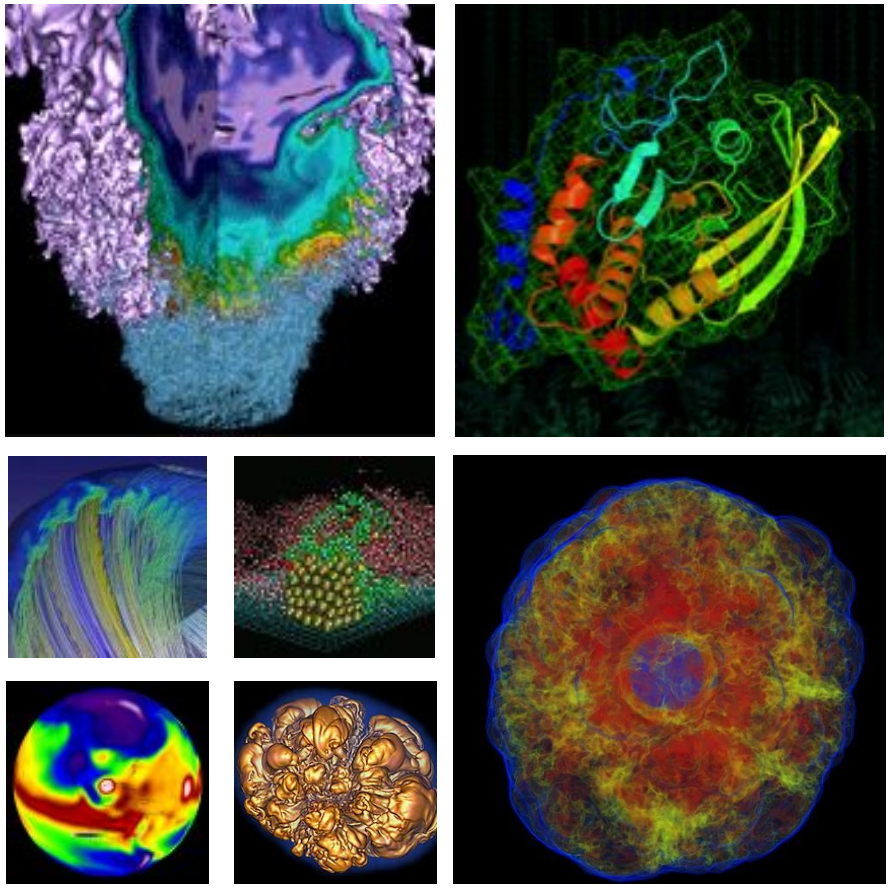
Running Containers at NERSC with Shifter



Shane Canon

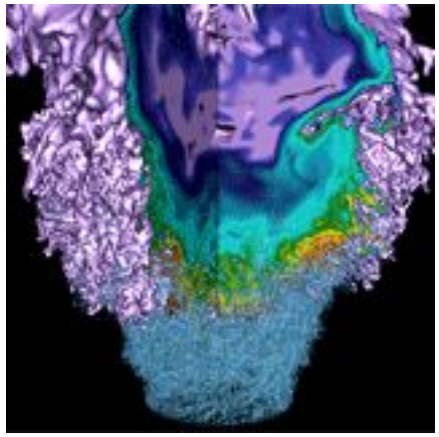
NERSC Early User Training Day 2019

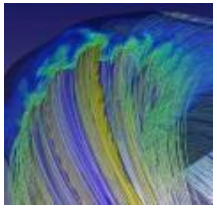
June 21, 2019

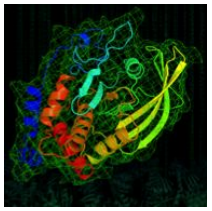
Outline

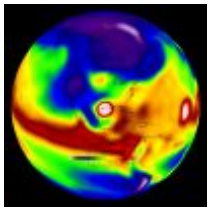
- Quick Intro to Containers
- Role of Shifter
- Walk through of using Docker and Shifter

