Project Status Report

High End Computing Capability
Strategic Capabilities Assets Program

June 10, 2015

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Intel Phi Nodes Available to HECC Users

- HECC engineers upgraded the Pleiades supercomputer with 32 Sandy Bridge nodes equipped with Intel Phi processing units (that came from the Maia system) for availability for the user community.
- The 32 Sandy Bridge nodes each contain 64 gigabytes (GB) of memory, and two Intel Phi processing units.
- The Intel Phi processing units, along with the NVIDIA Tesla K40 graphics processing unit (GPU) nodes that were deployed in April 2015, enable HECC users to test and evaluate the accelerators as a method to enhance the performance of their scientific applications.

Mission Impact: The addition of accelerator processing units enables NASA users to utilize new technology to speed up their demanding scientific applications running on HECC resources.

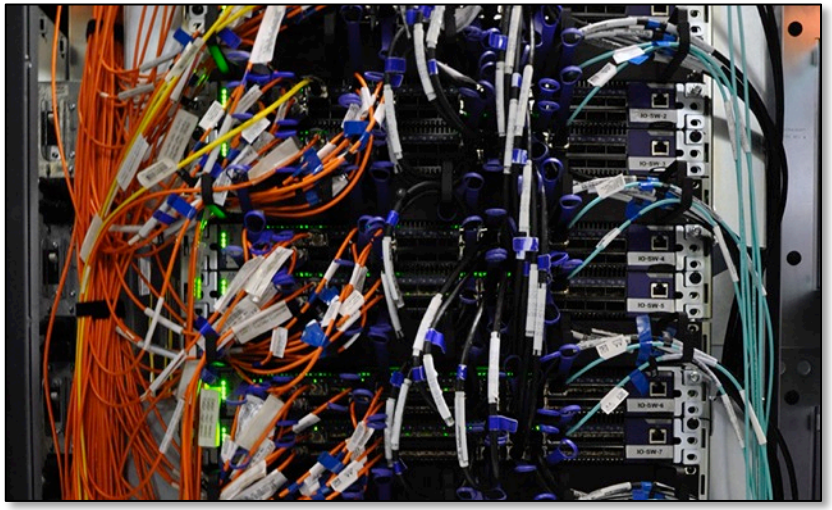
The Pleiades supercomputer's Sandy Bridge nodes, equipped with Intel Phi processing units, were integrated from a testbed system that was known as Maia.

POCs: Bob Ciotti, bob.ciotti@nasa.gov, (650) 604-4408, NASA Advanced Supercomputing (NAS) Division; Davin Chan, davin.s.chan@nasa.gov, (650) 604-4613, NAS Division, Computer Sciences Corp.

HECC Engineers Improve InfiniBand Stability

- HECC engineers resolved an InfiniBand (IB) issue that adversely impacted user job runs on Pleiades.
- The team, with support from vendors Mellanox and SGI, gathered and analyzed debugging information about an IB packet loss caused by packets being placed on the incorrect service levels for Quality of Service (QoS). The problem was traced to a firmware bug in the IB cards on the system.
- This troubleshooting effort took a significant amount of time, as initially it was not thought that the firmware could fail in this manner. But with detailed testing and validation, the issue was confirmed.
- Once the problem was correctly identified, Mellanox staff quickly provided a new firmware update to address it.

Mission Impact: Ensuring a stable I/O fabric is essential for providing reliable high-performance computing resources to NASA users.



The InfiniBand fabric on Pleiades utilizes Quality of Service (QoS) software to prioritize the level of service for InfiniBand packets, in order to improve responsiveness of network traffic within Pleiades.

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New Tools for Visualization of Cart3D Data Enable Rapid, Flexible Analyses

- HECC visualization experts released three new applications for the analysis of Cart3D data on Pleiades.
- The new apps improve on previous tools since they work with Cart3D data directly, with no resampling or preprocessing required.
- The new applications are:
  - **cutcart**: samples data on cutting planes.
  - **isocart**: generates isosurfaces from adaptive mesh refinement (AMR) "cell-centered" data.
  - **raycart**: produces ray-cast images with flexible control over fields for integration and image quality.
- The Cart3D team's initial interest in the raycart app was motivated by the need for shadowgraph visualizations.
  - Previous workflow for shadowgraphs involved a slower application with less flexibility and control.
- Flexibility in choice of field, including built-in support for standard Plot3D derived fields, means that raycart may have great utility in future analyses where ray integration through a simulation domain is required.

Mission Impact: Cart3D users in multiple mission directorates have employed HECC's new analysis applications in support of the Space Launch System and planetary protection missions.

A new HECC in-house ray-casting application, called raycart, enables scientists without visualization expertise to quickly produce quality visualizations on their own. This image shows the magnitude of the velocity cross vorticity field in a Cart3D simulation of a four-piece meteor fragmentation, moving at Mach 60. *Marian Nemec, NASA/Ames*

POCs: Patrick Moran, patrick.moran@nasa.gov, (650) 604-1660,
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NASA Advanced Supercomputing Division

GRAIL Project Enjoys Impressive Performance Gains with Haswell Migration

- HECC Application Performance and Productivity (APP) staff helped NASA's Gravity Recovery and Interior Laboratory (GRAIL) team migrate their "sfilter" code from the Ivy Bridge nodes to Haswell nodes on Pleiades to achieve multiple wins:
  - Jobs that previously took 4 days on 900 Ivy Bridge nodes completed in 2.2 days on 300 Haswell nodes after switching to a 2015 Intel compiler.
  - The sfilter code spends substantial time in the Intel ScaLAPACK math library. Previously, the GRAIL team used version 11.1.072 of the Intel library that was not Advanced Vector Extensions (AVX)-aware, limited to a maximum of 4 double-precision floating-point operations per clock period. With AVX, these limits increased to 8 and 16 for Ivy Bridge and Haswell nodes, respectively, and made up the bulk of the performance improvement.
  - Jobs using 900 Ivy Bridge nodes were wide and long enough to frequently encounter system issues during job runs. Switching to just 300 Haswell nodes decreased the probability of encountering a system issue, and still satisfied the memory requirements of the code. Fewer nodes also translated to fewer off-node MPI communications—another factor in the performance boost.
  - The 4-day long job on Ivy Bridge nodes consumed 218,000 Standard Billing Units (SBUs)* per run. The faster jobs on Haswell nodes consumed 53,000 SBUs per run, and will yield a savings of 2.47 million SBUs over 15 runs.

**1 SBU equals 1 hour of a Pleiades Westmere 12-core node*

Mission Impact: HECC experts improve overall efficiency of systems utilization by mapping user codes to those node types best suited for running specific applications, resulting in performance boosts and faster time-to-solution.

The Haswell nodes on the Pleiades supercomputer can perform twice as many floating point operations per cycle and have twice as much memory as the previous generation of Intel processors, making them well-suited for codes that are matrix-algebra-intensive and have a large memory footprint.

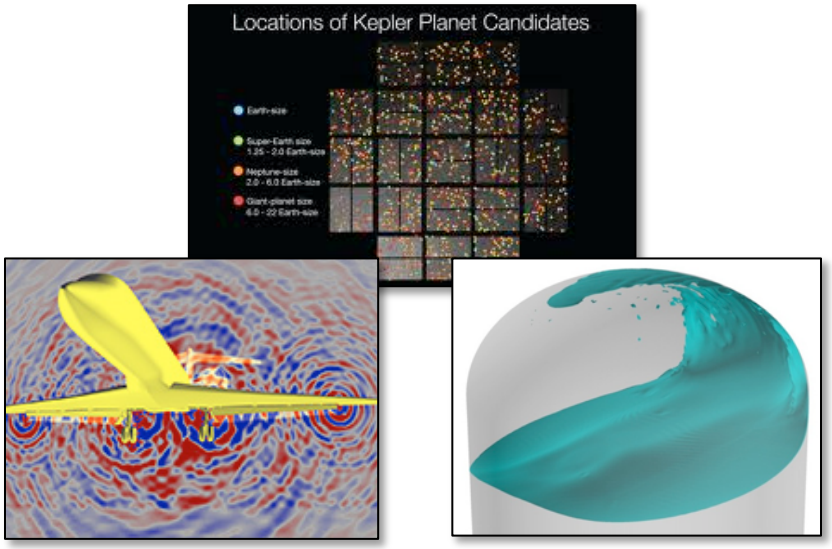
POC: Johnny Chang, johnny.chang@nasa.gov, (650) 604-4356, NASA Advanced Supercomputing Division, Computer Sciences Corp.

May 2015 Usage on Pleiades Sets New Monthly Record of 16.998 Million SBUs

- May usage on the Pleiades supercomputer set a new monthly record.
- 16.998 million Standard Billing Units (SBUs*) were used by NASA's science and engineering organizations, exceeding the previous record of 16.57 million SBUs (set in March 2015) by over 2.5%.
- This increase was enabled by high demand, system stability, and efficient operations that delivered over 83% system utilization (75% utilization is the target).
- Over 330 projects from all across NASA used time on Pleiades during May.
- The top 10 projects used from 383,880 to 1,425,701 SBUs, and together accounted for over 41% of total usage.
- The HECC Project continues to plan and evaluate ways to address the future requirements of NASA's users.

** 1 SBU equals 1 hour of a Pleiades Westmere 12-core node*

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



Images from projects that were among the top users in their respective Mission Directorates. Clockwise from bottom left: Simulated radiated sound field produced by a full-scale Gulfstream aircraft during landing. *E. Fares, Exa Corporation, P. Moran, NASA/Ames*; Kepler's planet candidates; *Kepler Science Team*; High-fidelity computational fluid dynamics simulation showing free surface waves for a high slosh amplitude inside a propellant tank. *H. Q. Yang, Jeff West, NASA/Marshall.*

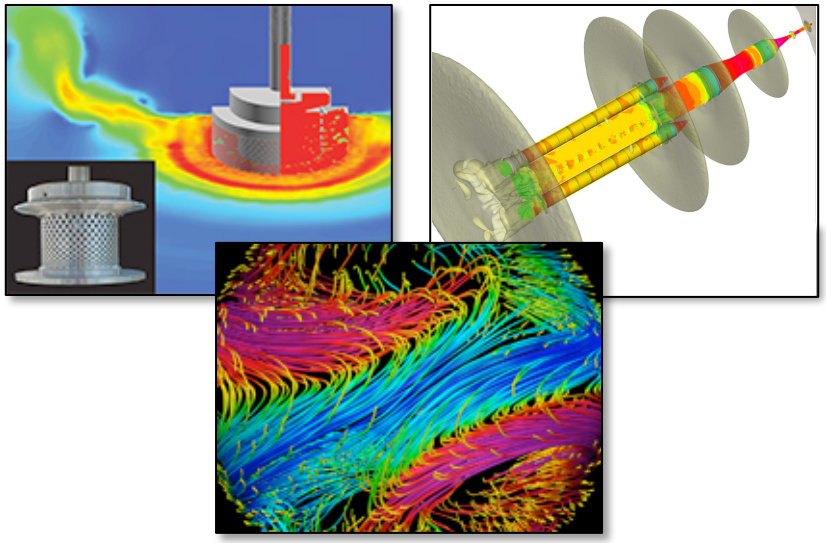
POC: Catherine Schulbach, catherine.h.schulbach@nasa.gov, (650) 604-3180, NASA Advanced Supercomputing Division

New Allocation Period Begins for NASA Mission Directorates

- May 1 marked the beginning of a new allocation period for the Human Exploration and Operations Mission Directorate (HEOMD), the NASA Engineering and Safety Center (NESC), and about half of the Science Mission Directorate (SMD).
- These organizations awarded new allocations of computing time on Pleiades and Endeavour to 275 computing projects.
- Combined awards exceeded 105 million Standard Billing Units* (SBUs) — an 11% increase over 2014.
- Requests for time from HEOMD and NESC were 125% of available time, and requests for time from SMD were more than 300% of available time.
- The new allocation period is an opportunity for each organization to assess demands for computing time and to rebalance allocations to meet computing needs for the next year.

** 1 SBU equals 1 hour of a Pleiades Westmere 12-core node*

Mission Impact: NASA programs and projects periodically review the distribution of supercomputer time to assess the demand for resources and assure consistency with mission-specific goals and objectives.



Representative images of HEOMD, NESC, and SMD projects supported by HECC resources. Clockwise from left: Simulated velocity magnitude contour and hardware of a prototype low-profile diffuser. *J. Brodnick, NASA/Marshall*. Surface pressure coefficient with sonic isosurfaces from an 11,640-processor computation of the transonic flow about a Space Launch System configuration. *S. Alter, NASA/Langley*. Night-side view of magnetic field lines in a simulation of a "hot Jupiter" exoplanet. *T. Rogers, J. Vriesema, University of Arizona.*

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

HECC Supports the 13th Annual SGI User Group Conference

- HECC supercomputing systems and storage experts participated in the 13th Annual SGI User Group (SGIUG) conference. The three-day event was held May 5–7 in Minneapolis.
- The SGIUG conference brought together experts from HPC sites from across the country and the world. The event provided an opportunity for SGI users to interact and share information, as well as to discuss and influence future products from SGI.
- The HECC team presented two session talks on work being done with the PBS batch scheduler and long-distance InfiniBand connectivity on Merope.
- In addition, a HECC team member served as vice-president and program chair for the 2015 conference.

Mission Impact: HECC staff supported NASA's outreach goals through participation at the SGIUG meeting by sharing information with counterparts at other high-performance computing sites.

HECC supercomputing systems experts participated in the 13th Annual SGI User Group Conference, held May 5–7 in Minneapolis. Above, Eng Lim Goh, SGI chief technology officer talks with attendees.

