

National Aeronautics and Space Administration



Project Status Report

High End Computing Capability Strategic Capabilities Assets Program

9 August 2011

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Significant Accomplishments – Current and Future



Current

- HECC Readied Resources for STS-135 and Supported 22 Shuttle Missions
- Support for Modeling of Protocellular Structure and Functions in the Origins of Life
- Prediction of Jet Engine Fan Noise Using Computational Aeroacoustics
- Error-Controlled Simulation Database for Orion Pad Abort Test
- Installation of GPU Nodes Provides New Graphics Capability for Pleiades Users
- New Pleiades Filesystem Deployed with 10x Increase in IOPS Performance
- Record Usage Shows Pleiades Provides Maximum Resources for NASA Missions
- SMD Usage of Pleiades Doubles in Six Months
- HECC Network Team Hosts Meeting With LBNL/NERSC For Information Exchange
- HECC Teams Respond Quickly to Facility Emergency Scenario

Future

- Complete file system migration
- Augment archive capability
- Participate in SMC-IT
- Participate in NASA IT Summit



HECC Readied Resources for STS-135 and Supported 22 Shuttle Missions

- HECC made available priority access to the Pleiades supercomputer for damage assessment during the final Space Shuttle mission (STS-135) in July.
- Fortunately, vehicle damage was minor, and damage assessments were completed without real-time computer simulations.
- Shuttle missions were not always so “clean”. When a 4-ft x 6-ft. corner of the thermal blanket peeled off an orbital maneuvering system pod during the launch of STS-117 (June 2007), computational analyses contributed to the decision to have astronaut John (Danny) Olivas spend two hours stapling and pinning the blanket.
- During the past 22 shuttle missions, over 200,000 Standard Billing Units (about 4 million wall-clock hours of a single-core computer) were used on the Columbia and Pleiades supercomputers.
- Atlantis landed safely at NASA’s Kennedy Space Flight Center in Florida on July 21.

Mission Impact: HECC supercomputers have enabled NASA groups to quickly perform high-fidelity Space Shuttle analyses. For 22 missions, starting with STS-114, groups supporting the damage assessment team had dedicated/priority access to resources for input into decisions to perform repairs and/or clear the orbiter for safe landing.



Figure: Atlantis making a picture-perfect landing to end the Space Shuttle Program.

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

Support for Modeling of Protocellular Structure and Functions in the Origins of Life



- Researchers at NASA Ames are performing molecular dynamics simulations on Pleiades to support astrobiology research into how life emerged from cosmic and planetary precursors.
- The formation of protein channels for transport across membranes was crucial for the emergence of cellular life.
- Simulations of antiameobin and trichotoxin ion channels (fungal antibiotic peptides that form conducting bundles in membranes) are being used to study the structure, stability, and conductivity of these channels; while these are modern, evolved proteins, they can be used as models of early channels because of their structural simplicity.
- Results show that computed conductance values agree well with experimental results.
- Computational studies of membrane systems require generating long trajectories (100M timesteps) for fairly large systems (~100K atoms). These calculations require large, parallel computers; and analyses of datasets require significant data storage.

POCs: Andrew Pohorille, andrew.pohorille@nasa.gov; Michael Wilson, michael.a.wilson@nasa.gov, (650) 604-5496, NASA Ames Research Center

Mission Impact: Goals to understand the origins of life are in the NASA Strategic Plan and the NASA Astrobiology roadmap; HECC resources support research that is an essential aspect of the origins of cellular life—the emergence and early evolution of protein structure and function.

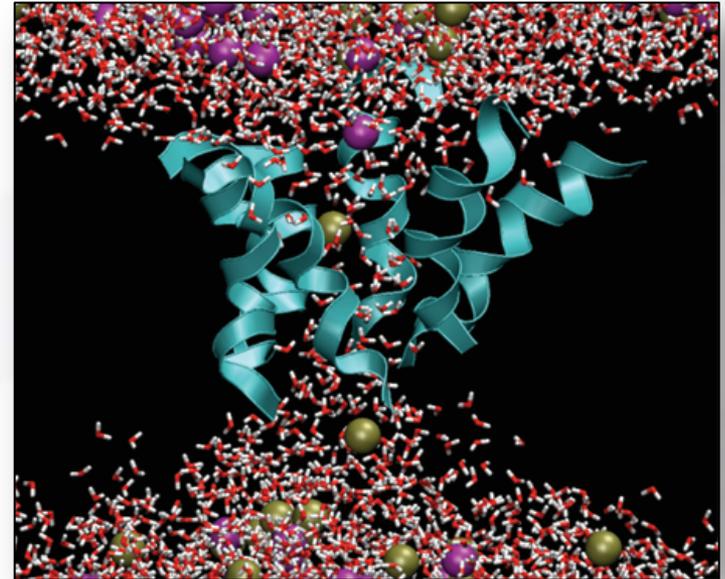


Figure: An antiameobin ion channel containing six helices (blue) surrounding a water-filled pore (oxygen in red, hydrogen in white). Potassium (gold) and chloride (magenta) are transported via the channel in the presence of an electric field. For clarity, membrane phospholipids are not shown (Michael Wilson, NASA/Ames)

Prediction of Jet Engine Fan Noise Using Computational Aeroacoustics



- Using HECC resources, researchers at NASA Glenn are running a state-of-the-art computational code to predict the noise signature of a realistic jet engine fan to support NASA's goal to improve aircraft performance.
- The NASA Broadband Aeroacoustic Stator Simulation (BASS) computational aeroacoustics (CAA) code is designed to accurately predict the unsteady flow and noise in highly complex flows such as those produced by jet engine fans.
- This tool will be invaluable for developing methods for reducing fan noise with minimal performance penalties.
- Even with the high-resolution capabilities of the BASS CAA code, a large number of grid points and time steps are required to accurately predict the unsteady flow and noise in a jet engine fan.
- HECC supercomputing and storage resources provide the enormous computational horsepower required to compute the flows and then store the resulting solutions.

Mission Impact: HECC supercomputing resources enable development of computational prediction methods for improving aircraft performance while reducing jet fan noise, emissions, and fuel burn.

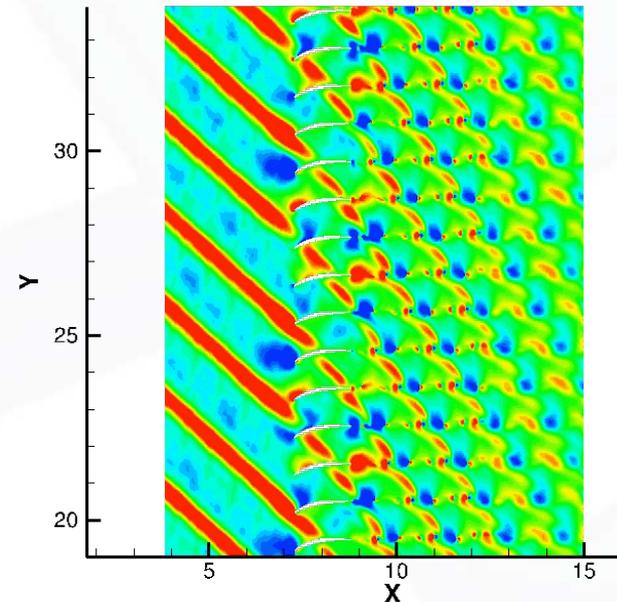


Figure: Snapshot of the interaction of rotor wakes with stator vanes at a radial location of 8.8 inches. (Duane Hixon, NASA/Glenn)

POC: Ray Hixon, duane.r.hixon@nasa.gov, (216) 433-2061, NASA Glenn Research Center

Error-Controlled Simulation Database for Orion Pad Abort Test



- Researchers at NASA Ames have run thousands of numerical simulations on Pleiades to generate an extensive, error-controlled database to support the Pad Abort 1 (PA-1) flight test of the Orion Multi-Purpose Crew Vehicle.
- Over 15,000 numerical simulations were performed to predict aerodynamic performance and flight loads on the vehicle for the PA-1 test flight.
- Simulations were performed primarily using NASA's Cart3D computational fluid dynamics code; analyses employed a new error-control capability that selectively adapts key regions of the computational mesh to minimize resolution-related error in the aerodynamic loads.
- Flight loads and aerodynamic performance data from these simulations were used to develop the guidance and control system for the vehicle, assess structural design criteria, and ensure the crew module could separate safely from the rest of the Launch Ascent Vehicle.
- HECC code optimization support resulted in executables that improved from ~8% of theoretical peak to ~25% for fully featured simulations of the complete vehicle.

Mission Impact: HECC supercomputing resources and support services enabled thousands of numerical simulations to be performed to give a detailed quantitative understanding of Orion's performance for several design iterations, from concept through the highly-successful flight-test.

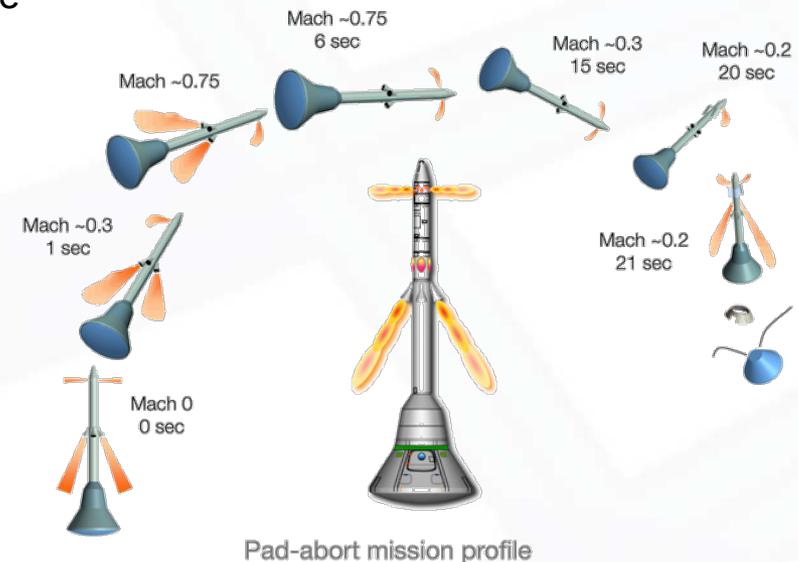


Figure: Pad Abort 1 (PA-1) flight test mission profile. (Michael Aftosmis, NASA/Ames)

POC: Michael Aftosmis, michael.aftosmis@nasa.gov, (650) 604-4499, NASA Ames Research Center



Installation of GPU Nodes Provides New Graphics Capability for Pleiades Users

- The Pleiades supercomputer has been expanded to include 64 new Intel Xeon 5600 (Westmere) nodes with graphics processing units (GPUs), which will be used for accelerated computation and visualization.
- The new nodes, with NVIDIA M2090 GPUs, provide a testbed for HECC users experimenting with using general-purpose graphics processing unit (GPGPU) programming methods to enhance the performance of their codes on Pleiades.
- These more powerful nodes will also allow the HECC visualization team to manage larger datasets and produce both traditional and concurrent visualizations more quickly.
- The new nodes are still in the testing and configuration phase; input from both HECC application and visualization experts, along with selected users, is being considered as the node configuration evolves.

Mission Impact: The incorporation of graphics processing units into the Pleiades supercomputer configuration provides a testbed for NASA users experimenting with GPGPU programming to test its viability for improving their application performance.

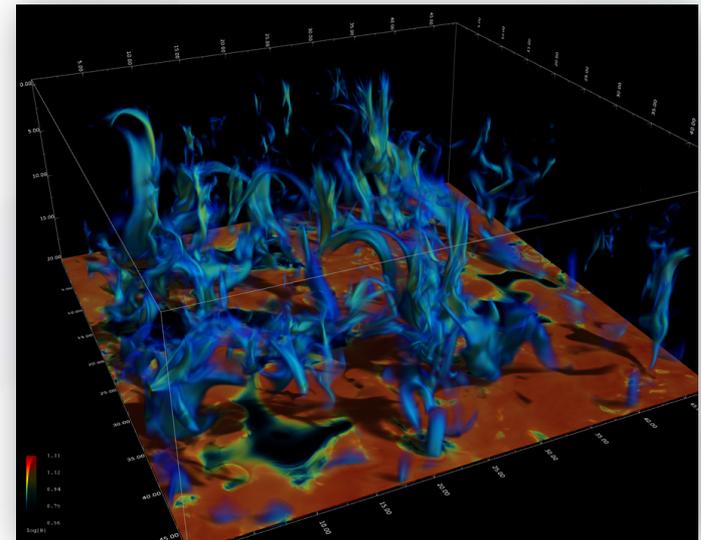


Figure: This visualization produced using solar magneto-hydrodynamics data was rendered in half the time on the new GPU (Westmere) nodes, compared to the older quad-core Opteron processors on the hyperwall-2 system.