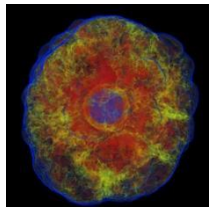
Intro to Containers and Shifter

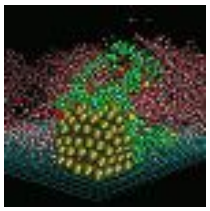












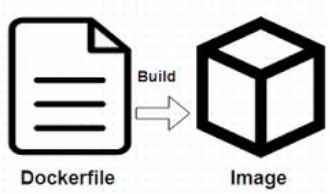
Docker Basics

Build

Ship

Run

- **Build images that captures applications requirements.**
- **Manually commit or use a recipe file.**
- **Push an image to DockerCloud, a hosted registry, or a private Docker Registry.**
- **Share Images**
- **Use Docker Engine to pull images down and execute a container from the image.**



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 (not relevant to Shifter)**
  - Network-related (e.g. ports)
  - Run User

Why not just run Docker

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

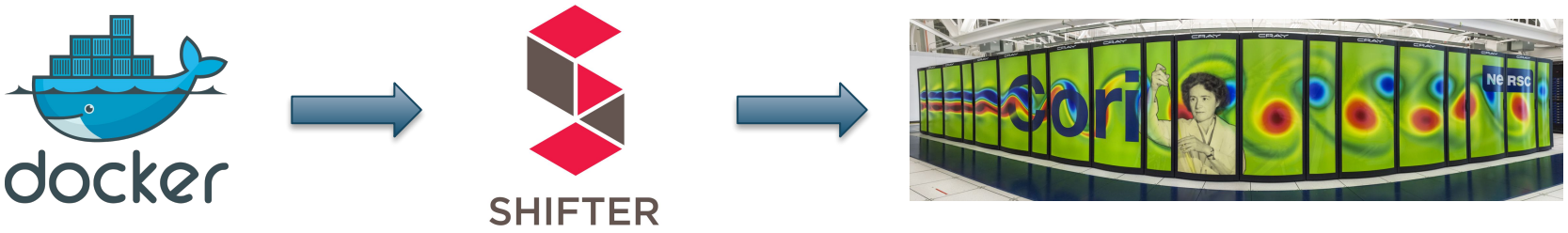
```
> docker run -it -v /:/mnt --rm busybox
```

- **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**

Shifter

- NERSC R&D effort, in collaboration with Cray, to support Docker Application images
- "Docker-like" functionality on the Cray and HPC Linux clusters
- Addresses security issues in a robust way
- Efficient job-start & Native application performance

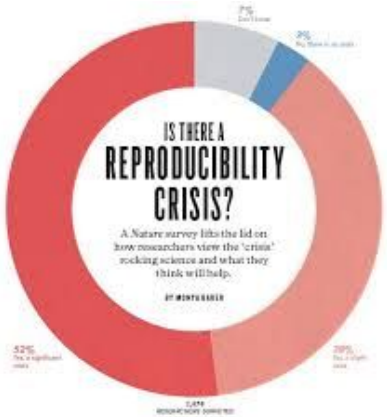


Why Users will like Containers and Shifter

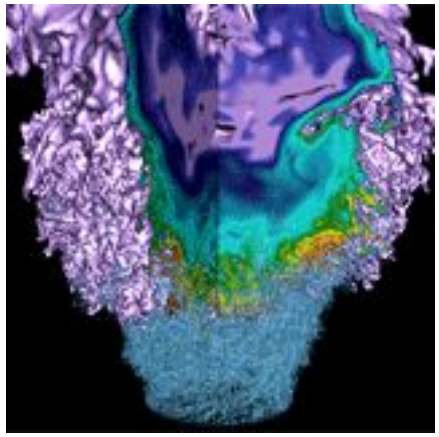
- Develop an application on your desk top and run it on Cori
- Enables you to solve your dependency problems yourself
- Run the (Linux) OS of your choice and the software versions you need
- Improves application performance in many cases
- Improve reproducibility
- Improve sharing (through sites like Dockerhub)

