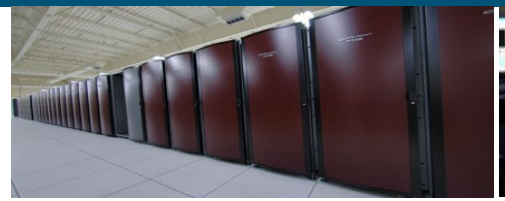
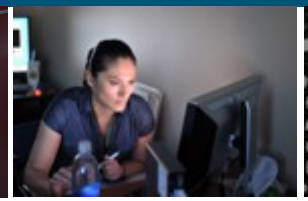
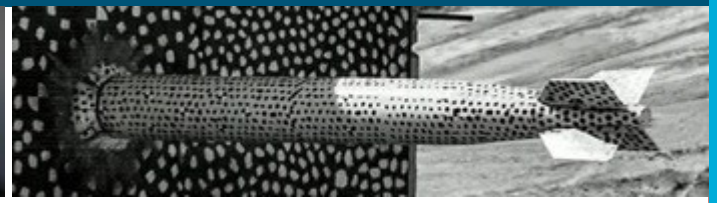
Leveraging Containerization for DevOps with Sandia's HPC Workloads

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Motivation

Multiple drivers exist for using containers in HPC

1. Containers to help with DevOps
   - Development of HPC apps on workstations which can port & scale to supercomputers
   - Utilize testbed/cloud resources for functionality and feature testing
   - Leverage latest Cloud craze in Docker containers
2. Containers to aid in emerging HPC workloads
   - Support for deep learning / machine learning software ecosystems
   - Large-scale data analytics & in-situ workload ensembles
   - Streaming analytics & non-batch jobs

Container features wanted in HPC

- **BYOE** - Bring-Your-Own-Environment.
  - Developers define the operating environment and system libraries in which their application runs.
- **Composability**
  - Developers explicitly define how their software environment is composed of modular components as container images
  - Enable reproducible environments that can potentially span different architectures
- **Portability**
  - Containers can be rebuilt, layered, or shared across multiple different computing systems
  - Potentially from laptops to clouds to advanced supercomputing re- sources
- **Version Control Integration**
  - Containers integrate with revision control systems like Git
  - Include not only build manifests but also with complete container images using container registries like Docker Hub.

Container features not wanted in HPC

- **Overhead**
  - HPC applications cannot incur significant overhead from containers
- **Micro-Services**
  - Micro-services container methodology does not apply to HPC workloads
  - 1 application per node with multiple processes or threads per container
- **On-node Partitioning**
  - On-node partitioning with cgroups is not necessary (yet?)
- **Root Operation**
  - Containers allow root-level access control to users
  - In supercomputers this is unnecessary and a significant security risk for facilities
- **Commodity Networking**
  - Containers and their network control mechanisms are built around commodity networking (TCP/IP)
  - Supercomputers utilize custom interconnects w/ OS kernel bypass operations

Container Vision @ Sandia

- Support software dev and testing on laptops
  - Working builds then can run on supercomputers
  - May also leverage VM/binary translation
- Let developers specify how to build the environment AND the application
  - Users just import a container and run on target platform
  - Many containers, but can have different code “branches” for arch, compilers, etc.
  - Not bound to vendor and sysadmin software release cycles
- Performance matters!
- Want to manage permutations of architectures and compilers
  - x86 & KNL, ARMv8, POWER9, etc
  - Intel, GCC, LLVM

