

## UDOCKER

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# Scientific computing and containers

Running applications across infrastructures may require considerable effort

#### Computers

- Several computing systems
- Laptops, Desktops, Farms, Cloud, HPC

#### OSes

- Several operating systems
- Linux flavors, Distribution versions

#### Environments

- Specific computing environments
- Compilers, Libraries, Customizations

#### Applications

- Multiple applications often combined
- > Portability, Maintainability, Reproducibility



#### Need a consistent portable way of running applications



## **Containers for batch processing**



- Challenges of batch systems?
  - Integrate it with the batch system (how to start/stop etc)?
  - Respect batch system policies (such as quotas/limits) ?
  - Respect batch system actions (job delete/kill) ?
  - Collect accounting ?
- Can we execute in a more basic way?
  - Can we download container images ?
  - Can we run without a layered filesystem ?
  - Can we run them as normal user ?
  - Can we still enforce container metadata ?





### udocker



- Run applications encapsulated in docker containers:
  - without using docker
  - without using (root) privileges
  - without system administrators intervention
  - without additional system software
  - Does not require Linux namespaces
- Run:
  - as a normal user
  - with the normal process controls and accounting
  - in interactive or batch systems
  - does not run as a service (for that use containerd)







# udocker How does it work ...









#### udocker is open source Developed under the Indigo-Datacloud and DEEP Hybrid-Datacloud projects

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

- https://github.com/indigo-dc/udocker/tree/master
- https://github.com/indigo-dc/udocker/tree/devel

#### **Documentation:**

https://github.com/indigo-dc/udocker/tree/master/doc







### udocker



- Run time to execute docker containers:
  - search
  - pull
  - images
  - create
  - rmi
  - ps
  - rm
  - run
  - login
  - logout



- load
- save
- import
- export
- setup
- clone
- verify
- Inspect
- mkrepo





# udocker How it was implemented ...





#### udocker



- Implemented
  - python, C, C++, go
- Can run:
  - CentOS 6, CentOS 7, Fedora >= 23
  - Ubuntu 14.04, Ubuntu 16.04
  - Any distro that supports python 2.6 and 2.7

#### Components:

- Command line interface docker like
- Pull of containers from Docker Hub
- Local repository of images and containers
- Execution of containers with modular engines





## udocker: run - Container

Computing



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## udocker: Execution engines



- udocker supports several techniques to achieve the equivalent to a chroot without using privileges
  - They are selected per container id via execution modes

| Base                       | Description   |
|----------------------------|---|
| PRoot                      | PTRACE accelerated (with SECCOMP filtering)  DEFAULT  |
| PRoot                      | PTRACE non-accelerated (without SECCOMP filtering)  |
| runC                       | rootless unprivileged using user namespaces   |
| Fakechroot                 | with loader as argument and LD_LIBRARY_PATH   |
| Fakechroot                 | with modified loader, loader as argument and LD_LIBRARY_PATH  |
| Fakechroot                 | modified loader and ELF headers of binaries + libs changed  |
| Fakechroot                 | modified loader and ELF headers dynamically changed   |
| Singularity                | where locally installed using chroot or user namespaces   |
| F<br>F<br>F<br>F<br>F<br>F | Base<br>PRoot<br>PRoot<br>PRoot<br>CunC<br>Fakechroot<br>Fakechroot<br>Fakechroot<br>Fakechroot<br>Fakechroot<br>Fakechroot<br>Fakechroot |







# udocker benchmarking





## udocker & Molecular dynamics





Computing

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

udocker P mode have lower performance udocker F mode same as Docker.

Using CUDA and OpenMP

udocker in P1 mode udocker in F3 mode



# udocker & Phenomenology



#### **Performance Degradation**

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

MasterCode connects several complex codes. Hard to deploy.

Scanning through large parameter spaces. High Throughput Computing

C++, Fortran, many authors,

#### udocker in P1 mode







# udocker Next ...





## udocker: What's next



- Ongoing:
  - <u>https://github.com/indigo-dc/udocker/tree/devel3</u>
  - Modularization of udocker (and unit tests)
  - Porting to Python3
  - pip install <u>https://pypi.org</u>





## udocker: What's next



- Next
  - Increase automation for MPI/infiniband applications
    - OpenMPI and MPICH
  - Better translation of "volume" directories
  - Command line interface enhancements
  - Improve root emulation









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





