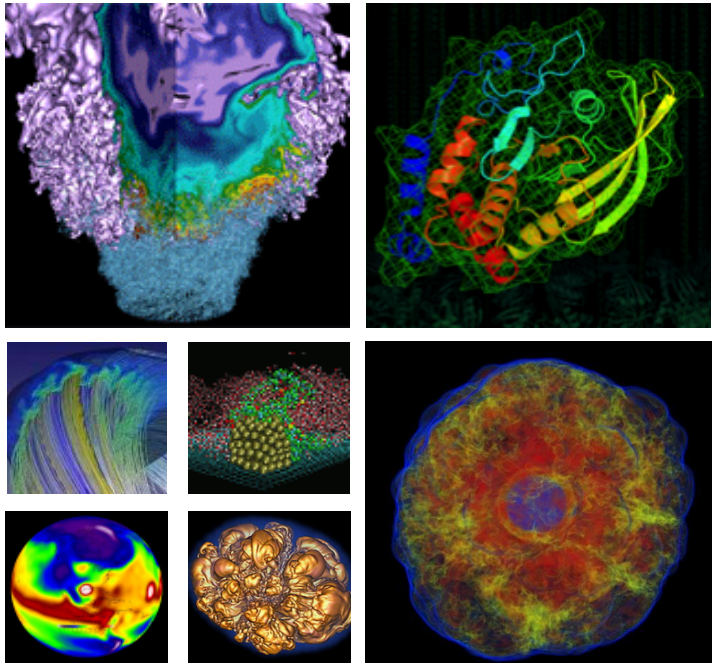
# The State of Containers in Scientific Computing




NERSC

Georg Rath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U.S. DEPARTMENT OF ENERGY | Office of Science

BERKELEY LAB

# NERSC

- Primary scientific computing facility of the office of science
- Two supercomputers (Cori, Edison), three clusters
  - Over 800.000 cores
  - Over 50 PB of storage in varying speeds
- Serving more than 6000 scientists
- Astrophysics, Climate & Earth Science, Chemistry, High Energy Physics, Genomics,…

# HPC in a nutshell

- A (large) number of compute nodes
- Connected by a **H**igh **S**peed **N**etwork
- Accessing data stored in a parallel filesystem
- Run as a shared resource
- Orchestrated by a workload manager

# What is the hardest problem in scientific computing?

# Installing Software

- Center provided software stack via Environment Modules
  - Lmod, Modules Classic, Modules4
- Error-prone
- Slow*
- Unique
- Not portable
- Leads to user maintained software stacks
  - That depend on system

# And then Docker hit…

- Simple
- Portable
- Reproducible
- Leveraging relatively stable Linux APIs
  - Namespaces
  - cgroups

# ...and we wept.

- High demand by users and admins alike
- Absolutely not built for HPC
- Security nightmare
  - access to Docker is root equivalent*
- A daemon on my compute node?
  - **No**

# What do we want?

- A way to run Docker images on HPC systems
- No fancy stuff
  - Overlay networks
  - Plugins
  - Swarm/Kubernetes
- No daemon
- Secure
- Scalable
- Bonus: works on older kernels

# Great minds think alike

| | Shifter | Charliecloud | Singularity |
|---|---|---|---|
| Governance | NERSC | LANL | SyLabs Inc (started at LBNL) |
| Mechanism | setuid | userns | setuid, userns |
| Image Format | squashfs | Tar File | squashfs (since 2.4) |
| Noteworthy | Focus on HPC | Lightweight | “Scientific Docker” |

# What is container, really?

```
debootstrap stable containerfs/ http://deb.debian.org/debian/
unshare --mount --pid –fork
mount --bind containerfs containerfs
mount --make-private containerfs
cd containerfs

mount -t proc none proc
mount -t sysfs none sys
mount -t tmpfs none tmp
mount -t tmpfs none run

pivot_root . mnt
umount -l mnt
exec bash -i
```

# Access to host hardware/libraries

- Violates containment
- Bind device file into container
- Inject host libraries into the container (eg. libcuda.so)
  - Manually or via libnvidia-container
- Requires ABI compatibility between host/container libs
- Does not work with static linking
- Glibc issues

# Do you see the problem?

```
FROM ubuntu:18.04

# install Tensorflow
RUN apt-get install python3-pip python3-dev
RUN pip3 install tensorflow

COPY ai.py /usr/bin/ai.py

CMD [“/usr/bin/ai.py”]
```

