udocker

Part 1 - Introduction

https://github.com/indigo-dc/udocker

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Scientific Computing Challenges I

Running applications across infrastructures often requires considerable effort

- **Heterogeneous Hardware**:
  - Several computing systems
  - Laptops, Desktops, Farms, Cloud, HPC
- **Multiple OSes and distributions**:
  - Several operating systems
  - Linux flavors, Distribution versions

Scientific Computing Challenges II

- **Software Environments**:
  - Specific computing environments.
  - Compilers, Libraries, Customizations, Drivers etc.
- **Applications**:
  - Multiple software codes often combined.
- **Issues**:
  - Portability, Maintainability, Reproducibility.

Using containers for applications I

Encapsulation:

- Applications, dependencies, configurations everything packed together.
- Enables portability across heterogeneous Linux systems.
- Easier distribution and sharing of ready to use software.

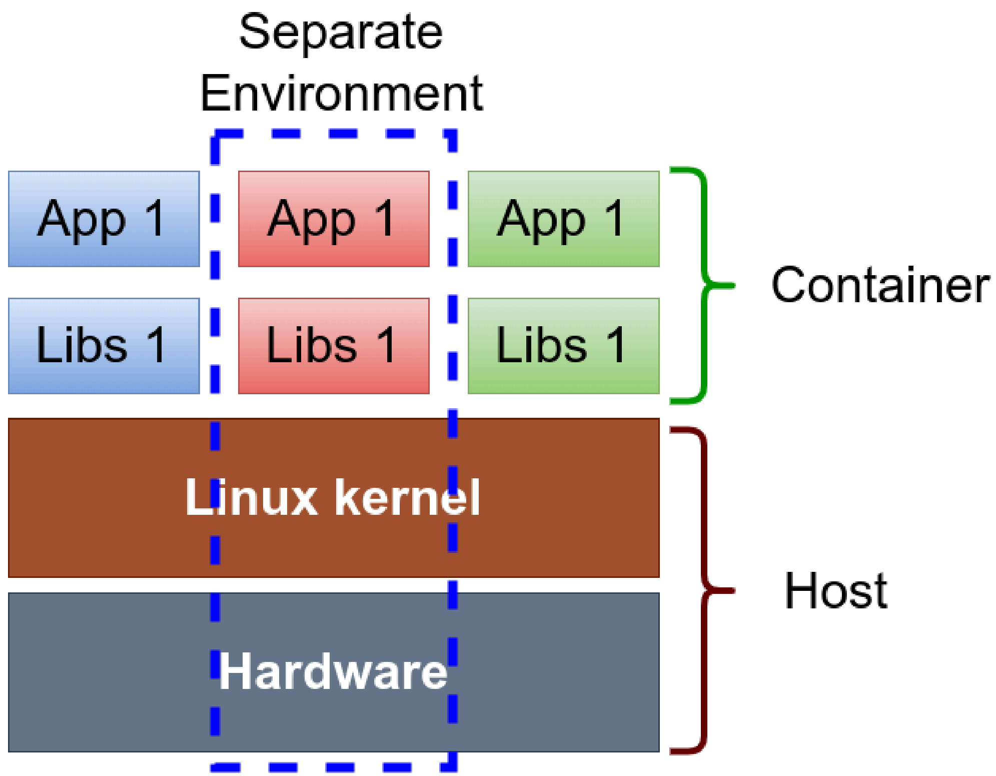
Efficiency:

- One single kernel, buffers etc shared by many applications.
- Performance and resource consumption similar to host execution.
- Take advantage of newer more optimized libraries and compilers.

Using containers for applications II

Reproducibility:

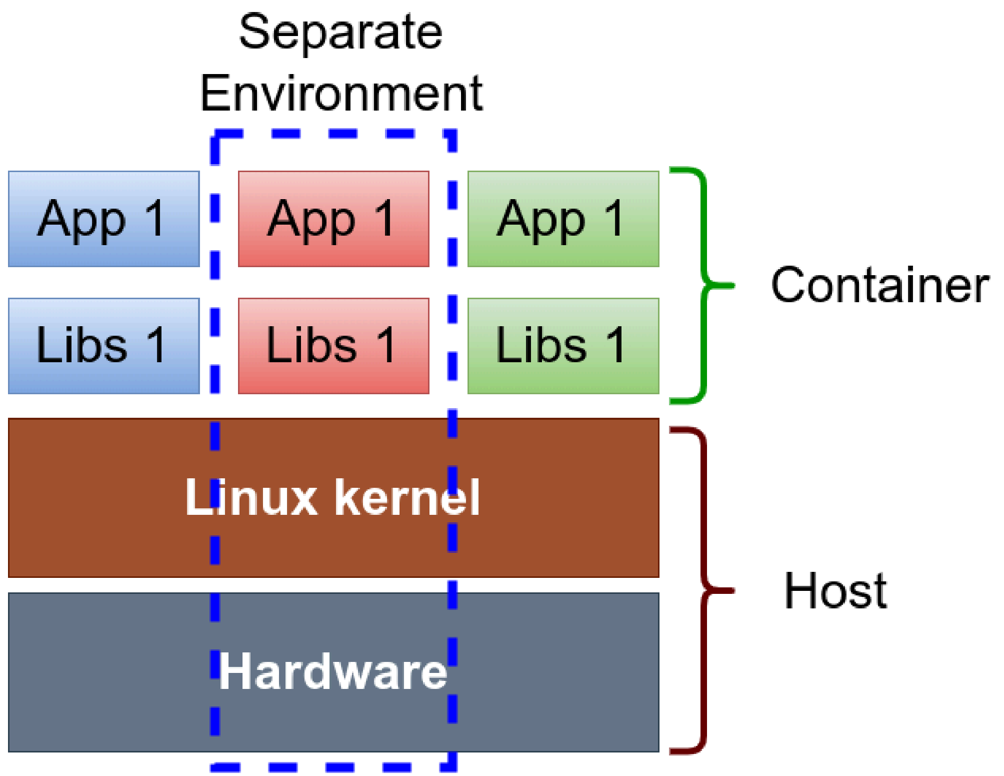
- The whole application and run-time environment is in the container.
- Can be easily stored for later replay, reuse and preservation.



Using containers for applications III

Maintainability:

- Easier application maintenance, distribution and deployment.
- No need to support applications across multiple OS distributions.
- Independance from software changes at the host level.



`udocker` - origin

- Need for a consistent portable way of running applications.
  - Running applications across different distributions and run-time environments.
- `udocker` began to be developed in 2015 in the Indigo-DataCloud project.
  - Proof of concept for running docker containers as a regular user.
- Focused on running scientific applications in Linux systems.
  - Batch or Interactive, HTC or HPC, across sites in grid infrastructures.

Containers for batch processing - I

- Challenges of running containers (docker) on batch systems:
  - Integration with the batch system (how to start/stop containers, etc.).
  - Respect batch system policies (such as quotas, time and resource limits).
  - Respect batch system actions (job management integration delete/kill).
  - Collect accounting (tight integration).

Containers for batch processing - II

- Can we execute in a more simple way?
  - Can we download container images (for instance, from Dockerhub or other registries)?
  - Can we run without a layered filesystem?
  - Can we run without namespaces?
  - Can we run without other complex kernel functionalities ?
  - Can we run as a regular user without privileges?

Containers for batch processing - III

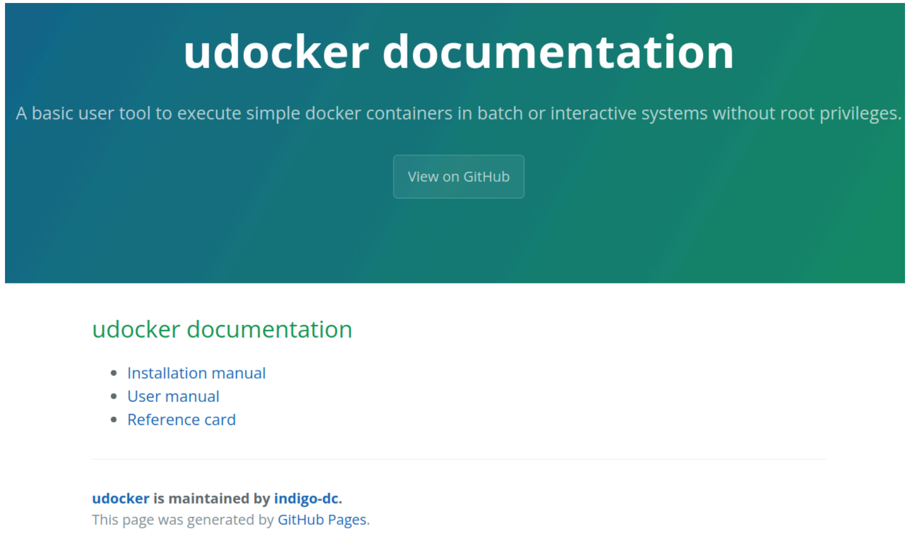
- When `udocker` started to be developed these were major limitations:
  - Now other tools can also address, at least partially, some of these issues.
    - singularity/apptainer, podman etc..
  - Yet they depend on kernel functionalities, that may not be available everywhere.

`udocker`: Introduction - I

- `udocker` can run applications encapsulated in docker containers **Without**:
  - Using docker.
  - Requiring (root) privileges.
  - System administrators intervention.
  - Additional system software.
  - Requiring Linux namespaces.
- Everything runs in user space:
  - As a regular user without privileges.
  - Subjected to the normal process controls and accounting.
  - Both in interactive or batch systems.

