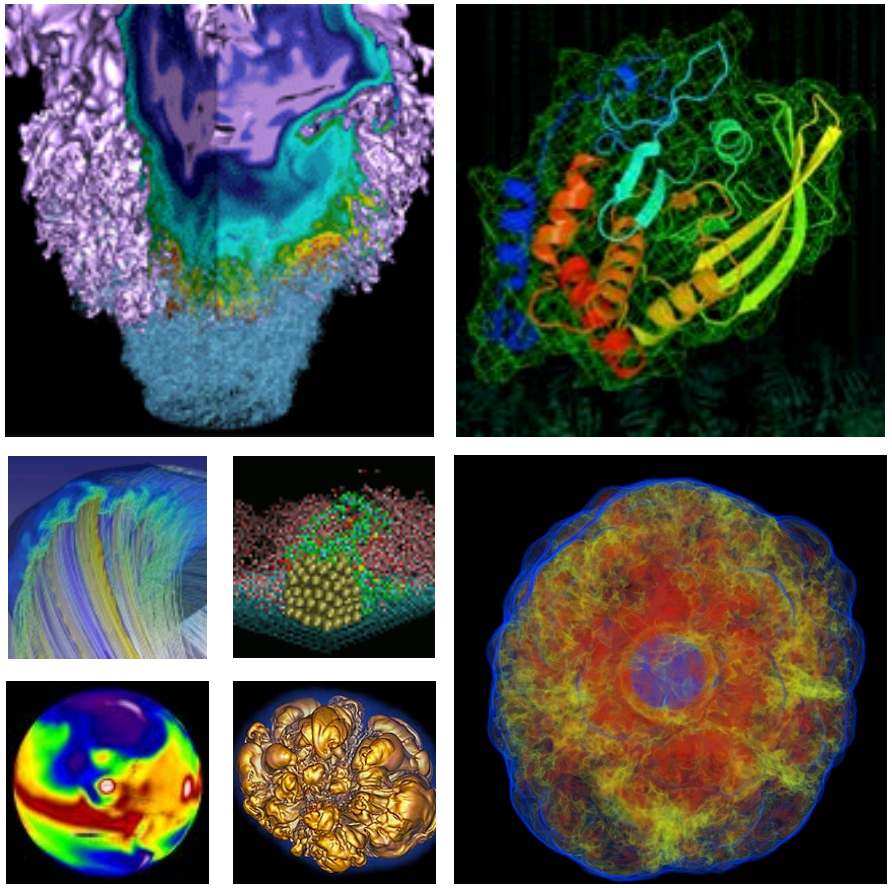
Containers in HPC



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Contents

- What are containers
- Why Containers
- Containers versus VMs
- What is Docker
- What is an image?
- Creating images

The Struggles

- **My software doesn't build on this system…**
- **I'm missing dependencies…**
- **I need version 1.3.2 but this system has version 1.0.2..**
- **I need to re-run the exact same thing 12 months from now…**
- **I want to run this exact same thing somewhere else…**
- **I want my collaborators to have the same exact software as me…**
- **I've heard about these Containers, can I just run that?**
- **Can I run docker on this HPC system?**

Solution - Containers

What are Containers?

- **Uses a combination of Kernel “cgroups” and “namespaces” to create isolated environments**
- **Long history of containers Solaris Zones (2005), LXC(2008), LMCTFY/Google and then Docker(2013)**
- **Docker provided a complete tool chain to simplify using containers from build to run.**
- **Entire ecosystem has grown around containers especially around orchestration.**

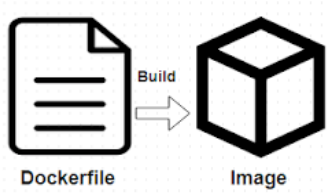
Docker Basic's

Build

Ship

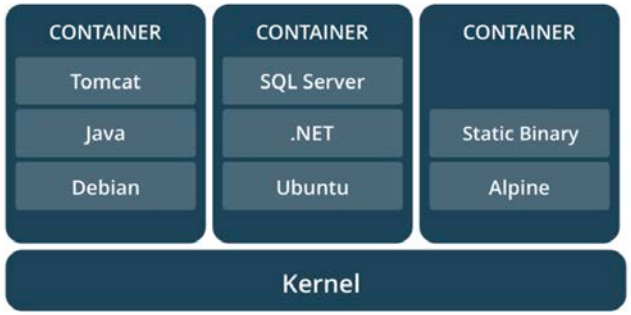
Run

- **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 Containers?

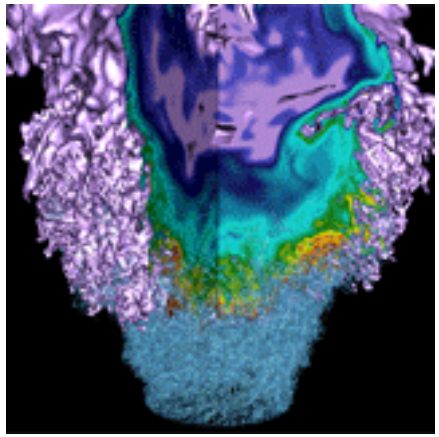
- **Light weight, executable piece of software that contains everything you need to run it**
  - Code, system libraries and tools, environment, settings
- **All software and processes are isolated from their surroundings**
- **Portable**
- **Typically used for single instance programs**

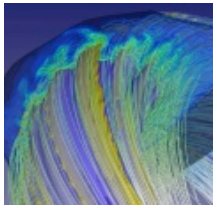


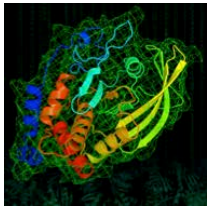
Containers and Science

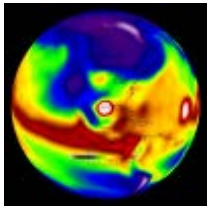
- **Reproducibility**
  - Everything you need to redo a scientific analysis
  - Image manifest contains all information about environment
    - Scripts, portable input files can be managed with version controller for greater control
- **Portability**
  - Runs on every system
- **Reduction of Effort**
  - Compile takes 10 hours? Just do it once and share it with everyone
  - System doesn't have the right library version? Yum install it yourself in the container

