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Opportunities for container environments on Cray XC30 with GPU devices

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Agenda

- Motivation
- Container technologies, Docker & Shifter
- Use case: High Energy Physics with containers on XC
- Use case: GPUs with containers on XC
- Conclusion

Motivation

Why do we at CSCS want to use containers on HPC?

- Containerizing applications provides an easy and portable way for packaging complex application setups
  - i.e. libraries, OS dependencies, etc.

- This allows us to support on our Cray systems a wider range of scientific applications and workflows
  - Reach communities beyond the common HPC use cases

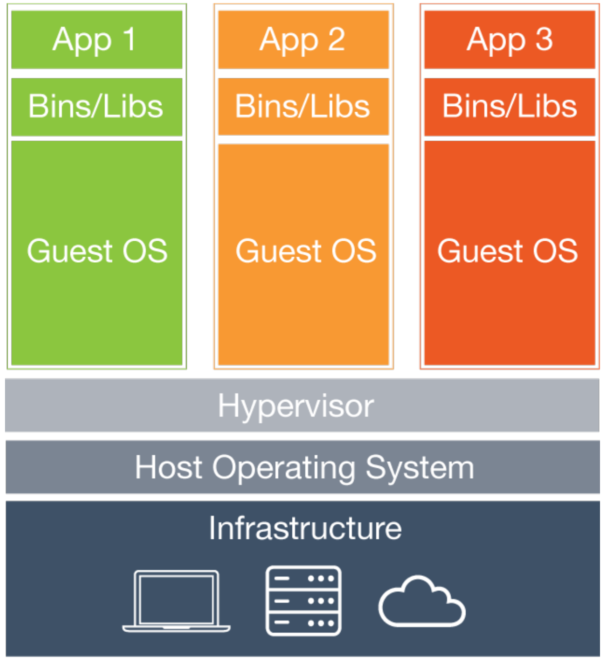
- This can also help consolidating our users and customers on fewer but elastic resources

- But, containers are not the solution for everything. Existing HPC workloads don't need to be containerized

Container technologies: Docker

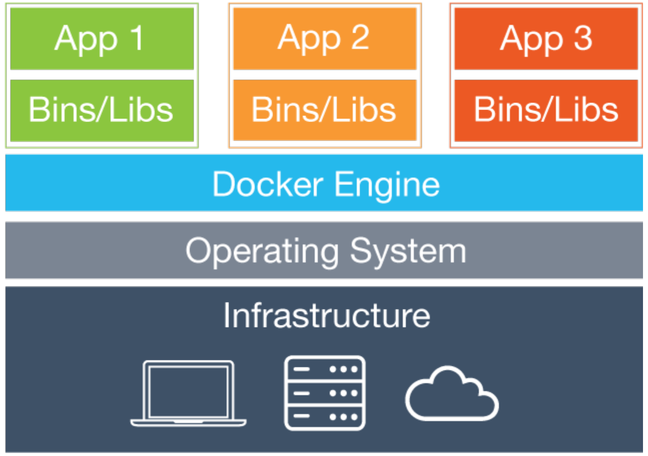
What is Docker and how does it work?

- "Docker containers wrap up a piece of software in a complete filesystem that contains everything it needs to run: code, runtime, system tools, system libraries – anything you can install on a server. This guarantees that it will always run the same, regardless of the environment it is running in." [*]



[*]

Virtual Machines



[*]

Containers

[*] https://www.docker.com/what-docker

What is Docker and how does it work?

- A Docker image is a file that contains a bunch of files on it. Usually libraries and application binaries
- Docker leverages the namespaces feature of the kernel to isolate processes

- On its simplest form, Docker basically
  1. Pulls an image to the local system
  2. Creates some sort of chroot environment with the image (=container)
  3. Runs our application in the container ('isolated' from the host thanks to kernel namespaces)

- However, it can also do *other* things:
  - Isolate network by creating NAT or bridge devices
  - *Can* use a *nice GUI*

Docker in HPC environments

- Docker is a nice tool, but it's not built for HPC environments, because:
  - Does not integrate well with workload managers
  - <u>Does not isolate users on shared filesystems</u>
  - Requires running a daemon on all nodes
  - Not designed to run on diskless clients
  - Network is by default NAT
  - Building Docker is done **within** a Docker container. It can be done outside, but is a complex task (Go language, seriously??)

