

BLUE WATERS

SUSTAINED PETASCALE COMPUTING

4/16/18

Blue Waters User Monthly Teleconference



GREAT LAKES CONSORTIUM
FOR PETASCALE COMPUTATION

CRAY®

Agenda

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

Recent Events and Outages

- No outages to report this period.

Recent Changes

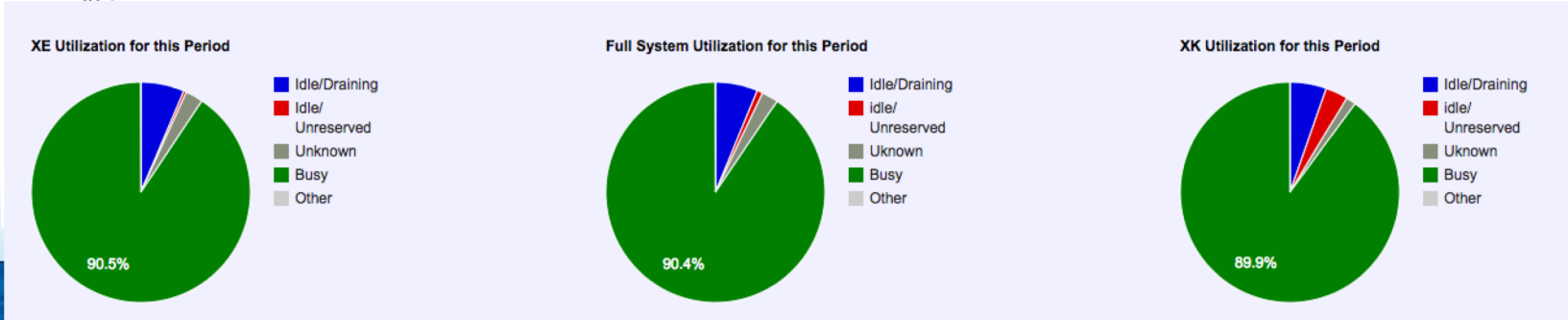
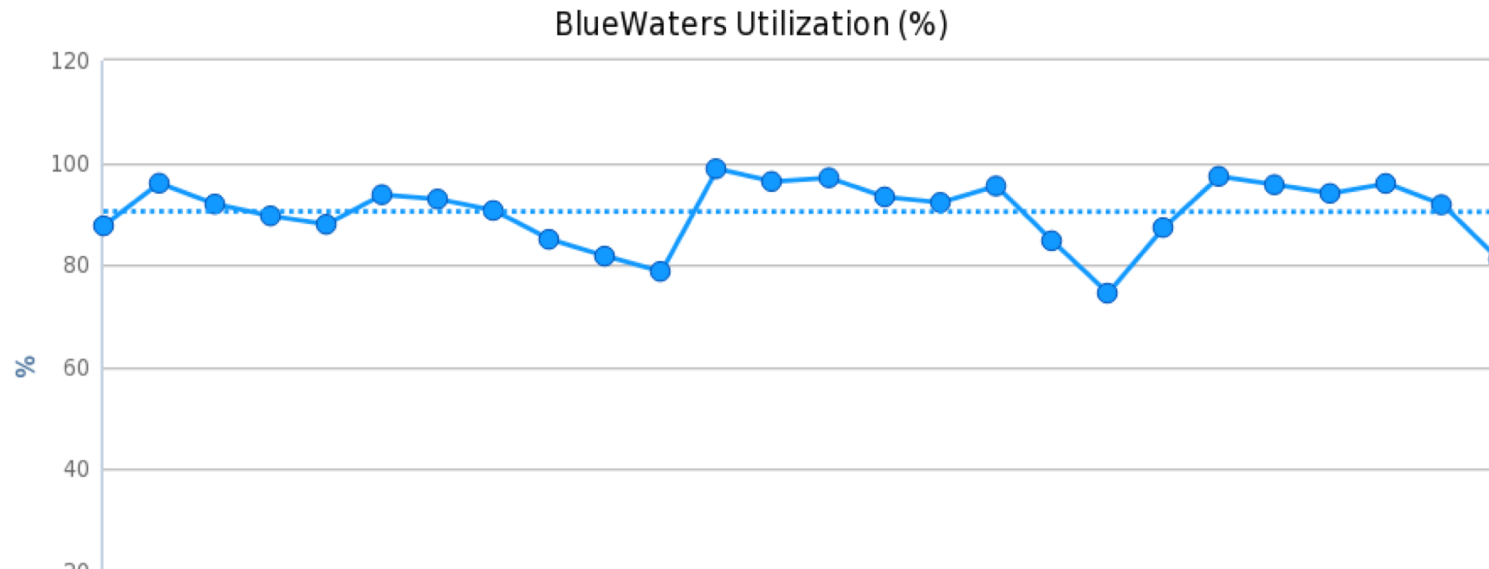
- Python
 - The default python has been changed from python2 to python3. All scripts which are not compatible with both major versions should explicitly use python2 or python3. See <https://python3statement.org/> for information on major package developer support timelines.
 - The pypy and pypy3 interpreters are now able to support numpy, scipy, and mpi4py. Some codes may benefit from the jit compilation these interpreters provide.
 - Tensorflow has been updated from 1.3.0 to 1.4.1
 - Python3.6 has been added as the non-default python3 compiler. As not all modules supported by 3.5 are installed for it, Python3.5 remains the default.
 - Numpy, scipy, and other modules which use BLAS routines now use Intel MKL rather than Cray libsci. DO NOT LET PIP INSTALL UPDATES TO THESE MODULES. The OpenBLAS versions installed by pip are **significantly slower**. Check your `~/.local/lib/*/site-packages` and your virtualenvs and delete any versions pip installed. When using pip `install`, it is recommended to use `--upgrade-strategy only-if-needed`
 - A note on virtualenvs: When a virtualenv is created, the version is written into the wrapper script according to the `BWPY_VERSION` environment variable. If created using `bwpy/latest-stable`, the virtualenv will always use the "default" image. If created using `bwpy/1.1.0`, it will always load the 1.1.0 image. This value can be manually changed by editing the wrapper script `[virtualenv]/bin/python`.