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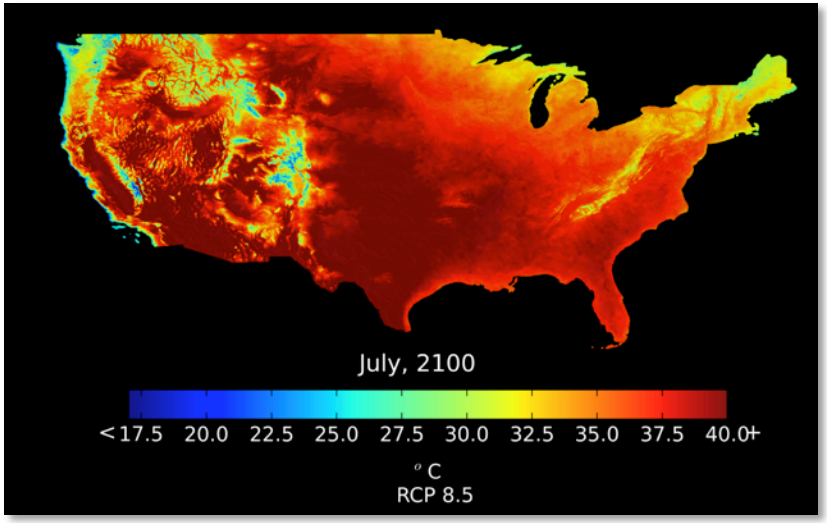
High-Resolution Climate Dataset Produced on Pleiades and Released to Scientists

- NASA Earth Exchange (NEX) scientists and their collaborators in the Climate Analytics Group created a new, high-resolution climate dataset, the NEX Downscaled Climate Projections (NEX-DCP30), and made it available to the Earth science community.
- The NEX-DCP30 dataset, based on the Coupled Model Intercomparison Project Phase 5 (CMIP5), is comprised of downscaled climate scenarios from 33 models.
  - NEX-DCP30 high-resolution climate change projections are used to evaluate climate impacts at the scale of individual neighborhoods and communities.
  - The dataset compiles over 100 climate projections downscaled over the conterminous U.S. at a spatial resolution of 800 meters.
  - The downscaled scenarios, as well as ensemble statistics calculated for four Representative Concentration Pathway (RCP) scenarios, were developed for the Fifth Assessment Report of the Intergovernmental Panel on Climate Change from all model runs available.
- NEX-DCP30 required almost 250,000 hours to produce on the Pleiades supercomputer, and resulted in more than 12 terabytes of data.

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

Mission Impact: The Pleiades supercomputer, along with HECC data storage and high-speed networks, enabled the NASA Earth Exchange (NEX) team to engage large scientific communities and provide capabilities to execute modeling and data analysis on a scale not previously achievable by most scientists.



The NEX-DCP30 predicted monthly mean of the daily maximum near-surface air temperature, for July 2100, downscaled to 800 meters.

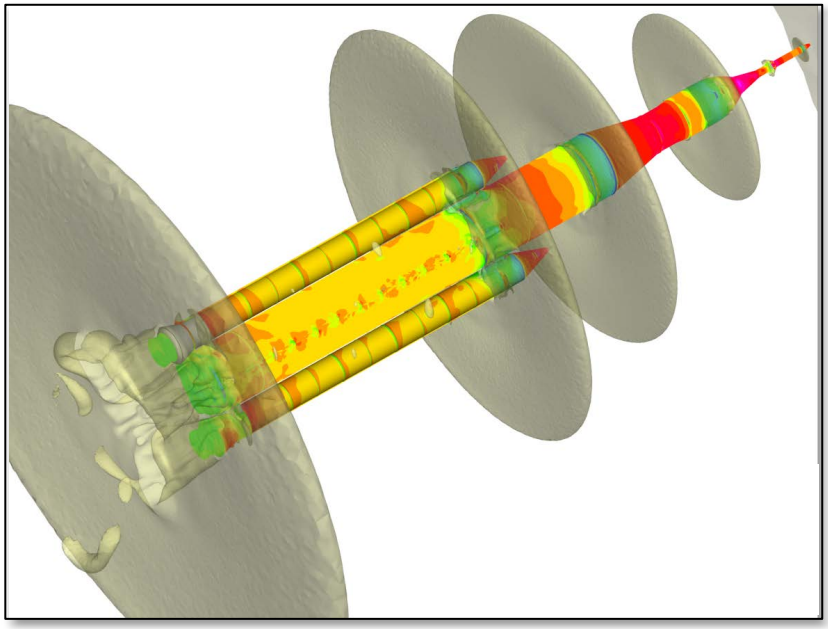
POCs: Ramakrishna Nemani, rama.nemani@nasa.gov, (650) 604-6185, NASA Ames Research Center; Forrest Melton, forrest.s.melton@nasa.gov, (650) 604-2787, NASA Ames Research Center, University Corporation at Monterey Bay

Pleiades Facilitates Studies of Space Launch System

- Using the Fully Unstructured Three-Dimensional (FUN3D) Navier-Stokes code, an engineer at Langley Research Center (LaRC) ran high-fidelity, time-accurate computational fluid dynamics (CFD) simulations to help understand the development of buffet loads on the Space Launch System (SLS).
- The time-accurate CFD simulations run on Pleiades enable engineers to better predict unsteady surface pressures on SLS and, ultimately, understand the development of buffet loads on the vehicle.
- Such detailed simulations require several hundred millions grid points, 10–20 thousand cores, and 4–6 months of computer time.
- Future simulations with better grid resolution will help engineers to further refine the design of SLS and improve vehicle safety and performance.

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

Mission Impact: Enabled by NASA's Pleiades supercomputer, new simulations help engineers understand the development of buffet loads on the Space Launch System.



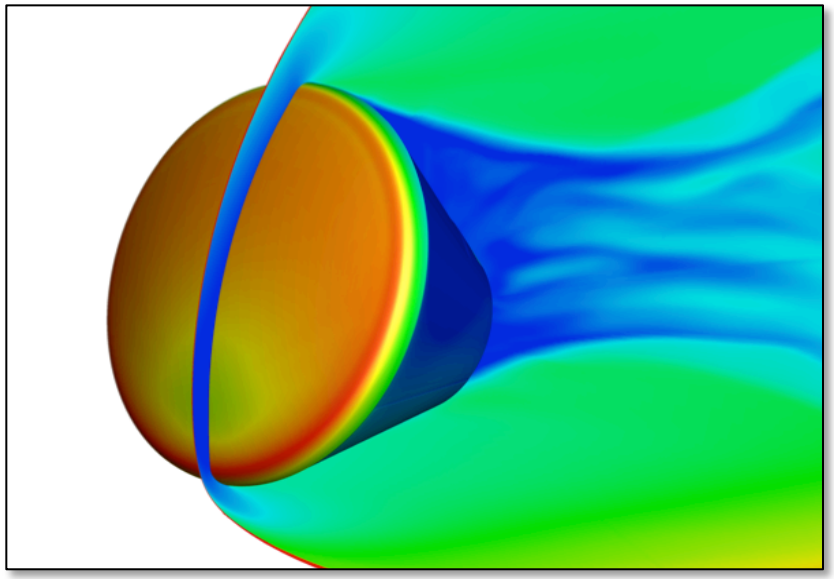
Surface pressure coefficient with sonic isosurfaces from a computation of the transonic flow about a Space Launch System configuration. The computation used 11,640 processors on the Pleiades supercomputer.

POC: Stephen Alter, stephen.j.alter@nasa.gov,
(757) 864-7771, NASA Langley Research Center

Aerothermal Simulations of the Orion Spacecraft for Reentry Analysis

- Using the Data Parallel Line Relaxation (DPLR) and the Langley Aerothermodynamic Upwind Relaxation Algorithm (LAURA) codes, engineers at Ames Research Center (ARC) ran high-fidelity computational fluid dynamics (CFD) simulations to update an aerothermal database for the Orion Multi-Purpose Crew Vehicle (MPCV).
- The simulations, run on Pleiades, enable engineers to estimate the heating environment of the Orion spacecraft for a wide range of reentry conditions.
- The estimates help engineers to predict the peak surface heat flux and heat loads on the MPCV during reentry. This information is critical for determining the type and thickness of the thermal protection system required to protect the spacecraft from harsh reentry conditions.
- Over 300 CFD simulations were computed to update the Orion database. Each simulation took about 3,000 Pleiades processor-hours to complete.
- Future simulations will help engineers to further refine the aerothermal models and improve the Orion MPCV design for deep space exploration.

Mission Impact: Enabled by NASA's Pleiades supercomputer, new simulations help engineers to update the Orion aerothermal database—crucial for accurate estimates of the heating environment for various reentry conditions.



Visualization of temperature contours on the surface of the Orion Multi-Purpose Crew Vehicle and Mach number contours (flow velocity divided by the speed of sound) on the symmetry plane.

POC: Chun Tang, chun.y.tang@nasa.gov, (650) 604-3480, NASA Ames Research Center

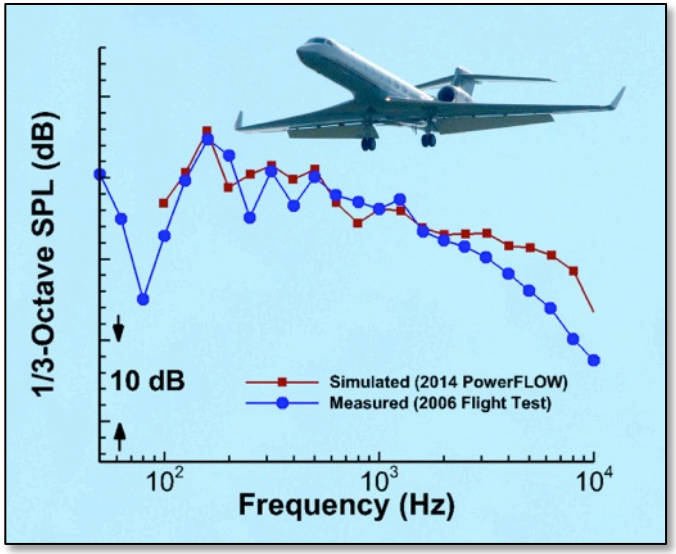
** HECC provided supercomputing resources and services in support of this work*

Extending Airframe Noise Simulations from Scale Models to Full-Scale Aircraft

- Researchers at Langley Research Center (LaRC) are performing simulations on Pleiades to study airframe-generated noise, a major source of aircraft noise during approach and landing.
- Building on their previous work, which was based on an 18% scale half-span model of a Gulfstream aircraft, the team simulated airflow over a full-span, full-scale aircraft in landing configuration (with wing flaps deflected 39 degrees, and main landing gear deployed).
  - This study is the first attempt to predict airframe noise radiating from a full-scale aircraft in landing configuration with most of the geometrical details included.
  - To capture the primary airframe noise sources, the simulations focused on accurately resolving the local flow fields at three locations: flap tips, areas near the main landing gear, and the interaction zones between them.
- LaRC results demonstrate that high-fidelity computer simulations can accurately predict the very complex fluid dynamic processes that generate airframe noise.
- Next steps include repeating the study using a finer-resolution grid, then extending the simulations to evaluate several noise reduction technologies for full-scale aircraft flaps and landing gear.

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

Mission Impact: In support of NASA's Environmentally Responsible Aviation Project, these simulations performed on the Pleiades supercomputer will help the agency develop and mature technologies that will reduce aircraft noise footprints.



Comparison between measured and simulated far-field noise spectra for a full-scale Gulfstream aircraft during landing. The measurement location corresponds to the flyover point the Federal Aviation Administration uses to evaluate noise from landing aircraft (396 feet altitude, 90° azimuth direction).

POC: Mehdi Khorrami, mehdi.r.khorrami@nasa.gov, (757) 864-3630, NASA Langley Research Center

HECC Facility Hosts Several Visitors and Tours in May 2015

- HECC hosted 6 tour groups in May; guests learned about the agency-wide missions being supported by HECC assets, and some of the groups also viewed the D-Wave Two quantum computer system. Visitors this month included:
  - Two science officers from the United Kingdom Consulate in San Francisco.
  - His Excellency, Mr. Pieter De Crem, Secretary of State for Foreign Trade, The Kingdom of Belgium.
  - Members of the Living with a Star (LWS) Steering Committee, who attended a meeting hosted at NASA Ames.
  - Rubén Del Rosario, manager of the Advanced Air Transport Technology(AATT) Project within Aeronautics Research Mission Directorate's Advanced Air Vehicles Program; and others on the AATT management team.
  - California community college faculty members working to enhance STEM preparation and provide opportunity for students to study STEM fields at the university level.

Bryan Biegel, deputy chief of the NASA Advanced Supercomputing (NAS) Division presented science and engineering results on the hyperwall system to faculty members from California community colleges collaborating with NASA Ames to promote Science, Technology, Engineering and Math (STEM) education.

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

Papers

- "**Simulated Solar Cycle Effects on the Middle Atmosphere: WACCM3 versus WACCM4**," E. D. Peck, C. E. Randall, V. L. Harvey, D. R. Marsh, Journal of Advances in Modeling Earth Systems (Accepted Article), May 6, 2015. *
  http://onlinelibrary.wiley.com/doi/10.1002/2014MS000387/full
- "**Cosmological Structure Formation**," J. Primack, arXiv:1505.02821 [astro-ph.GA], May 11, 2015. *
  http://arxiv.org/abs/1505.02821
- "**Development of the GEOS-5 Atmospheric General Circulation Model: Evolution from MERRA to MERRA2**," A. Molod, L. Takacs, M. Suarez, J. Bachmeister, Geoscientific Model Development, vol. 8, May 12, 2015. *
  http://www.geosci-model-dev.net/8/1339/2015/gmd-8-1339-2015.html
- "**A Simple Analytical Model for Gaps in Protoplanetary Disks**," P. Duffell, arXiv:1505.03514 [astro-ph.EP], May 13, 2015. *
  http://arxiv.org/abs/1505.03514
- "**Higher-Order and Length-Scale Statistics from DNS of a Decelerated Planar Wall-Bounded Turbulent Flow**," E. Jeyapaul, G. Coleman, C. Rumsey, International Journal of Heat and Fluid Flow, vol. 54 (Early Online Publication), May 14, 2015. *
  http://www.sciencedirect.com/science/article/pii/S0142727X15000302
- "**On Multiple Reconnection X-Lines and Tripolar Perturbations of Strong Guide Magnetic Fields**," S. Eriksson, et al., The Astrophysical Journal, vol. 805, May 20, 2015. *
  http://iopscience.iop.org/0004-637X/805/1/43

