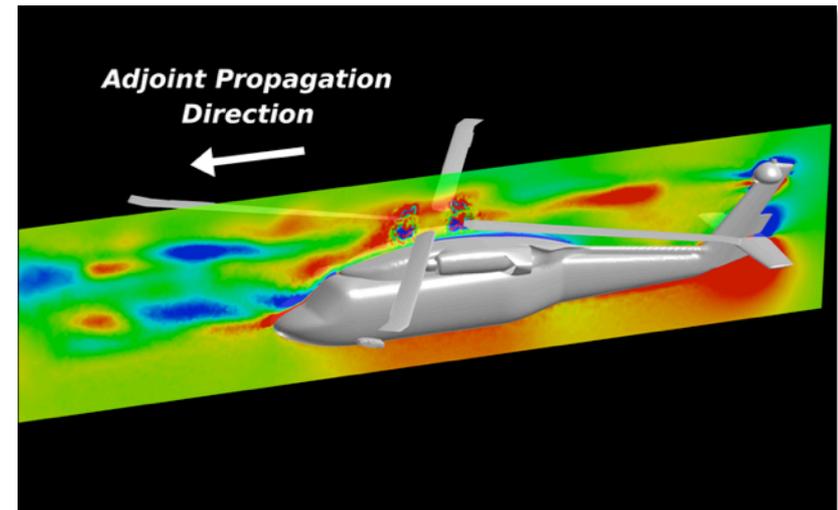
HECC Supports Adjoint-Based Design for Complex Aerospace Configurations



- Culminating two decades of development, software engineers at NASA Langley (LaRC) have introduced unique computational fluid dynamics (CFD) methods—enabled by Pleiades—to produce the world’s only CFD solver capable of adjoint-based sensitivity analysis for unsteady turbulent flows on dynamic, deforming, overset unstructured grids.
- Highly efficient asynchronous parallel I/O strategy manages the terabytes of data required to integrate backwards in time to establish sensitivities to all inputs using a single simulation.
- Coupled with the massively parallel Pleiades architecture, formal design optimization for extremely complex aerospace configurations becomes feasible, with compute times reduced from months/years to just a few days.
- The LaRC team successfully demonstrated their approach on a broad range of realistic design problems, including rotorcraft, fighter jets, flapping wing configurations, active flow control systems, and wind energy devices.

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

Mission Impact: Using computational tools and methods—enabled by HECC resources—to more accurately simulate and design complex vehicle configurations, researchers can speed up the design cycle and cut down on expensive wind tunnel experiments and flight testing, saving time and money.



Upstream propagation of adjoint solution for a UH-60 Black Hawk helicopter in forward flight. Contours indicate where the lift is sensitive to perturbations in both space and time. Conventional CFD solvers cannot identify these critical areas. (Eric Nielsen, NASA/Langley; Boris Diskin, National Institute of Aerospace)

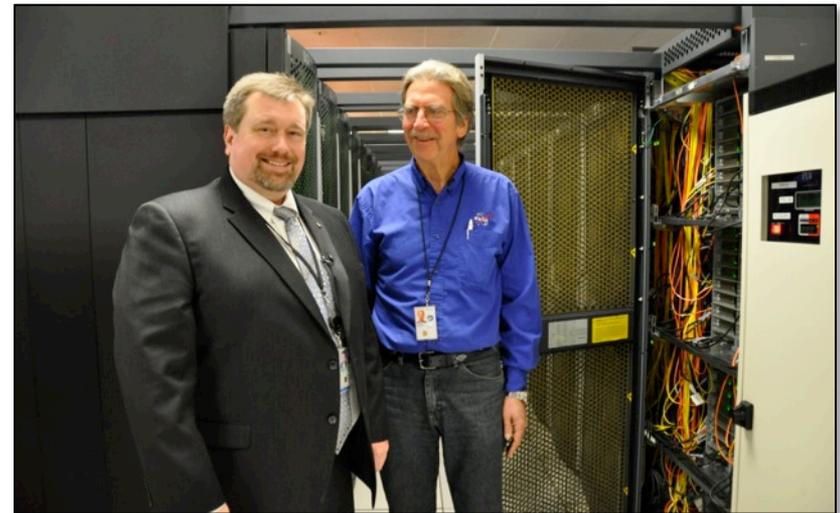
POC: Eric Nielsen, eric.j.nielsen@nasa.gov, (757) 864-2239,
NASA Langley Research Center.

HECC Facility Hosts Several Visitors and Tours in January 2013



•HECC hosted 6 tour groups in January; guests learned about the agency-wide missions being supported by Pleiades, and viewed scientific results on the hyperwall system. Visitors this month included:

- Bob Clay, Ground Infrastructure Manager/Program Specialist for the Human Exploration and Operations Mission Directorate (HEOMD) at Headquarters (HQ). Clay, who participates in Construction of Facilities Prioritization meetings and advocates projects that benefit HEOMD, met with HECC management for a briefing that highlighted how HECC benefits HEOMD science;
- Mason Peck, NASA's Chief Technologist, was briefed on HECC research by HECC management for an upcoming BBC documentary;
- Marshall Porterfield, HQ Division Director for Life and Physical Sciences, who is working with Ames staff to plan future International Space Station research, including a set of flight experiments (geneLAB) on genomics, proteomics, metabolomics and bioinformatics;
- The Right Honourable David Willetts, United Kingdom Minister for Universities and Science, visited as guest of the Ames director; Willetts is interested in supercomputing and future collaborations with Ames.



HECC Deputy Project Manager Bill Thigpen (at right) gave NASA Chief Technology Officer Mason Peck a tour of the NASA Advanced Supercomputing (NAS) facility main computer room, on January 22, 2013.

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

Papers and Presentations



- **Reliability and Maintainability Symposium (RAMS 2013)**, January 28–29, 2013, Orlando, Florida
<http://arxiv.org/abs/1210.4066>
 - “**Near-Earth Phase Risk Comparison of Human Mars Campaign Architectures**,” T. Manning, C. Mattenberger, H. Nejad. *
 - “**Top-down vs. Bottom-up Risk Assessment: Consistent, Contradictory or Complimentary?**,” H. Nejad, D. Mathias. *
 - “**Launch Vehicle Debris Models and Crew Vehicle Ascent Abort Risk**,” K. Gee, S. Lawrence. *
 - “**An Exploration of PRA Methodology used in Spacecraft Design**,” C. Mattenberger, H. Nejad. *
 - “**Human Space Mission Architecture Risk Analysis**,” S. Go, D. Mathias, H. Nejad. *
- “**The Ozone Response to ENSO in Aura Satellite Measurements and a Chemistry-Climate Simulation**,” L. D. Oman, et al., *Journal of Geophysical Research: Atmospheres*, January 24, 2013. *
<http://onlinelibrary.wiley.com/doi/10.1029/2012JD018546/full>
- “**The Maximum Energy of Accelerated Particles in Relativistic Collisionless Shocks**,” L. Sironi, A. Spitkovsky, J. Arons, arXiv:1301.5333 [astro-ph.HE], January 22, 2013. *
<http://arxiv.org/abs/1301.5333>
- “**Angular Momentum Transport by Acoustic Modes Generated in the Boundary Layer II: MHD Simulations**,” M. A. Belyaev, et al. arXiv:1301.4573 [astro-ph.SR], January 19, 2013. *
<http://arxiv.org/abs/1301.4573>

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

Papers and Presentations



- **“The Impact of Limiting Ocean Roughness on GEOS-5 AGCM Tropical Cyclone Forecasts,”** A. Molod, M. Suarez, G. Partyka, Geophysical Research Letters, January 18, 2013. *
<http://onlinelibrary.wiley.com/doi/10.1029/2012GL053979/full>
- **“Effects of Obliquity and Water Vapor/Trace Gas Greenhouses in the Early Martian Climate,”** M. A. Mischna, et al., Journal of Geophysical Research: Planets, January 18, 2013. *
<http://onlinelibrary.wiley.com/doi/10.1002/jgre.20054/abstract>
- **“Direct and Semi-Direct Aerosol Effects in the NASA GEOS-5 AGCM: Aerosol-climate Interactions Due to Prognostic Versus Prescribed Aerosols,”** C. A. Randles, P. R. Colarco, A. de Silva, Journal of Geophysical Research: Atmospheres, January 16, 2013. *
<http://onlinelibrary.wiley.com/doi/10.1029/2012JD018388/full>
- **“Spontaneous Formation Of Dipolarization Fronts And Reconnection Onset In The Magnetotail,”** M. I. Sitnov, et al., Geophysical Research Letters, January 16, 2013. *
<http://onlinelibrary.wiley.com/doi/10.1029/2012GL054701/full>
- **“Radio Light Curves During the Passage of Cloud G2 Near Sgr A,”** A. Sadowski, et al., arXiv:1301.3906 [astro-ph.HE], January 16, 2013. *
<http://arxiv.org/abs/1301.3906>

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

Papers and Presentations



- **“Spurious Behavior of Shock-Capturing Methods Below the CFL Limit: Problems Containing Stiff Source Terms and Discontinuities,”** H. Yee, Fourth Chilean Workshop on Numerical Analysis of Partial Differential Equations (WONAPDE 2013), January 14-18, 2013, Concepcion, Chile *
- **“Angular Momentum Acquisition in Galaxy Halos,”** K. Stewart, et al., arXiv:1301.3143 [astro-ph.CO], January 14, 2013. *
<http://arxiv.org/abs/1301.3143>
- **AIAA Aerospace Sciences Meeting**, January 7-10, 2013, Grapevine, Texas
 - **“Panel Discussion: Information Technology – Spin-On Technology for Aeronautics and Science,”** *Rupak Biswas (Moderator)*
 - **“Extension of the Time-Spectral Approach to Overset Solvers for Arbitrary Motion,”** J. Leffell, S. M. Murman, T. H. Pulliam *
 - **“Output Error Estimates and Mesh Refinement in Aerodynamic Shape Optimization,”** *M. Nemec; M. Aftosmis **
 - **“DPW-5 Analysis of the CRM in a Wing-Body Configuration Using Structured and Unstructured Meshes,”** A. J. Sclafani, et al. *
 - **“Integrated Nacelle-Wing Shape Optimization for an Ultra-High Bypass Fanjet Installation on a Single-Aisle Transport Configuration,”** *Stephen C. Smith; Marian Nemec; Steven E. Krist **
- **“Alignment of Magnetized Accretion Disks and Relativistic Jets with Spinning Black Holes,”** J. C. McKinney, A. Tchekhovskoy, R. Blandford, Science Magazine, Volume 339, No. 6115, pp. 49-52, January 4, 2013. *
<http://www.sciencemag.org/content/339/6115/49.full>