POC: Bob Ciotti, bob.ciotti@nasa.gov, (650) 604-4408,
NASA Advanced Supercomputing Division



New Pleiades Filesystem Deployed with 10x Increase in IOPS Performance

- A new Pleiades Lustre filesystem, named nobackupp1, has been deployed and will replace nobackupp10.
- The new filesystem has double the disk capacity and will provide 10x the Input/Output Operations Per Second (IOPS) performance of the old filesystem.
- The 10-fold improvement in IOPS addresses a deficiency in the previous RAID controller, and will provide better interactive filesystem performance to researchers.
- The remaining filesystems on Pleiades will also be upgraded to attain the 10x improvement in IOPS.
- Data is being transferred on a user-by-user basis, to minimize the disruption to researchers on the filesystem; all nobackupp10 users will be transitioned by mid-August 2011.

Mission Impact: Along with the increased computational capability of Pleiades, faster and larger scratch space is needed to enable researchers to more fully utilize the system.

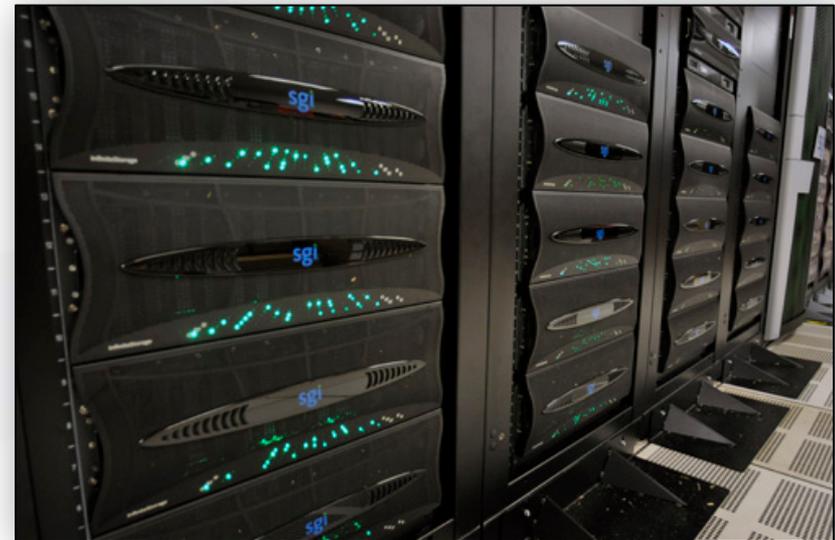


Figure: The new Data Direct Networks (DDN) RAID controllers provide a 10x improvement in IOPS performance, which, combined with increased hard drive storage density, substantially enhances HECC filesystem capabilities.

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NASA Advanced Supercomputing Division



Record Usage Shows Pleiades Provides Maximum Resources for NASA Missions

- July 2011 showed record high usage of HECC's Pleiades supercomputer.
- Over 4.5 million Standard Billing Units (SBUs) were used by NASA's Mission Directorates and Mission Support organizations.
- This increase was enabled by the recent installation and integration of new resources into the Pleiades system, increasing Pleiades capacity by 10% and providing more than 1 petaflop of computing power.
- Researchers in the Science Mission Directorate were the biggest users, almost doubling their usage from Feb 2011 (see slide #10).
- Computing resources continue to expand and are made available to users from all Mission Directorates to support their computing needs.

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

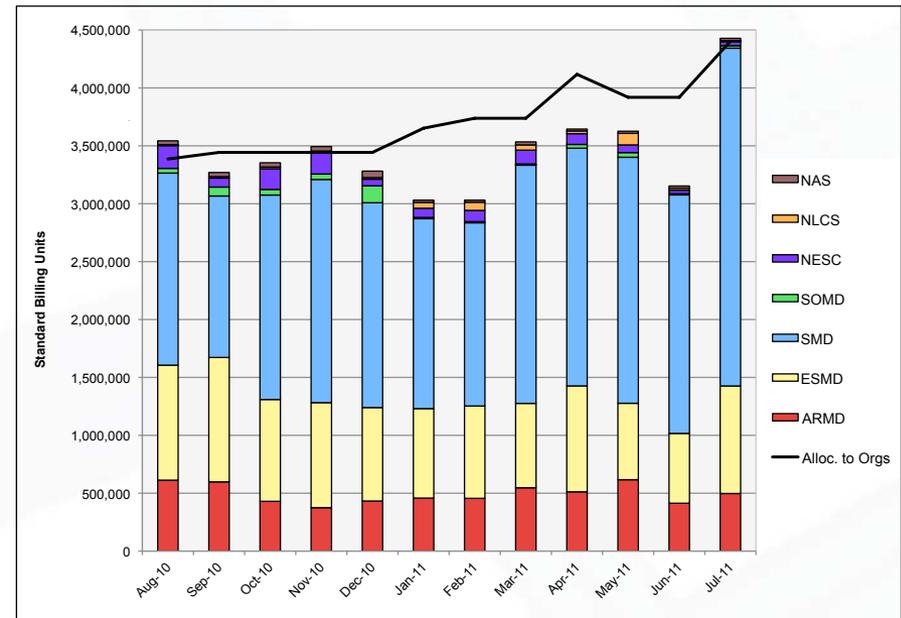


Figure: Utilization of Pleiades by all Mission Directorates and support organizations. Data is shown in Standard Billing Units (SBUs), where one SBU is equivalent to one node hour of a 12-core Westmere node of Pleiades. Data is normalized to 30-day months.

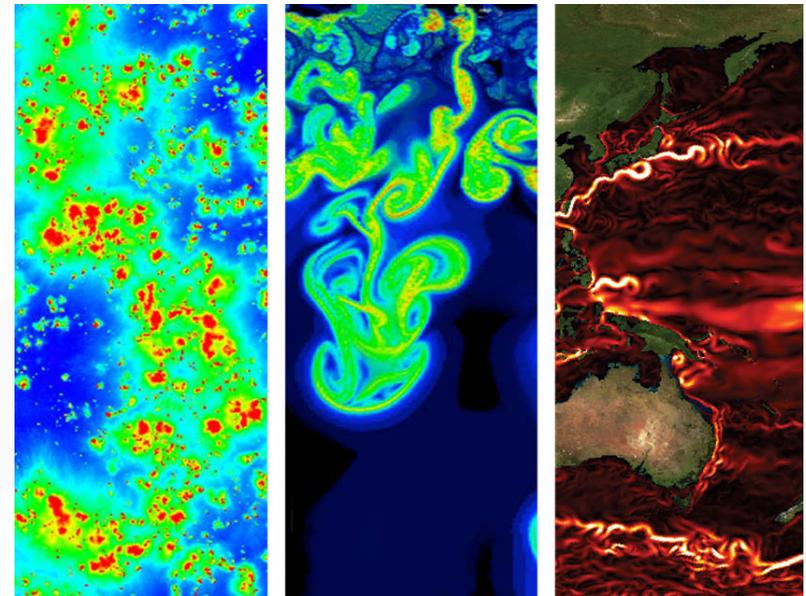
POC: Catherine Schulbach, catherine.h.schulbach@nasa.gov,
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SMD Usage of Pleiades Doubles in Six Months

- Since February 2011, the Science Mission Directorate (SMD) increased its usage of supercomputing resources provided by the HECC Project by 88%.
- SMD used over 3 million SBUs in July, compared to 1.6 million SBUs in February.
- July usage was also more than 0.75 million SBUs greater than the previous highest monthly usage (2.25 million SBUs in May 2011) – this represents an increase of 33% in 2 months.
- The increase was due to a recent 10% increase in the Pleiades' supercomputer resources, and to borrowing unused resources from other Mission Directorates.
- Within SMD, astrophysics work increased by 703K SBUs, Earth science by 494K, and heliophysics by 273 K; planetary science remained relatively flat with an increase of 55K.
- Seven projects increased usage by more than 100K SBUs during this six-month period.

Mission Impact: Increasing system capacity provides NASA Mission Directorates with the computational resources to support the research and engineering needed to accomplish their goals and objectives.



Figures: Samples of work of top users of SMD computer time. (Left to right) Digital signatures of cosmological reionization, R. Cen, Princeton Univ.; Solar convection zone, R. Stein, Michigan State Univ.; Earth's ocean and sea ice system, D. Menemenlis, JPL, and C. Hill, MIT.

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HECC Network Team Hosts Meeting With LBNL/NERSC For Information Exchange



- On June 15, the HECC Network team hosted a visit by network engineers from the National Energy Research Scientific Computing Center (NERSC), Lawrence Berkeley National Laboratory, and the Joint Genome Institute.
- Engineers discussed common problems encountered by users, as well as architecture and design, procedures, usability, security infrastructure, and network analysis tools.
- NERSC staff are particularly interested in the HECC-developed tools for network monitoring and analysis, and expressed interest in working with HECC network engineers to incorporate these tools into their environment.
- NERSC also expressed interest in HECC's cabling infrastructure, and has requested information about our approach and products used in the most recent build-out of the main computer room.
- The Network team is following up with NERSC to seek similar network design ideas for increased usability with remote file transfers, and more proactive security techniques.

Mission Impact: By meeting with other high-performance computing sites, HECC experts are able to exchange ideas and compare technique, ultimately improving the NASA user community environment .

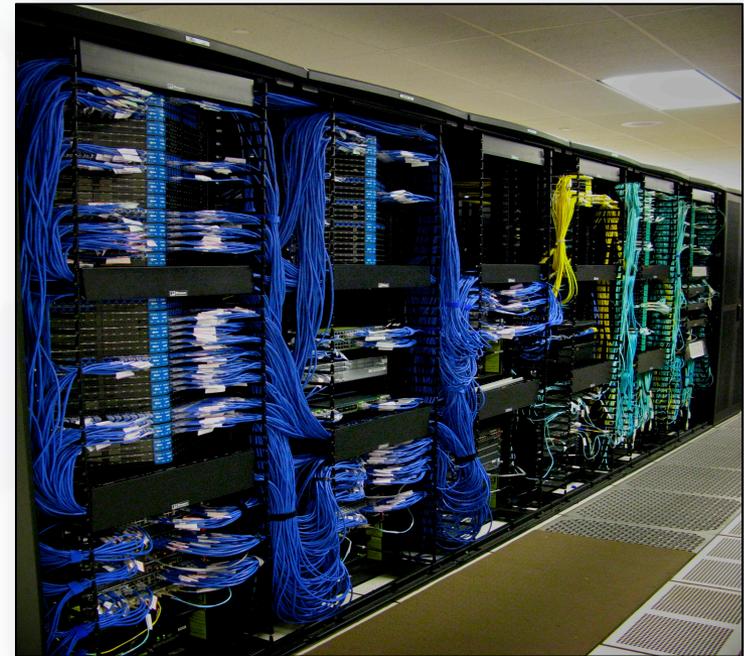


Figure: The photo above shows the HECC networking racks for the HECC Enclave.

POC: Nichole Boscia, nichole.k.boscia@nasa.gov, (650) 604-0891, NASA Advanced Supercomputing Division, Computer Sciences Corp.

HECC Teams Respond Quickly to Facility Emergency Scenario



- In June, a pump failure in the computing facility's chiller system caused chillers to immediately begin shutting down, and the computer room floor temperature to rise.
- The system that monitors the facility triggered alarms, and HECC Control Room staff (onsite 24x7), along with facility personnel, responded within 10 minutes to initiate emergency shutdown procedures.
- Process changes implemented after a previous nearly disastrous result to a cooling system failure were executed providing a "real world" validation of the process changes under high-stress conditions.
- HECC staff completed a smooth shutdown of all specified systems within 20 minutes of the initial alarm preventing the facility from ever reaching critical temperature set points and allowing all file systems to remain unaffected. Full service was restored later that afternoon, with no damage to equipment or hardware.