Upcoming Changes

- Awaiting possible software updates. Stay tuned.
- Spark testing continues. Preparing documentation. Inquire if interesting in testing.

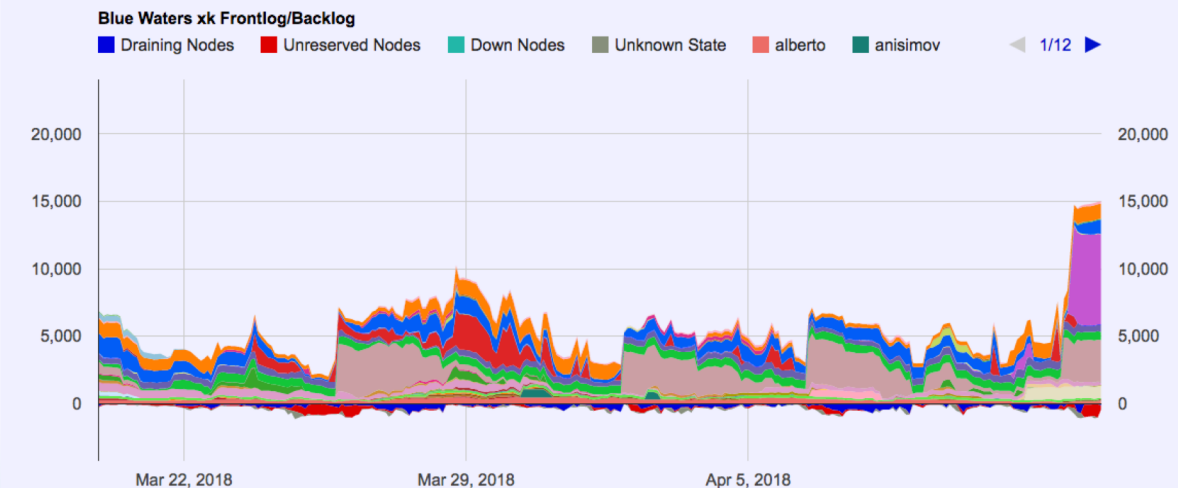
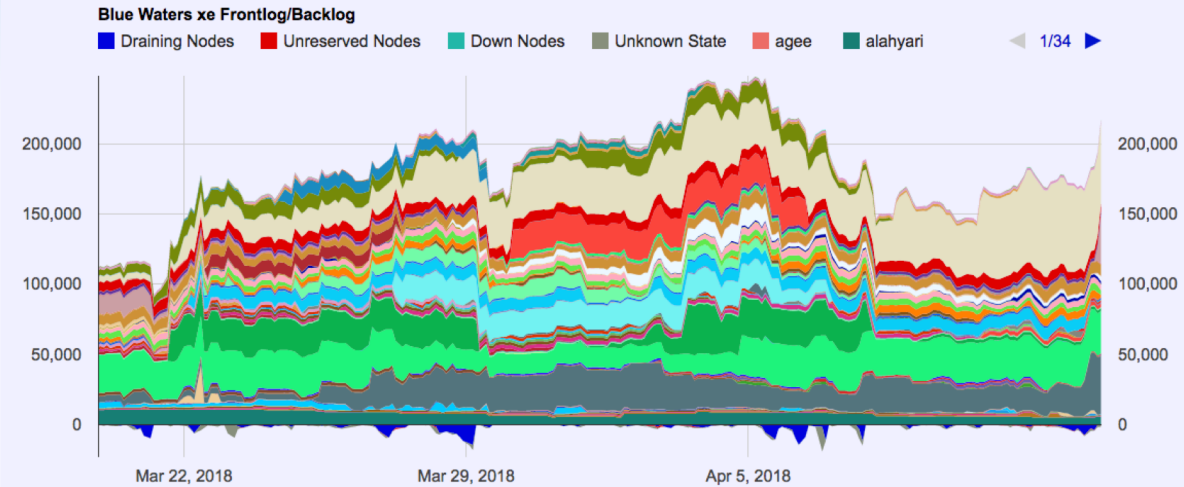
Usage, Utilization and other Items