Container Vision @ Sandia

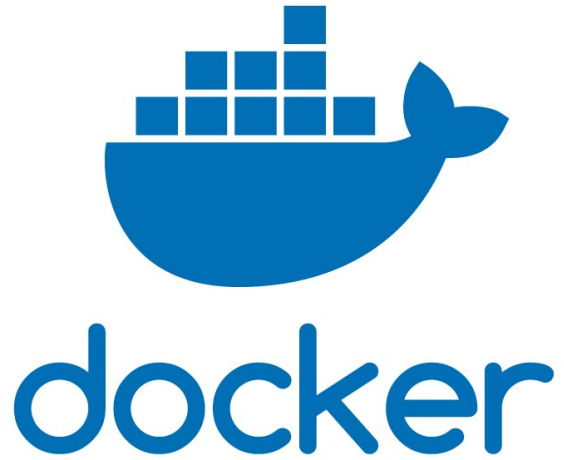
- Developers specify exactly their runtime environment
  - OS, version
  - Third-party libraries (TPLs)
  - How to compile
- Can share environment as a container with other developers
  - Quickly get env to new developer
  - Provide software as a container to analysts
  - Developer makes changes, triggerd container build with CI, validated image
- Leverage same container image on different clusters or supercomputers

Trilinos Muelu Container Example

```
FROM ajyounge/dev-tpl

WORKDIR /opt/trilinos

# Copy files to image

COPY do-configure /opt/trilinos/

# Download Trilinos source tarball

RUN wget -nv https://trilinos.org/oldsite/download/files/trilinos-12.8.1-Source.tar.gz -O /opt/trilinos/trilinos.tar.gz

# Extract Trilinos source file

RUN tar xf /opt/trilinos/trilinos.tar.gz -C /opt/trilinos/

RUN rm -f /opt/trilinos/trilinos.tar.gz

RUN mv /opt/trilinos/trilinos-12.8.1-Source /opt/trilinos/trilinos

RUN mkdir /opt/trilinos/trilinos-build

# Compile Trilinos

RUN /opt/trilinos/do-configure

RUN cd /opt/trilinos/trilinos-build && make -j 3

#Link in a directory, and then set the workdir

RUN ln -s /opt/trilinos/trilinos-build/packages/muelu/doc/Tutorial/src /opt/muelu-tutorial

WORKDIR /opt/muelu-tutorial
```

