



U.S. DEPARTMENT OF
ENERGY

Office of Science

Advanced Scientific Computing Research

FES/NERSC Requirements Gathering Workshop

August 3 and 4, 2010

Yukiko Sekine

Program Manager, Facilities Division

Advanced Scientific Computing Research

Office of Science, DOE



U.S. DEPARTMENT OF
ENERGY

Office of Science

Topics for Discussion

Advanced Scientific Computing Research

- Goal and Outcome of this Workshop
- Other approaches to NERSC requirements gathering
- Benefits of SC/HQ-centric requirements gathering for NERSC resources in the context of Programmatic mission needs
- NERSC requirements gathering workshop schedule
- Past NERSC Requirements WS's and NERSC Follow-on Actions



U.S. DEPARTMENT OF
ENERGY

Office of Science

Goal/Outcome of This Workshop

Advanced Scientific Computing Research

- The mission of NERSC is to **accelerate the pace of scientific discovery** by providing supercomputing capabilities, applicable software and middleware, expert consulting services, data analysis, visualization, and storage, and communications services for research sponsored by the Office of Science.
- The goal of this workshop is to **accurately characterize** and **document** FES' needs for NERSC resources for the next 5 years using a new mechanism (this workshop), and give input to:
 - **NERSC's new Five-Year Plan** and
 - **NERSC-7 requirements**
- The tangible outcome of the workshop will be a report that includes both the HPC requirements and a supporting narrative.

This workshop will help ensure that NERSC continues to provide world-class support for FES scientific discovery.

