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Building and Running HPC Containers across the US Department of Energy

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ECP **Supercontainers** activity as Packaging Technologies

- 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

There is a 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

HPC Container Runtimes today

- Docker is not good fit for running HPC workloads
  - Building with Docker on my laptop is ok!
  - Deployment issues: Security, scheduler integration, etc
- Several different container runtime options in HPC
- All our 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
  - Image signing, validation, registries, etc
- New tools emerging for rootless container *builds* as well!

Supercontainers investments in HPC container runtimes

Charliecloud

- multi-stage unprivileged build (0.19)
- fool distribution tools into thinking they're privileged (0.20)
- push to image repositories (0.22)
- architecture-aware pull (0.24)
- automatically make SSH secrets available to build (0.25)
- mount SquashFS images at runtime using FUSE (0.26, upcoming)

Singularity => Apptainer

- HPCng project renamed to Apptainer
- Managing ongoing fork issues in community
- Security fixes and bugfixes ongoing

Shifter

- Initial scalable container launch for Perlmutter
- Further integration with Podman being explored
- Bugfixes and registry compatibility upgrades

Podman

- Developing MOU Red Hat with DOE labs
- Rootless Podman builds on HPC login nodes
- Enabling SIF image support (Singularity compatibility)
- Investigating scalable launch of OCI images
  - Leveraging Shifter's squashfs experience
- Native overlay support

SUPERCONTAINERS

Container runtimes on different DOE systems

ALCF
- Theta: Singularity
- Aurora: Singularity

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

NERSC
- Cori: Shifter
- Perlmutter: Shifter & Podman

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

LANL
- Trinity: Charliecloud
- Linux clusters: Charliecloud
- Crossroads: Charliecloud

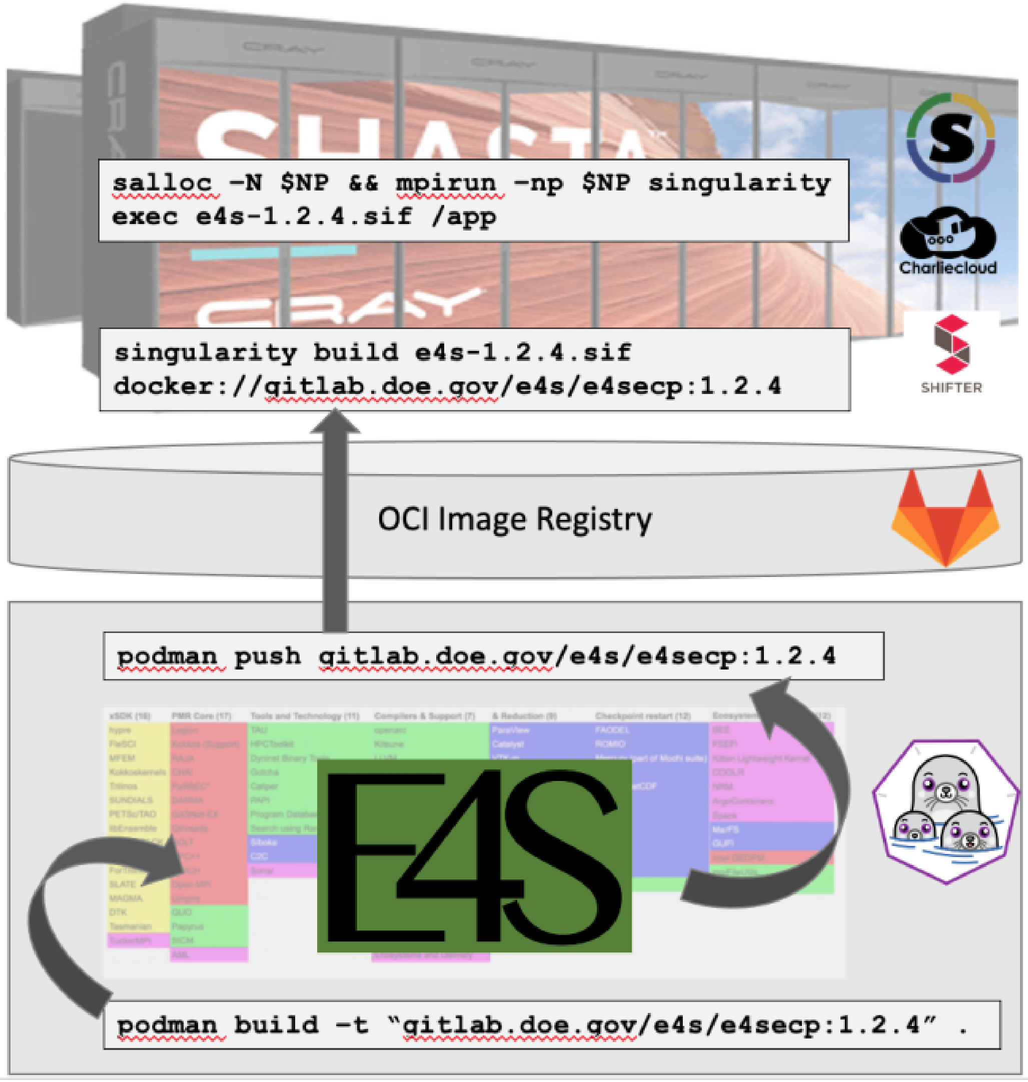
Sandia
- Astra: Singularity, Charliecloud, & Podman
- Linux clusters: Singularity & Podman

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

But what about *building* containers for HPC??

