Project Status Report

High End Computing Capability
Strategic Capabilities Assets Program

March 10, 2014

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Xeon Phi-based Maia Cluster Opened to User Community

- HECC management announced that Maia, a 128-node cluster in which each node has two Intel Sandy Bridge processors and two Intel Xeon Phi accelerator cards, is available to the user community.
- To prepare for this stage, HECC's Application Performance and Productivity team conducted an initial system performance characterization, and the Systems team configured Maia to a stability level suitable for user experimentation with this new architecture. Key findings include:
  - System stability is affected by Xeon Phi software, which is maturing gradually.
  - Architectural constraints and software overhead combine to make code transformations necessary to achieve high performance.
- By involving interested users, HECC hopes to characterize the types of NASA applications that are best suited to run on Xeon Phi processors.

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

The Maia system employs both conventional Xeon processors and "many-integrated core" (MIC) Xeon Phi coprocessors.

POCs: Henry Jin, haoqiang.jin@nasa.gov, (650) 604-0165; Jerry Yan, jerry.yan@nasa.gov, (650) 604-4381; NASA Advanced Supercomputing Division

HECC Tape Libraries Upgraded to Meet Increasing Data Storage Requirements

- HECC staff completed an upgrade to the tape libraries located on the primary computing floor at the NASA Advanced Supercomputing (NAS) facility, Building N258.
- The upgrade includes new robotics that enable HECC to take advantage of future improvements to tape library technology, resulting in faster tape media load times and providing a path for further growth of the library infrastructure.
- Original plans called for completing the upgrade over a three-week period (similar to the January 2014 tape library upgrade in the secondary computing facility). The vendor, Spectra Logic, completed the work several days ahead of schedule.
- The practice of maintaining two redundant copies of data on separate computer floors enabled the upgrade of the data archive infrastructure to be transparent to users.

Mission Impact: Enhancing the tape library infrastructure for NASA's largest supercomputing facility enables HECC to keep pace with the ever-increasing data storage requirements of science and engineering users supporting agency missions.

The data archive infrastructure now stores about 65 petabytes of data, and with current tape technology has the capacity to store up to 115 petabytes of data.

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

New Lustre Filesystem Increases Bandwidth for Temporary Storage

- HECC engineers deployed a new Lustre filesystem used for temporary ("scratch") storage while running user jobs on the Pleiades and Endeavour supercomputers.
- This 3.4 petabyte filesystem, designated nobackupp9, was created from hardware that was originally used for the nobackupp1 and nobackupp2 filesystems.
- The increased number of RAID controllers available on the combined filesystem provides higher bandwidth for data-intensive applications.
- The filesystem is currently being utilized to resolve Lustre bugs. Once that activity is complete, it will be available for general use by the HECC community.
- This upgrade, along with the work described in slides 4 and 7, continues HECC's ongoing efforts to provide an environment that facilitates NASA's requirements to handle big data.

Mission Impact: Increased temporary storage capacity will enable NASA researchers to more fully utilize the HECC computing resources and run more data-intensive applications.

The Lustre filesystems are the primary "scratch" systems used for running HECC computational jobs.

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Network Engineers Complete Upgrade to HECC Enclave Border Router

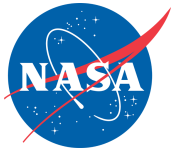
- HECC Network team completed an upgrade of the enclave border router to the newest technology from Cisco Systems.
- The upgrade provides 550 gigabit-per-second (Gbps) fabric switching per module. Previous hardware supported only 40 Gbps per module.
  - Each module can support up to forty-eight 1- or 10-Gigabit Ethernet (GE) connections. Previous modules could only support up to eight 10GE connections. This significantly increases the 10GE port density.
  - With the new fabric, no ports are over-subscribed. Previous ports were 2:1 over-subscribed, causing contention for high-usage hosts.
- Careful planning and redundancy built into the network design enabled the HECC network engineers to complete the transition without impacting users.
- Since virtually all traffic moving into and out of the HECC enclave passes through this border router, the added capability of this new hardware is essential to the current and future capacity of the enclave environment.

Mission Impact: HECC's upgrades to new network technologies prepare us for next generation Wide Area Network advancements.

The new enclave border router provides a faster backplane and higher port density preparing the enclave for future expansions.

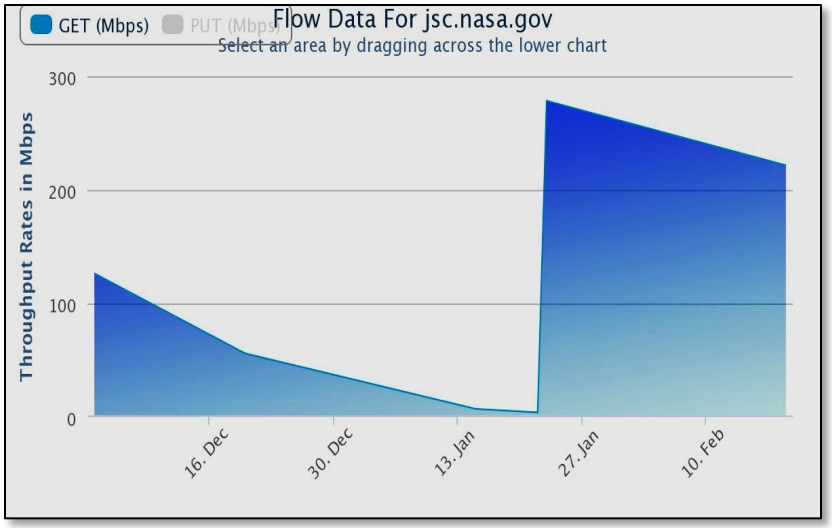
POCs: Nichole Boscia, nichole.k.boscia@nasa.gov, (650) 604-0891, Harjot Sidhu, harjot.s.sidhu@nasa.gov, (650) 604-4935, NASA Advanced Supercomputing Division, Computer Sciences Corp.

Network Solution Increases Data Transfer Performance to JSC by 40x



- The HECC Network team identified a packet loss issue on the Johnson Space Center (JSC) campus network after users reported issues with slow file transfers, and created a solution that resulted in significantly improved data transfer performance.
- Users running the secure copy protocol, SCP, to transfer files between JSC and Ames now experience file transfer rates up to 40x faster than available previously.
- HECC network engineers worked with NASA Integrated Communications Services and JSC engineers to test the network, isolate the problem to a bad fiber optics on a JSC switch, and validate the hardware replacement.
- Darby Vicker, HECC user from JSC, was extremely satisfied with the support from the HECC Network team. "We continue to get transfer rates of 20–30 megabytes/second. Thanks to everyone involved who helped find and fix this—it's a huge help for our lab!"

Mission Impact: HECC solves not only issues inside the enclave, but also user issues *outside* the enclave, in order to minimize their total time-to-solution in pursuing NASA mission goals.



Graph showing the network rates users received while transferring data from Johnson Space Center to Ames Research Center. Rates increased dramatically after HECC network engineers implemented a fix on January 23, 2014.

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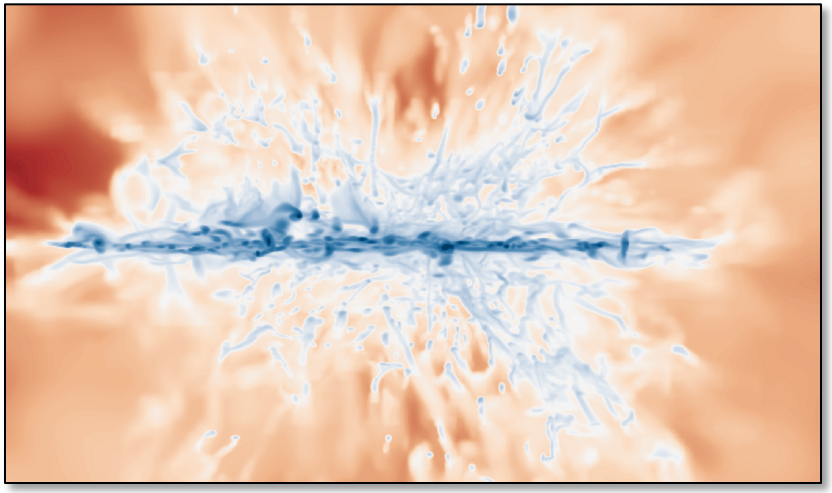
Advanced Simulations Track Formation and Evolution of Thousands of Galaxies *

- Modeling galaxy formation is a multi-scale, multi-physics problem that requires significant computational resources to incorporate a wide range of astrophysical phenomena and interactions.
- Using Pleiades, astronomers at Princeton University are running state-of-the-art 3D adaptive mesh refinement simulations that can, for the first time, follow the formation and evolution of thousands of galaxies simultaneously.
  - The simulations indicate that the earliest galaxies were remarkably mature, containing metals, dust, and a significant number of old stars.
  - Simulation results are in excellent agreement with observations from the Hubble Space Telescope (HST).
  - Predictions made by the simulations can be used to help guide further NASA observations by HST and the upcoming James Webb Space Telescope.
- Together, the Pleiades and Endeavour supercomputers provide the large-scale parallel cluster needed to perform the simulations and the shared-memory architecture for post-simulation data mining.

Mission Impact: State-of-the-art simulations made possible by HECC supercomputing resources enable astronomers to gain deep understanding of the formation and evolution of galaxies and the intergalactic medium—a central problem in the field of cosmology.



Visualization showing an edge-on projection of gas density in the inner 14-kiloparsec (kpc) region of a simulated galaxy. Dense clumps and filaments seen above the galactic plane are a clear indication of strong outflows. The rate of outflow measured through planes parallel to the disk at 5 kpc is comparable to the star formation rate (about three solar masses per year).

POC: Renyue Cen, cen@astro.princeton.edu, (609) 258-3806, Princeton University

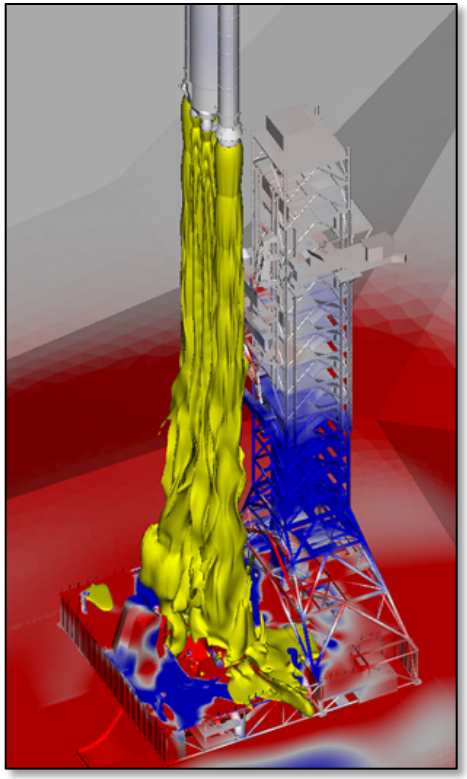
** HECC provided supercomputing resources and services in support of this work*

Computational Fluid Dynamics (CFD) Support for Space Launch Vehicles *

- Scientists in the NAS Division are running high-fidelity CFD simulations to support the design of next-generation space launch vehicles and launch environments.
- Enabled by Pleiades, these CFD simulations produce results for a large number aerodynamic performance databases and pad configurations possible before.
  - Launch vehicle aerodynamics simulations are conducted over the entire ascent trajectory.
  - Solid rocket booster separation simulations are used to assess the potential of re-contact between the boosters and core stage to ensure safe separation.
  - Launch environment simulations of ignition over-pressure and acoustic phenomena during liftoff ensure vehicle stability, payload safety, and pad durability for heavy-lift vehicles.
- Simulation results have provided critical data during two design analysis cycles of the Space Launch System.