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

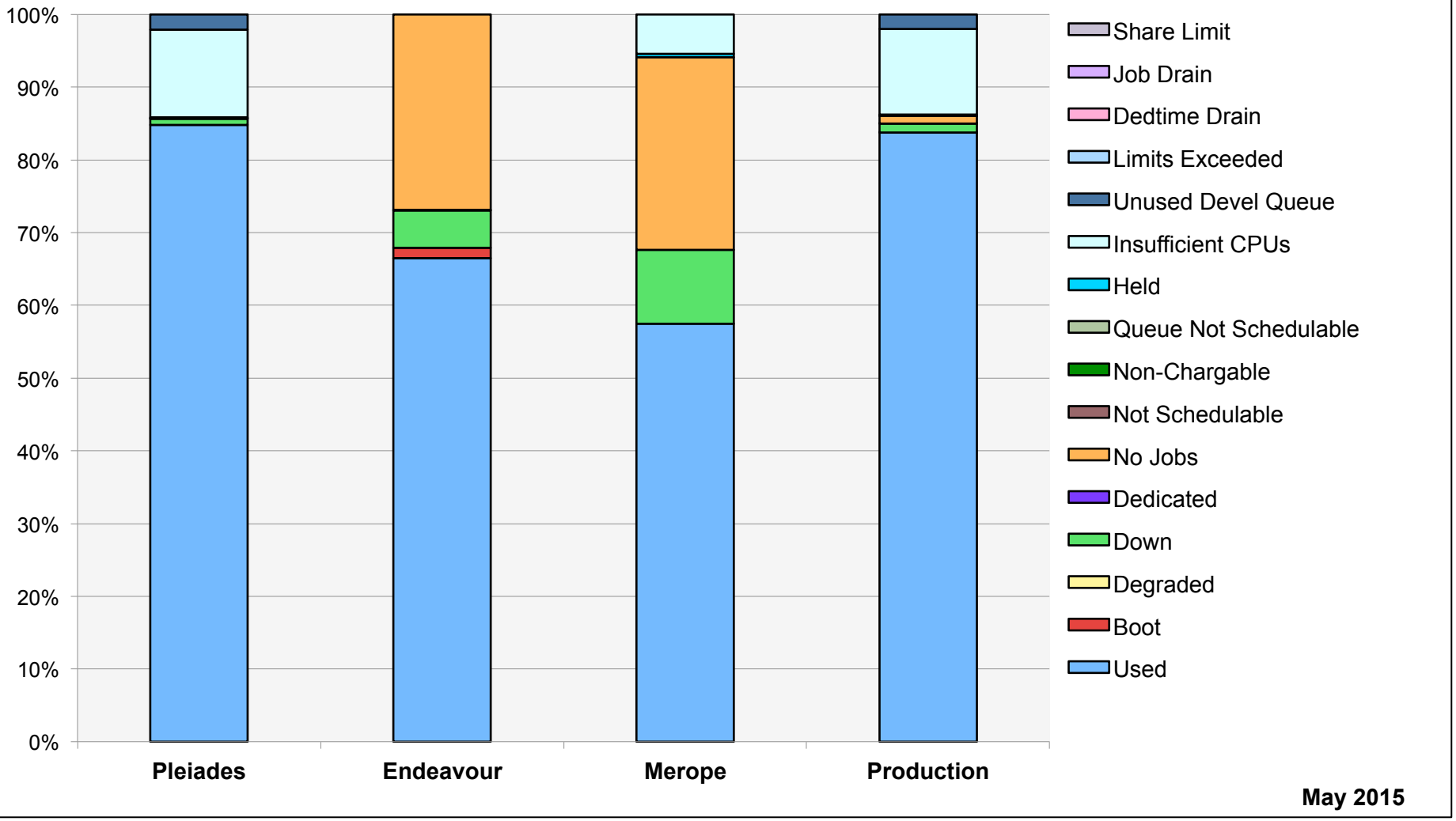
Presentations

- "**Navier-Stokes Assessment of Test Facility Effects on Hover Performance**," N. Chaderjian, J. Ahmad, presented at The American Helicopter Society (AHS) International 71st Annual Forum and Technology Display, Virginia Beach, Virginia, May 5–7, 2015.
- "**Long Haul Lustre**," M. Hartman, presented at the 2015 SGI User Group Conference, Minneapolis, Minnesota, May 5–7, 2015.
- "**Multiple Schedulers for Combining Quick-Turnaround and Batch Workloads in PBSPro**," G. Matthews, presented at the 2015 SGI User Group Conference, Minneapolis, Minnesota, May 5–7, 2015.
- "**Parallel Adaptive High-Order CFD Simulations Characterizing SOFIA Cavity Acoustics**," M. Barad, C. Brehm, C. Kiris, R. Biswas, presented at the International Conference on Parallel CFD, Montreal, Quebec, Canada, May 17–20, 2015.

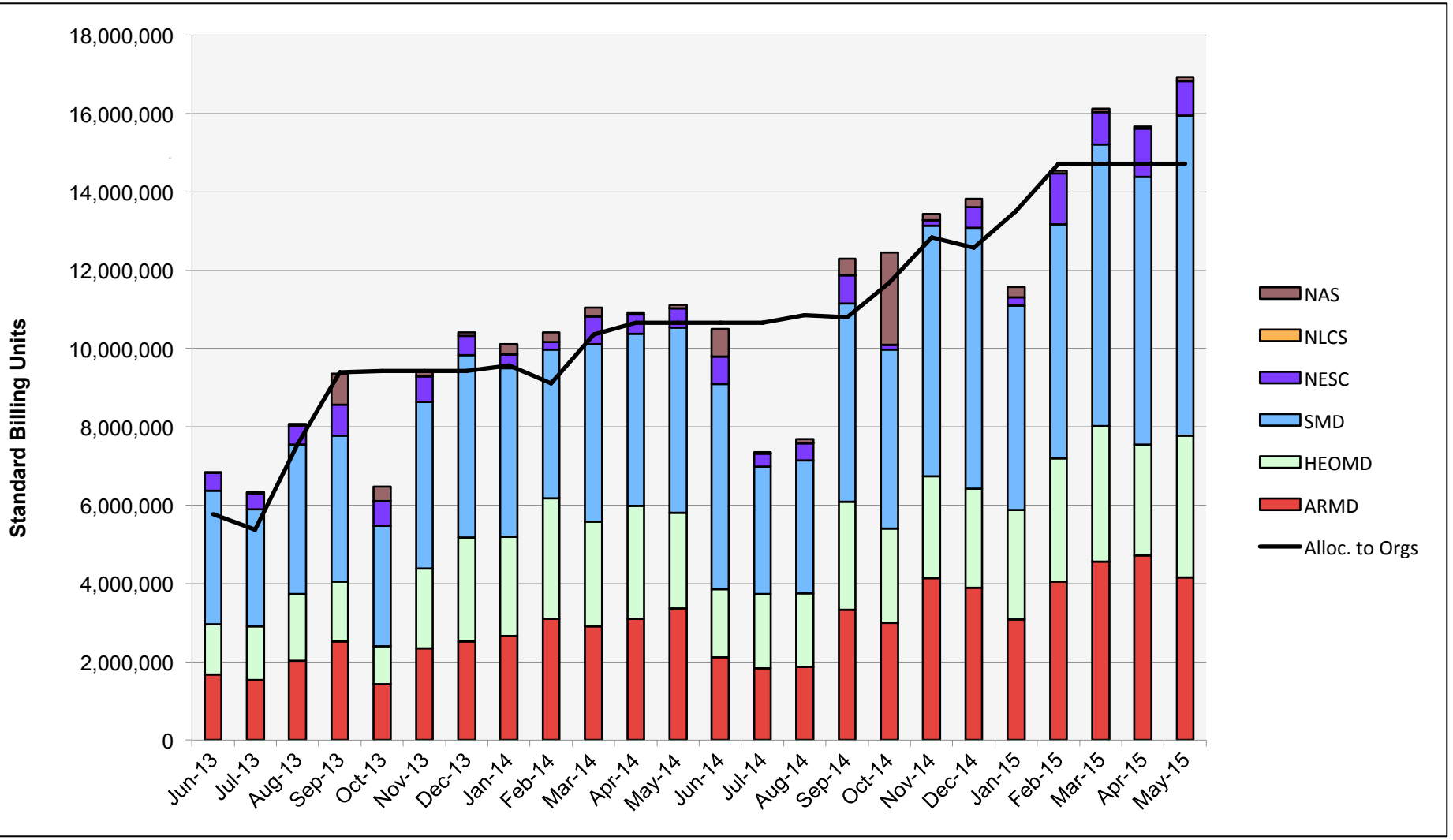
News and Events

- **Supercomputers a Hidden Power Center of Silicon Valley**, *San Jose Mercury News*, May 7, 2015—Silicon Valley companies support the ever-increasing hardware needs of supercomputing centers, working with government and industry partners to build and maintain high-end computing resources, like the supercomputing systems at the NASA Advanced Supercomputing (NAS) facility. (*Picked up by multiple media sources around the country*.)
  http://www.mercurynews.com/business/ci_28071868/supercomputers-hidden-power-center-silicon-valley
- **Living with a Star Heliophysics Science Technical Interchange Meeting (TIM) 2015**, May 19–21, 2015—NAS staff hosted the second annual technical meeting, which focused on the synergy between NASA space missions, ground-based missions, and the development of first-principles quantitative models that take advantage of the HECC resources.
  http://www.nas.nasa.gov/hms/2015tim.html
- **SC15 Selects Numerical Aerodynamic Simulation Program for the Test of Time Award**, *SC15 Blog*, May 20, 2015—The Supercomputing Conference Test of Time Award Committee has recognized the paper "The NAS Parallel Benchmarks – Summary and Preliminary Results," written and presented by NAS staff in 1991, for this year's award. The Test of Time Award recognizes an outstanding paper that has deeply influenced the HPC discipline and has made a historical impact on HPC trends.
  http://sc15blog.blogspot.com/2015/05/sc15-selects-numerical-aerodynamic.html
  - **SC15 Announces Test of Time Award Winners**, *insideHPC*, May 21, 2015.
    http://insidehpc.com/2015/05/sc15-announces-test-of-time-award-winners/
  - **SC15 Selects Numerical Aerodynamic Simulation Program for the Test of Time Award,** *HPCwire*, May 20, 2015.
    http://www.hpcwire.com/off-the-wire/sc15-selects-numerical-aerodynamic-simulation-program-for-the-test-of-time-award/

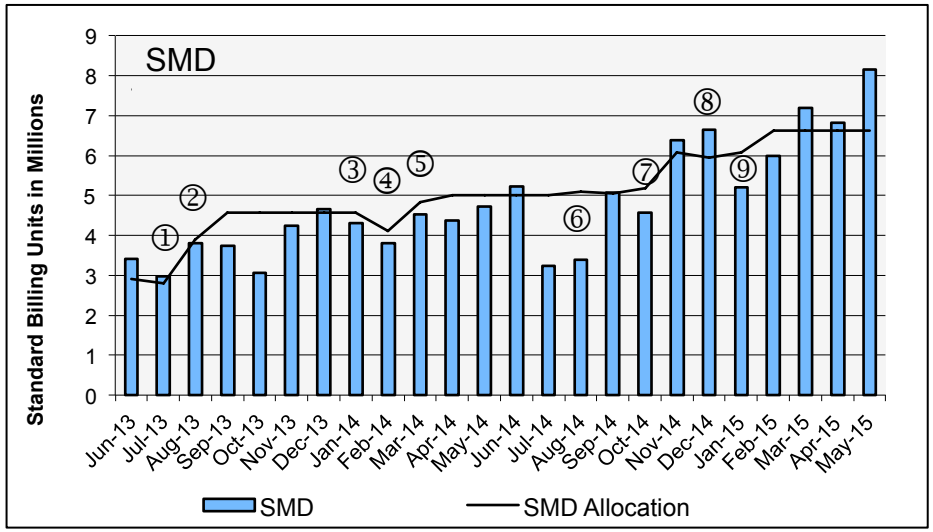
HECC Utilization

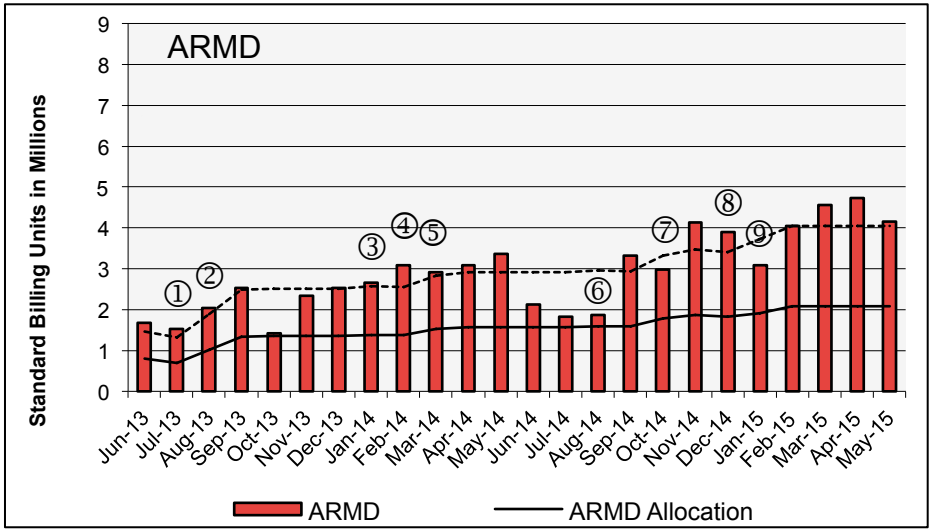


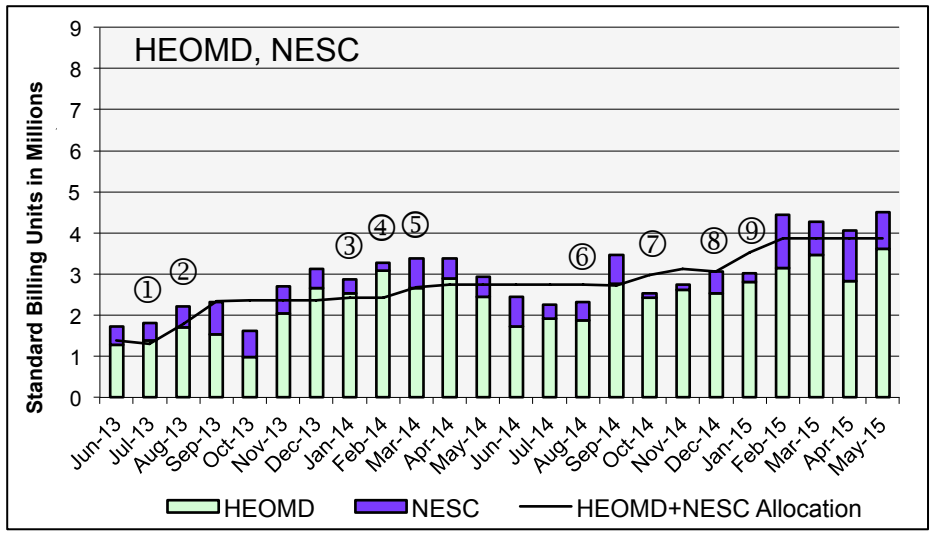
HECC Utilization Normalized to 30-Day Month



