Addressing Practical Aspects of Container-native Workflows with Popper

Ivo Jimenez

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UC Santa Cruz

What is a container?

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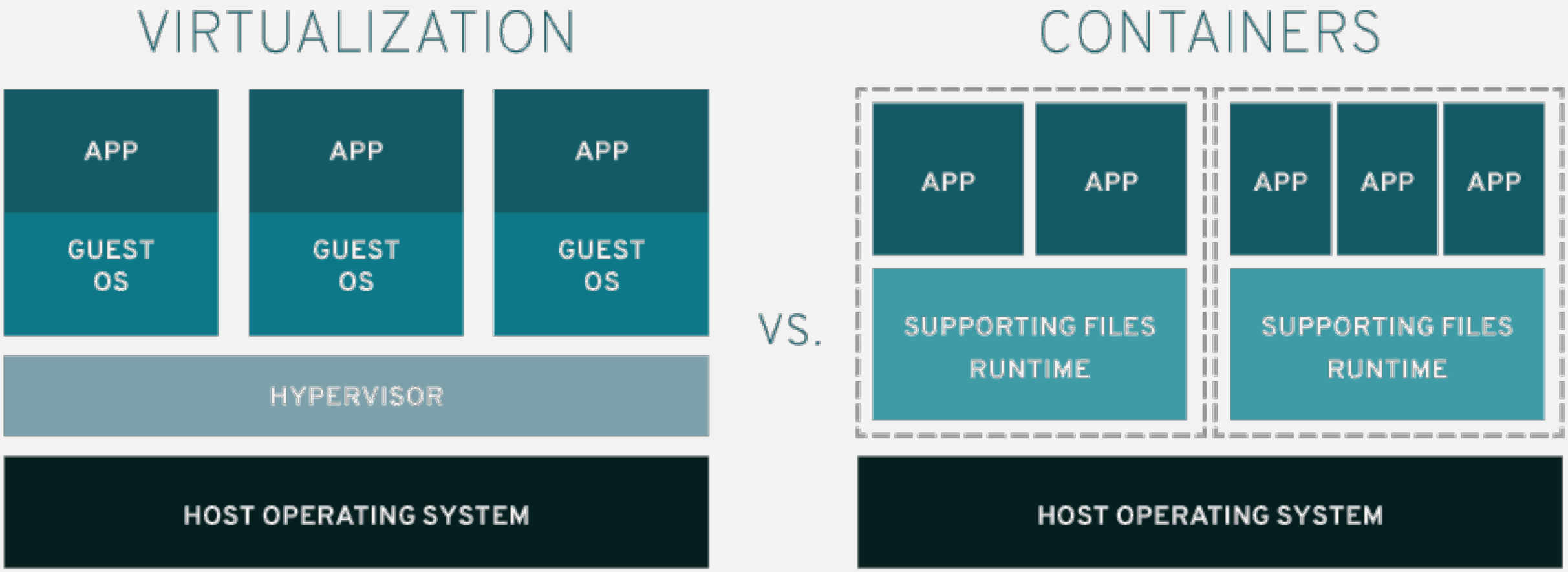

