Container technology for phenomenology tools: the `udocker` middleware suite

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INDIGO - DataCloud

28 November 2017
11th Annual Helmholtz Alliance Workshop on “Physics at the Terascale”
DESY, Hamburg

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Based on Gomes J. et al [1711.01758]

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Outline

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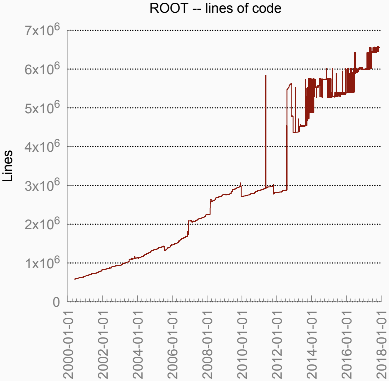
Motivations

- Complexity of phenomenology codes has risen consistently in the past years.
- Three drivers:
  1. (Precise) physics at the LHC requires sophisticated simulations.
  2. Large data set and complex analyses.
  3. Study of complex models of fundamental physics beyond the Standard Model.



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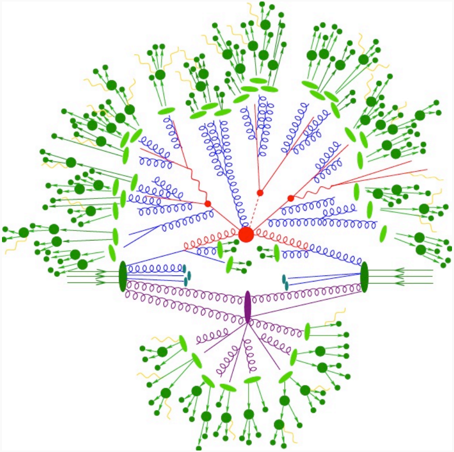

[SHERPA]

Examples

- Analysis (e.g. ROOT).
- Monte Carlo frameworks such as Madgraph_aMC@NLO, SHERPA, POWHEG-BOX, Whizard ...
- Lattice QCD computations.
- Global likelihood studies of BSM models (e.g. MasterCode, GAMBIT) ...
- Beyond HEP: molecular dynamics.

...

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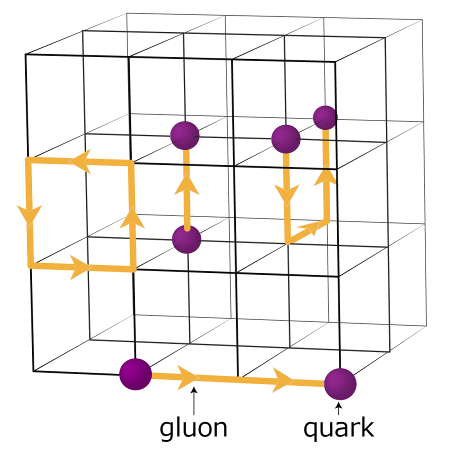

[Home page of G. Kossu]

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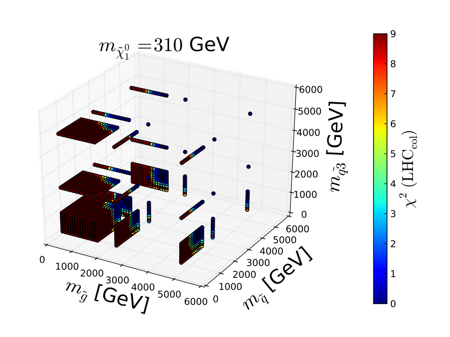

[MasterCode, 1504.03260]

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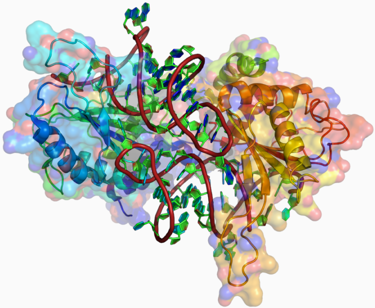