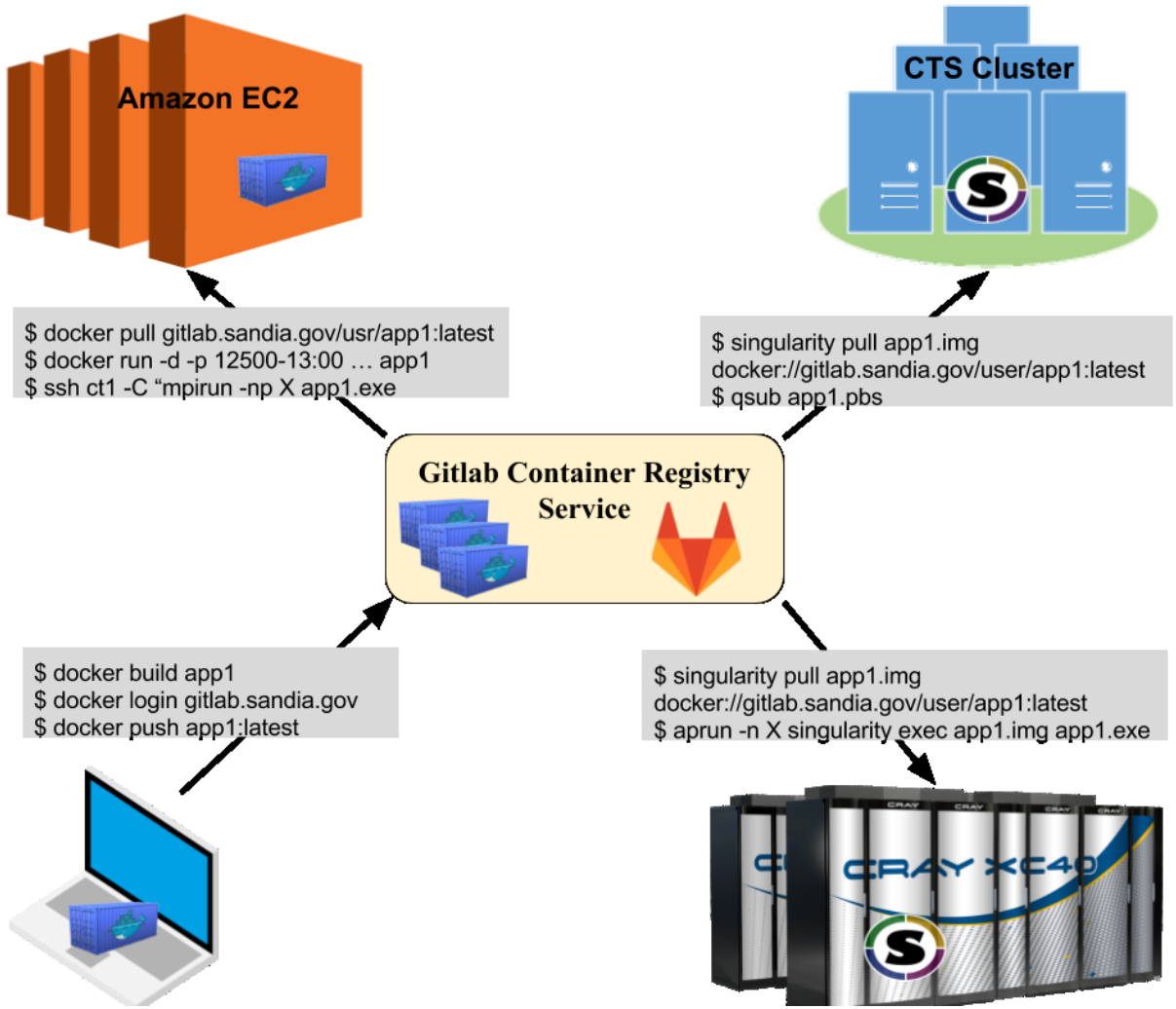
Container Runtimes

- Many different container options
  - Docker, Shifter, Singularity, Charliecloud, etc etc
- Docker containers useful for workstations
  - Allows root level builds and control on personal machine
  - NOT for HPC - Security issues, no shared resource integration
- Singularity best fit for our current HPC needs
  - OSS, publicly available, support backed by Sylabs
  - Simple image plan, support for HPC systems
  - Docker image support, as well as custom Singularity builds
  - Support for multiple architectures (x86, ARM, POWER)
  - Large HPC community support