HECC Utilization Normalized to 30-Day Month







① 32 Harpertown Racks retired

② 32 Harpertown Racks retired; 46 Ivy Bridge Racks added

③ 6 Ivy Bridge Racks added; 20 Nehalem, 12 Westmere Racks Retired

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

⑤ 4 Ivy Bridge Racks added mid-March

⑥ 6 Westmere Racks added to Merope, Merope Harpertown retired

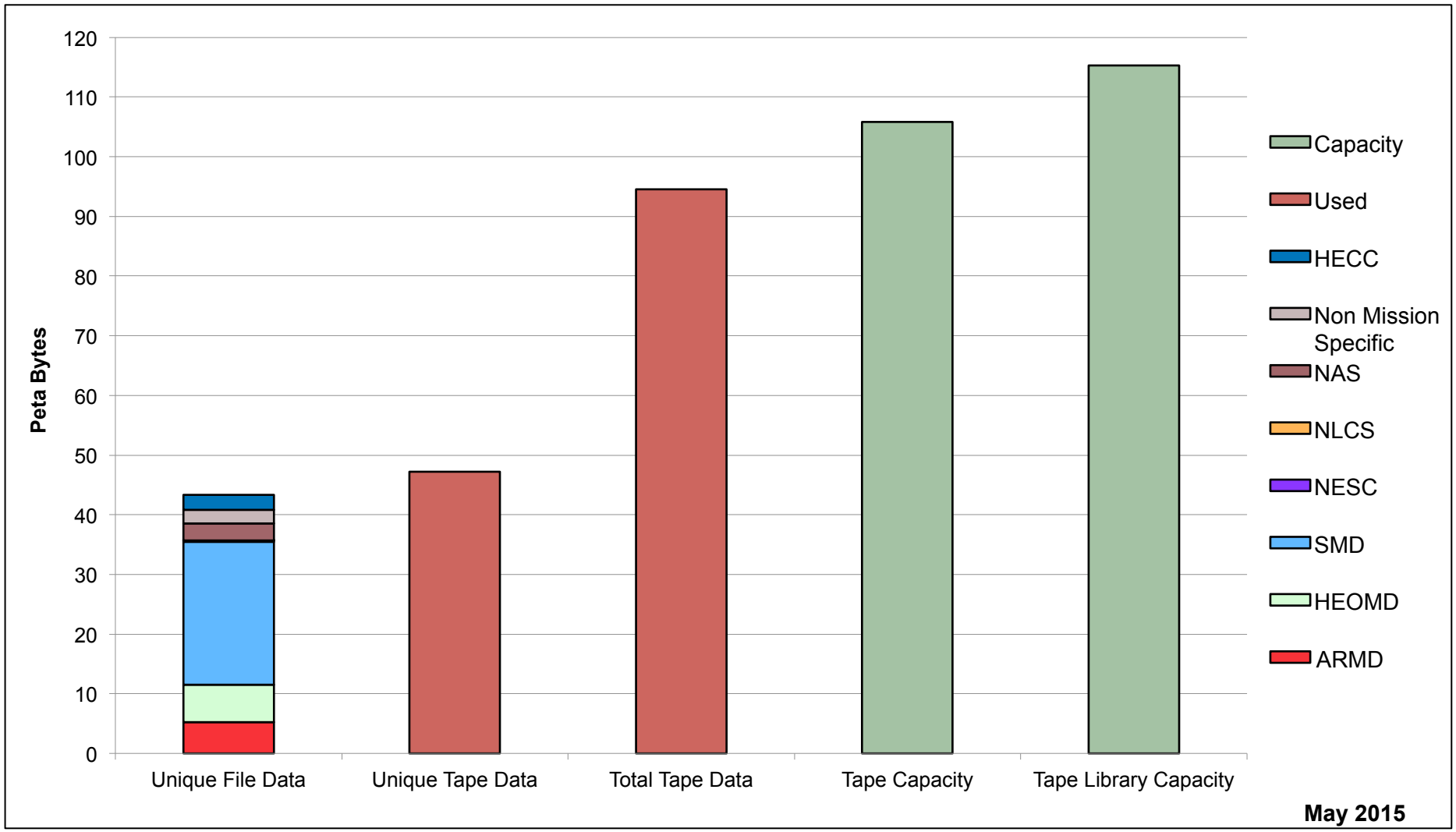
⑦ 16 Westmere Racks retired; 10 Nehalem Racks and 2 Westmere Racks added to Merope; 3 Ivy Bridge Racks added; 15 Haswell Racks added

⑧ 16 Westmere Racks retired

⑨ 14 Haswell racks added

Note The dashed line on the ARMD chart is the result of the 10% agency set aside being added

Tape Archive Status



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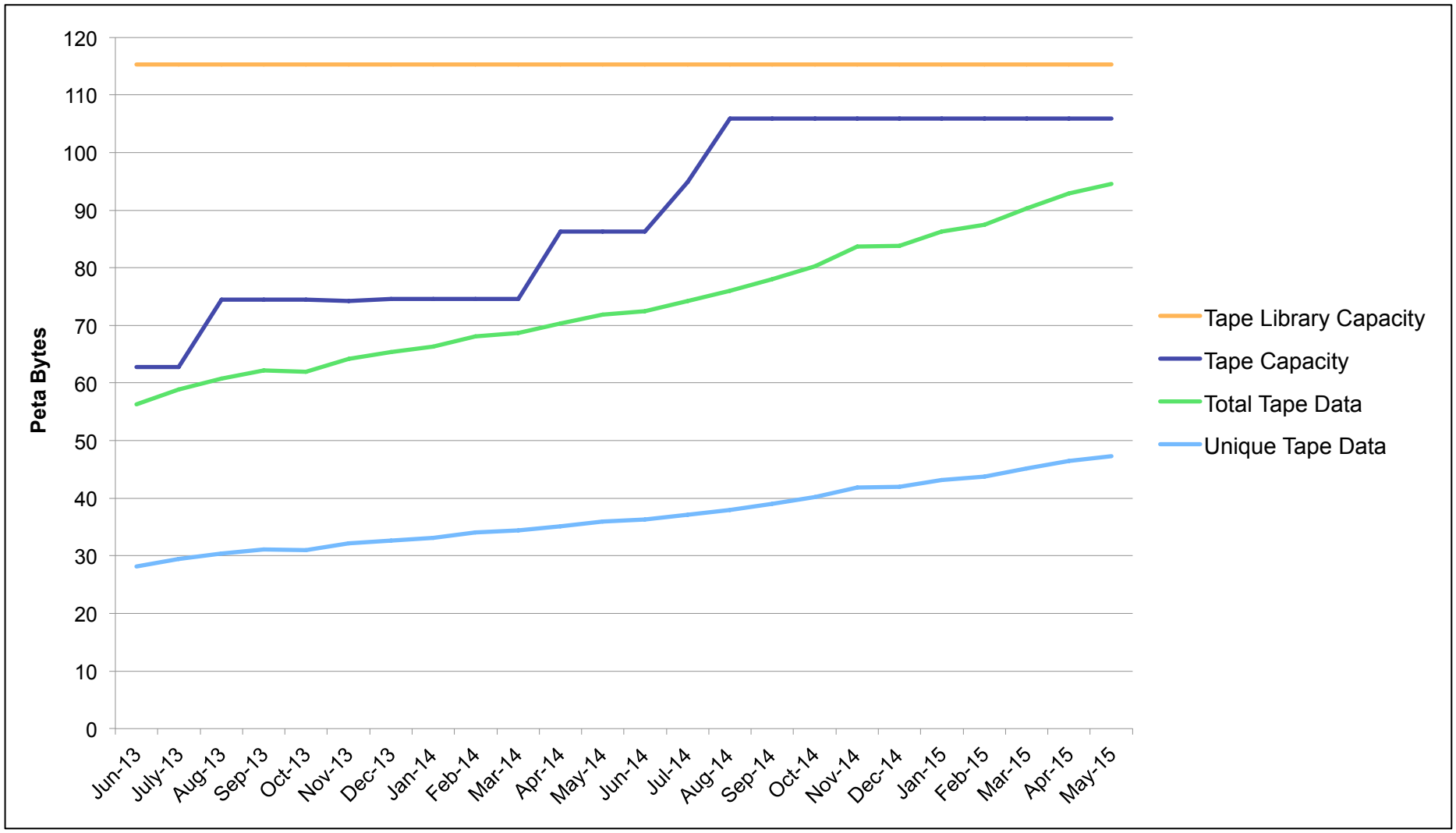
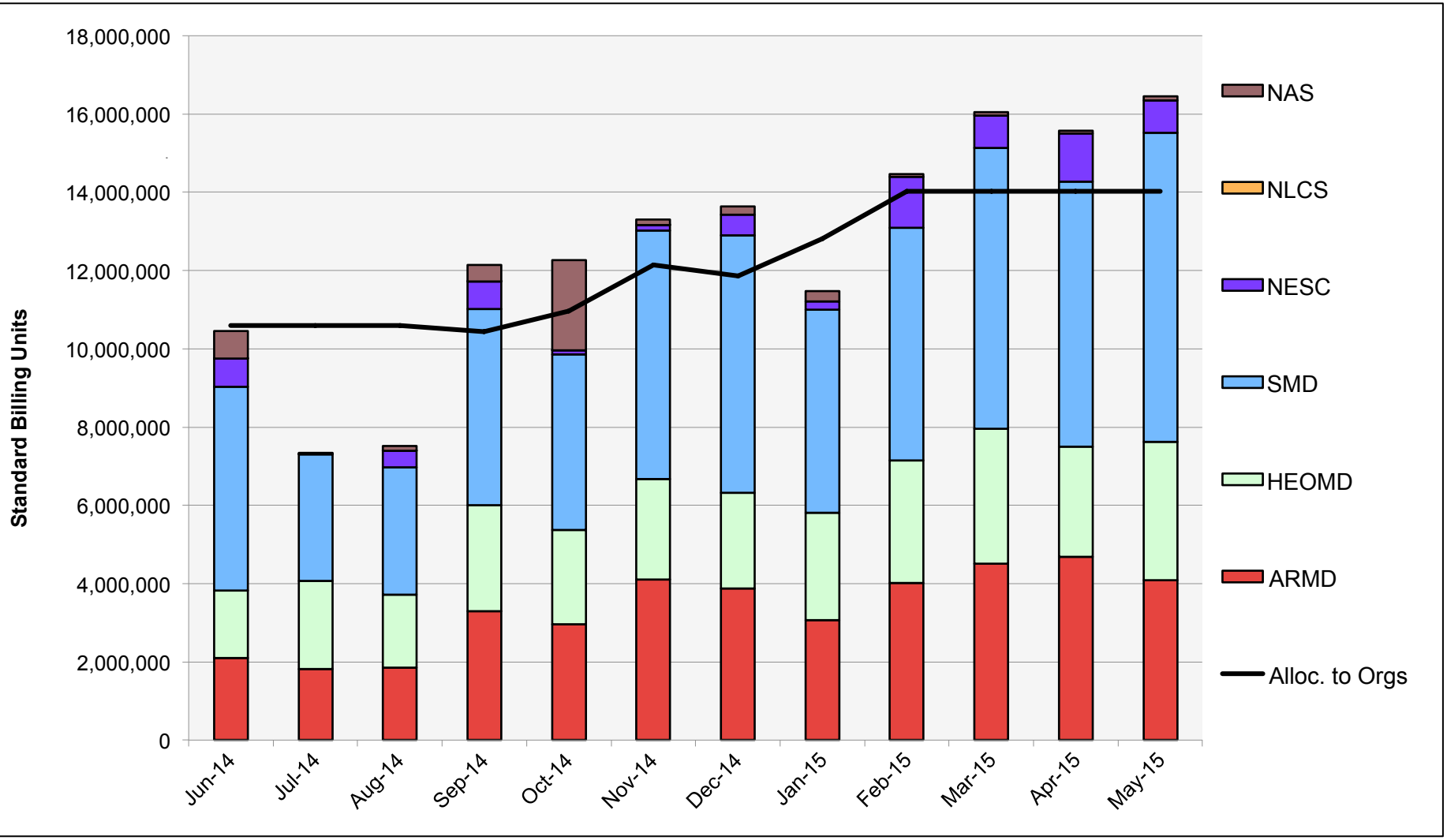
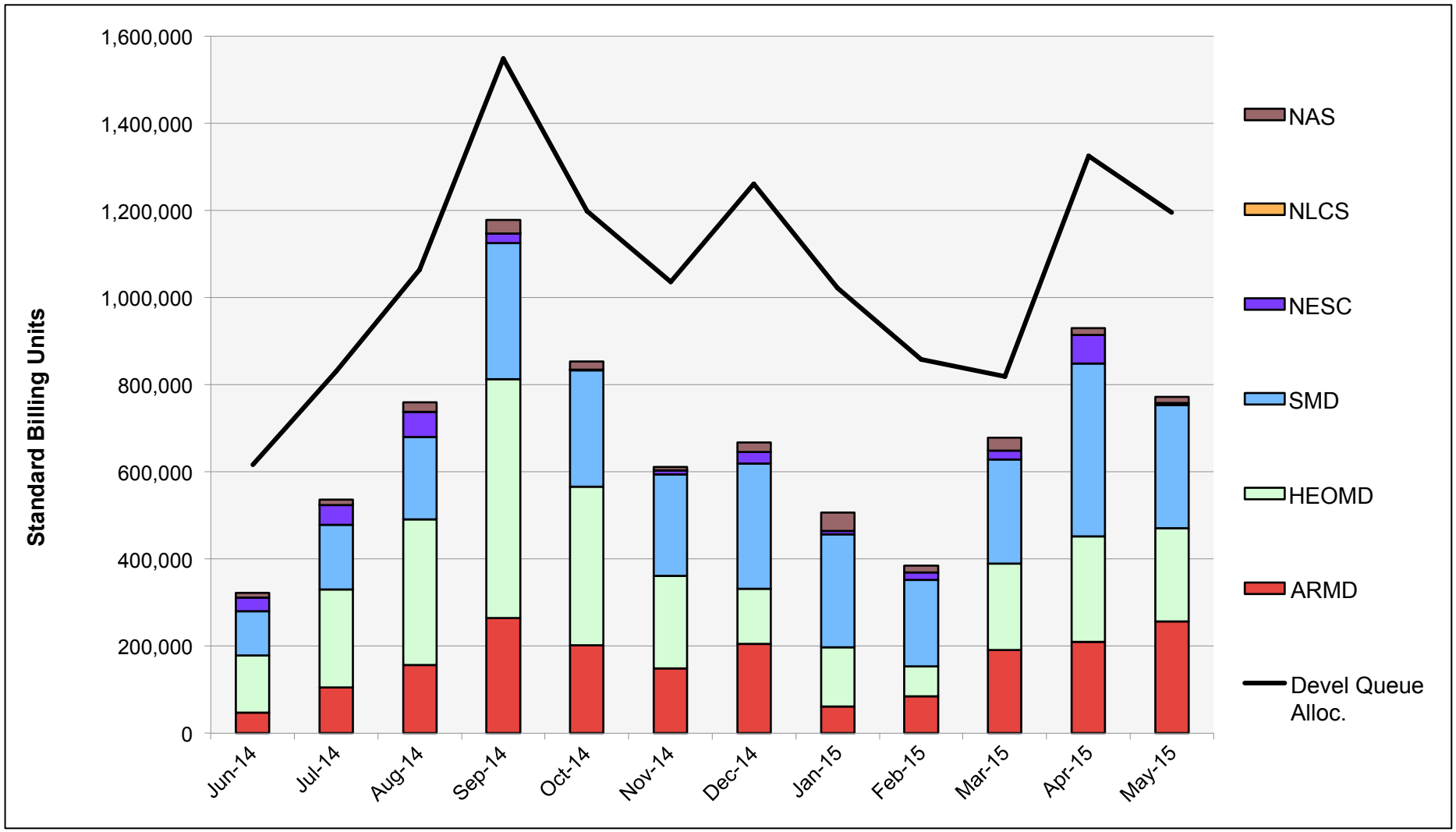