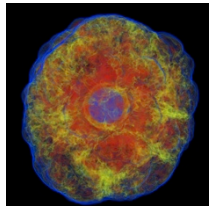
Containers in Action - Demo

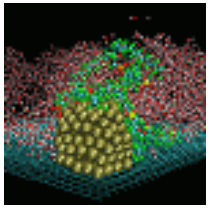




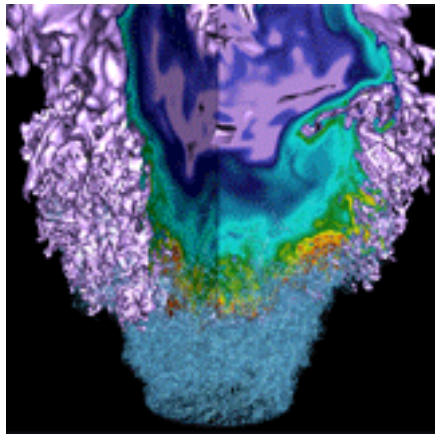


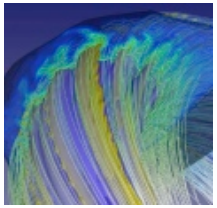


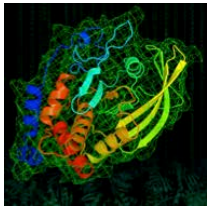


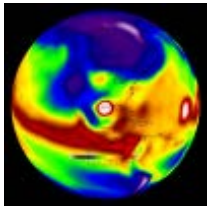


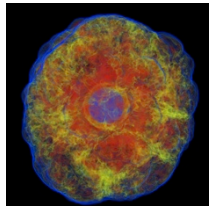
HPC Container Runtimes

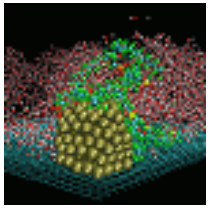






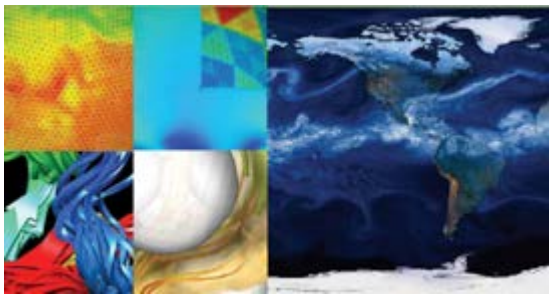


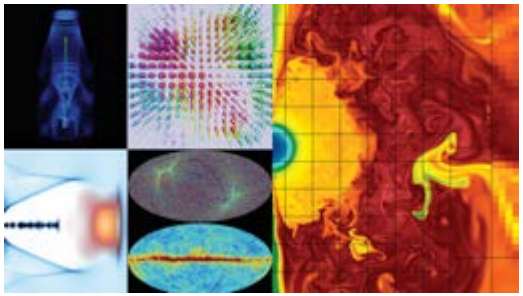


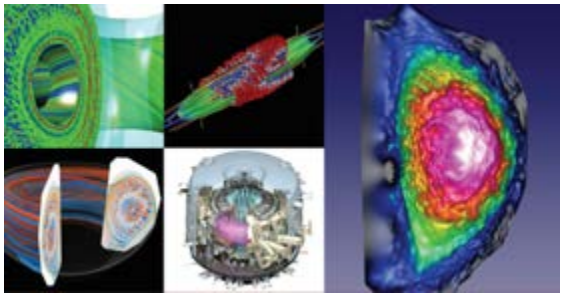


Why Containers at NERSC

- **NERSC deploys advanced HPC and data systems for the broad Office of Science community**
- **Approximately 6000 users and 750 projects**
- **Growing number of users around Analyzing Experimental and Observational Data, "Big Data" Analytics, and Machine Learning**
- **Shift towards converged systems that support traditional modeling and simulation workloads plus new models**







Why not just run Docker

- **Security: Docker currently uses an all or nothing security model. Users would effectively have system privileges**

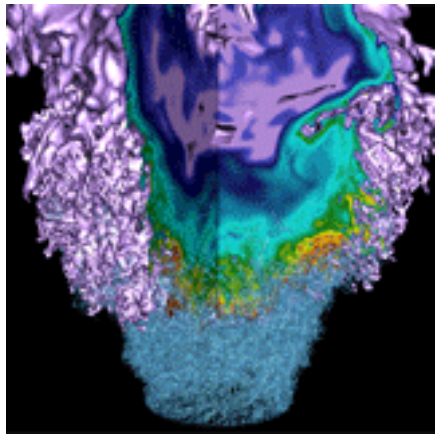
```
> docker run -it -v /:/mnt --rm busybox
```

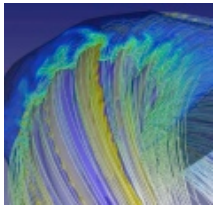
- **System Architecture: Docker assumes local disk**
- **Integration: Docker doesn't play nice with batch systems.**
- **System Requirements: Docker typically requires very modern kernel**
- **Complexity: Running real Docker would add new layers of complexity**

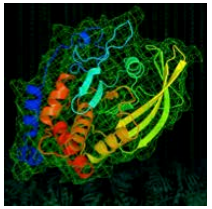
Solution: Shifter

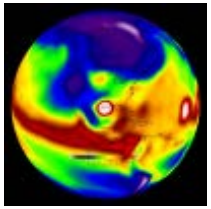
- **Design Goals:**
  - User independence: Require no administrator assistance to launch an application inside an image
  - Shared resource availability (e.g., file systems and network interfaces)
  - Leverages or integrates with public image repos (i.e. DockerHub)
  - Seamless user experience
  - Robust and secure implementation
- **Hosted at GitHub:**
  - https://github.com/nersc/shifter