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

Papers and Presentations



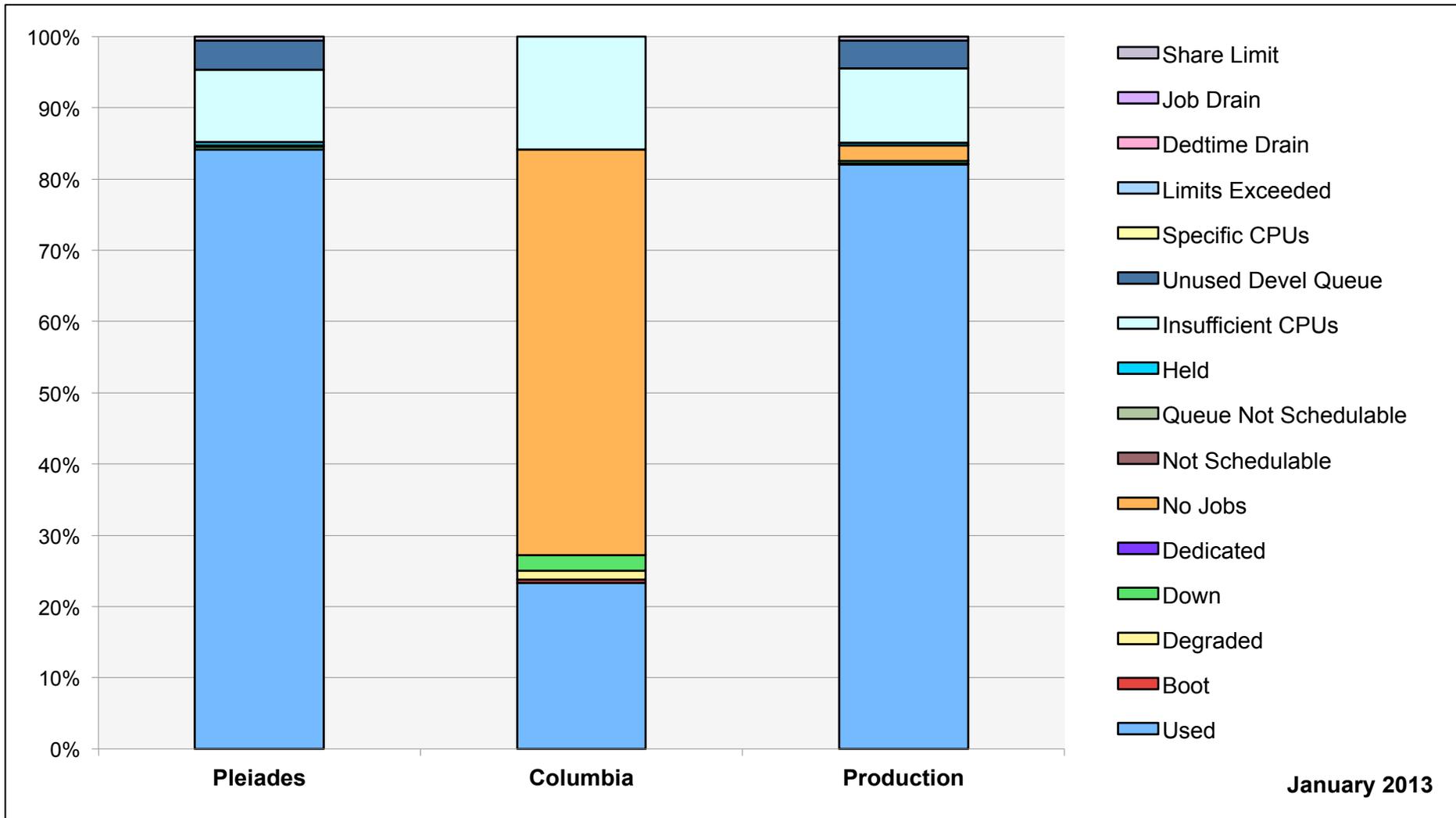
- **“Spectral Variability of Classical T Tauri Stars Accreting in an Unstable Regime,”** R. Kurosawa, M. M. Romanova, arXiv:1301.0641 [astro-ph.SR], January 3, 2013. *
<http://arxiv.org/abs/1301.0641>
- **“Spectral and Intermittency Properties of Relativistic Turbulence,”** J. Zrake, A. I. MacFadyen, arXiv:1210.4066 [astro-ph.HE], January 3, 2013. *
<http://arxiv.org/abs/1210.4066>
- **“Hybrid Large-Eddy/Reynolds-Averaged Simulation of a Supersonic Cavity using VULCAN,”** J. Quinlan, J. McDaniel, R. Baurle, University of Virginia, January 2013. *
<http://people.virginia.edu/~jrq2a/papers/ieee12.pdf>

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

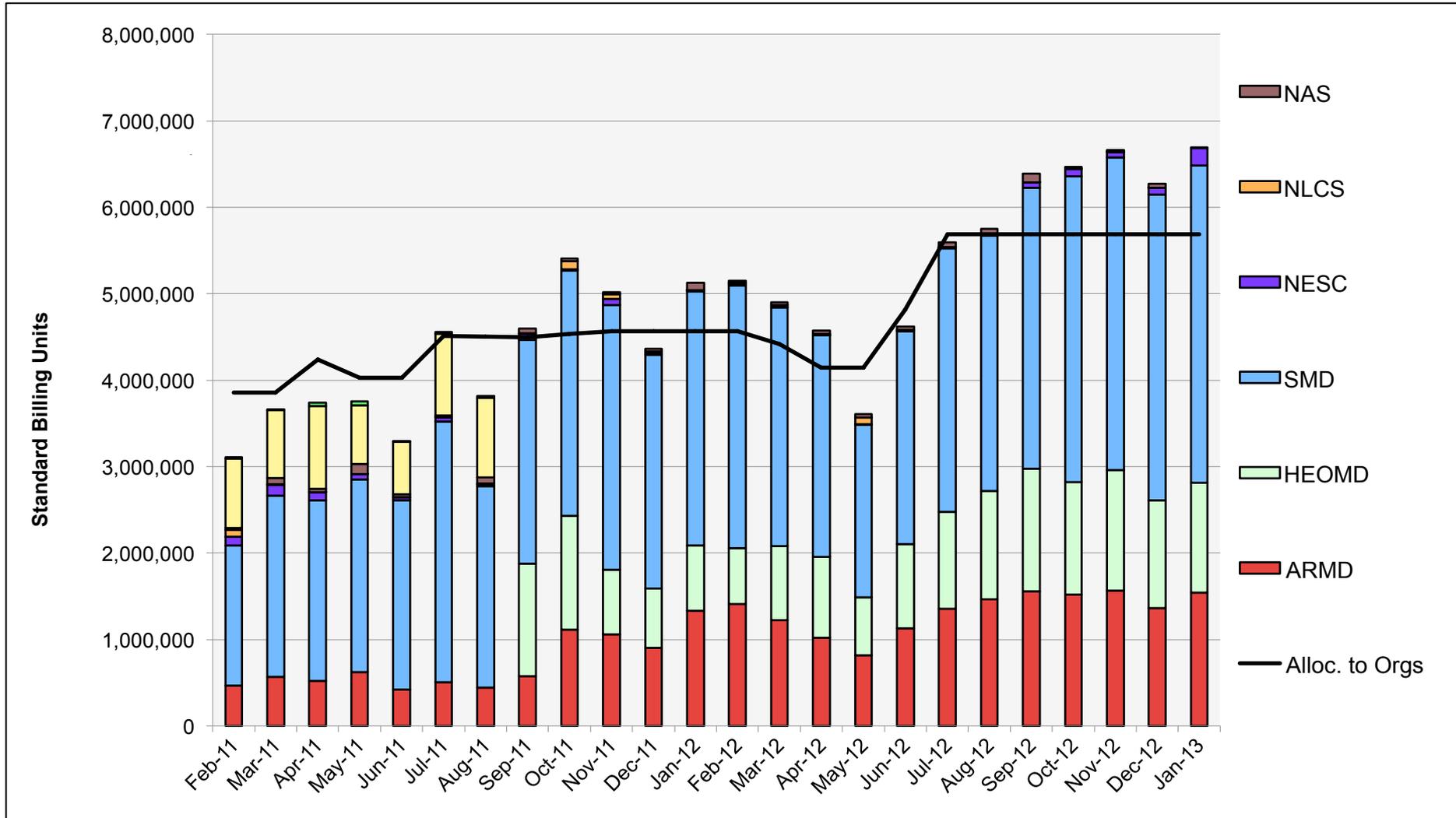


- **Improving Climate Change Predictions, One Cloud at a Time**, *JPL Center for Climate Studies Press Release*, January 7, 2013 – Climate scientists at JPL are developing more refined and accurate simulations of clouds using the Pleiades supercomputer. Cloud cover has an enormous effect on climate by reflecting sunlight or trapping heat emanating from the Earth's surface.
<http://climatesciences.jpl.nasa.gov/news-release/2013-01-cloud-modeling>
- **NASA's IRIS Spacecraft Is Fully Integrated**, *NASA Press Release*, January 18, 2013 – NASA's Interface Region Imaging Spectrograph (IRIS) will make use of high-resolution images, data, and advanced computer models run on Pleiades to investigate how energy moves from the sun's surface to its corona.
http://www.nasa.gov/mission_pages/iris/news/iris-integration.html
 - **NASA's IRIS Spacecraft Scheduled to Launch in April**, *Smithsonian Science*, January 23, 2013.
<http://smithsonianscience.org/2013/01/nasas-iris-spacecraft-scheduled-to-launch-in-april/>
 - **IRIS Looks to Shed Light on a Solar Puzzle**, *SEN.com*, January 24, 2013.
<http://www.sen.com/news/iris-looks-to-shed-light-on-a-solar-puzzle.html>
 - **NASA Spacecraft Readied for Sun Study**, *UPI.com*, January 18, 2013.
http://www.upi.com/Science_News/2013/01/18/NASA-spacecraft-readied-for-sun-study/UPI-84471358551676/
 - **A Narrow View of the Sun**, *Aviation Week*, January 21, 2013.
http://www.aviationweek.com/Article.aspx?id=/article-xml/AW_01_21_2013_p50-536575.xml&p=1#

