

BLUE WATERS

SUSTAINED PETASCALE COMPUTING

10/20/14

Blue Waters User Monthly Teleconference



GREAT LAKES CONSORTIUM
FOR PETASCALE COMPUTATION

CRAY®

Agenda

- Blue Waters Symposium 2015
- NSF PRAC CFP
- Blue Waters Fall User workshop
- Utilization and recent events
- Recent and upcoming changes.
- SC14 Conference
- XSEDE and VSCSE training opportunities.
- Requests for Science Successes.

2015 Blue Waters Symposium

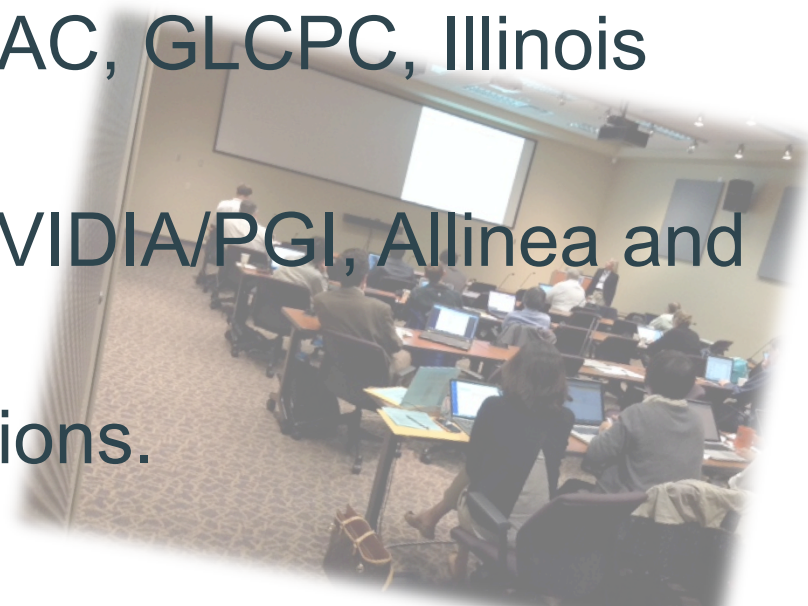
- May 10-14, 2015
- [Sunriver Resort](#) in Sunriver, OR



- Recreational opportunities: hiking, biking, fly fishing, rafting, canoeing, rock climbing, ...

Blue Waters Advanced User Workshop

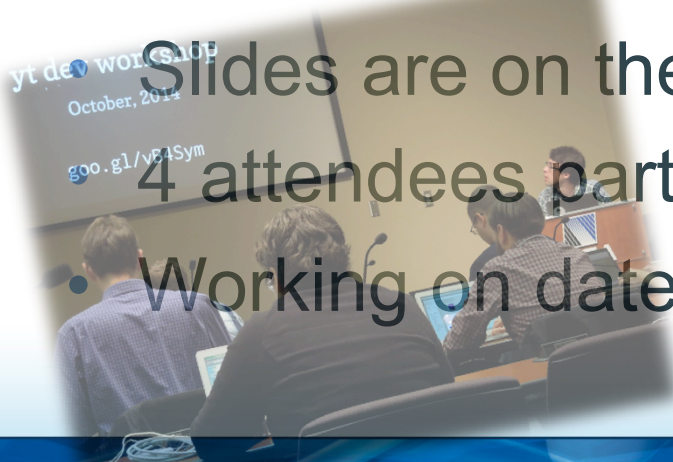
- 18 attendees from NSF PRAC, GLCPC, Illinois and Education allocations.
- Presentations from Cray, NVIDIA/PGI, Allinea and The HDF Group.
- Focused on hands-on sessions.



Slides are on the portal.

4 attendees participated in the yt dev. workshop

- Working on date for Spring 2015 workshop.



