BLUE WATERS
SUSTAINED PETASCALE COMPUTING

Blue Waters User Monthly Teleconference

Agenda

- Upcoming changes to the programming environment.
- Blue Waters Advanced User workshop: October 13-15.
- yt developer workshop October 16-17
- SC14 Conference
- XSEDE and VSCSE training opportunities.
- Requests for Science Successes.
- HPC Python – Omar Padron (SEAS)

PRAC CFP

Petascale Computing Resource Allocations (PRAC)

CONTACTS

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PROGRAM GUIDELINES

Solicitation 14-518

DUE DATES

Full Proposal Deadline Date: November 14, 2014

SYNOPSIS

In 2013, a new NSF-funded petascale computing system, Blue Waters, was deployed at the University of Illinois. The goal of this project and system is to open up new possibilities in science and engineering by providing computational capability that makes it possible for investigators to tackle much larger and more complex research challenges across a wide spectrum of domains. The purpose of this solicitation is to invite research

System Utilization
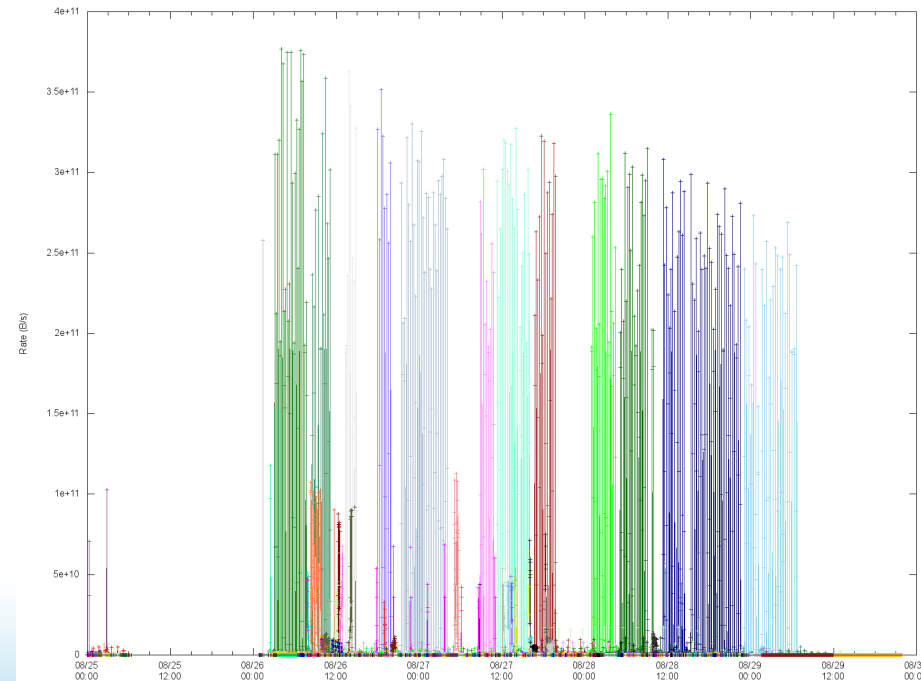
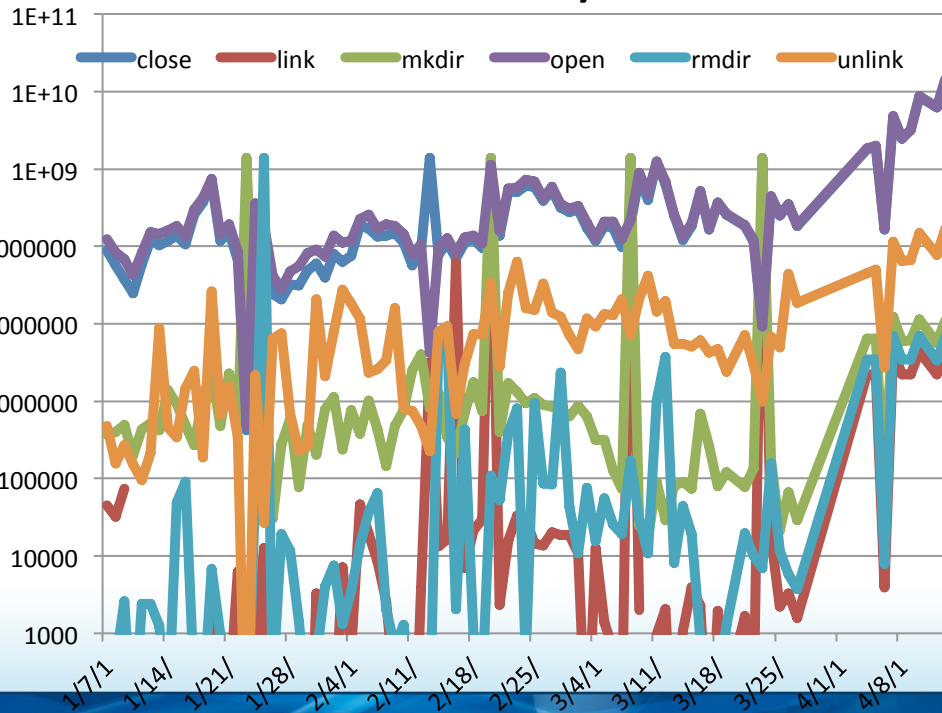- Utilization since last BW User Call (August 18)
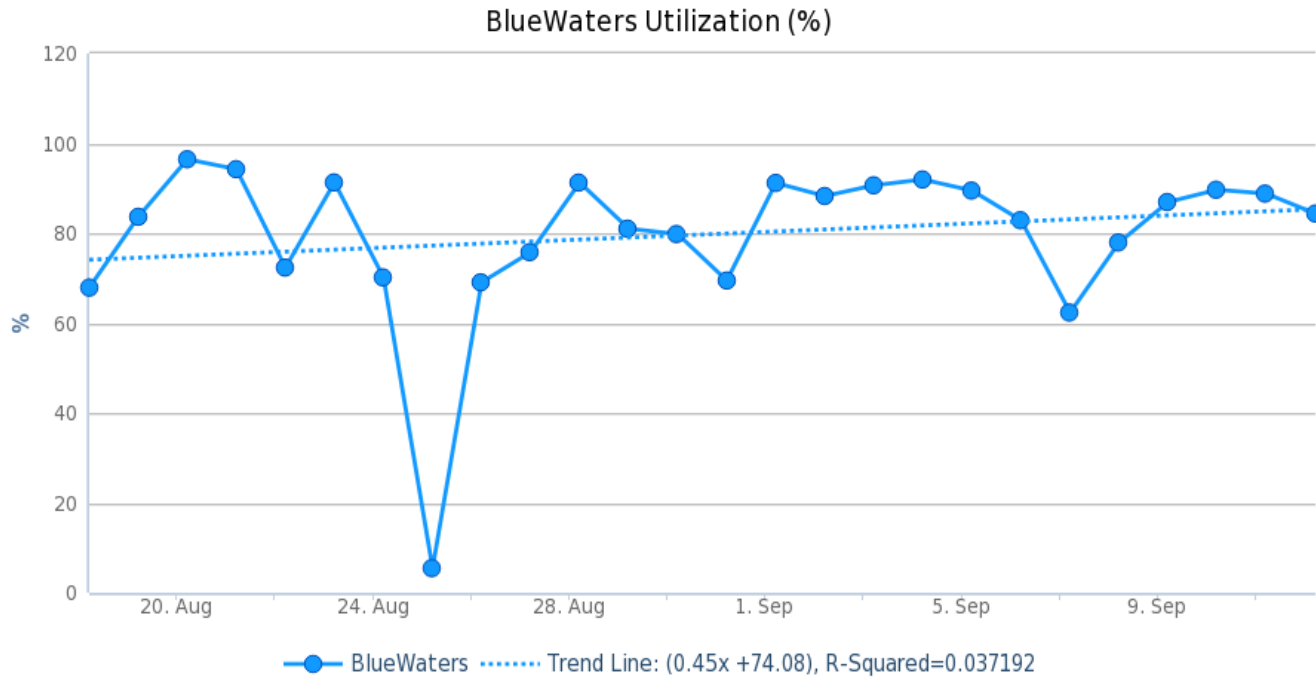
Recent System Events