`udocker`: Introduction - II

- `udocker` is open source.
- Developed under the Indigo-Datacloud, DEEP Hybrid-Datacloud, EOSC-Synergy, BigHPC
  and DT-Geo projects.
- Github repository: https://github.com/indigo-dc/udocker.
- Documentation: https://indigo-dc.github.io/udocker/.



`udocker` advantages: Deployment I

- `udocker` is meant to be deployed and used by the end-user:
  - Does not require root privileges.
  - Does not require system administrator intervention.
  - All operations can be performed in user space and in user accessible directories.
  - Deployed by default in the user `$HOME` directory.
  - Containers are in the user `$HOME` directory or other user chosen location.

`udocker` advantages: Deployment II

- `udocker` does not require compilation by the user:
  - Written in Python plus some binaries.
  - Has a minimal set of dependencies.
  - Required binaries are provided statically compiled.
- `udocker` deployment:
  - Just copy and untar into the user `$HOME` directory.
  - Ideal to execute containers across different sites and types of resources and infrastructures.
  - You can deploy `udocker` on the system where you run.

`udocker` advantages: Execution I

- `udocker` integrates several execution engines:
  - Allows execution using multiple different approaches.
  - Allows execution with and without using Linux namespaces.
  - Integrates several tools suitable to execute containers.
  - Makes these tools easier to use across systems.
- `udocker` can be submitted together with a batch job:
  - (Just fetch or ship the `udocker` tarball with the job.)

`udocker` advantages: Execution II

- `udocker` user interface:
  - Commands, syntax and logic are similar or even the same as docker CLI.
- `udocker` empowers users to use containers:
  - Ideal for heterogeneous computing environments.

`udocker`: Command Line Interface

`udocker` is mainly a run-time to execute docker containers:

clone	export	help	images	import
inspect	install	load	login	logout
mkrepo	name	protect	ps	pull
rm	rmi	rmname	search	setup
showconf	unprotect	verify	version	create
run	save			

By design `udocker` does not have container creation functionality. Containers can be created with other tools.

`udocker` : How does it work...

Programing languages and OS

- `udocker` is implemented:
  - Python
- the engines and other tools shipped with `udocker` are binaries:
  - C , C++, go
- Can run:
  - CentOS 7, RHEL8, RHEL9 (compatible distros)
  - Ubuntu >= 16.04
  - Any distro that supports python 2.7 and >= 3.6

Components - I

- The `udocker` Python code (this is what you need to fetch)
  - Command line interface.
  - Dockerhub API.
  - Container and image handling: import, load, save and export.
  - Local images repository.
  - Interface with the execution engines.

Components - II

- `udocker` tools:
  - Pulled and installed upon first invocation of `udocker`.
  - Set of binary executables and libraries that implement the engines.
  - Supporting different OSes and hardware architectures.
  - Executables: proot (Pn), runc (Rn), crun (Rn) and patchelf (Fn).
  - Libraries: fakechroot (Fn).

`udocker` in 4 steps - I

Step 1 - Installation:

- Get the `udocker` tarball using `curl`, `wget` or a browser.
- Extract the content of the tarball.
- No need to compile software.
- The first time `udocker` is run it will fetch the required binaries.

`udocker` in 4 steps - II

Step 2 - Get container images:

- Pull containers from docker compatible repositories.:
  - `udocker pull`
- Load and save in docker and OCI formats:
  - `udocker load`
  - `udocker save`
- Import and export tarballs:
  - `udocker import`
  - `udocker export`

`udocker` in 4 steps - III

Step 3 - Create from images:

- Create the container directory tree from the image:
  - `udocker create`

Step 4 - Execute containers:

- Run using several execution methods:
  - `udocker run`

`udocker` in 4 steps - IV

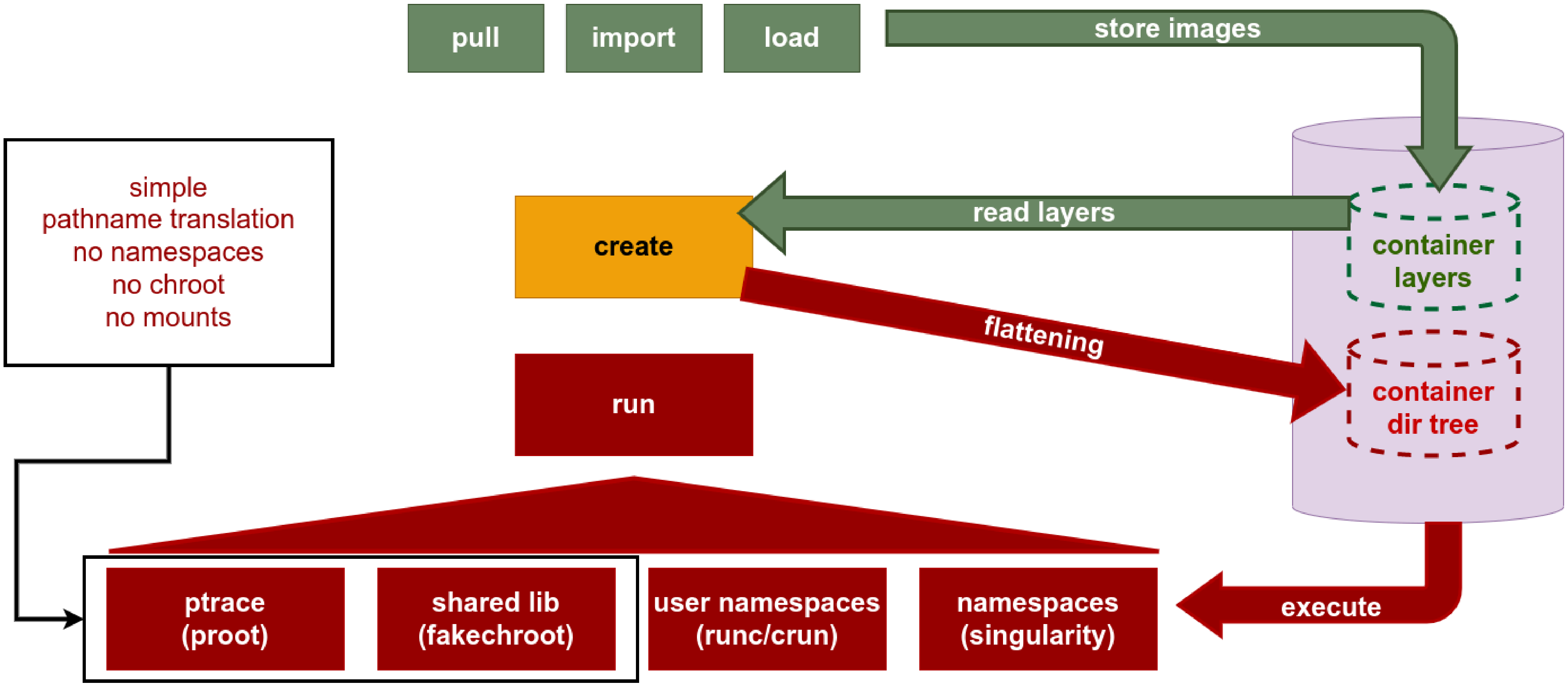
The steps to fetch and execute containers are important:

- `udocker pull <IMAGE>`
- `udocker create <IMAGE>`
- `udocker run <CONTAINER-ID-OR-NAME>`
- `udocker run <CONTAINER-ID-OR-NAME>`
- `udocker run <CONTAINER-ID-OR-NAME>`

The created container can be run as many times as you wish.

- You may call `udocker run` directly but this will create a new CONTAINER every-time.
- Will be slow and occupy much more space.