Main benefit of using containers

Bring Your Own Environment (BYOE) to shared infrastructure

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```
docker run mattrayner/lamp:latest-1804
```

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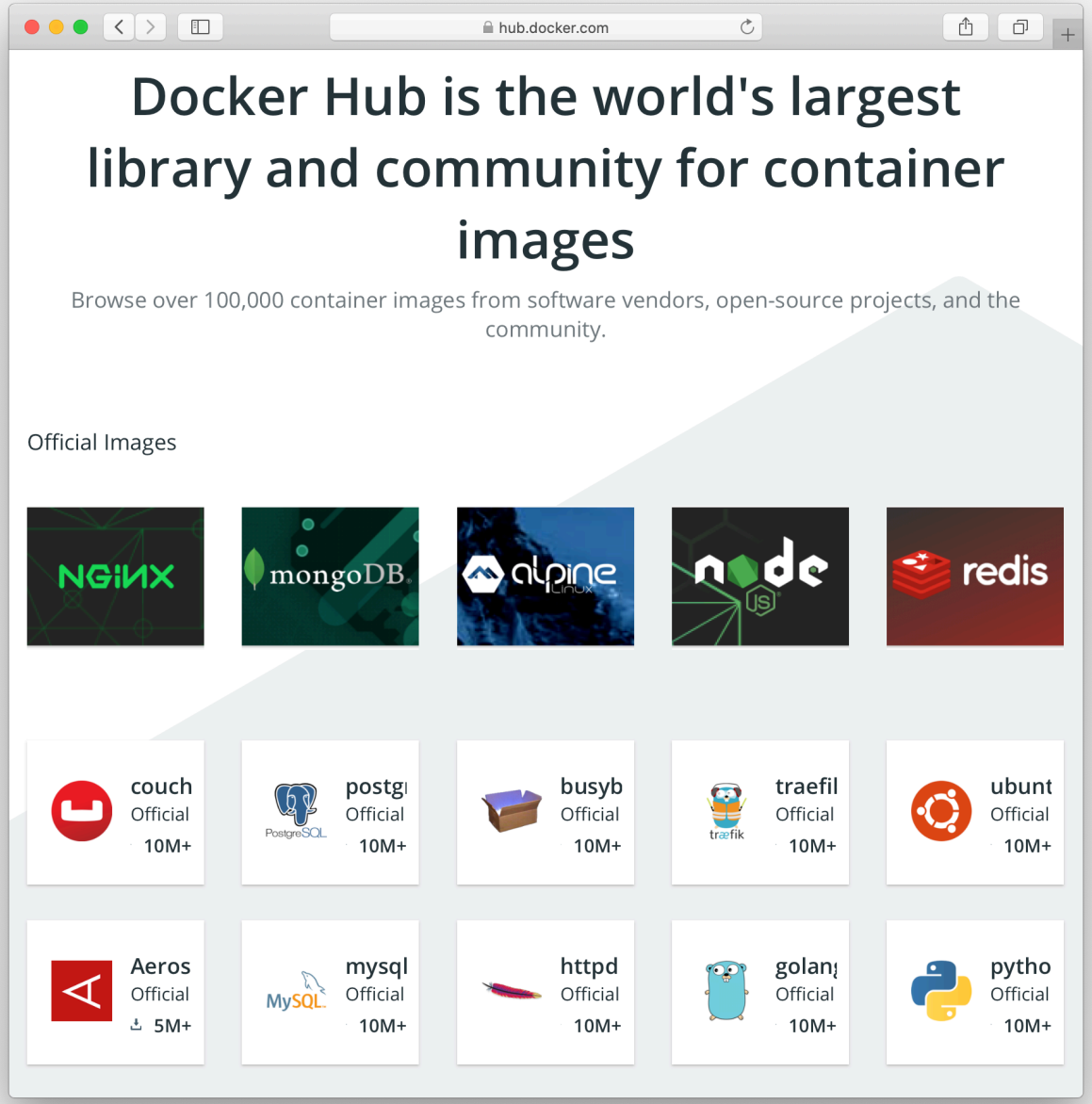
```
docker run tensorflow/tensorflow:2.1.1-gpu-jupyter
```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ubunt
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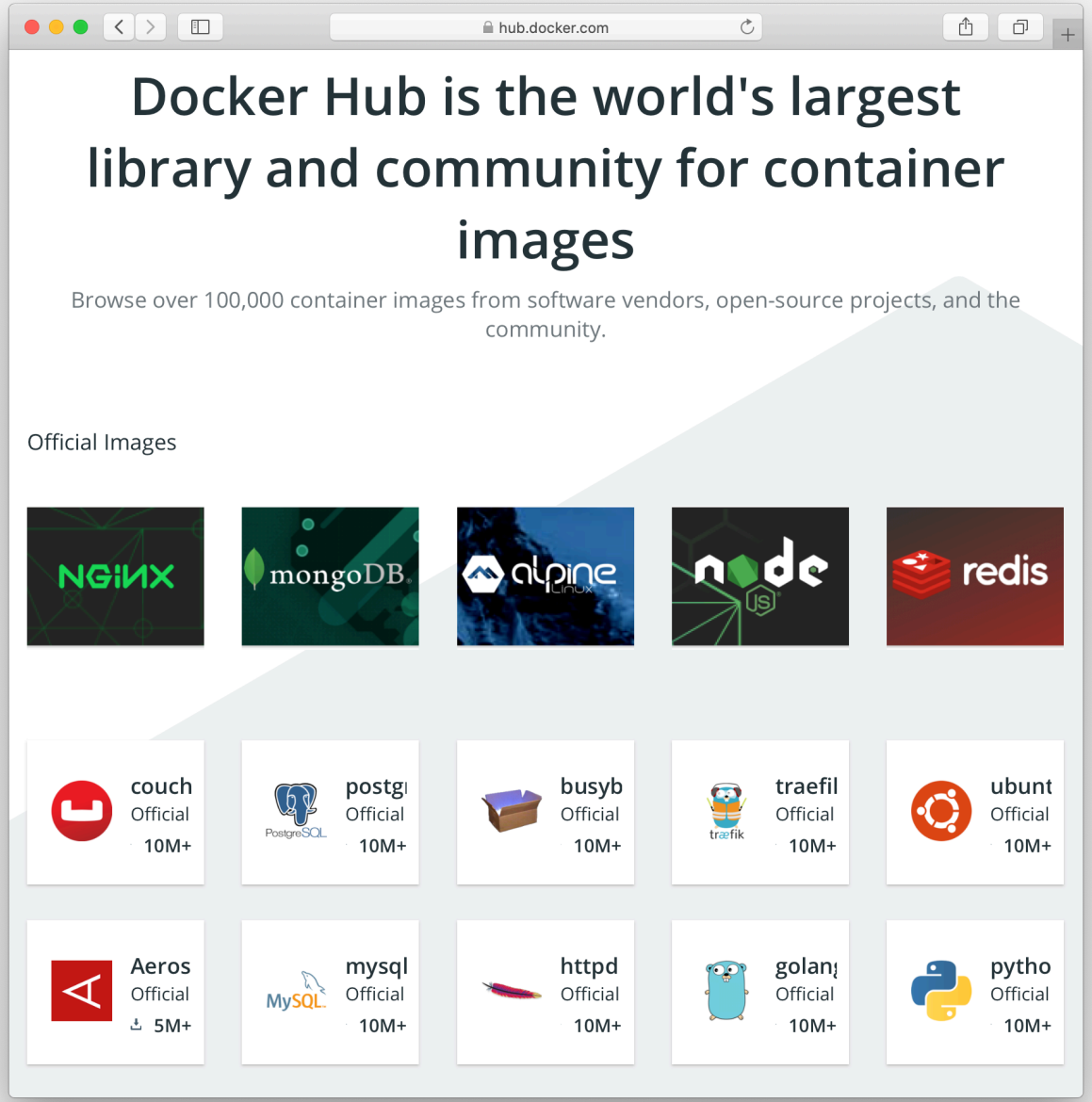
Aeros
Official
5M+
mysql
Official
10M+
httpd
Official
10M+
golan
Official
10M+
pytho
Official
10M+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Docker Hub is the world's largest library and community for container images
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mongoDB.
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sylabs/tests/not-default 99416
sylabs/tests/unsigned 46973
sylabs/tests/signed 21219
library/default/ubuntu 15126
library/default/centos 7544
sylabs/tests/busybox 7040
MOST STARRED
library/default/ubuntu 26
library/default/alpine 17
library/default/centos 13
sylabsed/examples/lolcow 11

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If you install software directly on your machine, then you are not following a container-native approach*

*other than personal productivity tools such as a text editor, web browser, email reader, calendar app, etc.

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Extreme Scale Multi-Physics Simulations of the Tsunamigenic 2004 Sumatra Megathrust Earthquake

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ABSTRACT

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To tackle the extreme size of this scenario an end-to-end optimization of the simulation code SeisSol was necessary. We implemented a new cache-aware wave propagation scheme and optimized the dynamic rupture kernels using code generation. We established a novel clustered local-time-stepping scheme for dynamic rupture. In total, we achieved a speed-up of 13.6 compared to the previous implementation. For the Sumatra scenario with 221 million elements this reduced the time-to-solution to 13.9 hours on 86,016 Haswell cores. Furthermore, we used asynchronous output to overlap I/O and compute time.