Chicken or Egg?

- But after all, a sysadmin can make *anything* to work on a cluster, right?
  - We can create (and hopefully maintain) **monstrous wrappers** to run Docker containers…

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Container technologies: Shifter

What is Shifter and how does it work?

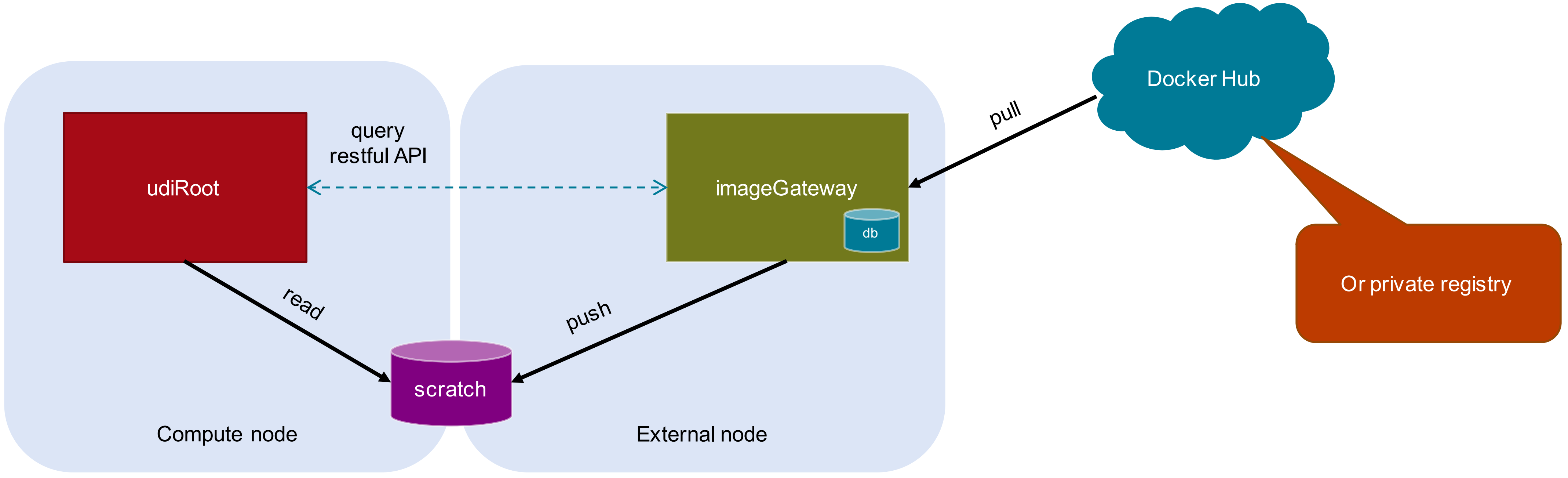
- Shifter is a container-based solution thought from the ground up for HPC environments and, in particular, Cray systems
- Open source tool created by NERSC. Available on Github
- It leverages the current Docker environment by using Docker images to create containers
- Shifter uses loop devices and chroot mechanisms as well as namespaces to provide the container environment