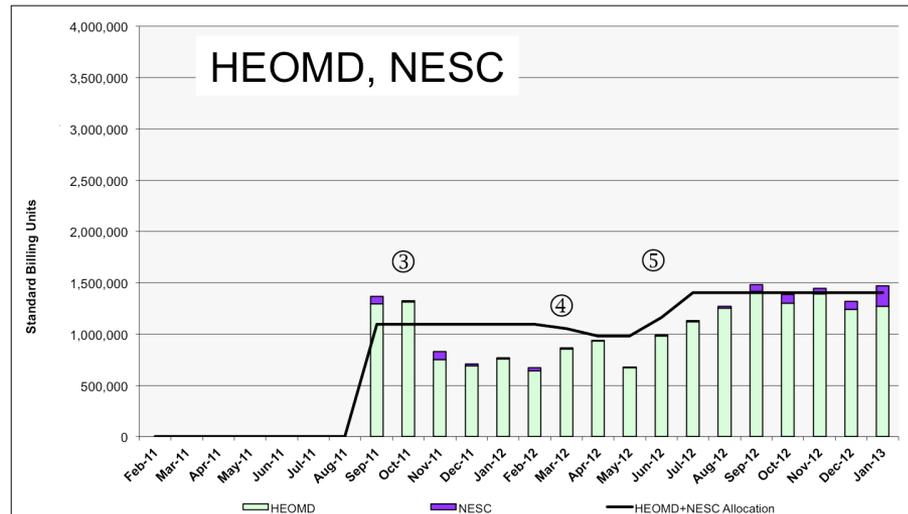
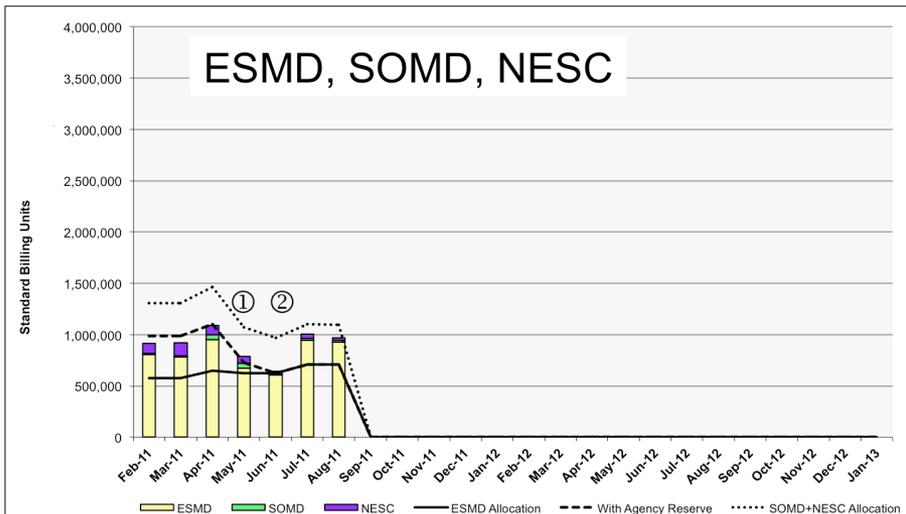
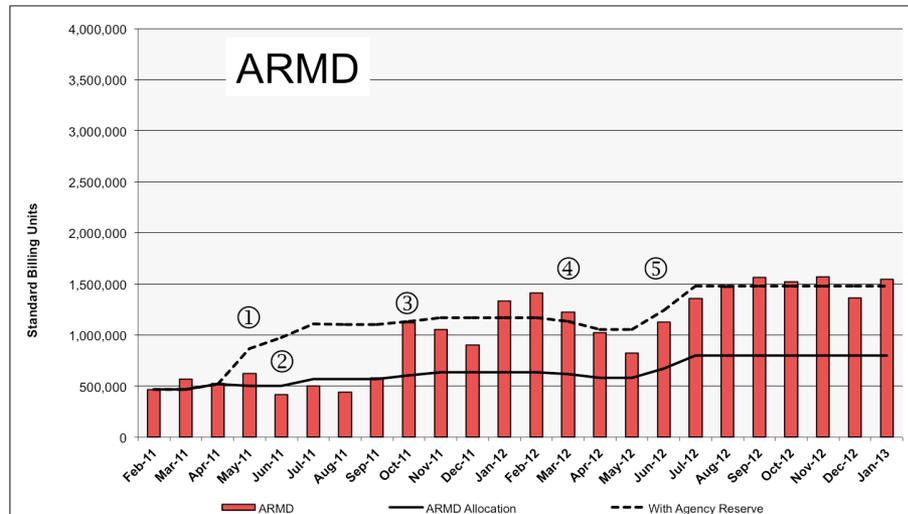
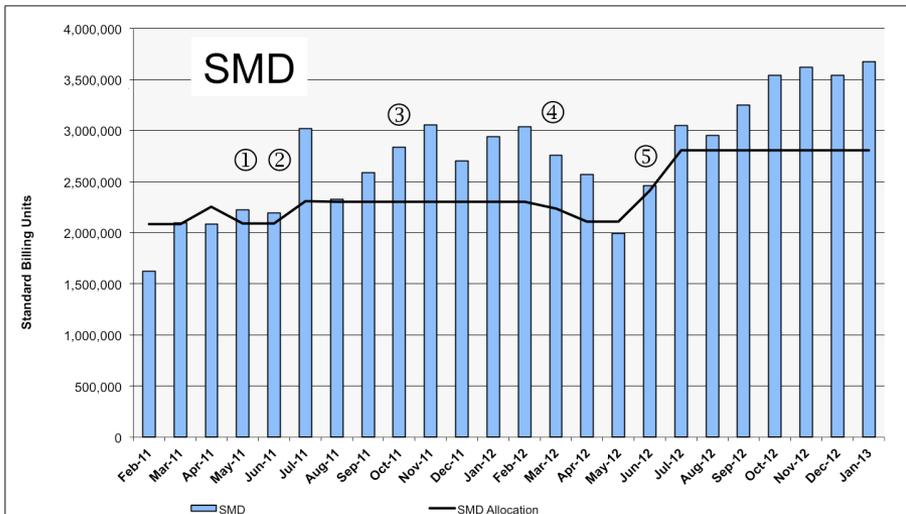
HECC Utilization