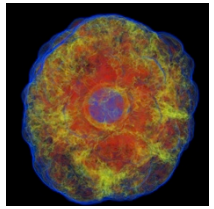
Implementation

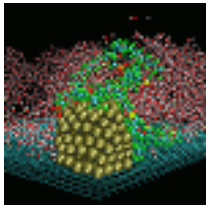






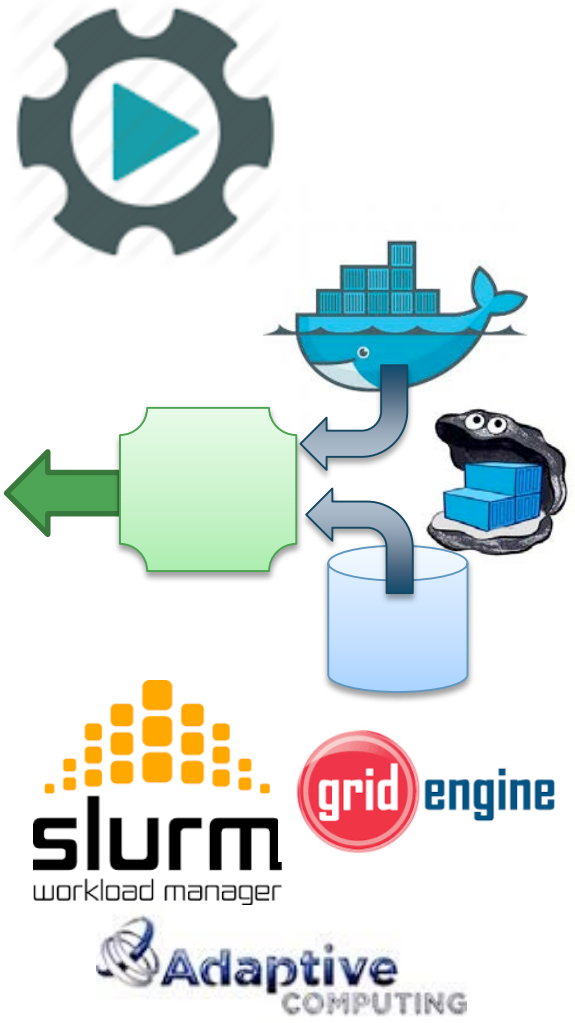




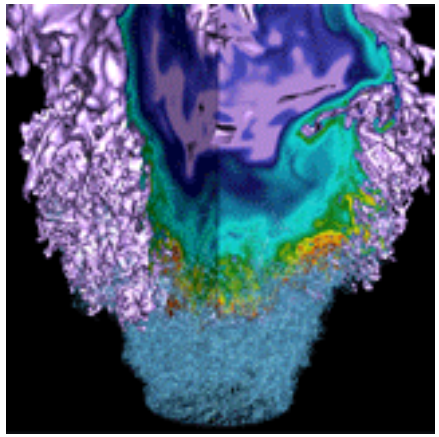


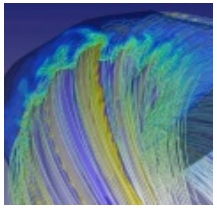
Shifter Components

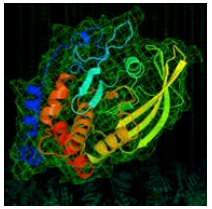
- **Shifter Image Gateway**
  - Imports and converts images from DockerHub and Private Registries
- **Shifter Runtime**
  - Instantiates images securely on compute resources
- **Work Load Manager Integration**
  - Integrates Shifter with WLM

