

BLUE WATERS

SUSTAINED PETASCALE COMPUTING

10/14/18

Blue Waters User Monthly Teleconference



GREAT LAKES CONSORTIUM
FOR PETASCALE COMPUTATION

CRAY®

Agenda

- Recent Events and Changes to Blue Waters
- Usage, Utilization and other Items
- Upcoming Opportunities
- Request for publications!

Recent Events and Outages

- 10/15 - 7:33 AM power loss to one feed (of 4) into the NPCF causing 3 rows to fail 27 minutes before maintenance was to start.

Recent Changes

- 10/15 - Security Update
 - Apply patch to address Mutagen Astronomy exploit.
 - Recently changed stack limits will revert to previous settings.
- Limit on open files set to 64K on compute nodes and MOM nodes. Used to be 1K/4K and 100000 respectively.

Outstanding Issues

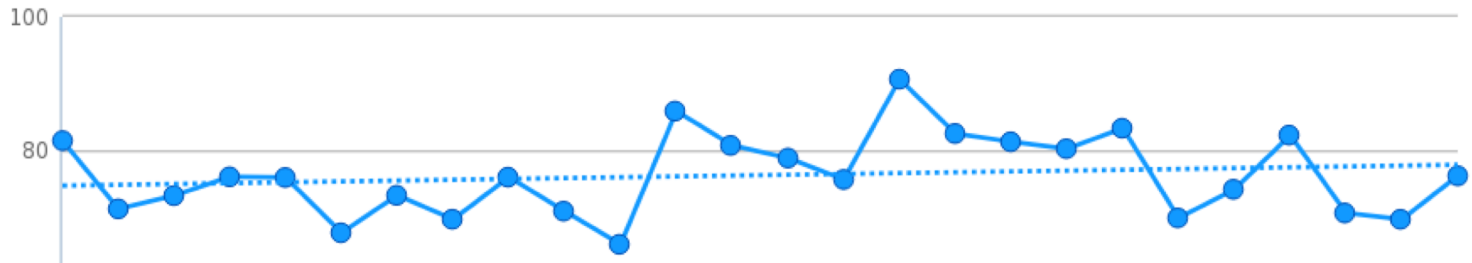
- CUDA 9.1 and GCC 6.3
 - broken `std::tuple` with GCC 6
- <https://devtalk.nvidia.com/default/topic/1028112/cuda-setup-and-installation/nvcc-bug-related-to-gcc-6-lt-tuple-gt-header-/>
- Work-around is to drop to GCC 5.3.
 - bwpy 2.0 pre-release for testing.
 - We are working with Cray and NVIDIA to get fix from CUDA 9.2 back-ported.

Upcoming Changes

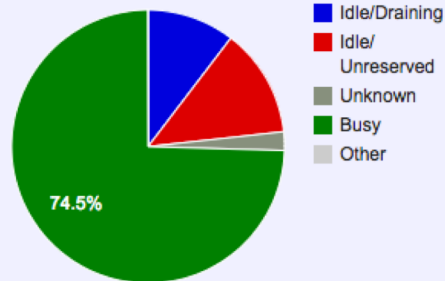
- Preparing to make PE 18-06 default. See [PE Changes page](#) on the portal.
- For testing ...
 - `module unload PrgEnv-cray; module load PrgEnv/cray-18_06-cuda-9.1`
 - `module unload PrgEnv-gnu; module load PrgEnv/gnu-6.3.0-cuda-9.1`
 - `module unload PrgEnv-intel; module load PrgEnv/intel-18.0.3.222-cuda-9.1`
 - `module unload PrgEnv-pgi; module load PrgEnv/pgi-18.3.0-cuda-9.1`
- Add as needed
 - OpenACC
 - `module add craype-accel-nvidia35`
 - CUDA
 - `module add cudatoolkit/9.1.85_3.10-1.0502.df1cc54.3.1`
 - HDF5
 - `module add cray-hdf5/1.10.2.0`
 - `module add cray-hdf5-parallel/1.10.2.0`

