

# BLUE WATERS

SUSTAINED PETASCALE COMPUTING

12/16/18

## Blue Waters User Monthly Teleconference



GREAT LAKES CONSORTIUM  
FOR PETASCALE COMPUTATION

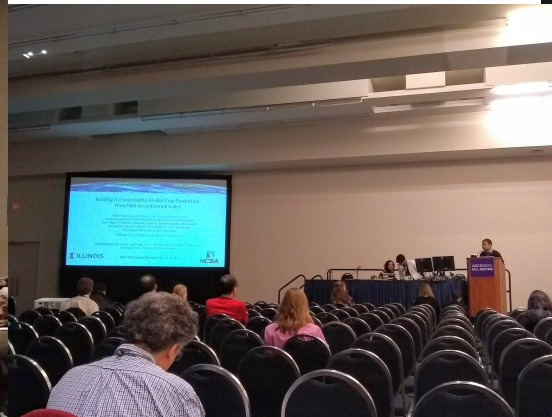
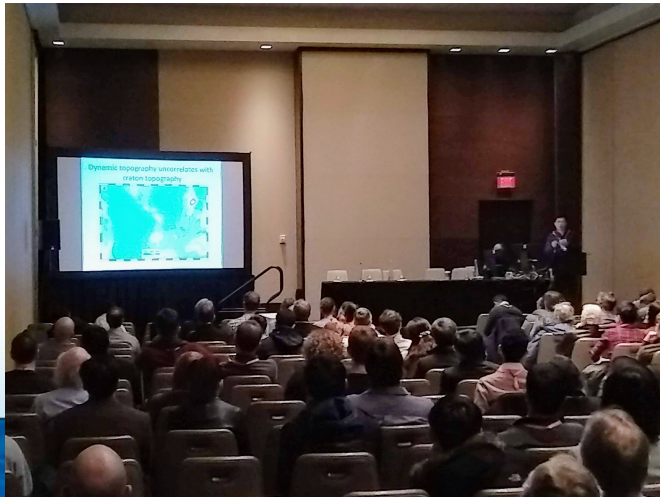
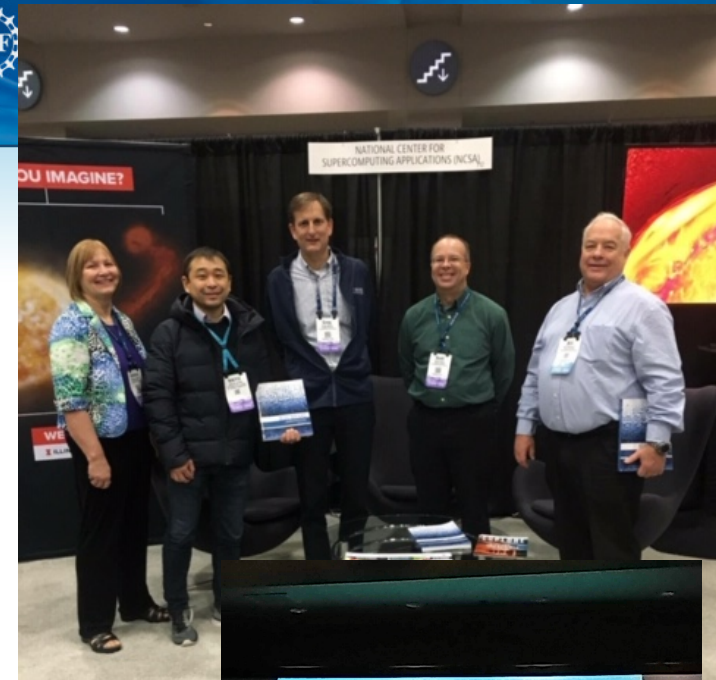
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# Agenda

- Blue Waters/NCSA at AGU
- NSF Dear Colleague Letter
- Discount Period
- Recent Events and Changes to Blue Waters
- Usage, Utilization and other Items
- Upcoming Opportunities
- Request for publications!

## AGU

- 4<sup>th</sup> year at AGU
- Visit our exhibitor booth.
- More than 10 posters and 15 talks by Blue Waters Science teams.



# NSF Dear Colleague Letter

- The two NSF leadership-class computing resources, Blue Waters and Frontera, will be available for allocation with an award start date of April 1, 2019.
- Allocations to be done via **supplemental funding requests**.
- Blue Waters
  - Up to 125 million node-hours will be available across **five to six** supplemental funding requests.
- Frontera
  - 34 million node-hours will be available across **15 to 20** supplemental funding requests.
- “For full consideration, supplemental funding requests should be submitted no later than February 1, 2019.”
- See <https://www.nsf.gov/pubs/2019/nsf19030/nsf19030.jsp> for more details.

