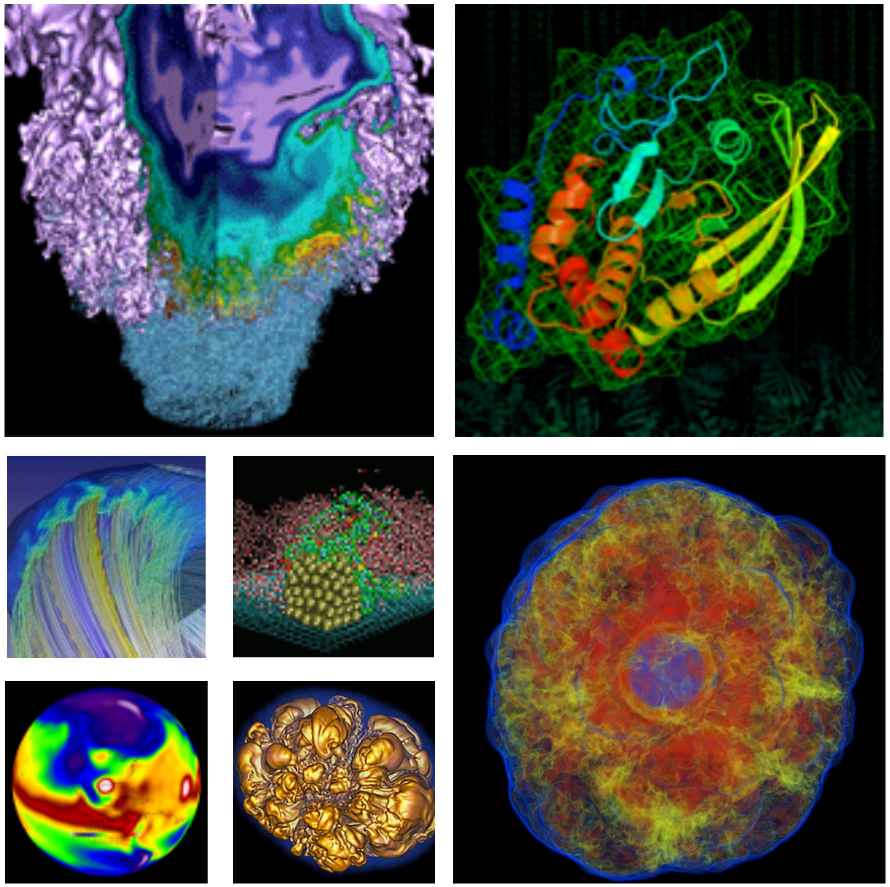
Shifter: Containers for HPC



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NERSC/Lawrence Berkeley Lab

Cray User Group 2016 May 12, 2016

Agenda

- Motivation and Background
- Shifter Architecture and Design
- Shifter in Action
- Discussion and Future Work

Acknowledgements

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Convergence of Disruptive Technology

- Increasing Role of Data
- Converging HPC and Data Platforms
- New Models of Application Development and Delivery

DOE Facilities Require Exascale Computing and Data

Astronomy

Particle Physics

Chemistry and Materials

Genomics

Fusion

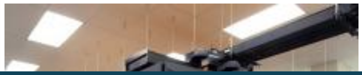
Petascale to Exascale

- **Petabyte data sets today, many growing exponentially**
- **Processing requirements grow super-linearly**
- **Need to move entire DOE workload to Exascale**

Converging Data Intensive Systems and HPC

Compute Intensive

Data Intensive


Carver

Why Convergence?

- Scale: Cori will have the scale needed to tackle current and emerging data challenges
- Coupling: Increasing Need to Couple Simulation and Analysis
- Capabilities: Access to the Burst Buffer
- Exascale: Helps place data intensive communities on exascale path

Popular features of a data intensive system and supporting them on Cori

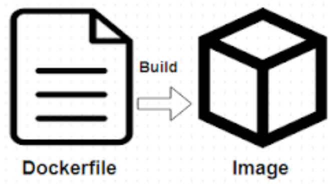
Data Intensive Workload Need	Cori Solution
Local Disk	NVRAM 'burst buffer' and ***Shifter***
Large memory nodes	128 GB/node on Haswell; Large memory login and service nodes
Massive serial jobs	NERSC serial queue
Complex workflows	***Shifter*** CCM mode Large Capacity of interactive resources
Communicate with databases from compute nodes	Advanced Compute Gateway Node
Stream Data from observational facilities	Advanced Compute Gateway Node
Easy to customize environment	***Shifter***
Policy Flexibility	Improvements coming with Cori: Rolling upgrades, CCM, above COEs would also contribute

Docker Basic's

- Build images that captures applications requirements.
- Manually commit or use a recipe file.

- Push an image to DockerHub, a hosted registry, or a private Docker Registry.
- Share Images

- Use Docker Engine to pull images down and execute a container from the image.