PRAC CFP

Petascale Computing Resource Allocations (PRAC)

CONTACTS

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PROGRAM GUIDELINES

Solicitation [14-518](#)

DUE DATES

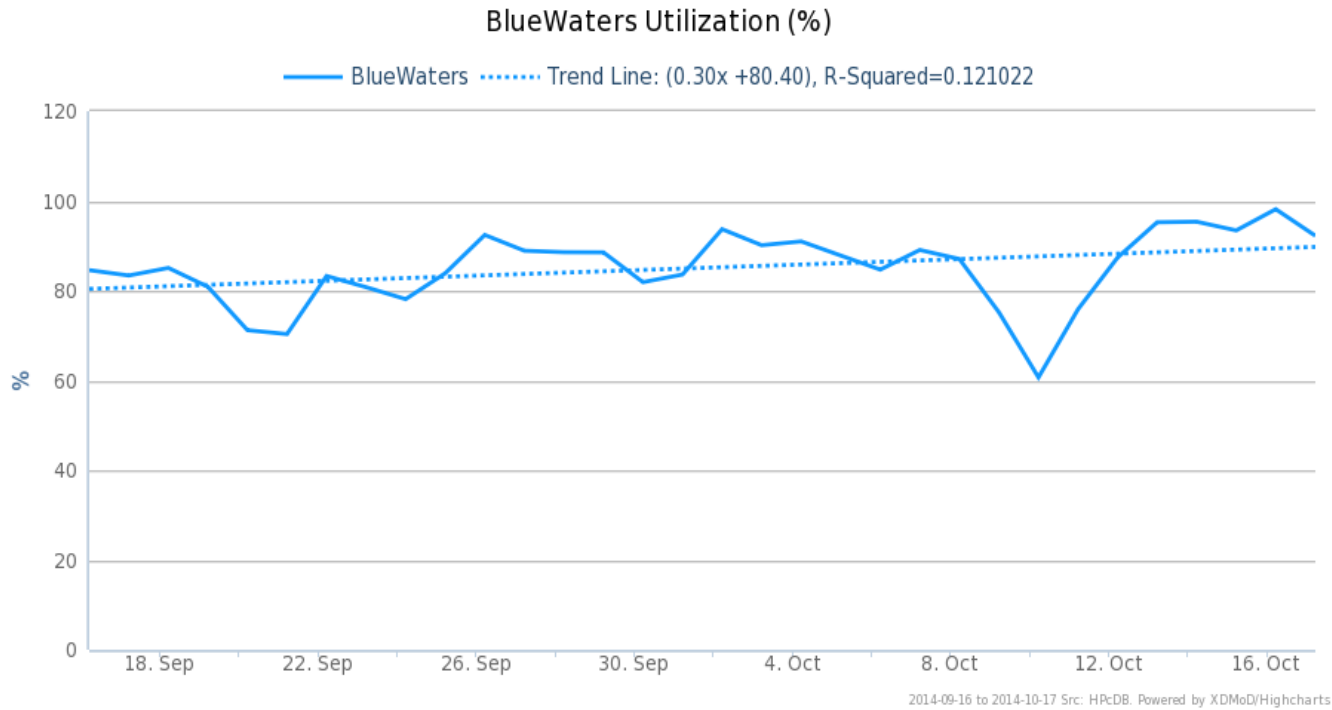
Full Proposal Deadline Date: November 14, 2014