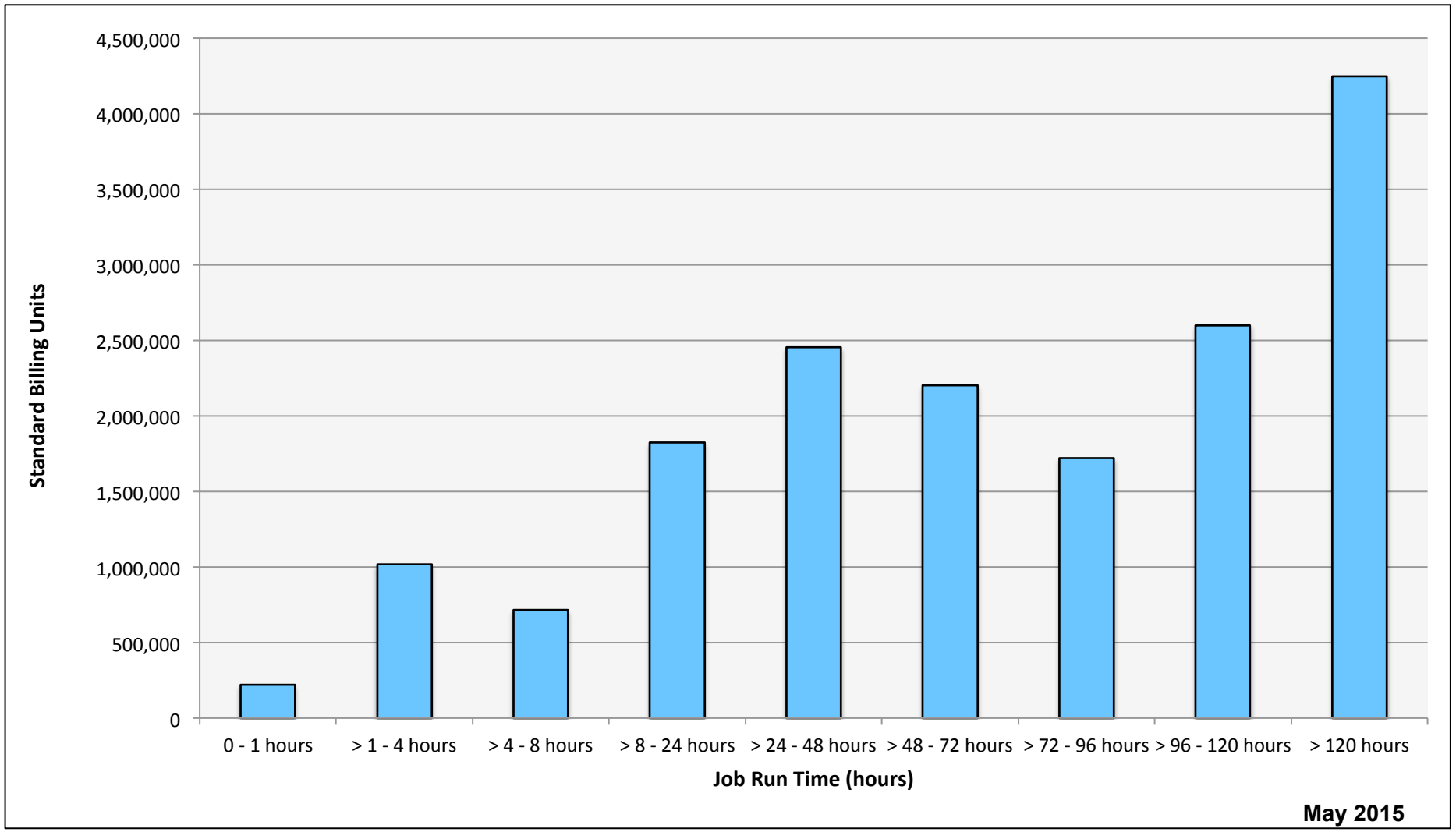
Pleiades:
SBUs Reported, Normalized to 30-Day Month



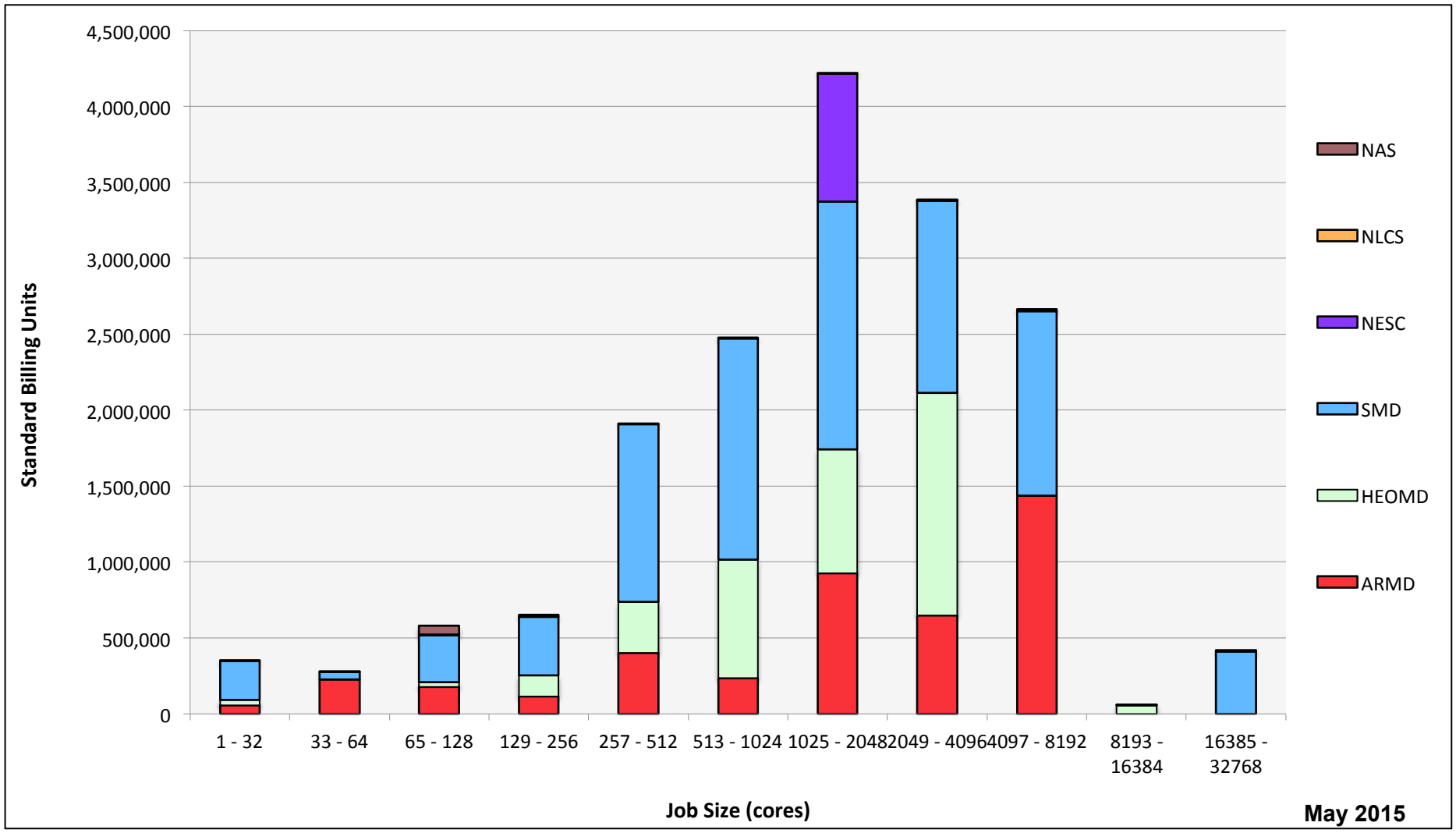
Pleiades:
Devel Queue Utilization



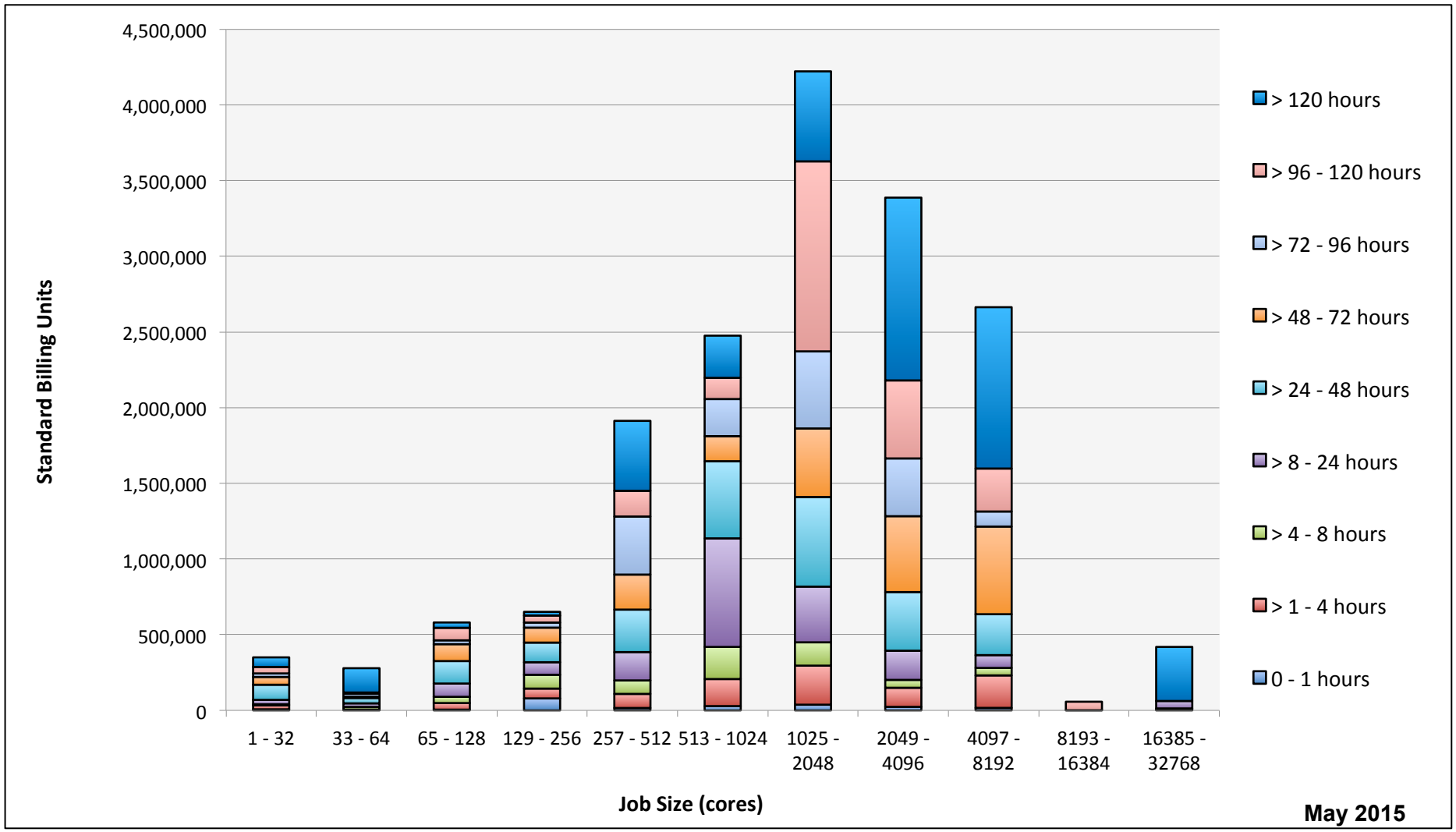
Pleiades:
Monthly Utilization by Job Length



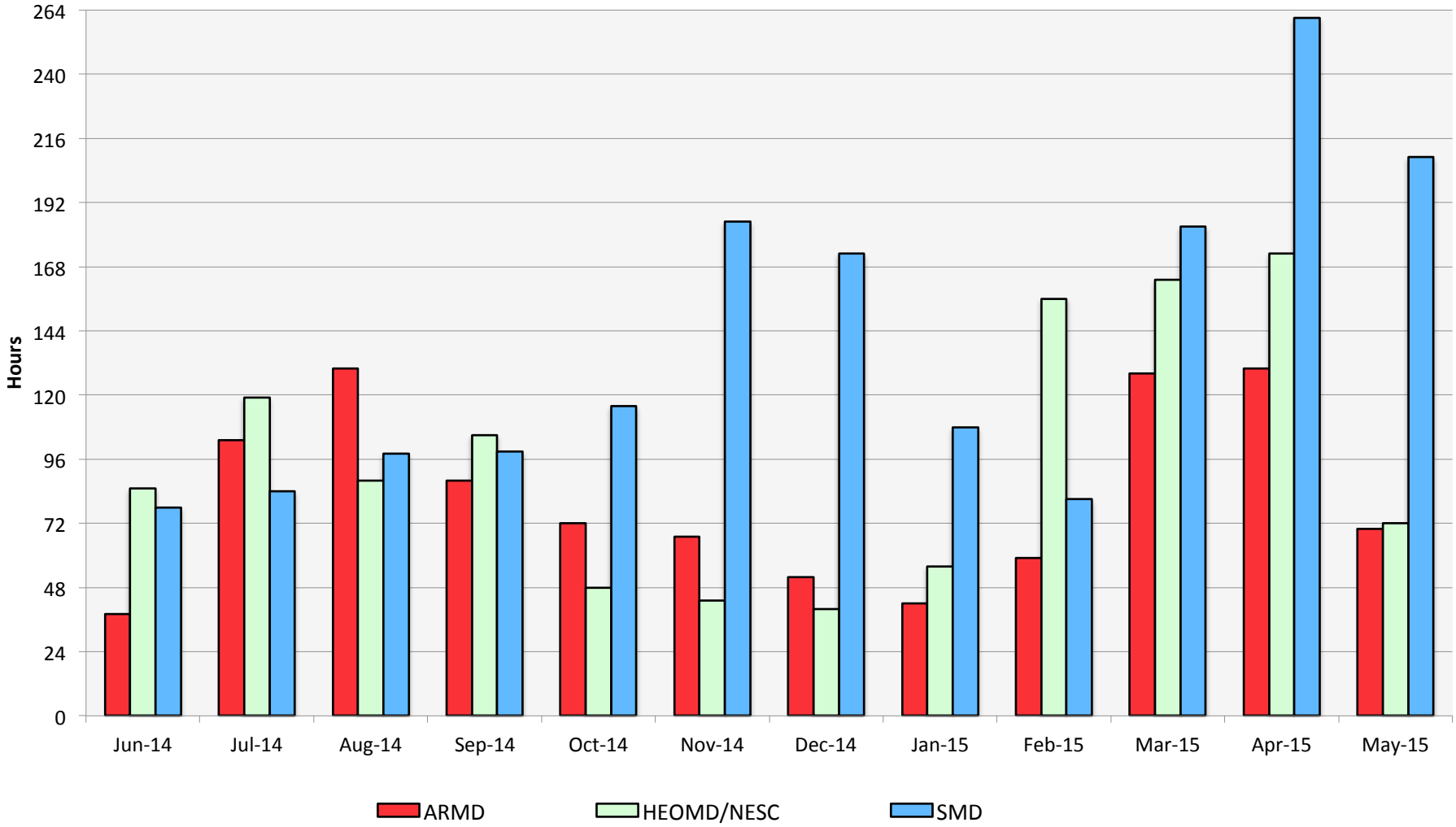
Pleiades:
Monthly Utilization by Size and Mission



