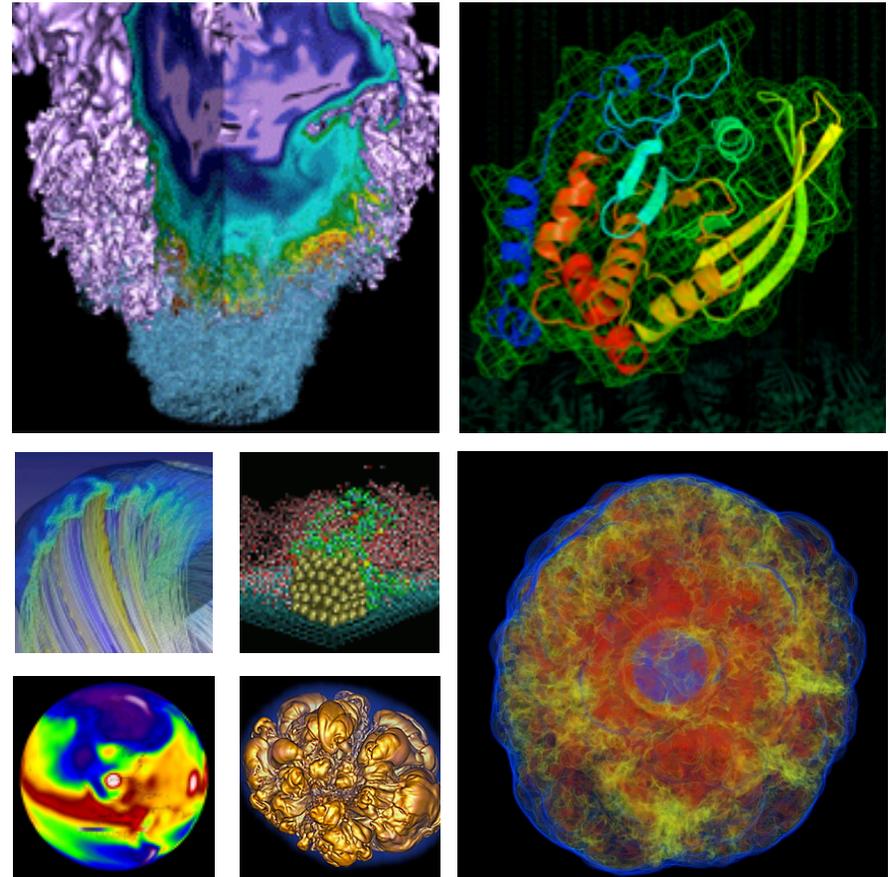


Review Overview, Goals & Process



Richard Gerber
NERSC Senior Science Advisor to the Director

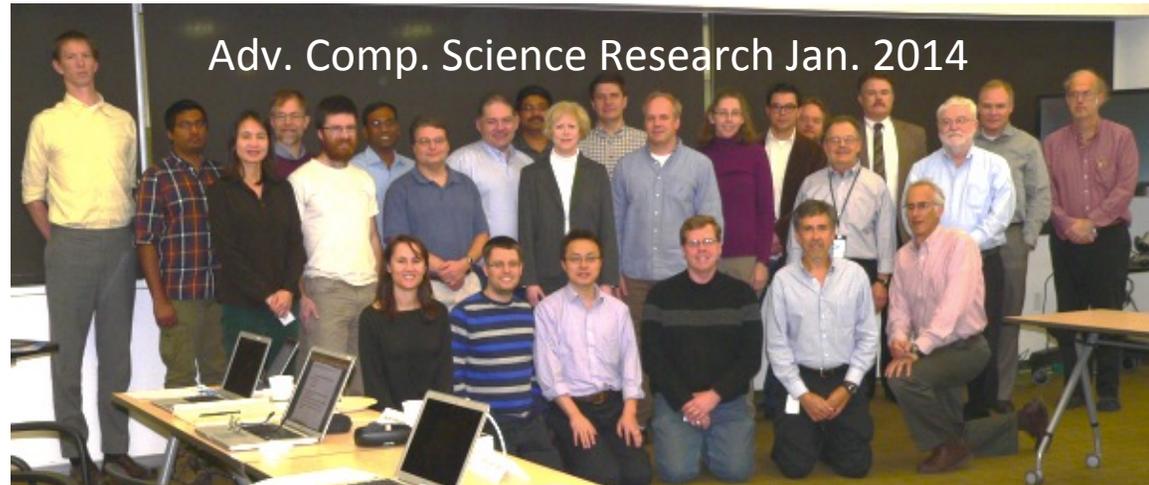
April 29, 2014

Requirements Reviews



1½-day reviews with each Program Office

Computing and storage requirements for next 5 years



- Participants
 - DOE Program Managers & ADs
 - Leading NERSC users & key potential users
 - NERSC staff