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A particularly devastating example is the M_w 9.1 2004 Sumatra-Andaman Earthquake and Indian Ocean Tsunami. The Sumatra earthquake ruptured the greatest fault length of any recorded earthquake and triggered a series of tsunamis, killing up to 280,000 people in 14 countries, and even displaced Earth's North Pole by 2.5 cm.

For the coming decades, there is no realistic hope to reliably predict earthquakes, such that the method of choice to mitigate earthquake- and tsunami-related damage to our societies is to forecast seafloor displacement and strong ground motions for likely earthquake scenarios. Dynamic rupture simulations combine non-linear frictional failure and seismic wave propagation in a multi-physics manner to produce physics-based forecasts [e.g. 5, 20, 30, 38, 65] and provide insight into the poorly understood fundamental processes of earthquake faulting [e.g. 2, 4, 29, 32, 33, 68].

A correct representation of subduction zone complexity is crucial, but, in concurrence with the giant spatial extent and temporal duration to be resolved, extremely challenging from a numerical point of view. Simulations must capture slip and seismic waves occurring for hundreds of seconds along hundreds of kilometers but at the same time resolve the meter-scale physical processes taking place at the rupture tip of the earthquake source.

A recent rise of 3D HPC earthquake simulation software [e.g. 18, 43, 48, 49, 72, 75, 76] allows for the simulation of various aspects of earthquake scenarios and enables researchers to answer geophysical questions complicated by the lack of sufficiently dense

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Meshes are usually constructed from CAD models using either the Simulation Modeling Suite from Simmetrix or Gmsh. To convert meshes to the custom netCDF format, the preprocessing tool PUMGen is available on Github https://github.com/TUM-I5/PUML/

