BLUE WATERS

SUSTAINED PETASCALE COMPUTING

10/14/16

Blue Waters User Monthly Teleconference

GREAT LAKES CONSORTIUM FOR PETASCALE COMPUTATION

Agenda

- Future Maintenance
- Recent Events and Changes
- Utilization and Usage
- Opportunities
- PUBLICATIONS!

Recent Changes

- None to report.

Reminder of Changes to Blue Waters

- Large memory nodes
  - 96 XE nodes with 128 GB (2x3x8 geometry)
  - 96 XK nodes with 64 GB
  - Slightly slower STREAM Triad for large *N*.

  - Add

```
#PBS -l feature=xehimem
#PBS -l feature=xkhimem
```

Future Maintenance

- In the near future (10/26)
  - Upgrade HPSS software; HSM functionality.
  - Blue Waters compute to be up. Stage your data as needed. Use PBS directive `-l gres=hpss` if your job requires HPSS and you do not want it to run during the HPSS outage.

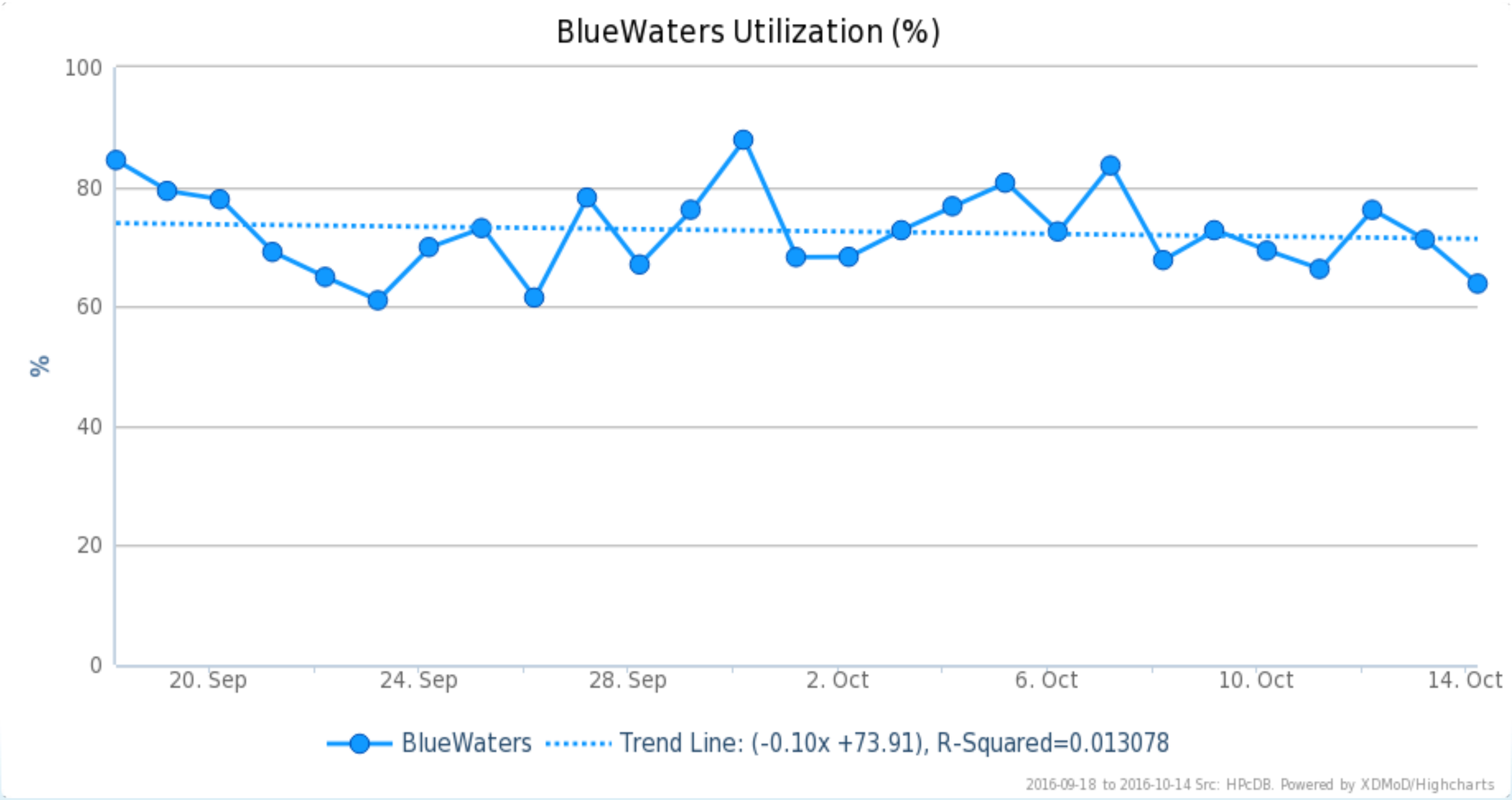
- In the next month
  - Blue Waters Core switch upgrade (not HSN).