PIs interested in submitting supplemental funding requests **must consult with the cognizant NSF program director** for this DCL: Edward Walker.

## Discount Period

- Nov 1 - Nov 15: 50% charge discount on all queues, all jobs completing during this period
- Nov 16 - Jan 2: 50% charge discount on all queues, all jobs completing during this period for projects that have consumed **at least 25%** of their current allocation.

## Recent Events and Outages

- No events to report.

## Recent Changes

- No changes to report.

## 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-/>
- Patch to `gcc/6.3.0`, as a work-around, available for testing.
  - Known issue with `namd` and optimization flag `-ftree-loop-vectorize`. Looking at impact of disabling flag by default.



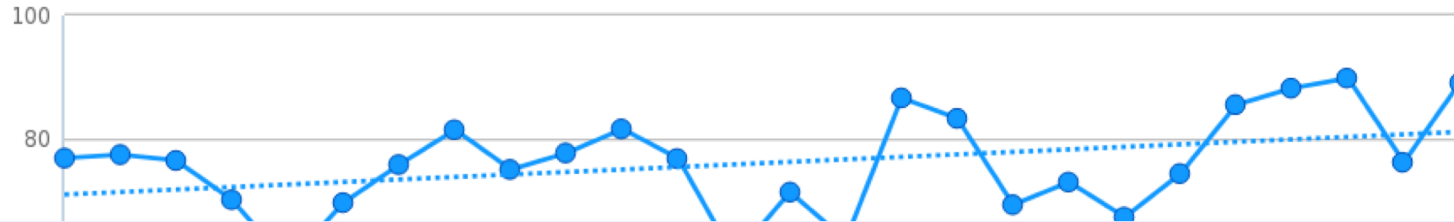
# Upcoming Changes

- 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`

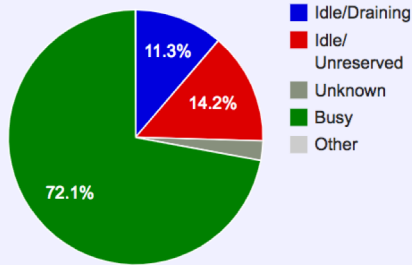
# Usage, Utilization and other Items

- Overall Utilization last 30 days

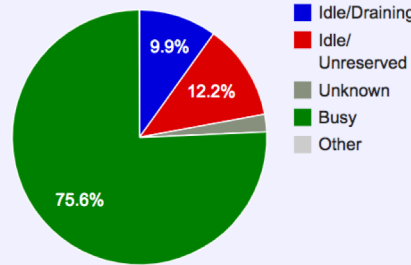
BlueWaters Utilization (%)