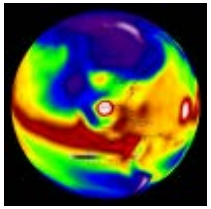


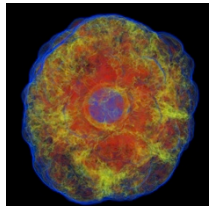
Shifter in Action

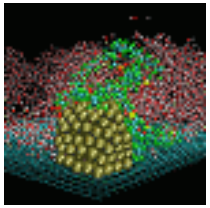












Usage slide

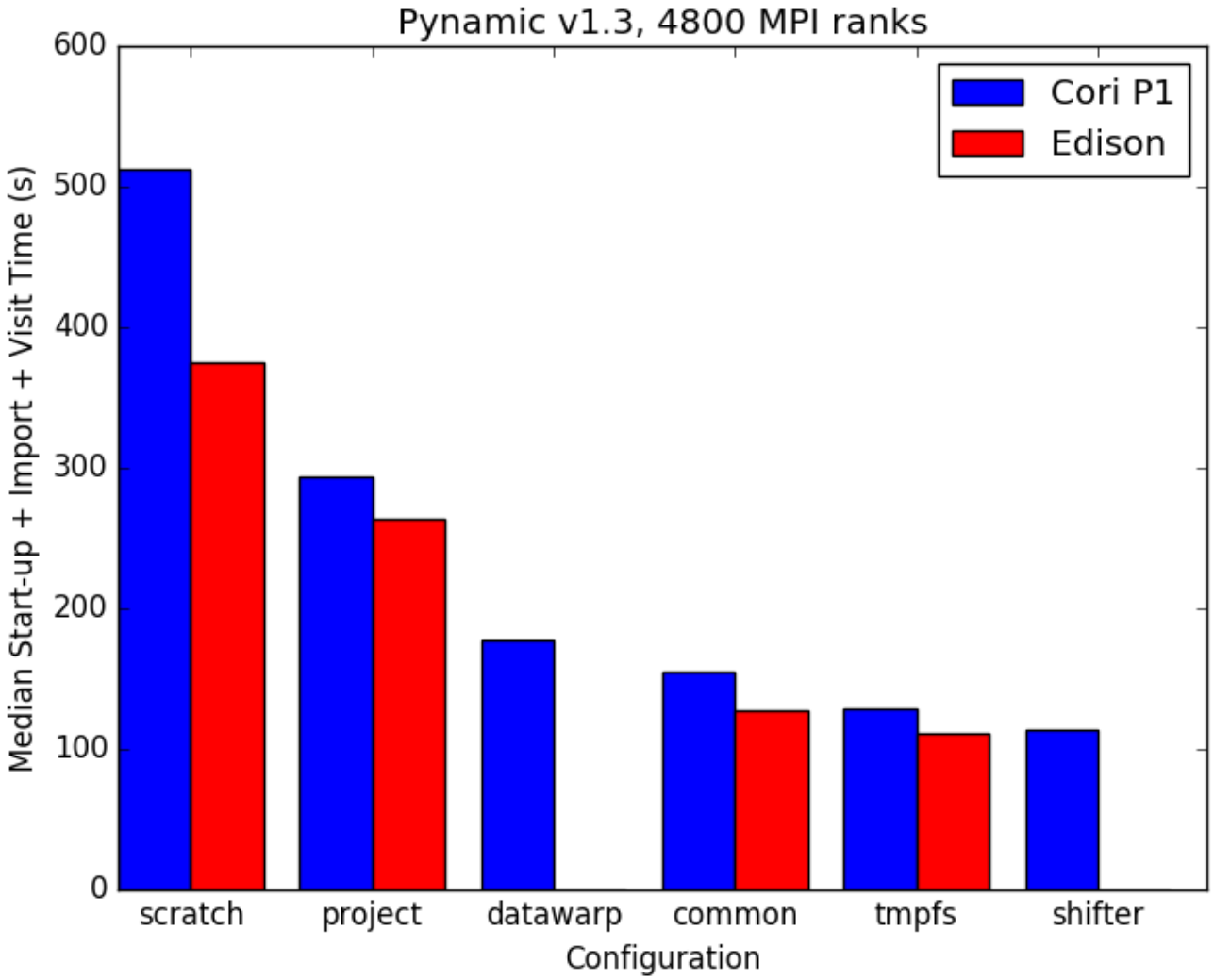
- **Use shifterimg pull to pull images from a registry**
  - Only do this once or after an update

```
> shifterimg pull ubuntu:14.04
```

- **Use shifter command to run a container with an image**

```
> shifter --image=ubuntu:14.04 bash
$ lsb_release -a
No LSB modules are available.
Distributor ID: Ubuntu
Description:    Ubuntu 14.04.5 LTS
Release:  14.04
Codename:     trusty
```

Shifter accelerates Python Apps



Why?

- **Python must walk through the python libraries to construct the namespace**
- **Python must load up (read) any dynamic libraries that are required**
- **The loader must traverse the LD_LIBRARY_PATH to find the libraries to load**
- **Result: Lots of metadata accesses which put a load on the file system Metadata server**

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.

Running an MPI Job – Building Image

```
FROM nersc/mpi-ubuntu:14.04

ADD . /app
RUN cd /app && \
    mpicc –o hello helloworld.c
```

Dockerfile

```
> docker build –t scanon/hello .
> docker push scanon/hello
```

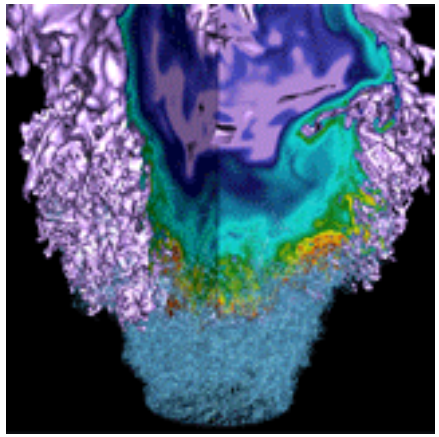
Running an MPI Job – Submit and run

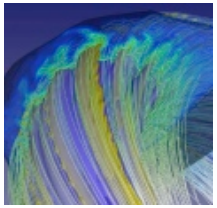
submit.sl

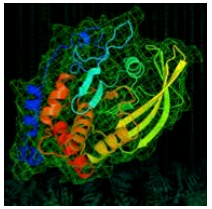
```
#!/bin/sh
#SBATCH --image=scanon/hello
srun -np 10 shifter /app/hello
```

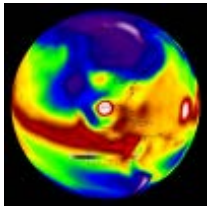
```
> sbatch submit.sl
```

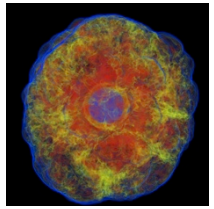
Related Work and Discussion

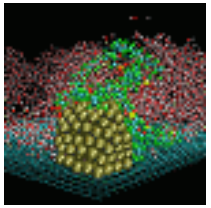












Other HPC Container Solutions

- **Singularity**
  - Very popular
  - Easy Installation
  - Runtime similar to Shifter
  - Native Image format in addition to Docker
  - Commercial company (Sylabs) now developing it
- **CharlieCloud**
  - Very light-weight
  - No special privileges required
  - Separate tools to unpack Docker images

How does Shifter differ from Docker?

Most Noticeable

- **Image read-only on the Computational Platform**
- **User runs as the user in the container – not root**
- **Image modified at container construction time (e.g. additional mounts)**

Less Noticeable:

- **Shifter only uses mount namespaces, not network or process namespaces**
- **Shifter does not use cgroups directly (integrated with the Workload Manager)**
- **Shifter uses individual compressed filesystem files to store images, not the Docker graph (slows down iterative updates)**
- **Shifter starts some additional services (e.g. sshd in container space)**

Why Users will like Shifter

Enables regular users to take advantage of Docker on HPC systems at scale.