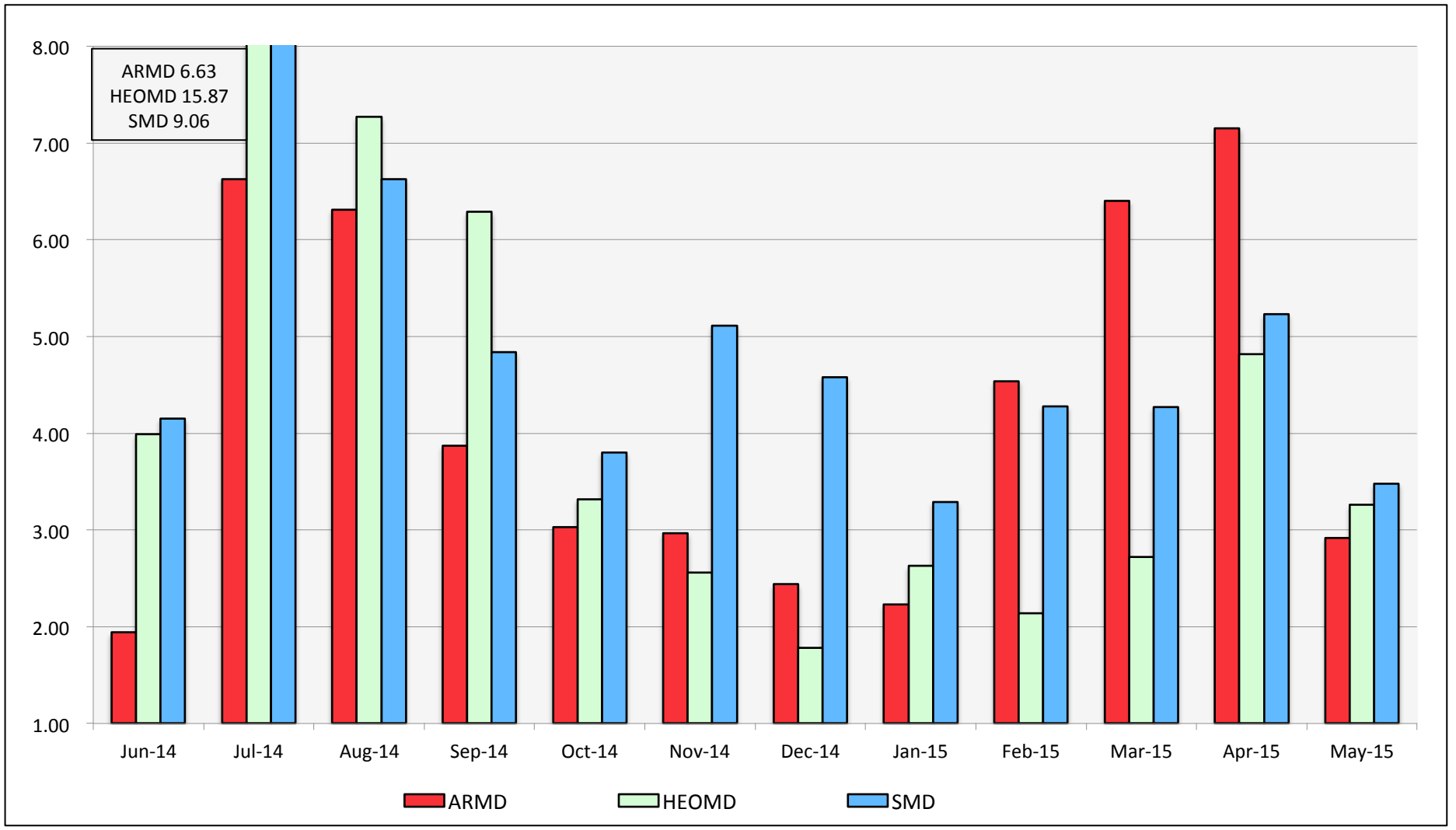
Pleiades:
Monthly Utilization by Size and Length



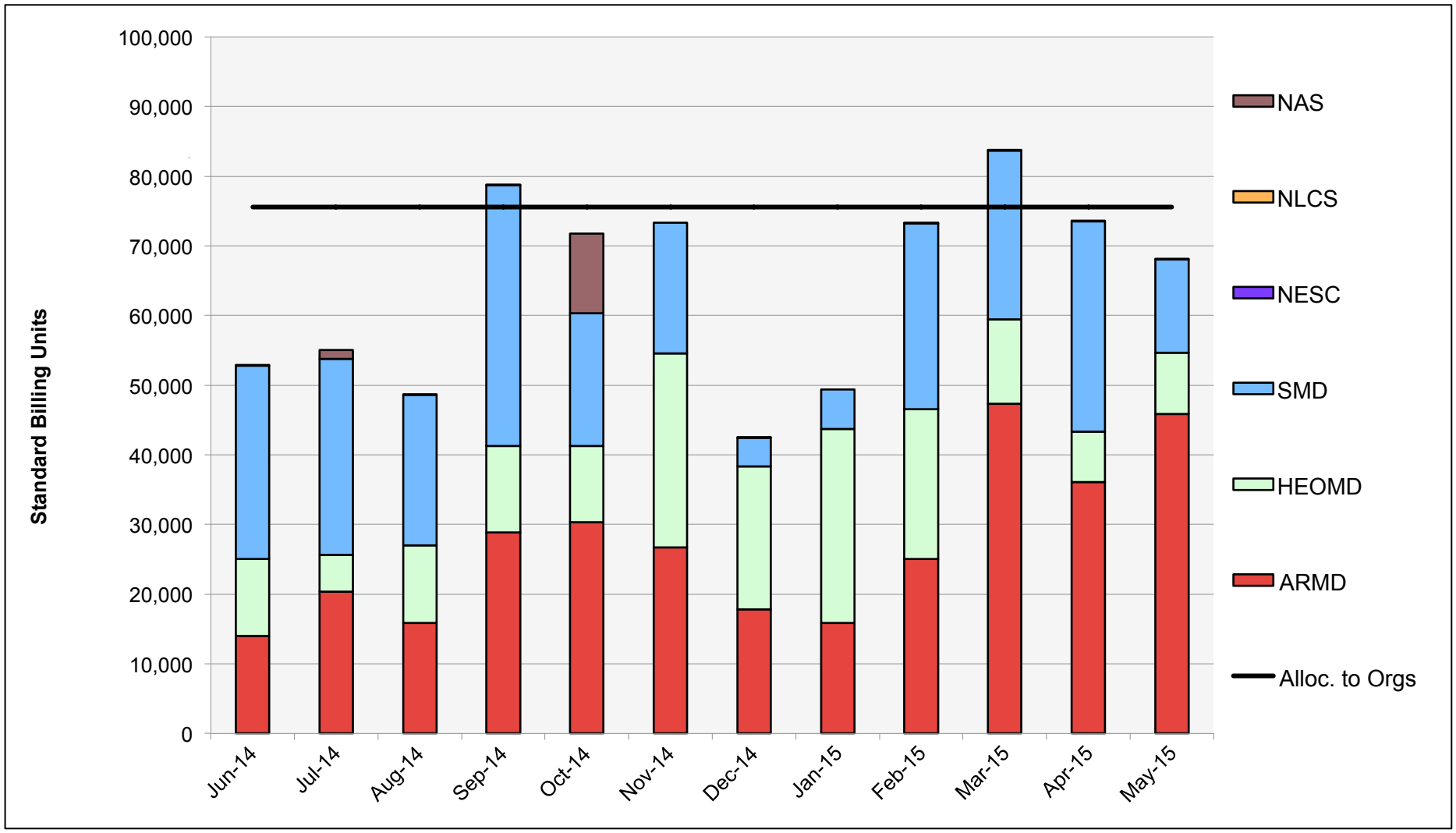
Pleiades:
Average Time to Clear All Jobs



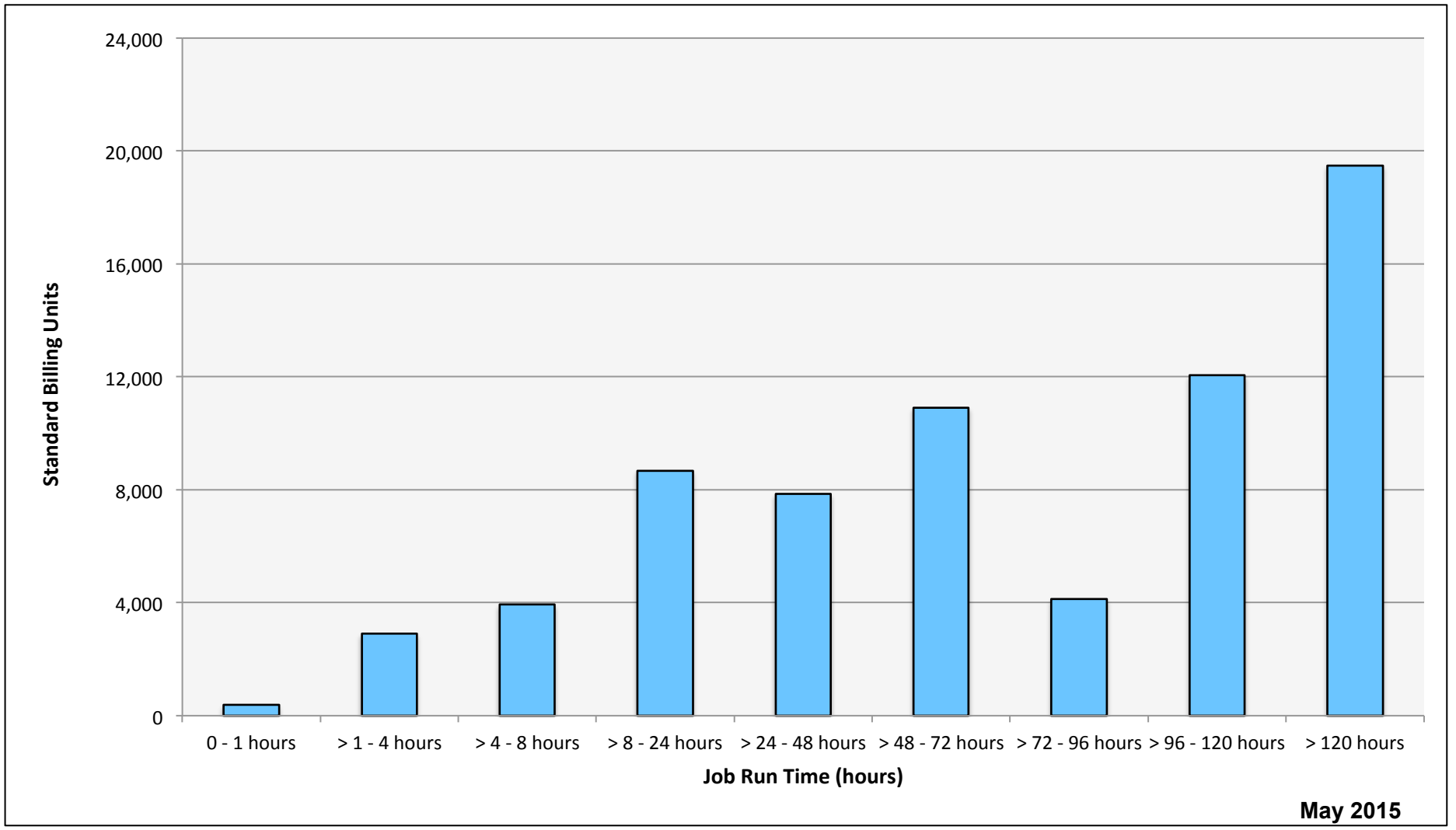
Pleiades:
Average Expansion Factor



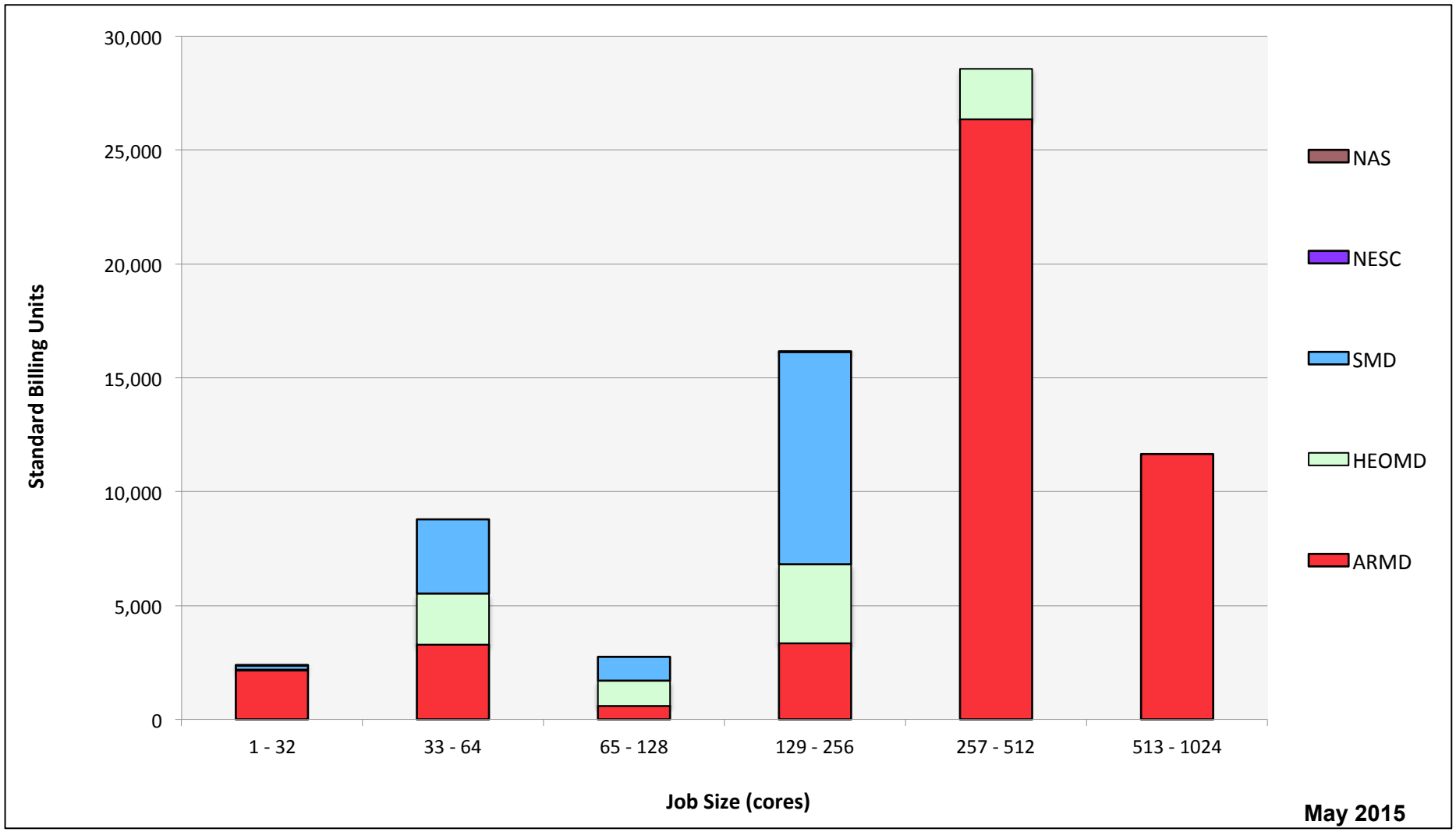
Endeavour:
SBUs Reported, Normalized to 30-Day Month