Shifter in HPC environments

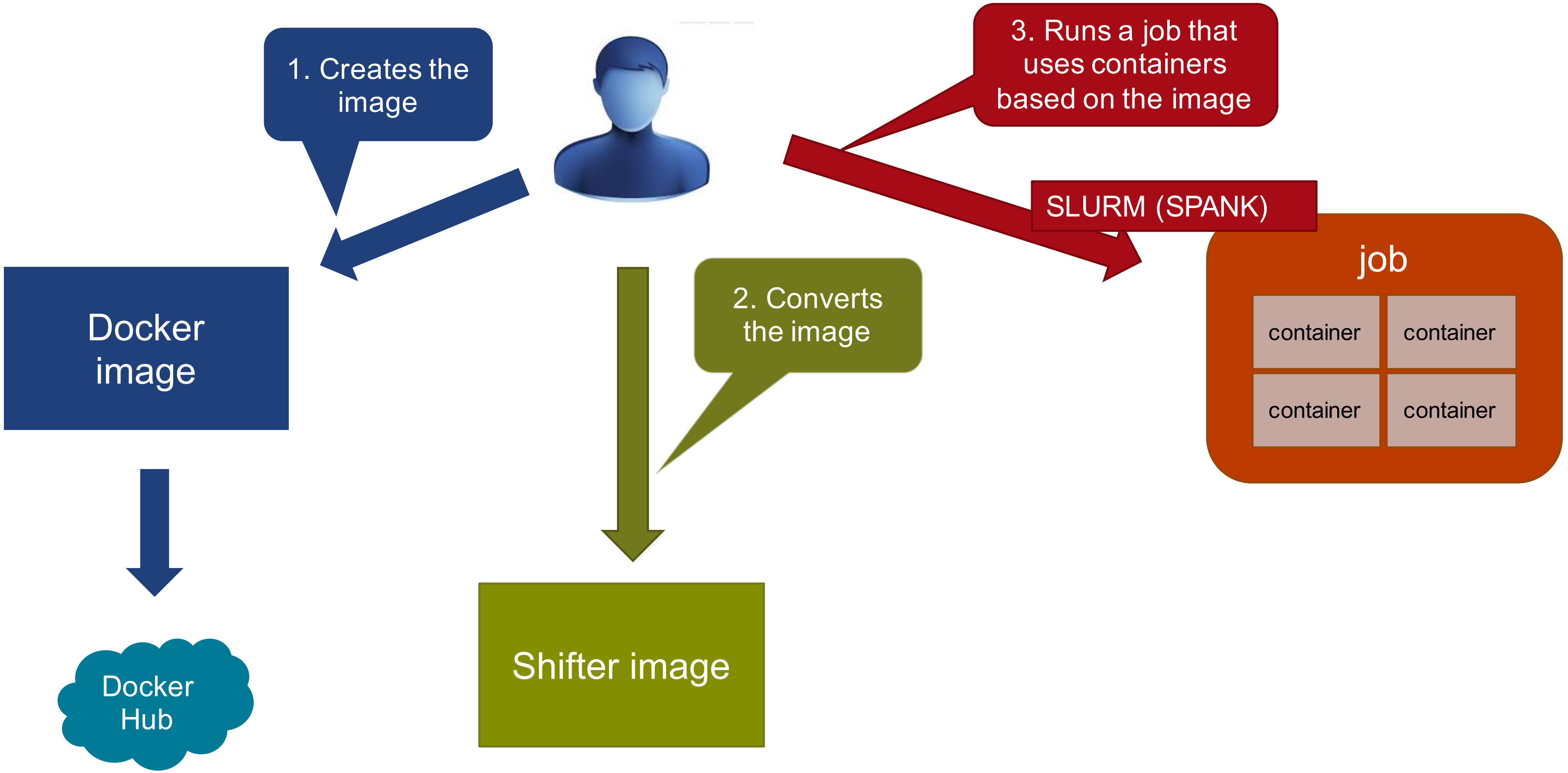
- Shifter is a great tool built for HPC!
- Integrates very well with workload managers (Slurm!)
- All user code is run in userland ☺
- No need for local storage ☺
- Can run off any mountpoint (/dsl/opt or /apps)
- Network and anything under /dev is exposed to containers
- Building Shifter is very easy
- Per-node caching (sparse xfs filesystems are awesome)

Architecture

- Shifter consists on two components:
  - imageGateway runs on an external server and converts any Docker image to a Shifter image. Built in Python, requires Redis & MongoDB.
  - udiRoot/Runtime runs on any compute node and chroots our application to run within the image constraints. Good old C.



