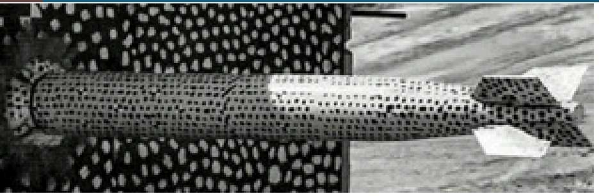
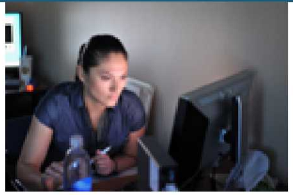
SAND2020-10317C

Towards Containerized HPC Applications at Exascale





PRESENTED BY

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E4S Forum 2020

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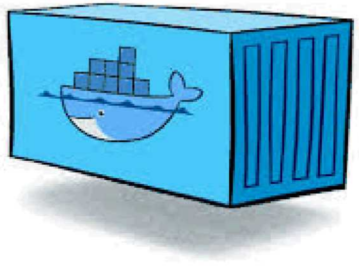
Outline

- Container background
- Introduction to *Supercontainers*
- Building HPC Containers
- Running HPC Containers
- Conclusion

What is a Container?

- Unit of software which packages up all code and dependencies necessary to execute single process or task
- Encapsulates the entire software ecosystem (minus the kernel)
- OS-level virtualization mechanism
  - Different than Virtual Machines
  - Think ”chroot” on steroids, BSD Jails
  - Dependent on host OS, which is (usually) Linux
  - Uses namespaces (user, mount, pid, etc)
- Docker is the leading container runtime
  - Used extensively in industry/cloud enterprise
  - Foundation for Kubernetes and Google cloud
  - Supported in Amazon AWS cloud



High Performance Computing

- DOE has a long history of investment in HPC
  - Stockpile Stewardship & simulation-based science
    - ASCI Red – first Teraflop Supercomputer
    - Red Storm - 100 Tflops and MPP
    - Summit/Sierra - 200 Pflops
  - Bulk synchronous parallel computing ~ HPC
    - 1 application spanning thousands of CPUs concurrently
    - Large-scale capability simulations
    - Also many capacity workloads
  - HPC represents the pinnacle of computing today

- Mission workloads computational requirements demand scale
  - Tightly coupled BSP simulation codes typically use MPI for communication
  - Many workload ensembles quickly expanding to ML/DL/AI

The Cloudy relationship with HPC

- Public cloud computing is often prohibitive
  - Cost – expensive to run millions of CPU hours
  - Security – Can we trust public clouds?
- However, HPC is not traditionally as flexible as “the cloud”
  - Shared resource models
  - Static software environments
  - Requires modification of many COTS tools
- Containers have become a primary cloud deployment model

- What about Containers in HPC?
  - Can we support containers in HPC in the same way as clouds do? *Yes and No*
  - Does this model fit for _both_ HPC and emerging workloads across DOE? *Yes and No*
  - Can we adapt our current programming environments into container images? *Yes*

HPC Container Vision

- Support HPC software development and testing on laptops/workstations
  - Create working container builds that can run on supercomputers
  - Minimize dev time on supercomputers
- Scale containers to leadership-class supercomputing resources
- Developers specify how to build the environment AND the application
  - Users/analysts just import and run on a supercomputer
  - Many containers, but with different manifests target platforms & deployments.
  - Not bound to vendor release cycles, sysadmin reqs, etc
- Enable full-scale software ecosystems = E4S
- Performance matters
  - Use mini-apps to “shake out” container implementations on HPC
  - Expand to exascale workloads & applications
  - Enable features to support emerging workflows (ML/DL/in-situ analytics)

ECP Supercontainers

- Joint DOE effort - LANL, LBNL, LLNL, Sandia, U. of Oregon
- Ensure container runtimes will be scalable, interoperable, and well integrated across DOE
  - Enable container deployments from laptops to Exascale
  - Assist Exascale applications and facilities leverage containers most efficiently
- Three-fold approach
  - Scalable R&D activities
  - Collaboration with related ST and AD projects
  - Training, Education, and Support
- Activities conducted in the context of interoperability
  - Portable solutions
    - Optimized E4S container images for each machine type
    - Containerized ECP that runs on Astra, A21, El-Capitan, …
  - Work for multiple container implementations
    - Not picking a “winning” container runtime
  - Multiple DOE facilities at multiple scales

SUPERCONTAINERS

ECP
EXASCALE COMPUTING PROJECT

Building HPC Container Images

Have to start from somewhere...

E4S: Extreme-scale Scientific Software Stack

- Curated release of ECP ST products based on Spack [http://spack.io] package manager
- Spack binary build caches for bare-metal installs
  - x86_64, ppc64le (IBM Power 9), and aarch64 (ARM64)
- Container images on DockerHub and E4S website of pre-built binaries of ECP ST products
  - Base images and full featured containers (GPU support)
  - GitHub recipes for creating custom images from base images
- GitLab integration for building E4S images
- E4S validation test suite on GitHub
- E4S VirtualBox image with support for container runtimes
  - Docker, Singularity, Shifter, Charliecloud
- AWS image to deploy E4S on EC2

https://e4s.io

Credit: Sameer Shende (U of Oregon)

E4S Container Images Available

- Providing E4S container images on Dockerhub
  - https://hub.docker.com/u/ecpe4s
- Multiple ISAs
  - x86_64, ppc64le, and aarch64
- Multiple OS distros
  - Centos, UBI (Red Hat), and Ubuntu images
- Enabling containerized CI in Gitlab (see T. Gamblin's talk)
- Additional GPU support incoming

There is a container performance-portability continuum

How do we strike the right balance?