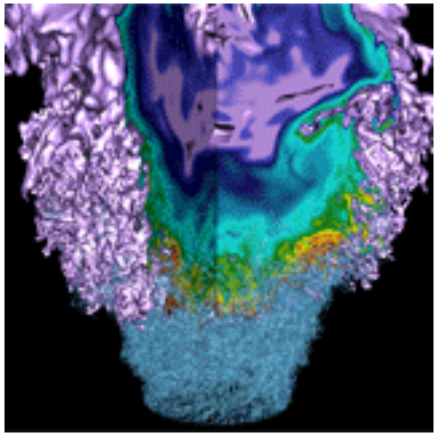
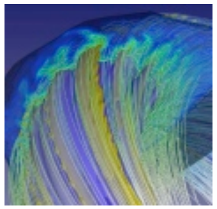
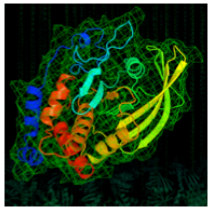
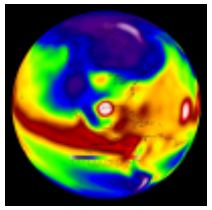
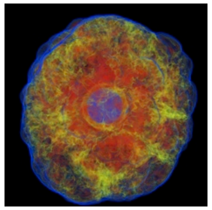
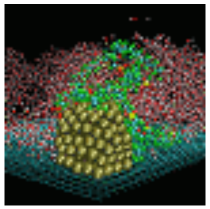
Why not just run Docker

- System Architecture: Docker assumes local disk
- Security: Docker currently uses an all or nothing security model. Users would effectively have system privileges
- Integration: Docker doesn't play nice with batch systems.
- System Requirements: Docker typically requires very modern kernel
- Complexity: Running real Docker would add new layers of complexity

Solution: Shifter

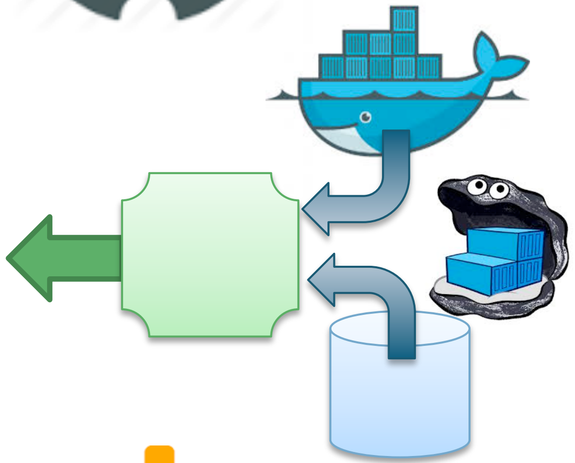
- **Partnership with Cray to design a solution to run containers on an HPC platform.**
- **Design Goals:**
  - User independence: Require no administrator assistance to launch an application inside an image
  - Shared resource availability (e.g., PFS/DVS mounts and network interfaces)
  - Leverages or integrates with public image repos (i.e. DockerHub)
  - Seamless user experience
  - Robust and secure implementation

Implementation

Shifter Components

- **Shifter Image Gateway**
  – Imports and converts images from DockerHub and Private Registries
- **Shifter Runtime**
  – Instantiates images securely on compute resources
- **Work Load Manager Integration**
  – Integrates Shifter with WLM