Using shifter



Use case: High Energy Physics with containers on XC

WLCG Swiss Tier-2

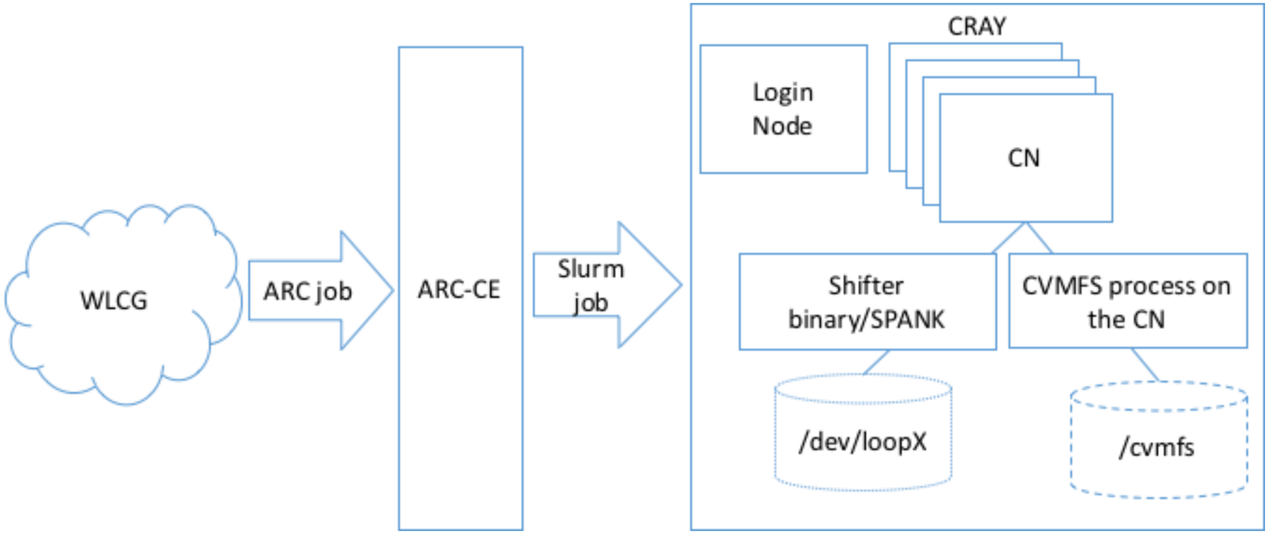
- CSCS operates the cluster Phoenix on behalf of CHIPP, the Swiss Institute of Particle Physics
- Phoenix runs Tier-2 jobs for ATLAS, CMS and LHCb, 3 experiments of the LHC at CERN and part of WLCG (Worldwide LHC Computing Grid)
- WLCG jobs need and expect RHEL-compatible OS. All software is precompiled and exposed in a cvmfs[*] filesystem
- But Cray XC compute nodes run CLE, a modified version of SLES 11 SP3

- So, how do we get these jobs to run on a Cray?

[*] https://cernvm.cern.ch/portal/filesystem

How do we get WLCG jobs to run on a Cray?

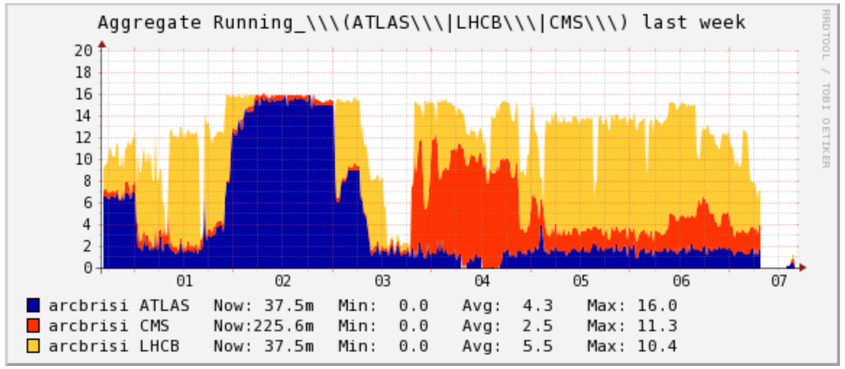
- Mount cvmfs natively on the compute nodes using a preloaded cache
  - Cvmfs process runs in the compute nodes, within dsl environment
  - Cvmfs cache is located on scratch and contains all the cache that CERN exposes
  - Compute nodes see /var/cvmfs/{atlas,cms,lhcb}.cern.ch and have 100% success hits
- Use shifter to contain the environment of a job to a RHEL-compatible image with a bunch of Grid packages (globus* and few others) installed
- Connect all this to WLCG with ARC

