BLUE WATERS

SUSTAINED PETASCALE COMPUTING

6/20/16

Blue Waters User Monthly Teleconference

NCSA

NSF

GREAT LAKES CONSORTIUM
FOR PETASCALE COMPUTATION

CRAY

Agenda

- Symposium
- File System Upgrade Status
- Maintenance Changes
  - CUDA 7.5
  - Programming Environment
- Utilization
- Recent Events
- XSEDE
- Opportunities
- PUBLICATIONS!

Blue Waters Symposium

- 160 attendees and 4 parallel sessions
- Ed Walker and Jim Kurose from NSF.
- 10 new graduate fellows.
- Four short tutorials.
- Plenary Speakers
  - Peter Ungaro
  - David Abramson
  - Paul Morin
  - Wen-mei Hwu

New SEAS team – Roland Haas

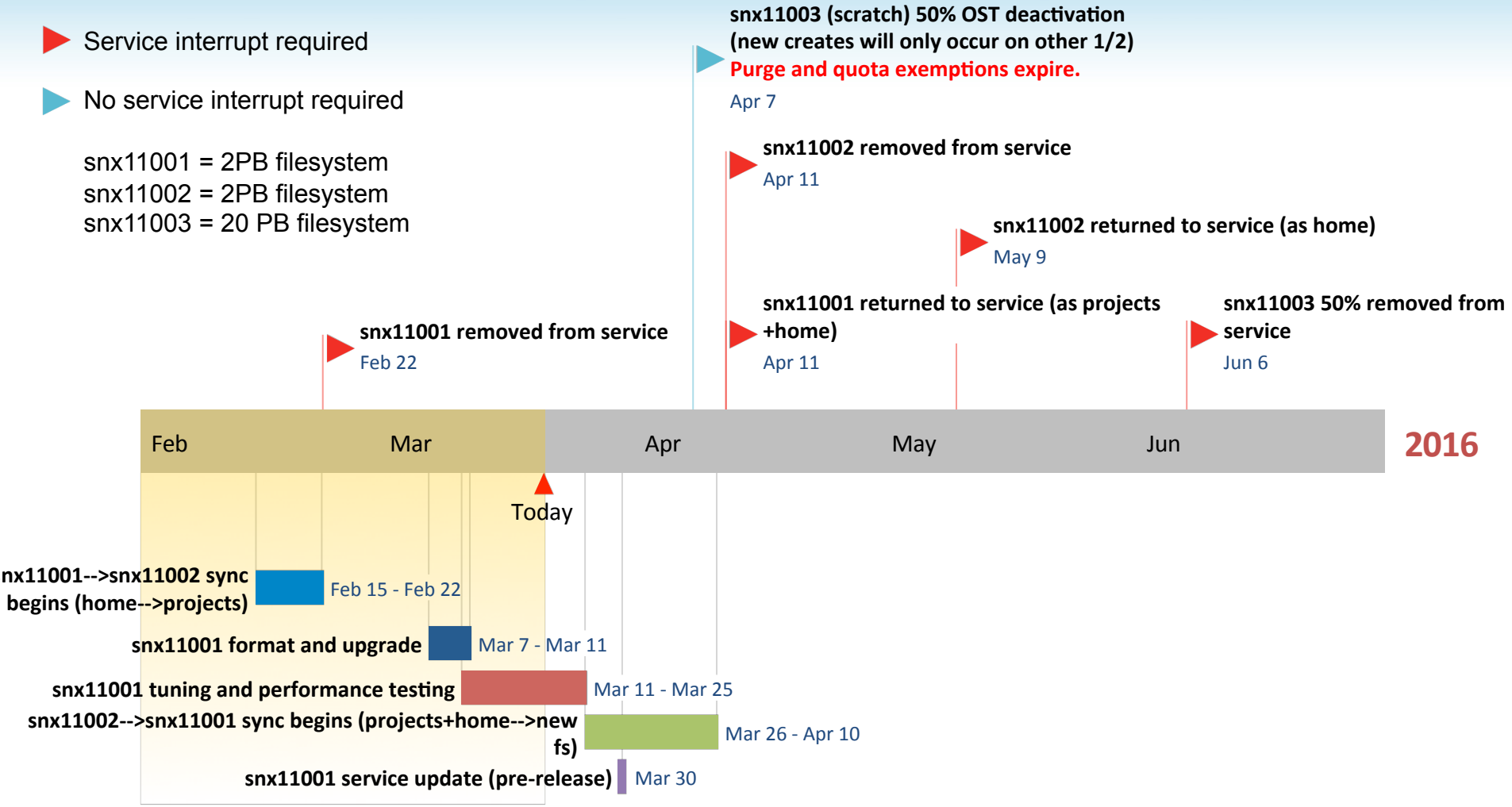
- Numerical relativity
- Relativistic (magneto-)hydrodynamics
- Extreme mass ratio inspirals and self-force problems
- Black hole perturbation theory
- Gravitational and electromagnetic emission from mixed black hole—star systems
- The Einstein Toolkit
- Numerical techniques for mesh refinement, and elliptic problems