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

Mission Impact: HECC supercomputing resources enable fast and efficient turnaround times for CFD simulations of space vehicles and launch environments, at minimal cost to the agency.



Computational fluid dynamics simulation of a Space Launch System drift scenario with the vehicle plume impinging on the launch tower and platform. This simulation was used to provide engineers with unsteady pressure forces to assist in the redesign of the tower and "umbilical" hardware.

POC: Cetin Kiris, cetin.c.kiris@nasa.gov, (650) 604-4485, Michael Barad, michael.f.barad@nasa.gov, (650) 604-0550, NASA Ames Research Center

HECC Facility Hosts Several Visitors and Tours in February 2014

- HECC hosted three tour groups in February. Guests learned about the agency-wide missions being supported by Pleiades, and viewed scientific results on the hyperwall system. Visitors this month included:
  - Amber Harmon, U.S. desk editor, International Science Grid this Week, visited Ames for an interview with Rupak Biswas to discuss the quantum computing project. She also visited the NAS facility for an overview and hyperwall-2 demonstration.
  - A group of students participating in the NASA Spring Intern program visited the facility as part of their NASA Ames tour. These students are majoring in science, technology, engineering & mathematics (STEM) fields at universities across the U.S.
  - A group from In-Q-Tel (D-Wave System investors) and some of their U.S. government partners toured the quantum computing room and received an overview of the facility, including a hyperwall-2 demonstration.

Bryan Biegel, NAS deputy division chief, presented scientific results on the hyperwall-2 to STEM students from major universities across the country who are participating in the NASA Spring Intern program.

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

Papers and Presentations

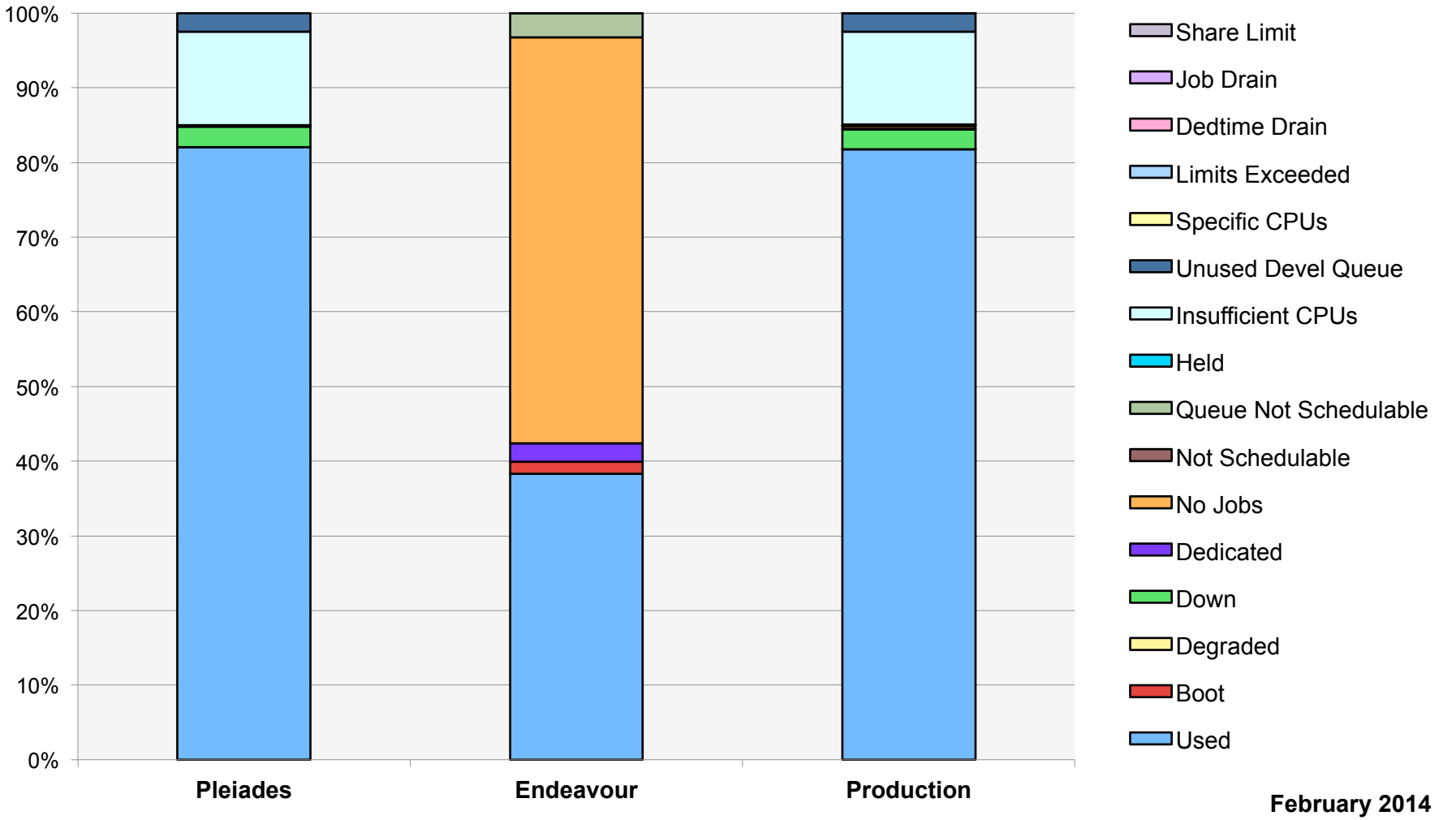
- "**Electromagnetic Energy Conversion in Downstream Fronts from 3D Kinetic Reconnection**," G. Lapenta, M. Goldman, D. Newman, S. Markidis, A. Divin, arXiv: 1402.0082 [physics.plasm-ph], February 1, 2014. * *http://arxiv.org/abs/1402.0082*
- "**Spatial Growth of the Current-Driven Instability in Relativistic Jets**," Y. Mizuno, P. E. Hardee, K.-I. Nishikawa, arXiv:1402.2370 [astro-ph.HE], February 11, 2014 * *http://arxiv.org/abs/1402.2370*
- "**Radiation Magneto-hydrodynamic Simulations of the Formation of Hot Accretion Disk Coronae**," Y.-F. Jiang, J. M. Stone, S. W. Davis, arXiv:1402.2979 [astro-ph.HE], February 12, 2014. * *http://arxiv.org/abs/1402.2979*
- "**Challenges in Supporting Big Data Analytics at the NASA Advanced Supercomputing (NAS) Division**," P. Mehrotra, L. H. Pryor, presented at the Workshop on Big Data and Extreme Computing (BDEC), Fukuoka, Japan, February 27, 2014. *http://www.exascale.org/bdec/sites/www.exascale.org.bdec/files/whitepapers/mehrotra.pdf*