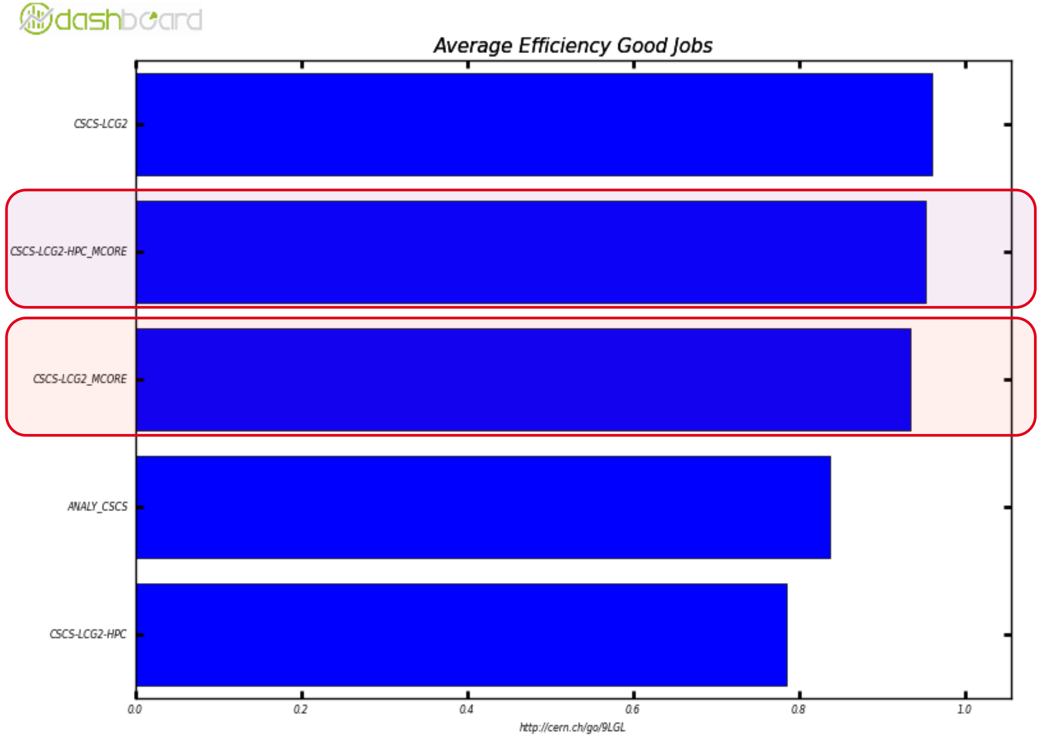


[*] https://cernvm.cern.ch/portal/filesystem

That's it!

- Using Shifter, we are able to run unmodified ATLAS, CMS and LHCb production jobs on a Cray XC TDS
- Jobs see standard CentOS 6 containers
- Nodes are shared: multiple single-core and multi-core jobs, from different experiments, can run on the same compute node
- Job efficiency is comparable in both systems