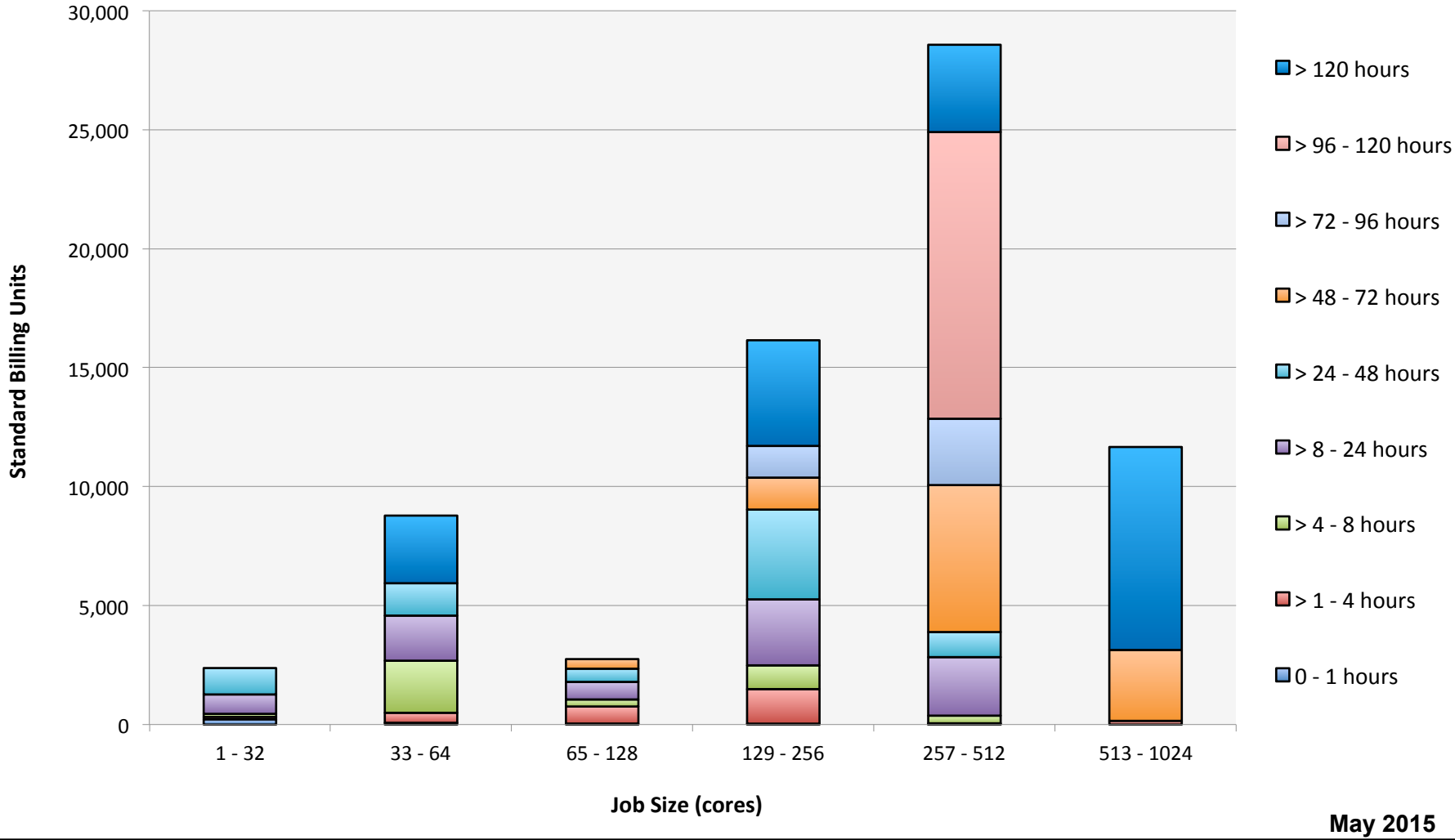
Endeavour:
Monthly Utilization by Job Length



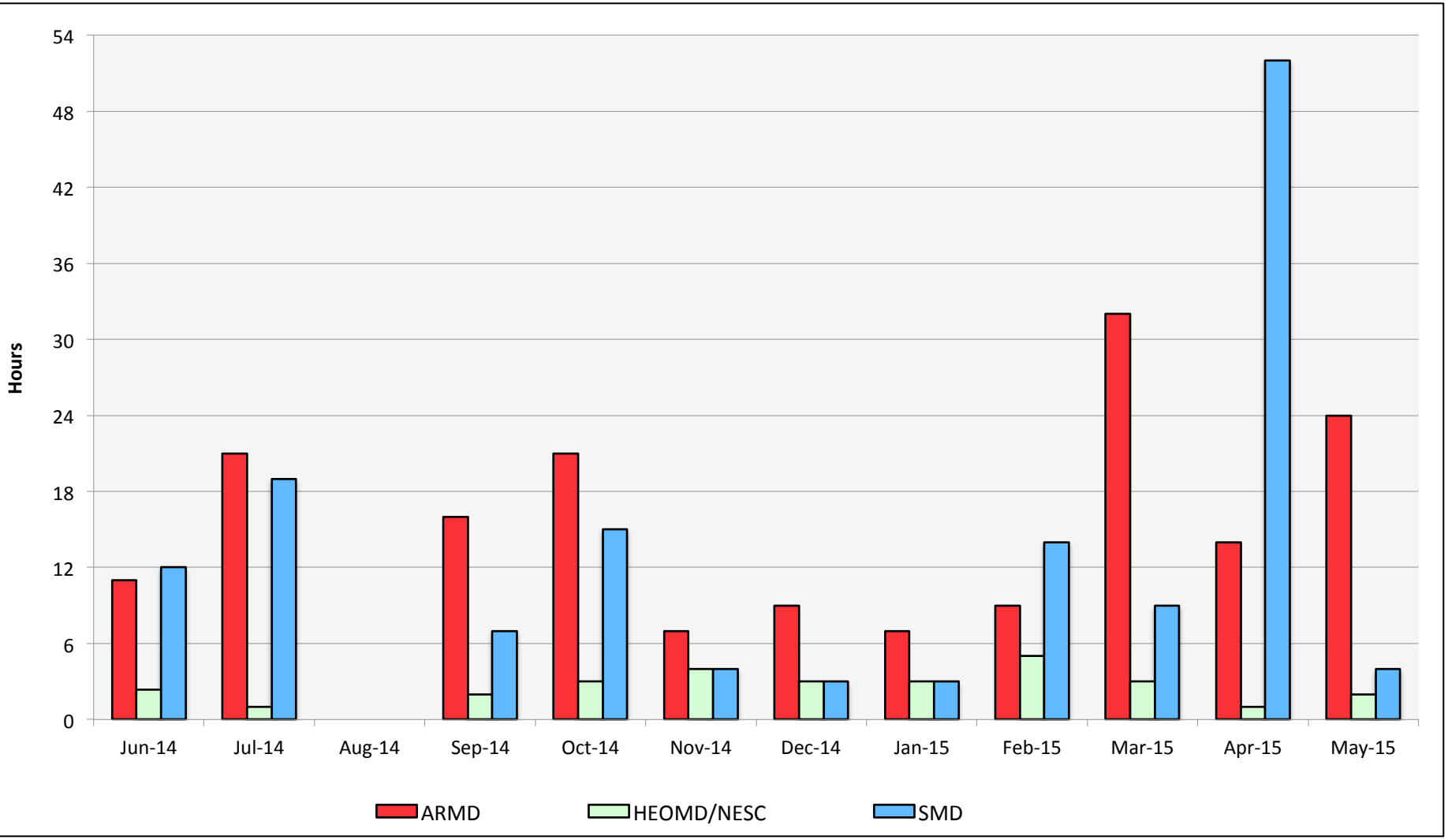
Endeavour:
Monthly Utilization by Size and Mission



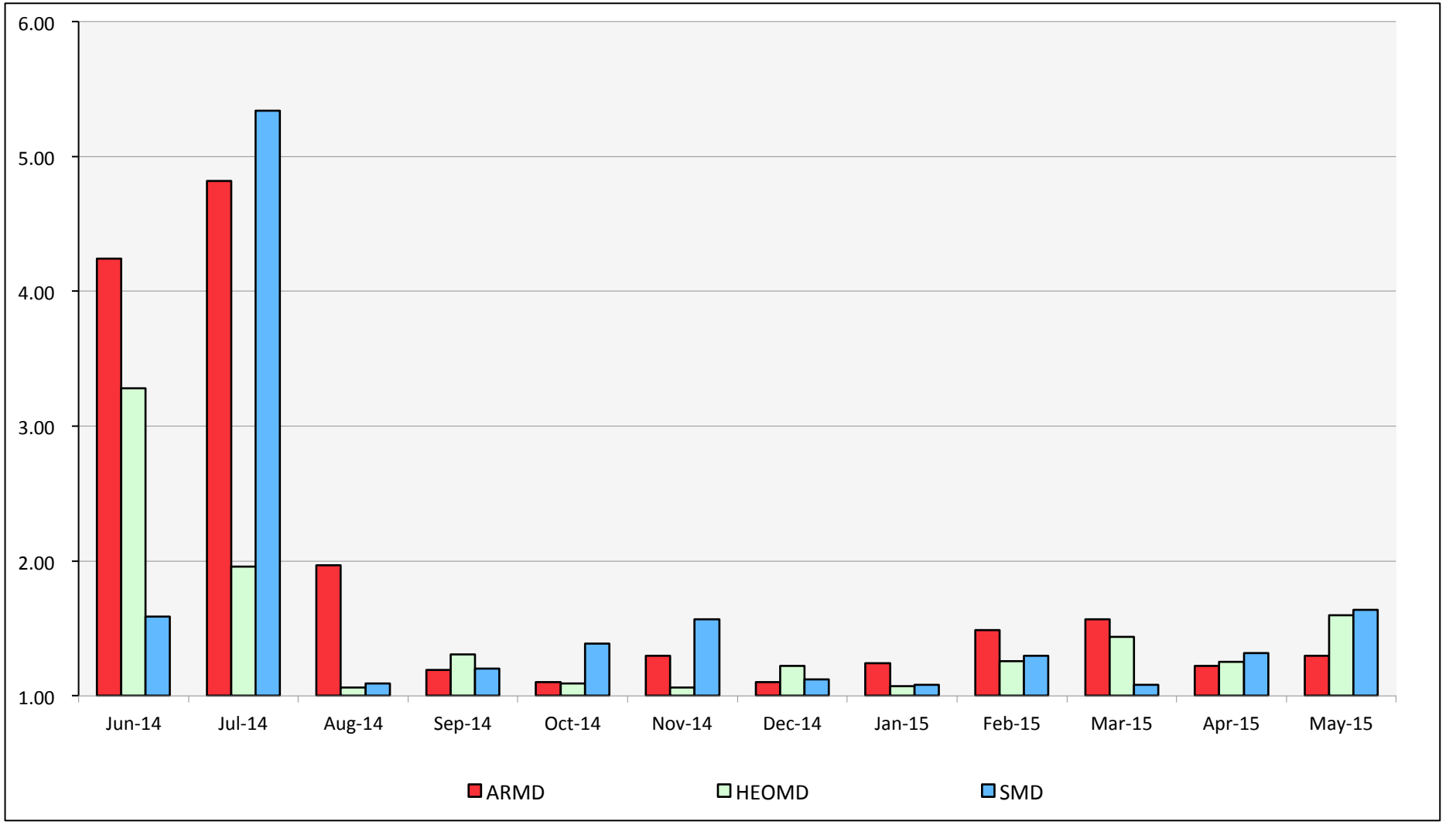
Endeavour:
Monthly Utilization by Size and Length



