BLUE WATERS

SUSTAINED PETASCALE COMPUTING

2/17/14

Blue Waters User Monthly Teleconference

NCSA

GREAT LAKES CONSORTIUM
FOR PETASCALE COMPUTATION

CRAY

Agenda

Topics for this webconference:

- Recent changes to Blue Waters.
- User Experience.
- Current usage.
- Requests for information on Science Successes
- NSF PRAC request for proposals
- Blue Waters Symposium
- Blue Waters SETAC
- Blue Waters Internships
- XSEDE/Blue Waters Extreme Scaling Workshop

System Changes

- Last month (1/21)
  - Software updates to Sonexion (Lustre) servers to improve resiliency and reliability. Lustre client update.
  - Hardware maintenance.
  - SLES and NVIDIA security fixes.
  - Nearline software (HPSS) and firmware updates.
  - Change to default PE versions.
- Last week (2/10)
  - Facility and Hardware maintenance.
  - NVIDIA graphics engine patch.
  - Verified esMS reliability.
  - Lustre client regression
- Upcoming
  - Changes to job policies.
  - Addition of project space links in Nearline.
  - Darshan (ANL) for IO profiling.

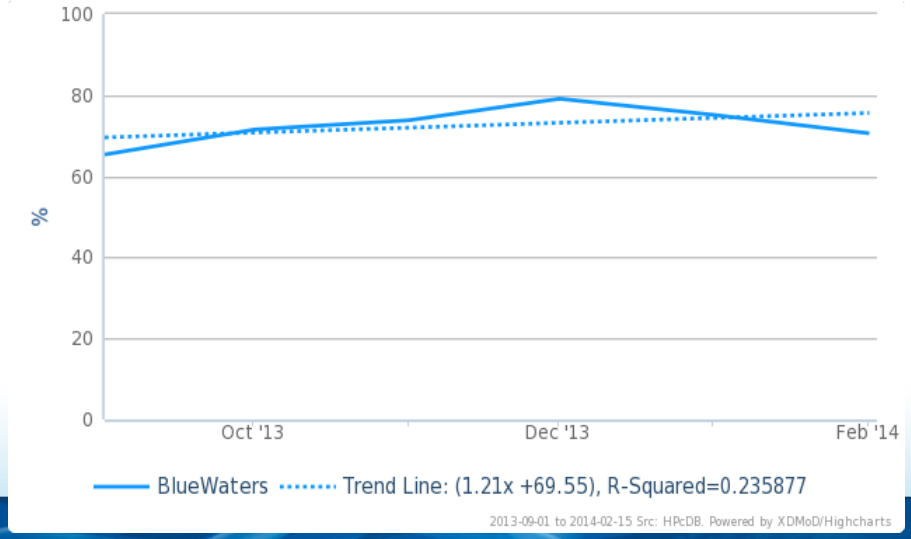
User Experience

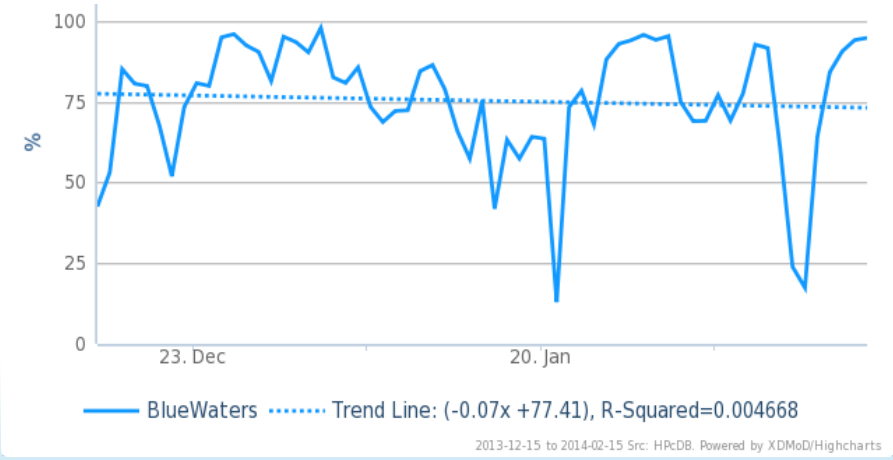
- No immediate reports of performance issues after 1/21 PM and PE changes. One compiler issue with GNU 4.8.2 reported.
- Several user reports of degraded performance a few days prior to PM on 2/10. Application performance restored after PM reboot. Cray and NCSA looking into possible causes for degraded performance.