Mission Impact: HECC personnel averted a potential disaster during a chiller pump failure that could have resulted in costly equipment damage and many hours of lost computational time for Mission Directorate projects by learning from past mishaps and implementing processes that prevent future occurrences.



Figure: Screenshot of the Facility Monitoring and Control system used to monitor the NASA Advanced Supercomputing facility.

POC: Leigh Ann Tanner, leighann.tanner@nasa.gov, (650) 604-4468, NASA Advanced Supercomputing Division, Computer Sciences Corp.

HECC Facility Hosts Several Visitors and Tours in July 2011



- HECC hosted 12 scheduled tour groups in July; guests received an overview of the HECC Project, demonstrations of the hyperwall-2 visualization system, and tours of the computer room floor:
- Steven Cain, NASA KSC, Commercial Crew Program Office (CCPO) and Partner Insight Development (Space X), met with Ames staff to discuss how we assist CCPO when needed for SpaceX-related activity; this group received a tour and demo during their visit.
- SGI CEO Mark Barrenechea, and SGI Board of Directors member Doug King, met with Bill Thigpen and toured the facility.
- 101 Ames summer students from various internship programs toured the facility.
- 25 participants in the Teacher Professional Development Program, hosted by the NASA Ames Aeronautics Directorate, gathered ideas for encouraging their students to pursue education in Science, Technology, Engineering, and Mathematics (STEM) fields.
- 22 Singularity University students representing 14 countries expressed excitement about their tour of the supercomputing facility and hyperwall-2 system.



Figure: Singularity University students attend a demonstration of the hyperwall -2 visualization system, as part of their tour of the NASA Advanced Supercomputing facility.

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

Presentations and Papers



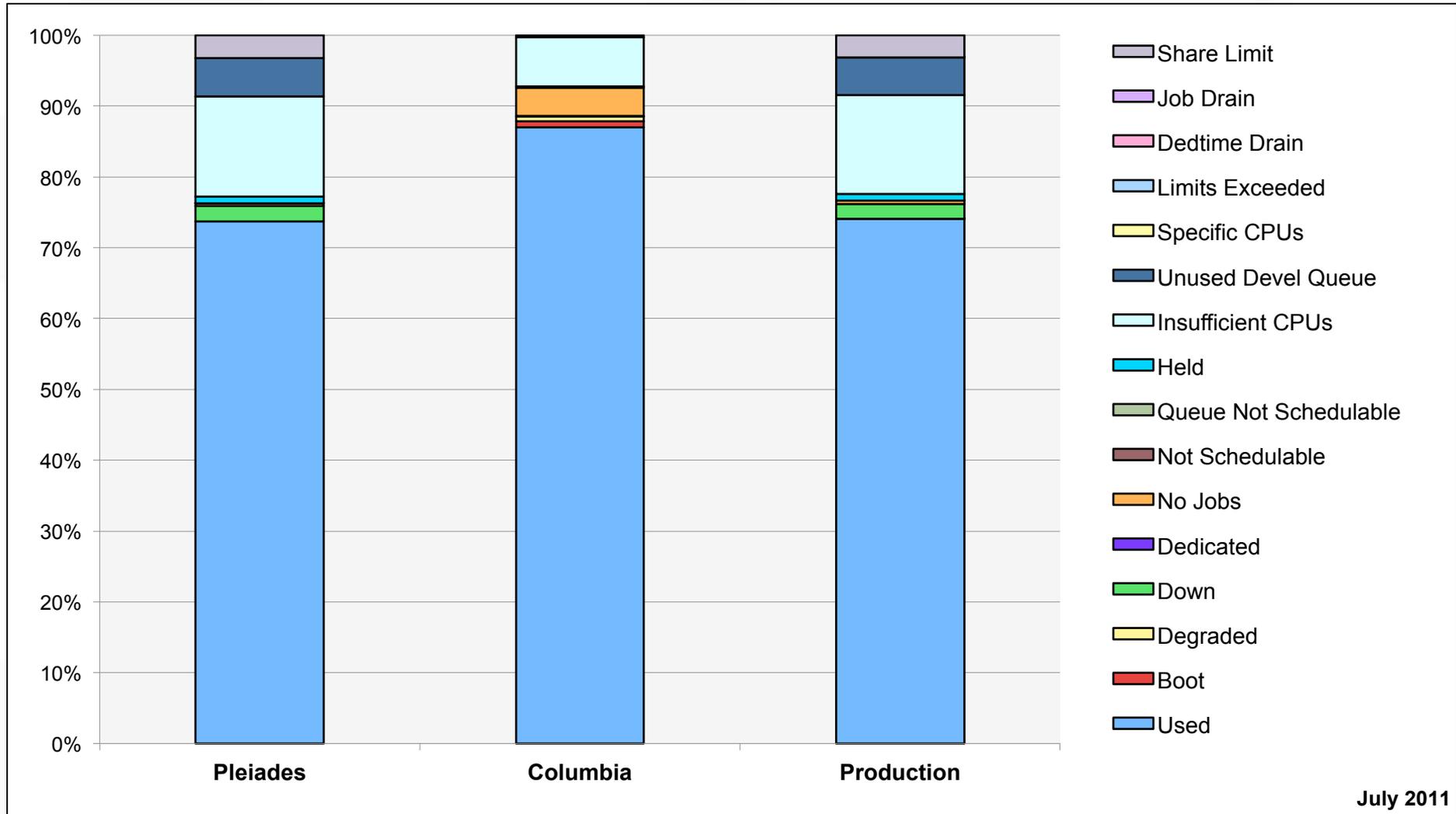
- “Engineering Analysis and the Safety Case,” D. Mathias, presented at the NASA System Safety Steering Group F2F, July 12-14, Washington, D.C.*
- “Particle simulations of space weather,” G. Lapenta, Journal of Computational Physics, * in progress, corrected proof at:
<http://www.sciencedirect.com/science/article/pii/S0021999111001860>
- “Magnetic Fields: Modeling and ATST Observations,” R. Stein et al, 200th American Astronomical Society, SPD meeting, Bulletin of the American Astronomical Society, Vol. 43, 2011, abstract at:
<http://adsabs.harvard.edu/abs/2011SPD....42.0804S> *

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



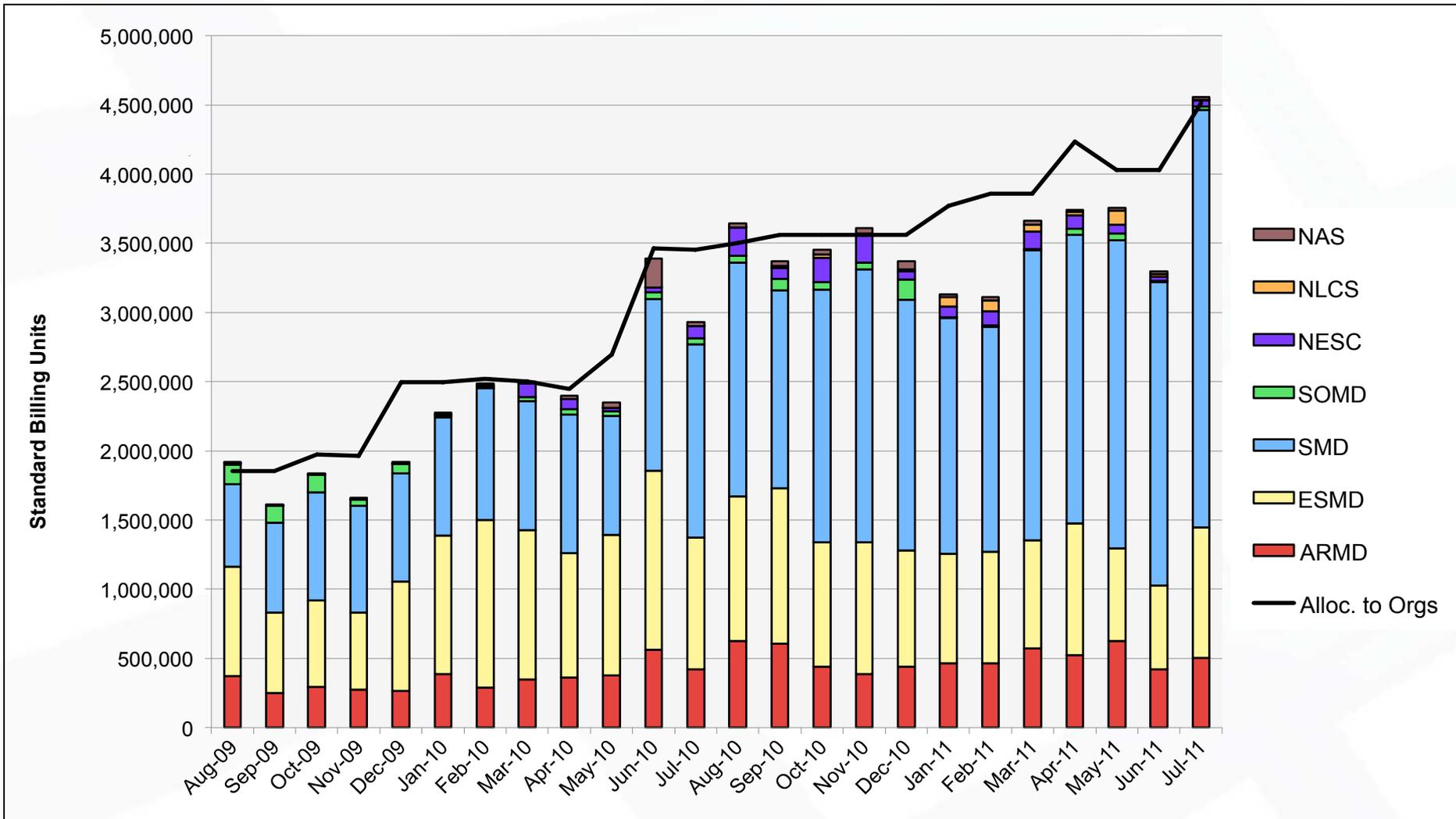
- **Space Shuttle, Silicon Valley have long and deep ties**, *San Jose Mercury News*, July 2, 2011 – Feature story with explanation of supercomputing's role in shuttle safety, with a quote from NAS researcher Stuart Rogers.
http://www.mercurynews.com/science/cj_18399027?nclick_check=1
- **SGI Revamps Altix ICE Design**, *HPCwire*, July 5, 2011 – Feature article on SGI's plans for fifth-generation Altix design, with a description of Pleiades and speculation about future performance enhancements.
http://www.hpcwire.com/hpcwire/2011-07-05/sgi_revamps_altix_ice_design.html?featured=top
- **Adler Planetarium Completes Massive NV-Powered Digital Projector**, *HotHardware.com*, July 11, 2011 – Multimedia feature that explains the HECC Visualization team's extensive work to create high-definition photos and animations for the Sky Theater.
<http://hothardware.com/News/Adler-Planetarium-Completes-Massive-NVPowered-Digital-Projector/>
- **Black Hole Collision May Have Set Off Fireworks in the Milky Way**, *Science*, July 27, 2011 – Article with link to paper citing Pleiades as resource used.
<http://news.sciencemag.org/sciencenow/2011/07/black-hole-collision-may-have-se.html?ref=hp>