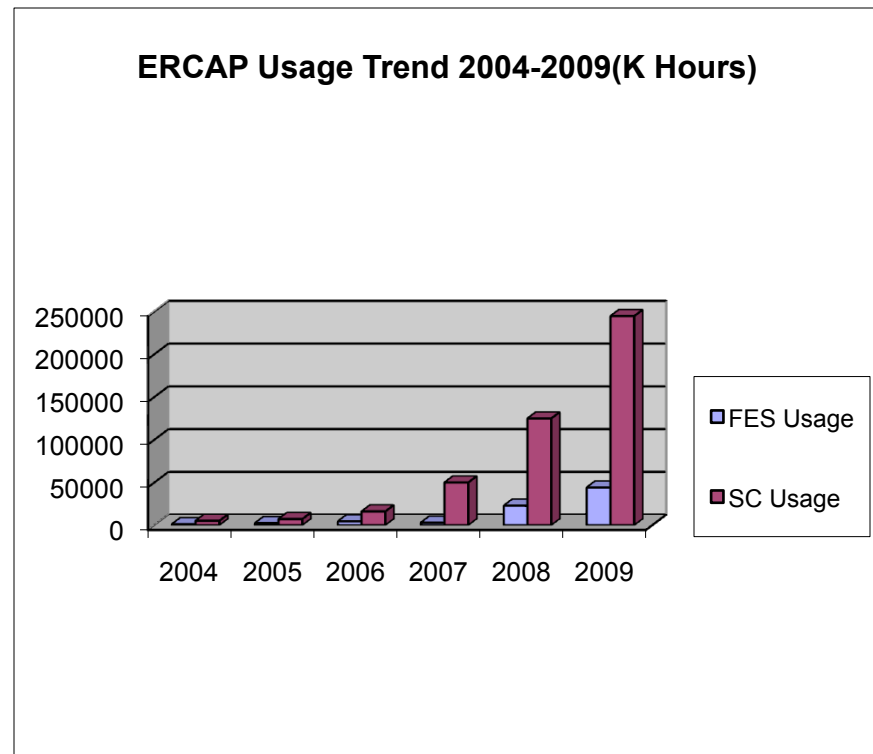


FES Usage Trend

Advanced Scientific Computing Research

In K Hours

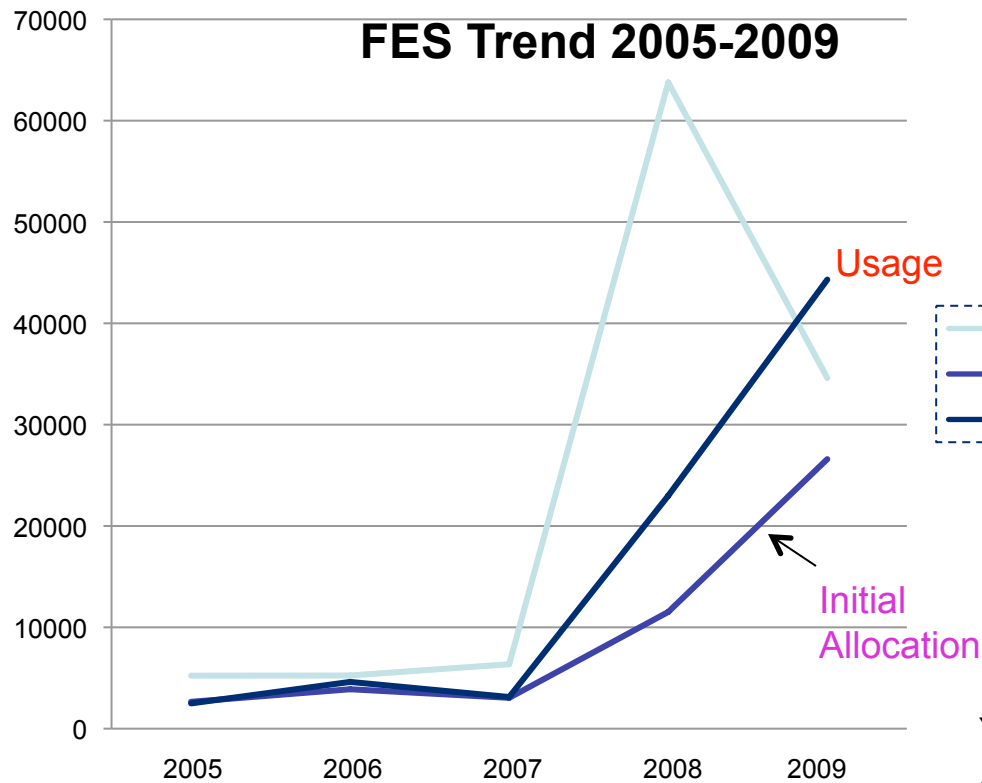
FY	FES Usage	SC Usage
04	1344	5315
05	2493	7385
06	4614	16248
07	3122	50134
08	22988	125015
09	44317	244697



Cray XT-4 (Franklin Equivalent Hours)



FES Request-Initial Allocation-Usage



?

Your real needs in
2013, 2015



Other Tools for Requirements Gathering for NERSC

Advanced Scientific Computing Research

Document or Action	Owner/Perspective	Frequency
DOE Greenbook – Needs and Directions in High-Performance Computing for the Office of Science, June 2005	NERSC User Group (NUG)/NERSC users	Once every ? - five years
NERSC “Visualization Greenbook,” October 2002	NUG/NERSC users	Not set
Science-Driven Computing: NERSC’s Plan for 2006-2010, May 2005	LBNL NERSC/LBNL NERSC	Once every five years



NUG Executive Board (NUGEX)*

Advanced Scientific Computing Research

Program	Representatives			
ASCR	Kirk Cameron (Virginia Tech)	Mike Lijewski (LBNL)	Ravi Samtaney (PPPL)	
BER	David Beck (University of WA)	Brian Hingerty (ORNL)	Adrienne Middleton (NCAR)	
BES	Bas Braams (Emory University)	Eric Bylaska (PNNL)	Thomas Miller (UC Berkeley)	
FES	Andris Dimits (LLNL)	Stephane Ethier Chair (PPPL)	Jean-Luc Vay (LBNL)	
HEP	Julian Borrill (LBNL)	Cameron Geddes (LBNL)	Frank Tsung Vice Chair (UCLA)	
NP	David Bruhwiler (Tech-X)	Peter Messmer (Tech-X)	James Vary (Iowa State Univ.)	
At Large	Angus Macnab (Woodruff Scientific)	Ned Patton (NCAR)	Jerry Potter (LLNL)	Xingfu Wu (Texas A&M)

