NERSC Workload Analysis on Hopper

Katie Antypas, Brian Austin, Tina Butler, Richard Gerber, Cary Whitney, Nick Wright, Woo-Sun Yang, Zhengji Zhao

February 22, 2013
Understanding the NERSC workload is key to procuring productive, high performing systems for science

- Conducted workload analysis to understand application requirements and guide future system procurements
- Important for understanding efforts needed to transition workload to future architectures
- Analyzed the workload by:
  - Science area
  - Application code
  - 3rd party application usage
  - Algorithm
  - Job size
  - Memory usage
  - Threading usage
  - Library usage
- I/O workload analysis is in progress and will be ready in Mid-March 2013
Methods

• Data collected in this presentation came from a variety of sources
  – System accounting logs
  – NIM database
  – ALPS command line capture log
  – Automatic Library Tracking Database (ALTD)
  – Application Resource Usage (ARU) Tool
NERSC serves a broad range of science disciplines for the DOE Office of Science

NERSC serves:
- Over 4500 users
- Over 650 projects

2012 Allocation Breakdown

- Fusion Energy
- Materials Science
- Lattice QCD
- Chemistry
- Climate
- Astrophysics
- Biosciences
- Earth Sciences
- Math and CS
- Accelerator Science
- Engineering
- Nuclear Physics
- Combustion Science

NERSC services include:
- Over 4500 users
- Over 650 projects
Over 650 applications run on NERSC resources

Approximately 80% of the workload needs to transfer to NERSC-8 (20% can remain on Edison)
NERSC installs and directly supports software used by over 20% of workload

Percent of workload using NERSC installed and supported application codes
(On Hopper by Number of Hours)
In addition to science area and code diversity, NERSC supports a broad range of algorithms.
NERSC users run applications at every scale to conduct their research.

Approximately 15% of computational cycles use more than 40% of the compute nodes and 40% of cycles use more than 10% of the system.
80% of the Hopper workload uses less than or equal to 1 GB of memory per task

And >90% of the Hopper workload uses 2GBs or less per task
Over 20% of hours used on Hopper run with more than a single thread

% of Hours Used by Thread Count
(Hopper system 11/2012-2/2013)

- 1 Thread; 79%
- 2 Threads; 3%
- 3 Threads; 5%
- 4 Threads; 10%
- 6 Threads; 1%
- 24 Threads

Other

Node Hours used by Application Thread Count
(Hopper system 11/2012-2/2013)

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24

Threads
NERSC users require an array of software to conduct their research

**Library usage on Hopper**
*(June 21, 2012 - Jan 17, 2013)*

MPICH, parallel-I/O and math libraries are crucial packages to a large number of NERSC users
NERSC has new tools to capture memory, threading, and library usage on Cray systems

New tools will allow workload characterization on both Hopper and Edison systems

Understanding workload is key to quantifying the effort that will be required to transition applications to future architectures

Stay tuned for I/O workload analysis
Journal Cover Stories from NERSC-Enabled Research
2012

Devanathan, PNNL: BES
Jiang, ORNL: BES
Jiang, ORNL: BES
Daggett, U. Washington: BER

Dupuis, PNNL: BES
Petrik, PNNL: BES
Jiang, ORNL: BES
Smit, UCB: BES
Varga, Vanderbilt: BES

Sugiyama, MIT: FES
Snurr, Northwestern: BES
Striolo, U. Oklahoma: BES
Liang, U. Maryland: BER
In addition to science area and code diversity, NERSC supports a broad range of algorithms.

- **DFT Proxies:** Quantum Espresso, Berkeley GW
- **Fusion PIC Proxy:** GTC
- **Lattice QCD Proxy:** MILC
- **Climate Proxies:** POP, SE-CAM, MPAS, WRF
- **Molecular Dynamics Proxies:** NAMD, Amber
- **Fusion Continuum Proxy:** GYRO
- **QMC Proxy:** Zori
- **Fast Math Proxies:** FLASH, MAESTRO
- **CMB Proxy:** MADAM
- **Bioinformatics Proxy:** BLAST
- **Accelerator PIC:** Impact
- **Other codes**
In addition to science area and code diversity, NERSC supports a broad range of algorithms.