- Overall Utilization last 30 days



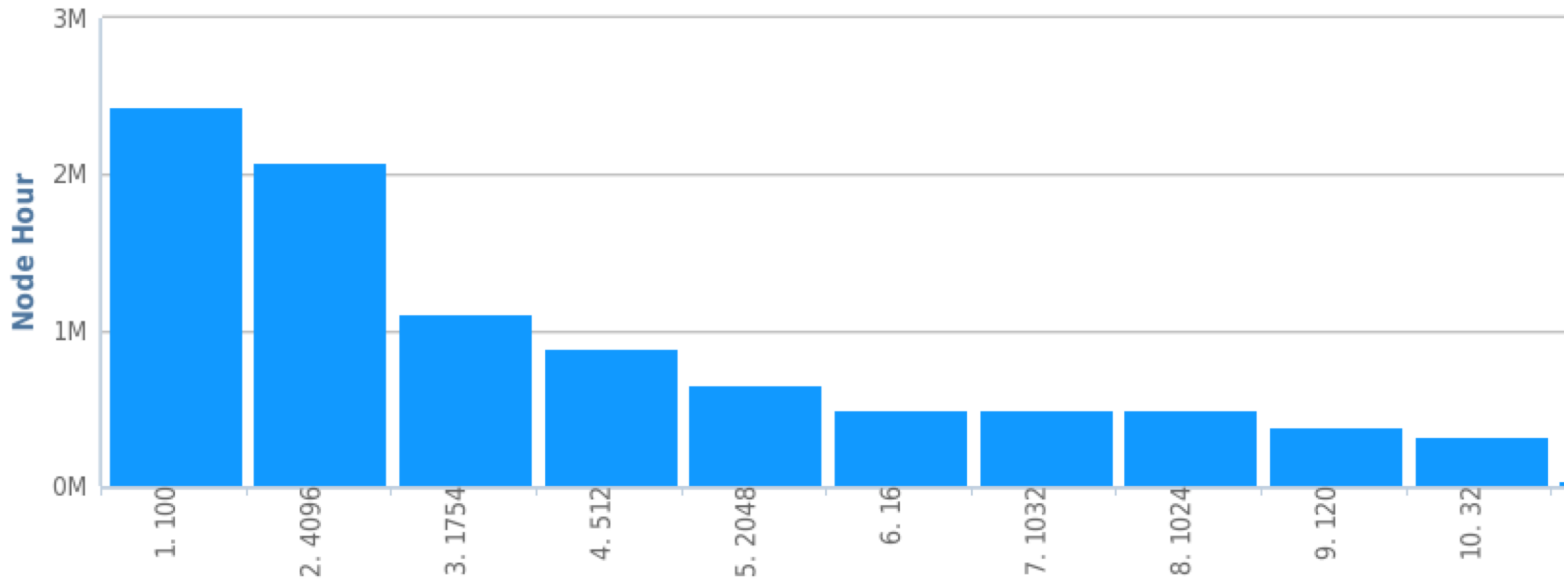
Backlog

- 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.