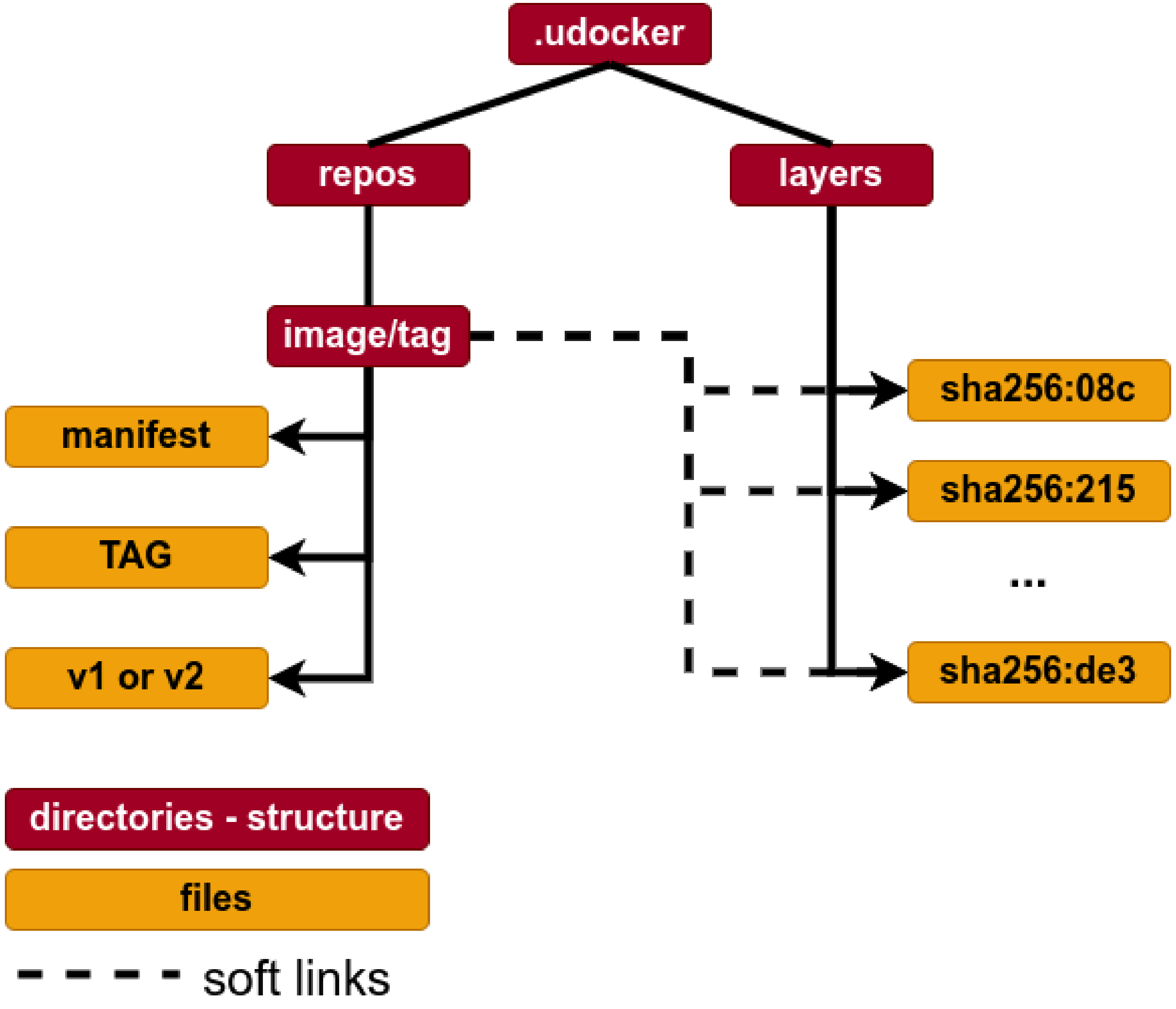
udocker is an integration tool



`udocker` : pull - Images I

- Docker images are composed of:
  - Metadata describing the images content and how to run.
  - Multiple file-system layers stored as tarballs.
- `udocker` pulls the metadata and layers:
  - Using the DockerHub REST API.
  - Image metadata is parsed to identify the layers.
  - Layers are stored in the user home directory under `${UDOCKER_DIR}/.udocker/layers`
  - Image information with links to the layers is under `${UDOCKER_DIR}/.udocker/repos`