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

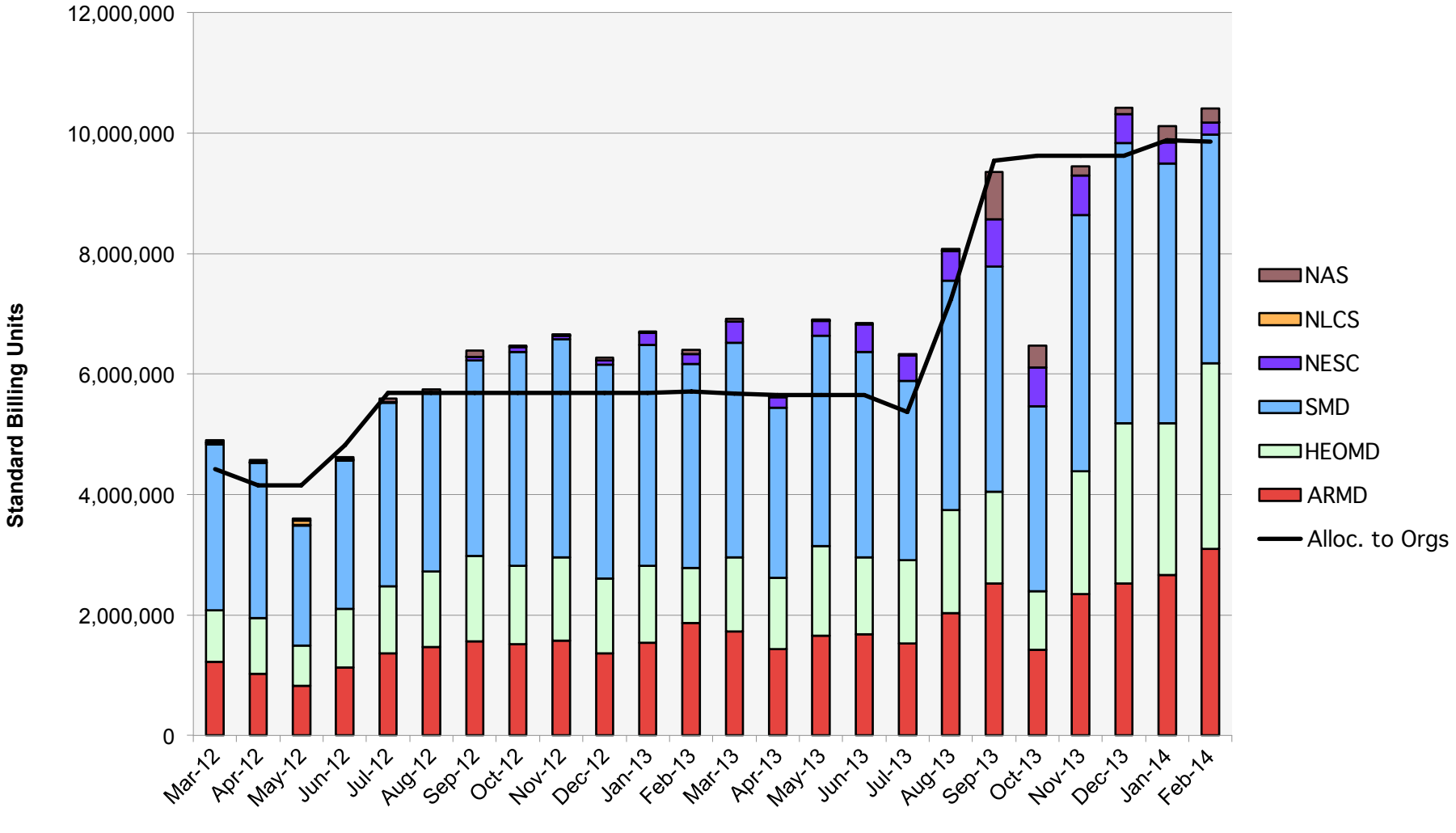
News and Events

- **A Brave New Ocean World**, *Oceans at MIT*, February 14, 2014—MIT's Department of Earth, Atmospheric, and Planetary Sciences spotlights a detailed visualization of ocean behavior from the output of the highest-ever resolution run of a global ocean model, which was processed using the Pleiades supercomputer.
  http://eaps-www.mit.edu/paoc/about/spotlights/brave-new-ocean-world
- **The Quantum Quest for a Revolutionary Computer**, *Time Magazine,* February 17, 2014—This cover article describes how quantum computing uses strange subatomic behavior to exponentially speed up processing; however, it could be a revolution or wishful thinking. Dr. Rupak Biswas is quoted in the article.
  http://time.com/4802/quantum-leap
- **NASA's IRIS Spots Its Largest Solar Flare**, *NASA*, February 21, 2014—NASA's Interface Region Imaging Spectrograph (IRIS) mission, which utilizes the Pleiades supercomputer to carry out numerical simulations, witnessed an M-class solar flare in late January, the largest flare the spacecraft viewed since its launch June 2013. Picked up by *Space Daily* and other media sources.
  http://www.nasa.gov/content/goddard/nasas-iris-spots-its-largest-solar-flare/index.html
- **NASA Helps Growers During California's Drought**, *NASA,* February 25, 2014—NASA discusses plans to use Earth satellite imaging, including the NASA Earth Exchange project database, which utilizes HECC resources at the NASA Advanced Supercomputing facility, to address the expected water shortage to California farmers.
  http://www.nasa.gov/ames/nasa-helps/growers-during-californias-drought

HECC Utilization



HECC Utilization Normalized to 30-Day Month



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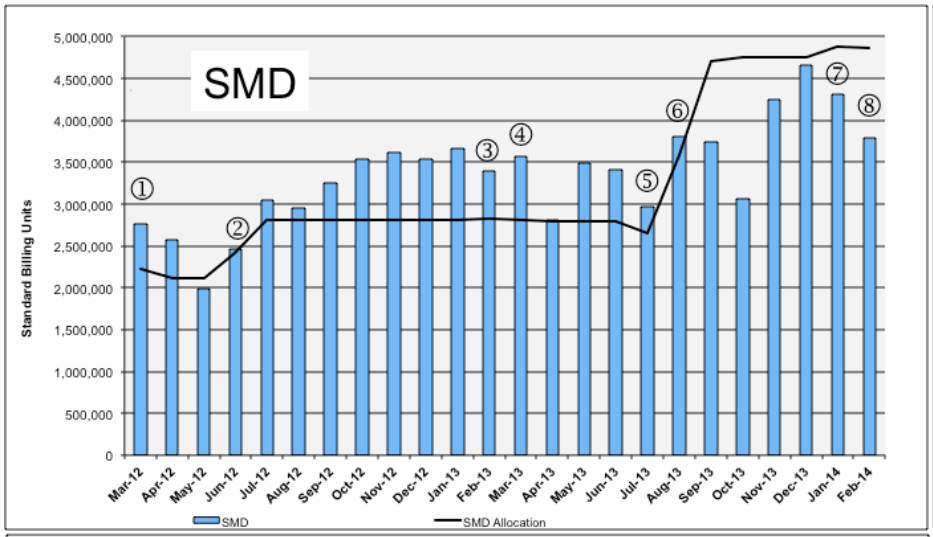
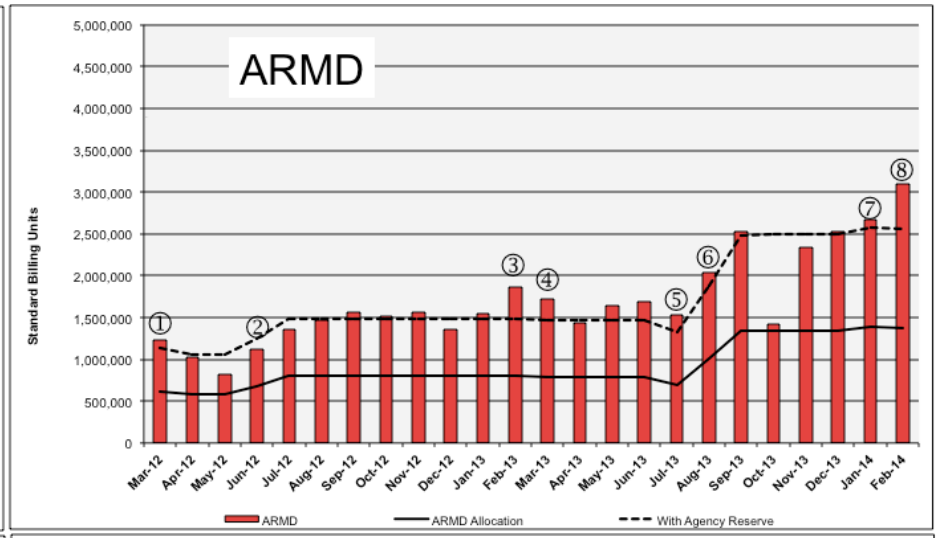
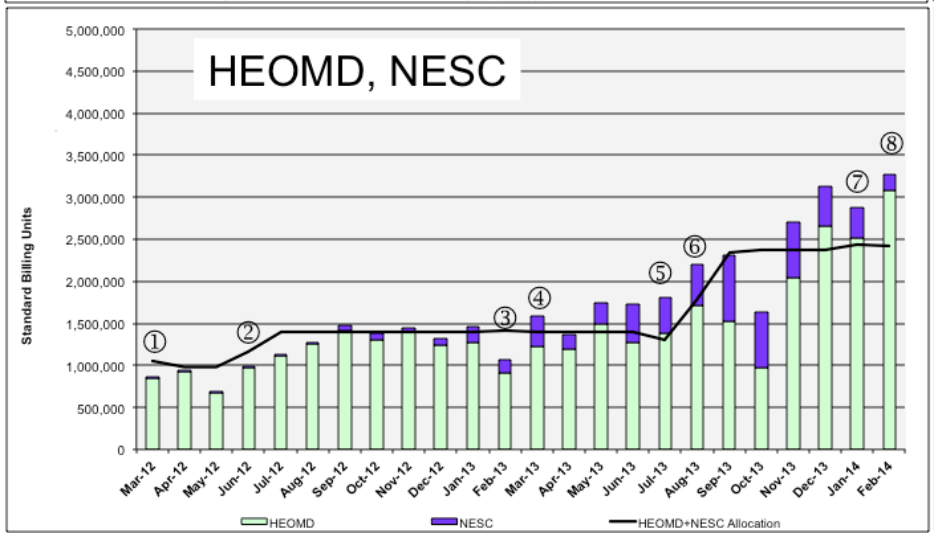