NAS Utilization

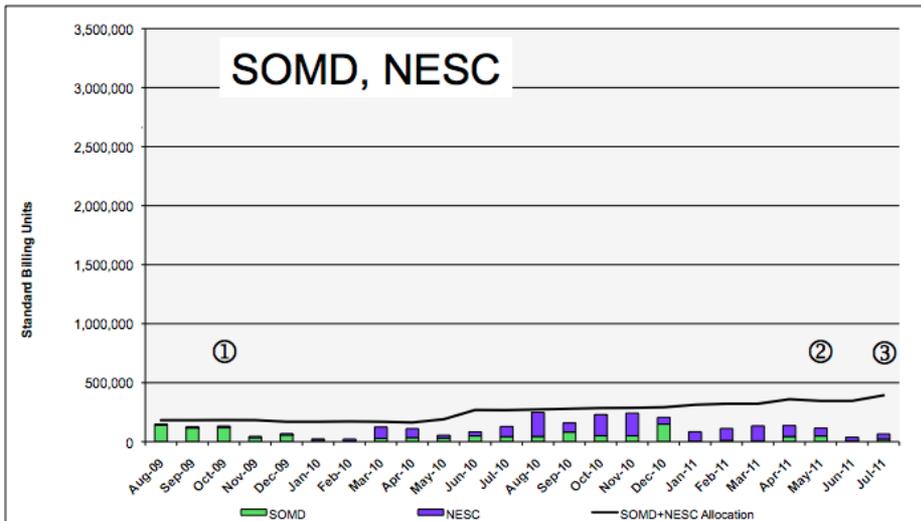
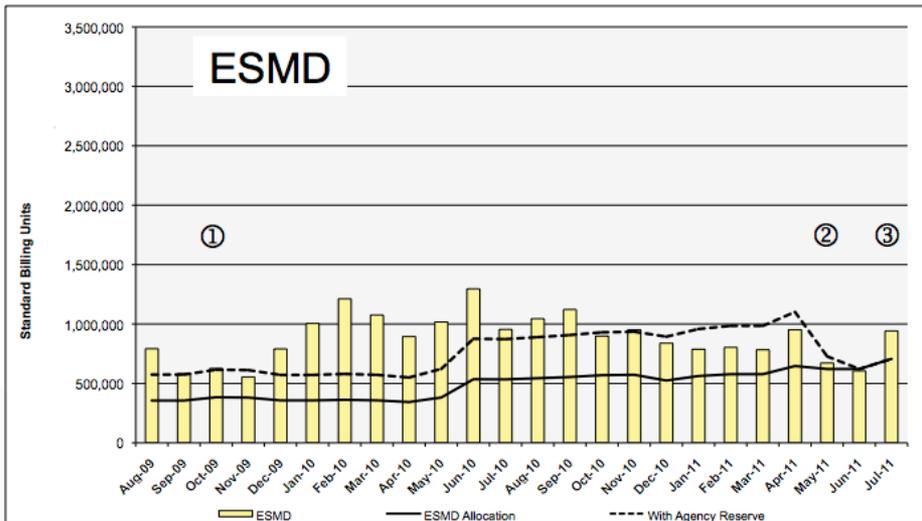
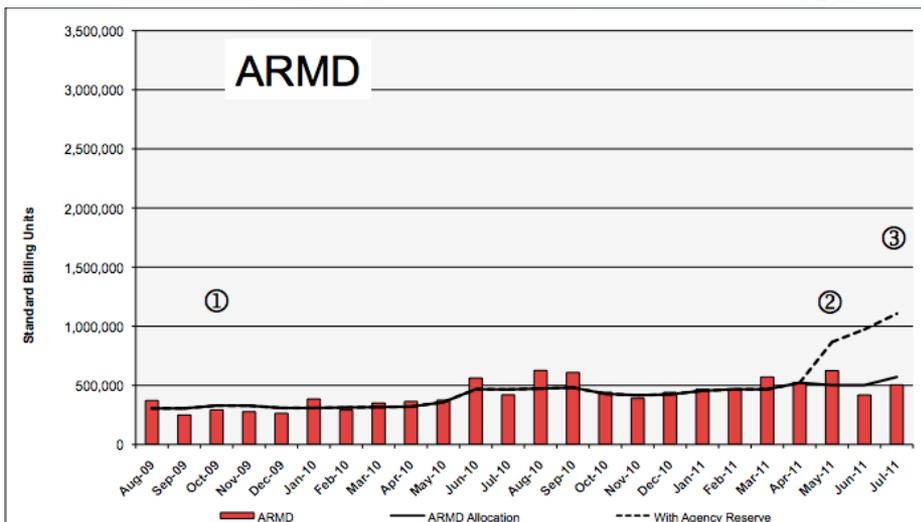
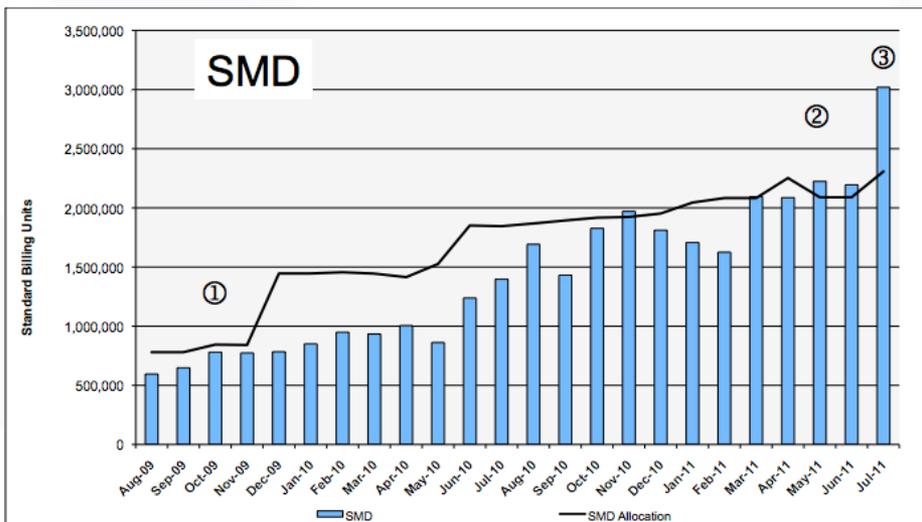


July 2011

NAS Utilization Normalized to 30-Day Month

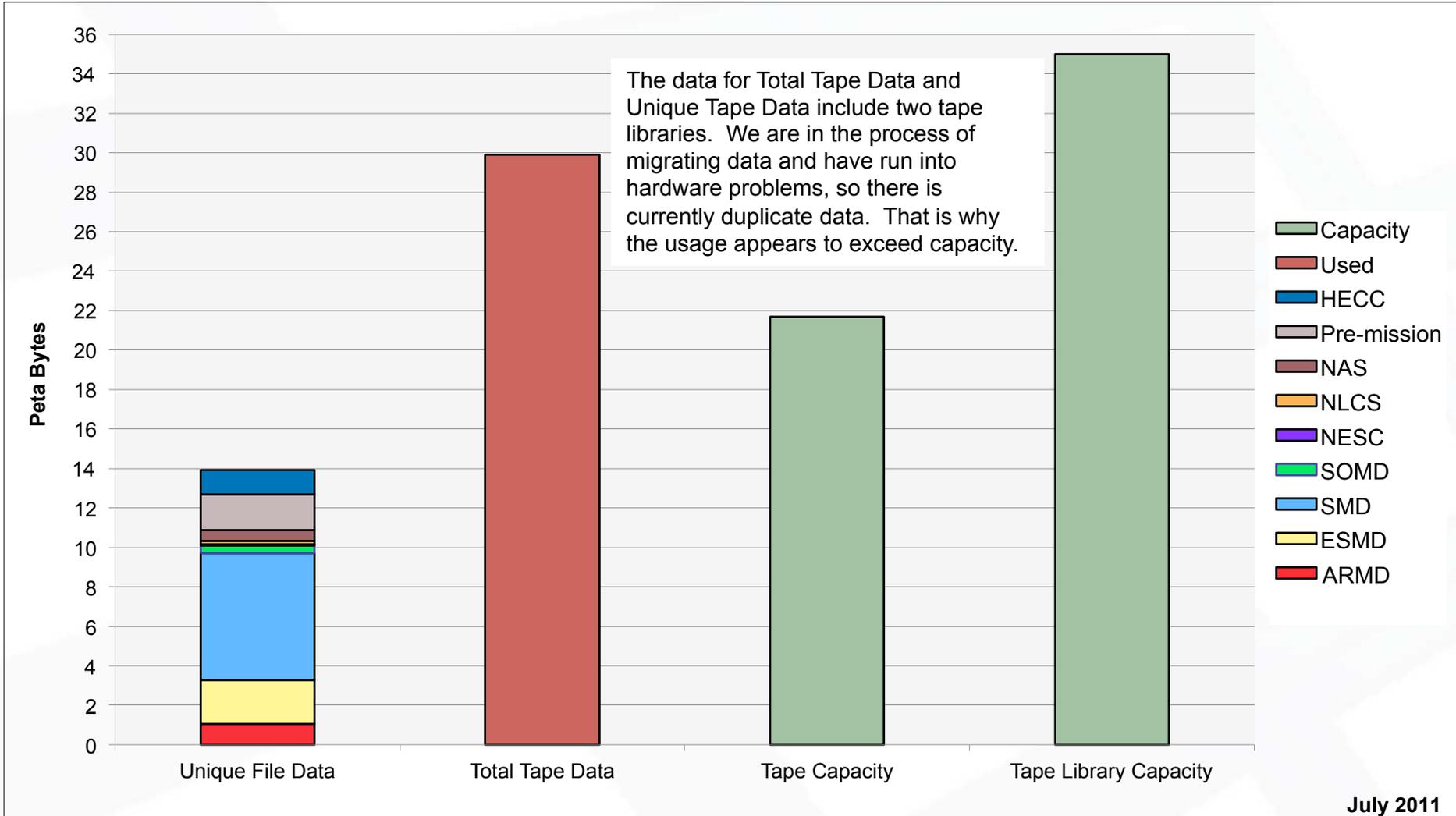


NAS Utilization Normalized to 30-Day Month



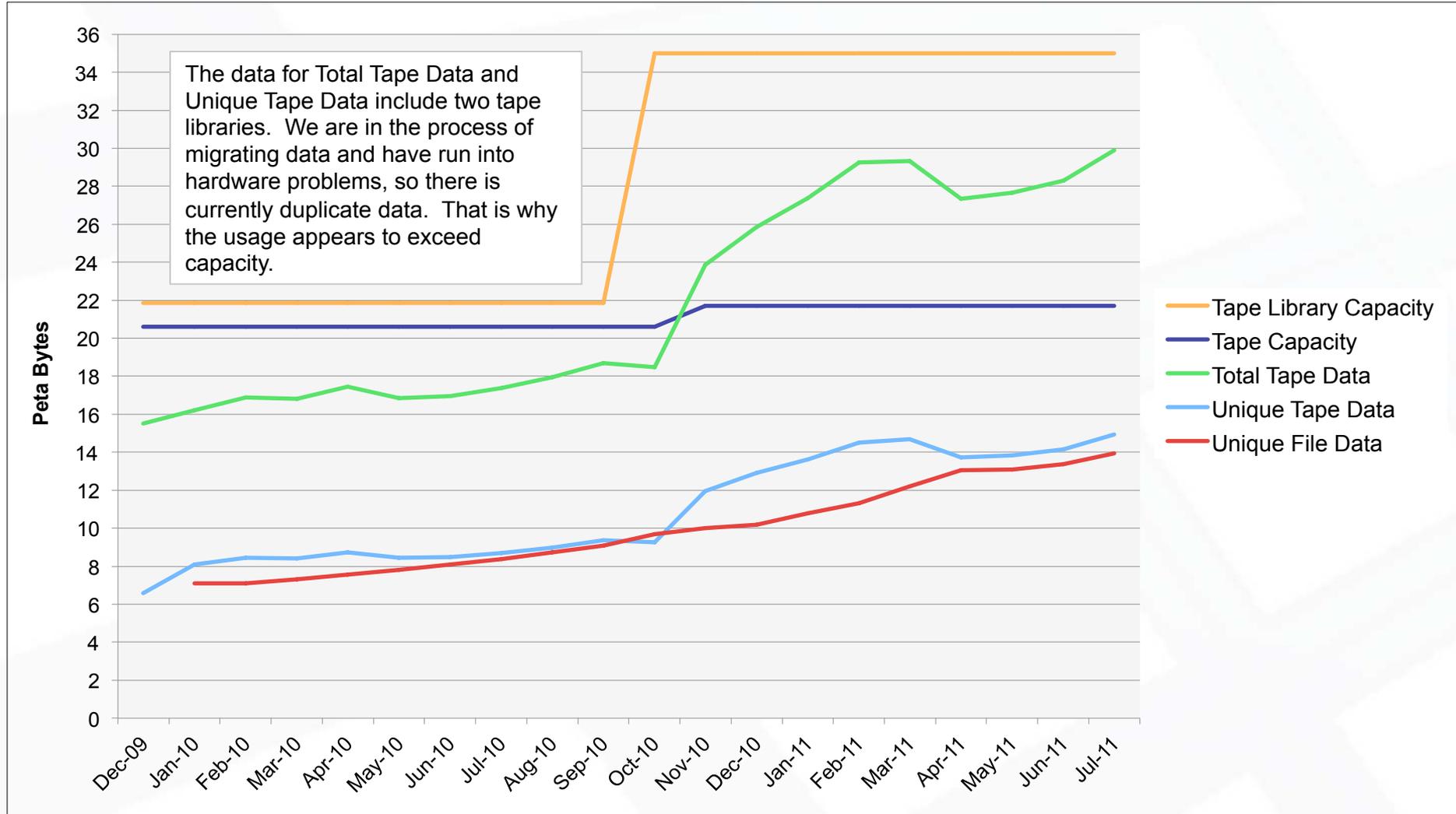
- ① Allocation to orgs. increased to 80%
- ② Allocation to orgs. decreased to 75%, Agency reserve shifted to ARMD
- ③ 14 Westmere racks added