This enables users to:

- **Develop an application on the desktop or laptop and easily run it on a cluster or Supercomputer**
- **Solve their dependency problems themselves**
- **Run the (Linux) OS of their choice and the software versions they need**

And…

- **Improves application performance in many cases**
- **Improves reproducibility**
- **Improves sharing (through sites like Dockerhub)**

Acknowledgements

Cray

NERSC – Benchmarks and Use Cases

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Others – Contributors and Use Cases

CSCS, Vakho Tsulaia, Ted Kisner

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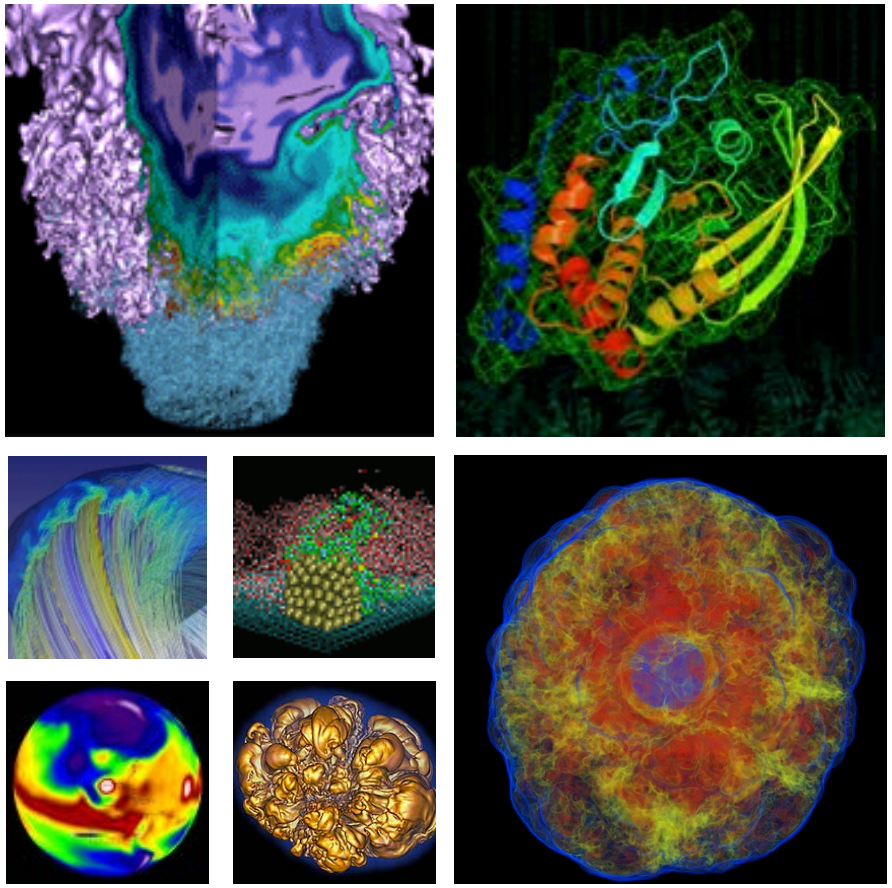
Summary

- **Shifter enables HPC systems to easily and securely run Containers even at large scale**
- **Shifter provides 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.**

Shifter – Advanced Usage



Shane Canon

NERSC Data and Analytics Services

January 14, 2019

Volume Mounts

- **Volume Mounts provide a way to map external paths into container paths.**
- **This allows paths in the container to be abstracted so it can be portable across different systems.**
- **Basic syntax is:**

```
-volume <external path>:<container path>
```

- **Shifter places some constraints on what paths can be mapped and where they can be mapped for added security.**

Using Volume Mounts

```
anon@cori06:~> ls $SCRATCH/myjob
config   data.in

canon@cori06:~> shifter --image=ubuntu --volume=$SCRATCH/myjob:/data bash
canon@cori06:~$ ls /data/
config   data.in

canon@cori06:~$
```

PerNode Write Cache

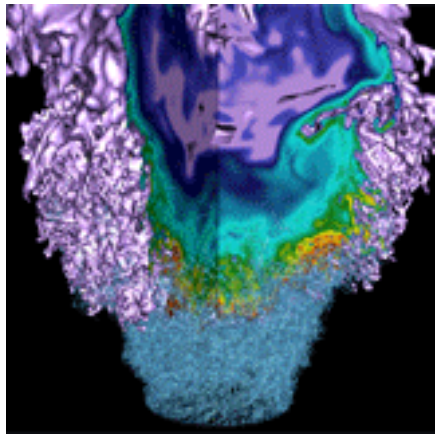
- **PerNodeWrite extends the volume concept to create temporary writeable space that aren't shared across nodes.**
- **These spaces are ephemeral (removed on exit)**
- **These are node local and the size can be adjusted**
- **Performs like a local disk but is more flexible**
- **Basic syntax is**

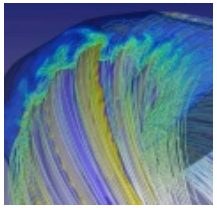
```
--volume <external path>:<container path>:perNodeCache=size=XXG
```

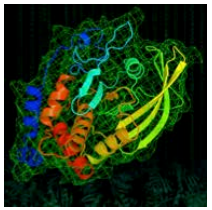
Using Volume Mounts

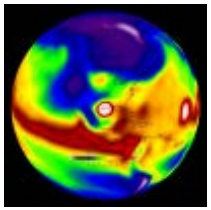
```
canon@cori06:~> shifter --image=ubuntu \
      --volume=$SCRATCH:/scratch:perNodeCache=size=100G /bin/bash
canon@cori06:~$ df -h /scratch/
Filesystem      Size  Used Avail Use% Mounted on
/dev/loop4      100G   33M  100G   1% /scratch
canon@cori06:~$ dd if=/dev/zero bs=1k count=10M of=/scratch/output
10485760+0 records in
10485760+0 records out
10737418240 bytes (11 GB, 10 GiB) copied, 22.2795 s, 482 MB/s
canon@cori06:~$ ls -lh /scratch/output
-rw-r--r-- 1 canon canon 10G Nov  9 23:38 /scratch/output
canon@cori06:~$ exit
exit
canon@cori06:~> shifter --image=ubuntu \
     --volume=$SCRATCH:/scratch:perNodeCache=size=100G /bin/bash
canon@cori06:~$ ls -l /scratch
total 0
```