JOBID	USER	ACCOUNT	NAME	NODELIST	ST	REASON	START_TIME	END_TIME	TIME_LEFT	NODES	CPU
82471	atlasprd	atlas	a53eb5f8_34f0_	nid00043	R	None	15:03:33	Thu 15:03	1-23:54:18	1	8
82476	cms04	cms	gridjob	nid00043	R	None	15:08:39	Tomorr 03:08	11:59:24	1	2
82451	lhcbplt	lhcb	gridjob	nid00043	R	None	15:00:10	Tomorr 03:00	11:50:55	1	2
82447	lhcbplt	lhcb	gridjob	nid00043	R	None	14:59:31	Tomorr 02:59	11:50:16	1	2
82448	lhcbplt	lhcb	gridjob	nid00043	R	None	14:59:31	Tomorr 02:59	11:50:16	1	2
82449	lhcbplt	lhcb	gridjob	nid00043	R	None	14:59:31	Tomorr 02:59	11:50:16	1	2
82450	lhcbplt	lhcb	gridjob	nid00043	R	None	14:59:31	Tomorr 02:59	11:50:16	1	2
82446	lhcbplt	lhcb	gridjob	nid00043	R	None	14:49:01	Tomorr 02:49	11:39:46	1	2
82444	lhcbplt	lhcb	gridjob	nid00043	R	None	14:48:01	Tomorr 02:48	11:38:46	1	2
82445	lhcbplt	lhcb	gridjob	nid00043	R	None	14:48:01	Tomorr 02:48	11:38:46	1	2

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Use case: GPUs with containers on XC

Containerizing GPU applications

- Containerizing GPU applications provides and easy and portable way for packaging complex application setups

- Take advantage of several benefits:
  - Facilitate collaboration
  - Reproducible builds
  - Isolation of individual GPU devices
  - Running across heterogeneous CUDA toolkit environments
  - Requires only the NVIDIA driver installed on the host

The Docker catch

- Docker containers are both hardware-agnostic and platform-agnostic *by design*.

- This is not the case when using GPUs since:
  - it is using specialized hardware (that shows on your system as special character device), and
  - it requires the installation of the NVIDIA kernel driver

Collaboration with NVidia

- Mutual engineering and testing efforts to find a solution for Docker and Shifter

- Early prototype solution: to fully install the kernel driver inside the container, but:
  - the version of the host driver had to exactly match driver version installed in the container
  - container images had to be built locally on each machine, i.e., could not be shared
  - one needs to adhere to intellectual property regulations, i.e., not embedding proprietary code on a potentially sharable image without proper consent

Collaboration with NVidia: solution

- Shifter already provides the required character devices (/dev/nvidiaX) to the container 👍
- The driver files are mounted when starting the container on the target machine using the pre-mount hooks made available by Shifter
- Then we alter the runtime library search configuration to make the container aware of the new libraries available
- This makes images agnostic to the NVIDIA driver and capable of running on our environment without embedding any driver on the image

No overhead

- Testing done so far shows no overhead in terms of GPU performance when running within Shifter containers