Tape Archive Status

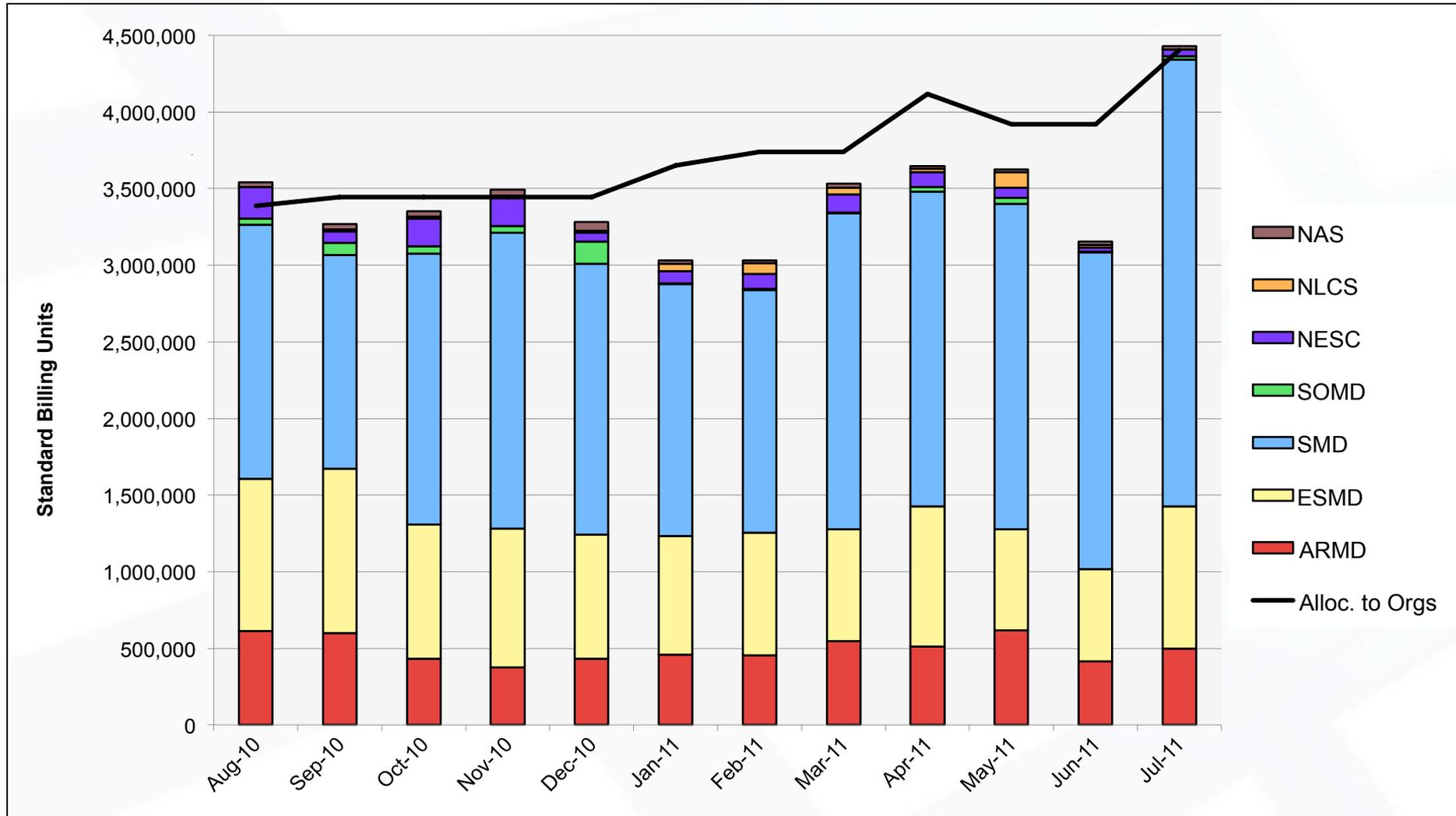


July 2011

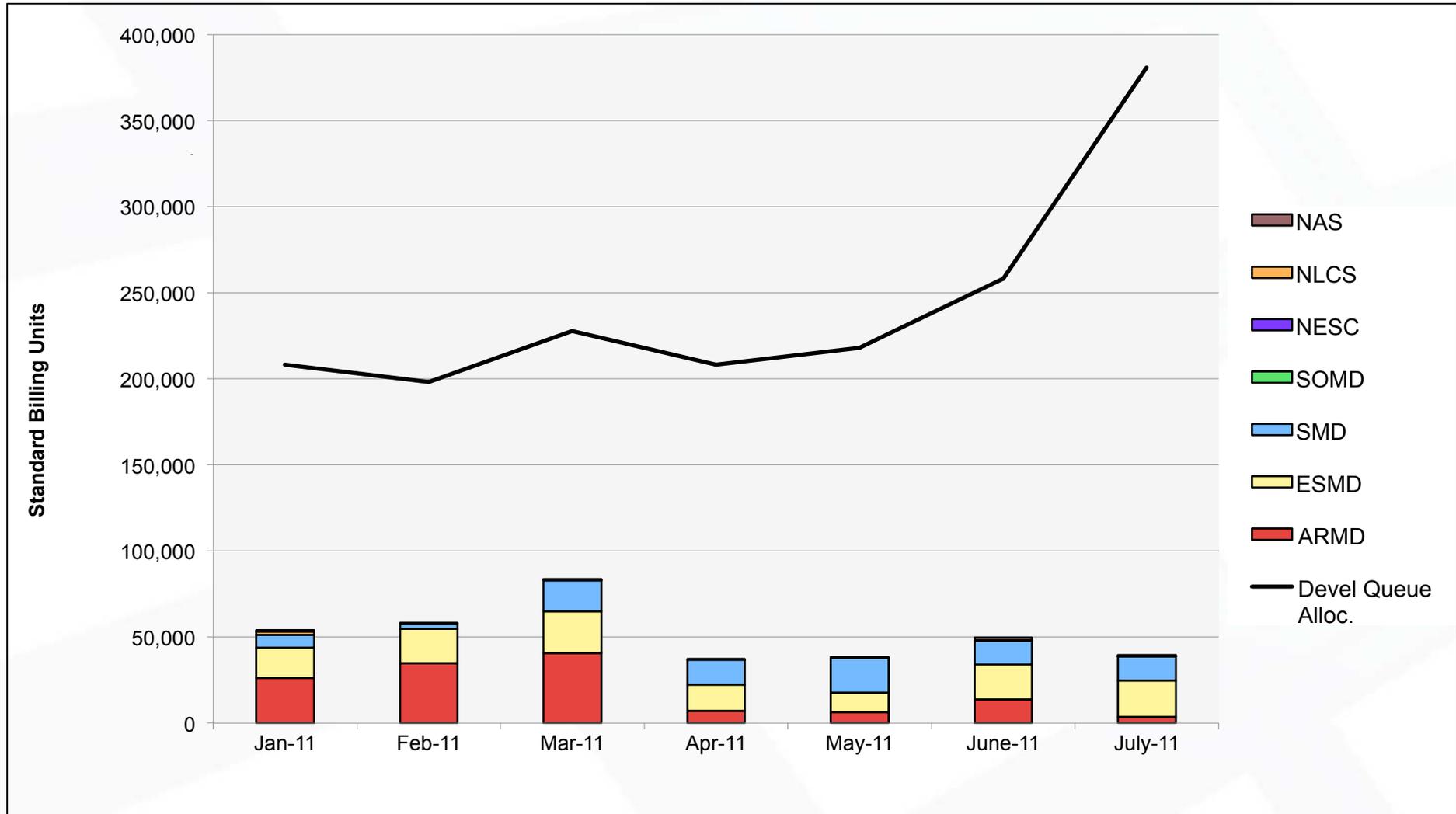
Tape Archive Status



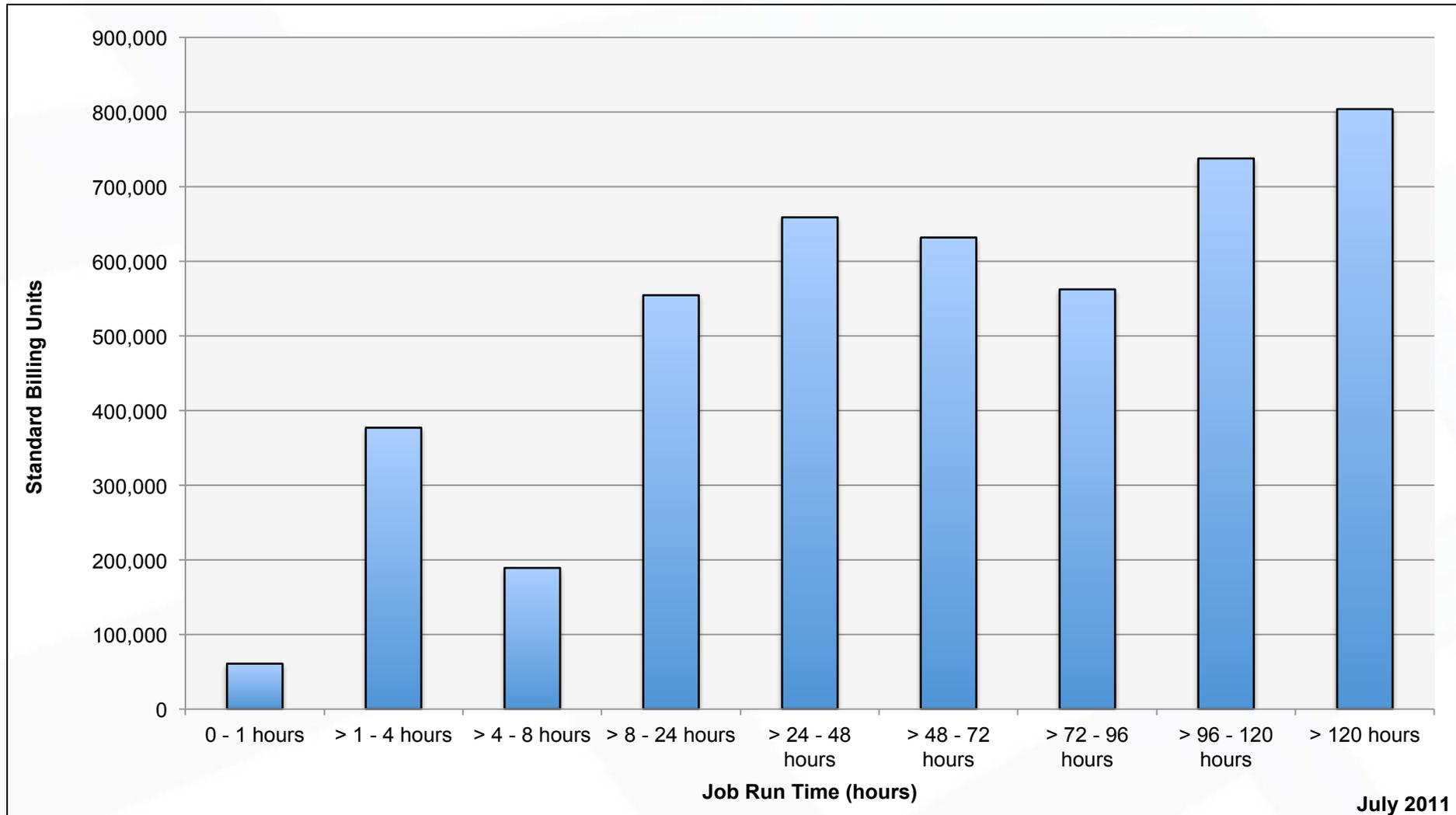
Pleiades: SBUs Reported, Normalized to 30-Day Month