```yaml
steps:
- id: install lulesh
  uses: popperized/spack@master
  args: [spack, install, -j8, lulesh+mpi]

- id: delete existing jobs
  uses: popperized/bin/sh@master
  args: [rm, -fr, sweep/jobs]

- id: install sweepj2
  uses: popperized/python-actions@master
  args: [pip, install, sweepj2]

- id: generate sweep
  uses: jefftriplett/python-actions@master
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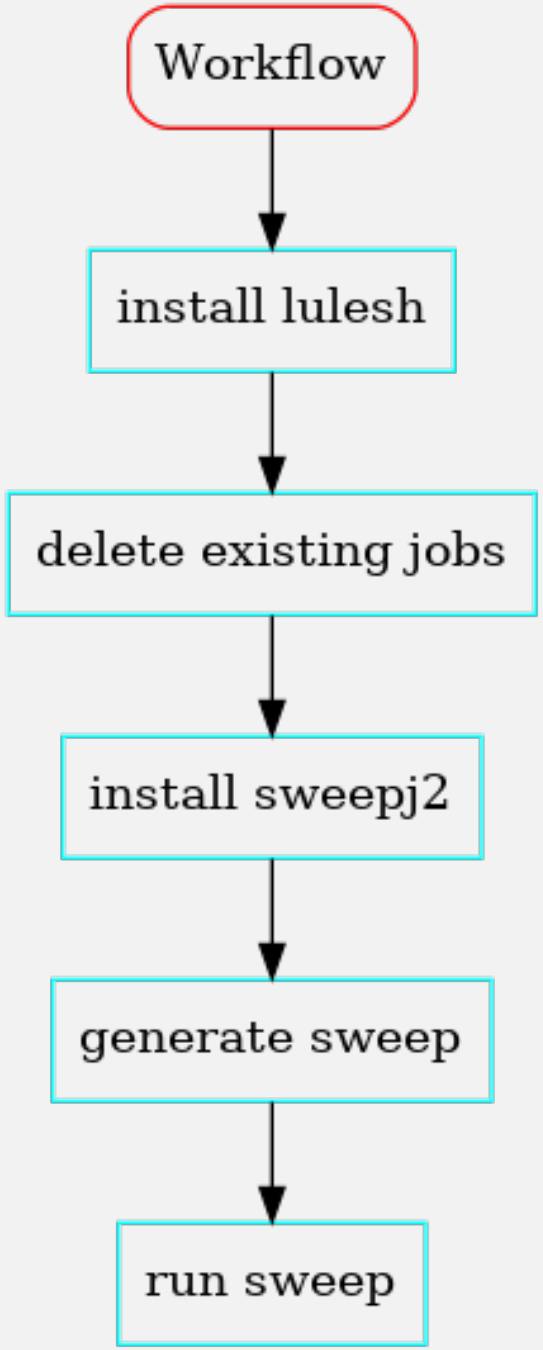