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

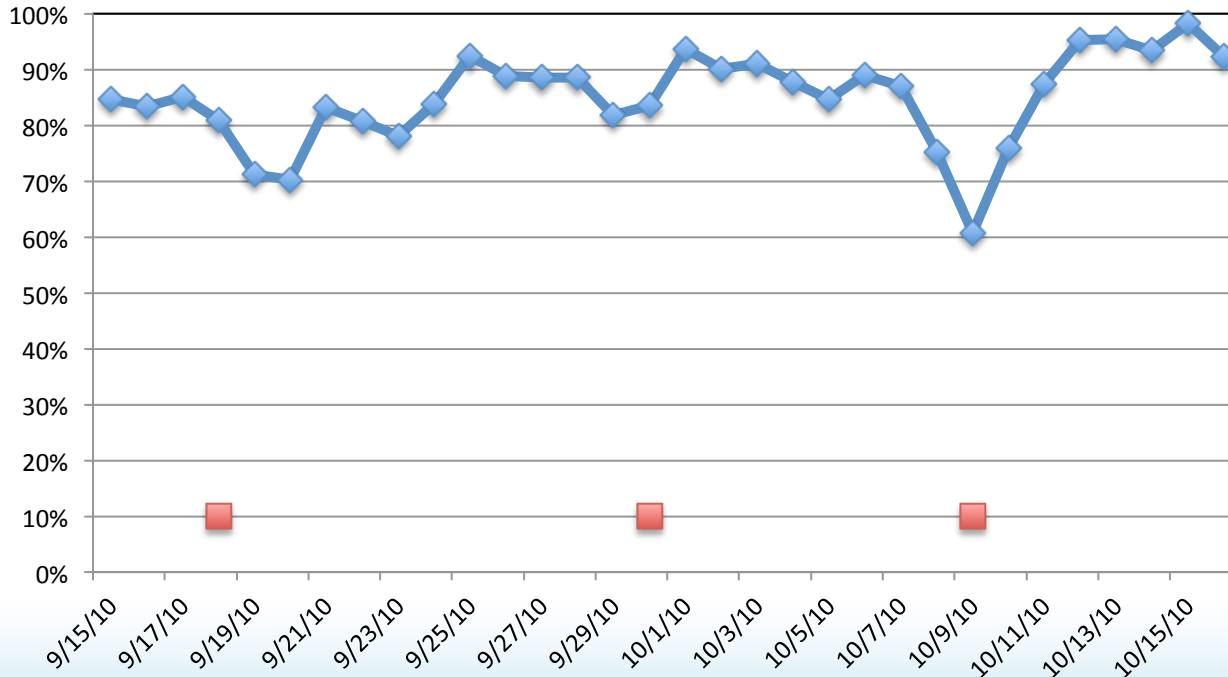
System Utilization

- Utilization since last BW User Call (September 15)



Recent System Events

- Hardware / Power related.
 - 9/18 and 10/1 – single cabinet emergency power off
 - 10/10 – larger power issue, sourced to loose connection



Recent Issues

- NVIDIA cuBLAS DGEMM
 - Observed only with sm_35 Kepler GPUs
 - $N * ldb \geq 536870912$ or $(1 \ll 29)$ or $2^{**}29$
 - "NN" (non-transposed) case only
- NVIDIA has a fix that should make its way to Blue Waters in a week or two.
- Use CPU equivalents to check results.

Recent Changes

- Programming Environment (PE) changes
 - September PE will not be default.
 - 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>
 - Some dynamically linked applications will need to be rebuilt or use the cray-mpich-compat/v6 module
 - Many changes to default versions.
 - CCE 8.3, PGI 14.2 (issue with LibSci), GNU 4.8.2 (4.9 CUDA conflicts)

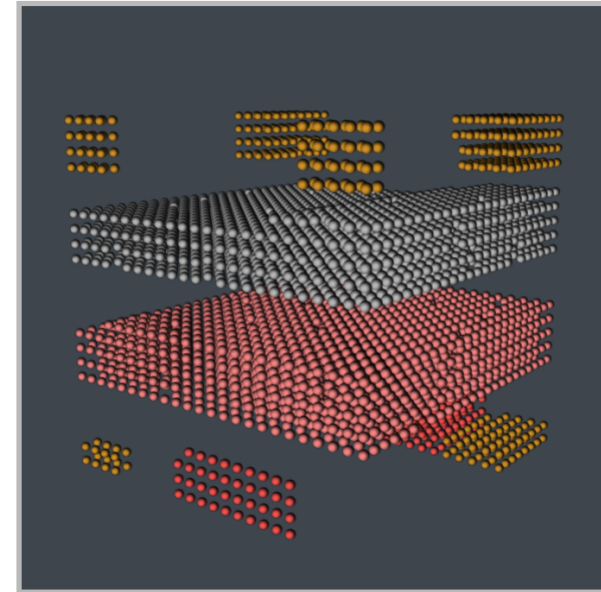
Upcoming Changes

- Modules
 - Enhancements by NCSA (Craig Steffen)
 - module output to stdout rather than stderr
 - tab-completion within module shell function
 - module load PrgTAB
 - 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.
 - Awaiting results of our application testing from this morning.