- Portable container images can be moved form one resource deployment to another with ease
- Reproducibility is possible
  - Everything (minus kernel) is self-contained
  - Traceability is possible via build manuscripts
  - No image modifications
- **Performance can suffer - no optimizations**
  - Can't build for AVX512 and run on Haswell
  - Unable to leverage latest GPU drivers

- Performant container images can run at near-native performance compared to natively build applications
- Requires targeted builds for custom hardware
  - Specialized interconnect optimizations
  - Vendor-proprietary software
- Host libraries are mounted into containers
  - Load system MPI library (glibc issues!?)
  - Match accelerator libs to host driver
- **Not portable across multiple systems**

Spack environments help with building containers

- We recently started providing base images with **Spack** preinstalled.
- **Very** easy to build a container with some Spack packages in it:

spack-docker-demo/
    Dockerfile
    spack.yaml

```
FROM spack/centos:7

WORKDIR /build
COPY spack.yaml .
RUN spack install
```

Base image with Spack in PATH

Copy in spack.yaml
Then run spack install

```
spack:
  specs:
    - hdf5 @1.8.16
    - openmpi fabrics=libfabric
    - nalu
```

List of packages to install, with constraints

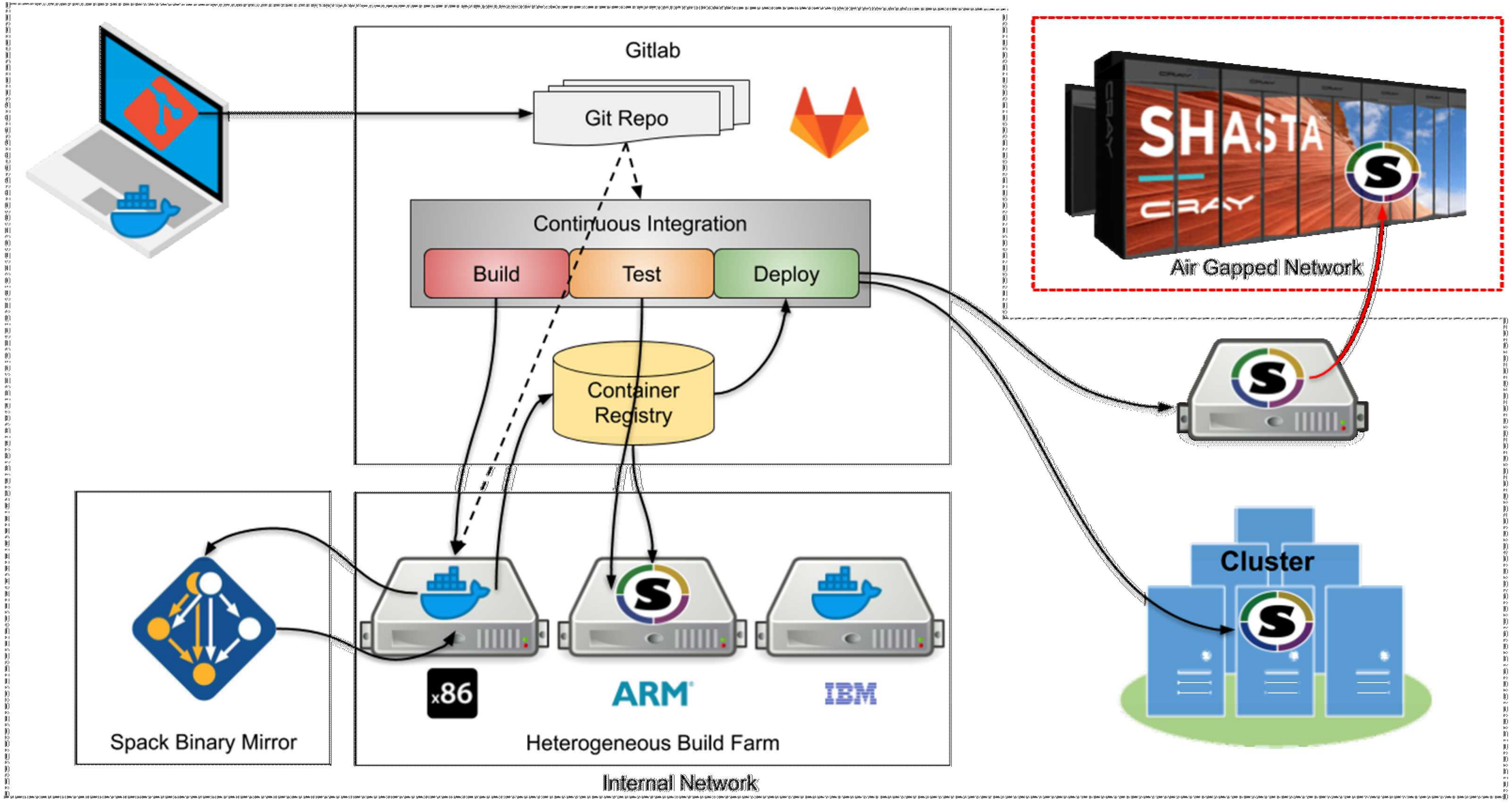
Build with docker build .

Run with Singularity (or some other tool)

Credit: Todd Gamblin (LLNL)

A Containerized CI Pipeline

- As a *developer* I want to *generate container builds from code* ~~*pull requests*~~ *releases* so that *containers are used to test & deploy new code on target HPC machines.*



Focus on OCI-spec Container Images

- Container runtime diversity does not mean diversity in container image types!
- Directed focus only on Open Container Initiative (OCI) images
- Effectively build from Docker v2.2 format
  - Uses Dockerfiles
  - Follows community-driven image conventions
- Can be *built* with several modern container runtimes
  - Docker, Podman, Buildah, …
- Can be *run* on several HPD container runtimes
  - Singularity, Shifter, Charliecloud, SARUS, …
- Can be *stored* across many DOE container registry services:
  - Gitlab, OpenShift, Harbor, …
- Allow for ECP to integrate and share containers across wider community
  - Deploy ECP software in the cloud?

OPEN CONTAINER INITIATIVE

https://github.com/opencontainers/image-spec

Custom OCI Image Labels

SHIFTER

- HPC apps require special system libraries
  - CrayMPI linked in at runtime
- Fix: Leverage OCI-compatible image LABELs
  - Insert directly in Dockerfile
  - Embedding metadata into spec
- Labels specify expectations from the host
  - HPC container runtime intercepts labels, makes appro
  - Specify MPI version, Glibc expectation, etc
- Implemented prototype solution in Shifter
- Working with OCI container community

```
FROM centos:7

LABEL org.supercontainers.mpi=mpich
LABEL org.supercontainers.glibc=2.17

RUN yum -y update && \
    yum -y install gcc make gcc-gfortran \
           gcc-c++ wget curl

RUN B=mpich.org/static/downloads && V=3.2 && \
    wget $B/$V/mpich-$V.tar.gz && \
    tar xf mpich-$V.tar.gz && \
    cd mpich-$V && \
    ./configure && \
    make && \
    make install

ADD helloworld.c /src/helloworld.c

RUN mpicc -o /bin/hello /src/helloworld.c
```

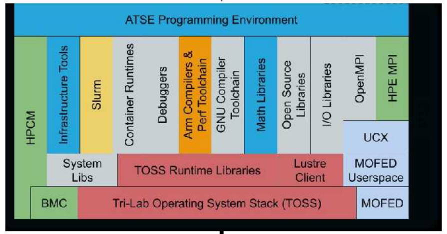
Label	Values	Comment
org.supercontainers.mpi	{mpich,openmpi}	Required MPI support, ABI compatibility
org.supercontainers.gpu	{cuda,opencl,rocm, etc}	Required GPU library support
org.supercontainers.glibc	Semantic version: XX.YY.Z	Specific version of GLIBC