Shifter Architecture and Flow

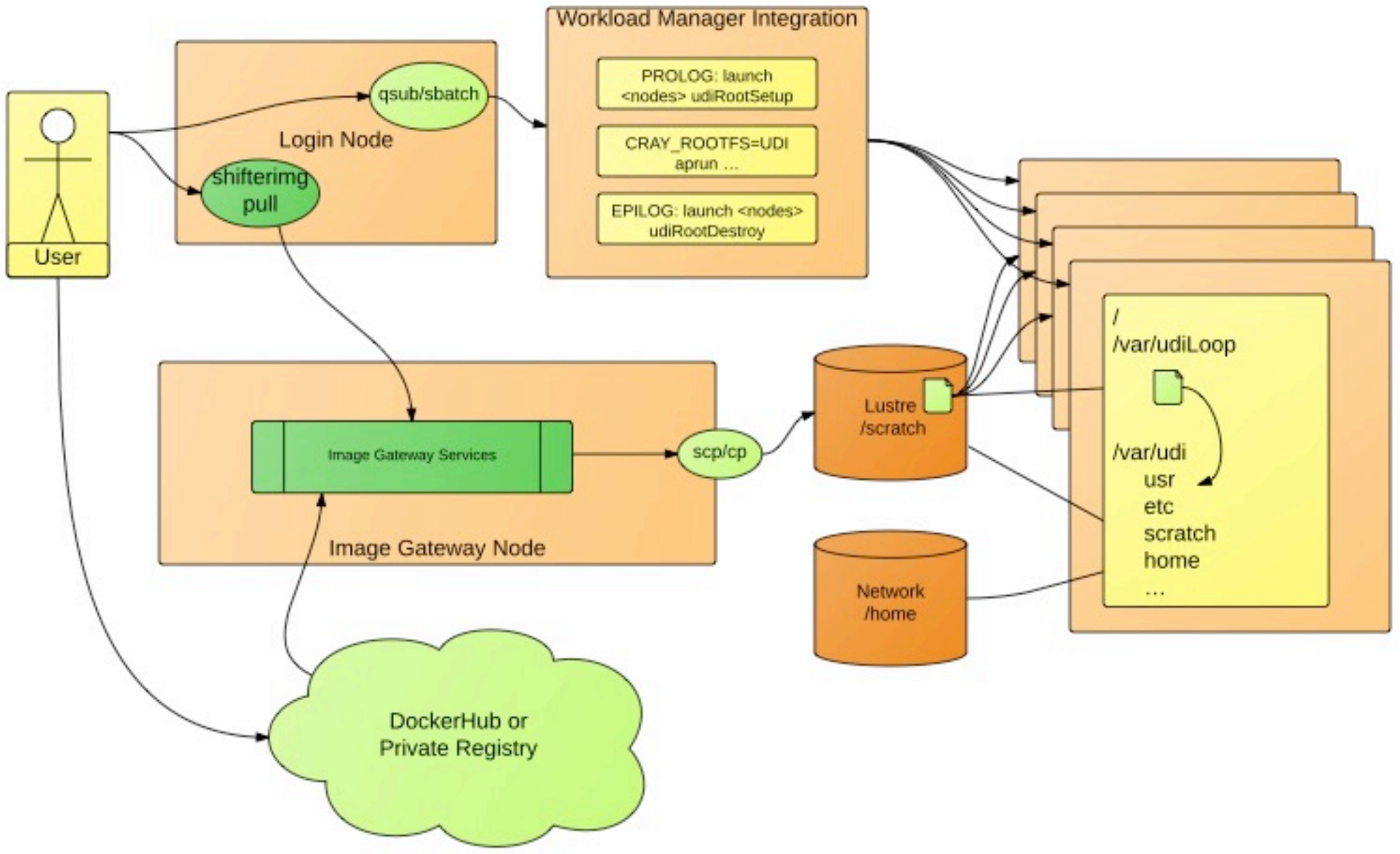
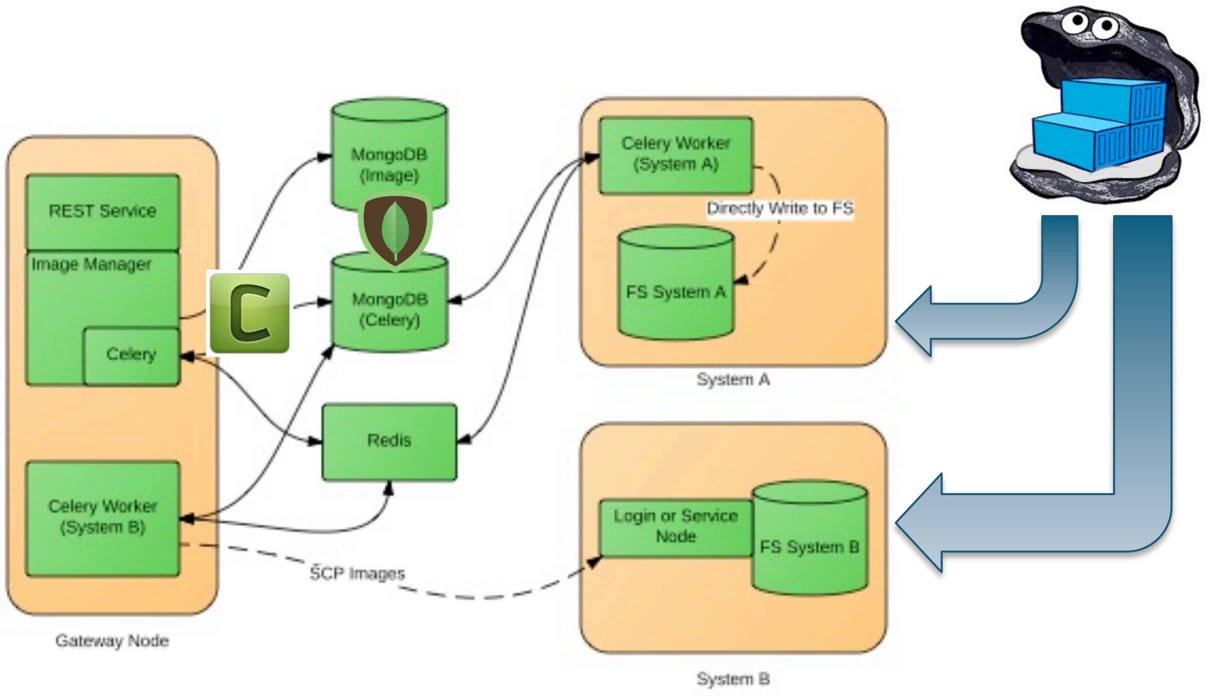