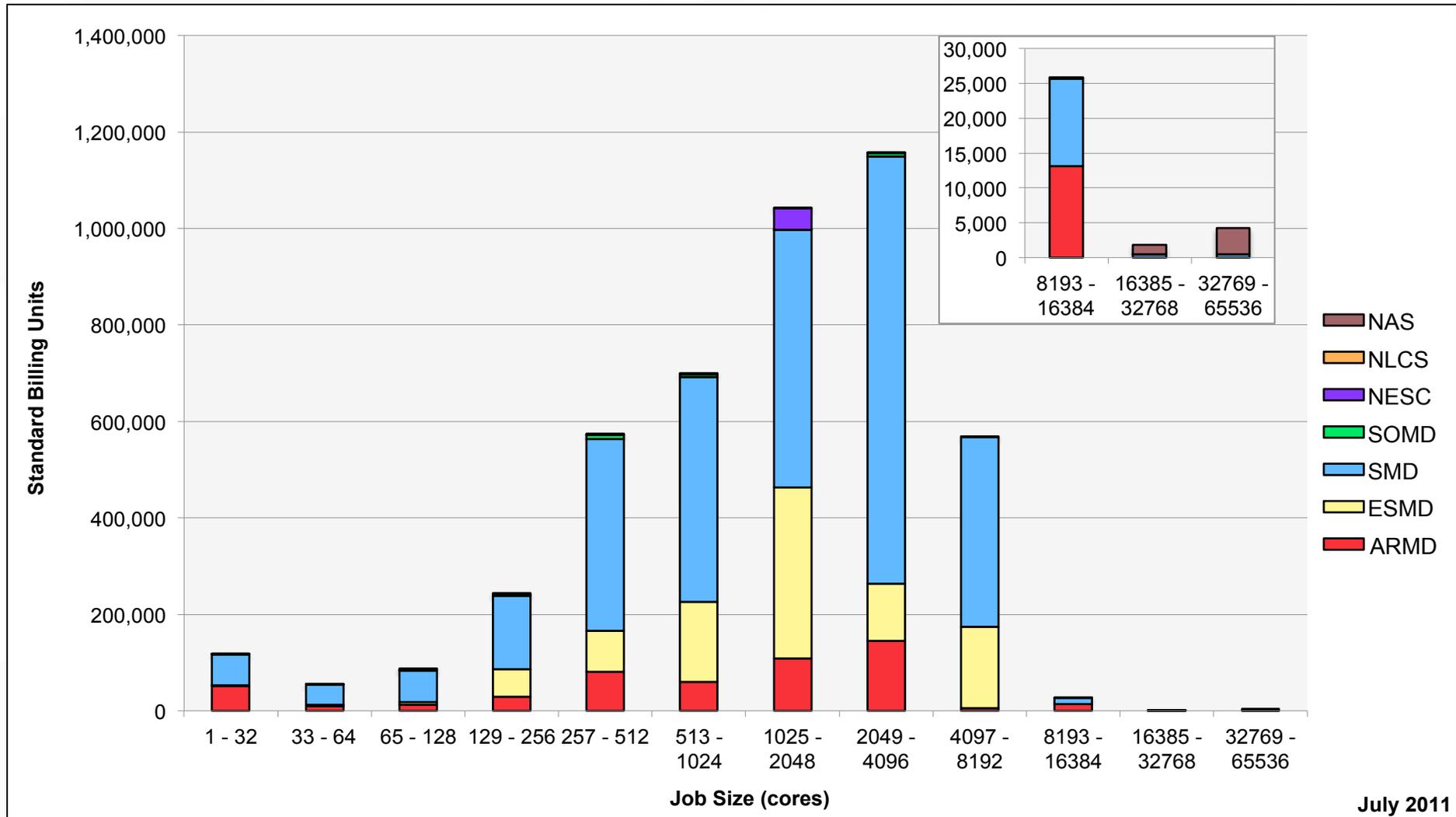
Pleiades: Devel Queue Utilization



Pleiades: Monthly SBUs by Run Time

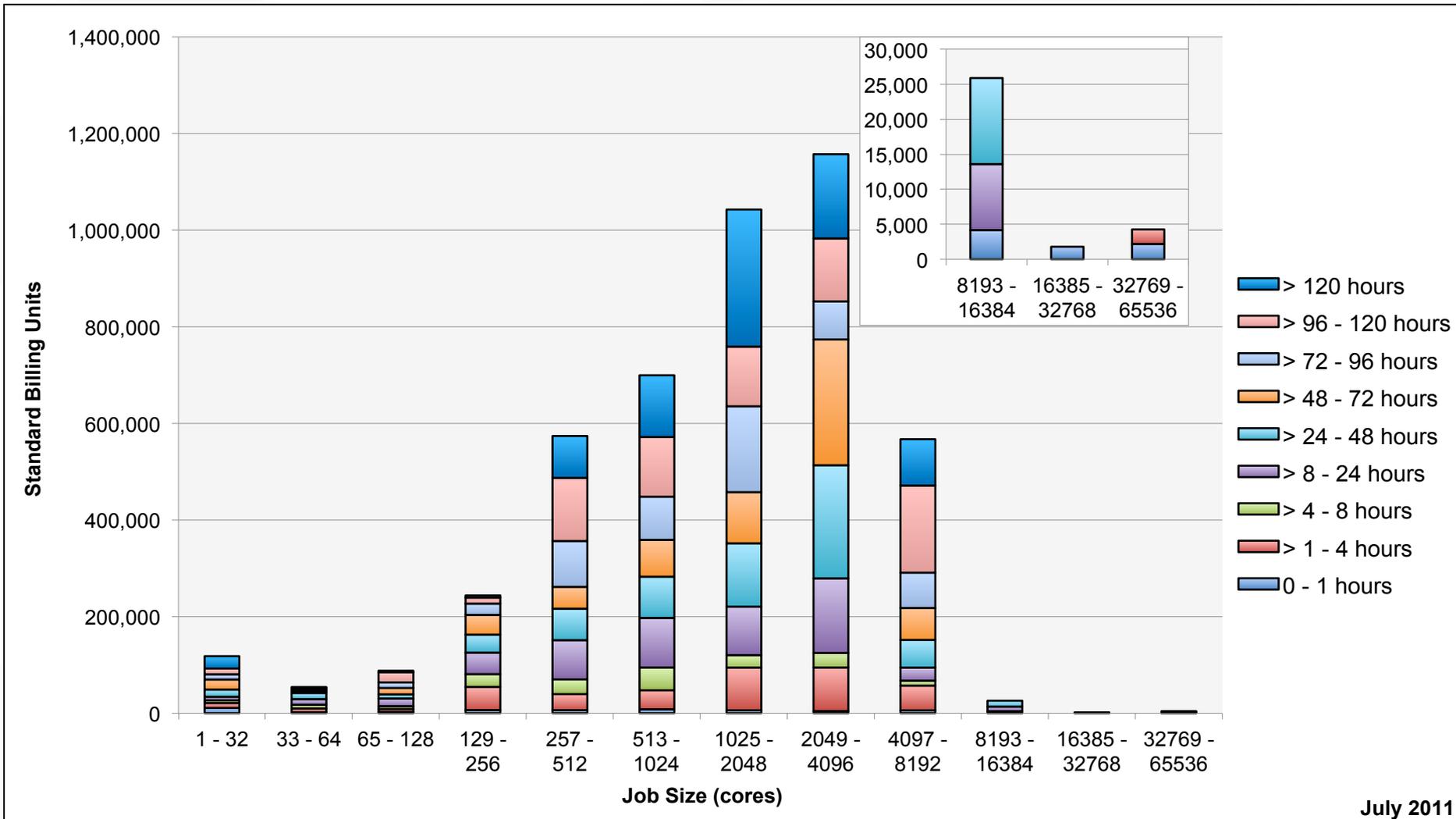


Pleiades: Monthly Utilization by Size and Mission



