BLUE WATERS

SUSTAINED PETASCALE COMPUTING

Blue Waters User Monthly Teleconference

Agenda

Topics for this webconference:

- NSF announces call for PRAC proposals.
- Upcoming changes to Blue Waters: Purging, Ordering of nodes for jobs (nid order), and Programming Environment defaults.
- Current usage and the new usage tool on the portal.
- Reminder for NSF PRAC teams to work with Point of Contact on Science Team details.
- Data Management Best Practices using Globus Online and Blue Waters Nearline.

Petascale Computing Resource Allocations (PRAC)

- PROGRAM SOLICITATION NSF 14-518

- Deadline March 10, 2014

  - November 14, 2014

  - November 13, 2015

  - November 09, 2016

- Program Officer

  - Rudolf Eigenmann reigenma@nsf.gov

  This description should include the number and type of system nodes needed for your runs, the anticipated memory usage, the expected number and duration of runs required for each phase of the research, the total number of node-hours required, the anticipated I/O requirements, the amount of data that you anticipate transferring to or from the Blue Waters.
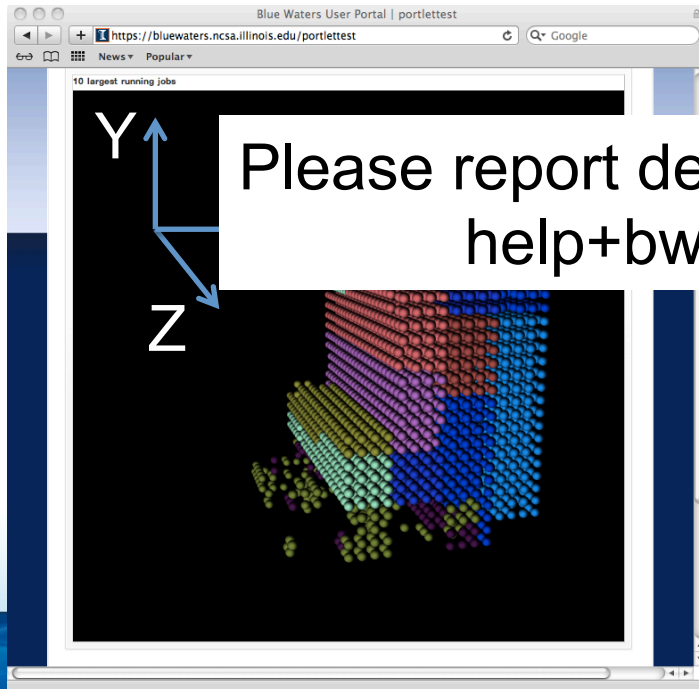
System Changes

- This Week (Tuesday 12/10/2013)
  - Changes to purging of scratch file system.
  - NID Ordering change.
- Next Month
  - Default modules to latest release of packages.
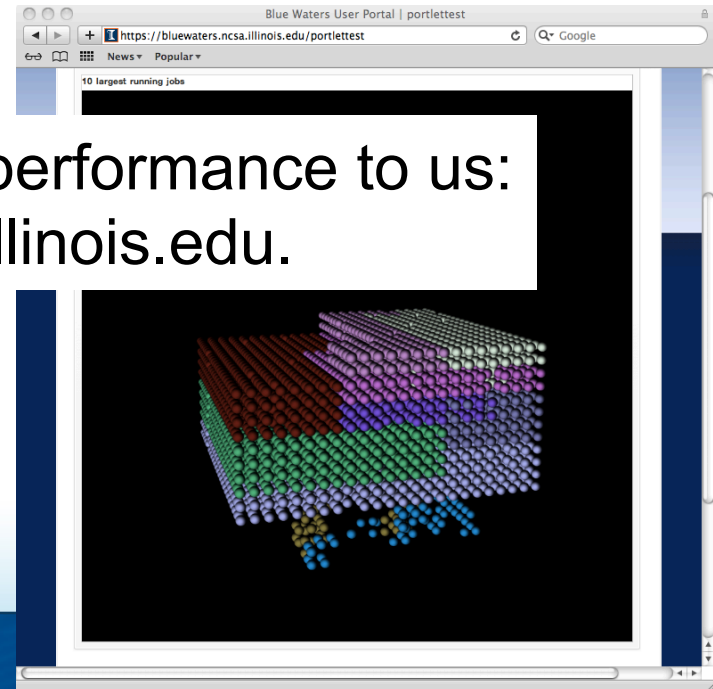
Scratch purging

- Now includes empty directories.
- Same policy as with files:
  - Last access and last modified greater than 30 days.
- Be sure to check job scripts that assume directories in scratch exist.
- Documented on the Blue Waters portal.

Changes to NID Ordering

- Change in order nodes are presented to Moab/Torque by ALPS. Current order gives a YZ preference.
- New order will give a XZ preference that will provide better aggregate interconnect bandwidth. Tests show marked improvement in application performance for many applications.
- Special attention to XK region.

Please report degraded performance to us: help+bw@ncsa.illinois.edu.

Changes to Programming Environment

- In January
  - CCE 8.2.2 - Supports the use of AVX intrinsic/built-in functions.
  - PGI 13.10.0 – Improved OpenACC support.
  - GNU 4.8.2
  - MPT 6.2.0 (cray-mpich) – GPU2GPU improvements.
  - LibSci/LibSci_acc
  - Perftools

Usage To Date

Project Group	Allocated (M node-hrs)	% of Allocation Used
NSF PRAC	177.36	41.0
IL	8.88	21.3
GLCPC	3.59	15.6

- 60% into "year" starting April 4, 2013, corrected for XK upgrade outage.

- Two largest projects > 70% used. Next 12 projects at < 50% used.

- Will be difficult for all teams to fully use allocation.

Portal Usage Tool

- Open access
- Dive-down
- Tables
- see Usage

Request for publications, presentations, …

- We need to be current on products that result from time on Blue Waters such as:
  - Publications, Preprints (e.g. arXiv.org 🙂), Presentations.
- Appreciate updates sooner than annual reports.
- NSF PRAC teams send information to PoCs.
- See the Share Results section of the portal as well.

Data Management Best Practices

- Ryan Mokos (NCSA)

Future Topics?

- Please send us your suggestions on topics for future teleconferences / webinars