BLUE WATERS

SUSTAINED PETASCALE COMPUTING

Supporting Containers on Blue Waters

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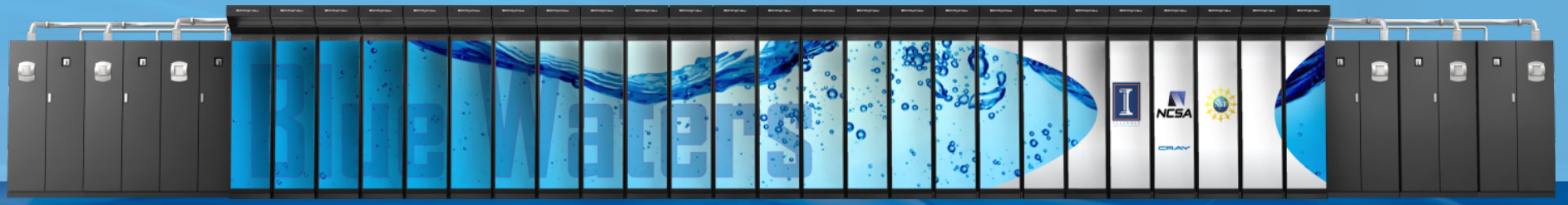


NCSA NSF GREAT LAKES CONSORTIUM FOR PETASCALE COMPUTATION CRAY

Outline

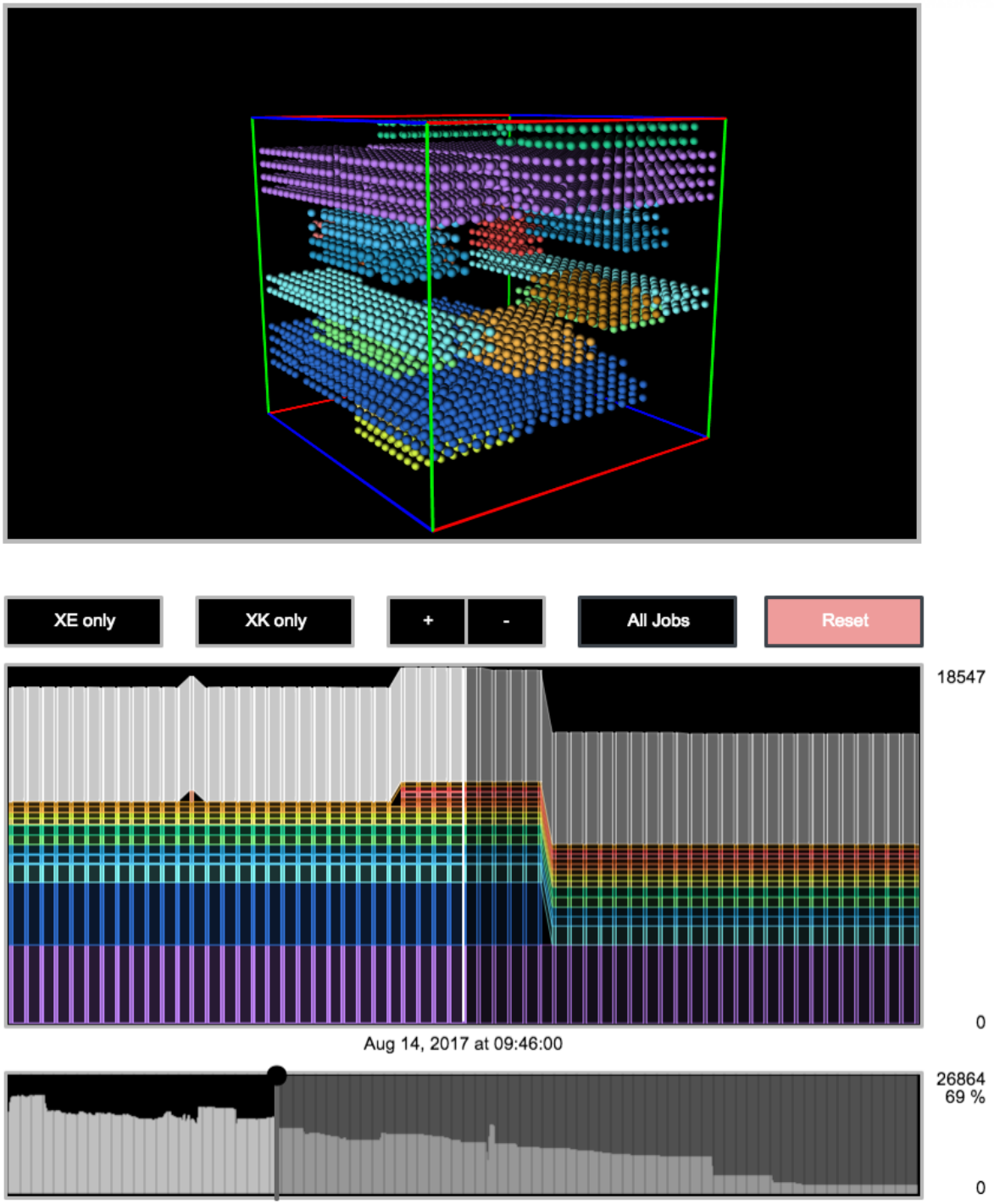
- Blue Waters: what is it, anyway?
- Do we need containers?
- Containers in HPC.
- Who is using containers on Blue Waters?