File System Upgrade Status

- Home & Projects are still sharing hardware resources. Final sync delayed.
- Issue encountered in sync of home to upgraded file system.
- Current outage to split scratch only.
- Two more service interruptions later this summer to complete scratch work and home final sync.
- Continue to expect degraded service on filesystems during periods of double duty (home and projects) or reduced resource (scratch).

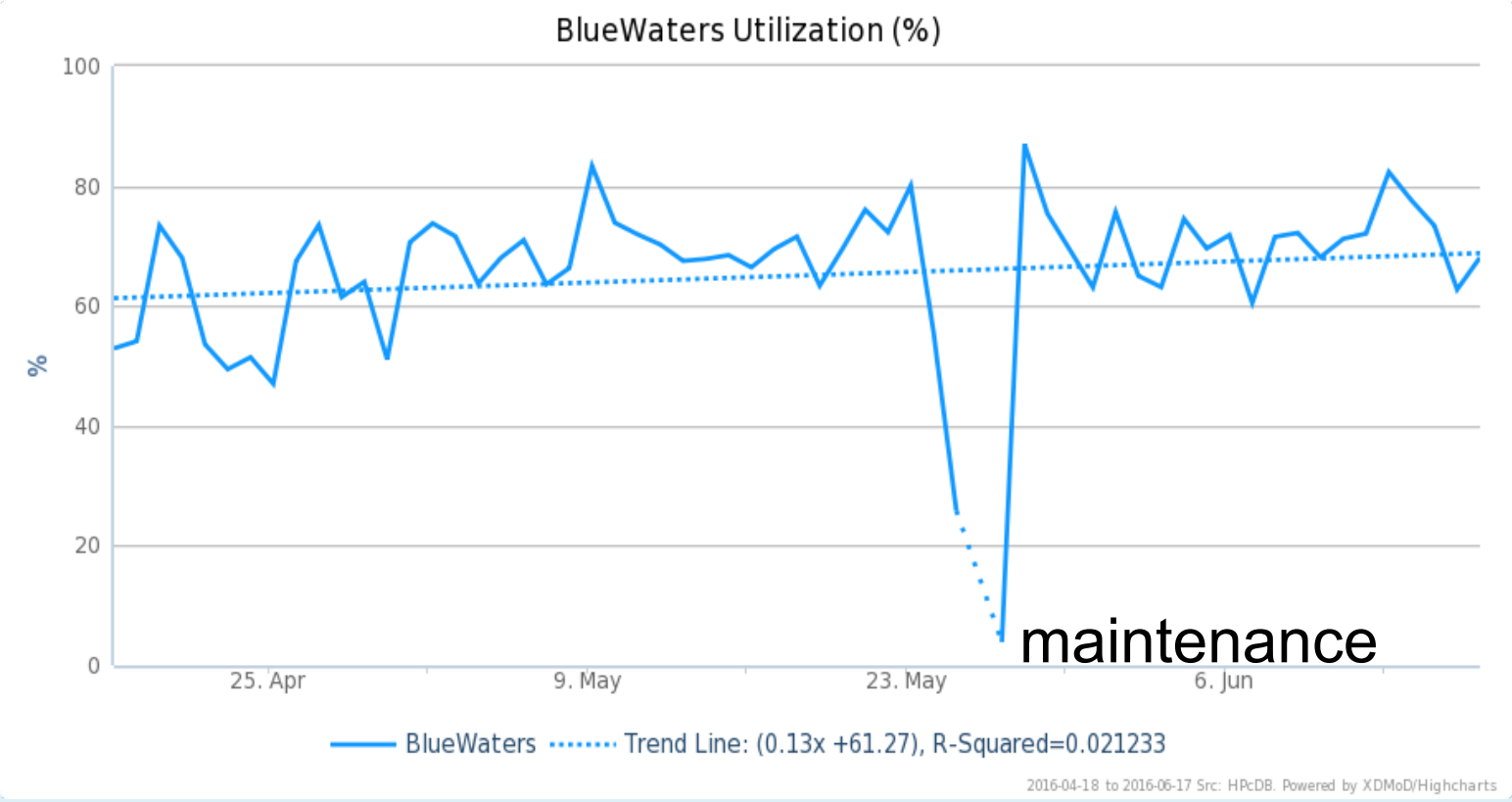
- Service interrupt required
- No service interrupt required