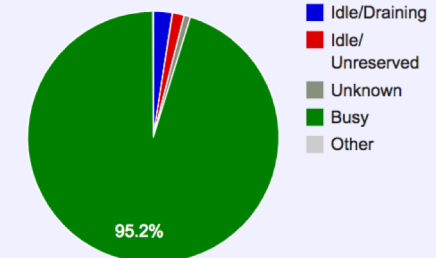
XE Utilization for this Period



Full System Utilization for this Period



XK Utilization for this Period



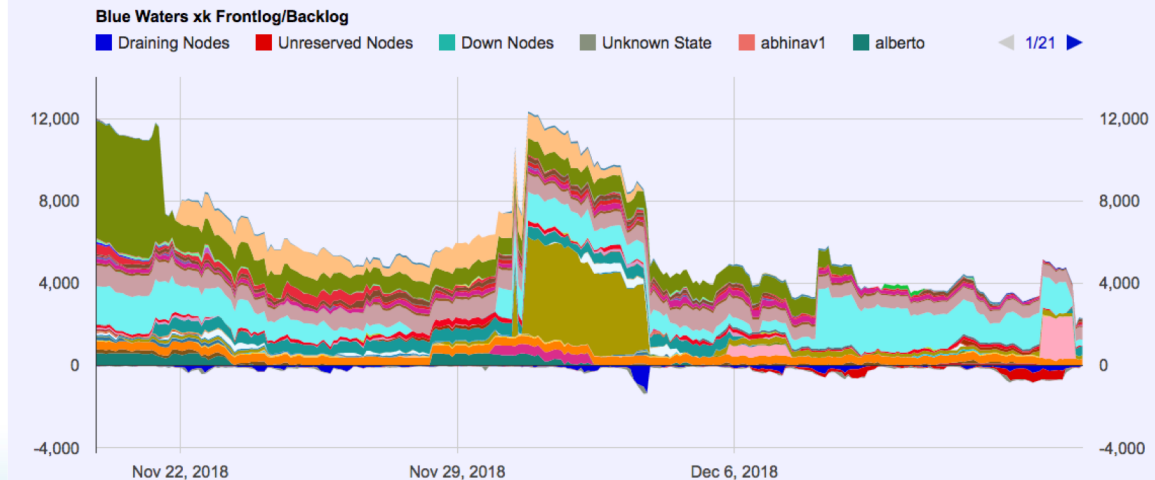
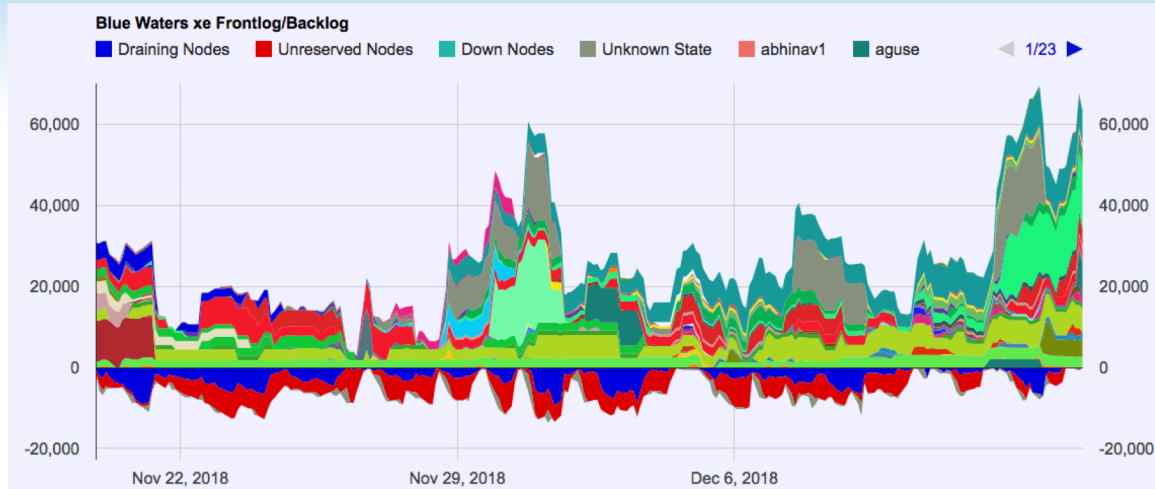
0 20. Nov 24. Nov 28. Nov 2. Dec 6. Dec 10. Dec 14. Dec

—●— BlueWaters ..... Trend Line:  $(0.41x + 70.73)$ , R-Squared=0.140999

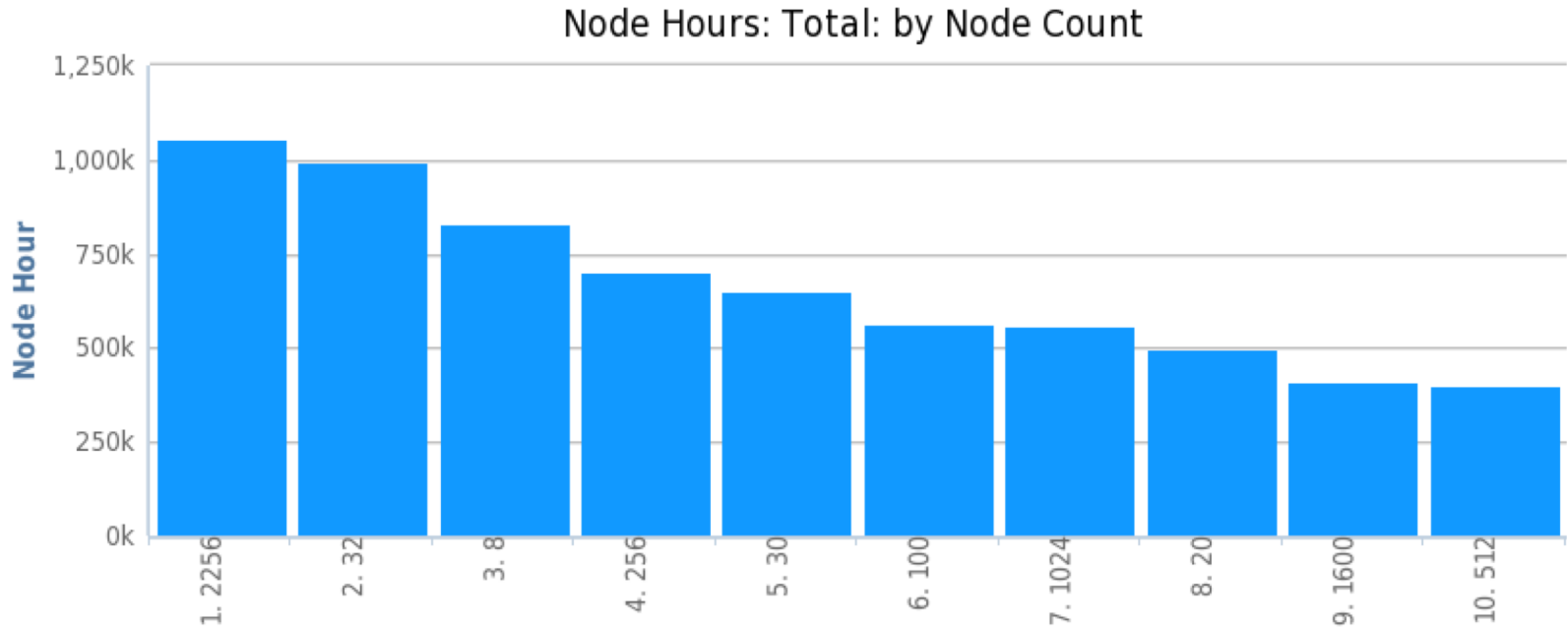
2018-11-19 to 2018-12-14 Src: HPcDB. Powered by XDMoD/Highcharts