Upcoming Changes

- System upgrades
 - CLE 5.2 – mid to late November
 - CUDA 6.5 – December
- Move to newer Lustre software.
- Puts Blue Waters on similar stack as newer XC systems.

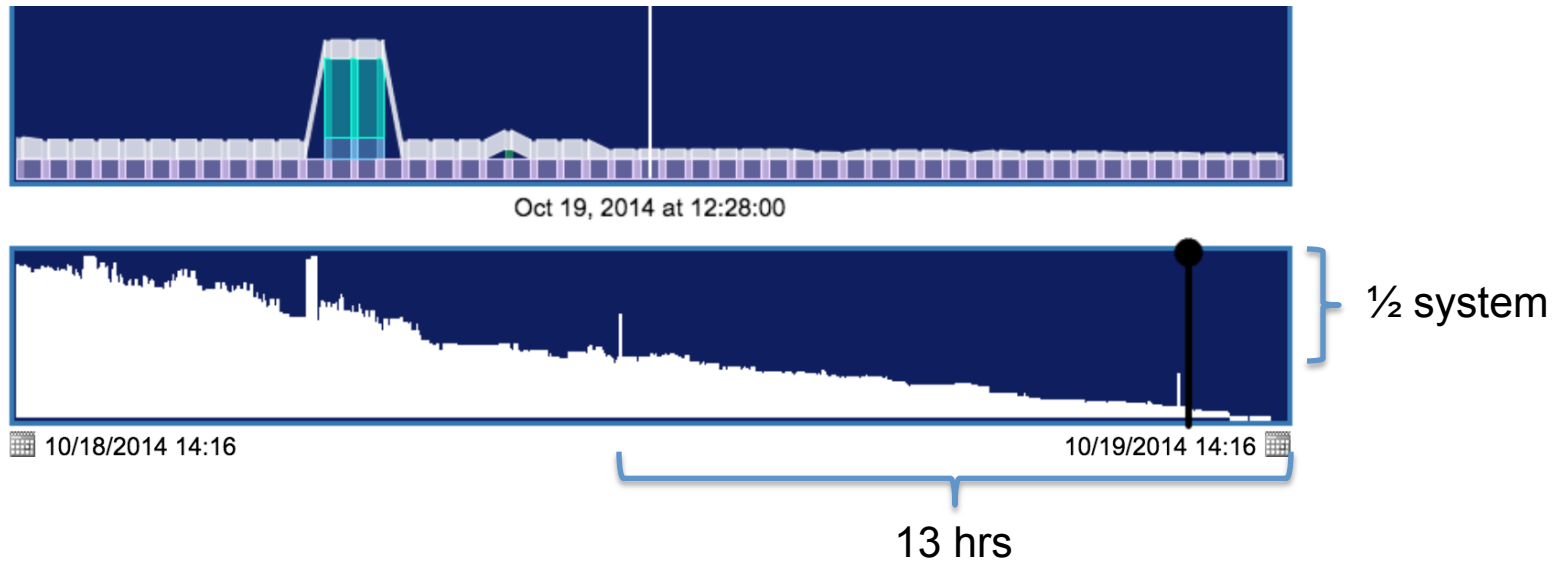
New software

- Intel Compiler
 - Installed.
 - module swap PrgEnv-XYZ PrgEnv-intel
 - Portal page in progress.
 - Includes TBB and MKL.
 - No Intel MPI.

Data Sharing Service Update

- Globus Online (GO) and Web service based access.
 - Resolving an issue with GO sharing.
- Finalizing procedural aspects.
 - DOI

Reminder to backfill ...



- Watch for maintenance notices.
- Realtime chart of backfill opportunities

<https://bluewaters.ncsa.illinois.edu/why-isn-t-my-job-running#backfill>

SC14

- Blue Waters Graduate Fellows will be in attendance, working the NCSA booth.
- Several Blue Waters staff will be there.
- Let us know if you will be there.

VSCSE and XSEDE Events


VSCSE

- [Call for sites.](#)

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](https://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

- No topic this month.
- Next topic (in December) – IO practices for efficient Nearline usage.

Future Topics?

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