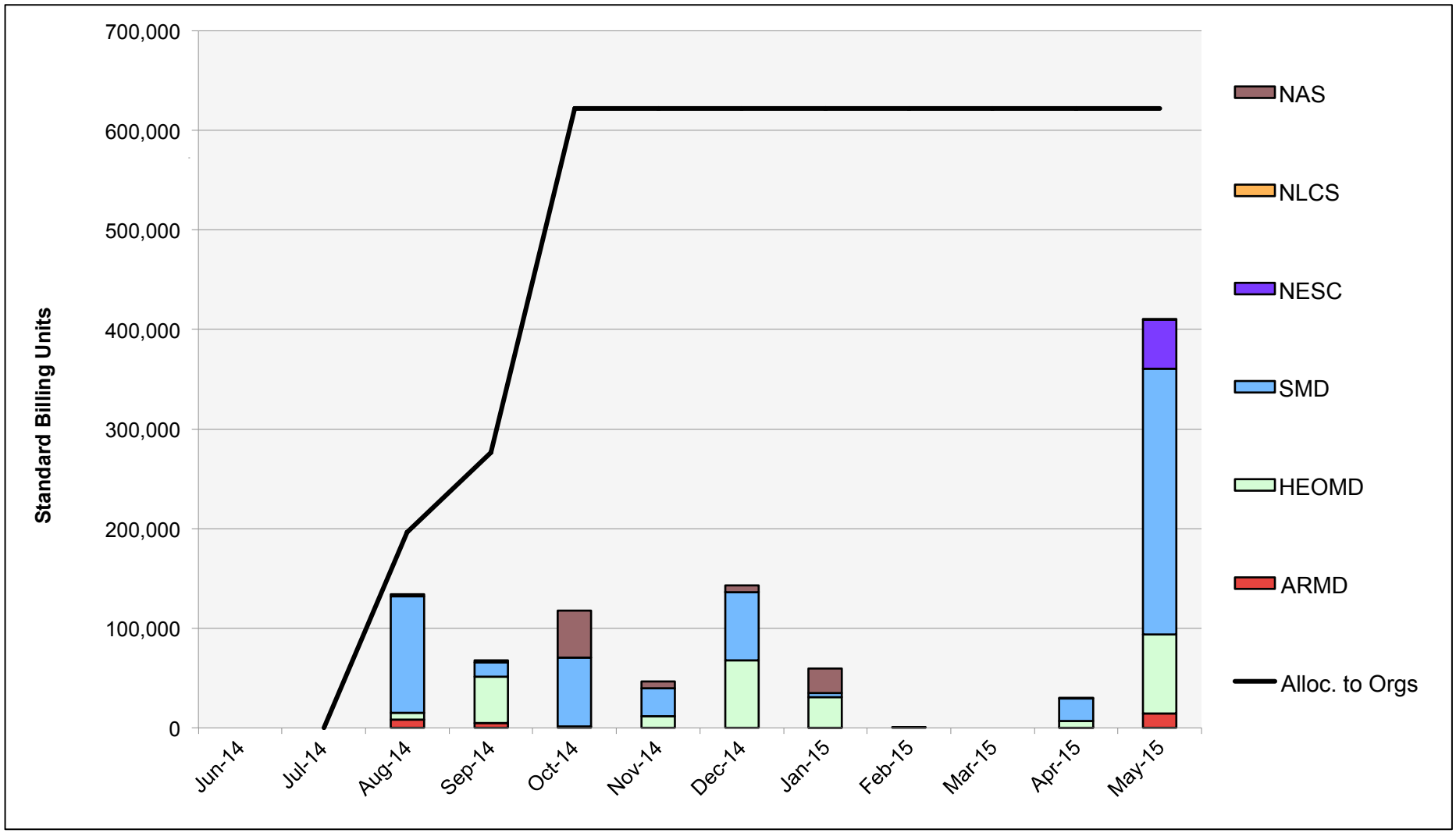
Endeavour:
Average Time to Clear All Jobs



Endeavour:
Average Expansion Factor

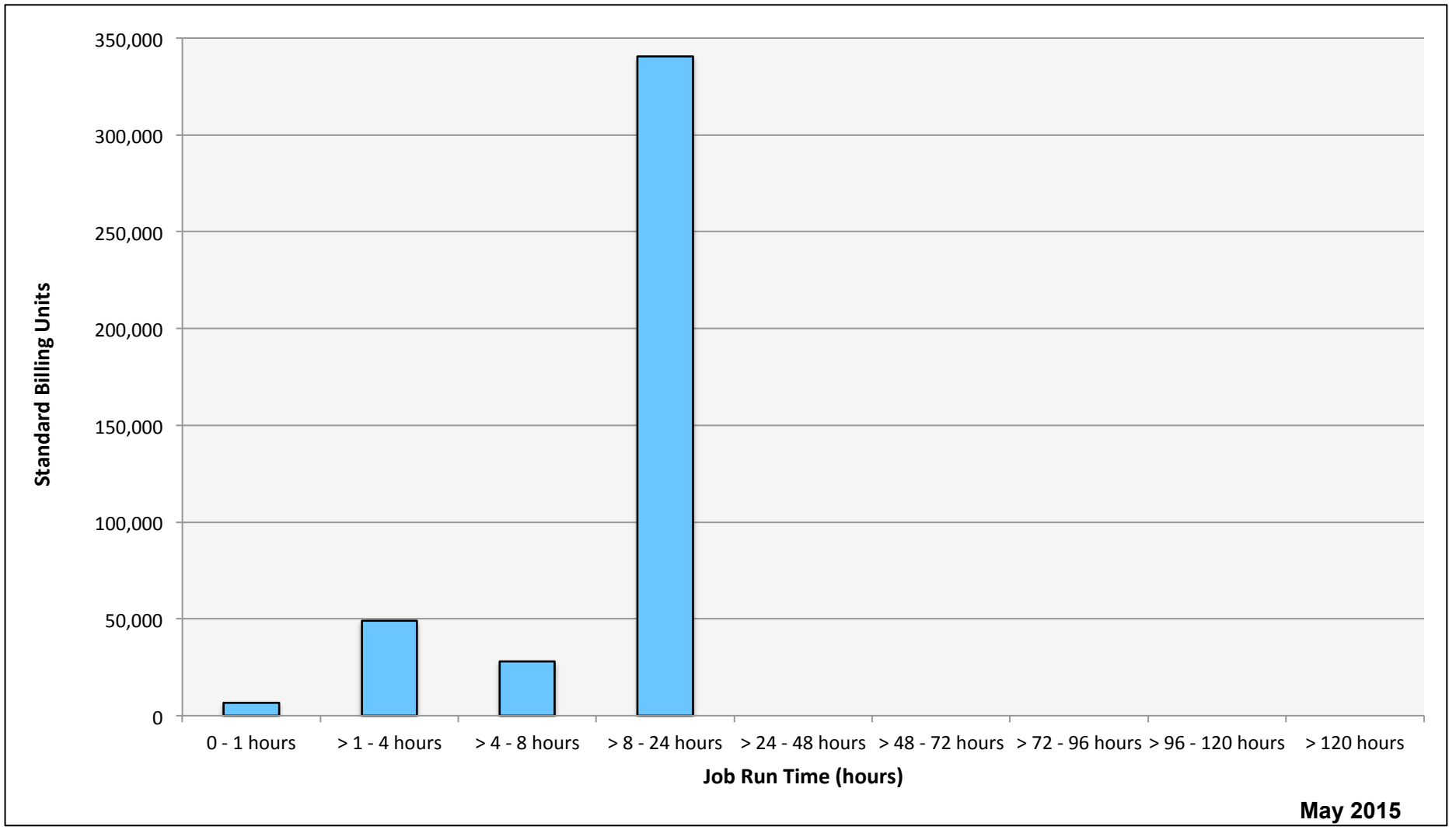


Merope:
SBUs Reported, Normalized to 30-Day Month

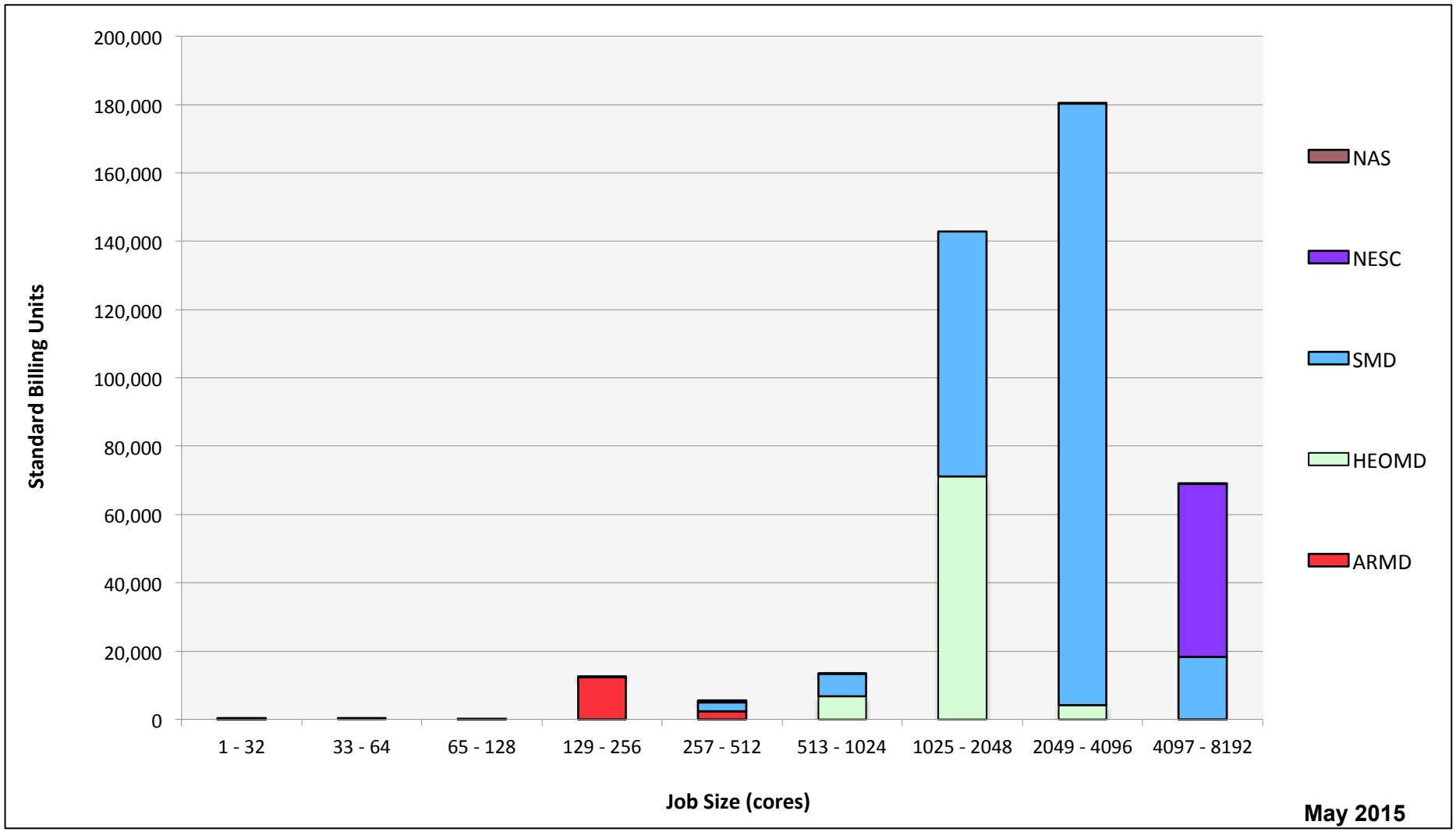


Note The low utilization of Merope was due to unstable connectivity to the file systems. The issues were resolved.

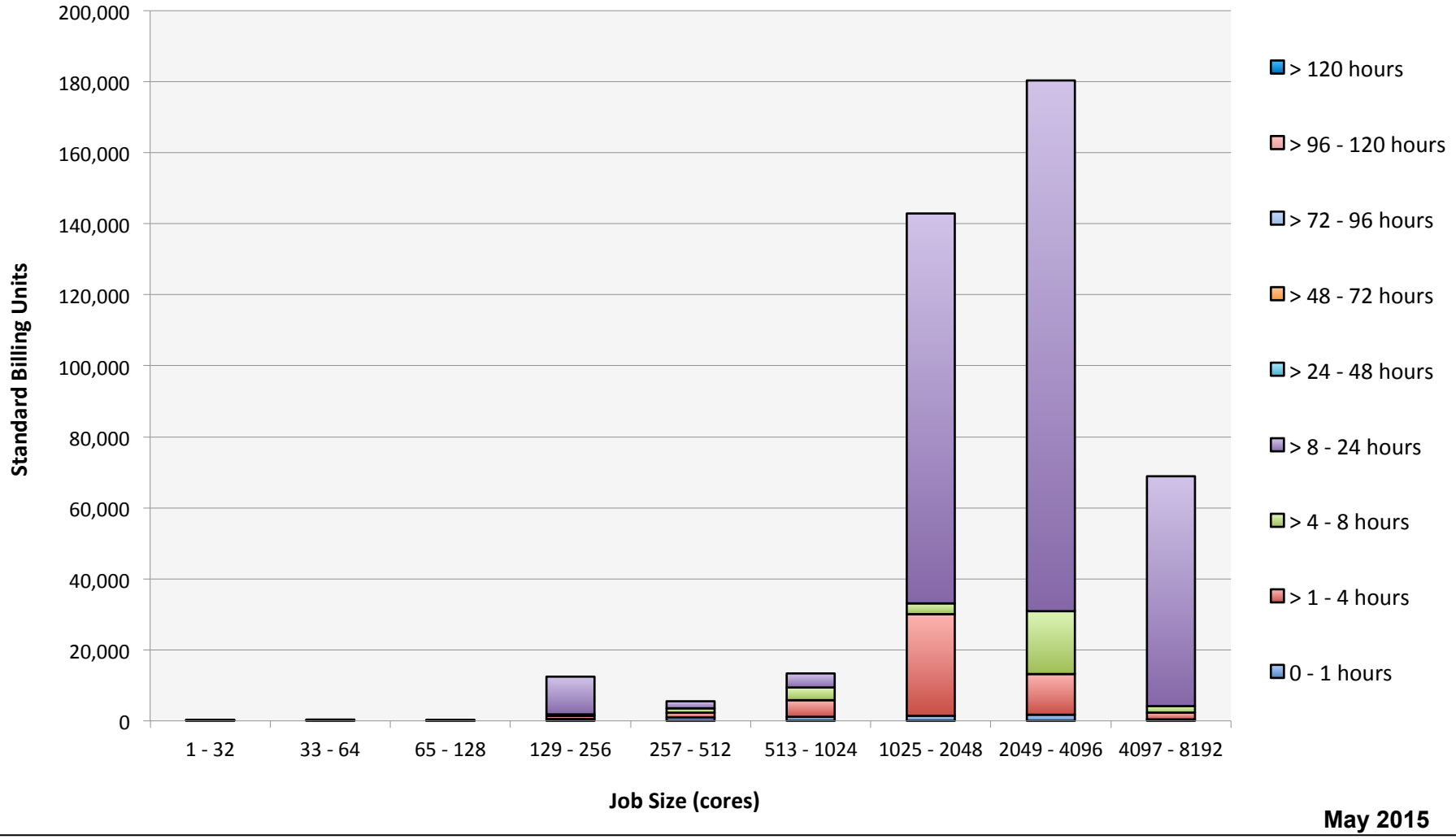
Merope:
Monthly Utilization by Job Length



Merope:
Monthly Utilization by Size and Mission



Merope:
Monthly Utilization by Size and Length



Merope:
Average Expansion Factor