Credit: Shane Canon (LBNL)

Podman for Un-privileged Container Builds

- Build containers directly on HPC nodes
  - Doing so w/ Docker requires root
  - Need user functionality for building containers
- Leverage user namespaces for _building_ containers
- Podman and Buildah to provide container builds functionality while maintaining user-level permissions
  - User namespaces
  - Set uid/gid mappers
  - TBD Overlay & FUSE for mount
- *Next: Enhanced E4S builds for ECP*

```
podman build -t "gitlab.sandia.gov/atse/astra:1.2.4" .
```




```
podman push gitlab.sandia.gov/atse/astra:1.2.4
```

```
singularity build atse-astra-1.2.4.sif docker://gitlab.sandia.gov/atse/astra:1.2.4
```


```
salloc -N 2048 && mpirun -np $NP singularity exec atse-astra-1.2.4.sif /app
```

Pedretti, Younge, et. al, *Chronicles of Astra: Challenges and Lessons from the First Petascale Arm Supercomputer* , to appear in SC20

Running Containers at scale

Petascale? Exascale?

HPC Container Runtimes

- Docker is not good fit for running HPC workloads
  - Building with Docker on my laptop is ok
  - Security issues, no HPC integration
- Several different container options in HPC

SHIFTER Charliecloud

- All 3 HPC container runtimes are usable in HPC today!
- Each runtime offers different designs and OS mechanisms
  - Storage & mgmt of images
  - User, PID, Mount namespaces
  - Security models
  - OCI vs Docker vs Singularity images
  - Image signing, validation, registries, etc

HPC container runtimes are rapidly emerging at DOE sites

ALCF
- Theta: Singularity
- Aurora: Singularity (TBD)

OLCF
- Summit: Singularity (trial)
- Frontier: Singularity (2022)

NERSC
- Cori: Shifter
- Perlmutter: Shifter or Singularity (2020)

LLNL
- Sierra/Lassen: Singularity (trial)
- Linux clusters: Singularity
- El Capitan: Singularity (2023)

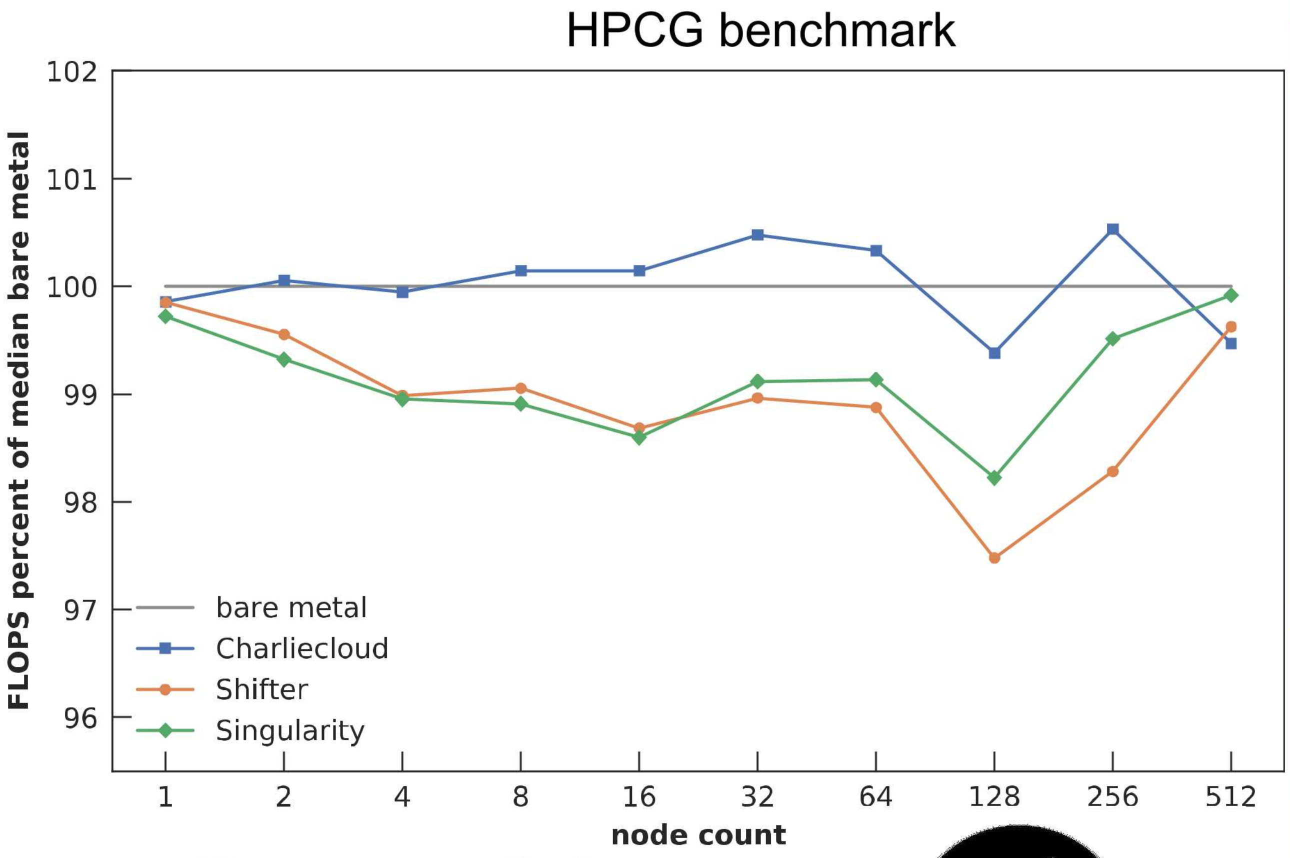
LANL
- Trinity: Charliecloud
- Linux clusters: Charliecloud
- Crossroads: Charliecloud (2021)

Sandia
- Astra: Singularity, Charliecloud, & Podma
- Linux clusters: Singularity

Many sites are rolling out container runtimes for users.
We are developing resources to facilitate consistent, performant deployment across sites.