Future Changes to Blue Waters

- Shifter (coming soon)
    - Docker-like container allowing user-defined images.
    - Improved security model.
    - Testing on Blue Waters now. Should be available in a few weeks.
    - Watch for announcement.

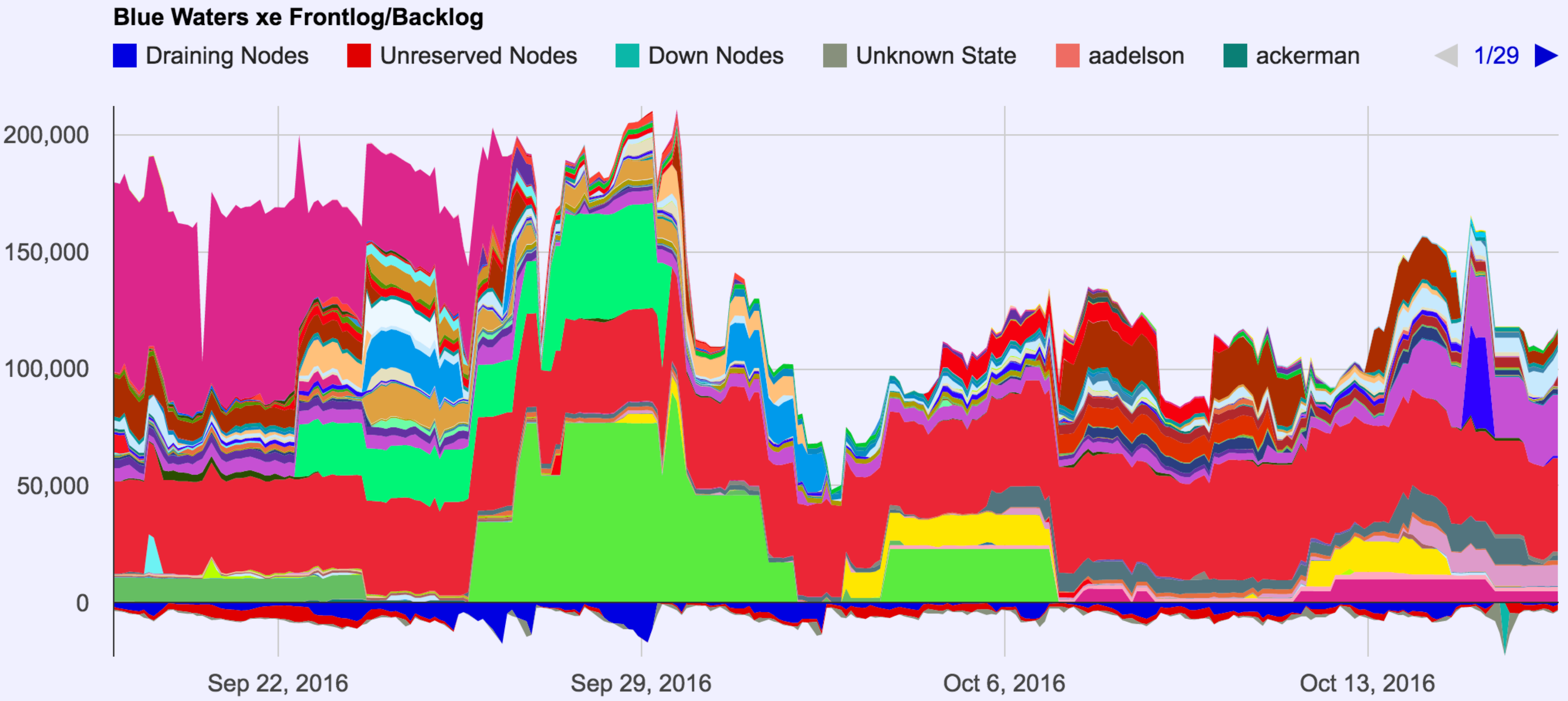
Usage, Utilization and other Items

- Utilization since last BW User Call (Sept 19)