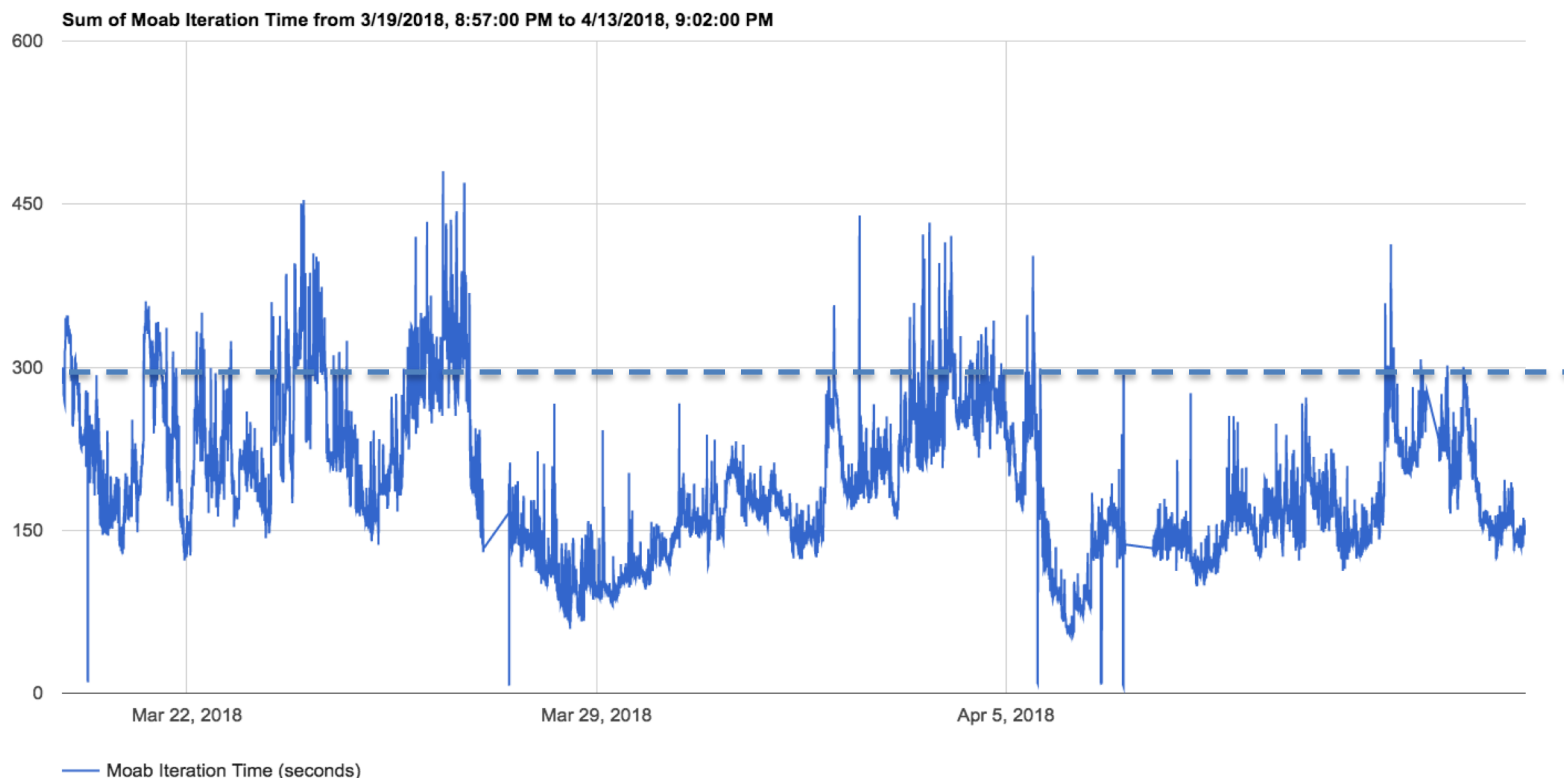
Workload Details

Node Hours: Total: by Node Count



- Less contribution from full system jobs.
- Data combines XE and XK jobs.
- Last 30 days.

Job scheduler iteration time



- Working to keep iteration time < 300 seconds.


Blue Waters Weekly Webinar Series

- 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](#).
- Our next offering is a Blue Waters Webinar that will focus on the XSEDE Service Provider Forum and feature Dr. Dan Stanzione, the Executive Director of the Texas Advanced Computing Center (TACC) at the University of Texas at Austin.
- Please find the full abstract and biography below, and make sure to [RSVP on Facebook](#) and on the [Blue Waters Portal](#)
- **When:** 10:00 CDT, April 18, 2018
- We welcome suggestions for topics that will benefit the petascale community. Send your suggestions to bw-eot@ncsa.illinois.edu.

XSEDE Training Events

- May 1-2 – Big Data
- Series run from 11AM-5PM Eastern Time each day.
- NCSA hosting local site for Illinois partners.
- <https://portal.xsede.org/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