HECC Utilization Normalized to 30-Day Month

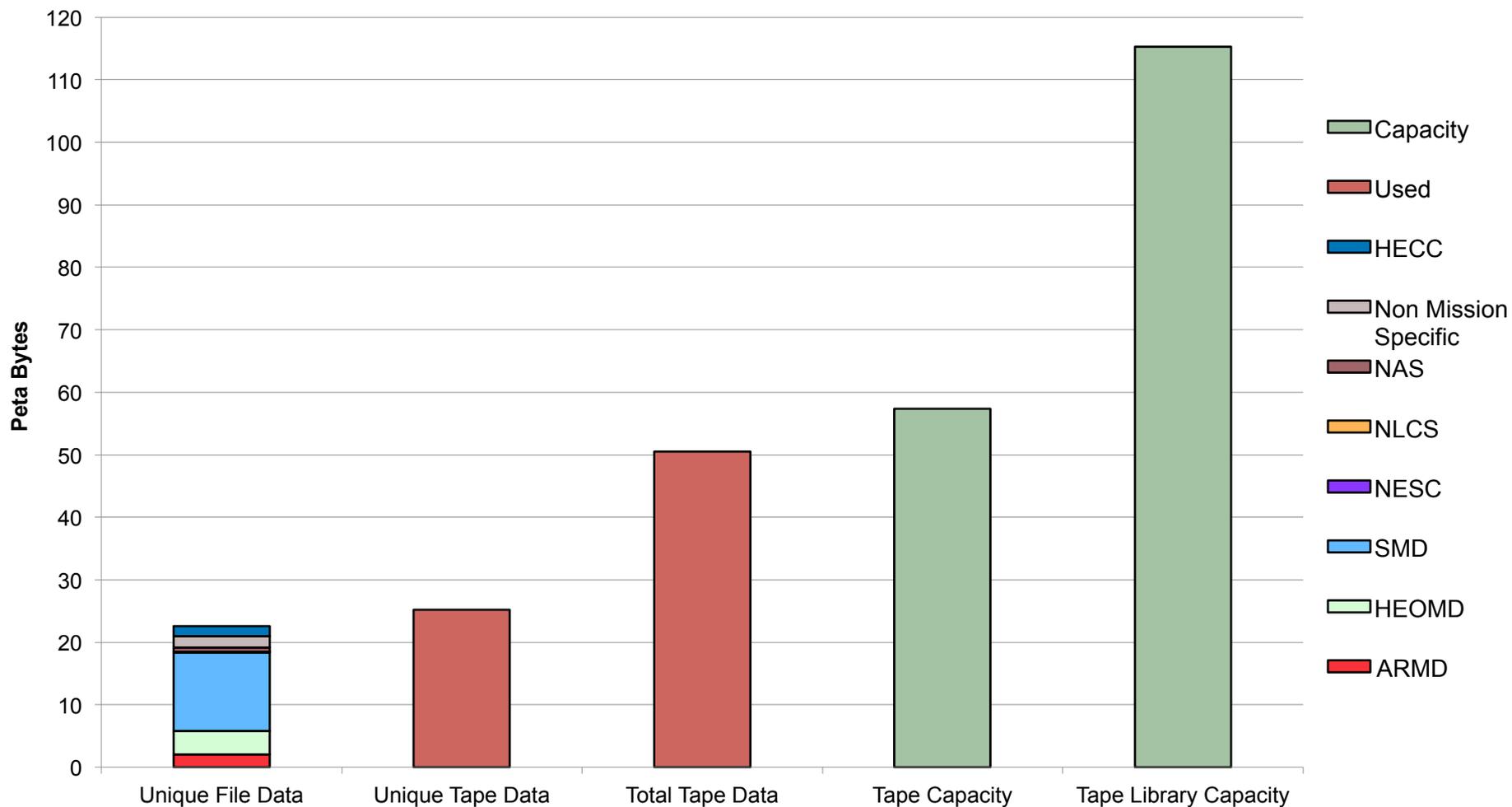


HECC Utilization Normalized to 30-Day Month



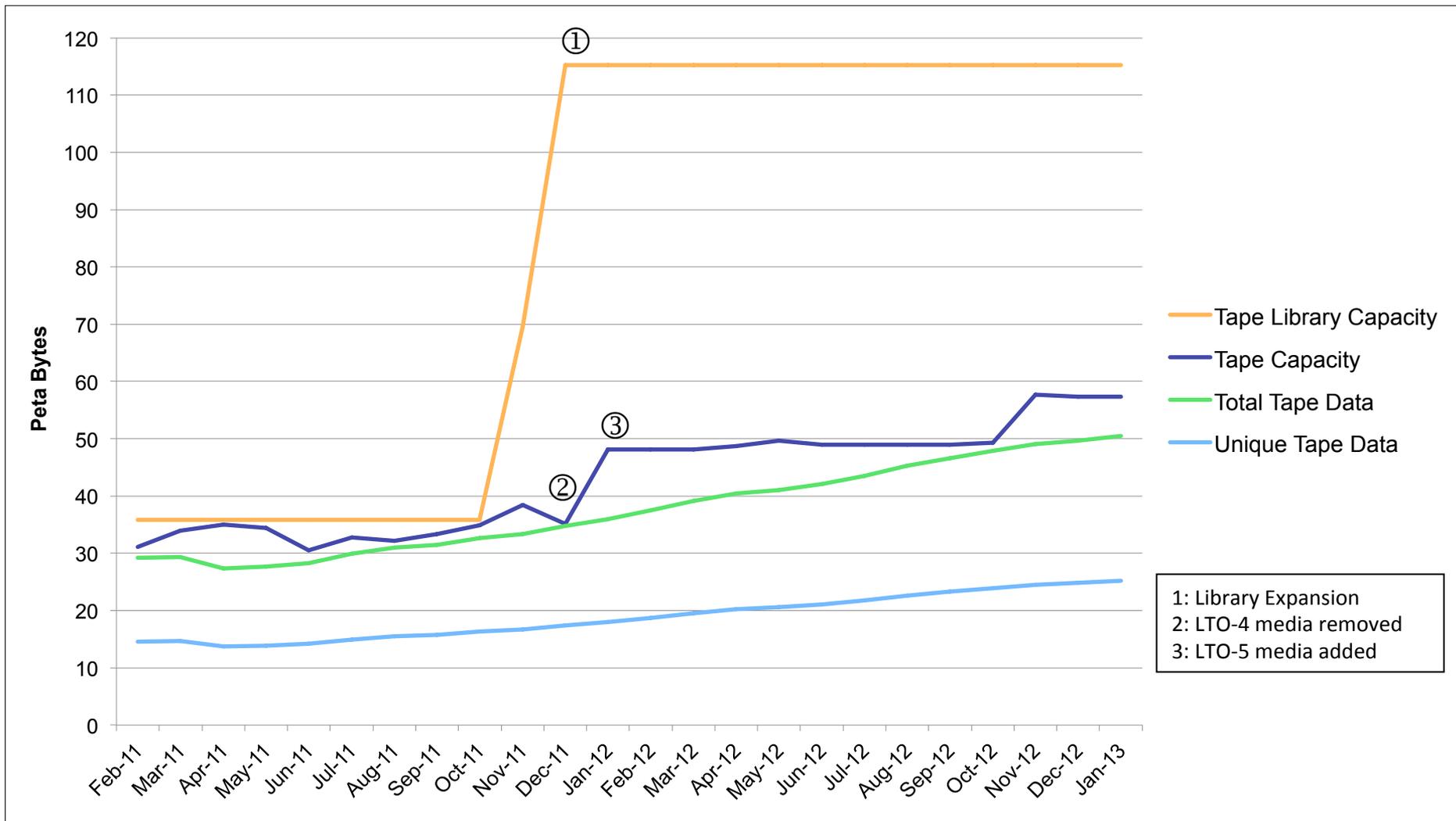
- ① Allocation to orgs. decreased to 75%, Agency reserve shifted to ARMD
- ② 14 Westmere racks added
- ③ 2 ARMD Westmere racks added
- ④ 28 Harpertown racks removed
- ⑤ 24 Sandy Bridge racks added

Tape Archive Status



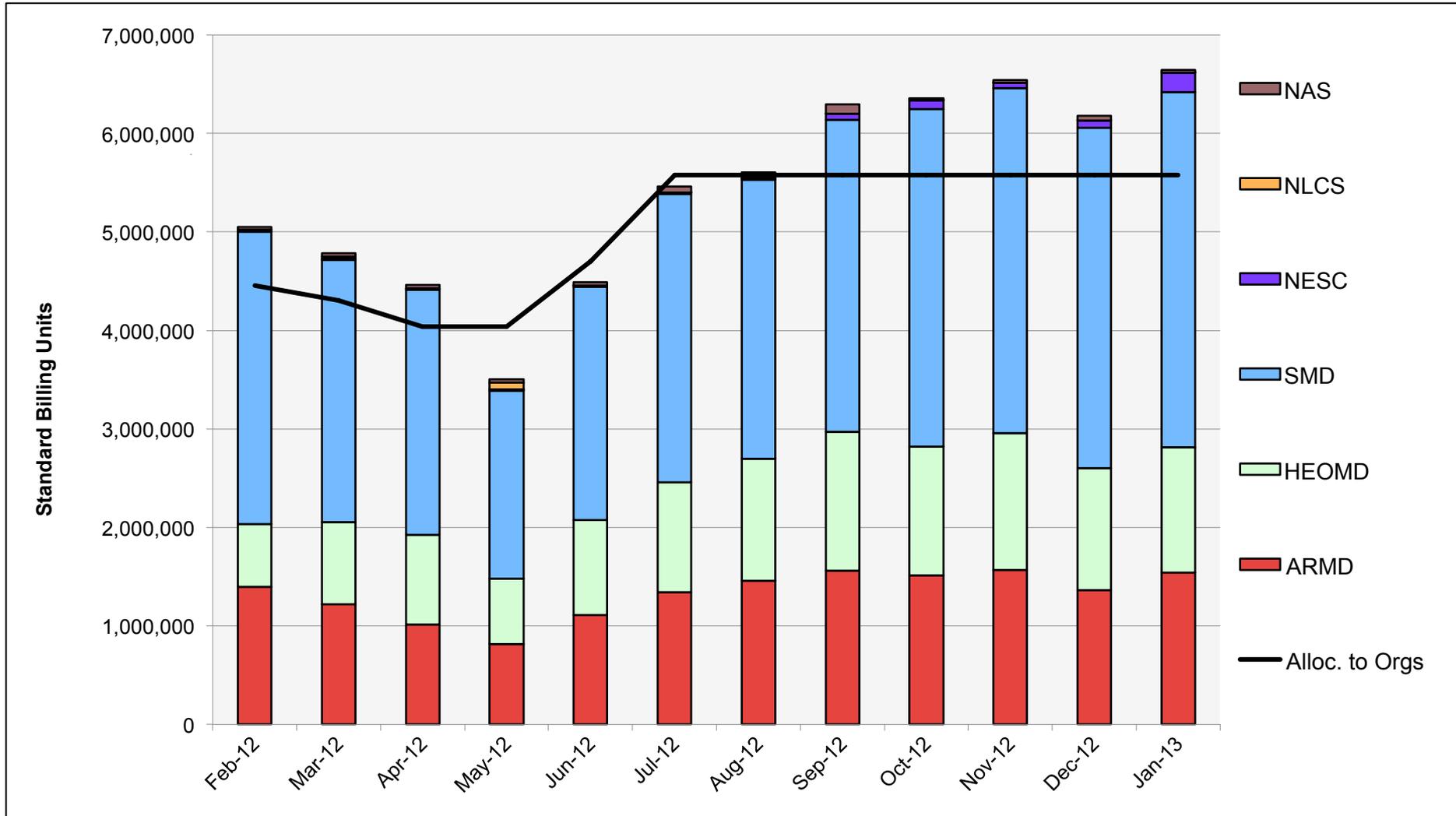
January 2013

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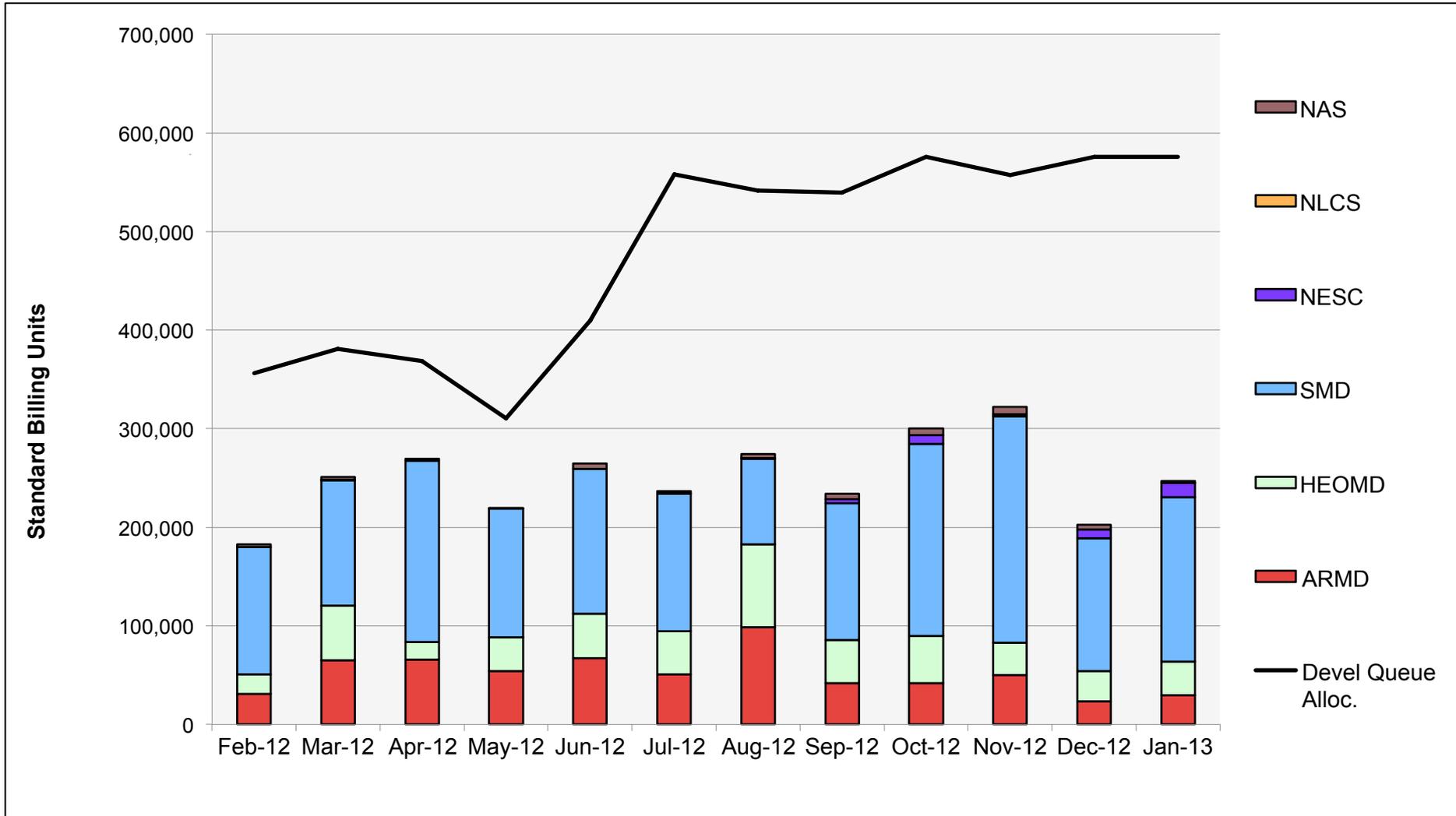