"HPC container runtimes have minimal or no performance impact"

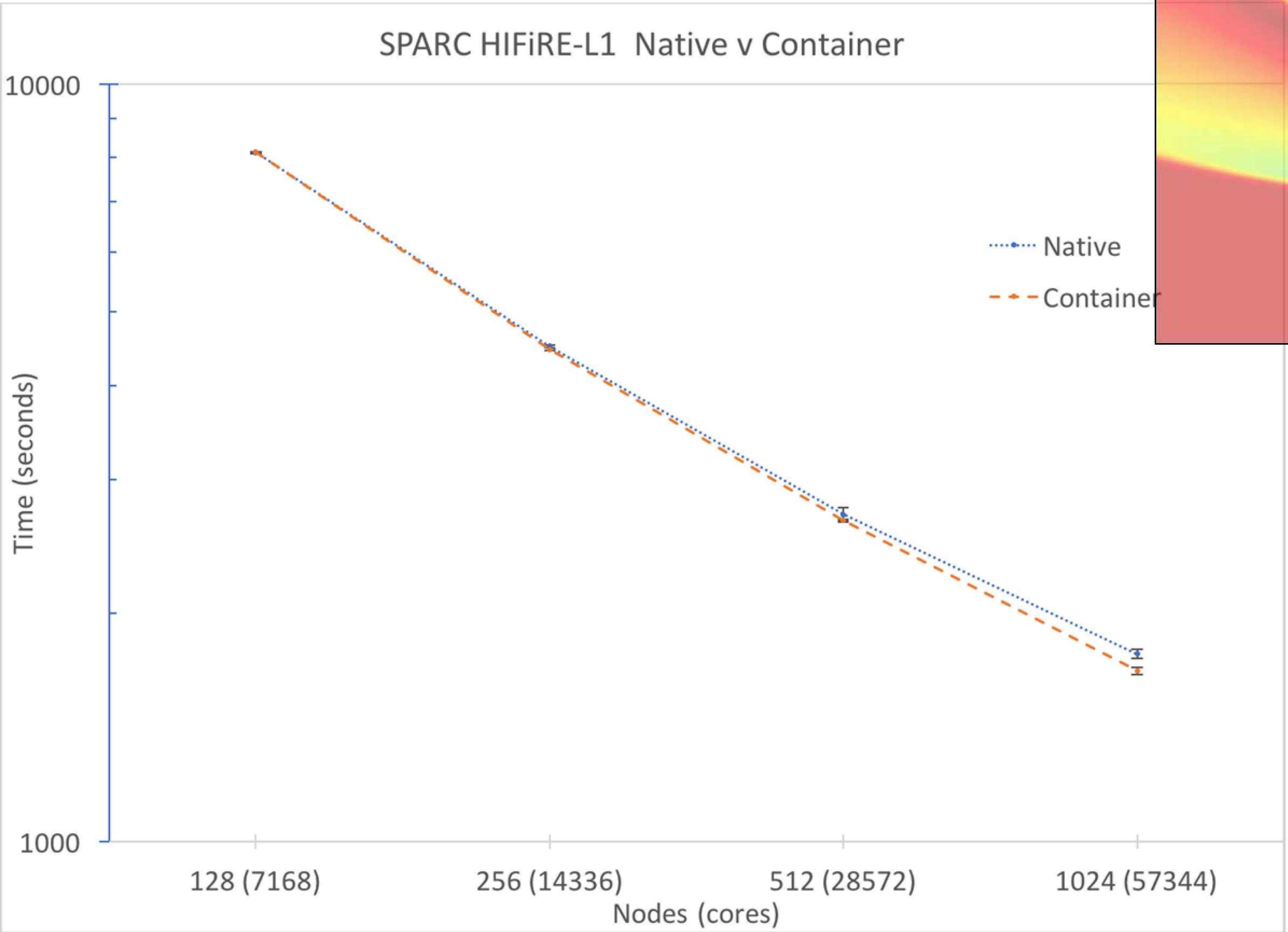
- LANL team confirms all HPC container runtimes perform well
  - Performance delta < 1% @ 512 nodes
  - "*we hypothesize that the performance impact of containerization itself is nil*."
  - Memory consumption may differ
- Pick a container runtime, any runtime!
  - More about features and experience
- Need to confirm experiments to Exascale

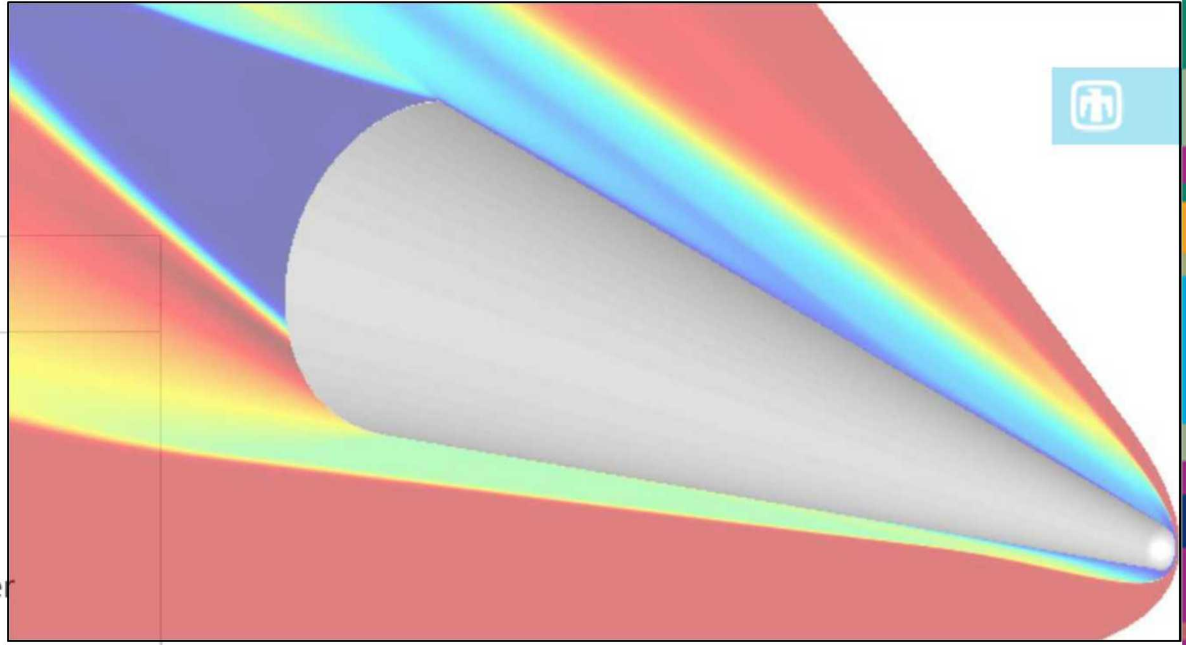


Charliecloud

From: Alfred Torrez, Tim Randles, and Reid Priedhorsky, *"HPC Container Runtimes Have Minimal or No Performance Impact"*, IEEE CANOPIE-HPC Workshop @ SC19, Nov 2019.