① 28 Harpertown Racks retired

② 24 Sandy Bridge Racks added

③ Columbia 21, 23, and 24 retired, Endeavour 2 added

④ Columbia 22 retired; Endeavour 1 added

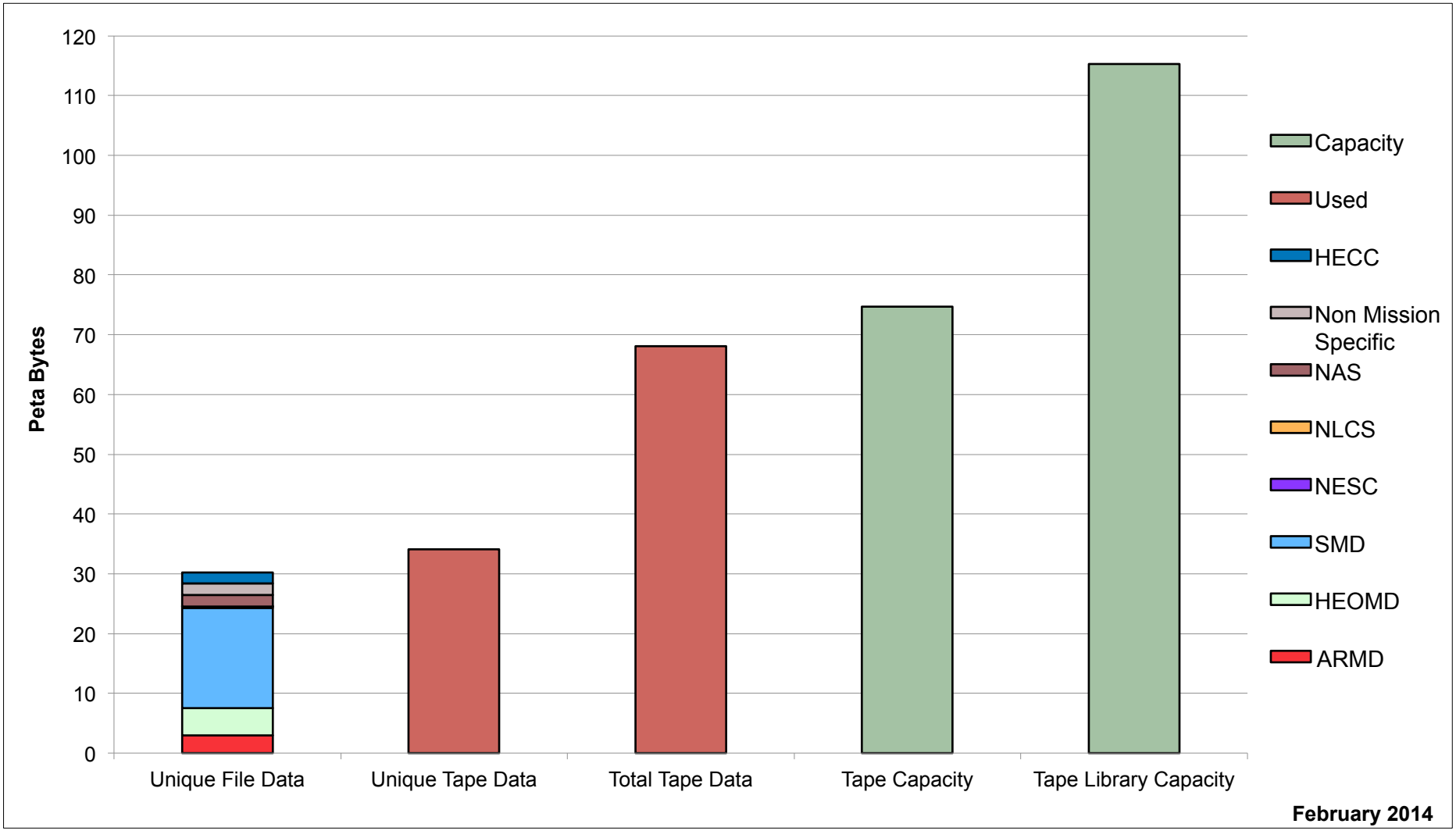
⑤ 32 Harpertown Racks retired

⑥ 32 Harpertown Racks retired; 46 Ivy Bridge Racks added

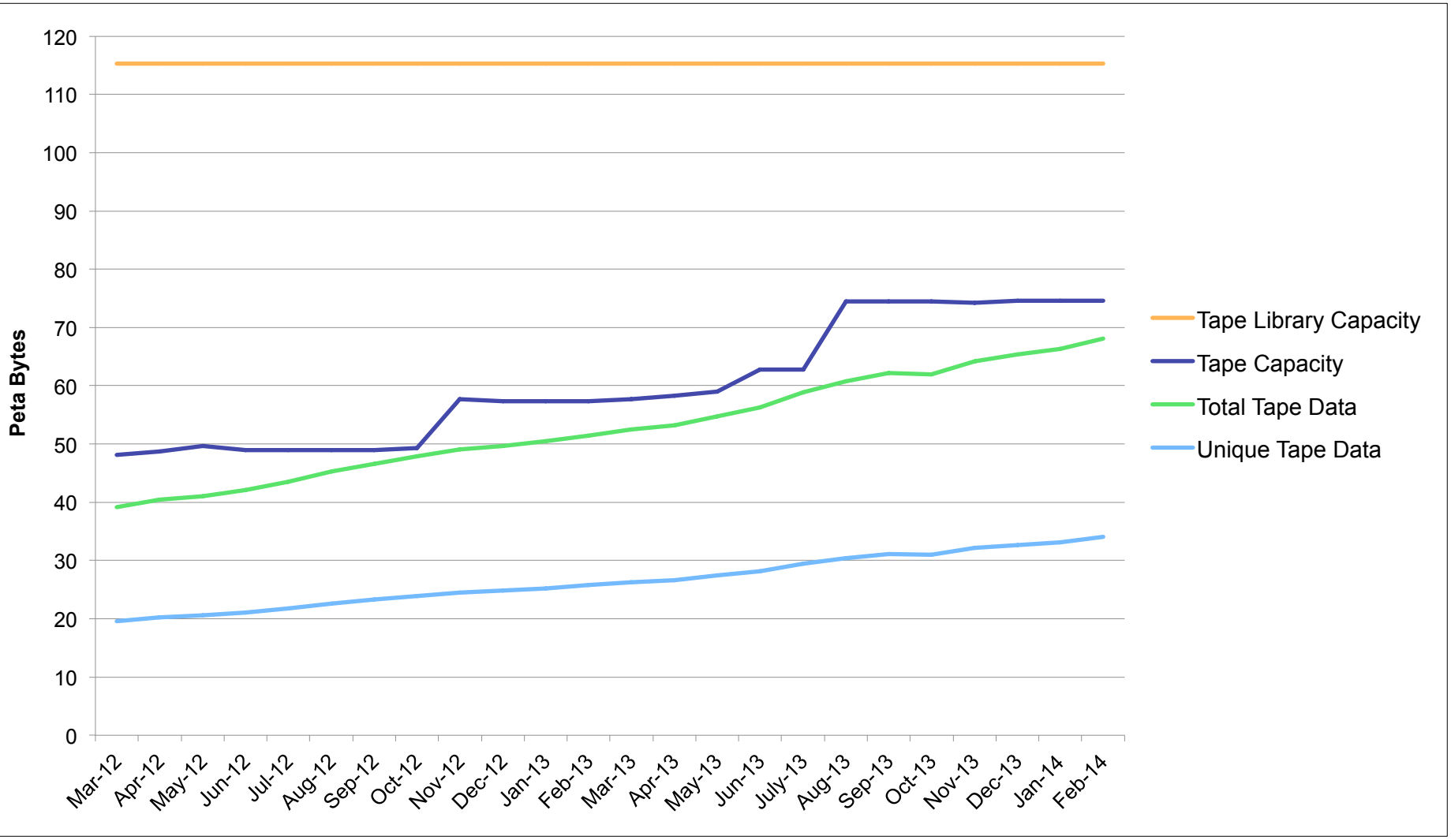
⑦ 6 Ivy Bridge Racks added; 20 Nehalem and 12 Westmere Racks Retired

⑧ 8 Ivy Bridge Racks added mid-Feb; 8 additional Ivy Bridge Racks late Feb.