- 1: Library Expansion
- 2: LTO-4 media removed
- 3: LTO-5 media added

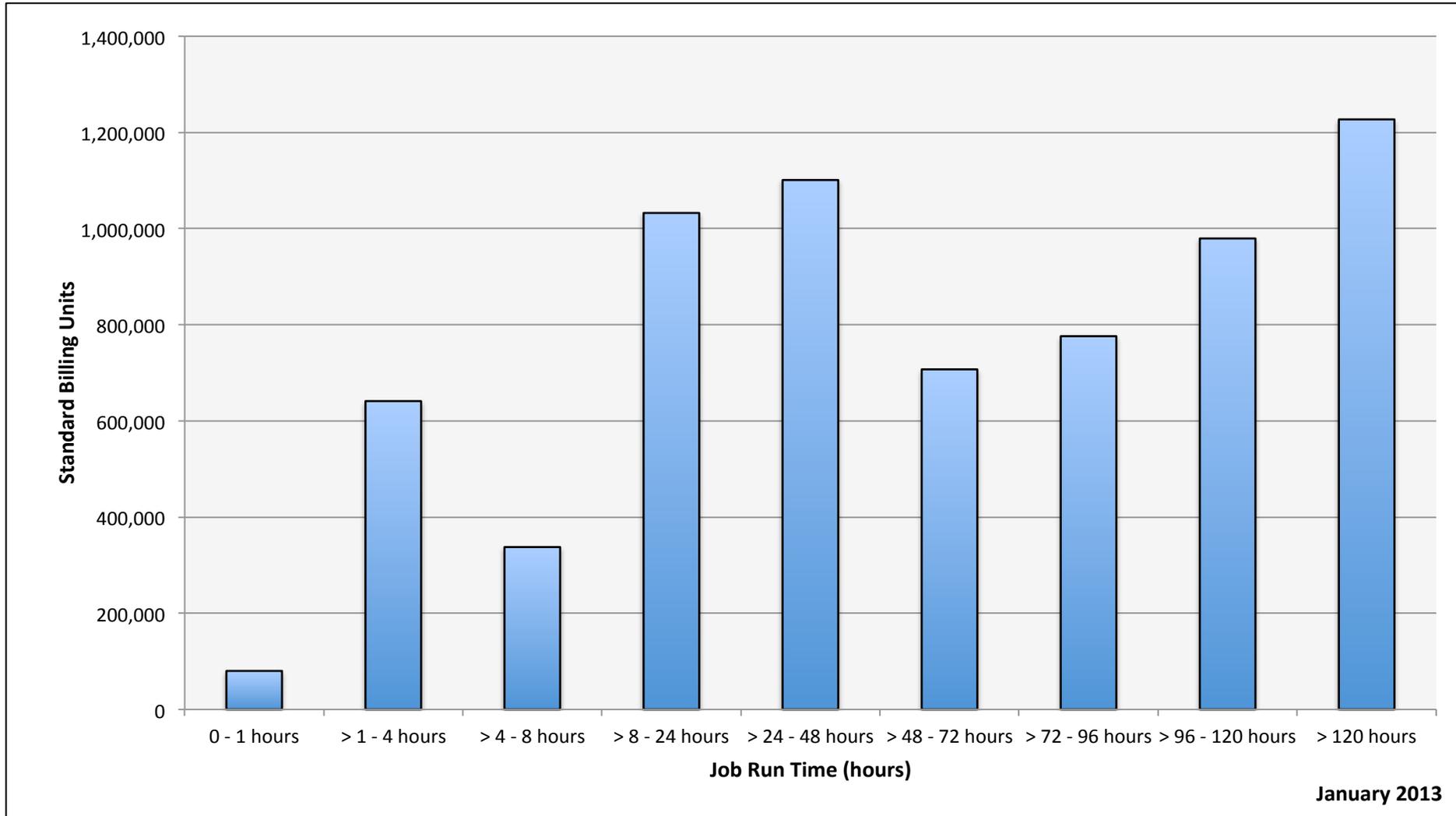
Pleiades: SBUs Reported, Normalized to 30-Day Month