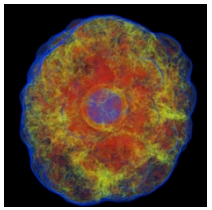
Optimizations

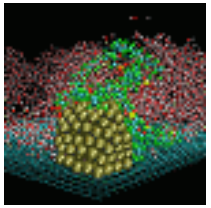












Dockerfile Best Practices

Bad:

```
RUN wget http://hostname.com/mycode.tgz
RUN tar xzf mycode.tgz
RUN cd mycode ; make; make install
RUN rm -rf mycode.tgz mycode
```

Good:

```
RUN wget http://hostname.com/mycode.tgz && \
 tar xzf mycode.tgz && \
 cd mycode && make && make install && \
 rm -rf mycode.tgz mycode
```

Dockerfile Best Practices

Bad:

```
RUN wget http://hostname.com/mycode.tgz ; \
 tar xzf mycode.tgz ; \
 cd mycode ; make ; make install ; \
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```

Good:

```
RUN wget http://hostname.com/mycode.tgz && \
 tar xzf mycode.tgz && \
 cd mycode && make && make install && \
 rm -rf mycode.tgz mycode
```

Dockerfile Best Practices

Bad:

```
ADD . /src

RUN apt-get update –y && atp-get install gcc

RUN cd /src && make && make install
```

Good:

```
RUN apt-get update –y && apt-get install gcc

ADD . /src

RUN cd /src && make && make install
```

Multi-Stage Builds

- **Added in Docker 17.05**
- **Allows a build to progress through stages**
- **Files can be copied from a stage to later stages**
- **Useful for splitting images between build and run-time to keep image sizes small**
- **Can be used to make public images that make use of commercial compilers**

Dockerfile – Multistage build

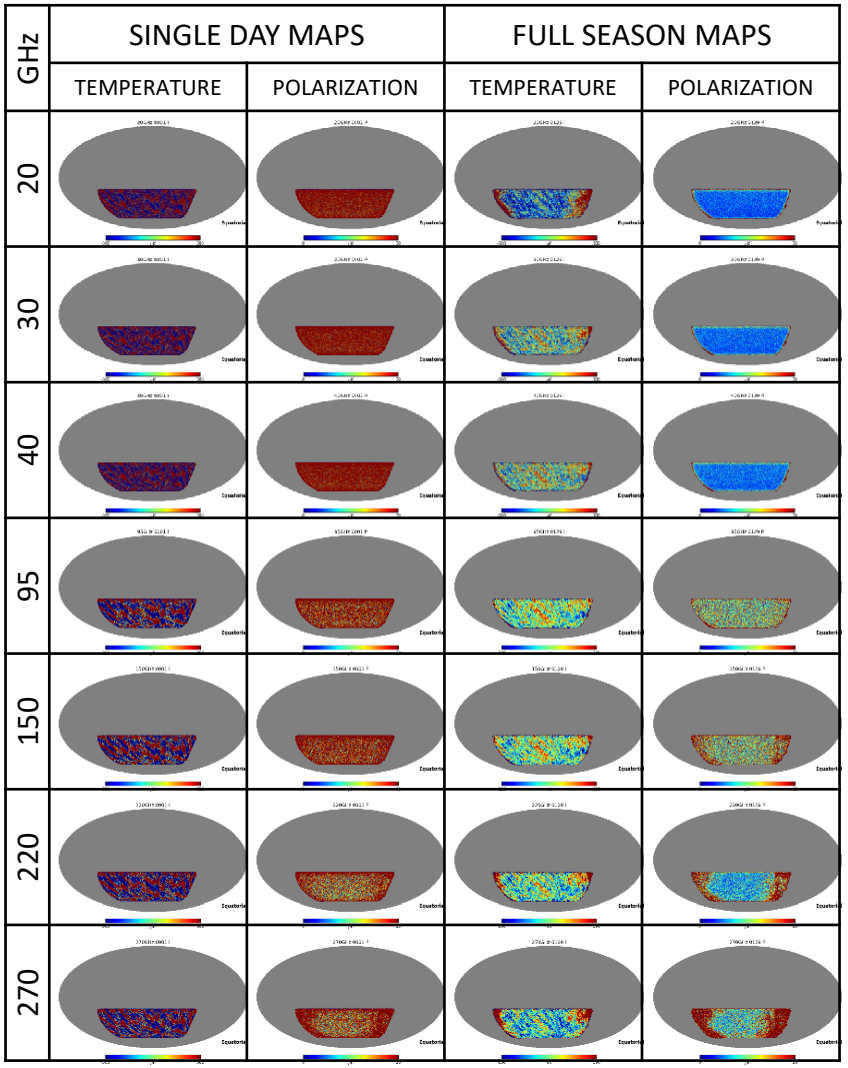
```
FROM centos:7 as build
RUN yum -y install gcc make
ADD code.c /src/code.c
RUN gcc -o /src/mycode /src/code.c

FROM centos:7
COPY --from=build /src/mycode /usr/bin/mycode
```

Other Considerations

- **Avoid very large images (> ~5 GB)**
- **Keep data in $SCRATCH and volume mount into the container if data is large**
- **Use volume mounts for rapid prototyping and testing, then add that into the image after code stabalizes**

Measuring the Composition of the Universe

- **CMB – S4**
  - Ambitious collection of telescopes to measure the remnants of the Big Bang with unprecedented precision
- **Simulated 50,000 instances of telescope using 600,000 cores on Cori KNL nodes.**
- **Why Shifter?**
  - Python wrapped code needs to start at scale



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Questions?

Create an image with Docker

Dockerfile