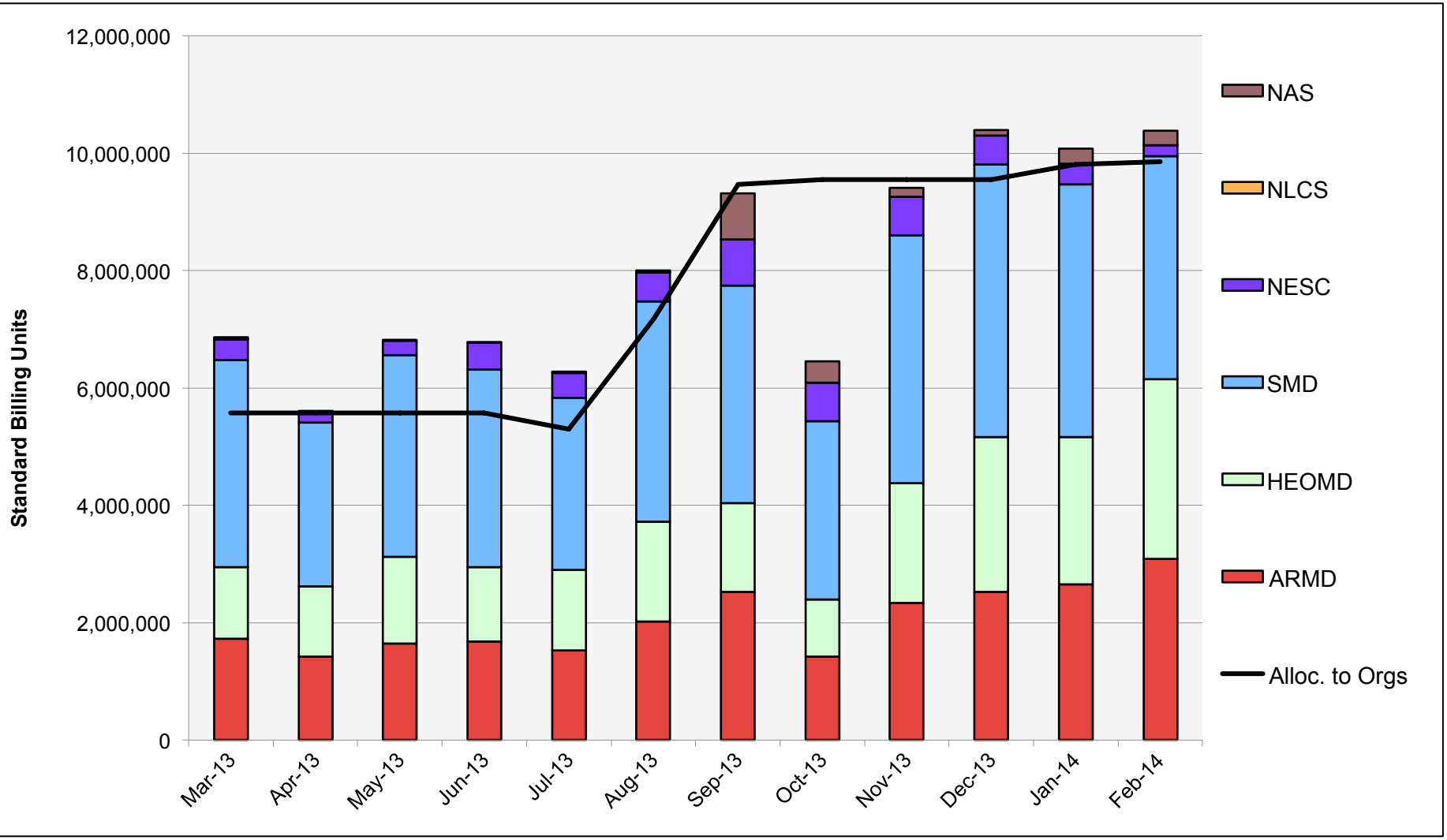
Tape Archive Status



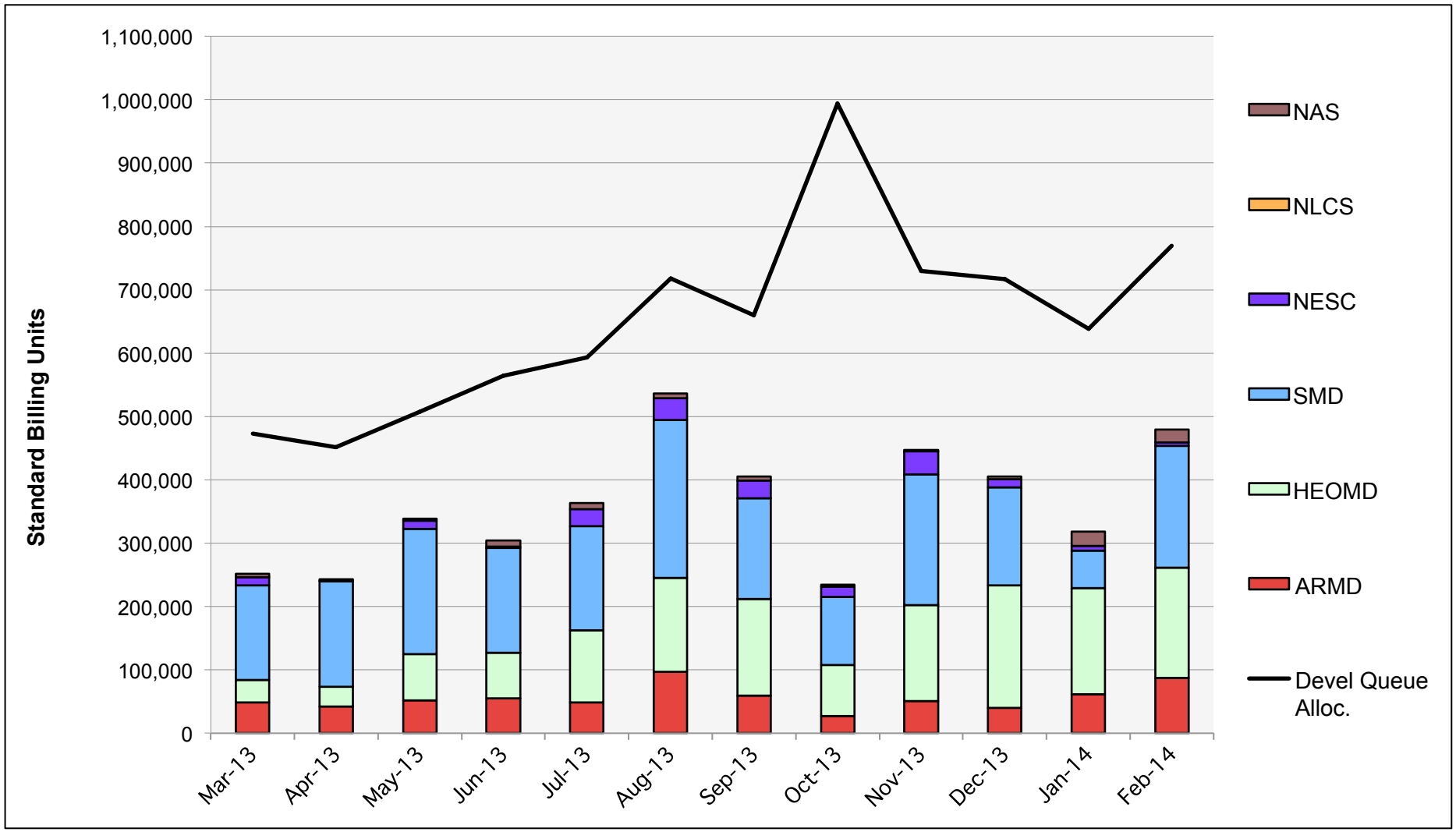
Tape Archive Status



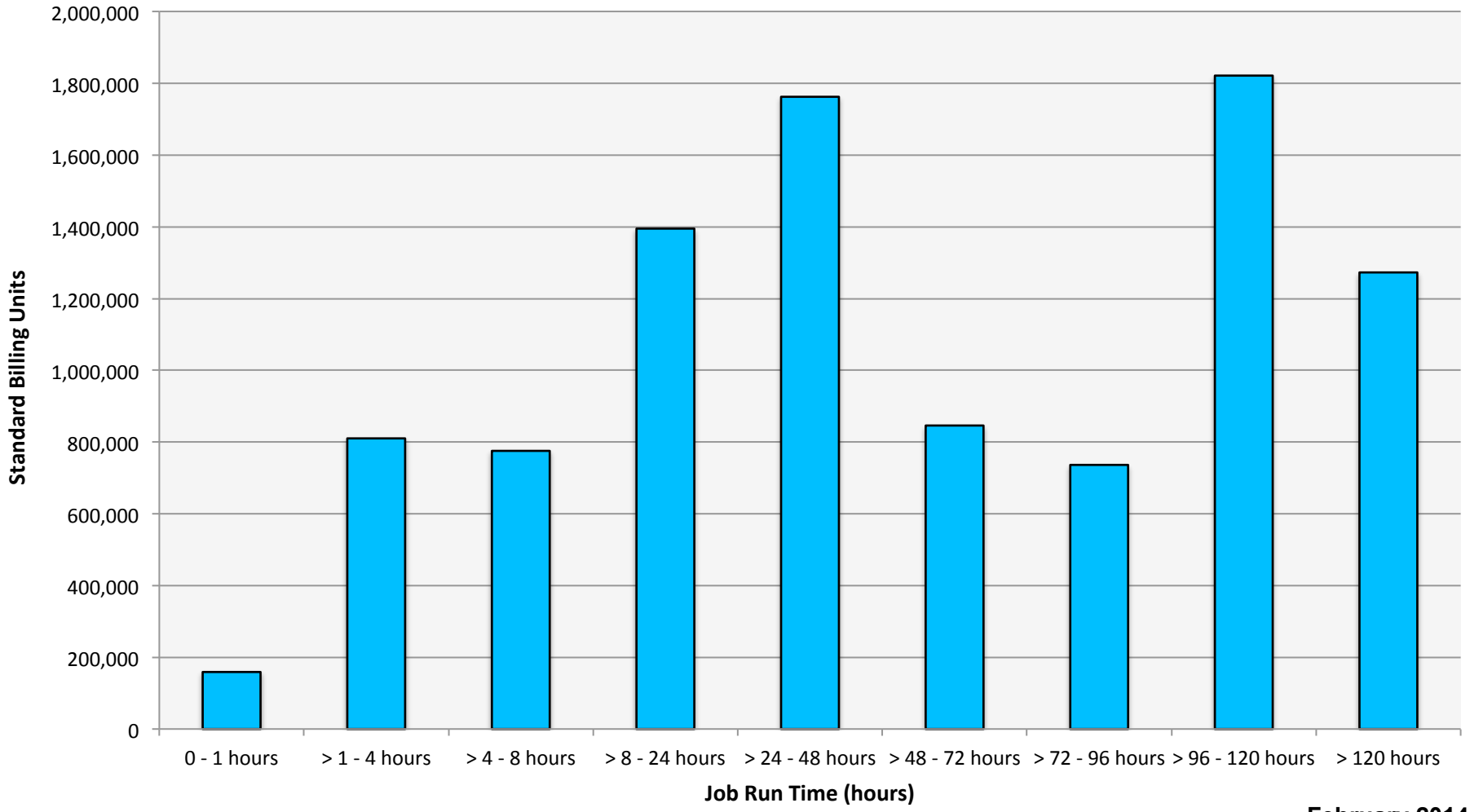
Pleiades:
SBUs Reported, Normalized to 30-Day Month



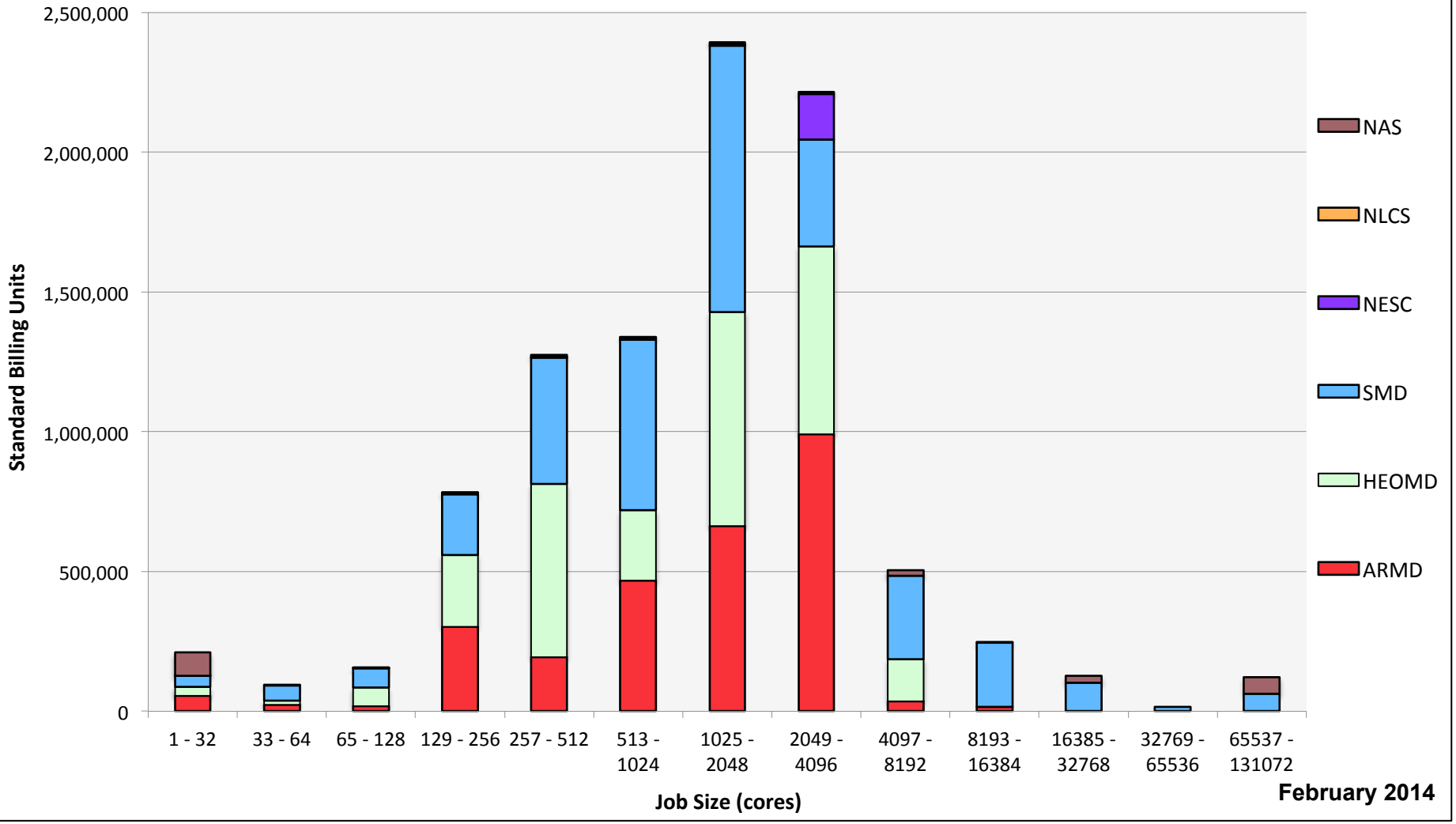
Pleiades:
Devel Queue Utilization



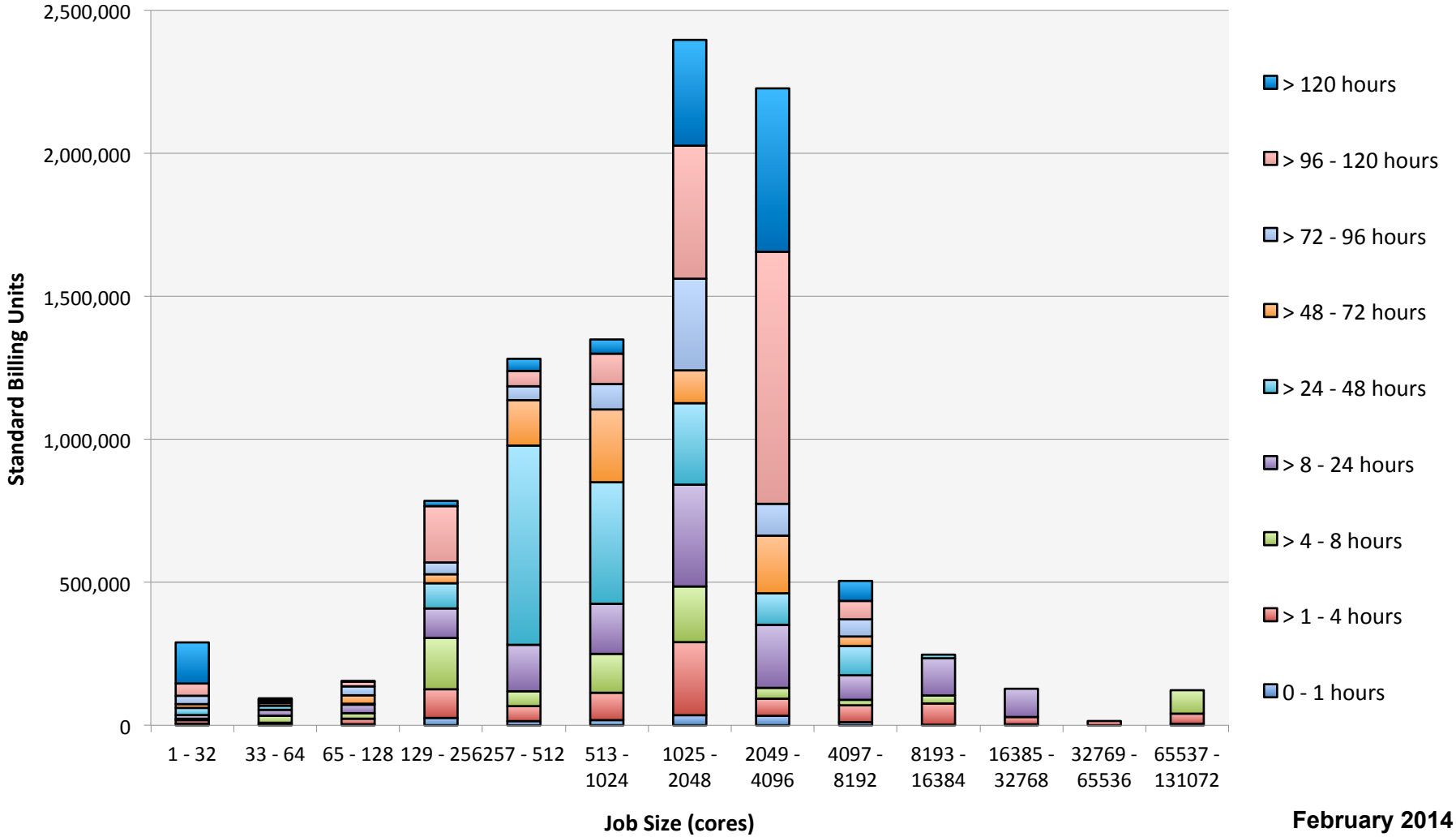
Pleiades:
Monthly Utilization by Job Length