Image Gateway Design

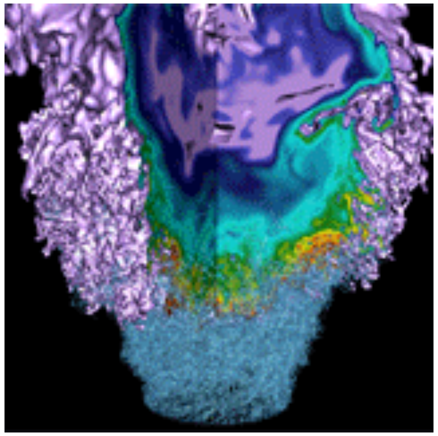


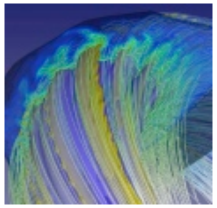
- Python Flask Application provides REST interface
- Mongo Database stores image metadata and provides an index of available images
- Python Celery provides a distributed queueing system
- Celery "Workers" do the actual image manipulation including pulling Docker Images from DockerHub or Registries

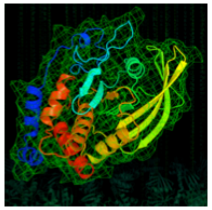
Workload Integration - Slurm

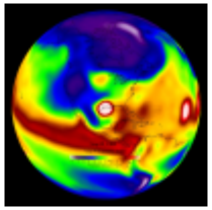
- Custom Plugin using the Spank plugin architecture
- Allows users to specify images, volumes and other options directly in the batch submission.
- Extensions will pre-create a common Shifter area (best for MPI applications).
- See Doug for more details.

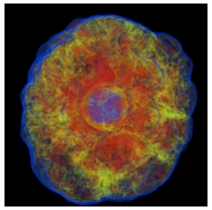
Shifter in Action

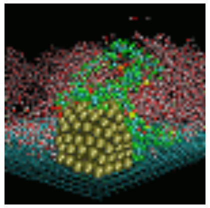












Create an image with Docker

Dockerfile

```
FROM ubuntu:14.04
MAINTAINER Shane Canon scanon@lbl.gov
# Update packages and install dependencies
RUN apt-update -y && \
   apt-get install -y build-essential

# Copy in the application
ADD . /myapp
# Build it
RUN cd /myapp && \
    make && make install
```

```
> docker build –t scanon/myapp:1.1 .
> docker push scanon/myapp:1.1
```

Use the Image with Shifter

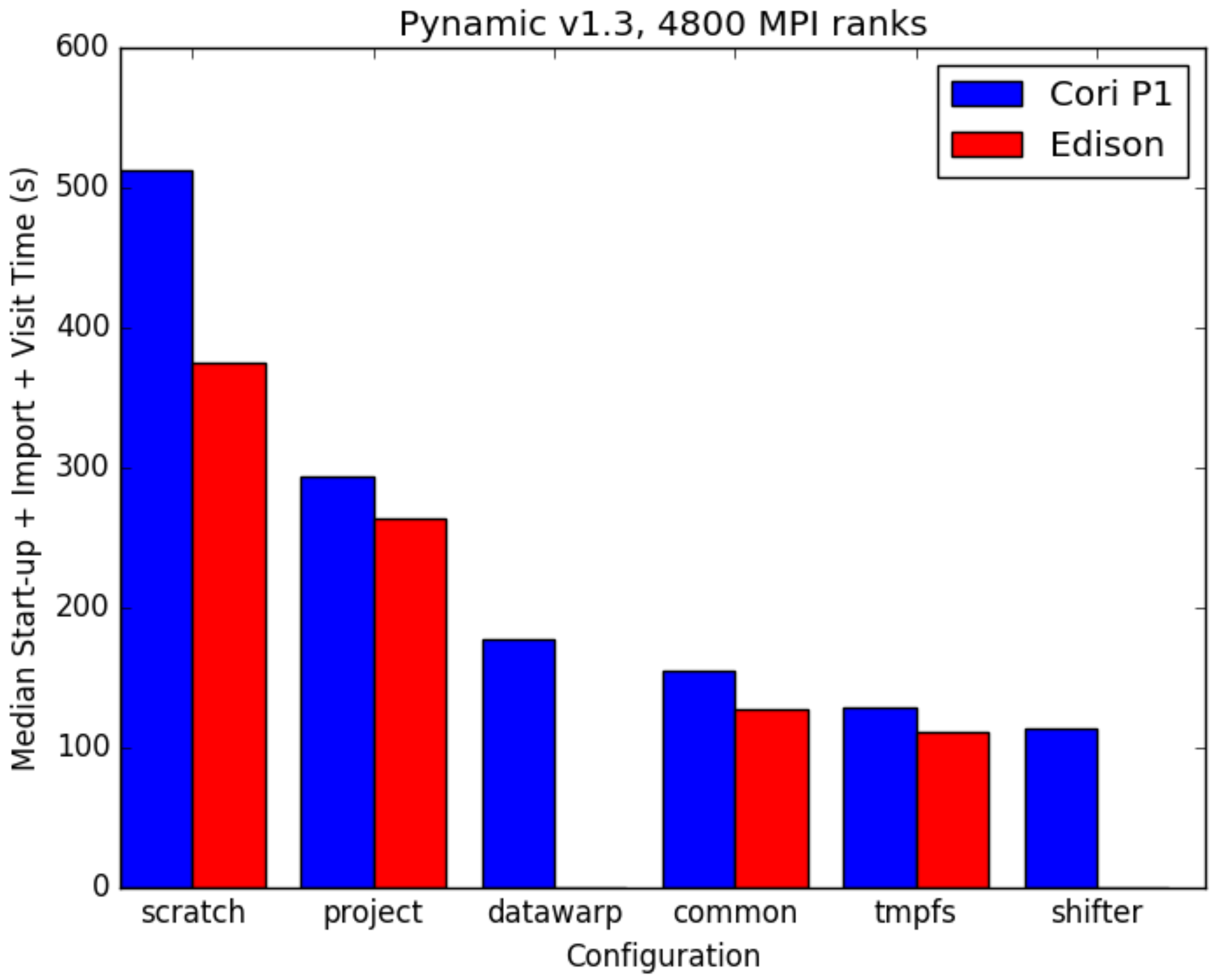
Submit script

```
#!/bin/bash
#SBATCH -N 16 -t 20
#SBATCH --image=docker:scanon/myapp:1.1
#SBATCH --volume=/global/cscratch1/sd/canon/
backingFile:/mnt:perNodeCache=size=100G


module load shifter
export TMPDIR=/mnt
srun -n 16 shifter /myapp/app
```

```
> shifterimg pull docker:scanon/myapp:1.1
> sbatch ./job.sl
```