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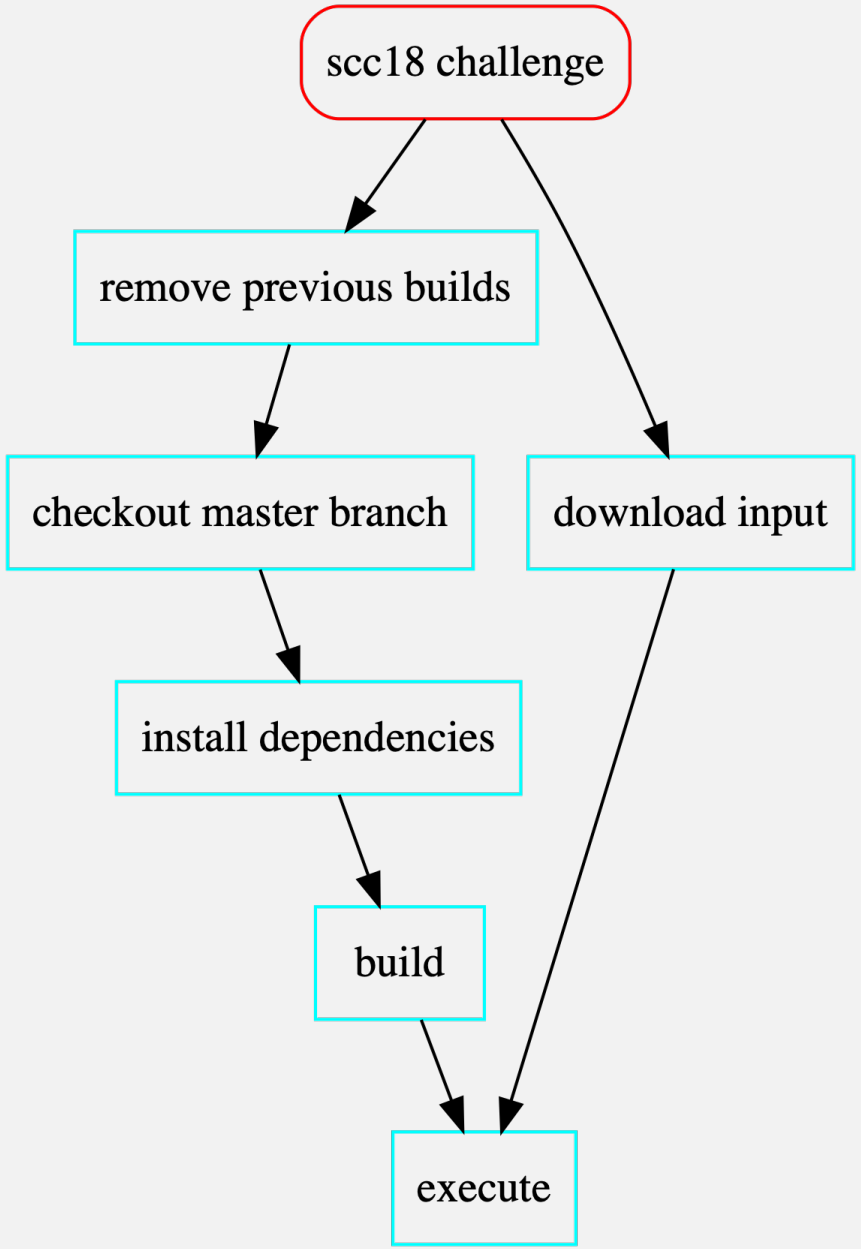