Case Study 1: SNL ATDM App





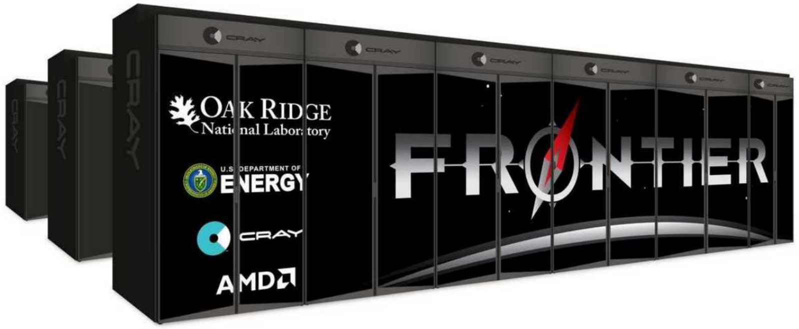
Points:

- Supporting SPARC containerized build & deployment
- Deployed on **Astra** with **Singularity**
- Near-native performance using a container
  - Container faster due to testing new optimizations for TX2
- Testing HIFiRE-1 Experiment (MacLean et al. 2008)
  - UNCLASSIFIED problem

Younge, et. al, *(U) Practice and Experience with Containers and ARM64 on Astra*, NNSA/AWE JOWOG 34

Vendor Engagement is a continual activity

- Starting working with Vendors & HW providers to enable container deployment
- Solutions must be both functional AND performant!
  - Scale is critical to success
  - Handle the growing heterogeneity in the HPC marketplace
- Working with vendors to provide optimized base container images
  - How do I build a my container to use CrayPE tools?
  - How do I use the latest GPU toolchain for my exa-app in a container?
- Enable new capabilities for controlling HPC software stack management [facilities]
  - Release testing, Rollback debugging, and cross-system software synchronization
- Fix some previous container issues moving forward
  - Can we stop runtime library hot-swapping?
  - Can we avoid `glibc` compatibility issues indefinitely?



Containers and Reproducibility?

- Reproducibility is a cornerstone of science!
  - Consistent results across studies aimed at answering the same **scientific** question
  - Critically important in conducting computational science today
- DOE/NNSA must extend the lifecycle without underground testing
- Rely on modeling and simulation apps to perform this task
  - Incorporate a multitude of physics and engineering models
  - Executed on leadership-class supercomputers
- Long-term studies take years
  - Any particular simulation may not seem important at the time
  - Later analysis may prove to demonstrate value in an old simulation
  - Need to reproduce & reevaluate runs many months or years later!
- Containerized builds can help future reproducibility efforts
- Containers alone are not the answer
  - Can be part of the solution

Conclusion

- Containers *will* be a viable software deployment model for the first Exascale platforms
- Demonstrated value of container models
  - Deployments in testbeds to production Petascale
  - Modern DevOps approach with containers useful
- Supercontainers = Container enablement at Exascale
  - Enable efficient *build* and *execution* of container images
  - Simplify HPC application development via modern DevOps
- E4S will prove-out containerized SW deployments at Exascale
  - Support next generation AI & ML apps
- Containers can increase software flexibility in HPC
- Could be the new-default mechanism for software deployment?

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Questions?

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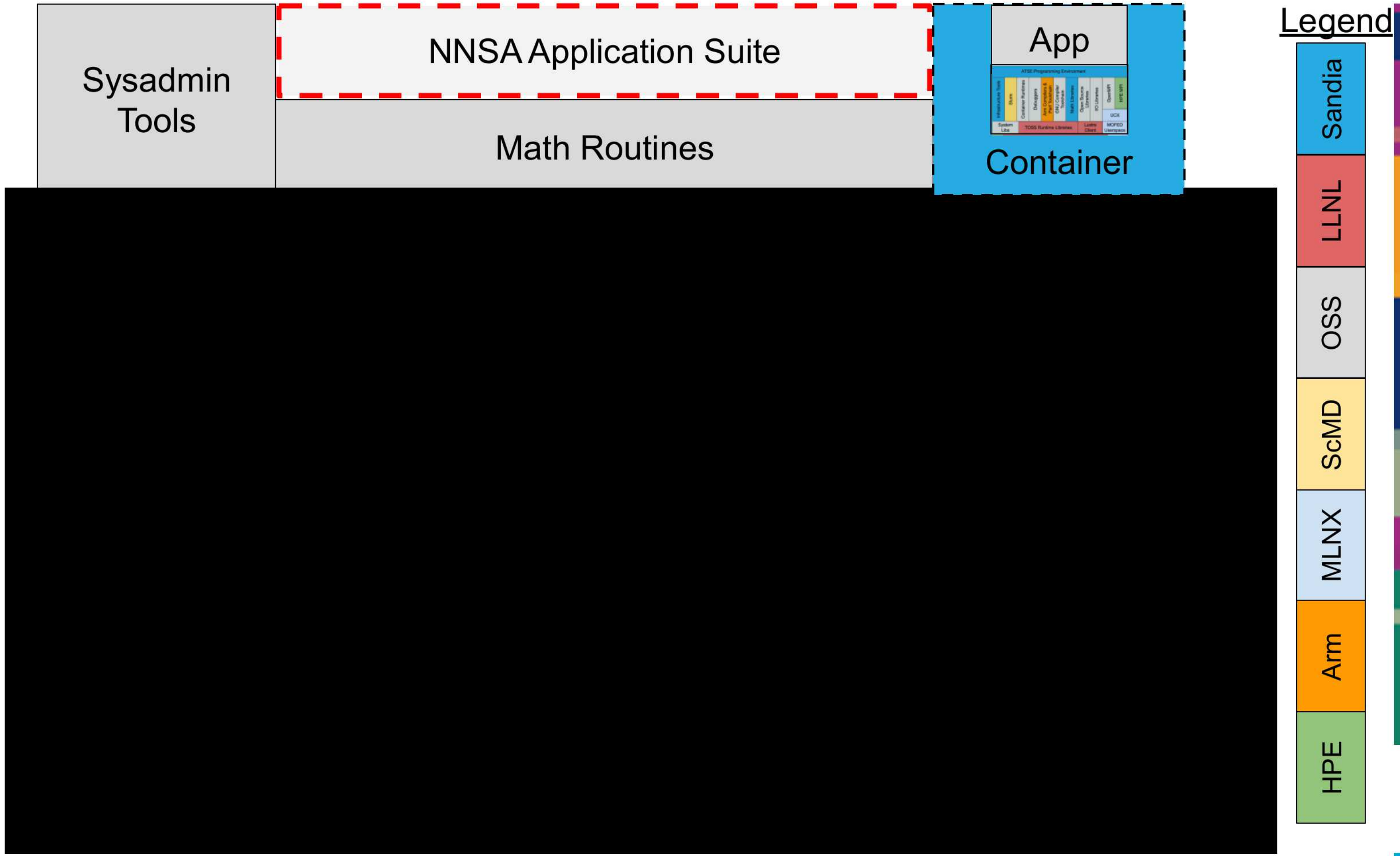
ARM SUPERCOMPUTER
ASTRA
"Per aspera ad astra"
Hewlett Packard
Enterprise
ATSE
stack
VANGUARD
2.3 PFLOPs peak
>5000 TX2 ARM CPUs, ~150k cores
885 TB/s memory bandwidth peak
332 TB memory
1.2 MW