Blue Waters

- **Largest** academic **supercomputer**
  - **22,640 CPU** nodes with 2 x AMD Interlagos processors and 32 *cores* per node
  - **4,228 GPU** nodes with 1 x AMD Interlagos processor + 1 x NVIDIA K20x GPU.
  - 3D torus Cray Gemini interconnect with **9.6 GB/s** per node. Use topology aware scheduling.
  - **26 PB** of Lustre parallel file system storage with **1 TB/s**

https://bluewaters.ncsa.illinois.edu/blue-waters

- Largest jobs shown.
- Shows range of jobs in ribbon.
- Bottom shows jobs with future reservations.



Blue Waters continued

- No local disk on compute nodes.
- Most nodes have 64 GB (CPU) and 32 GB (GPU) RAM per node. 96 nodes with 2x memory.
  - IOP intensive workloads need to use /tmp (*tmpfs*) or /dev/shmem.
- No ssh access to or between compute nodes unless using a cluster compatibility mode (CCM).
- CCM has some scalability limits and memory consumption.

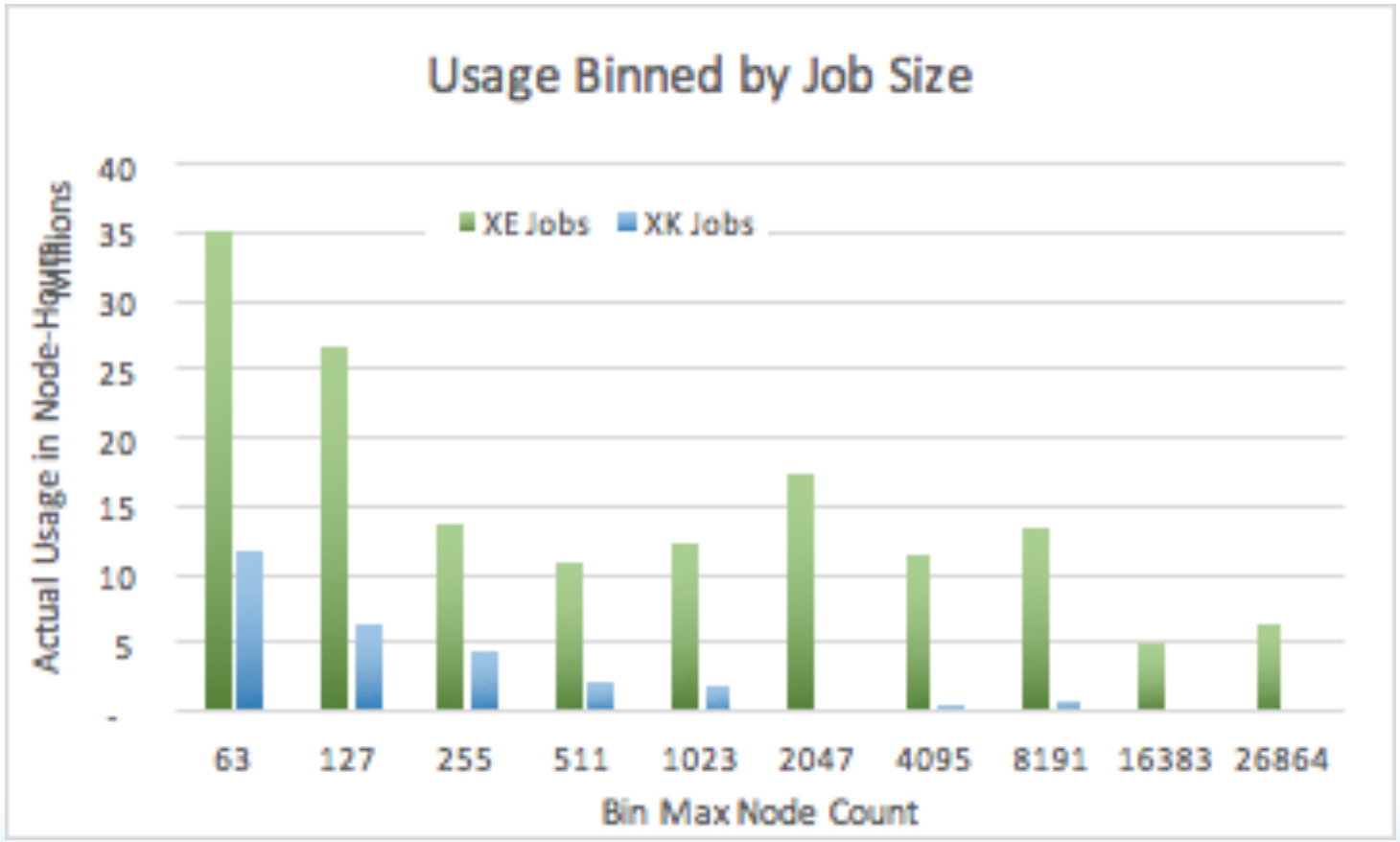
Blue Waters continued

- Blue Waters OS *frozen* at SLES11SP3
  - Linux kernel 3.0
  - GCC 4.3.4
  - glibc 2.11.3
  - python 2.6.8
- Software stack realized via Modules
  - GCC 4.4 - 6.3 along with Intel, PGI, Cray compilers.
  - python 2.6 - 3.5