```
FROM ubuntu:14.04
LABEL 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 .
```

Running an image with Docker

```
> docker run -it –rm scanon/myapp:1.1 /myapp/myapp
…
App Output
….
```

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

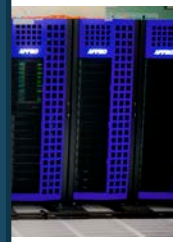
Data Intensive Workload Need	Cori Solution
Local Disk	NVRAM 'burst buffer' and ***Shifter***
Large memory nodes	128 GB/node on Haswell; Large memory login and service nodes
Massive serial jobs	NERSC serial queue
Complex workflows	***Shifter*** CCM mode Large Capacity of interactive resources
Communicate 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

Converging Data Intensive Systems and HPC

Compute Intensive

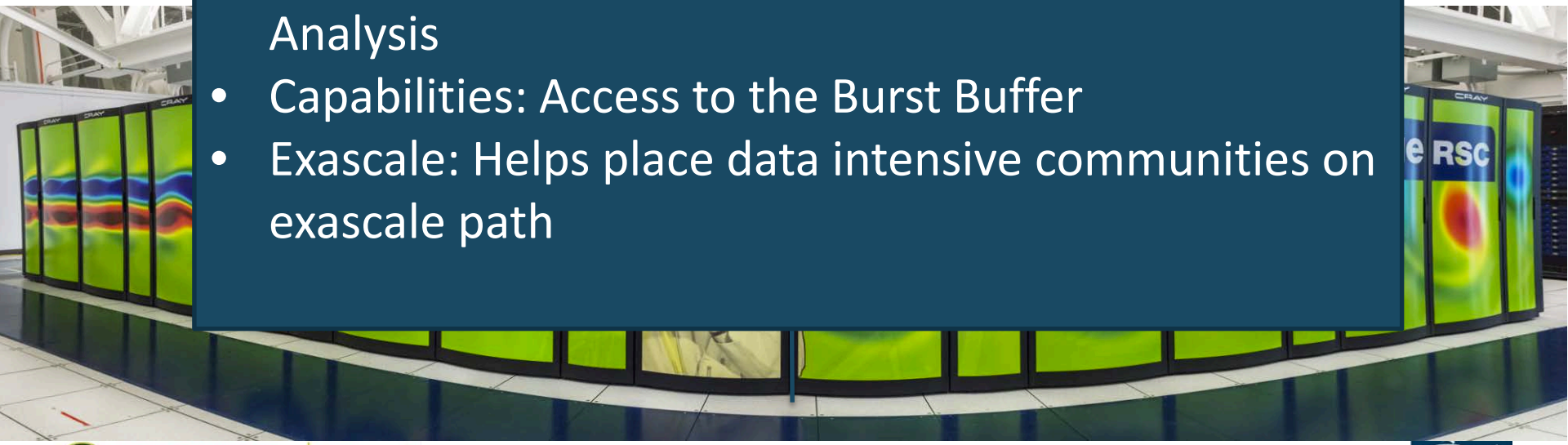
Data Intensive

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



What's in an Image

- **Directory tree**
  - Base Linux OS
  - Libraries, binaries, tools, scripts, etc
  - User code
  - Data
- **Run-time Settings**
  - Environment variables
  - Working Directory
  - Default execution and parameters
- **Other things**
  - Network-related (e.g. ports)
  - Run User

Singularity

- **Can pull and use Docker images. Converted to a singularity file.**
- **Has its own recipe file and build tools**
- **Images are flat (no layers)**
- **Images can be copied like regular files**

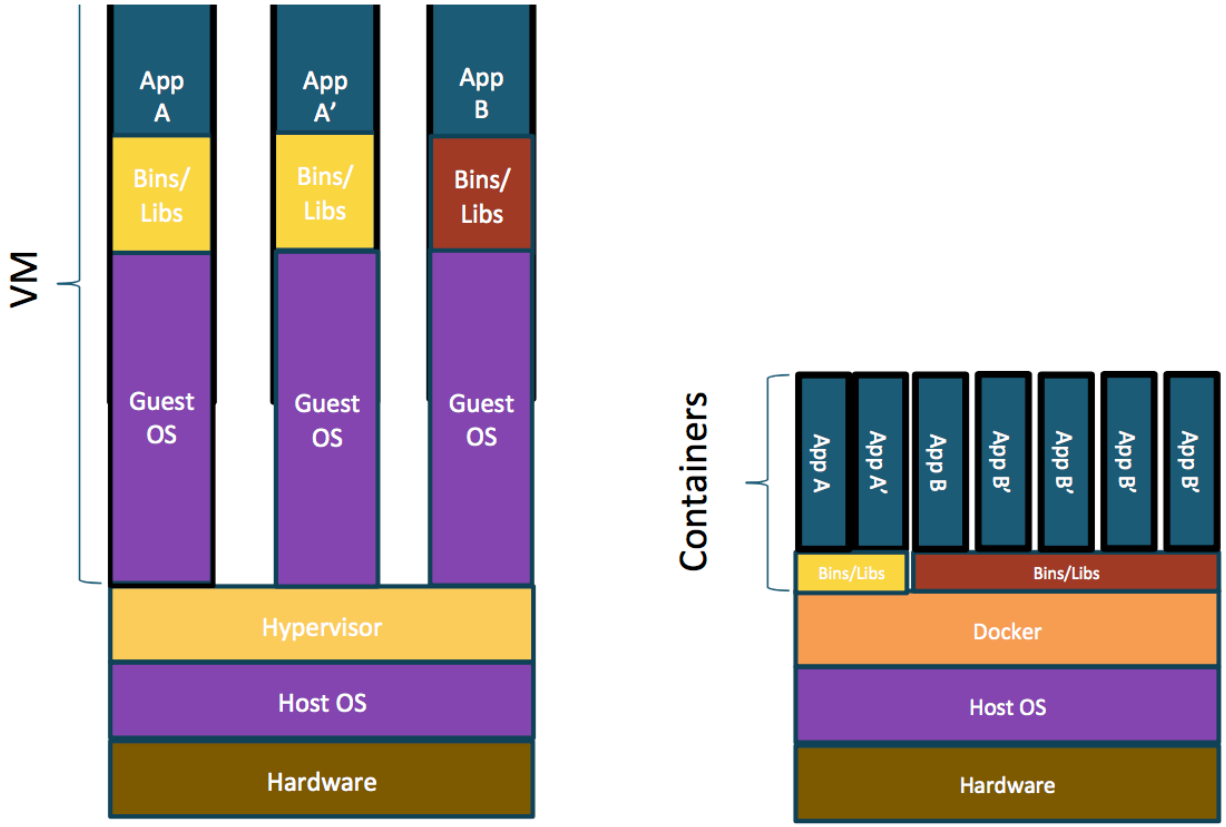
Singularity Recipe File Example