[Gromacs, courtesy of R. Capelli]

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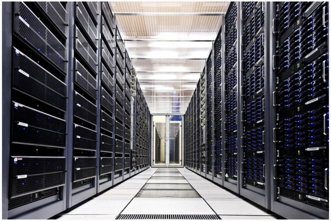
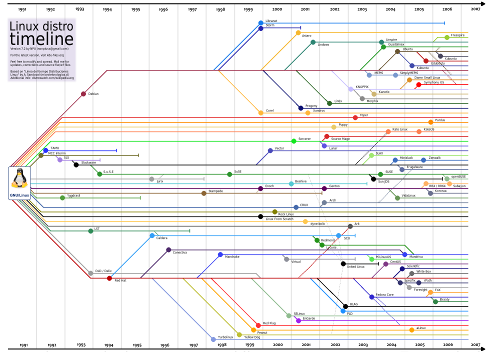
Deployment issues

Deployment issues

- Complexity means that these codes have a lot dependencies.
- Heterogeneous batch clusters.
- Large collaborations run at different sites.

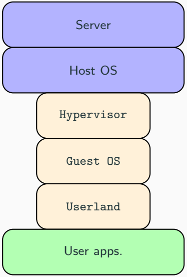




Possible solutions

Virtual machines

- *Emulation* of a full computer system.
- Many different hypervisors exist today: `KVM`, `VirtualBox`, `XEN` etc.



Operating-system level virtualization

- Old idea, e.g. `chroot`, `FreeBSD` ($>$ 4.0) `jails`.
- Linux containers: cgroups ($>$ 2.6.24), namespace support ($>$ 2.4.19).

Advantages over VMs

- Lightweight approach to virtualization (less resource hungry, more running in parallel on a single host).
- `Linux container`: easy to deploy on recent `Linux` systems (kernel version $>$ 3.8).

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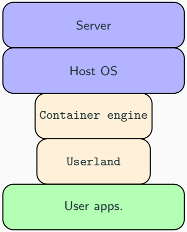

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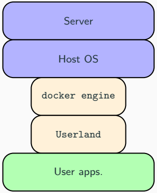
Docker containers and the udocker suite

Docker and udocker

- As suggested by the name, `udocker` uses `docker` containers.
- `Docker`: software framework to automatize the deployment of application inside Linux containers.
- Other options, such as `LXC`, are available to use the Linux container infrastructure.



- Middleware suite developed in the context of the `INDIGO data-cloud` project to run `docker` containers in userspace, without requiring root privileges (both for installation and execution).

Udocker inner workings

Features

- udocker pre-compiled code and the containers are download to ${UDOCKER_DIR}, by default ${HOME}/.udocker.
- Docker layered FS is UnionFS based. Images are pulled by downloading the corresponding layers and metadata (docker Hub REST API).
- udocker implements parsing of docker container and of a subset of metadata.
- Different execution engines: PTRACE, LD_PRELOAD, runC, Singularity.
- Tested with GPGPU and MPI aware applications.

PTRACE engine

- Implements through PRoot.
- PRoot uses PTRACE to change the pathnames dynamically and to execute the binary transparently inside the container (P2 mode).
- Patches have been written to make SECCOMP works with PTRACE (P1 mode).

Mode	Description	Changes container
P1	PRoot+SECCOMP	No
P2	PRoot	No

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LD_PRELOAD engine

- Based on the Fakechroot library.
- Implemented several workarounds to address Fakechroot shortcomings and to avoid letting the containerized application load system libraries.
- Modified version of PatchELF to perform the modifications of the binaries.

Mode	Description	Changes container
F1	exec w/ direct loader	symlinks
F2	F1 + mod. loader	F1+ld.so
F3	ELF header mod.	F2+ELF headers
F4	F3 + new execs and libs	as F3

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RunC engine

- Support for unprivileged User Namespace and rootless container using RunC.
- udocker performs the translation between docker metadata and cli args and the OCI specs to run the container in unprivileged mode.