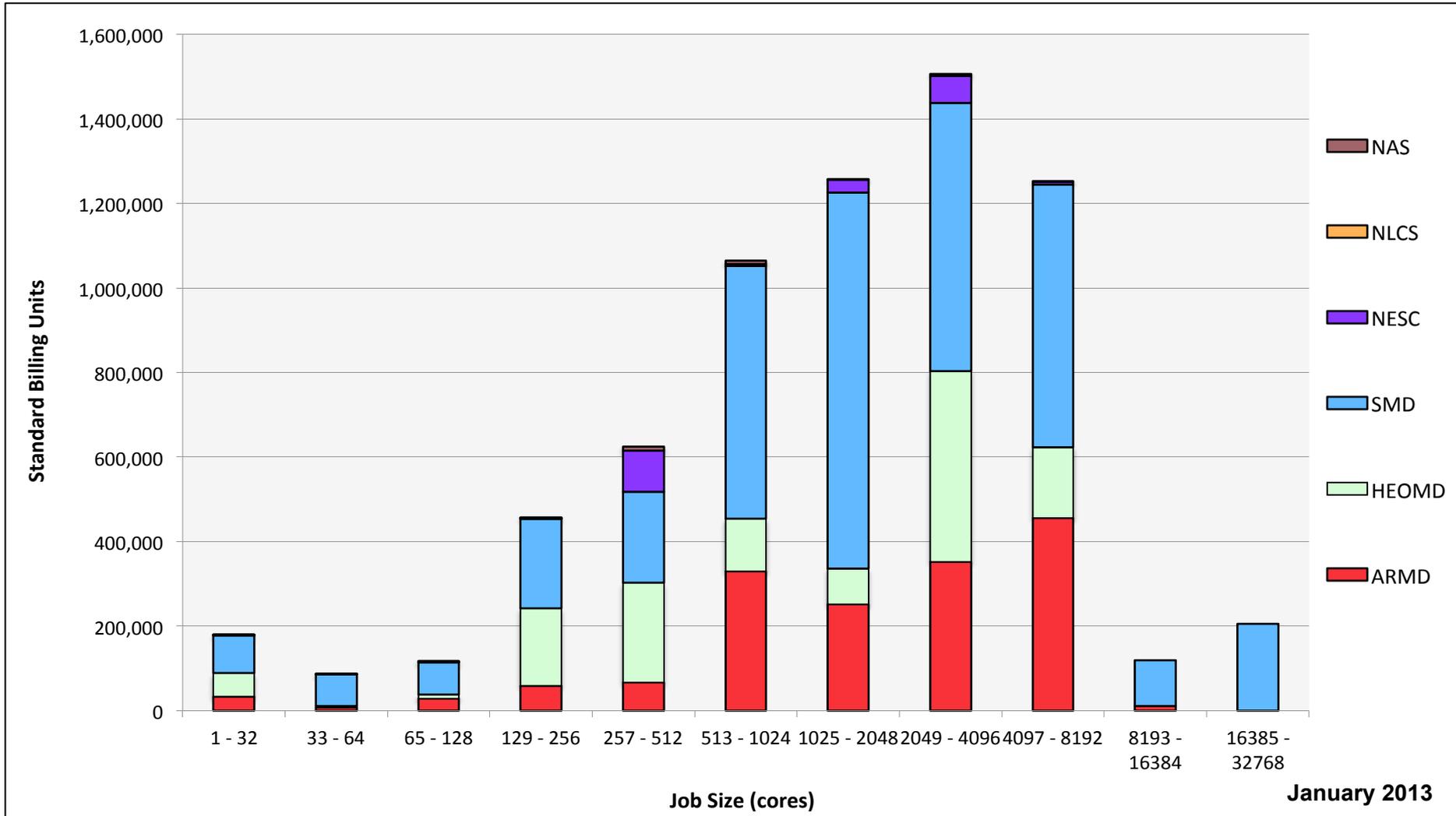
Pleiades: Devel Queue Utilization



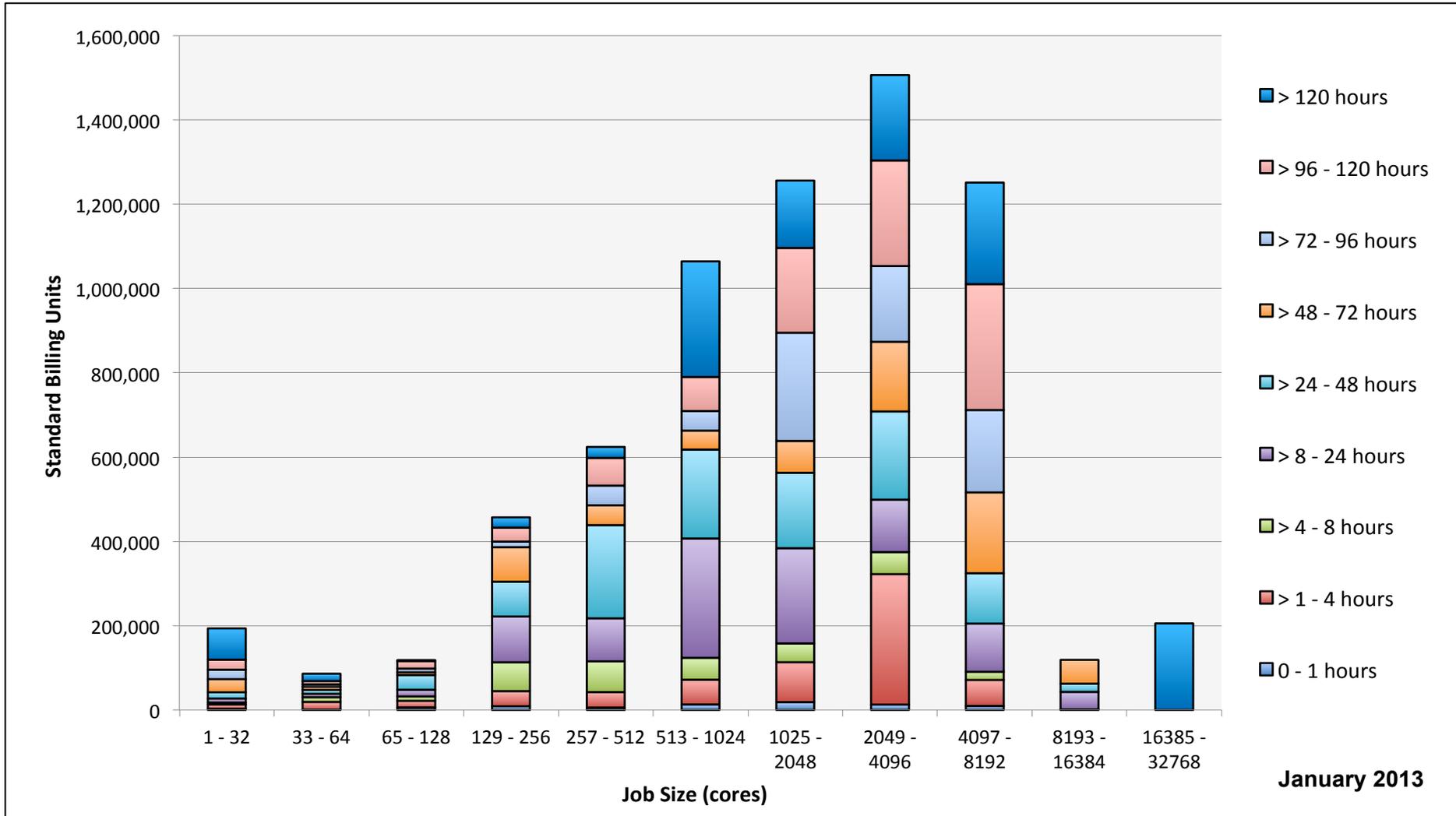
Pleiades: SBUs Reported, Normalized to 30-Day Month



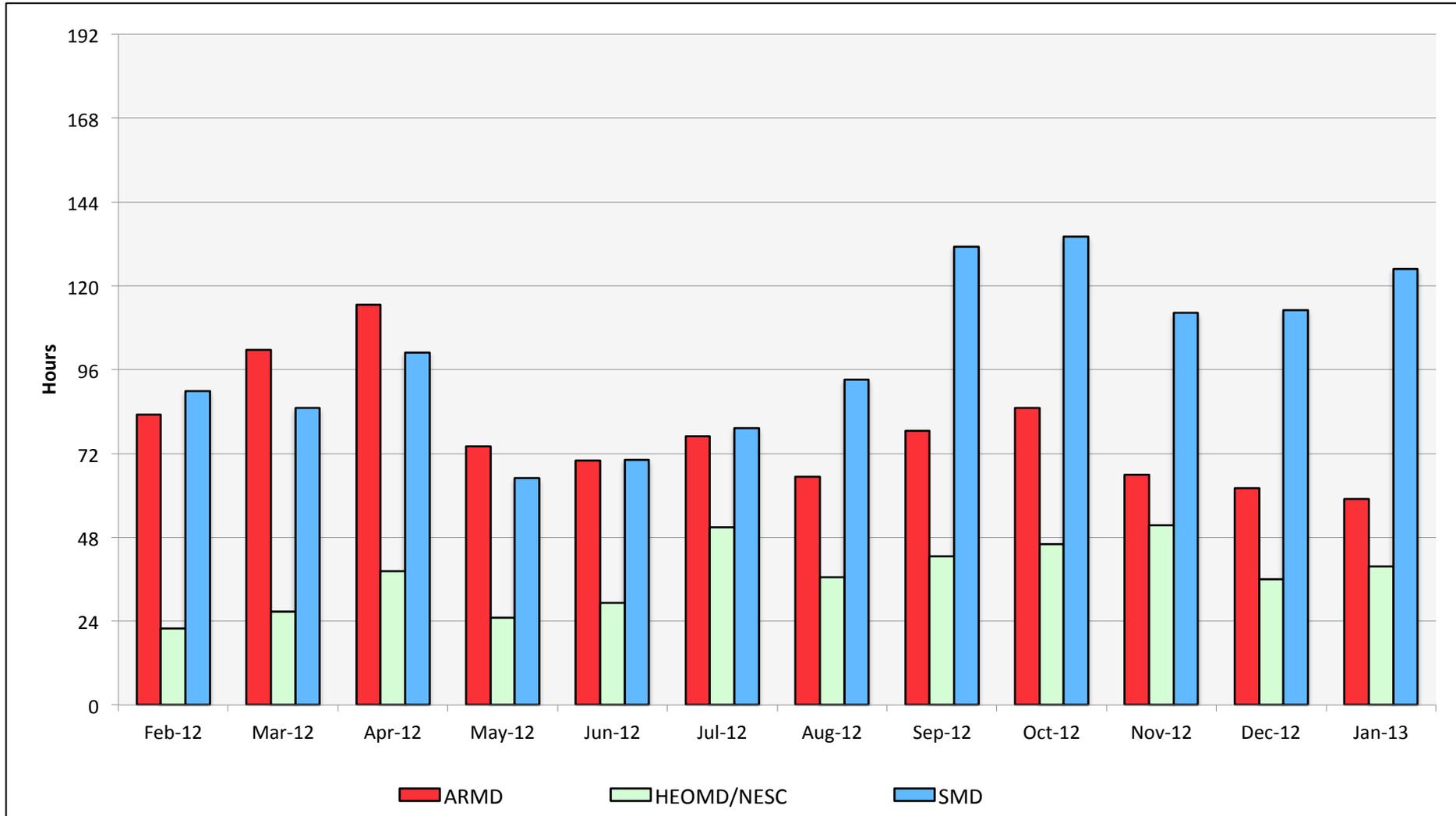
Pleiades: Monthly Utilization by Size and Mission



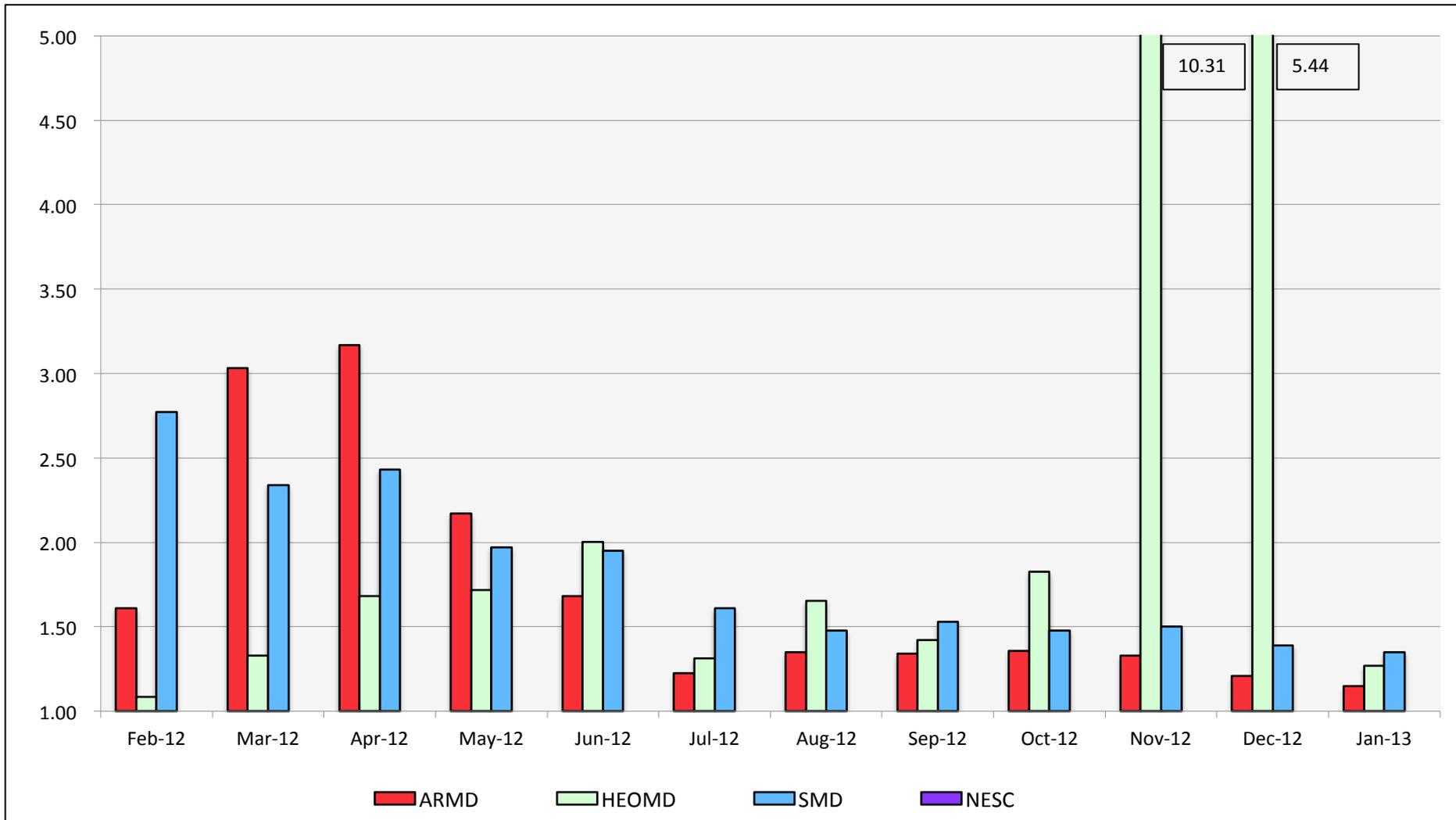
Pleiades: Monthly Utilization by Size and Length