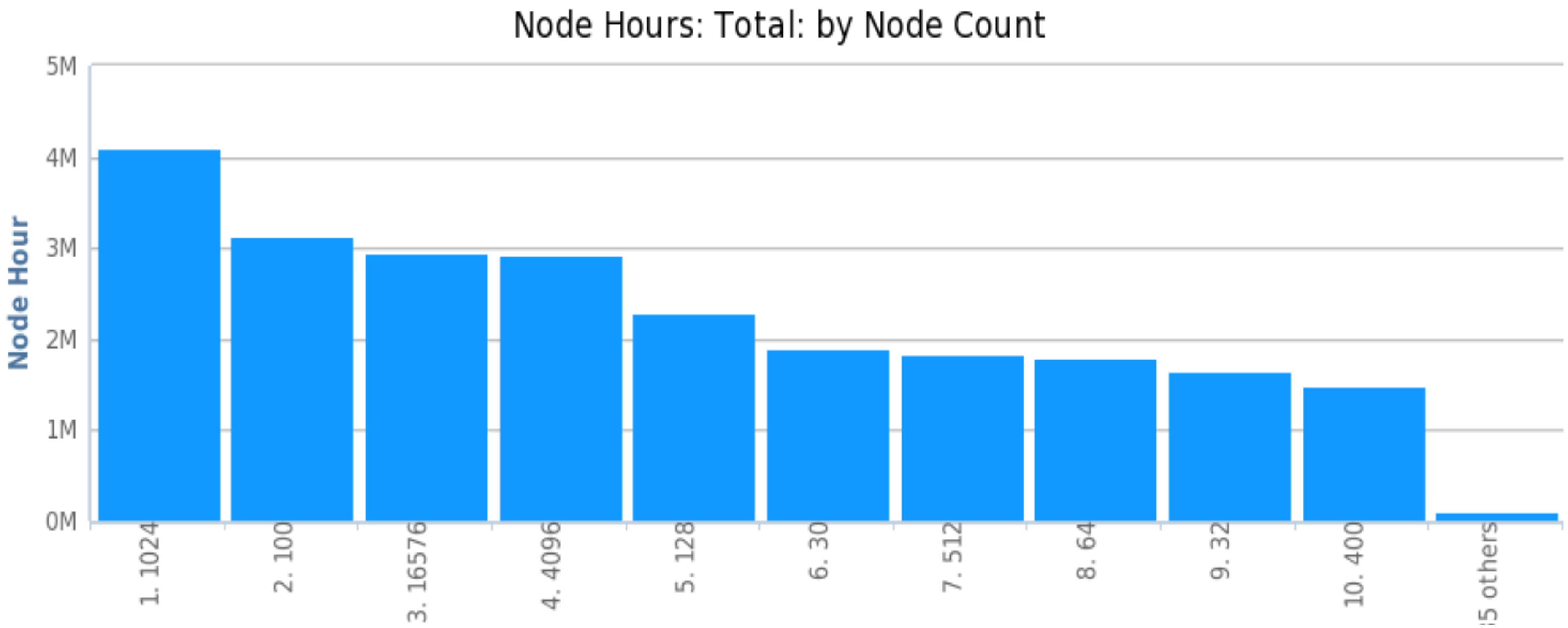
2016-09-18 to 2016-10-14 Src: HPcDB. Powered by XDMoD/Highcharts

Workload backlog



- Vertical axis in units of nodes. Colors are different users.
- 28% reduction in XE backlog after Sept 31st. Larger reduction for XK backlog.

Workload Details



- Data combines XE and XK jobs.