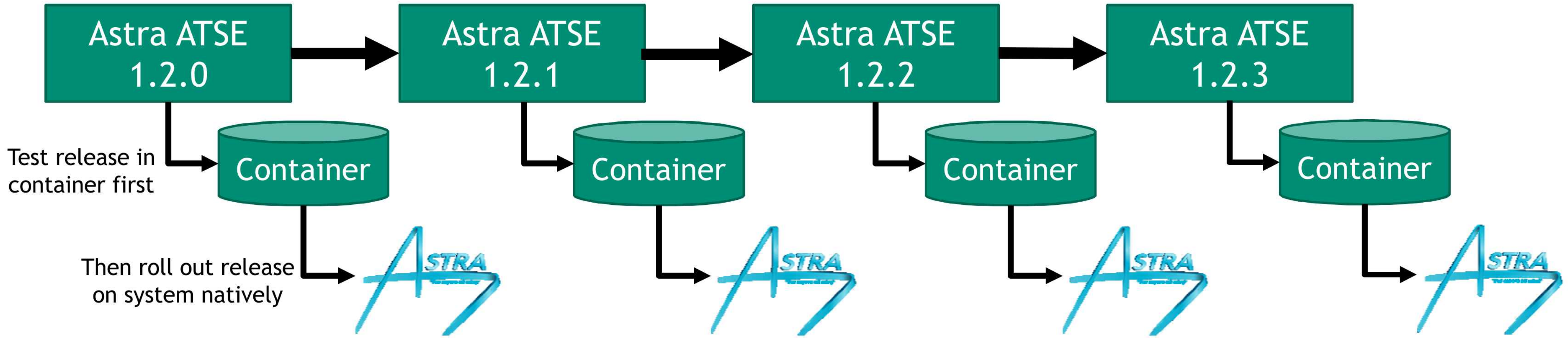
ATSE & Collaboration with HPE, OpenHPC, and ARM

- Advanced Tri-lab Software Environment = ATSE
- Many pieces to the software stack puzzle
- HPE's HPC Software Stack
  - HPE Cluster Manager
  - HPE MPI (+ XPMEM)
- Arm
  - Arm HPC Compilers
  - Arm Math Libraries
  - Allinea Tools
- Open source tools - OpenHPC
  - Slurm, OpenMPI, etc
- Mellanox-OFED & HPC-X
- RedHat 7.x for aarch64 - TOSS



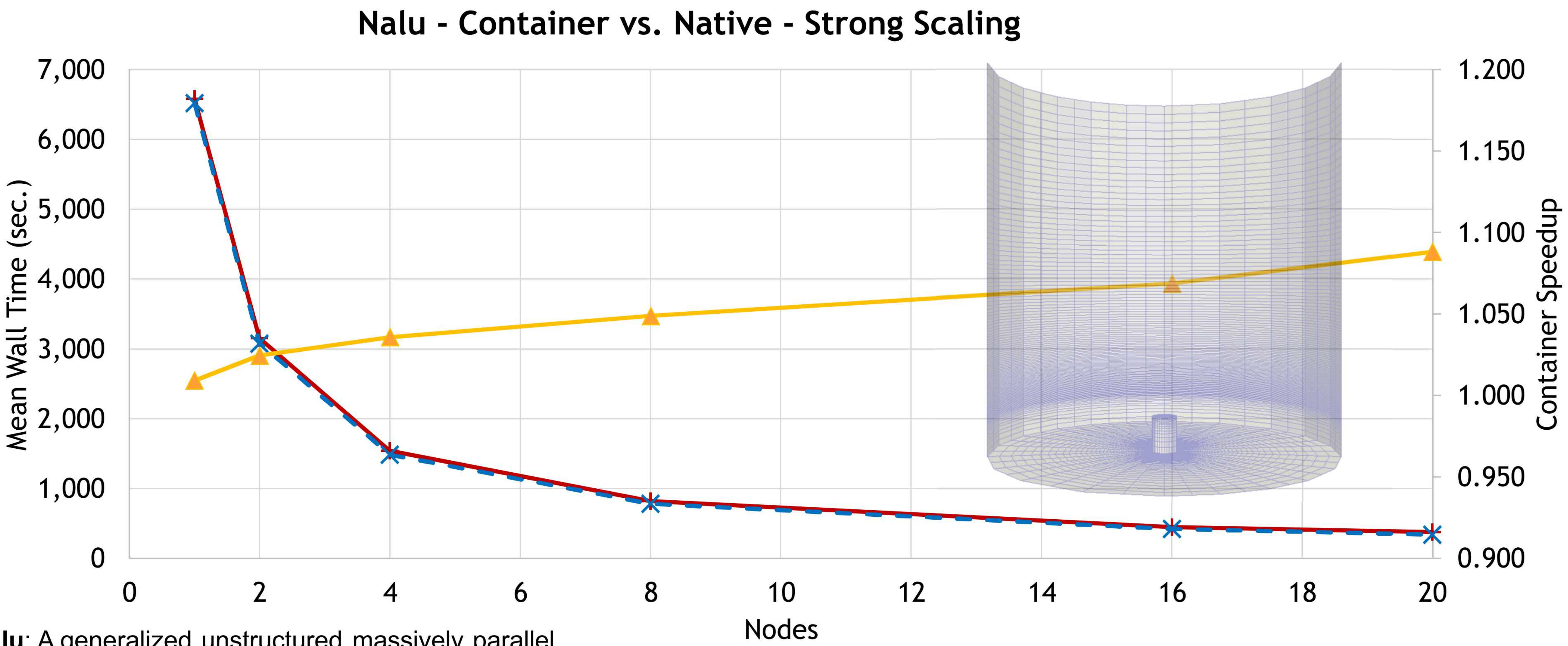
System Software Stack Testing & Debugging

- Astra ATSE programming environment release consists of:
  - TOSS base operating system + Mellanox InfiniBand stack
  - {2 compilers} * {3 mpi implementations} * {~25 libraries} = 150 packages
  - Each release packaged as a container for testing and archival purposes



- ATSE Container use cases:
  - **Release testing:** Enables full applications to be built and run at scale (2048+ nodes) before rolling out natively
  - **Rollback debug:** If issues are identified, ability to easily go back to a prior software release and test
  - **Cross-system synchronization**: Move full user-level software environments between systems. In one instance, this allowed an Astra InfiniBand library bug to be debugged off platform on another Arm cluster.