Scientific Objectives

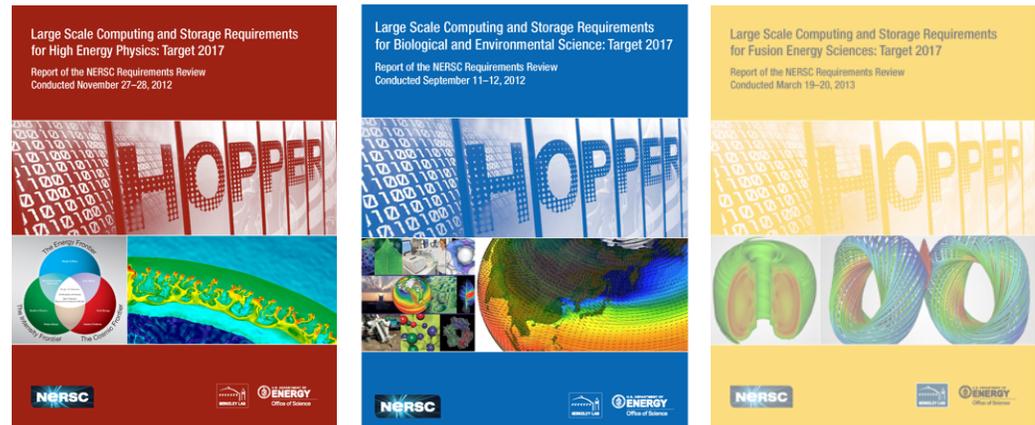


Computing, Storage, Software, Services Requirements

Reports From 9 Requirements Reviews Have Been Completed



- Computing and storage requirements for 2014 & 2017
- Executive Summary of requirements
- Case studies
- Second round, for 2017 requirements, will be completed in April 2014 (NP)



<http://www.nersc.gov/science/hpc-requirements-reviews/reports/>



- **Scientific justification for ASCR budget requests**
 - Quantitative requirements
 - Description of scientific benefit
 - Documented needs from science teams
- **Basis for NERSC 7 and NERSC 8 Mission Need**
 - Demand for hours beyond available resources
 - Science at scale, support for ensemble runs & HTC
 - Rich development environment
- **Guides NERSC services directions**
 - Application readiness teams
 - Queues for science at scale & HTC
 - Support for standard tools, libraries, applications
 - Planning for NERSC data services

Meeting Goals



- **Gather computing, storage, and HPC services required to support NP research through 2017**
- **Collect a set of project-based “case studies” with scientific goals and how HPC requirements support achieving those goals**
- **Before we leave: high-level findings**
- **Ultimately: a written report for DOE**

PRRs Influenced the Selection of Edison & N8



- **Findings from first round of PRRs (Program Requirements Reviews)**
 - The NERSC community would not be ready to effectively use accelerators in production by 2014
 - There is a need for improved I/O rates and disk storage
 - Many codes benefit from more memory per node, faster single-processor performance, and a high-bandwidth, low-latency interconnect
 - Productivity is more important than “feeds and speeds”
- **PRRs findings formed basis of NERSC 7 Mission Need Statement**
 - Edison has fast commodity Intel x86 processors, 64 GB/node memory, 6+ PB of /scratch, and novel high bandwidth, low-latency Aries interconnect
 - Adoption by NERSC community was immediate, with little porting effort
 - Performance is running 2X-4X that of Hopper on a per-core basis

Process



- **Collect and refine requirements for 2017**
 - Case study worksheets
 - Discussions at this meeting lead to high-level findings
 - Post-meeting refinement of case studies
- **Draft a written report (Richard & Harvey)**
 - Assemble case studies and check for internal consistency and compare against historical trends
 - Aggregate requirements and summarize
 - Create draft report for you & NP to review
- **Send final draft to NP & ASCR for final approval**
- **Publish final report**

Strategy Overview



Tell how these are needed to achieve your scientific goals – as specifically as possible

- Computational and storage resources
- HPC services
- Software

Additional important info: Are your codes ready for many-core? If not, what do you need?