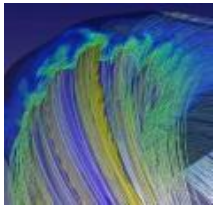
Containers and Science

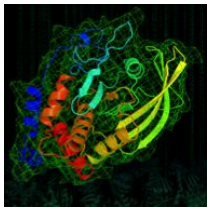
- **Reproducibility**
  - Everything you need to redo a scientific analysis
  - Image manifest contains all information about environment
    - Scripts, portable input files can be managed with version controller for greater control
- **Portability**
  - Runs on every system
- **Reduction of Effort**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

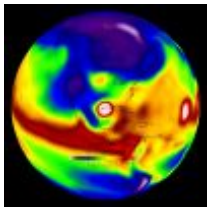


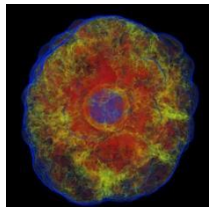
Shifter in Action

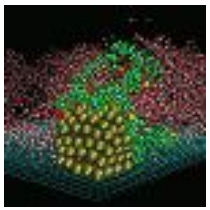












Create an image with Docker

Dockerfile

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

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

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

Use the Image with Shifter

Submit script

```
#!/bin/bash
#SBATCH -N 16 -t 20
#SBATCH --image=scanon/myapp:1.1

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

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

Shifter and MPI

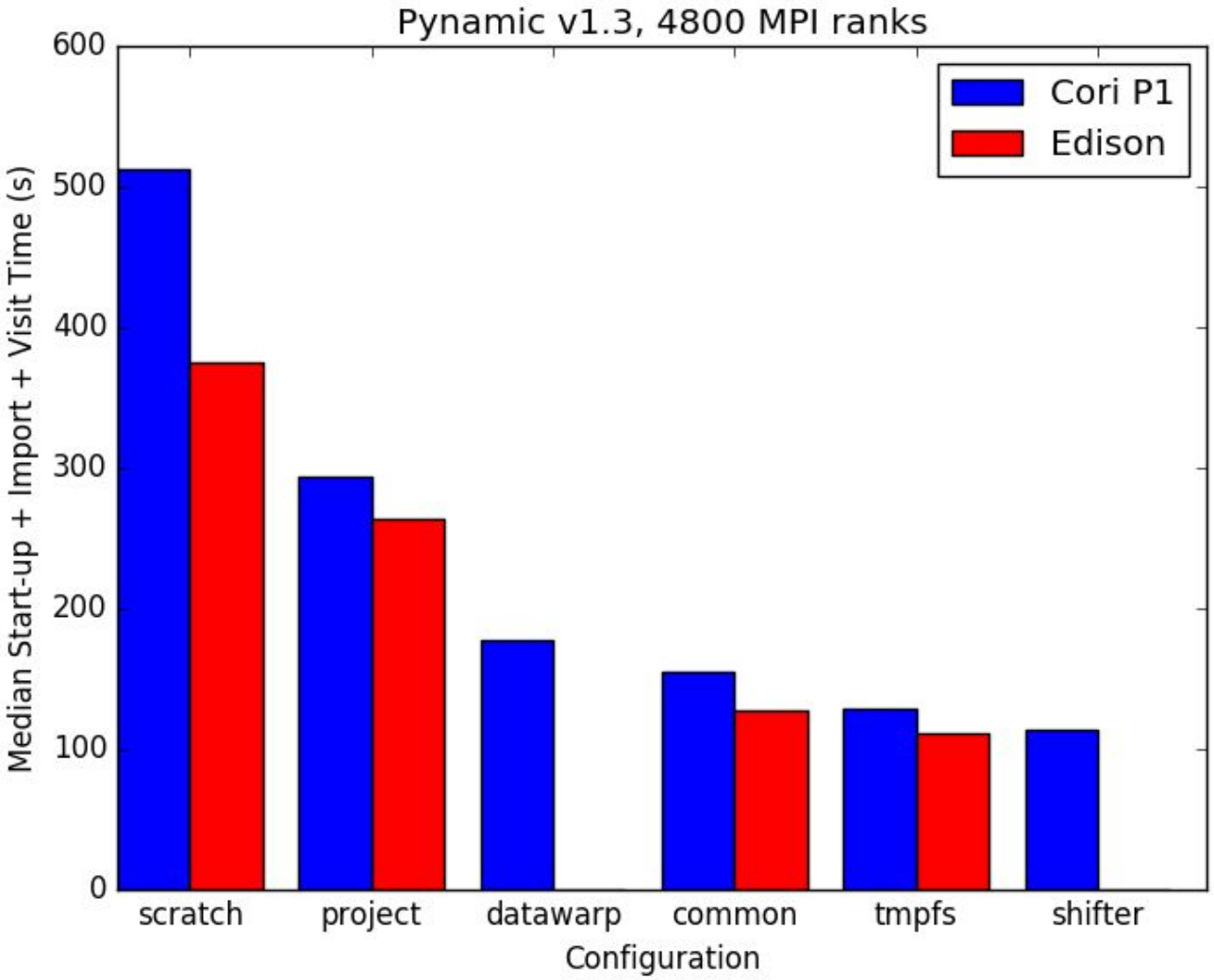
- Shifter has a “built-in” approach for supporting MPI applications in containers.
- Build Applications using ABI compatibility.
- Shifter automatically maps in appropriate libraries at run time.
- No rebuild required, but may not work for all cases.
- Can provide native MPI performance.

Shifter and MPI