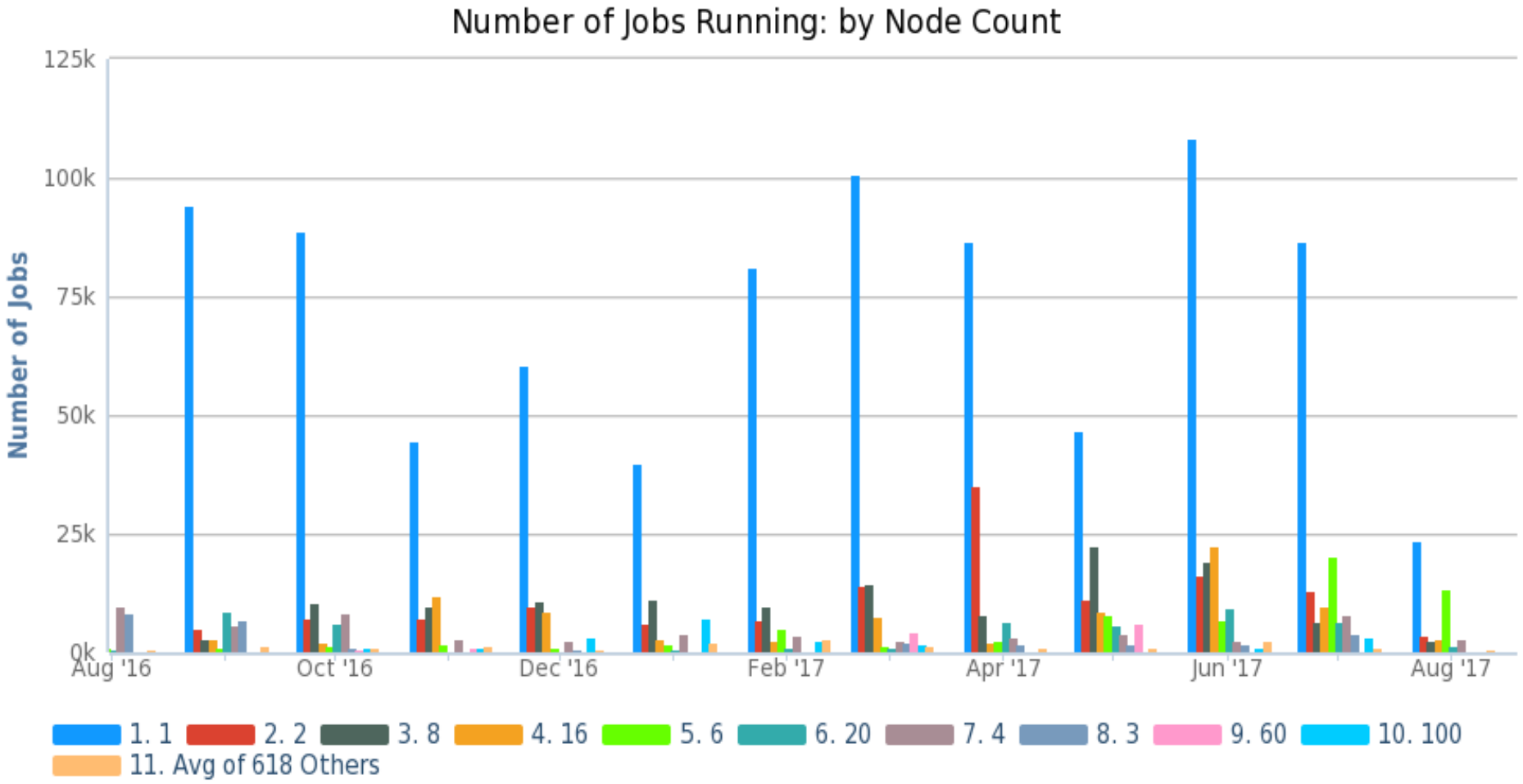
Why containers?

- Keep system current.
- Be able to accommodate new workloads that can help use Blue Waters efficiently.
- For example ArcticDEM workload
  - 300 TB of satellite imagery processed to produce elevation models.
  - 10s of millions of “jobs”.
  - Used swift workflow to bundle, launch and monitor.

Blue Waters usage by job node count