Supercontainers created two HPC build solutions: Podman & Charliecloud

- Podman/Buildah provide container build functionality through low privilege
  - UID/GID mappers with shadow-utils
  - Overlay & FUSE for mount operations
- Charliecloud for fully unprivileged build with single UID/GID mapping to UID0
  - Simpler setup, remains entirely unprivileged
  - Requires `fakeroot` injection in container
- Both implementations prototyped and working
- Next Steps
  - Enable E4S container builds directly on DOE/ECP resources
  - Integrate with CI activities & DevOps
- Able to work with facilities to help roll out new capability



Supercontainers team leading container build technologies

New taxonomy of container privilege levels

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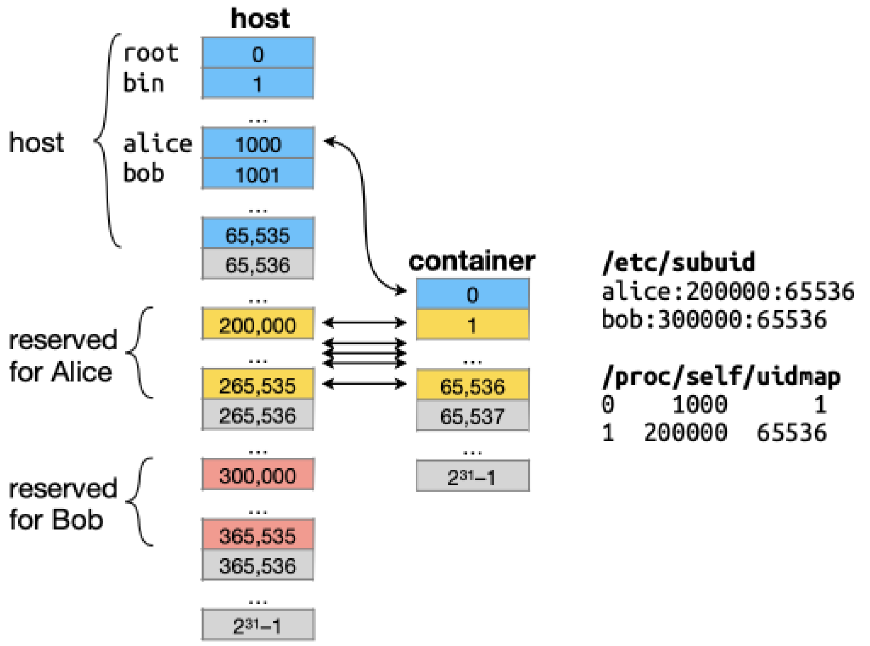
type	namespaces	setup	IDs in container	examples
I	mount	privileged	UIDs and GIDs shared with host	docker, podman, SHIFTER
II	mount + privileged user	privileged	arbitrary UIDs and GIDs separate from host (but pitfalls)	docker, podman
III	mount + unprivileged user	unprivileged	host EUID & EGID aliased (supplemental GIDs partially functional)	Charliecloud, podman

HPC-focused

only Type III containers are fully unprivileged throughout the container lifetime



Example of Type II user namespace mapping used by container runtimes

From: Reid Priedhorsky, Shane Canon, Tim Randles, and Andrew Younge, Minimizing privilege for building HPC containers, in SC '21: Proceedings of the International Conference for High Performance Computing, Networking, Storage and Analysis, Nov 2021.

Podman – in – Podman for containerized CI

- Many DOE codes use Gitlab for developing HPC applications
- Need to leverage Continuous Development and Continuous Integration capabilities
  - {build,test,deploy} HPC apps in containers
  - Automatic building container images
- Gitlab CI has git-lab runners, but expect elevated privileges
- Solution: **Podman-in-Podman**
  - The gitlab runner built in a OCI container image
  - Run Rootless Podman to have gitlab-runner think it has root privs
  - Gitlab-runner auto-starts a container build within the 1st container
  - Push resulting container to Gitlab container registry
- Simplified container build & deploy infrastructure with Gitlab
- Solution appliable to SNL as well as greater DOE infrastructure
  - Future integration with DOE Jacamar runners

Extreme-scale Scientific Software Stack (E4S)

- E4S: HPC Software Ecosystem – a curated software portfolio
- A **Spack-based** distribution of software tested for interoperability and portability to multiple architectures
- Available from **source**, **containers**, **cloud, binary caches**
- Leverages and enhances SDK interoperability thrust
- Not a commercial product – an open resource for all
- E4S over time:

• Oct 2018:	E4S 0.1	24 full, 24 partial release products
• Jan 2019:	E4S 0.2	37 full, 10 partial release products
• Nov 2019:	E4S 1.0	50 full, 5 partial release products
• Feb 2020:	E4S 1.1	61 full release products
• Nov 2020:	E4S 20.10	67 full release products
• Feb 2021:	E4S 21.02	67 full release, 4 partial release
• May 2021:	E4S 21.05	76 full release products
– Aug 2021:	E4S 21.08	88 full release products
– **Nov 2021:**	E4S 21.11	91 **full release products**

https://e4s.io

Lead: Sameer Shende (U Oregon)

Also include other products .e.g.,
AI: PyTorch, TensorFlow (CUDA, ROCm)
Co-Design: AMReX, Cabana, MFEM

Our strategy is to focus on Exascale systems

- **We aim to leverage the new containerized PE to enable CI for these environments.**
  - We are experimenting with containerized builds for the Cray environment
- **We have worked with HPE/Cray to enable Spack to autodetect PE components**
  - Metadata for Spack now ships with the PE itself, can be automatically used via spack install --reuse
- **GPU integration across the stack will be an ongoing focus**
  - We are improving our compiler and GPU support model – compiler interoperability is a major focus
- **We aim to have a distribution of *optimized* Spack binaries for these systems by the end of ECP**
  - Spack will work on Exascale systems out of the box
- **We will also have optimized container images that can use these binaries**
  - Users will be able to construct images from E4S packages on demand, run optimized on exascale machines