Singularity

- Support running singularity containers.

Mode	Description	Changes container
R1	rootless usermod namesp.	resolv,passwd
S1	singularity	passwd

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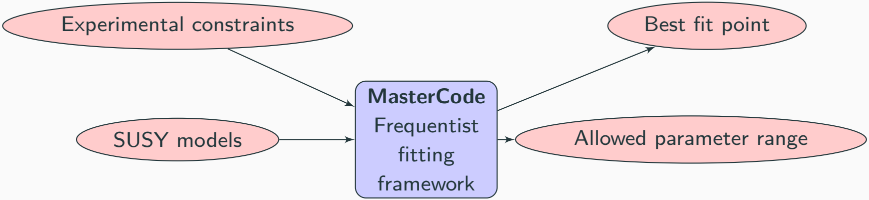
Complex libraries dependencies: `MasterCode`

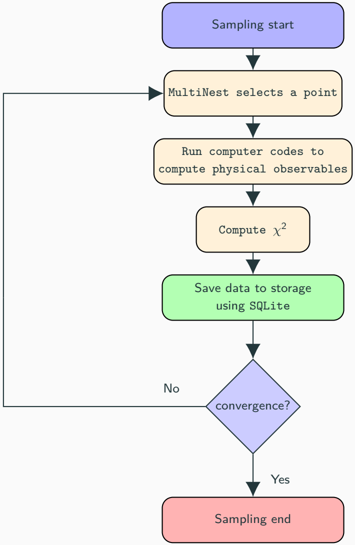
MasterCode

Global likelihood studies of BSM models

- Mixed collaboration of experimentalists and theorists to understand the status of BSM models in light of current constraints.
- Use of the available collider data, electro-weak precision observables and DM constraint to fit the best value and the likelihood profile of the model parameters.
- See my talk in the BSM-session this morning for our latest pMSSM study.



Structure of the framework


Sampling start
MultiNest selects a point
Run computer codes to compute physical observables
Compute χ^2
Save data to storage using SQLite
convergence?
No
Yes
Sampling end

Codes

Spectrum generation
SoftSUSY
Higgs sector and $(g-2)_\mu$
FeynHiggs, HiggsSignals, HiggsBounds
B-Physics
SuFla, SuperISO
EW precision observables
FeynWZ
Dark matter
MicrOMEGAs, SSARD

- During our last study, we sampled a total of 2×10^9 points.
- We thank DESY for the resources provided by the NAF2/BIRD cluster.

Running MasterCode with (u)docker

- Due to its complex structure, MasterCode is a perfect test case to show the advantages of using containerization to ease the deployment.
- We have built a docker container to support MasterCode.

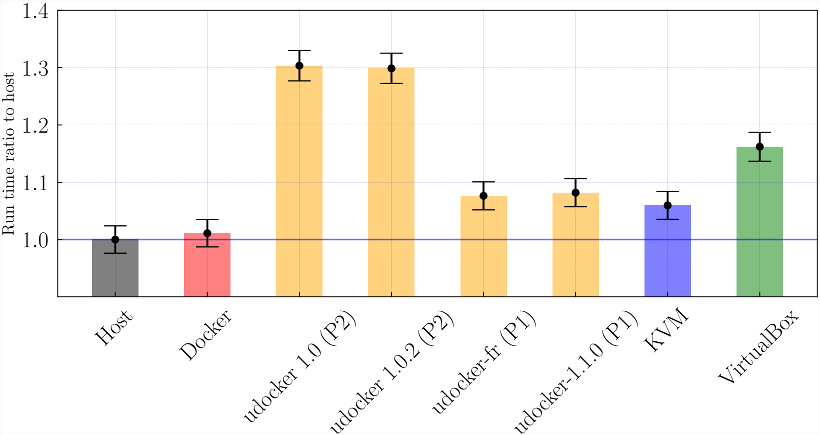
Docker

```
emanuele [0]> docker pull \
 indigodatacloud/docker-mastercode

emanuele [0]> docker run -t -i \
 -v ${HOME} \
 -w ${HOME}/my_mc_dir \
indigodatacloud/docker-mastercode \
 /bin/bash
```