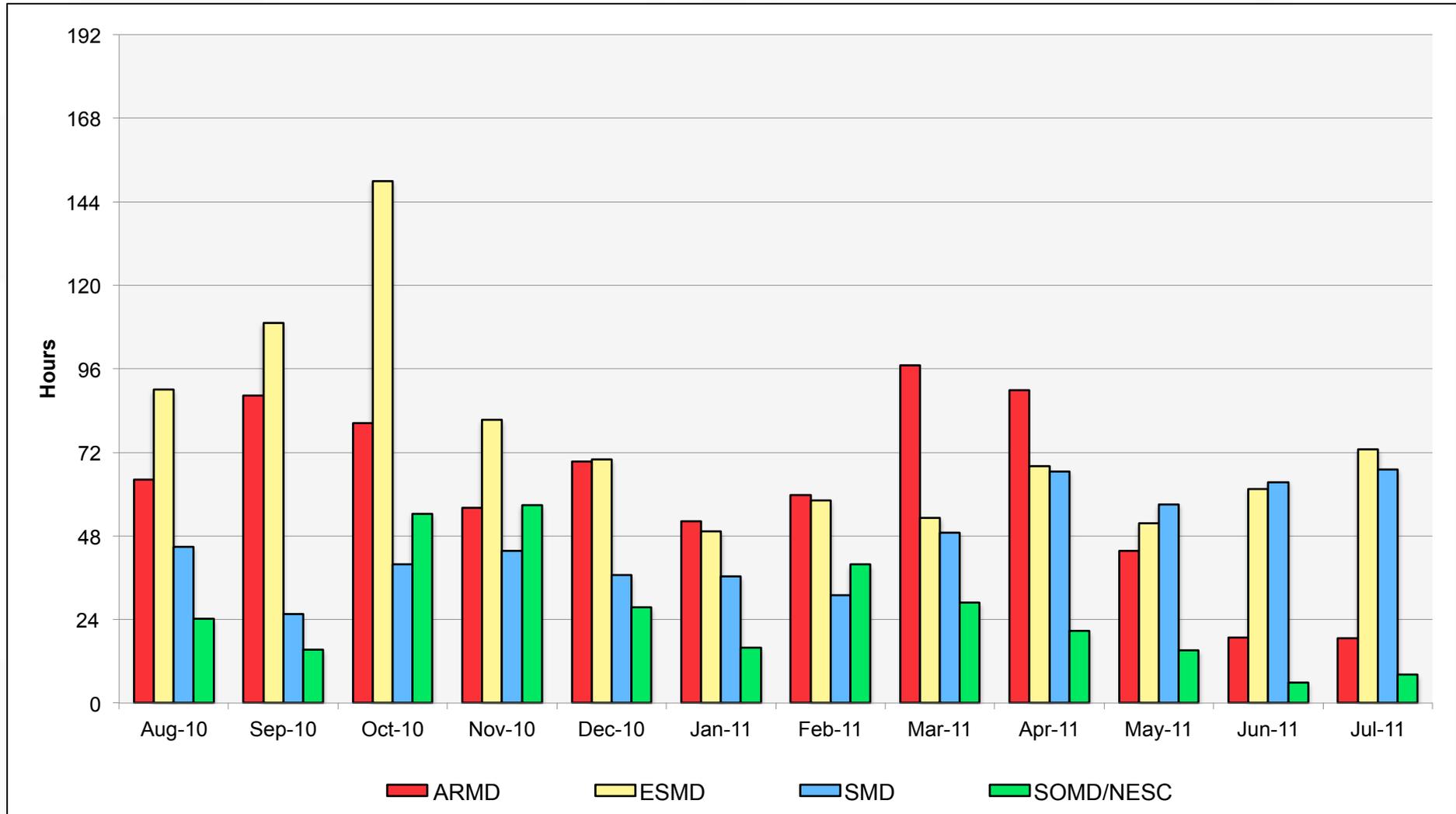
July 2011

Pleiades: Monthly Utilization by Size and Length

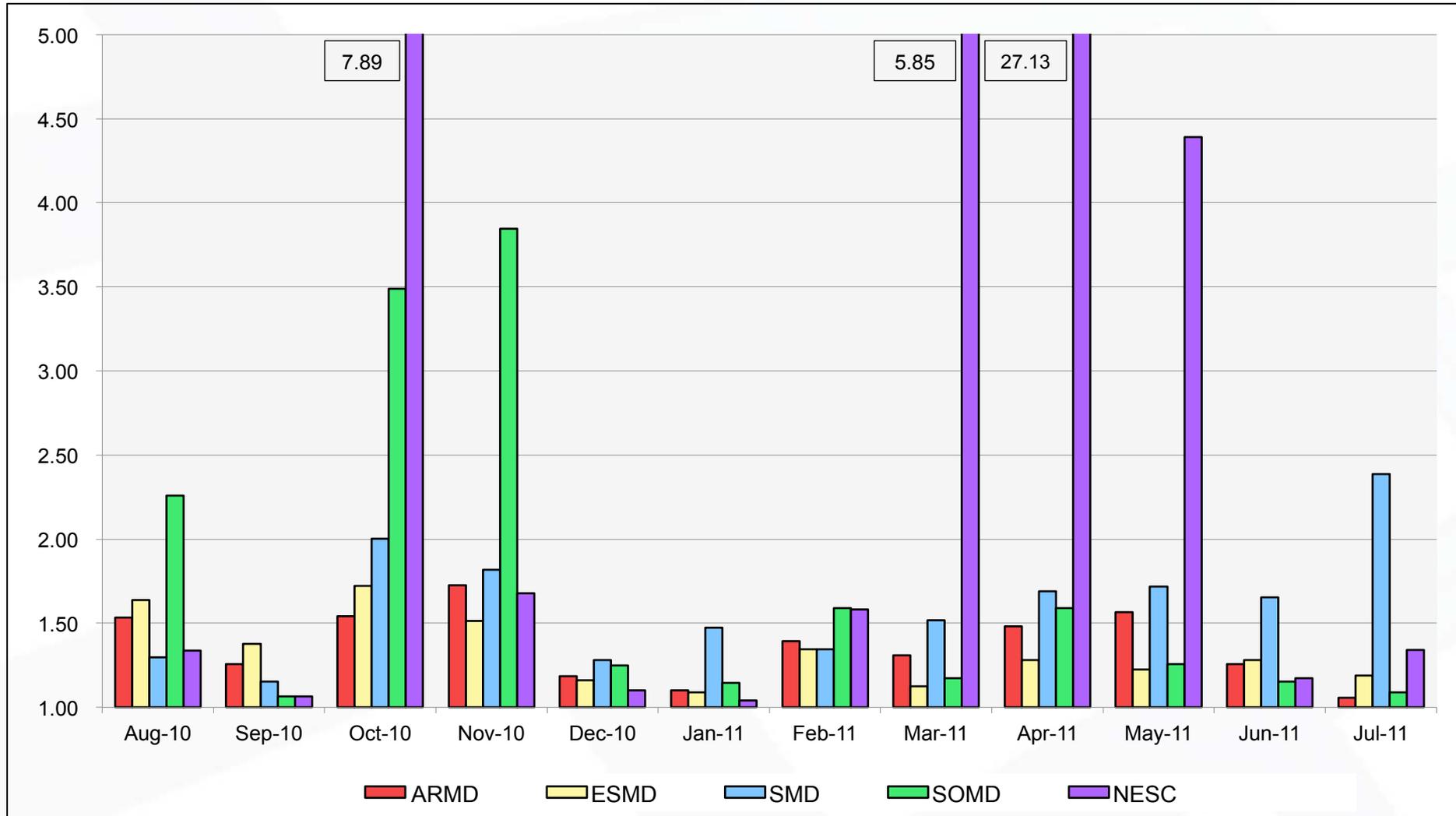


July 2011

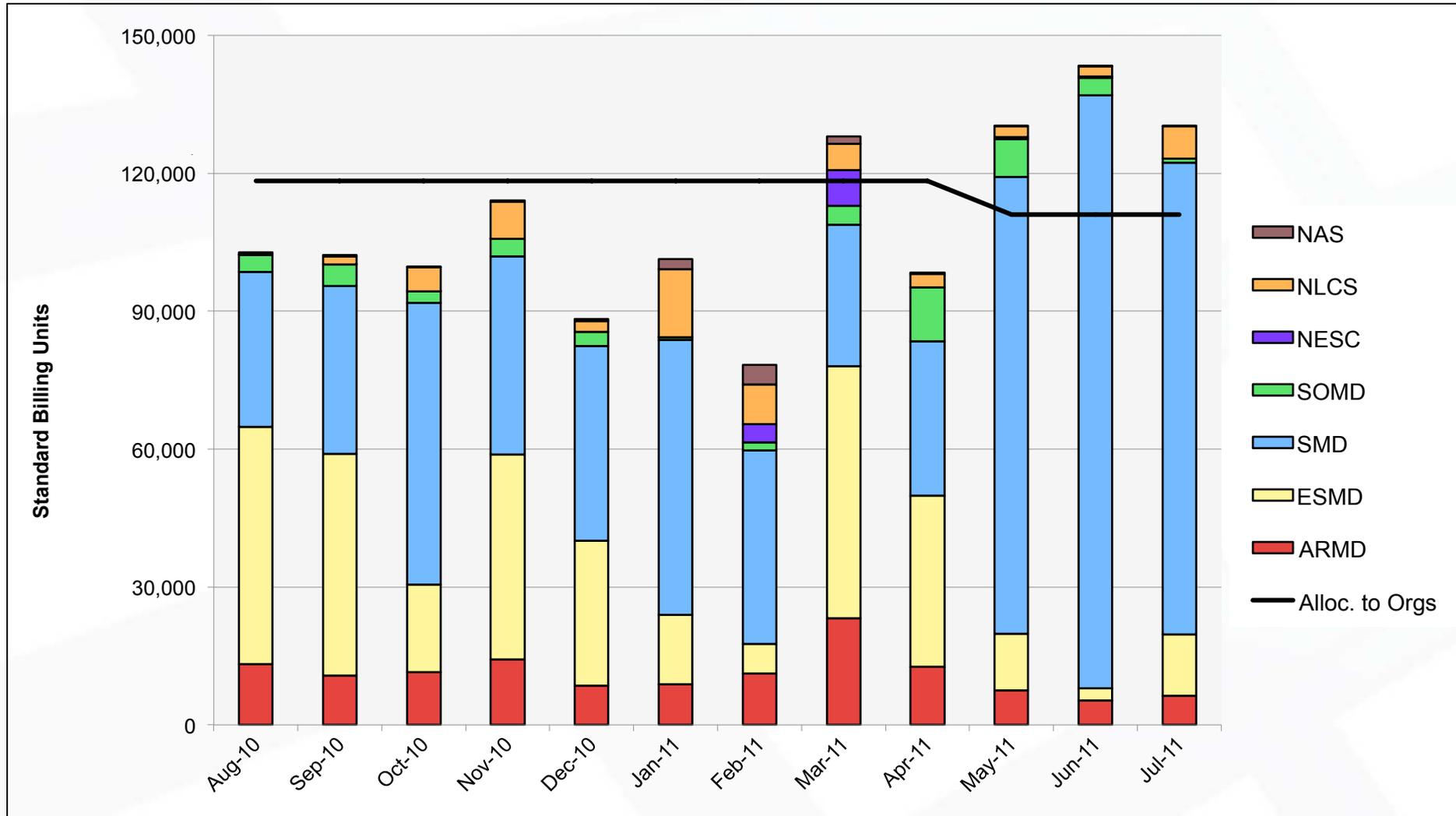
Pleiades: Average Time to Clear All Jobs