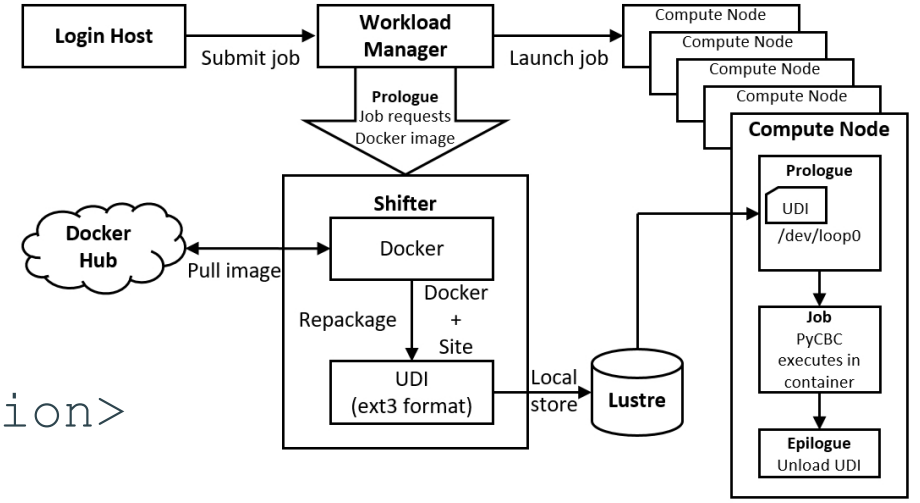
Blue Waters usage continued



Containers in HPC

- **Modules** do not solve all the problems…
  - **Old** or **complex** software stacks
- **Containers**
  - Use **any** software stack (**full control** over environment)
  - Develop on a laptop, deploy on a cluster
  - **Reproducible science**
  - **Shifter** (NERSC), **Singularity** (LBL)