udocker

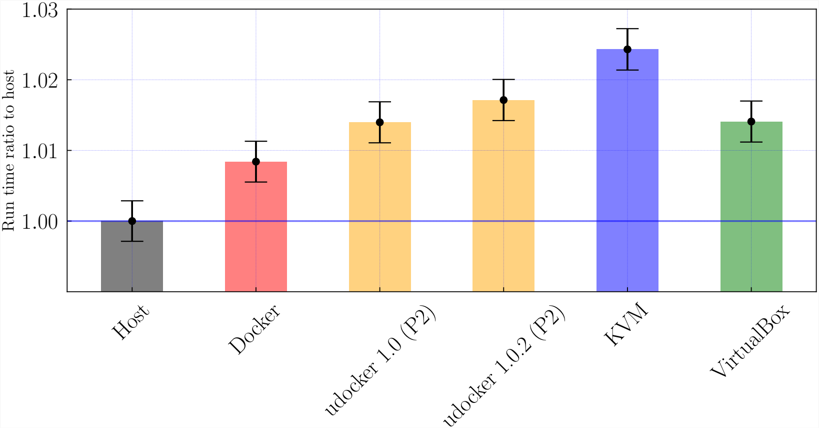
```
emanuele [0]> git clone \
 https://github.com/indigo-dc/udocker.git

emanuele [0]> cd udocker.git

emanuele [0]> ./udocker.py \
 pull indigodatacloud/docker-mastercode

emanuele [0]> ./udocker.py \
 create indigodatacloud/docker-mastercode

emanuele [0]> ./udocker.py \
-v /home/emanuele/mastercode \
-w /home/emanuele/mastercode \
'/bin/bash -c "run_mastercode_container.sh"'
```

Benchmarking: compilation



- P2 (PTRACE) mode slower by about 30% w.r.t. to host. Expected, since compilation implies a lot of syscalls.
- The PTRACE mode with SECCOMP filtering (P1 – the default) improves a lot the situation, making udocker as fast as the VMs.

Benchmarking: sampling



- The sampling phase is characterized by less I/O activity.
- `udocker` close to `docker` performances, only $\mathcal{O}(1.5\%)$ performance hit even in P2 mode.

MPI simulations: `OpenQCD`

MPI simulations: Open QCD

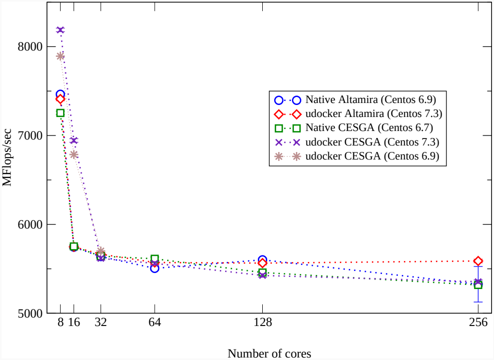
- Lattice QCD is a strongly computing-characterized discipline (hundreds of millions of CPU hours/year).
- Current simulations run spread over thousands of processor cores in parallel.
- OpenQCD is a very advanced GPL-licensed code to run lattice simulations.