## 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.
- **Still seeing red.**

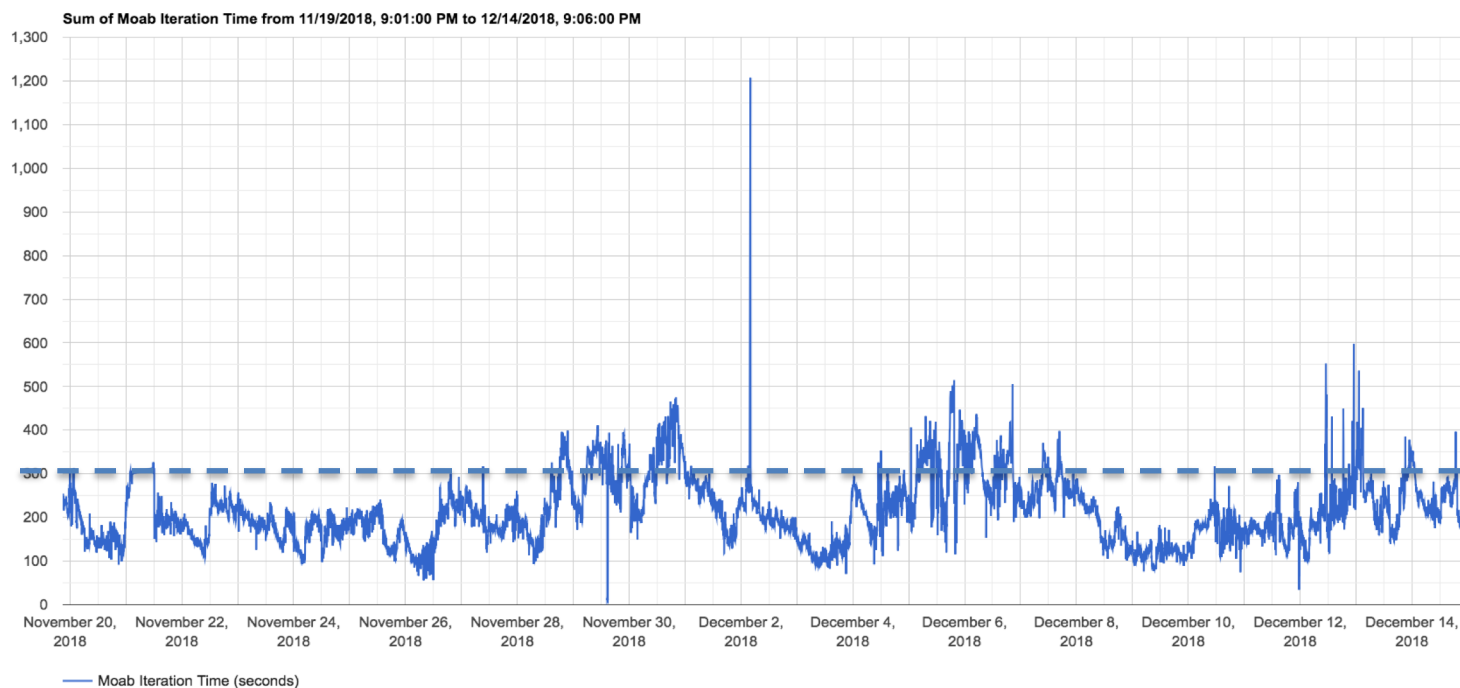


# Workload Details



- Fewer, full XE jobs.
- Data combines XE and XK jobs.
- Last 30 days.

# Job scheduler iteration time




# XSEDE Training Events

- <https://portal.xsede.org/course-calendar>

# 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](#).
- 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](mailto: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](mailto: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