Usage, Utilization and other Items

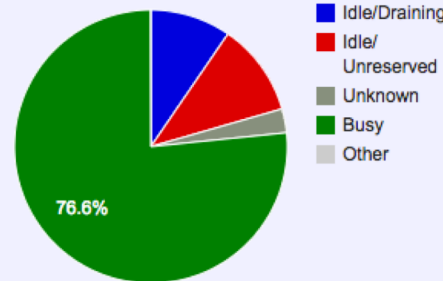
- Overall Utilization last 30 days



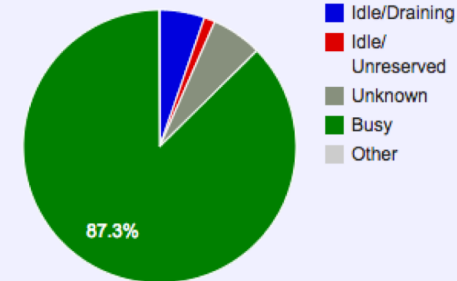
XE Utilization for this Period



Full System Utilization for this Period



XK Utilization for this Period

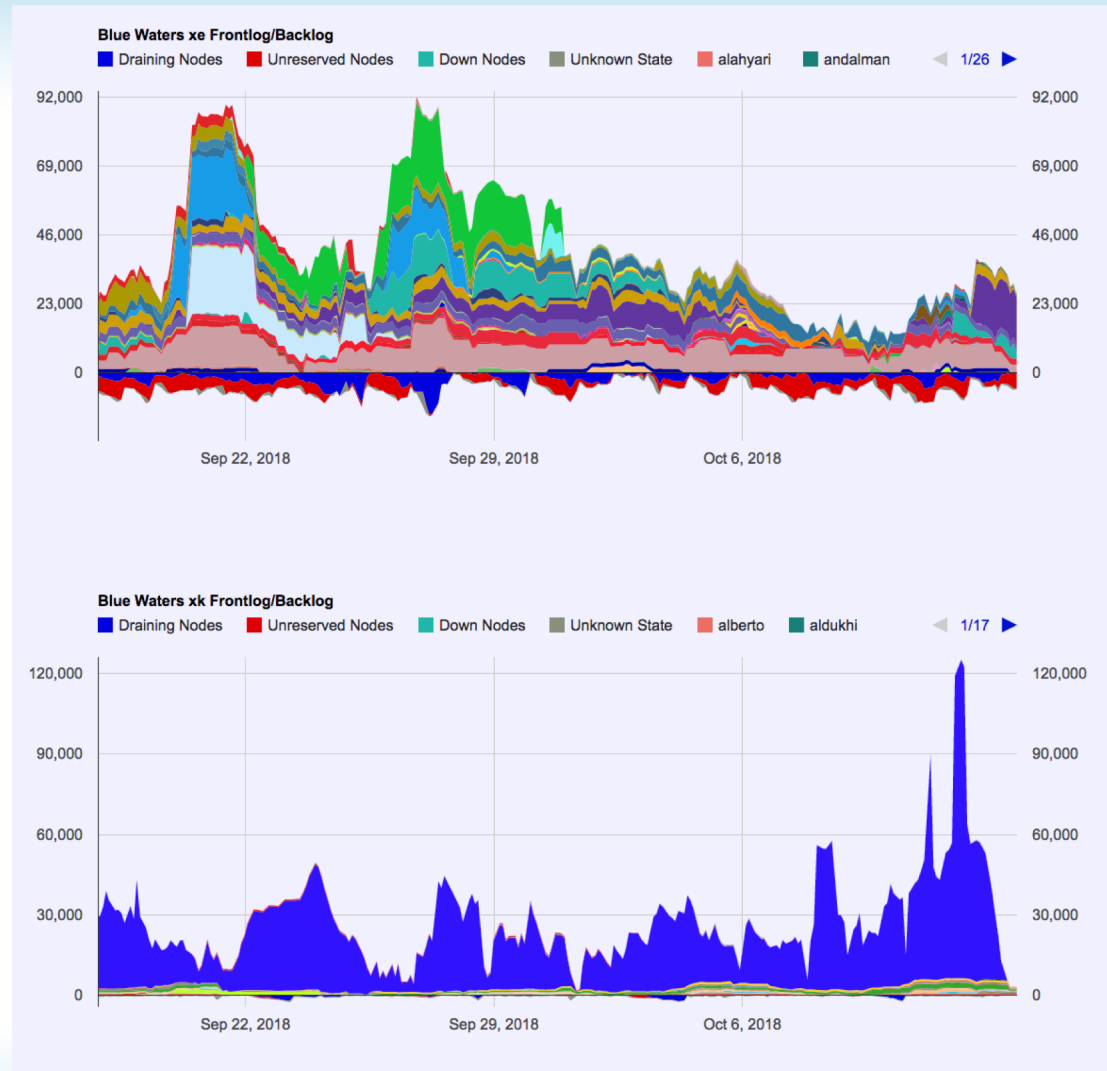


0 18. Sep 22. Sep 26. Sep 30. Sep 4. Oct 8. Oct 12. Oct