Running MPI codes w/ udocker

- Download and install the container as with MasterCode.
- caveat: exactly the same version of MPI on the host and in the container.
- With udocker, the mpiexec of the host system is used to submit the MPI processes.

```
emanuele [0]> ${HOST_OPENMPI_PATH_BIN}/mpiexec \
 -np 128 udocker run \
 --hostenv --hostauth --user=${USERID} \
 --workdir=${OPENQCD_CONTAINER_DIR} \
 openqcd \
 ${OPENQCD_CONTAINER_DIR}/ym1 -i ym1.in
```

Scaling test



- Scaling performance as a function of the cores for the computation of application of the Dirac operator to a spinor field (Practically, it is a sparse-matrix-matrix × vector multiplication).
- `udocker` at *least* as fast as the host.
- At CESGA `udocker` *faster* than host because of newest libraries for 8 and 16 cores.

GPU-accelerated simulations: DisVis and Gromacs

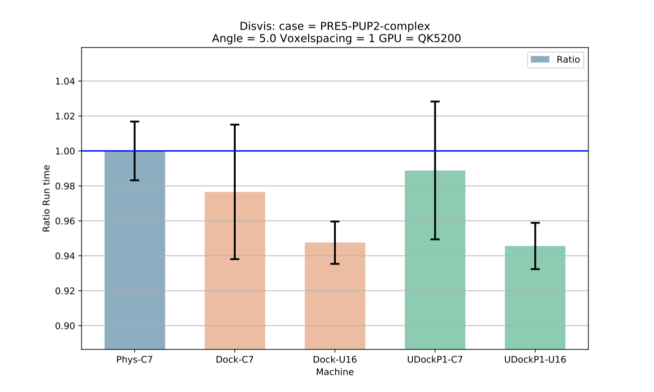
Biomolecular complexes: DisVis, Powerfit and Gromacs

- `DisVis` and `Powerfit` are MIT-licensed codes available on `GitHub` to model biomolecular complexes.
- They leverage GPUs through `OpenCL`, via `PyOpenCL`
- `Gromacs`is a molecular dynamics package for both biochemical and non-biochemical systems.

Running w/ `udocker`

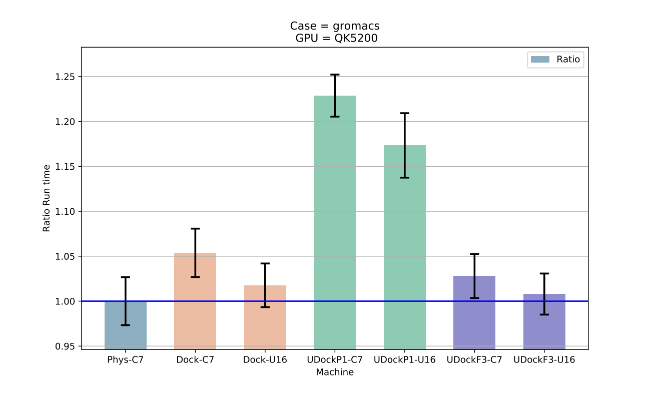
- Download and install the container as with `MasterCode`.
- caveat: exactly the same version of the NVIDIA drivers and libraries needs to be installed on the host and the container.

DisVis



- `udocker` and `docker` have same performance as the host when using `CentOS7`.
- Improved performance due to newer userland libraries when using `Ubuntu16`.

Gromacs



- `udocker` and `docker` are worse than the host when using `CentOS7` of $\mathcal{O}$(3-5%).
- Same performances when using `Ubuntu16`.
- Use of P1 mode results in $\mathcal{O}$(22%) performance hit (due to communication between the GPGPU and the CPU threads – Gromacs spawns 8 OpenMP threads / GPU).

Conclusions

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- We have presented the udocker middleware suite, which allow to run seamless docker container in user-space without root access.
- The goal of udocker is to ease the deployment of complex frameworks on (heterogeneous) clusters.
- Requires no intervention from a system administrator (no root access required!).
- For CPU intensive application, there is basically no performance hit.
- I/O bounded applications require more care (use of Fn modes vs Pn modes to reduce the performance hit).
- Available on GitHub at https://github.com/indigo-dc/udocker/.

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