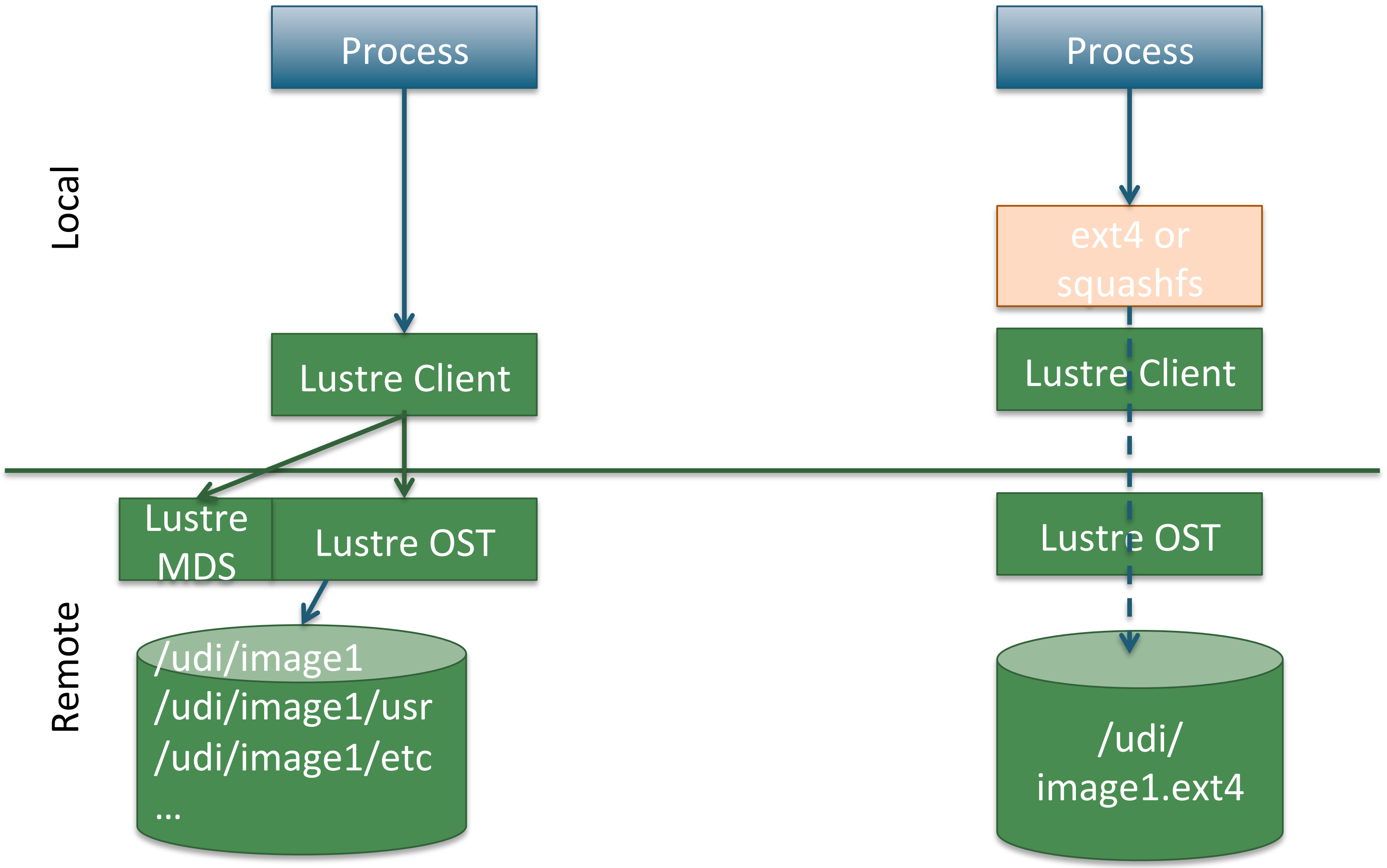
Shifter accelerates Python Apps



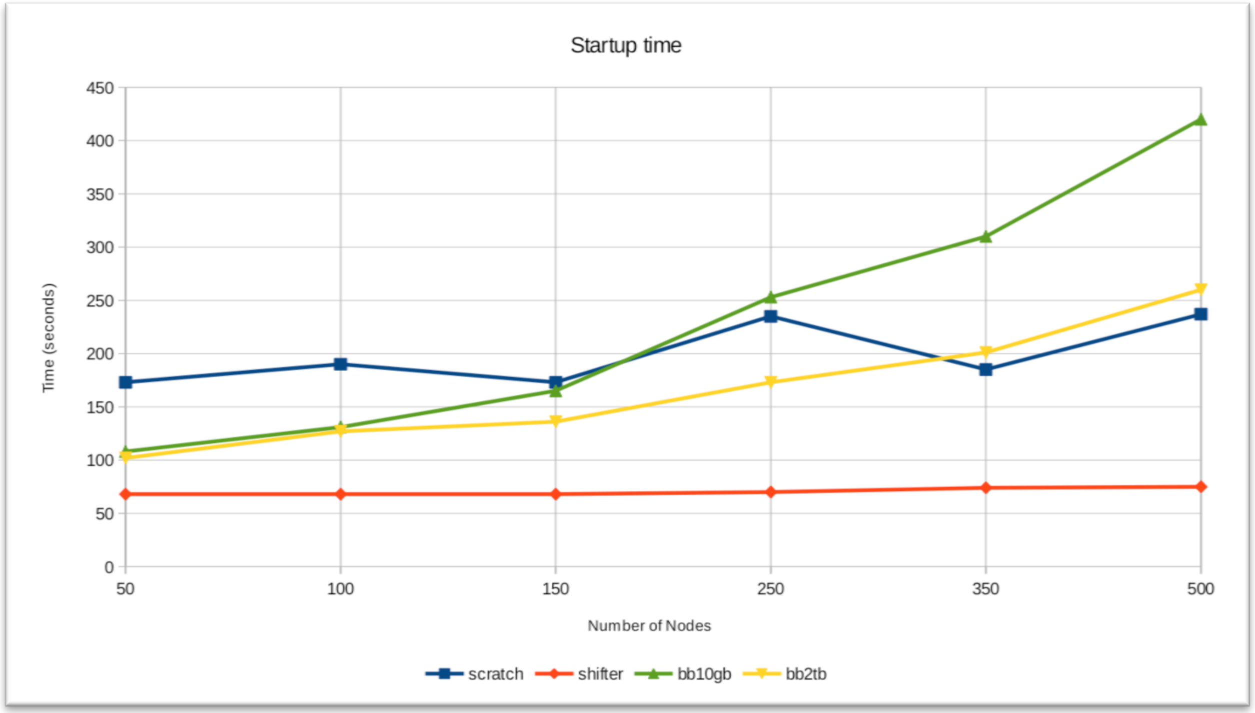
Why?

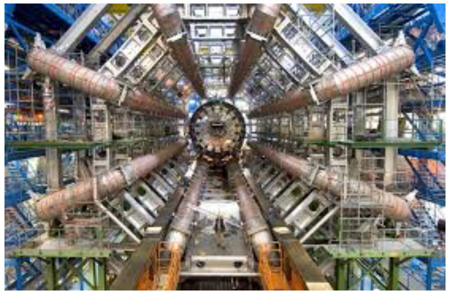
- Python must walk through the python libraries to construct the namespace
- Python must load up any dynamic libraries that are required
- The loader must traverse the LD_LIBRARY_PATH to find the libraries to load

File System flow – Traditional vs Shifter



Shifter and Atlas





- ATLAS software built and maintained by the international collaboration.
- Makes heavy use of "CVMFS" a software distribution system.
- Complete ATLAS CVMFS distro is O(TB) in size.
- Shifter provides linear startup times and requires no additional integration to run on the Cray systems.
- Images range from ~200GB to 3 TB!!