Case Study 2: Nalu CFD

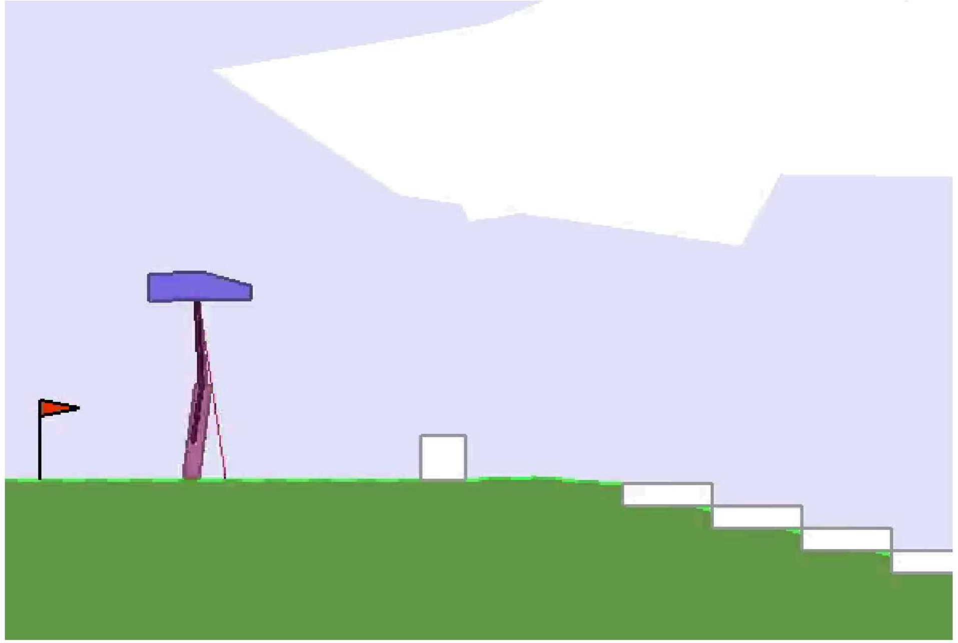


Nalu: A generalized unstructured massively parallel low Mach CFD flow code designed to support energy applications of interest

Agelastos, Younge, et. al, *(U) Quantifying Metrics to Evaluate Containers for Deployment and Usage of NNSA Production Applications,* NECDC 2018

Case Study 3: Reinforcement Learning Algorithms

- An evolutionary approach for multi-objective optimization
  - Evolutionary Algorithms are gradient-free population-based methods
  - EA benefits from parallelization and does not require GPU acceleration
    - Population of agents is generated and attempts a problem in parallel
    - High performance agents are used for next population generation
- Astra has been ideal for experimenting with EA
- We are using Astra for scaling of ASTool
  - Coevolves an agent's decision making policy and body
- Built Singularity container
  - Ubuntu 16.04, NumPy, PyBullet, …
  - Simple to use and modify
- 500 nodes - 7.5 hours



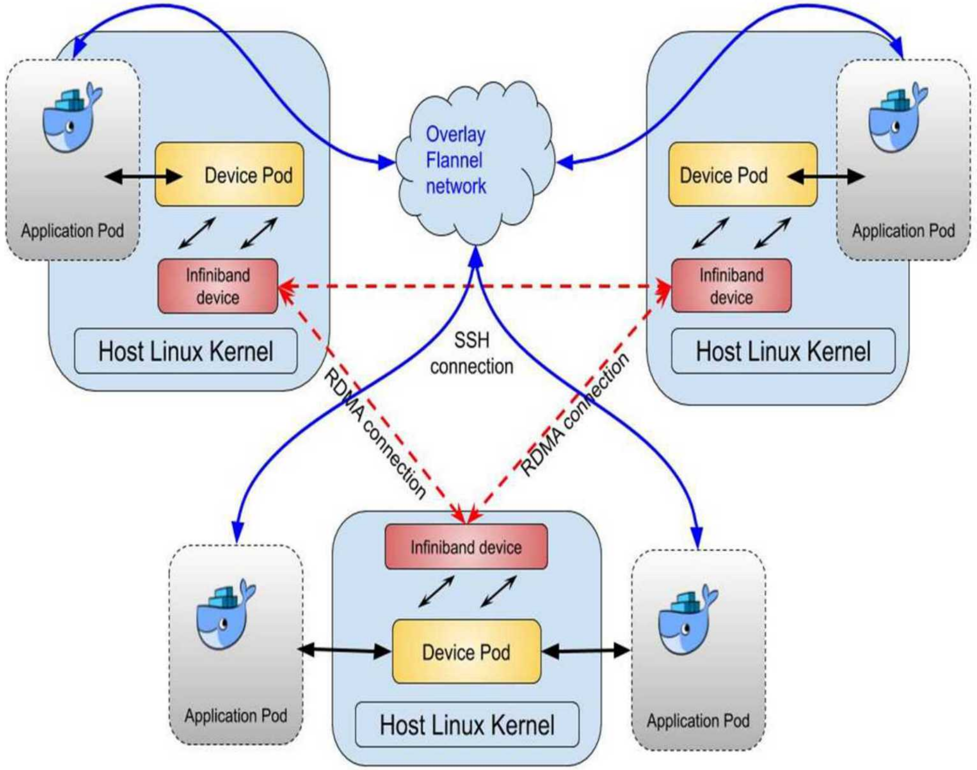
Credit: https://designrl.github.io/

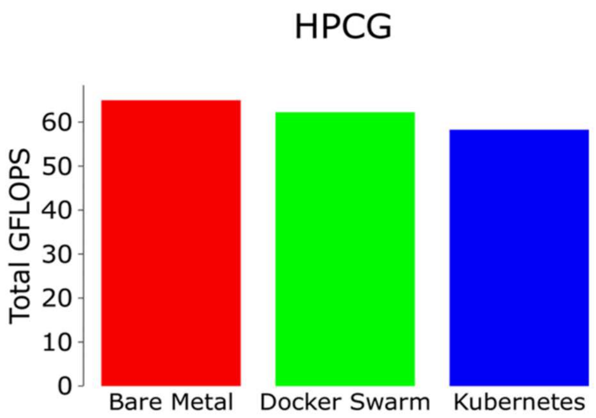
Takeaway: Containers help support Emerging HPC workloads like Reinforcement Learning

Kubernetes is coming…

kubernetes

- Containers are changing the software ecosystem for application deployment
- Container orchestration tools are now mainstream
  - VERY different than traditional HPC
  - No batch job scheduler, no jobs, just services and and orchestrator
- **Study Opportunities container orchestration frameworks in HPC**
  - Performance, Usability, and Constraints
- Orchestration and batch?
  - Separate solutions deployed today
  - Orchestration _and_ batch!