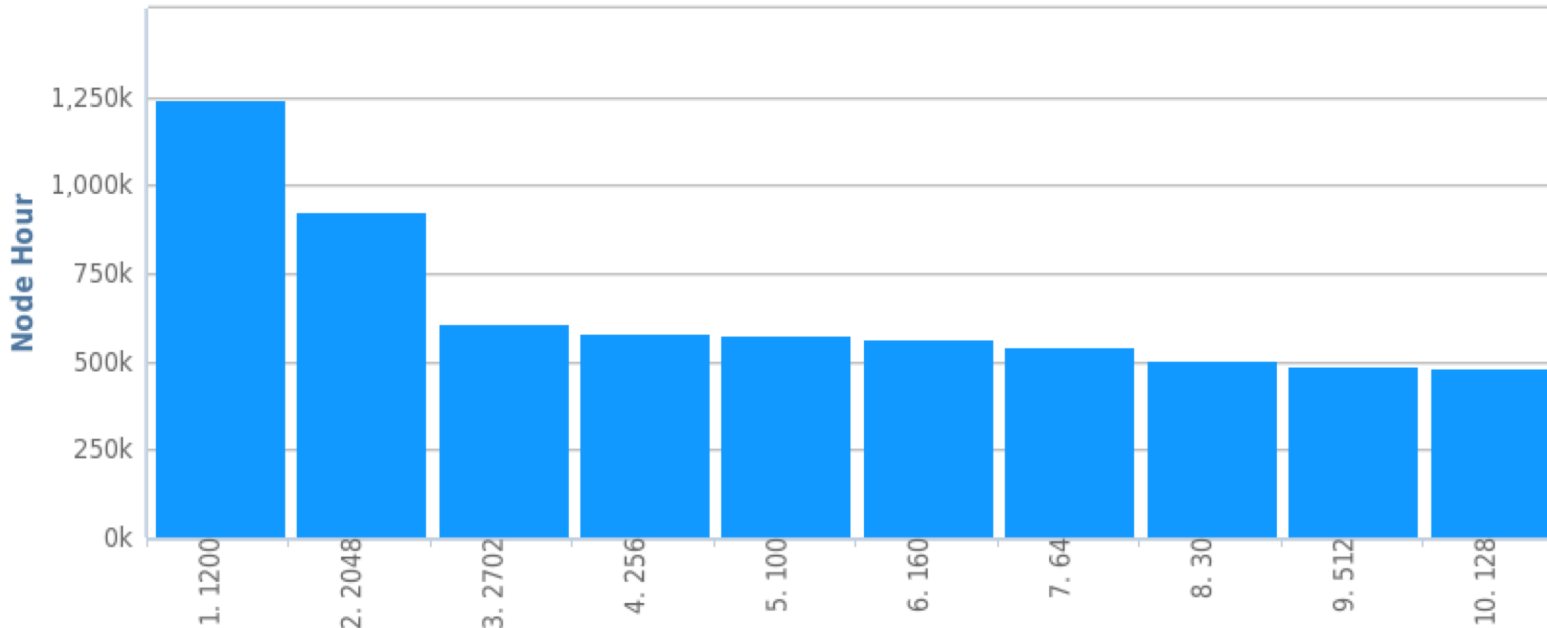
—●— BlueWaters Trend Line: $(0.13x + 74.53)$, R-Squared=0.024342

Backlog

- Last 30 days.
- Vertical axis in units of **nodes**. Colors are different users.
- Red **below** the x-axis indicates unreserved nodes. Blue **below** the x-axis indicates draining.
- **Decreased backlog. Good turn-around time for jobs.**