Per-Node Write Cache (New Feature)

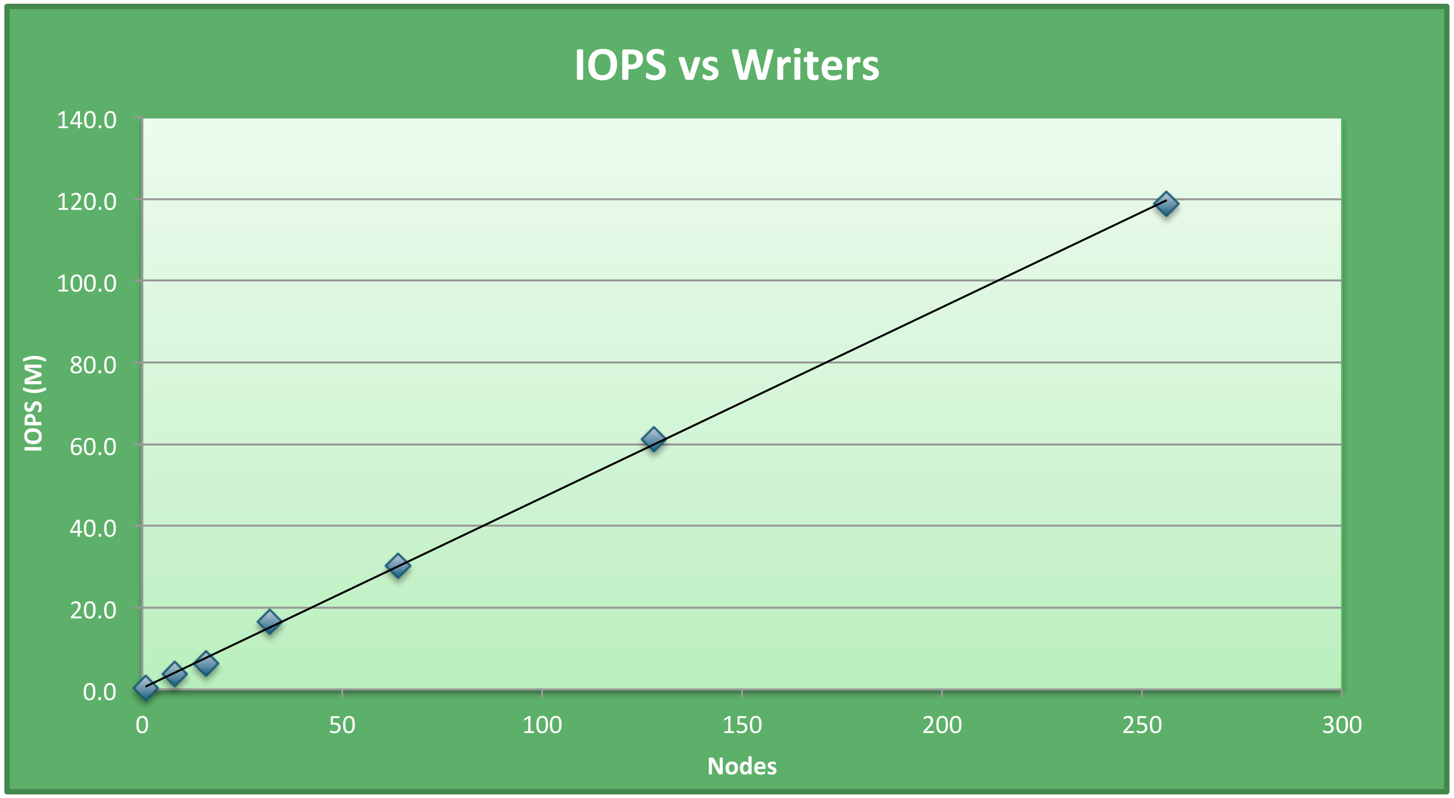
Per-Node Write Cache provides local disk like functionality but is backed by the Parallel File System.

Nodes/Writers per node	Lustre (MB/s) per writer	Shifter (MB/s) per writer	Real Local Disk (MB/s) per writer
1/1	83	594	416
10/10	87	625	416*
10/20	67	616	165*
10/40	55	589	53*
20/40	71	627	165*
20/80	55	588	53*

Results of a simple “dd” test to simulate writing ~5GB of small transaction I/O (`dd if=/dev/zero of=$TARGET bs=512 count=10M`)

* Extrapolated from a single node test

Per-Node Write Cache (IOPS)



Results of an IOR File per-process, 2 tasks per node, 512B transfer size, 2GB write. 100x faster than Lustre at the same scale.

Spark

- “Big Data” high productivity analytics Framework
- Designed around commodity clusters (Ethernet network and local disk)
- Shifter image: lgerhardt/spark-1.6.0
- Uses per-Node write cache for spills and other temporary per-node file caches.
- Tested up to full scale of Cori Phase 1 (1600 nodes) with multiple Spark applications.

Shifter and MPI

- **In Image**
  - Add required libraries directly into image.
  - Users would have to maintain libraries and rebuild images after an upgrade.
- **Managed Base Image (Golden Images)**
  - User builds off of a managed image that has required libraries.
  - Images are built or provided as part of a system upgrade.
  - Constrained OS choices and a rebuild is still required.
- **Volume Mounting**
  - Applications built using ABI compatibility.
  - Appropriate libraries are volume mounted at run time.
  - No rebuild required, but may not work for all cases.