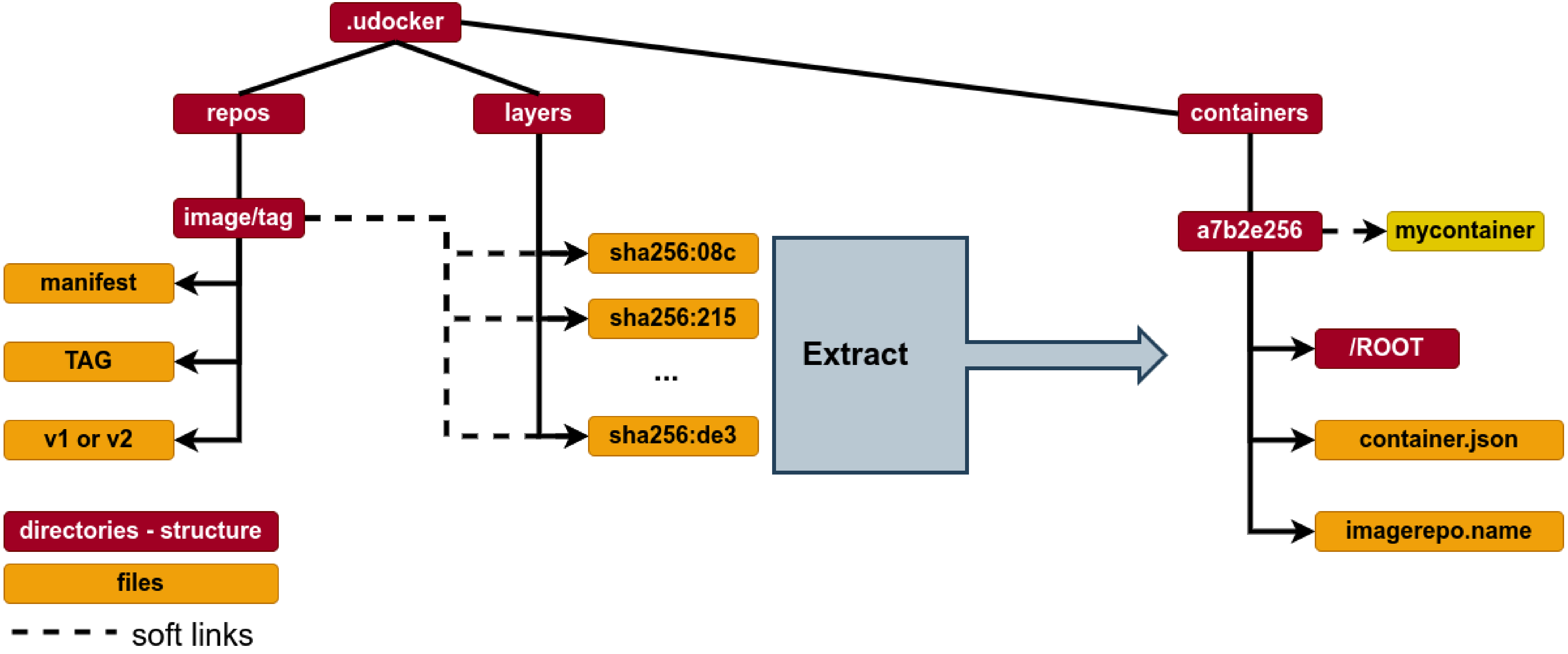
udocker : pull - Images II



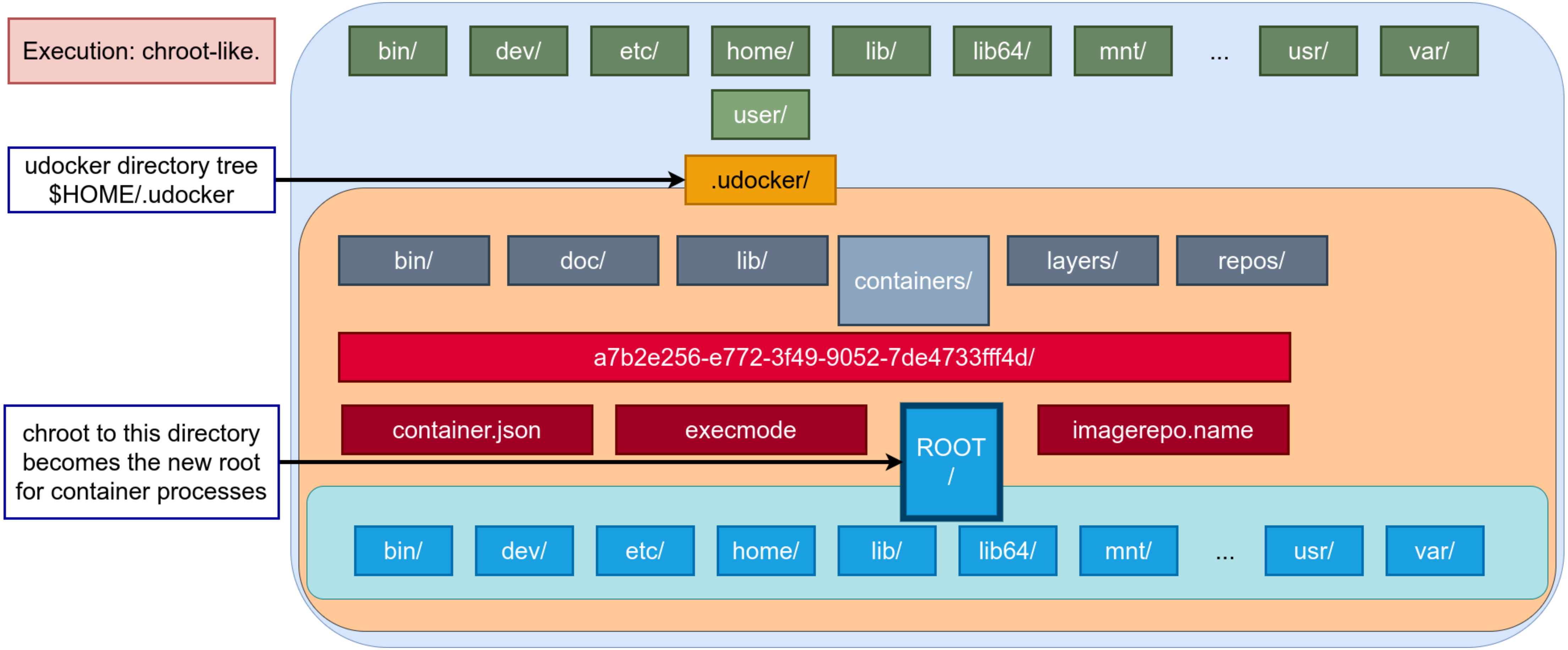
`udocker`: Create containers - I

- Containers are produced from the images in a process called flattening.
  - Each image layer is extracted on top of the previous.
  - UnionFS Whiteouts are applied before each layer extraction.
  - Protection changes are applied to make files accessible.
  - The resulting directory tree is stored under `${UDOCKER_DIR}/.udocker/containers`
- Accessing files is easy:
  - just cd into `${UDOCKER_DIR}/.udocker/containers/CONTAINER-ID/ROOT`.
- The creation can be slow depending on underlying filesystem (e.g. Lustre, GPFS):
  - Alternative use the /tmp or some partition local to the host.