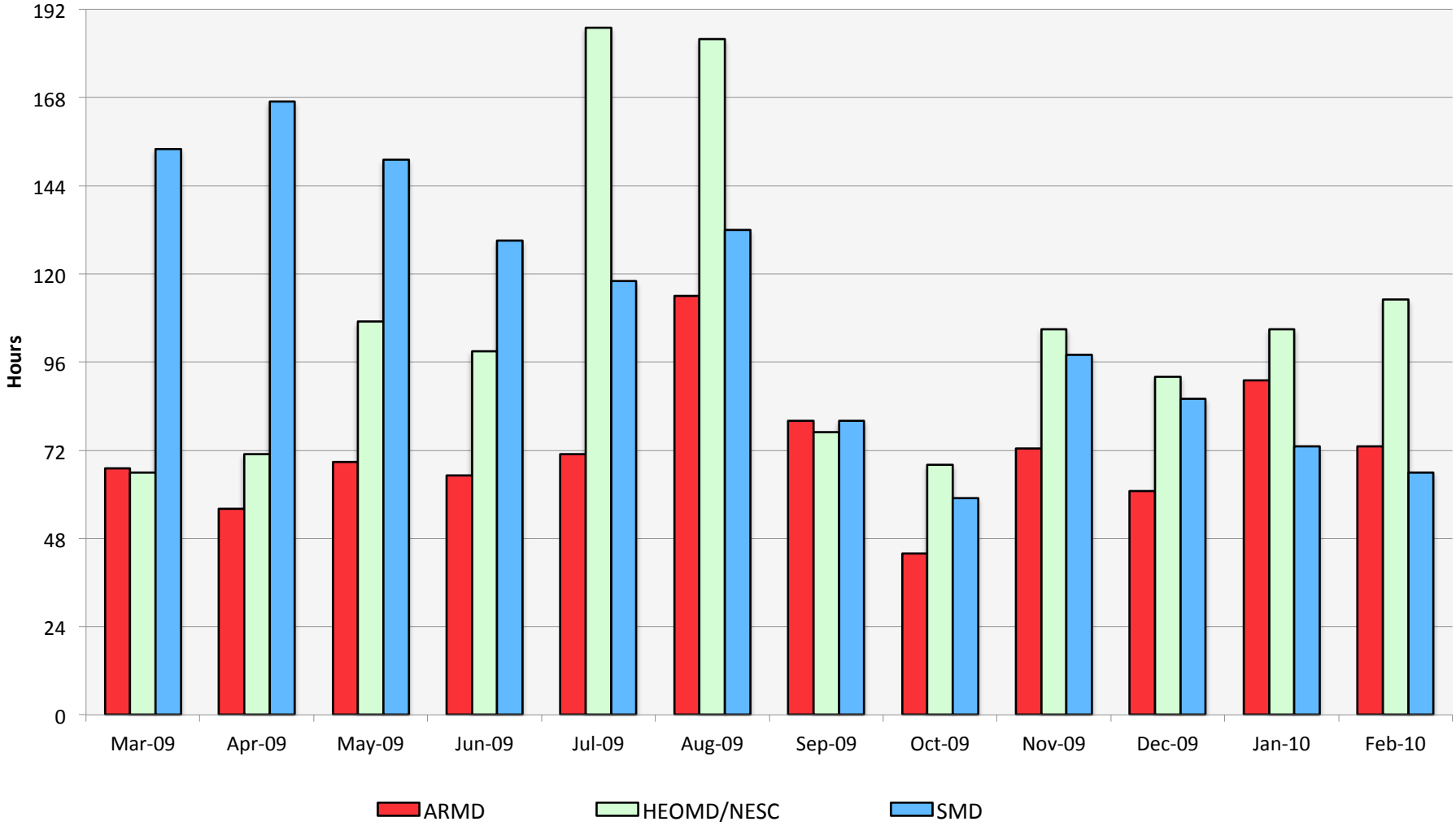
Pleiades:
Monthly Utilization by Size and Mission



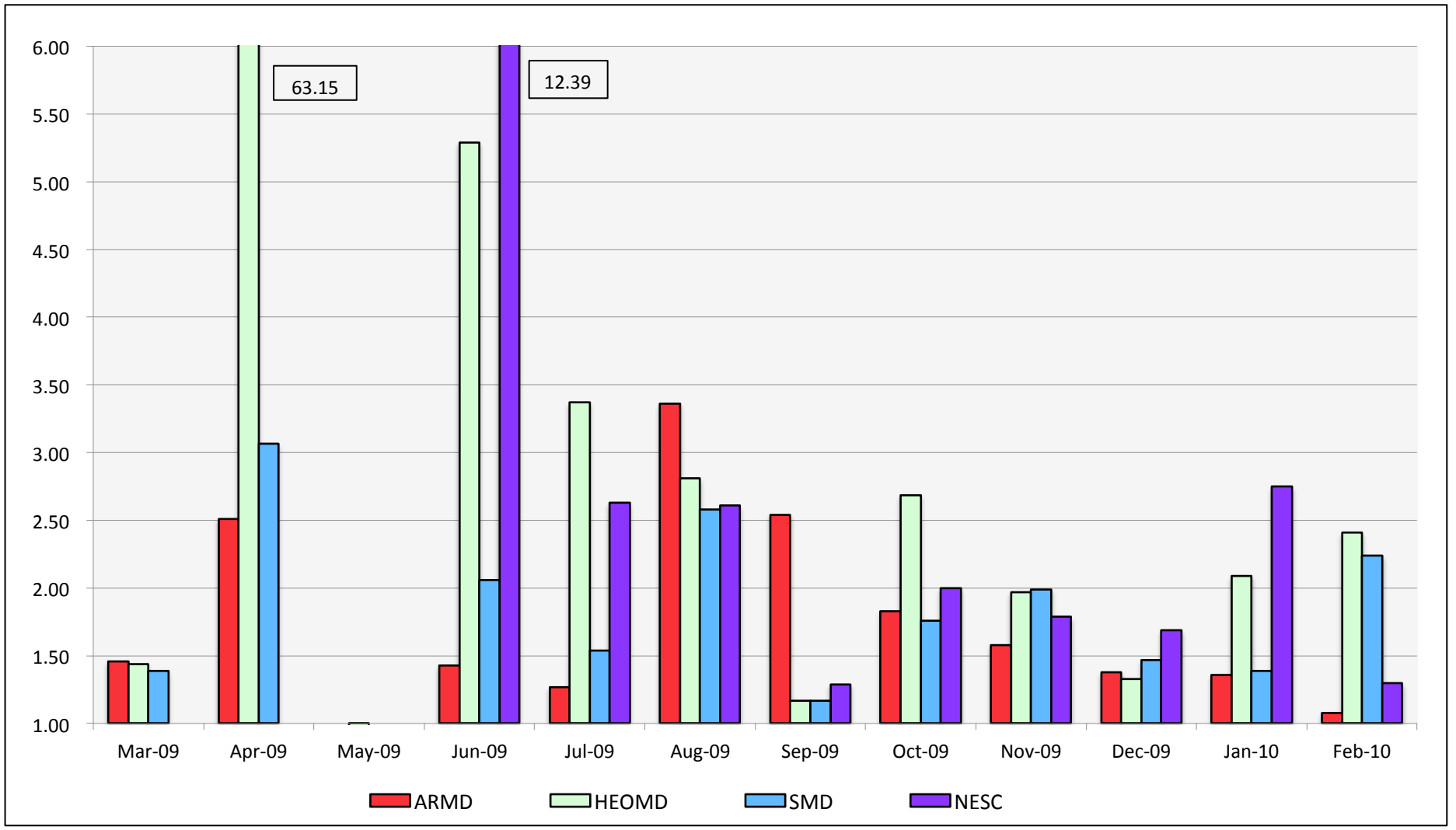
Pleiades:
Monthly Utilization by Size and Length