Container DevOps @ Sandia

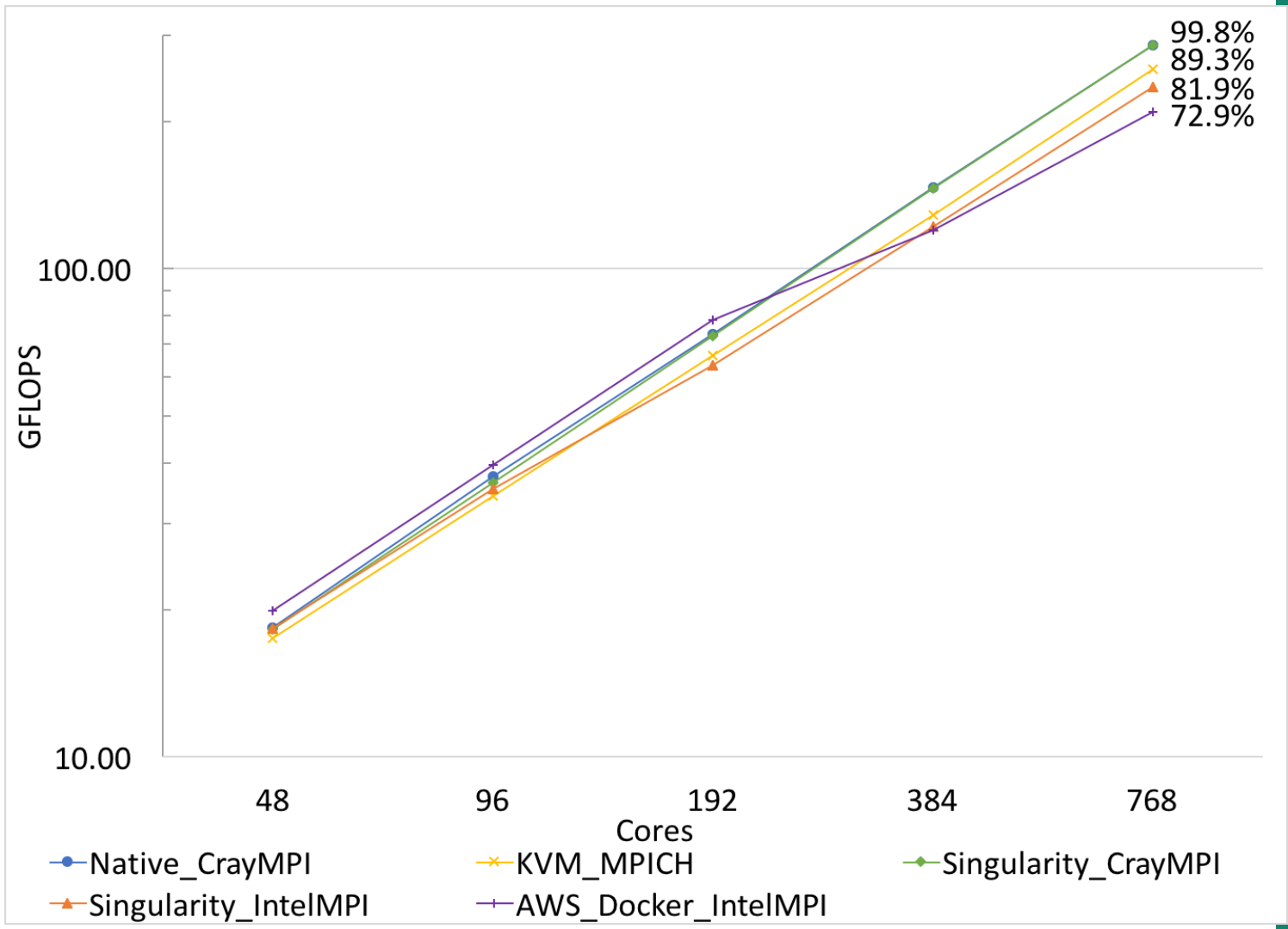
- Impractical for apps to use large-scale supercomputers for DevOps and/or testing
  - HPC resources have long batch queues
  - Dev time commonly delayed as a result
- Create deployment portability with containers
  - Develop Docker containers on your laptop or workstation
  - Leverage Gitlab registry services
    - Separate networks maintain separate registries
  - Import to target deployment
    - Leverage local resource manager
- Deployment to Cray supercomputer now possible



Younge et. al, *A Tale of Two Systems: Using Containers to Deploy HPC Applications on Supercomputers and Clouds*, IEEE CloudCom 2017

HPCG Container Performance

- Modified Cray XC supercomputer to run Singularity containers
- Create `/opt/cray` and `/var/opt/cray` on all images
- Link in Cray system software
  - XPMEM, CrayMPI, uGNI, etc
- HPCG Benchmark in Container
  - Compare Singularity on Cray
  - Compare KVM on Cray
  - Compare Amazon EC2
- Near-native (99.8%) efficiency when using Singularity on a Cray
  - Poor scalability on EC2



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Discussion

- Containers in HPC are different than containers in the cloud
  - Running Docker alone is unacceptable on HPC
  - Need for HPC-centric containerization – Singularity
- Developing DevOps models for custom software ecosystems
- Performance _*can*_ be near native
  - Leveraging vendor libraries within a container is critical
  - Cray MPI on Aries most performant
  - Best-practices are necessary
- Leveraging container model into current & future integrated code teams deployment and testing strategy

Future Directions

Many opportunities & challenges moving forward:

- Container and library interoperability is key
  - Vendor-blessed base images
  - Facilities-blessed user-defined images – container signing?
  - Standardization on image format and ABI compatibility is necessary
- Better system software architecture is needed
  - Containers are a piece of a larger puzzle
  - Better integration with HPC scheduling systems
  - Experiment provenance possible?
- Support emerging HPC software ecosystems
  - Large-scale data analytics
  - Deep Neural Networks on supercomputers
  - Non-batch streaming workloads
  - etc etc

Questions?

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