Workflow of Shifter job



- Job submission requests for "shifter" resource.

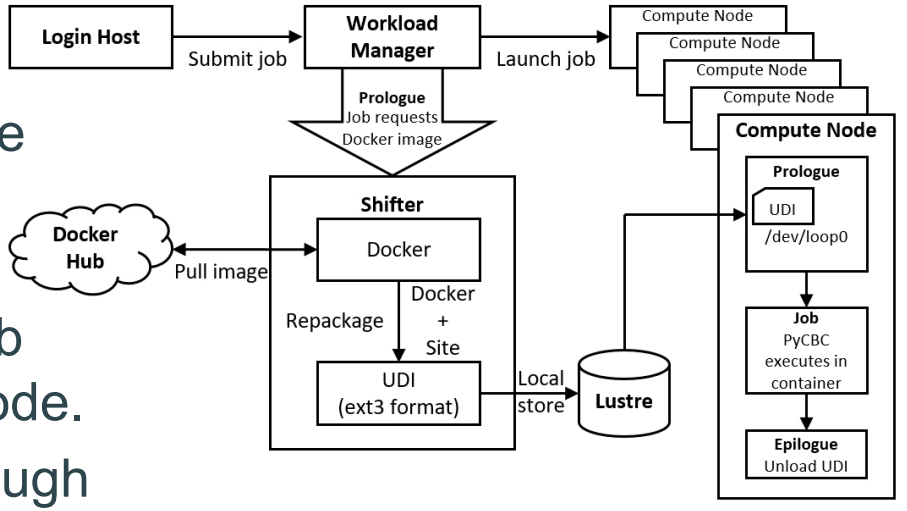
```
$ qsub -l nodes=4:ppn=32
  -l gres=shifter
  -v UDI=<dockerimg>:<version>
  shifter.job.sh
```

- Resource Manager detect "shifter" request, call Shifter prologue to pull docker image from Docker Hub, convert it to UDI and load it into compute nodes.
- Call from job script directly, without "gres=shifter" request.

```
$ aprun -b -- shifter --image=docker:osimage:version
  -- program args
```

- Internet access to Docker Hub.

Workflow of Shifter job



- Epilogue script to clean up compute nodes after job ends.
- Risk of improper cleanup due to timeout, and may affect the next job scheduled to the same compute node.
- Direct "SSH" to compute node through Shifter "port".

```
$ ssh -F ~/.shifter/config nid00002
```

- Shared storage space to store User-Defined Images (UDI) files.
- UDI files owned by 'root'. Could be exploited by users to download all kind of images from Docker Hub that fill up disk space.
- All UDI files accessible to all users, no access control.

Blue Waters continued

- Two-factor user authentication using RSA.
- Support Globus based methods like gsissh, globus-url-copy, myproxy.
- Prefer use of Globus Online for data transfer.
- Compute nodes can initiate connection to outside via RSIP/NAT. Finite number of ports out.

Users of containers on Blue Waters

- LSST/DES (previous talk)
  - HTCondor
- LIGO (next talk)
  - OSG
  - Pegasus and Condor
- ATLAS - OSG All Hands Meeting presentation
  - OSG
  - CVMFS – limited by lack of *fuse*

HPC uses of containers

- Support MPI model for communication between processes running on multiple containers
  - native MPI possible when using MPICH2 API
  - up to 800 node jobs (9000 in future release)
- Bundle code and dynamic libraries in image
  - reduce load on metadata server, speed up application startup time