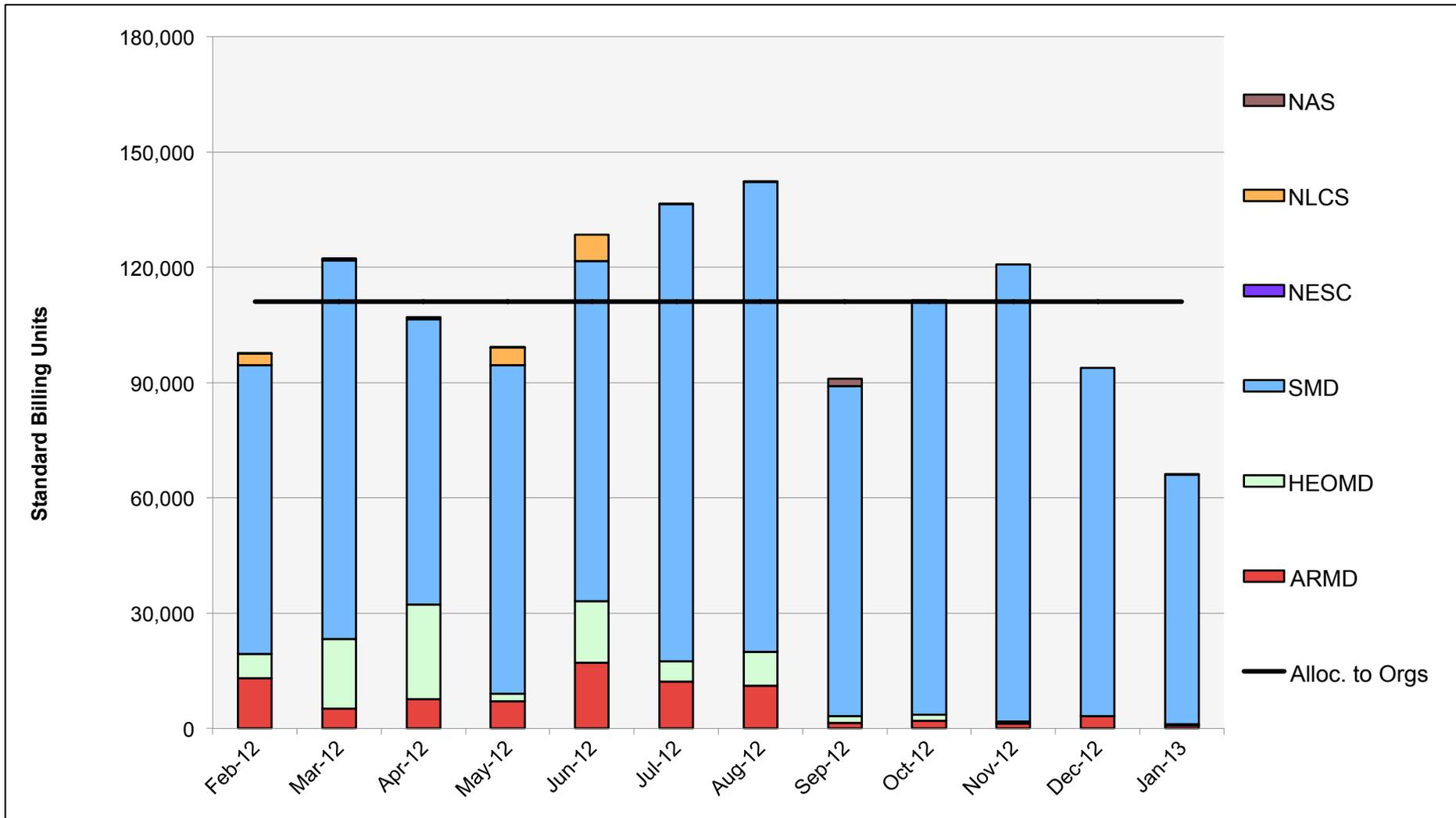
Pleiades: Average Time to Clear All Jobs