Quantitative Method



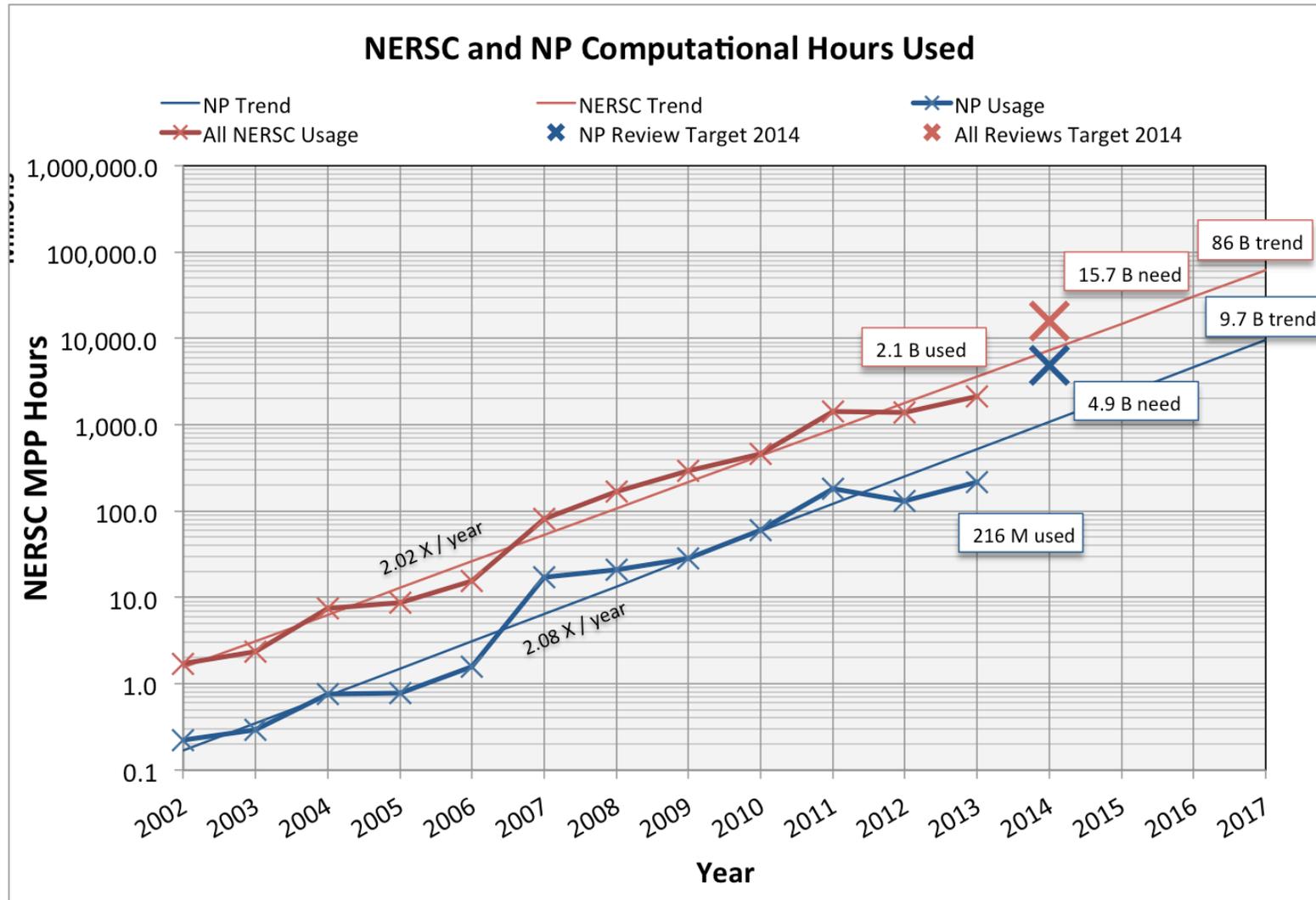
- **Quantitative requirements are very important**
 - Hours needed
 - Archival data (HPSS) storage needed
 - Disk storage needed
- **For hours and archival storage**
 - Requirements from this review are summed
 - Scaled to full NP need by the fraction of 2013 NP usage represented by case studies
 - **Important: Associate each case study with 2013 NERSC repo or repos**
 - New/potential projects' requirements added in separately
- **Like to do the same for Scratch and Project shared disk**
 - Please state 2013 usage and 2017 need so we can create a ratio