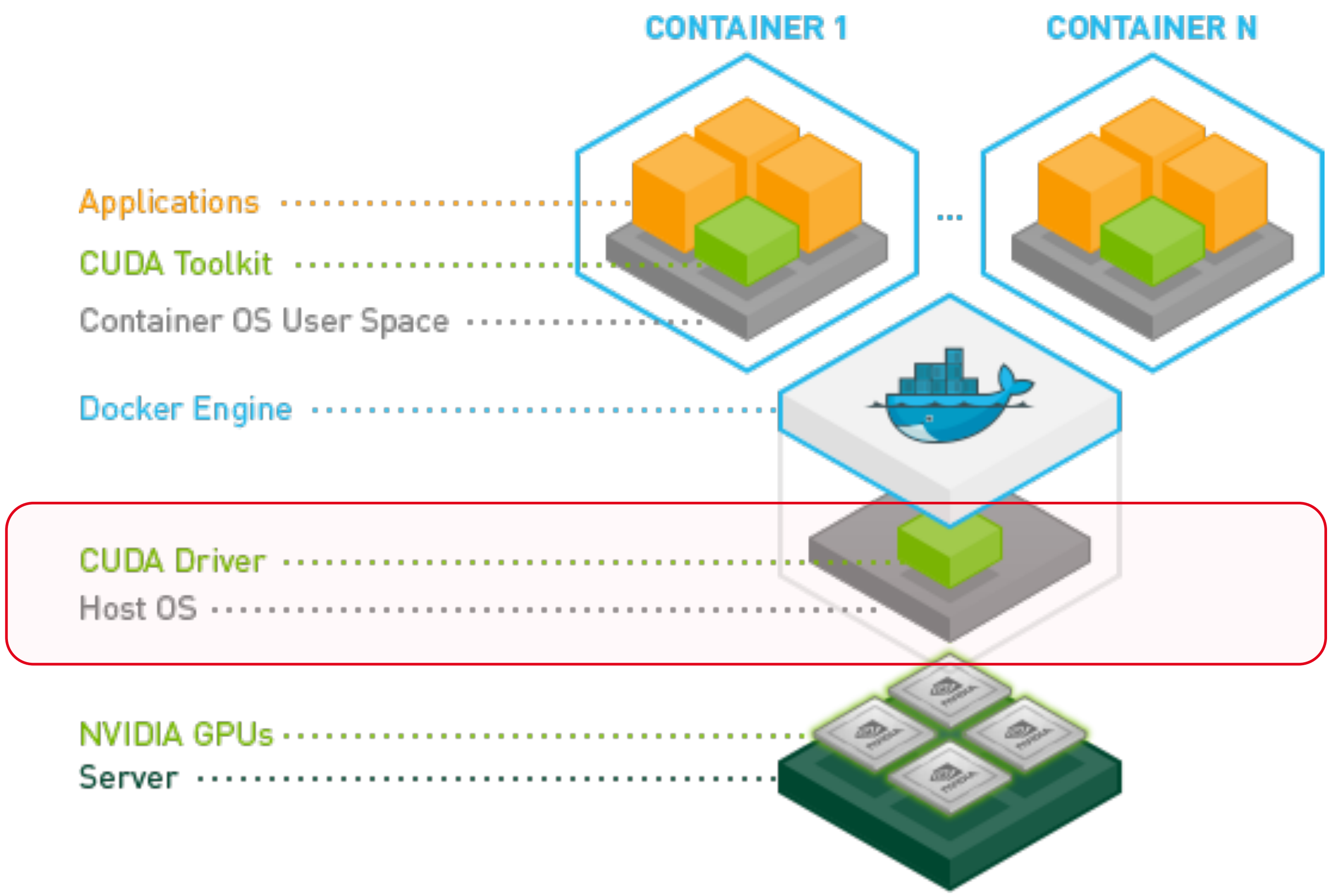
Stream benchmark within Shifter

```
lucasbe@santis01 ~/shifter-gpu> sbatch ./nvidia-docker/samples/cuda-
stream/benchmark.sbatch
Submitted batch job 496

lucasbe@santis01 /scratch/santis/lucasbe/jobs> cat shifter-gpu.out.log
Launching GPU stream benchmark on nid00012 ...
STREAM Benchmark implementation in CUDA
Array size (double precision) = 1073.74 MB
using 192 threads per block, 699051 blocks
Function      Rate (GB/s)   Avg time(s)   Min time(s)   Max time(s)
Copy:         184.3169      0.01167758    0.01165104    0.01170397
Scale:        183.1849      0.01175387    0.01172304    0.01178598
Add:          180.3075      0.01790012    0.01786518    0.01792288
Triad:        180.1056      0.01790700    0.01788521    0.01794291
```

A common approach

- NVIDIA DGX-1 uses the engineered solution for the management of its software stack



https://github.com/NVIDIA/nvidia-docker

Conclusion

Conclusion

- We like Shifter!
- It allows us to run workloads that traditionally have been difficult to port on Cray systems
- It helps our users to package complex applications and be able to reproduce results over time
- It's easy to use ☺

- But this is not all or nothing: things that already run on our Cray systems don't need to change

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Questions?

Thank you for your attention.

Extra slides