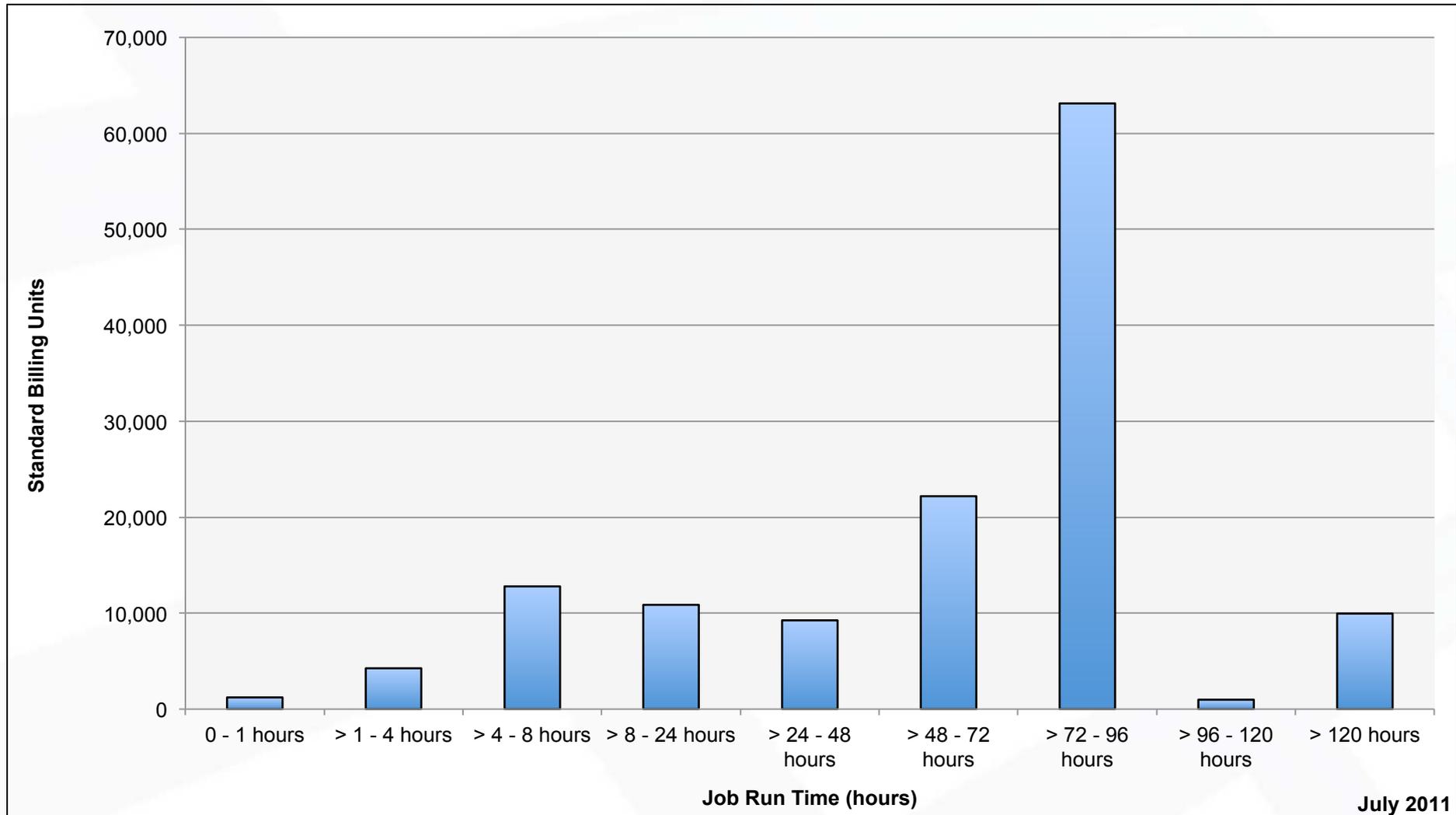
Pleiades: Average Expansion Factor



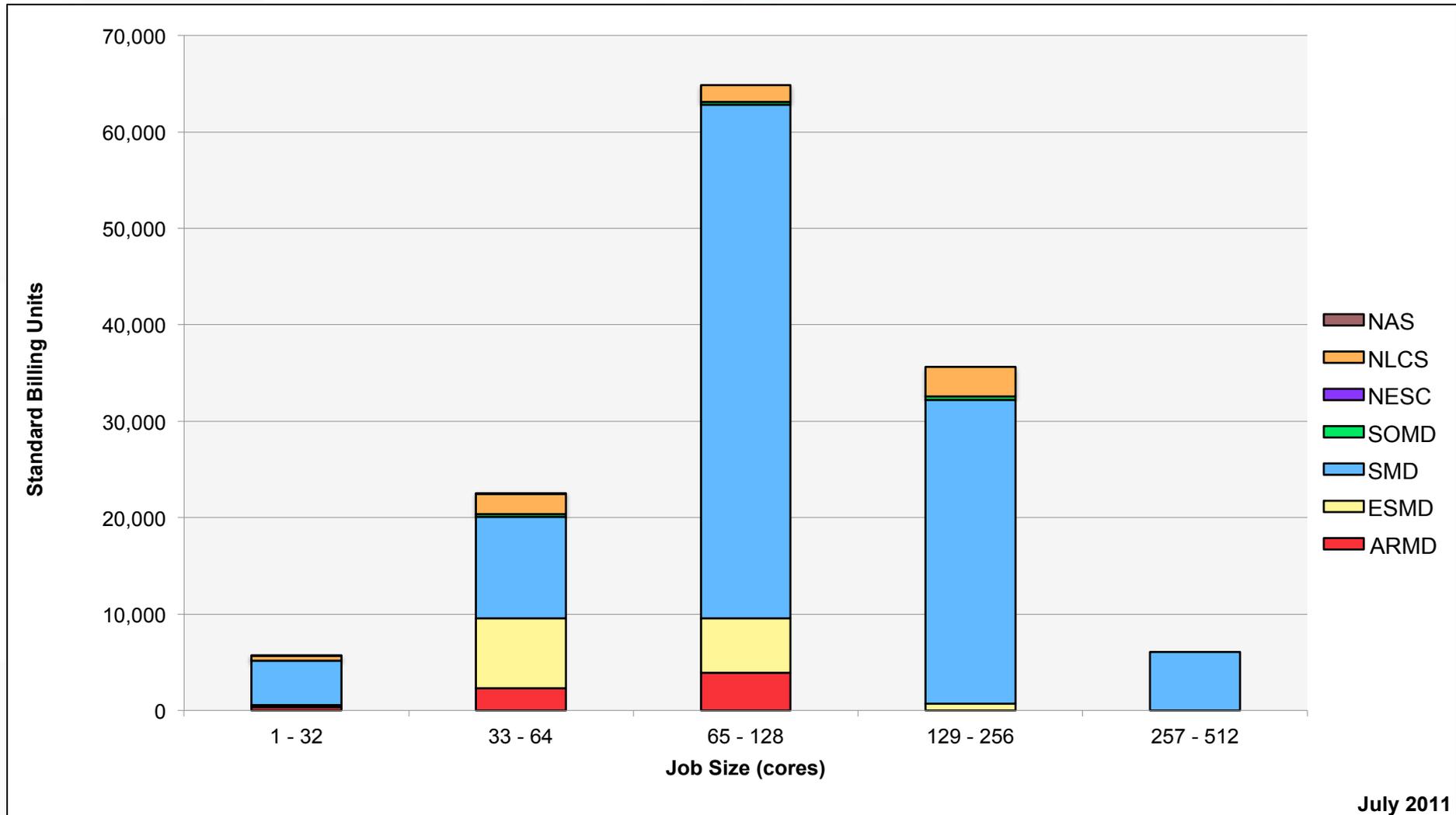
Columbia: SBUs Reported, Normalized to 30-Day Month



Columbia: Monthly SBUs by Run Time

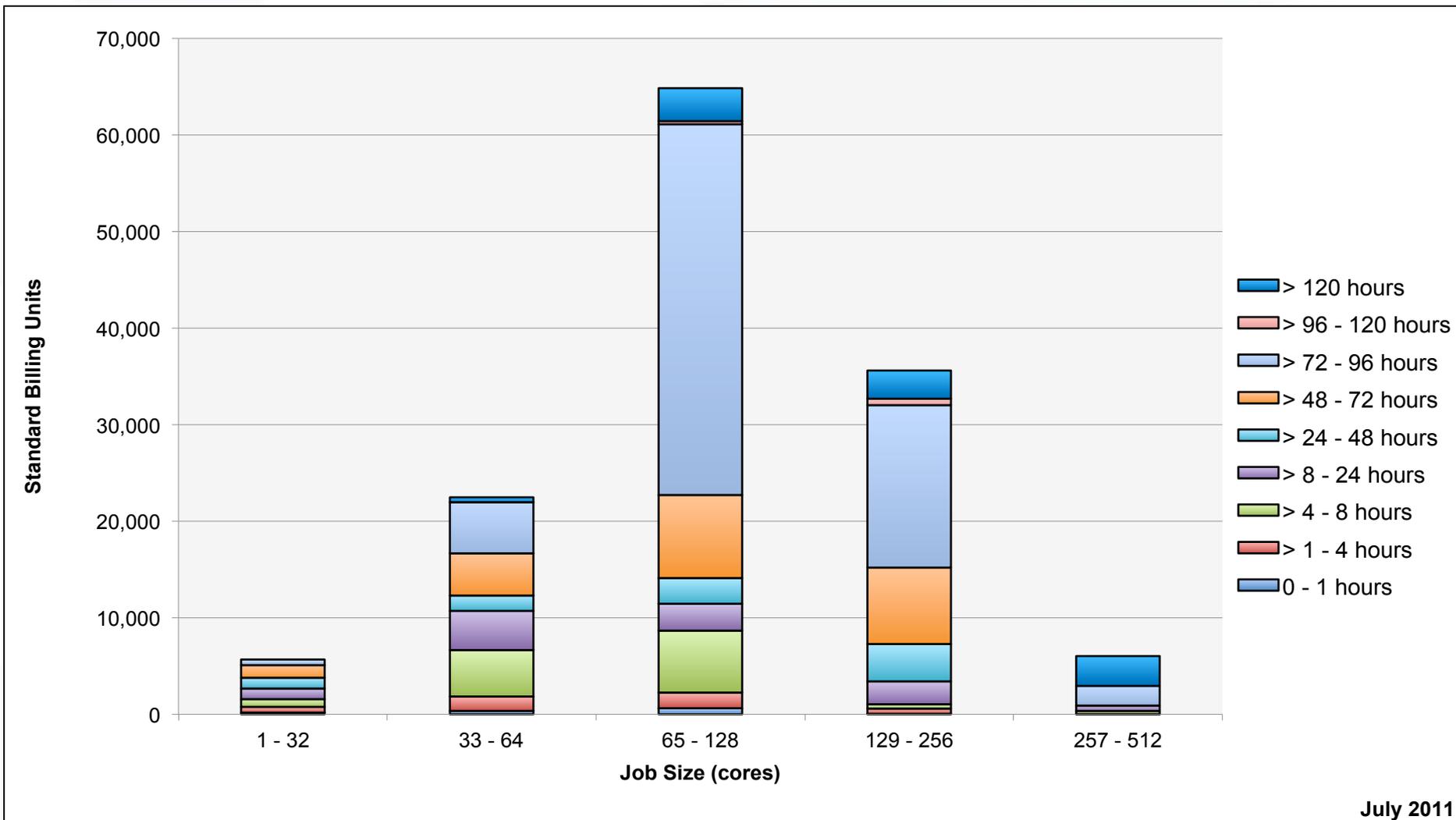


Columbia: Monthly Utilization by Size and Mission



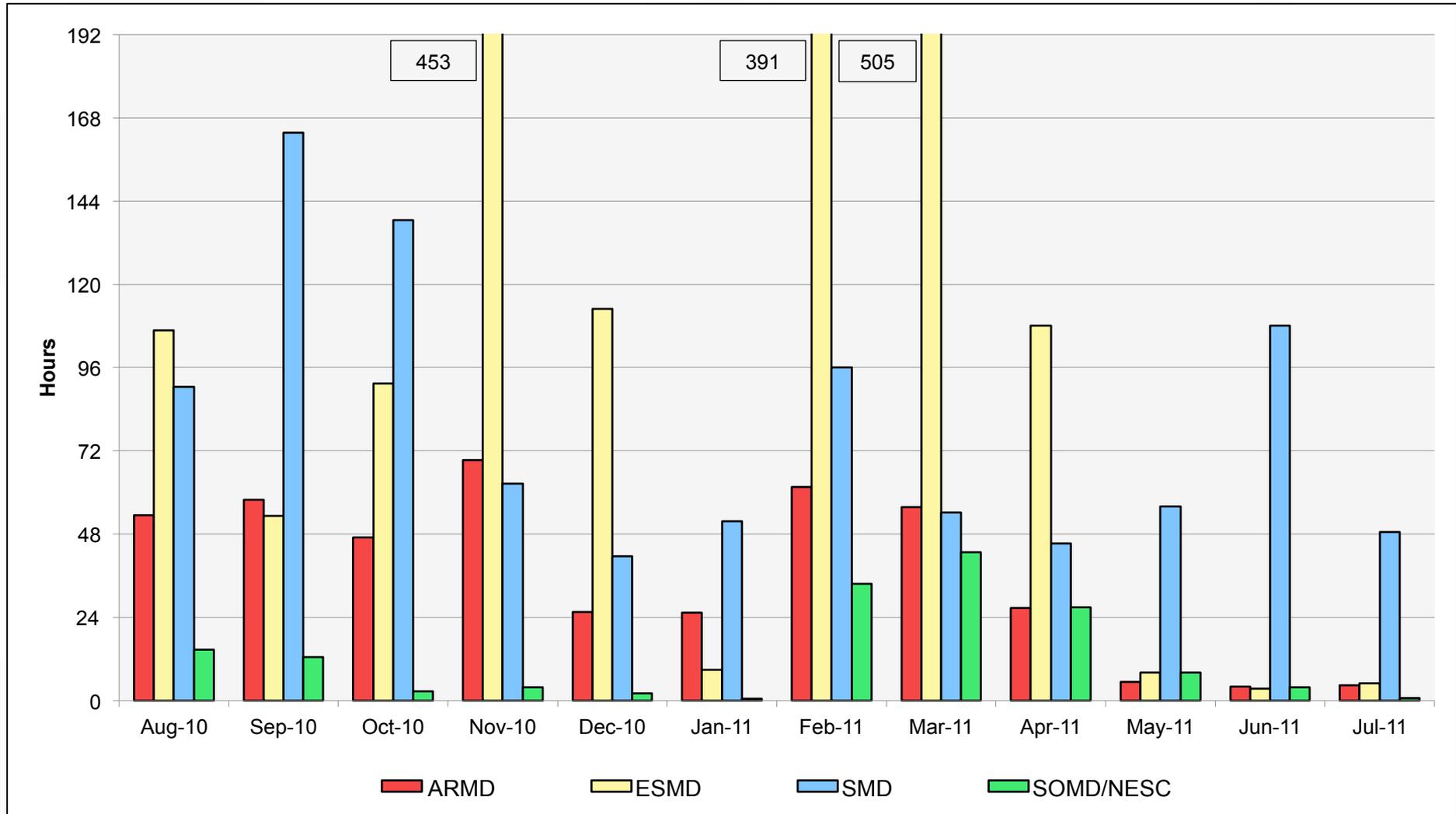
July 2011

Columbia: Monthly Utilization by Size and Length



July 2011

Columbia: Average Time to Clear All Jobs



Columbia: Average Expansion Factor