# The need for speed

- Binary build of Tensorflow is not optimized
- Modern processors need vector instructions for performance
- Theoretical Peak Performance Intel Haswell
  - Scalar: ~ 130 GFLOPS
  - AVX: ~ 500 GFLOPS
- Let's fix this…

# An easy fix?

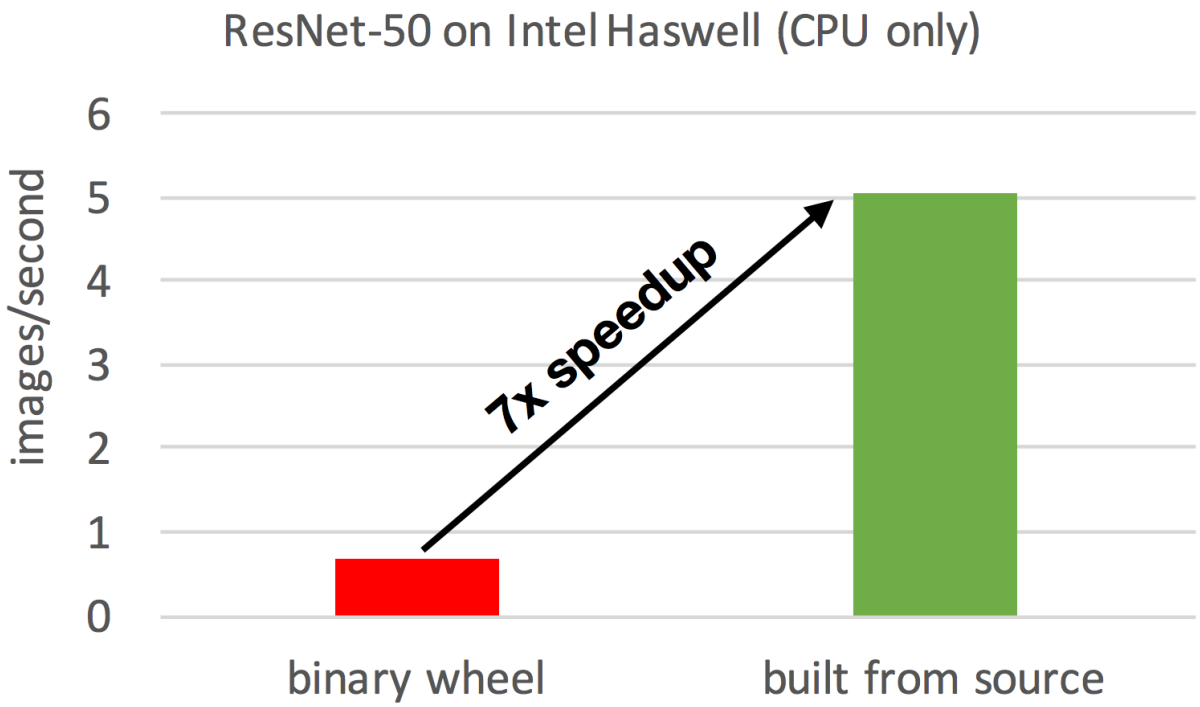
```
[…]

RUN LD_LIBRARY_PATH=${LD_LIBRARY_PATH} \
    bazel build --config=mkl \
                --config="opt" \
                --copt="-march=haswell" \
                --copt="-O3" \
                //tensorflow/tools/pip_package:build_pip_package && \
    mkdir ${WHL_DIR} && \
    bazel-bin/tensorflow/tools/pip_package/build_pip_package ${WHL_DIR}

[…]
```

* actual Dockerfile around 80 lines lot more sophisticated
** EasyBuild/Spack highly recommended

# Does it pay off?



# Portability

- Requires ”cross-compiling”
- Different containers with different tags
- Or leverage Docker “fat manifest” containers
  - Introduced with Image Manifest v2.2
  - Specifies architecture and features
  - Not integrated yet

# Conclusion

- Containers are a valuable tool for scientific computing
  - User defined software stack
- Containers are not a panacea
  - Portability and performance require work
  - Reproducibility over time will be challenging as well
- Leveraging proven tools in conjunction with containers provides great benefit

# Questions?


# Thank You