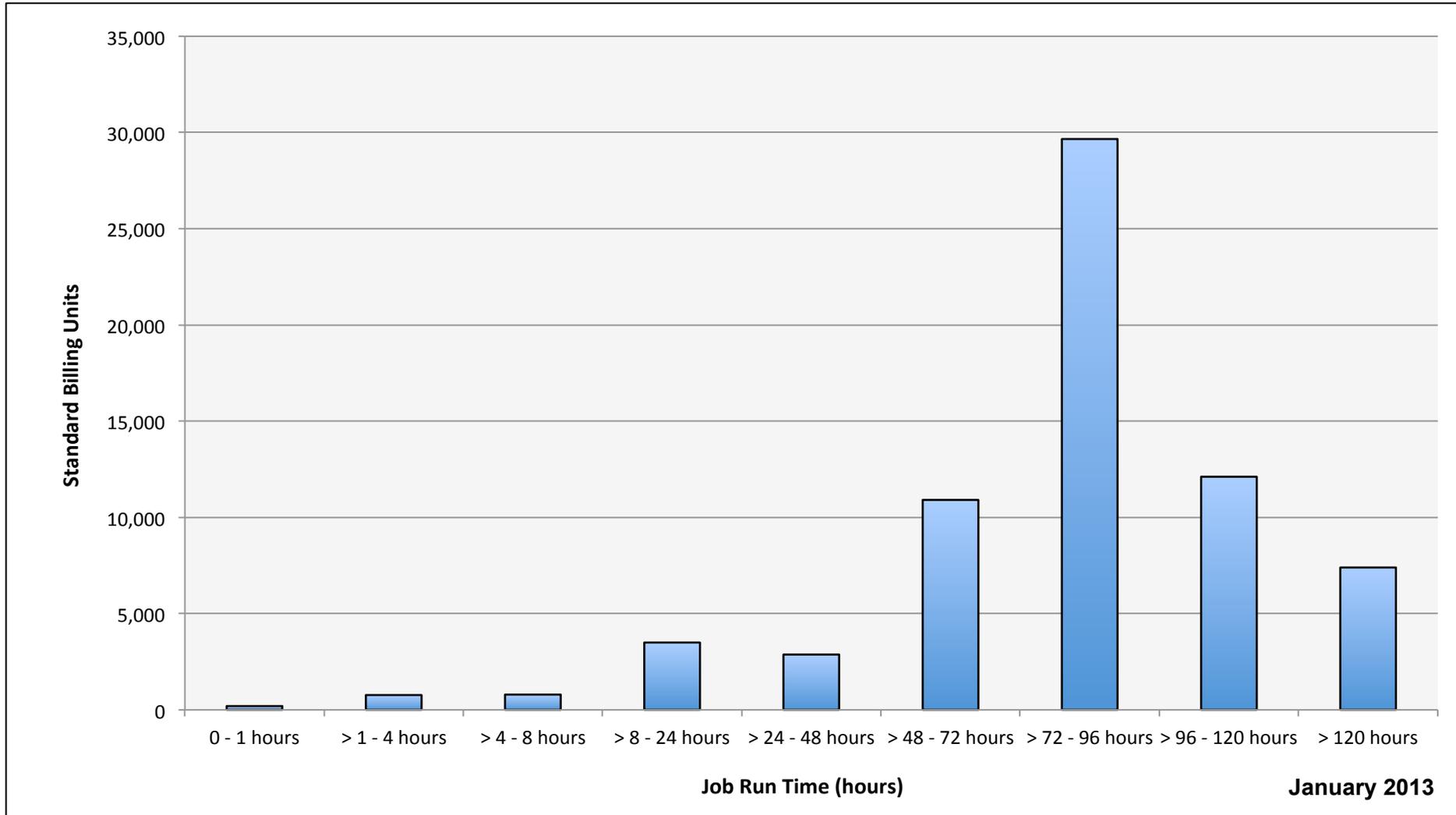
Pleiades: Average Expansion Factor



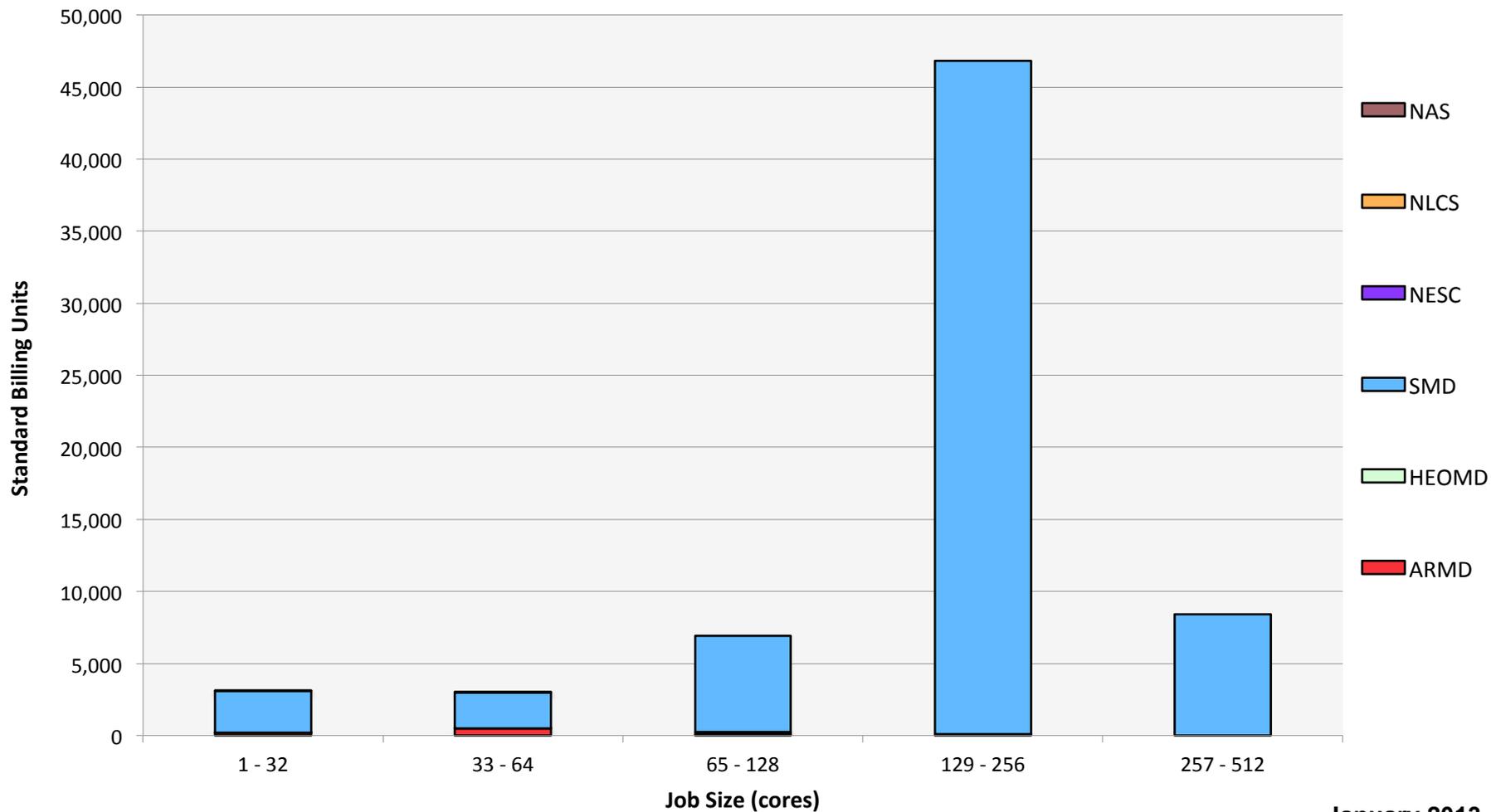
Columbia: SBUs Reported, Normalized to 30-Day Month



Columbia: SBUs Reported, Normalized to 30-Day Month

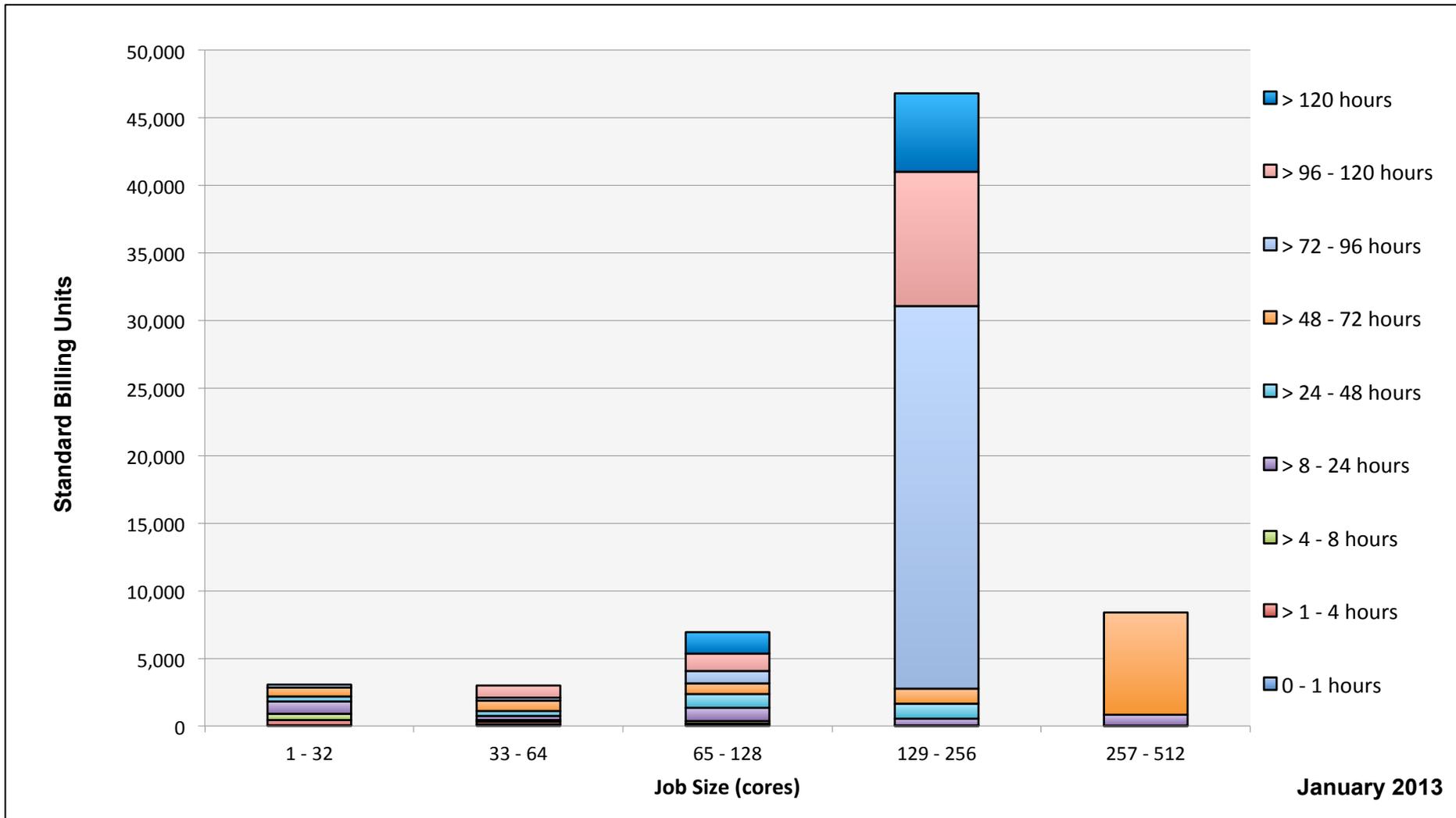


Columbia: Monthly Utilization by Size and Mission

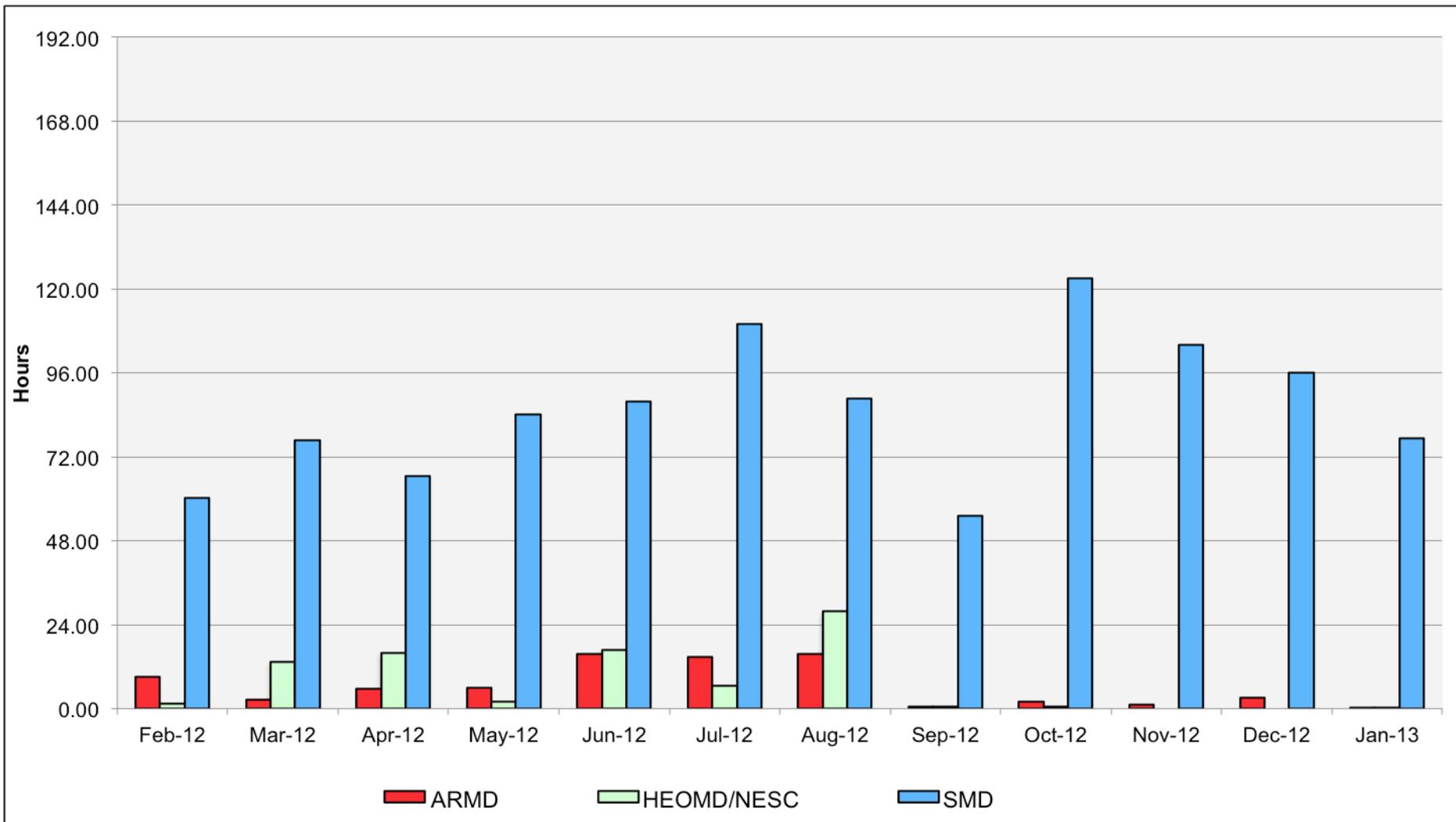


January 2013

Columbia: Monthly Utilization by Size and Length



Columbia: Average Time to Clear All Jobs



Columbia: Average Expansion Factor