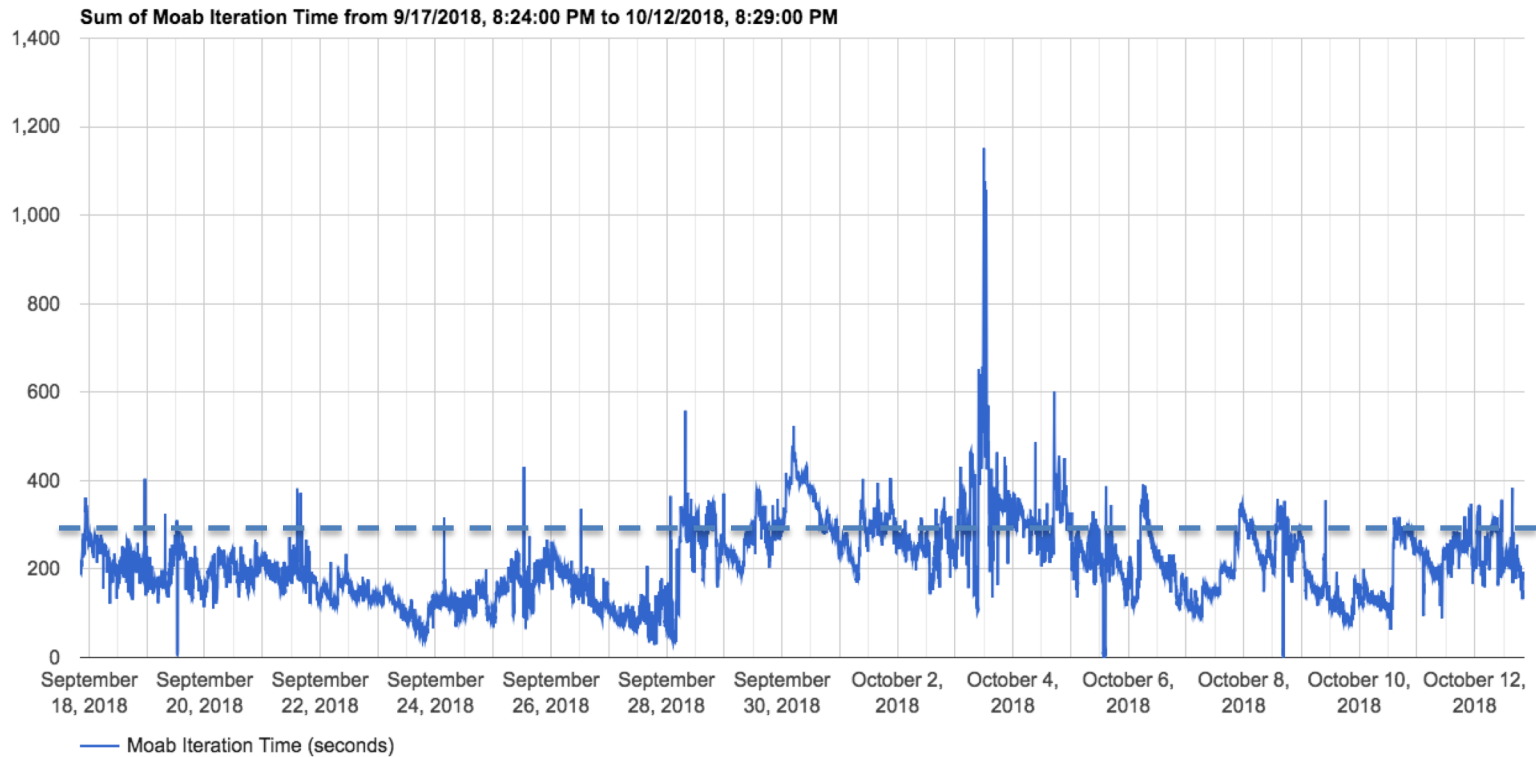


Workload Details



- Large contribution from 1K to 3K XE jobs, 1200 XK jobs.
- Data combines XE and XK jobs.
- Last 30 days.

Job scheduler iteration time



XSEDE Training Events

- <https://portal.xsede.org/course-calendar>
 - November 6, OpenACC.

NVIDIA Online Training Event

- [New OpenACC Online Course Will Help You Quickly Accelerate Your Code on GPUs](#)
 - October 18, 2018 – Analyzing and Parallelizing with OpenACC
 - October 25, 2018 – GPU Programming with OpenACC
 - November 1, 2018 – Optimizing and Best Practices with OpenACC


Blue Waters Weekly Webinar Series

THE NEXT SCHEDULED WEBINARS

- October 10, 2018: [Developing Interactive Parallel Workflows in Python using Parsl](#)
- October 24, 2018: [Introduction to Performance Tuning with Cray Perftools](#)
- November 7, 2018: [Introduction to NVIDIA Nsight Systems - A Performance Analysis Tool](#)
- November 21, 2018: [Getting started with WDL and Cromwell for workflow management on multiple platforms](#)

- For more information about the webinar series, including registration, abstracts, speakers, as well as links to Youtube recordings, please visit the [Blue Waters webinar series webpage](#).
- Make sure to [RSVP on Facebook](#) and on the [Blue Waters Portal](#)
- We welcome suggestions for topics that will benefit the petascale community. Send your suggestions to bw-eot@ncsa.illinois.edu.

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