Hours Required



- **The unit of “Hour” is defined as 1 Hopper core hour**
- **Please state your requirements in these units**
 - How much computing will you need in multiples of a Hopper hour?
 - For this exercise, ignore the architecture – we will normalize this when future systems arrive, based on average application performance
- **Give your best estimate for 2017 specifically**
 - Remember that each year’s usage has historically been 2X the previous year’s

Computational Hours

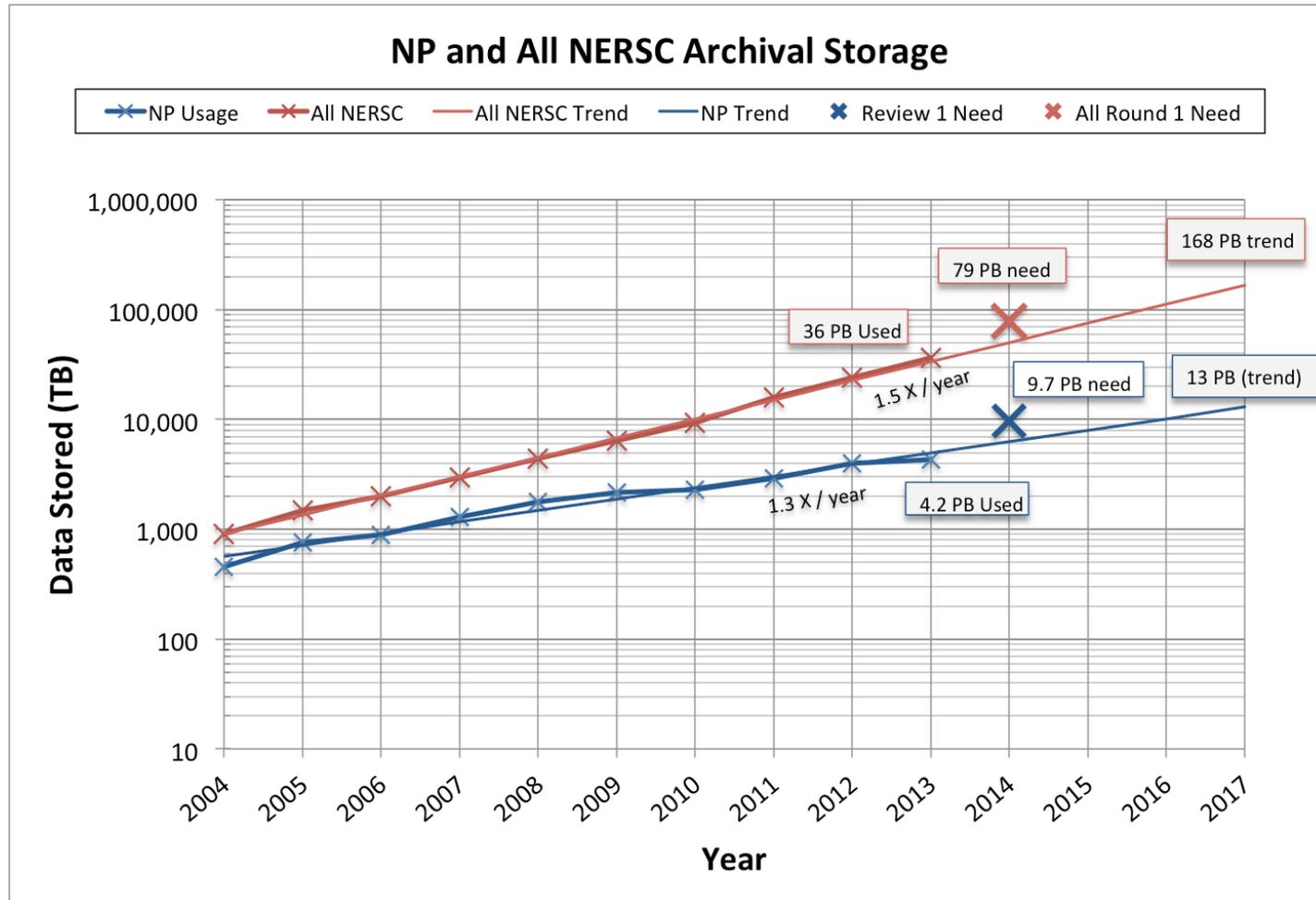


Data Storage Requirements



- **Archival storage estimate for 2017**
 - This is an aggregate number, not what you will add in 2017
 - Historical trend: 1.5-1.7 X / year
- **Scratch (temporary)**
 - What is the maximum you will need at any given time during 2017?
 - Not just what you will need for a single run
- **Project shared disk space (permanent)**
 - What will you need for source code, data files or executables that will be constantly accessed and/or shared, etc.

Archival Storage



Logistics: Schedule



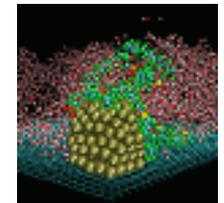
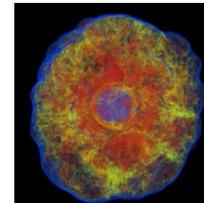
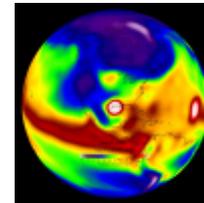
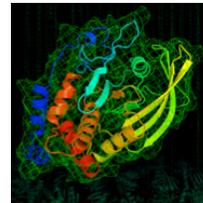
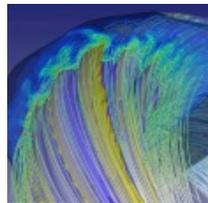
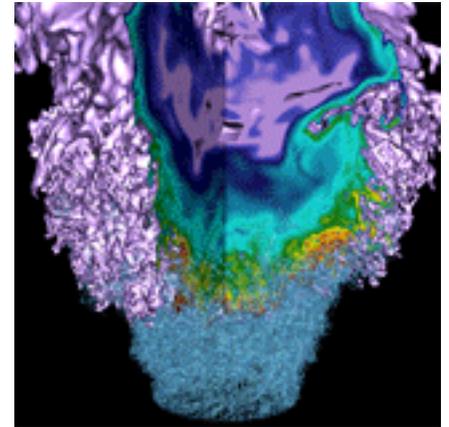
- **Agenda on workshop web page**
 - <http://www.nersc.gov/science/requirements/NP/>
- **Mid-morning / afternoon break, lunch**
- **Today: Case study presentations & discussions**
- **Self-organization for dinner**
- **Wednesday: overview, review, and discuss key findings**
- **Report: NP Intro + PI case studies + NERSC summary**
 - Final Case Studies due June 1