udocker : Create containers - II



udocker : Run container



`udocker`: Execution engines I

- Like in other container tools execution is achieved by providing `chroot` like functionality.
- `udocker` supports several techniques to achieve the equivalent to a `chroot` without using privileges.
- These techniques can be selected per container via execution modes implemented by execution engines.

udocker: Execution engines II

Mode	Base	Description
P1	PRoot	PTRACE accelerated (with SECCOMP filtering): *DEFAULT*
P2	PRoot	PTRACE non-accelerated (without SECCOMP filtering)
R1	runC	rootless unprivileged using user namespaces
R2	runC	rootless unprivileged using user namespaces + P1
R3	runC	rootless unprivileged using user namespaces + P2
F1	Fakechroot	with loader as argument and LD_LIBRARY_PATH
F2	Fakechroot	with modified loader, loader as argument and LD_LIBRARY_PATH
F3	Fakechroot	modified loader and ELF headers of binaries + libs changed
F4	Fakechroot	modified loader and ELF headers dynamically changed
S1	Singularity	where locally installed using chroot or user namespaces

Selection in terms of performance

Mode	Base	Description
P1	PRoot	System call intensive applications may suffer degradation
P2	PRoot	Same limitations as P1 apply. All system calls are traced causing higher overheads than P1
R1	runC	Same performance as namespace based applications
R2	runC	Only for software installation and similar. Same performance as P1
R3	runC	Only for software installation and similar. Same performance as P2
F1	Fakechroot	All Fn modes have similar performance during execution. Frequently the Fn modes are the fastest
F2	Fakechroot	Same as F1
F3	Fakechroot	Same as F1. Setup can be very slow
F4	Fakechroot	Same as F1. Setup can be very slow
S1	Singularity	Similar to Rn

Selection in terms of interoperability I

Mode	Base	Description
P1	PRoot	PTRACE + SECCOMP requires kernel >= 3.5. Can fall back to P2 if SECCOMP is unavailable
P2	PRoot	Runs across a wide range of kernels even old ones. Can run with kernels and libraries that would fail with kernel too old
R1	runC	User namespace limitations apply
R2	runC	User namespace limitations apply. Same limitations as P1 also apply, this is a nested mode P1 over R
R3	runC	User namespace limitations apply. Same limitations as P2 also apply, this is a nested mode P2 over R

Selection in terms of interoperability II

Mode	Base	Description
F1	Fakechroot	May escape and load host libraries. Requires shared library compiled against same libc as in container
F2	Fakechroot	Same as F1
F3	Fakechroot	Requires shared library compiled against same libc as in container. Binary executables and libraries get tied to the user HOME pathname
F4	Fakechroot	Same as F3. Executables and libraries can be compiled or added dynamically
S1	Singularity	Not part of `udocker` must already exist on the system, may use user namespaces or chroot

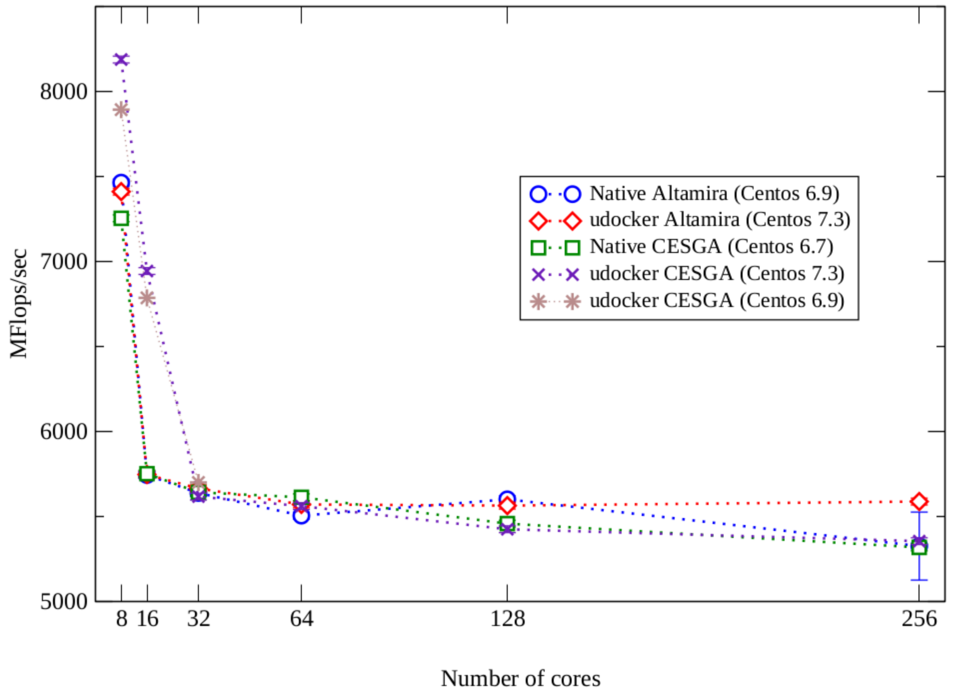
`udocker` : Running applications ...

udocker & Lattice QCD

OpenQCD is a very advanced code to run lattice simulations.