```
# This example makes use of an Ubuntu-based NERSC base image
# that already has MPI built and installed.
#
FROM nersc/ubuntu-mpi:14.04

ADD helloworld.c /app/

RUN cd /app && mpicc helloworld.c -o /app/hello

ENV PATH=/usr/bin:/bin:/app:/usr/local/bin
```

```
> shifterimg pull scanon/myapp:1.1
> salloc –n 128 –image=scanon/myapp:1.1 –C haswell
# srun -n 128 shifter /myapp/app
```

Shifter accelerates Python Apps



Shifter behavior versus Docker

- Processes run as your user id (not root).
- Images are mounted read-only (so you modify files in the image).
- Home directories and global file systems are automatically mounted.
- Some handling of special Dockerfile directives isn't yet supported

Other things of Note

- Shifter supports volume mounts that allow you to map a directory (e.g. $SCRATCH) into another location in your image.
- Shifter supports per-Node write-able scratch spaces that work well for apps that want a local disk.
- NERSC runs a private registry (registry.services.nersc.gov) that can be used to store private images that you can't put in DockerHub.

Shifter versus Spin

Shifter

- Runs processes as the user
- Runs on the HPC systems

Best for:

- Simulation or analysis runs
- Need to run at scale
- Need to read/write a lot of data

Spin

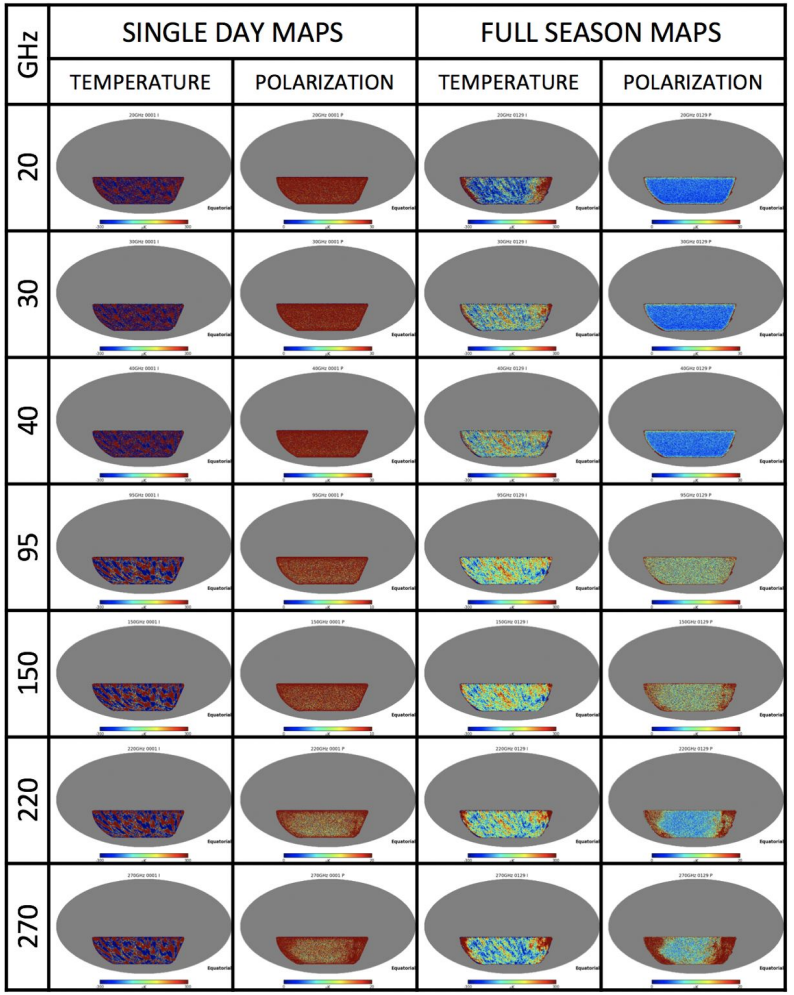
- Runs with stock Docker and Rancher
- Runs on dedicated hardware

Best for:

- Running services or processes that need to run "indefinitely"
- Services that need to be externally accessible

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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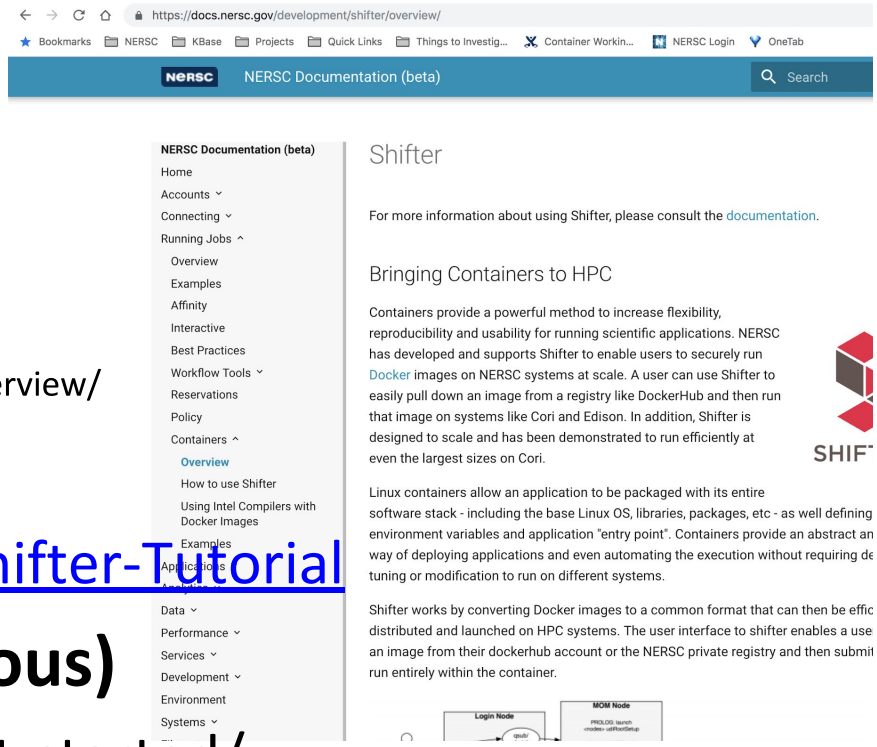
Where can you learn more

- **NERSC Docs Website**
  - docs.nersc.gov
  - Running Jobs
    Containers
    Overview
  - https://docs.nersc.gov/development/shifter/overview/
- **Previous Training**
  - https://github.com/nersc/Shifter-Tutorial
- **Docker Resources (Numerous)**
  - https://docs.docker.com/get-started/



Questions