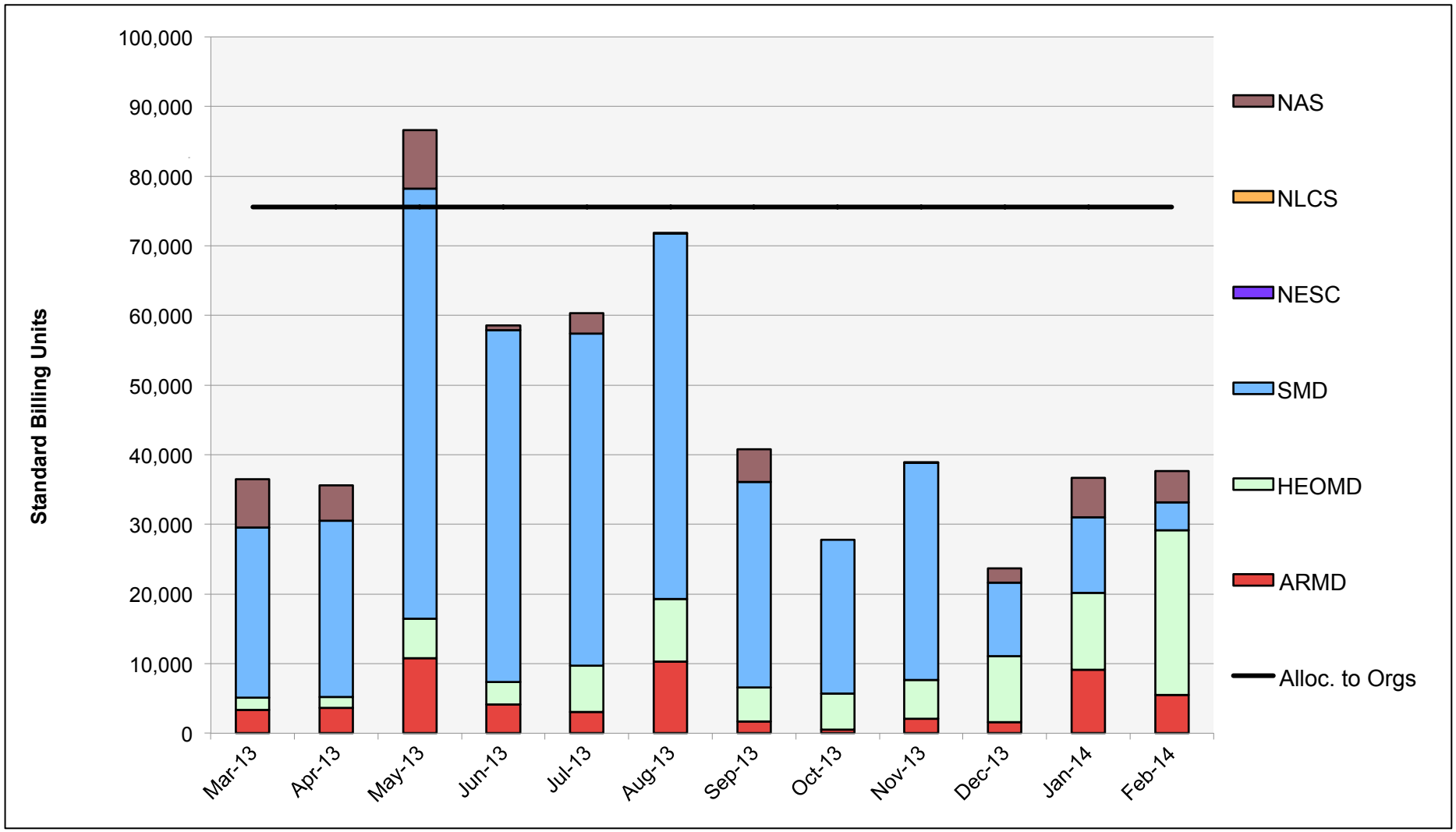
Pleiades:
Average Time to Clear All Jobs



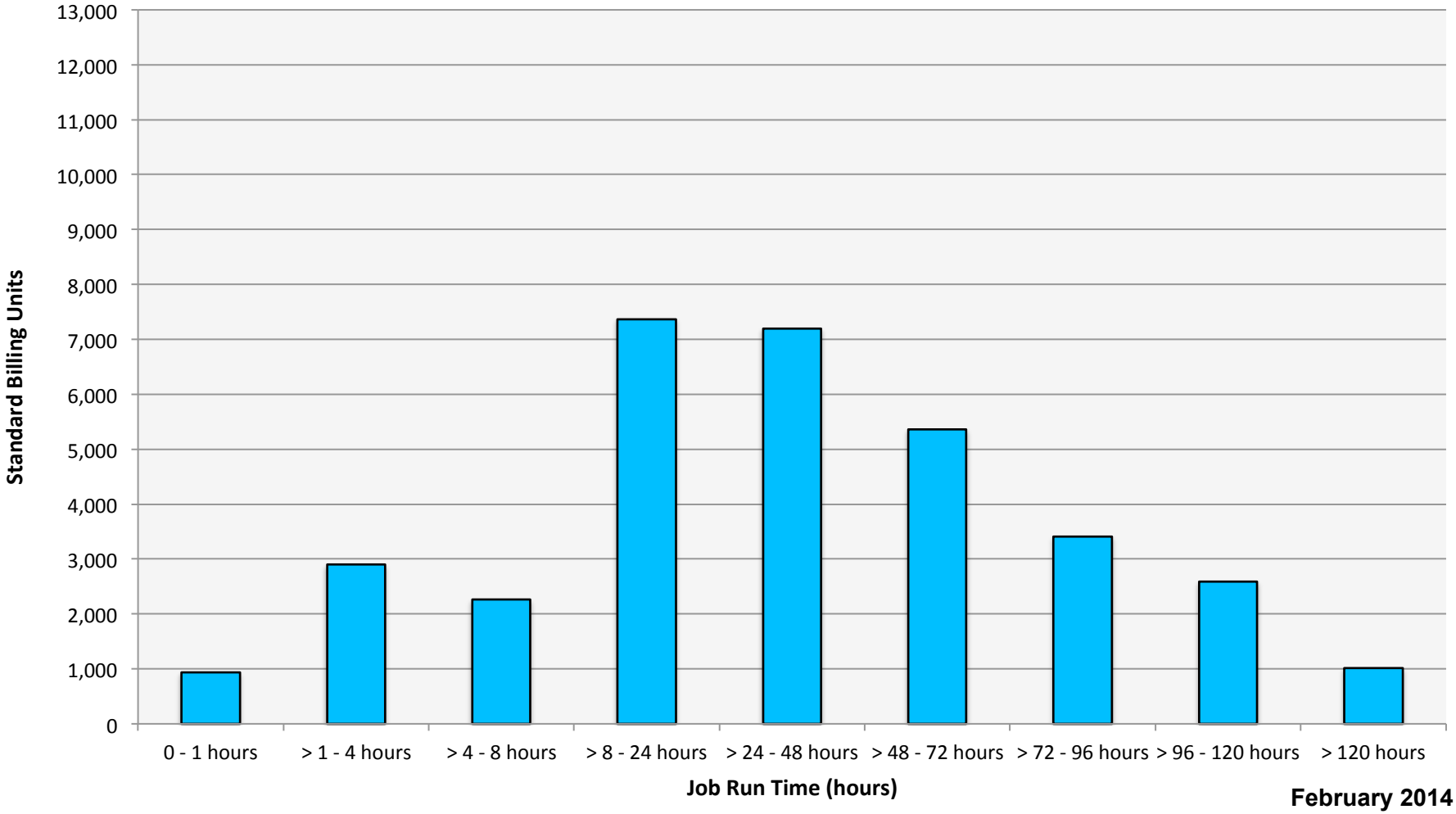
Pleiades:
Average Expansion Factor



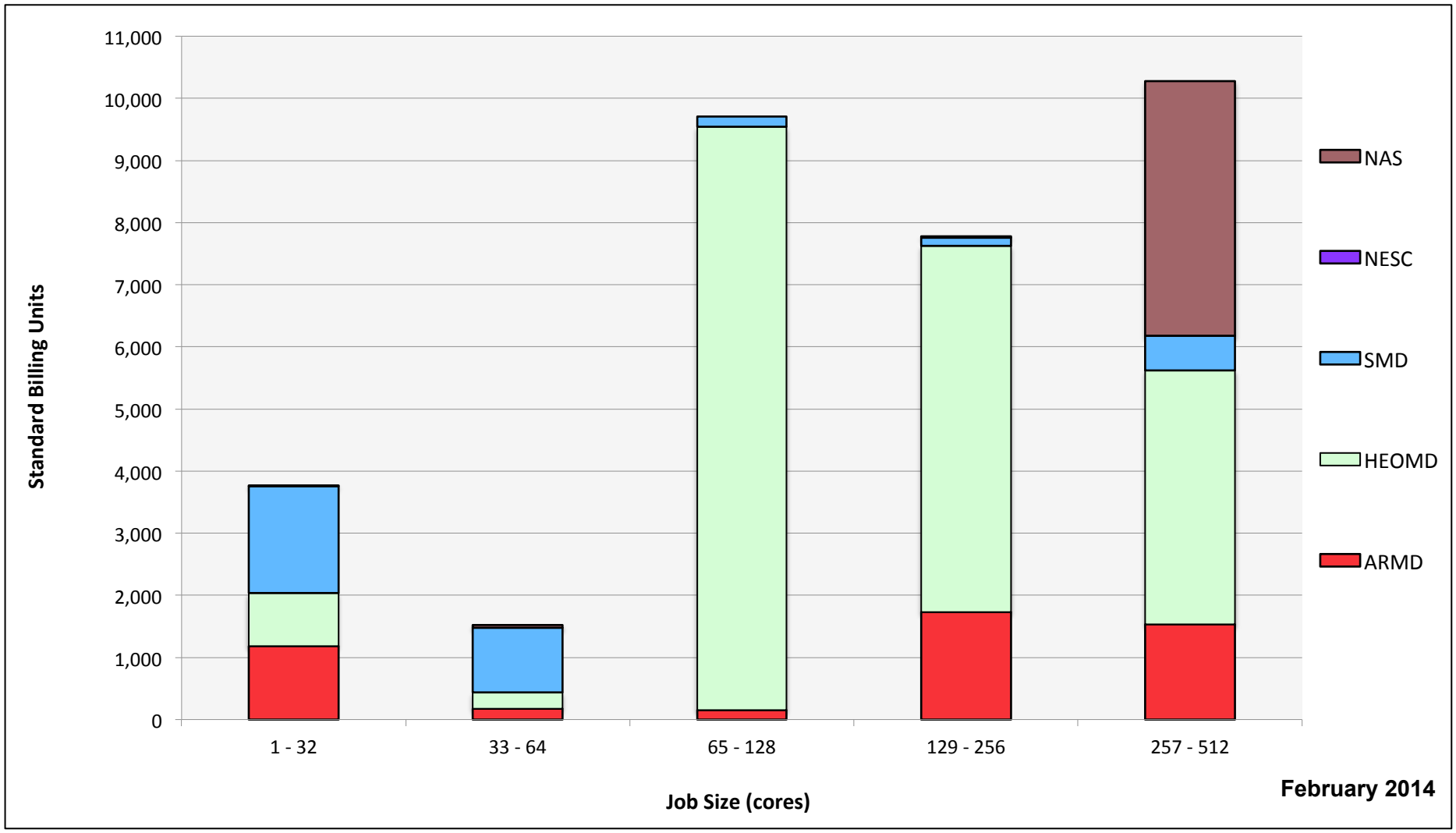
Endeavour:
SBUs Reported, Normalized to 30-Day Month



