Workshop Goals & Process

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Overview

• **We’re holding this review to ensure that**
  – you have the HPC resources you need to be successful in your research
  – NERSC can fulfill its mission to accelerate scientific discovery within the Office of Science

• **Your input helps NERSC**
  – create science-based justification for acquiring needed resources
  – focus on delivering the services that are important to you
  – make technology decisions

• **Result: NERSC can better provide what you need for your work**

• **This exercise benefits the Office of Science, FES, ASCR, NERSC, & you**
Process

• Collect and refine requirements for 2017
  – Case study worksheets
  – Discussions at this meeting
  – Post-meeting refinement of case studies

• NERSC editors (Richard & Harvey)
  – Check case studies for internal consistency and compare against historical trends
  – Aggregate requirements and summarize
  – Create draft report for you & FES to review

• Send final draft to DOE FES office for final approval
• Publish final report
Key Strategy

• Key is to tie computational, storage, and services needs to achievement of scientific goals – as specifically as possible.
  – Science -> codes & algorithms -> computation parameters
    -> resources needed
Quantitative Method

• **Quantitative requirements are very important**
  – Hours needed
  – Archival data storage needed
  – Disk storage needed

• **For hours and archival storage**
  – Requirements from this review are summed
  – Scaled to full FES need by the fraction of 2012 FES usage represented by case studies
  – Important: Associate each case study with 2012 NERSC repo or repos
  – New projects’ requirements added in separately

• **Like to do the same for Scratch and Permanent Disk**
  – Please state 2012 usage and 2017 need so we can create a ratio
• 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
Data Storage Requirements

- **Archival storage estimate for 2017**
  - This is an aggregate number: $\Sigma$ all years
  - 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

- **Permanent disk space**
  - What will you need for source code, data files or executables that will be constantly accessed and/or shared, etc.
Archival Storage

![Graph showing archival storage trends]

- FES Usage
- All NERSC
- All NERSC Trend
- FES Trend
- Round 1 Need
- All Round 1 Need

Data Stored (TB)


- 23 PB Used
- 700 TB Used
- 1.8 PB need
- 79 PB need
- 168 PB trend
- 4.1 PB trend
Logistics: Schedule

- Agenda on workshop web page
  - http://www.nersc.gov/science/requirements/FES
- Mid-morning / afternoon break, lunch
- Today: Case study presentations & discussions
- Self-organization for dinner
- Wednesday: overview, review, and reach agreement on key findings
- Report: FES Intro + PI case studies + NERSC summary
  - Final Case Studies due May 1
  - Richard / Harvey review
  - PI/DOE draft review June 15\textsuperscript{b}
  - Final: August 1 (?)
- Final reports from 2009-2011 workshops (Target: 2014) on web
  - http://www.nersc.gov/science/requirements
Logistics: Presentation to Remote Participants

• We need your view graphs in advance
  – Email
  – Web download
  – USB stick

• The laptop at the front is sharing its screen with remote participants
  – We’ll load your presentations onto it
Questions?
National Energy Research Scientific Computing Center
Terms

• “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