A ARTIFACT DESCRIPTION: EXTREME SCALE MULTI-PHYSICS SIMULATIONS OF THE 2004 SUMATRA MEGATHRUST EARTHQUAKE

A.1 Abstract

This artifact description contains information about the complete workflow required to set up simulations with the Shaking Corals version of SeisSol. We describe how the software can be obtained and the build process as well as necessary preprocessing steps to generate the input dataset for the node level performance measurements. Input datasets for the scaling and production runs are not publicly available due to their size. In addition, the artifact description outlines the complete workflow from the raw input data to the final visualization of the output.

A.2 Description

A.2.1 Check-list (artifact meta information).

- **Algorithm:** Arbitrary high-order DERivative Discontinuous Galerkin (ADER-DG) with clustered local time stepping.
- **Program:** SeisSol (www.seissol.org); version: *Shaking Corals*.
- **Compilation:** Intel C/C++ and Fortran Compiler.
- **Binary:** -
- **Data set:** CAD model of Sumatra subduction zone and Bay of Bengal assembled with GoCAD; Mesh generated with the Simulation Modeling Suite from Simmetrix (http://simmetrix.com/); see Section 5.1 for input data sets concerning topography, etc.
- **Run-time environment:** Lenovo NeXtScale nx360M5 WCT with IBM MPI (SuperMUC), Cray XC40 with Cray MPI (Shaheen II and Cori)
- **Hardware:** Optimized code is available for Intel Haswell, Intel Knights Landing and other Intel architectures. An unoptimized fallback version is also available.
- **Output:** Timings from the log file; optional receiver (seismic stations) and visualization output.
- **Experiment workflow:** See below.
- **Publicly available?** Code and example datasets are publicly available. The original input datasets for this paper are available

A.2.5 Datasets. A setup including a mesh with over 3 million elements for the 2004 Sumatra-Andaman earthquake can be obtained from Zenodo https://dx.doi.org/10.5281/zenodo.439946. Due to the large size of the production-run meshes, these are only available upon request.

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Shaking Corals uses SCons for compilation and supports various options to customize the binary. The following command compiles the release version using optimized Intel Haswell kernels for convergence order 6. The resulting binary will support a hybrid MPI+OpenMP parallelization and netCDF for mesh initialization. Note that netCDF is optional but recommended for large runs.