See Cray talk at 4:30

Advanced example with MPI support

Dockerfile

```
FROM cern/slc6-lite:latest
## update packages and install dependencies
RUN yum upgrade -y && \
    yum -y install csh tar numpy scipy matplotlib gcc
WORKDIR /
## replace mpi4py with cray-tuned one
ADD optcray_cori.tar /
ADD mpi4py-1.3.1.tar.gz /usr/src
ADD mpi.cfg /usr/src/mpi4py-1.3.1/
RUN cd /usr/src/mpi4py-1.3.1 && \
    chmod -R a+rX /opt/cray && chown -R root:root /opt/cray && \
    python setup.py build && \
    export MPI4PY_LIB=$( rpm -ql $(rpm -qa | grep mpi4py | head -1) | egrep "lib$" ) && \
    export MPI4PY_DIR="${MPI4PY_LIB}/.." && \
    python setup.py install && \
    cd / && rm -rf /usr/src/mpi4py-1.3.1 && \
    echo "/opt/cray/wlm_detect/default/lib64/libwlm_detect.so.0" >>/etc/ld.so.preload && \
    (echo "/opt/cray/mpt/default/gni/mpich2-gnu/48/lib\n/opt/cray/pmi/default/lib64”;\
     echo “/opt/cray/ugni/default/lib64\n/opt/cray/udreg/default/lib64”;\
     echo “/opt/cray/xpmem/default/lib64\n/opt/cray/alps/default/lib64”) \
     >> /etc/ld.so.conf && \
    ldconfig
```

```
> docker build –t scanon/myapp:1.1 .
> docker push scanon/myapp:1.1
```

Advanced example with Golden Image

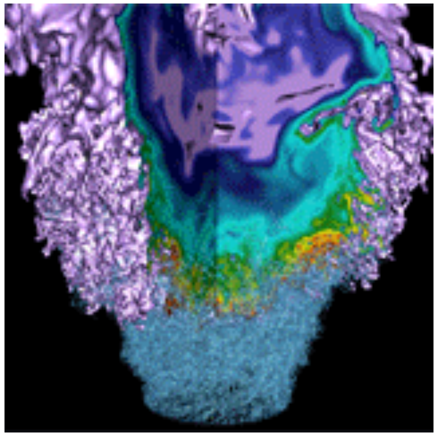
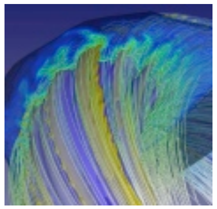
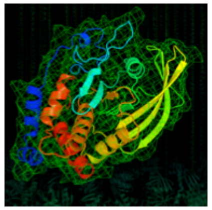
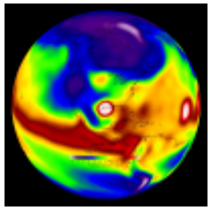
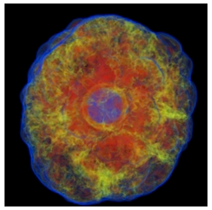
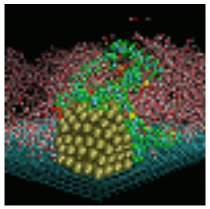
Dockerfile

```
FROM nersc/cori:latest

ADD . /myapp
RUN cd /myapp && \
    make
```

```
> docker build –t scanon/myapp:1.1 .
> docker push scanon/myapp:1.1
```

Discussion and Future Work

Why Users will like Docker and Shifter

- Develop an application on your desktop or laptop and easily run it on a Cray or other Supercomputer
- Enables the user to solve their dependency problems themselves
- Run the (Linux) OS of their choice and the software versions they need
- Improves application performance in many cases
- Improves reproducibility
- Improves sharing (through sites like Dockerhub)

Roadmap

- **16.05 Release:**
  - Support for RHEL 6/7, SLES 11/12, Rhine/Redwood
  - RPM builds
  - Improved scaling
  - UI Improvements
  - Per-node write cache
  - Bug Fixes
- **16.08 Release**
  - ACL support (private and authenticated images)
  - Image expiry and removal
  - Image usage statistics and metrics
  - Overlayfs support (stretch)
  - Debian packages for Ubuntu LTS

Future Work (beyond the roadmap)

- Continue to simplify installation and increase test coverage
- Expand support for other image types and batch systems (with outside help)
- Create a base image for running MPI applications in a NERSC private Docker registry
- Continue to promote Docker and Shifter within the HPC community to increase access

Conclusions

- Shifter is enabling and improving support for Data Intensive Workloads
- “Shifter” implementation demonstrates that centers can provide the flexibility of Docker without sacrificing security, scalability or performance.
- Shifter opens the door to the many benefits of Docker including easy sharing of images, reproducibility, etc.

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