 - Richard / Harvey review
 - PI/DOE draft review August 1
 - Final: September 1
- **Final reports from previous workshops on web**
 - <http://www.nersc.gov/science/requirements>

Logistics



- **Get your presentations to us (Harvey/Richard)**
 - Email
 - Web download
 - USB stick
- **The laptop at the front will be used to display presentations**
- **We will stay on time**
 - Descriptive and concise science justification
 - Please emphasize requirements and application readiness for manycore
 - Watch countdown timer

Questions?



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Science





National Energy Research Scientific Computing Center

- **“Memory”**
 - Volatile or “RAM”
 - Each “node” has a pool of RAM shared among all cores on the node
 - “Global memory requirement” means the sum of all the RAM on the nodes on which your job is running
- **“Many Core”**
 - “Processors” with 100s+ of “light-weight” cores
 - Slower clock speeds (energy efficient)
 - Not self-hosted; need a master CPU (today)
 - Special ways needed to write programs
 - GPUs and Intel Phi

Storage Terms



- **“Scratch storage”**
 - Temporary, purged after ~6 weeks
 - Fast: 10s – 100s of GB/sec
 - Not backed up
 - Access from a single system (at least at high performance)
 - Default quotas: ~ 10s TB + today
- **“Permanent storage”**
 - Not purged
 - Usually backed up (feasible into the future?)
 - Somewhat less performant
 - Maybe sharable
 - Center-wide access
 - Default quotas: ~10s GB (Home) to ~10-100 TB (Project) today
- **“Archival Storage”**
 - Permanent & long term
 - Much slower access time
 - No quotas: up to 10 PB today

Burst Buffers