* http://www.nersc.gov/about/NUG/nugex_members.php



Assessment of Other Tools

- These documents are very informative.
- They represent either NERSC's User Group's perspective, or LBNL/NERSC Team's perspective.
- *Science-Driven Computing: NERSC's Plan* is the closest to capture SC's needs, and is published once every 5 years.
- Science needs are changing rapidly, and the five-year cycle does not capture the changing needs very effectively.
- We also need **more computation-oriented data** for NERSC needs than those currently collected using the existing mechanisms.



U.S. DEPARTMENT OF
ENERGY

Office of Science

Benefits of Conducting NERSC Requirements Workshops in Three- Year Cycle

Advanced Scientific Computing Research

- SC Program Offices will have direct input on the requirements and can provide forecasts of needs aligned with mission priorities.
- Requirements gathering workshops in the DC area in the three-year cycle can capture rapidly changing Program-specific needs for NERSC resources better.
- We can document SC programmatic needs for NERSC resources that may not be captured in the five-year cycle planning tools (in 5 years; beyond 5 years).
- Scientists can get direct feedback on Program mission priorities.
- NERSC Staff can help quantify scientists' needs interactively.
- The new workshops will augment the existing, user-oriented requirements documents.
- We can leverage the successful structure and approach used for the ESnet requirements workshops.



U.S. DEPARTMENT OF
ENERGY

Office of Science

Program/NERSC Requirements Gathering Workshops

Advanced Scientific Computing Research

- **Program's active involvement is critical in all phases of the workshop: in pre-workshop planning, conducting the workshop, and writing the final report -- Own the Workshop**
- **Timeframe and location: Two – three workshops/year, in the DC Area. BER May 2009; HEP November 2009; BES February 2010; FES August 2010.**
- **NERSC Facilitators (NERSC staff) have the knowledge of end products; and translate Program's needs in quantitative ways; can help Scientists articulate and quantify their needs if necessary; and help Program and NERSC Management forecast Program's future needs.**
- **Program Office representative John Mandrekas has been working very closely with NERSC Program Manager and Workshop Facilitators.**
- **NERSC prepares templates ("Business Cases") for information gathering and report writing for participants' convenience (similar to those used in ESnet WS).**
- **Prior to the workshop, participants develop business cases to: (1) capture information and (2) use them as a backbone of the workshop report.**



U.S. DEPARTMENT OF
ENERGY

Office of Science

Requirements WS's and NERSC Follow-on Actions

Advanced Scientific Computing Research

- We held BER/NERSC Requirements Workshop in May 2009.
- BER scientists told us that they wished to be able to reserve NERSC resources recurrently at specific Interval.
- NERSC Response: New Service for Franklin Dedicated Time Reservation:
 - NERSC is testing a new service which will allow users who need access to a large number of nodes to make a reservation for a certain date, time and duration.
 - http://www.nersc.gov/nusers/systems/franklin/running_jobs/reservation.php
- BER, HEP, and BES WS participants told NERSC that they wanted a testbed to try new architectures and or languages.
- NERSC Response: Have a testbed available as part of NERSC-6.
- We Listen to you!



U.S. DEPARTMENT OF
ENERGY

Office of Science

Contact Information

Advanced Scientific Computing Research

Yukiko Sekine, Ph.D.

NERSC Program Manager

Advanced Scientific Computing Research

Office of Science, Department of Energy

Yukiko.sekine@science.doe.gov

301-903-5997

E235, Germantown