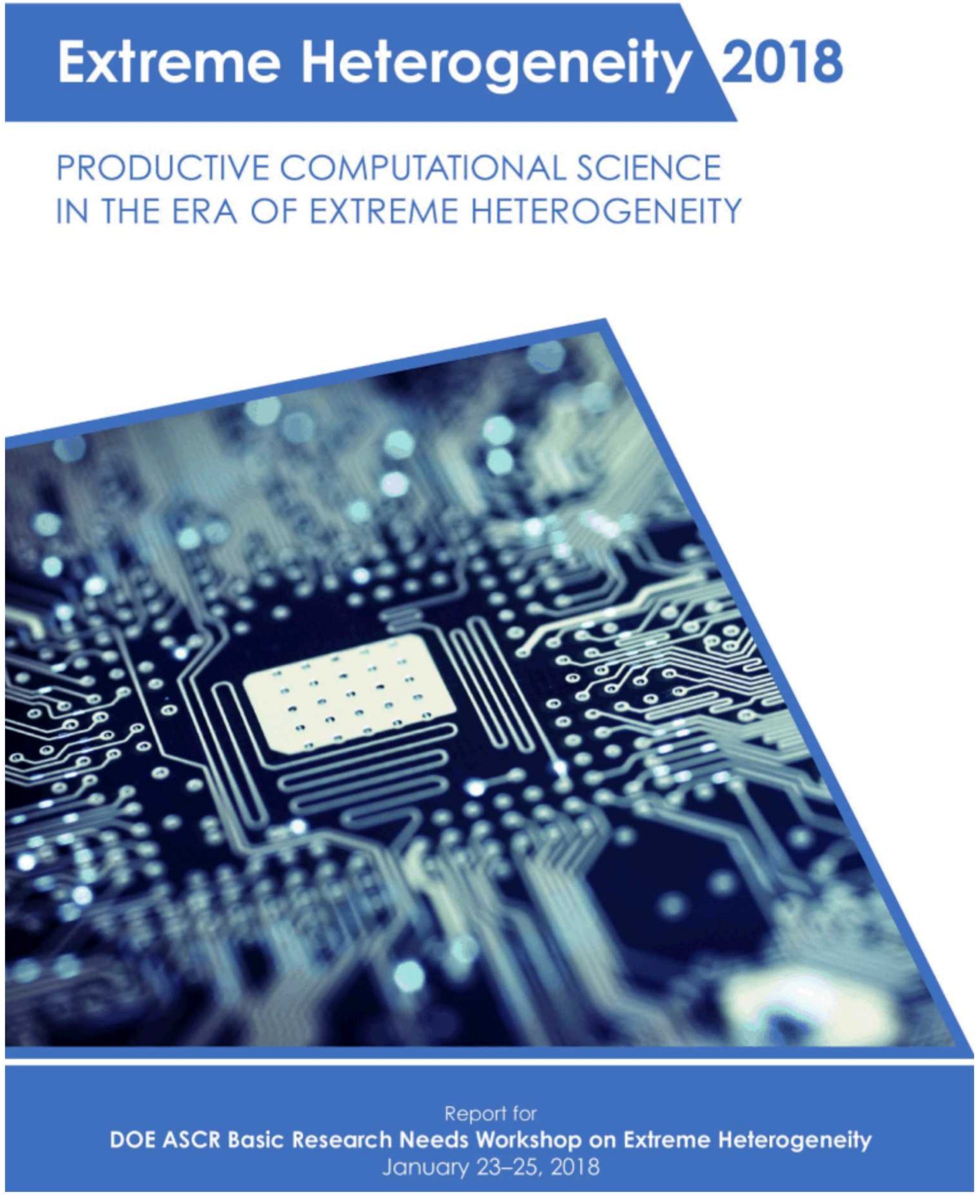




Credit: Angel Beltre (Binghamton University)

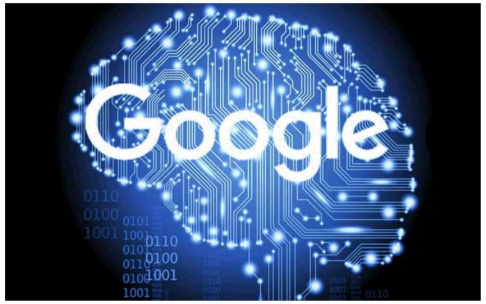
Position 1: Heterogeneity is the Future of HPC…

- HPC workloads are becoming more diverse
  - It's not just BSP simulations any more
  - Data is a cornerstone in ML, analytics, …
- And HPC hardware will be more diverse
  - "Era of predictable [hardware] improvements is ending."
  - Expecting custom aggregated components at the system level
- How will system software cope and support system-level heterogeneity?
  - How will programmers be efficient in such a landscape?
  - Will abstractions help or hinder performance?
- We need more APIs…



Position 2: … and so is the Cloud

- The hyperscalers are finally paying attention to HPC
  - *"The physical network topology does affect performance; particularly important is the performance of MPI Allreduce, grouped by splitting the mesh by a subset of the dimensions, which can be very efficient [5] [6] if each such group is physically connected."* – Shazeer et al Google Brain, Mesh-TensorFlow: Deep Learning for Supercomputers.
  - As learning techniques grow in scale, HPC becomes more important.



- HPC cannot compete with the hyperscalers
  - Let's stop trying and start *integrating*
    - *That doesn't mean adopting Cloud as-is*
    - *That doesn't dissolving HPC either*
  - The closer HPC and cloud paradigms get, the better we all are
    - Encourage open source infrastructure
    - Collaborative partnerships
  - Avoid boutique solutions without sacrificing performance