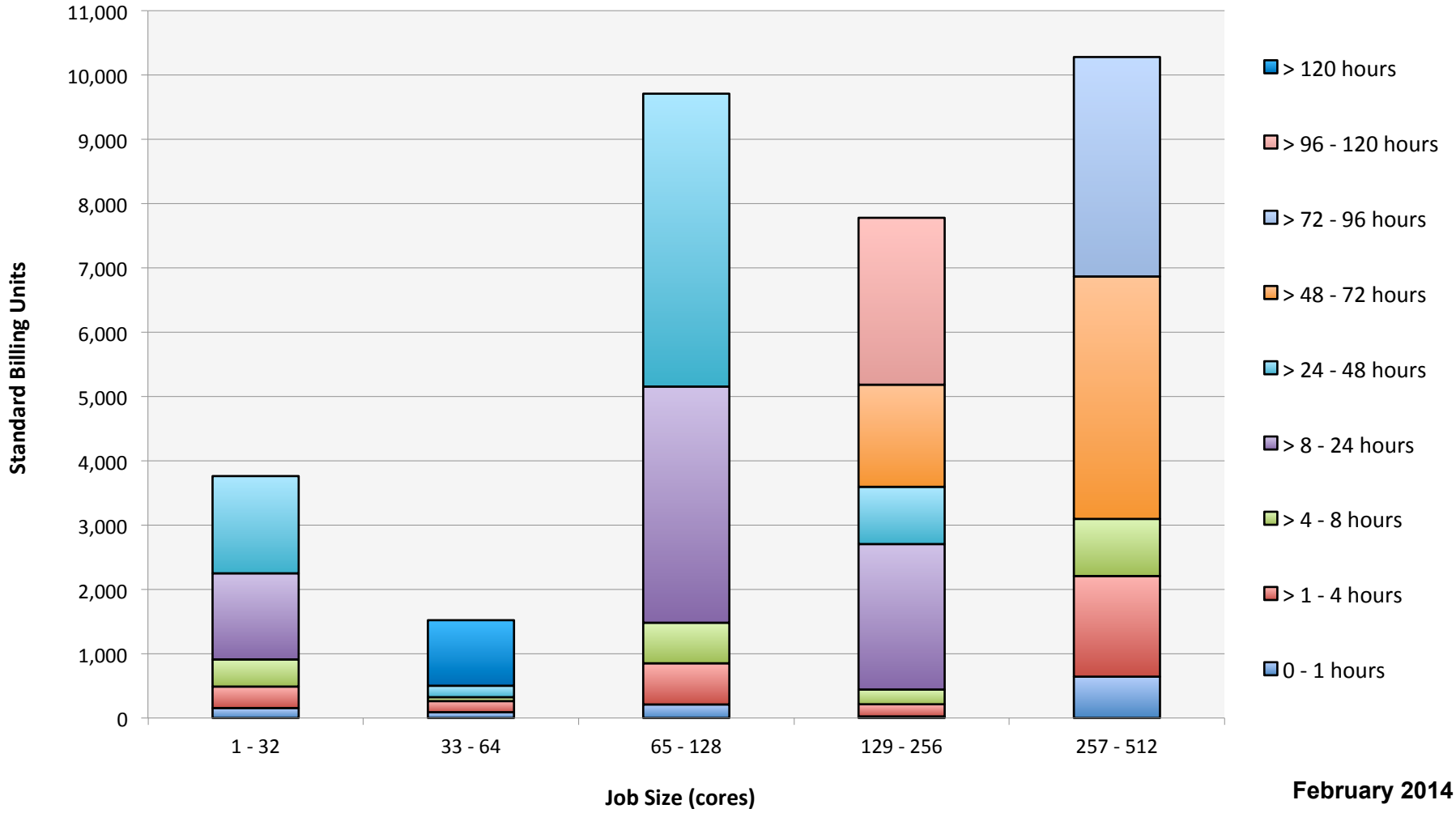
Endeavour:
Monthly Utilization by Job Length



Endeavour:
Monthly Utilization by Size and Mission



Endeavour:
Monthly Utilization by Size and Length



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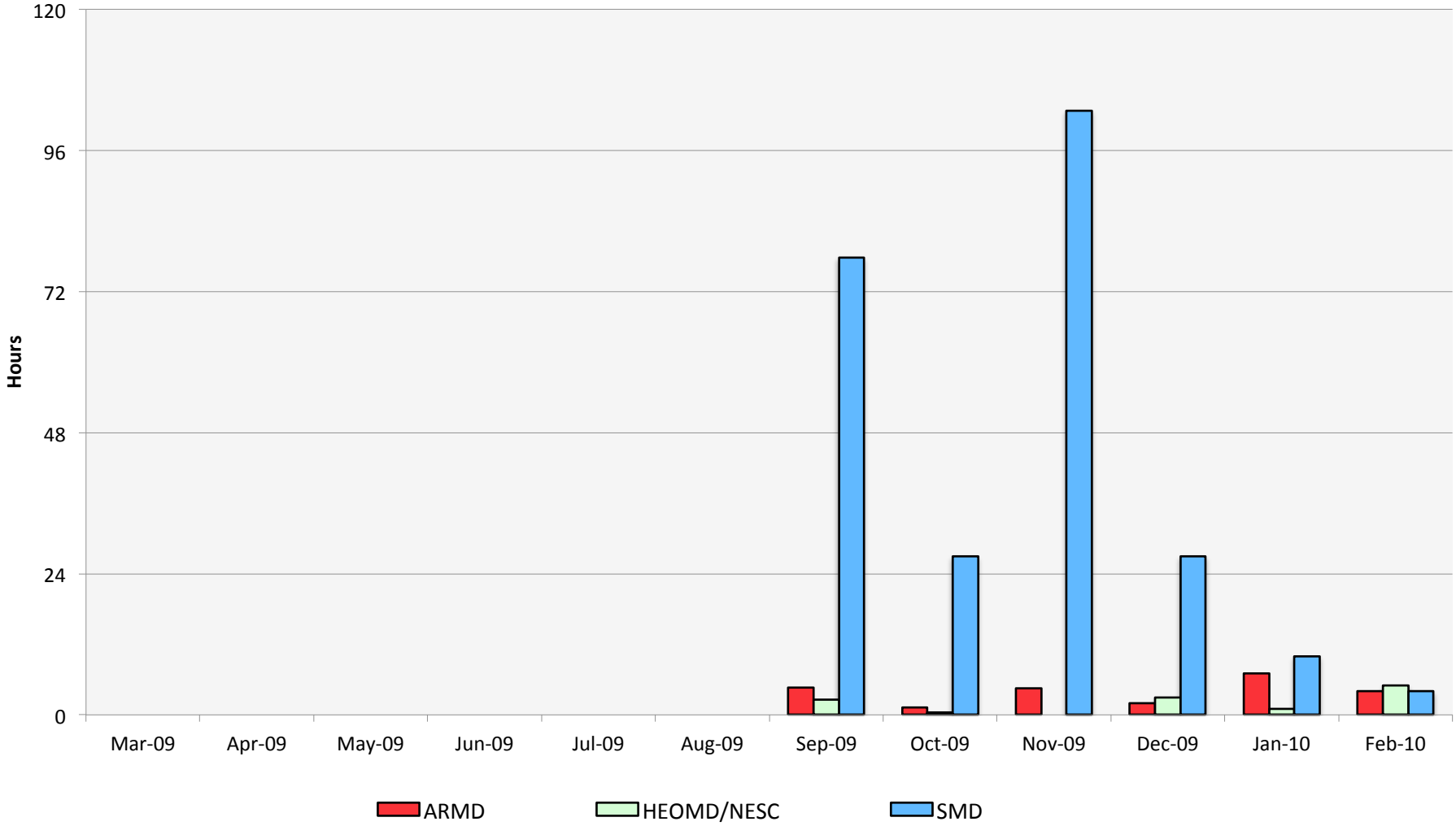
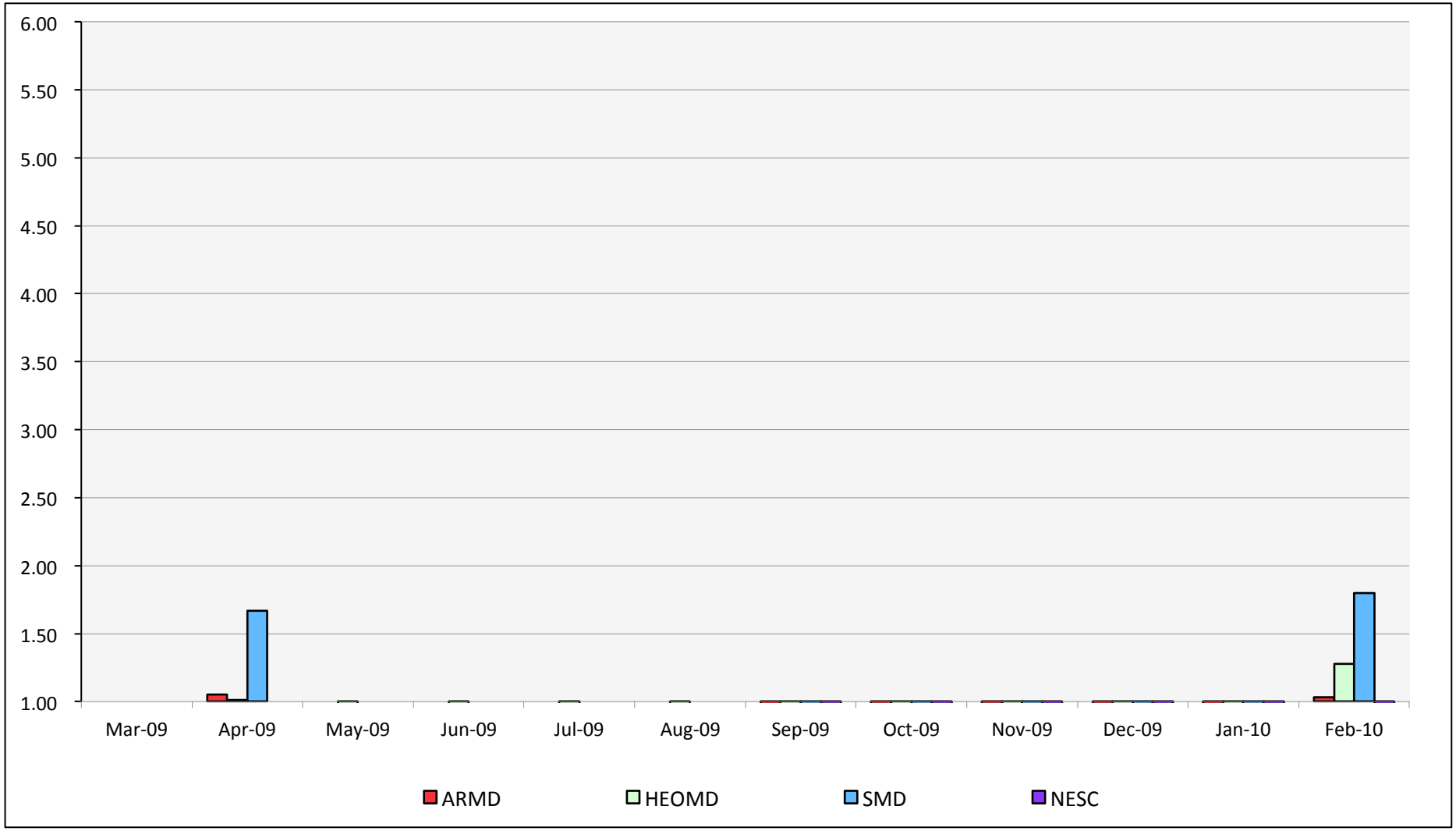
Average Time to Clear All Jobs



Endeavour:
Average Expansion Factor



Maia:
SBUs Reported, Normalized to 30-Day Month