- Scratch responsiveness
  - Monitoring of "user" commands: login, MOM, i/e nodes.
  - Compute node Lustre client counter data.

Metadata Online /scratch

Recent System Events

- Saturday Lustre scratch unavailability
  - Analysis still in progress.
  - System reboot to clear state of essential services.

Recent Changes

- Previously

Upcoming Changes

- Modules
  - Enhanements by NCSA (Craig Steffen)
    - module output to stdout rather than stderr
    - tab-completion within module shell function
      - module load Prg*TAB*
    - shell prompt module context dependent
      - $ _D_-___-Gnu-_ module swap PrgEnv-gnu PrgEnv-pgi
      - $ _D_-___-PGI-_
  - Try it out. Feed back appreciated.

  See https://bluewaters.ncsa.illinois.edu/modules

Upcoming Changes

- Moab/Torque (PBS) 8.0 testing
  - Preparation for topology aware production scheduling evaluation period.
  - Two-day run with production jobs default settings.
  - Date not set yet but coming soon.
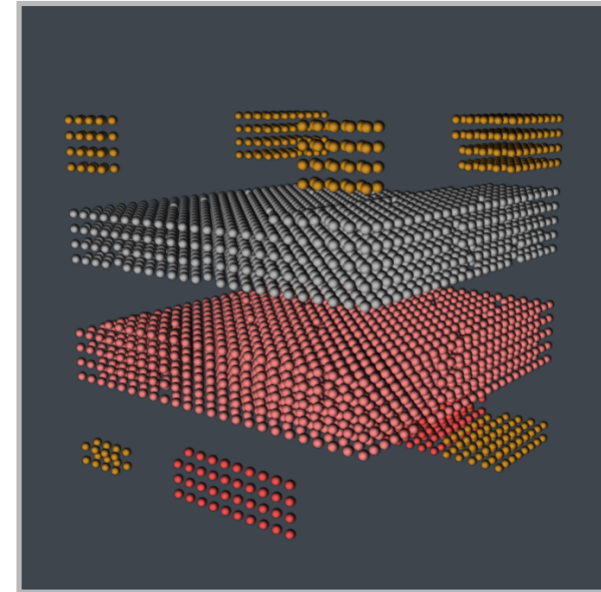
Upcoming Changes

- Planned Programming Environment (PE) changes
  - Next PE will require rebuild of MPI based applications.
  - Please try the new release. See
    https://bluewaters.ncsa.illinois.edu/pe-updates
  - MPT 7.0.X release adheres to the "MPICH ABI Compatibility Initiative" - https://www.mpich.org/abi
  - Fixes to some bugs from initial release.

New software

- IDL – Installed
  - module load idl
- Intel Compiler
  - On test system.
  - Installing on production system.

Data Sharing Service Update

- Globus Online and Web service based access.
- Finalizing procedural aspects.
    - DOI
    - Metadata Collection

Blue Waters Advanced User Workshop

- The week of October 13th at NCSA.

- More hands-on section oriented

  - Monday: Cray Tools: Reveal and Topaware

  - Tuesday: Allinea DDT and PGI

  - Wednesday: NVIDIA and Cray, HDF

- Bring your own code.

- Tie in with YT visualization workshop from Matthew Turk (NCSA).

VSCSE and XSEDE Events

VSCSE

- To resume in 2015.

XSEDE

- Check out XSEDE training Course Calendar

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

Special Topic

- HPC Python – Omar Padron
  - PRACE/XSEDE material

Future Topics?

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