Why isn’t my job running

- Check system status page for utilization.
- Check backfill at above url or on system
  - `showbf -p bwsched -f xe`
- Check top jobs
  - `showq -i`
  - Ordered by priority. Jobs with * have a reservation on nodes.
- Check start times of jobs with reservations using `showres`.

```
> showbf -f xe -p bwsched
Partition      Tasks  Nodes      Duration   StartOffset       StartDate  Geometry
---------     ------  -----  ------------  ------------  --------------  --------
bwsched        12032    376       2:26:17      00:00:00  14:21:45_08/14  4x6x8
bwsched         7168    224       4:09:44      00:00:00  14:21:45_08/14  8x2x7
bwsched         1536     48       5:56:17      00:00:00  14:21:45_08/14  3x2x4
bwsched         1536     48       6:01:17      00:00:00  14:21:45_08/14  3x2x4
bwsched         1024     32       6:06:17      00:00:00  14:21:45_08/14  1x2x8
bwsched          640     20      INFINITY      00:00:00  14:21:45_08/14  1x2x5
```

```
> showq -i | grep -v xk | grep \*
5207970*      10321211     99.0 to  dtoussai     baea   4096     3:30:00    normal   Wed Jul 20 07:08:18
5276564*      10125901     99.0 to     yeung      jmo  16512    00:30:00      high   Wed Aug 10 20:59:04
5207973*       9587740     99.0 to  dtoussai     baea   4096     3:30:00    normal   Wed Jul 20 07:08:27
5275602*       7617711     99.0 to      guo2      jna   8000    00:30:00      high   Wed Aug 10 14:14:31
5271992*       7307965     99.0 to   pinelli      jno   9216    00:05:00      high   Tue Aug  9 13:44:27
5273294*       7200637     99.0 to   pinelli      jno  18432    00:05:00      high   Tue Aug  9 17:05:50
5246922*       5689508     99.0 to  dtoussai     baea   4096     3:30:00    normal   Sun Jul 31 01:51:04
5246923*       5642442     99.0 to  dtoussai     baea   4096     3:30:00    normal   Sun Jul 31 01:51:12
5269231*       5637764      4.9 to     clay1      jmo   8340  2:00:00:00      high   Sat Aug  6 19:06:02
5246924*       5600588     99.0 to  dtoussai     baea   4096     3:30:00    normal   Sun Jul 31 01:51:19
```

```
> showres 5207970 ...
5207970      Job I    00:33:05     4:03:05     3:30:00 4096/131072 Sun Aug 14 14:54:44
5276564      Job I     6:06:23     6:36:23    00:30:00 16512/528384 Sun Aug 14 20:28:02
5207973      Job I     2:26:23     5:56:23     3:30:00 4096/131072 Sun Aug 14 16:48:02
5275602      Job I     4:09:50     4:39:50    00:30:00 8000/256000 Sun Aug 14 18:31:29
5271992      Job I     5:56:23     6:01:23    00:05:00 9216/147456 Sun Aug 14 20:18:02
5273294      Job I     6:01:23     6:06:23    00:05:00 18432/147456 Sun Aug 14 20:23:02
5246922      Job I     6:36:23    10:06:23     3:30:00 4096/131072 Sun Aug 14 20:58:02
5246923      Job I     6:36:23    10:06:23     3:30:00 4096/131072 Sun Aug 14 20:58:02
5269231      Job I    10:06:22  2:10:06:22  2:00:00:00 8340/266880 Mon Aug 15 00:28:02
5246924      Job I  2:10:06:22  2:13:36:22     3:30:00 4096/131072 Wed Aug 17 00:28:02
```

Recent Events (since last User call)

- 10/15 – LNET module failure (supports file system IO from compute nodes to OSS/OSTs for the file system. Separate issue impacting scheduler operation.

Looking forward

- Two webinar series being planned
  - Workflows - follow up to the virtual workshop
  - Visualization and Analytics
- Broad target audience and wide range of potential solutions.
- Help with technology adoption.

SC16 Salt Lake City

NCSA

- Let us know if you will be there.
- Stop by the NCSA booth.
- Several Blue Waters staff will be there.

SC16
Salt Lake City, Utah | hpc matters.

Review of Best Practices

- Improper use of login nodes
  - Use compute nodes for all production workloads.
- Avoid excessive calling of job scheduling commands
  - Unintentional denial of service may result otherwise.
- MOM node use should be limited to aprun launch.
  - All other commands can be run on compute nodes via aprun.
- Bundling of Jobs
  - Independent jobs bundled from 2 node to 32 nodes.
  - Avoid excessive, single nodes jobs.
  - Use a workflow.
- Small files usage
  - Use directory hierarchies, less than 10,000 files per directory.
  - Avoid many concurrent writers to same directory.
  - Tar up files before transferring to Nearline.

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