Usage and Utilization

Project Group	Allocated (M node-hrs)	% of Allocation Used
NSF PRAC	177.36	49
IL	8.88	35
GLCPC	3.59	22

- Now 80% into "year" starting April 4, 2013, corrected for XK upgrade outage.
- Utilization has steadily improved.





Request for Science Successes

- We need to be current on products that result from time on Blue Waters such as:
  - Publications, Preprints (e.g. arXiv.org ), Presentations.
  - Very interested in data product sharing.
- Appreciate updates sooner than annual reports.
  - Send to gbauer@illinois.edu
- NSF PRAC teams send information to PoCs.
- See the Share Results section of the portal as well.
- Be sure to include proper acknowledgment
  - Blue Waters - National Science Foundation (ACI 1238993)
  - NSF PRAC – OCI award number

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.

Blue Waters Symposium

- 2nd Annual - Petascale Science and Beyond
- May 12-15, 2014 in Champaign-Urbana.
- Keynotes, panels, posters, and breakout sessions.
- Blue Waters science teams are expected to have a senior representative.

Blue Waters SETAC

Science and Engineering Team Advisory Committee (SETAC)

- PRAC
  - Physics and Astrophysics: Paul Woodward, University of Minnesota
  - Chemistry: Tom Cheatham, University of Utah
  - Civil and Environmental Engineering — Systems Optimization: Patrick Reed, Cornell
  - Physics and Molecular Dynamics: Klaus Schulten, University of Illinois Urbana-Champaign
  - Physics and Material Science: David Ceperley, University of Illinois Urbana-Champaign
  - Physics and Cosmology: Tiziana Di Matteo, Carnegie Mellon University
  - Atmospheric Sciences and Climate: Dave Randall, Colorado State University
- GLCPC
  - Academic & Research Technologies in Information Technology: Joe Paris, Northwestern University (Chair for 2013/2014, followed by Structural Mechanics and Biophysics: Jorge Vinals, University of Minnesota, Chair for 2014/2015)
- UNIVERSITY OF ILLINOIS AT URBANA-CHAMPAIGN
  - Chemistry: So Hirata, University of Illinois at Urbana-Champaign
- INDUSTRY
  - Computer and Software Engineering: Rick Authur, General Electric Global Research

Membership on the SETAC will be for staggered two-year terms, with rotations beginning after year two. The committee will meet three to four times each year, producing one report per year that will include an evaluation of the project's performance and recommendations for the next year.

For more information see NCSA web page.

Blue Waters Internships

- 20 undergraduate research interns in 2014. The goal is to engage undergraduate students in petascale computing research and development projects.
- The program provides each student a stipend totaling $5000, a two-week intensive high-performance computing workshop, and travel to The Blue Waters Symposium 2015.
- This program includes support for undergraduate internship activities at any accredited degree granting institution in the United States.
- Applications must be submitted by March 21, 2014
- Notifications will be made by April 15,2014
- Also looking for Faculty interested in Mentoring
- For more information see

https://bluewaters.ncsa.illinois.edu/internships

XSEDE/Blue Waters Extreme Scaling Workshop

- Topic: The Intersection of Big Data and Large-Scale Computing
  - Data intensive applications running on HPC style architectures
  - Big data analytical applications running on HPC style architectures
  - Computationally intensive applications running on big data or data intensive architectures
  - Using GPU/many-core processors for big data applications
  - System architectural features that can support big data and high performance computing
- The Extreme Scaling Workshop 2014 will showcase the discoveries, innovations, and achievements of those who use, build, and/or support advanced architectures at extreme scales around the world.
- The workshop will also provide a forum among researchers, professional staff, students, HPC center staff, and representatives from funding agencies.
- August 14-15, 2014 in Boulder, CO.
- See https://www.xsede.org/web/xscale/xscale14 for more information.
- After the RMACC High Performance Computing Symposium.

Future Topics?

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