```
Bootstrap: docker
From: ubuntu

%help
Example Singularity Image

%files
    script.sh /script.sh

%labels
    Maintainer I. M. Maintainer
    Version v1.0

%environment
    FOO=bar
    export FOO

%post
    apt-get update -y
    apt-get install -y curl
    echo 'export BAR=blah' >> $SINGULARITY_ENVIRONMENT

%runscript
    exec /script.sh
```

Singularity

```
> singularity build myimage.simg Singularity
```

Containers versus VMs



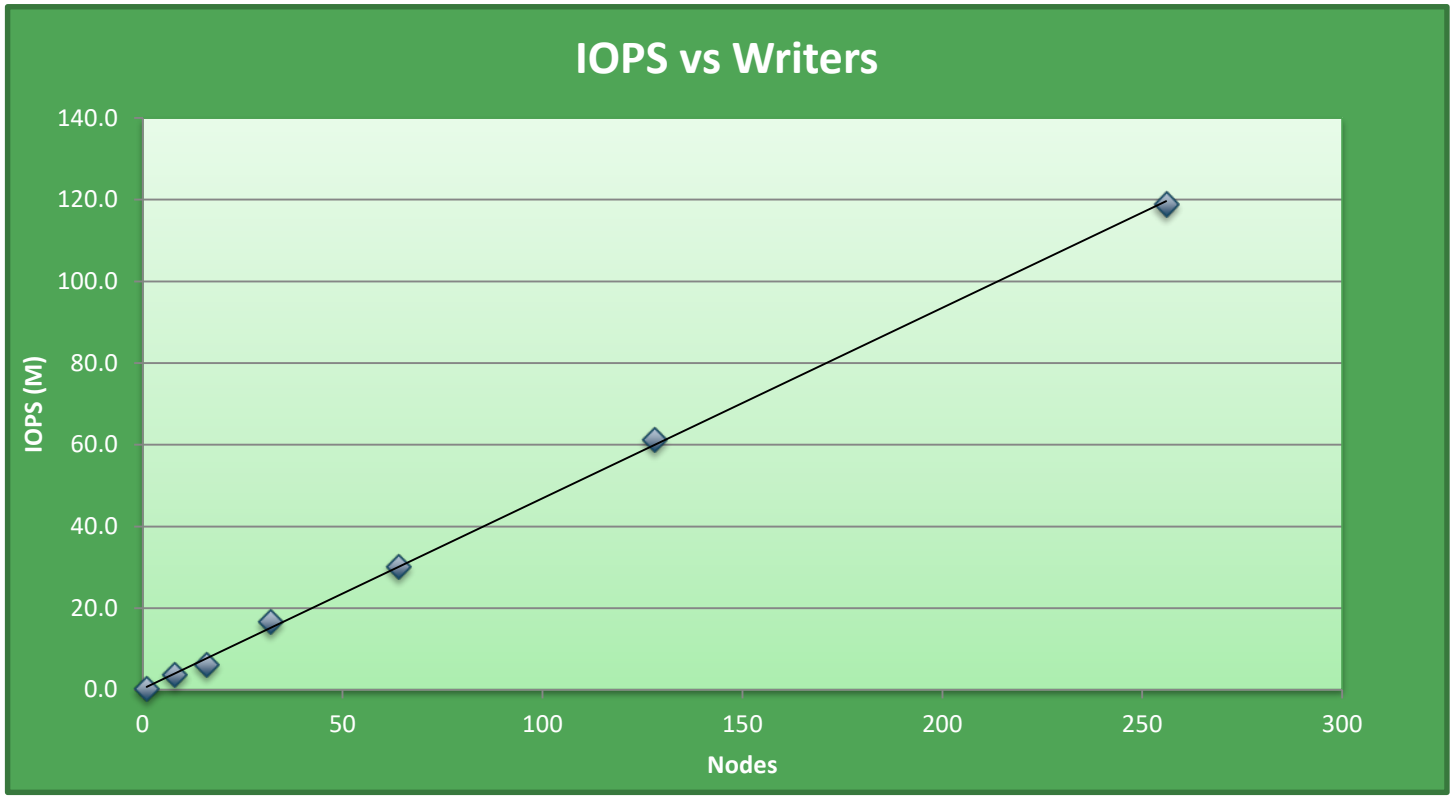
Singularity Execution

```
> singularity shell myimage.simg
Singularity myimage.simg:~>

> singularity run myimage.simg
Hello World

> singularity shell docker://ubuntu:latest
 Singularity ubuntu:~>
```

Charliecloud

- https://github.com/hpc/charliecloud
- **No root privs required for installation**
- **Does require user namespace report (increasingly common now)**
- https://hpc.github.io/charliecloud/index.html

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.