snx11001 = 2PB filesystem
snx11002 = 2PB filesystem
snx11003 = 20 PB filesystem



System Utilization

- Utilization since last BW User Call (April 18)



Recent Events

- 5/28 and 5/29 – Scratch metadata server (MDS) not responding. Failed over MDS to clear issue.
- 6/14 – Failed high speed network (HSN) gemini module triggered scratch issue.
- 6/15 – Single cabinet issue.
- 6/17 – Cooling issue caused 5 cabinets to emergency power off.

Changes

- CUDA 7.5
  - Default after maintenance. No need to rebuild applications.
- Programming Environment
  - craype - 2.5.4
  - cray-mpich - 7.3.3
  - CCE - 8.4.6
  - GNU – No change in default (4.9.3). 5.3.0 available.
  - Intel - 16.0.3.210
  - PGI - 16.3.0

Previous Changes

- Scheduler and discount changes
  - Chained jobs (jobs using scheduler dependencies) beyond the first eligible job will no longer accrue queue time priority.
  - Job walltime will no longer contribute to job priority.
  - The combined use of `minwclimit` and `preemptee` will count as only one discount factor instead of two.
- File systems
  - Default quotas restored for scratch.
  - Discontinued short term purge exemptions.
  - Home directory permissions restored to default for **some** users with 777 set.

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.
- Bundling of Jobs
  - Independent jobs bundled from 2 node to 32 nodes.
  - Avoid excessive, single nodes jobs.
- Small files usage
  - Use directory hierarchies, less than 10,000 files per directory.
  - Avoid many writers to same directory.
  - Tar up files before transferring to Nearline.

Reminder of discounted job charging

Charge factors for completed jobs that meet one or more of the following criteria below are discounted by 25% for each of the following opportunities with a resulting maximum discount of 69% when compounded.

1. job backfills available nodes.
2. use flexible wall clock time with preemption.
3. job wall clock accuracy of 75% or better

- For more information see the July 9th blog entry Charge Factor Discounts for jobs on Blue Waters.

Virtual School events

- Blue Waters Virtual Course Announcement
  - Introduction to High Performance Computing
  - Autumn 2016
  - Contact: Steve Gordon (sgordon@osc.edu)
  - https://www.osc.edu/~sgordon/IntroHPC
  - Instructor Dr. David E. Keyes
- Workflow software
  - Under development. After XSEDE.

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