Scaling performance as a function of the cores for the computation of application of the Dirac operator to a spinor field.

Using OpenMPI, `udocker` in P1 mode.

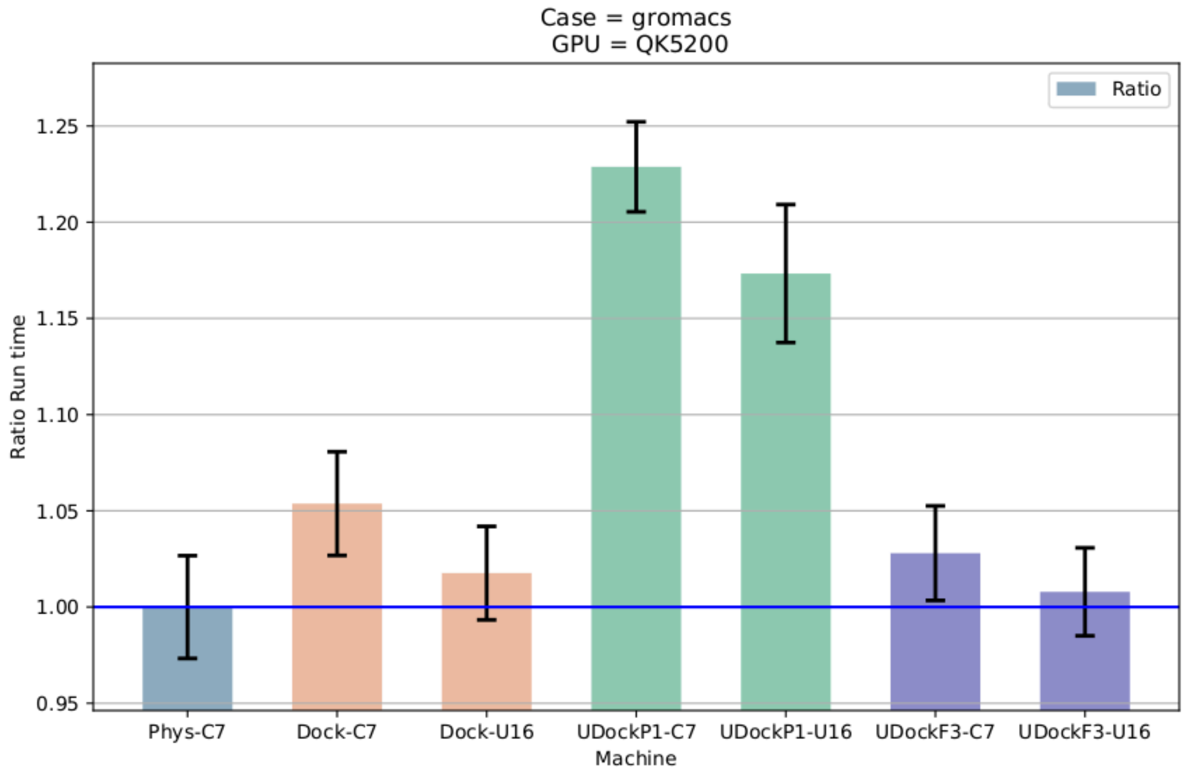


`udocker` & Molecular dynamics

Gromacs is widely used both in biochemical and non-biochemical systems.

In this comparison Gromacs was run using CUDA and OpenMP:

- `udocker` using P mode has lower performance with Gromacs.
- `udocker` using F mode has same or better performance as Docker.



`udocker` & Phenomenology I

MasterCode connects several complex codes:

- Hard to deploy.
- Scanning through large parameter spaces.
- High Throughput Computing.
- C++, Fortran, many authors, legacy code.

udocker & Phenomenology II

Performance Degradation (*udocker in P1 mode*)

Environment	Compiling	Running
HOST	0%	0%
DOCKER	10%	1.0%
udocker	7%	1.3%
VirtualBox	15%	1.6%
KVM	5%	2.6%

Thank you!

Questions ?

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Backup slides

Other container technologies

- Singularity/Apptainer (LBL) https://apptainer.org/ - `udocker` currently supports it as execution mode.
- Charliecloud (LANL) https://charliecloud.io/.
- Shifter (NERSC) https://docs.nersc.gov/development/containers/shifter/how-to-use/.
- Podman (RedHat) https://www.redhat.com/en/topics/containers/what-is-podman.