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$ scons order=6 compileMode=release \
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      parallelization=hybrid commThread=yes \
      netcdf=yes
```

To get a full list of all available options, run:

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For a more detailed description, see https://github.com/SeisSol/SeisSol/wiki.

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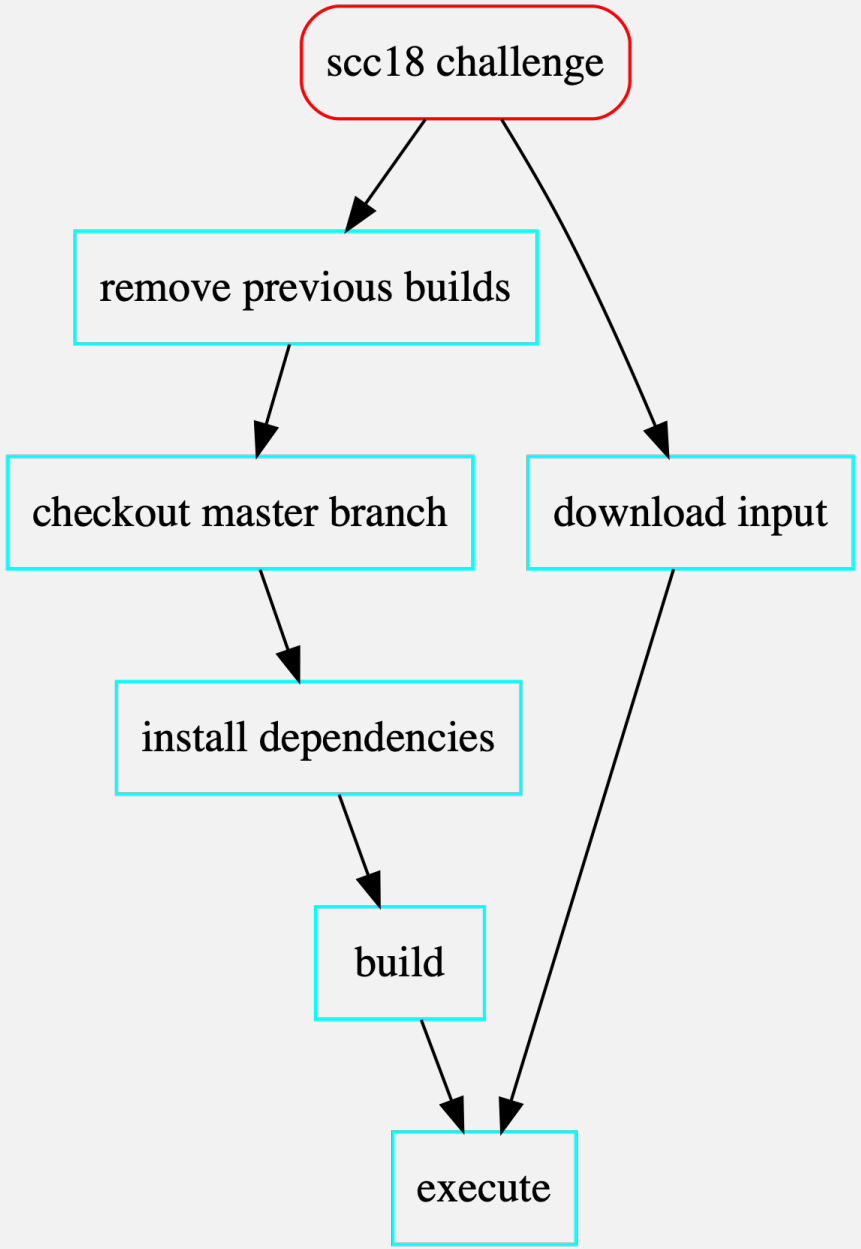

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SCC18: https://github.com/getpopper/seissol-workflows
SCC19: https://github.com/getpopper/normalmodes-workflows

Practical problems that arise when working under the container-native paradigm

- Dealing with multi-container workflows
    - Complex application testing and prototyping becomes difficult to reproduce if done by hand
- Myriad of container runtimes
    - Docker, Podman, LXD, Singularity, Charliecloud, …
- Lack of common orchestration platform support
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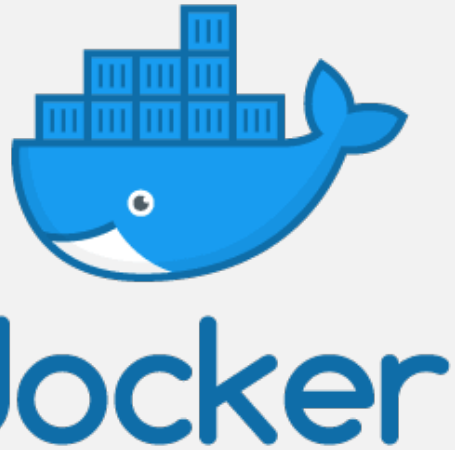
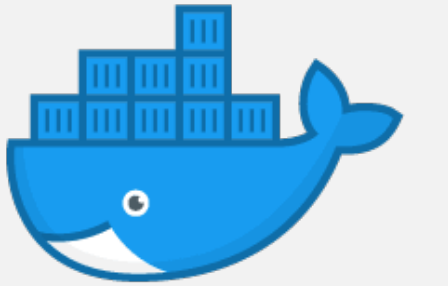
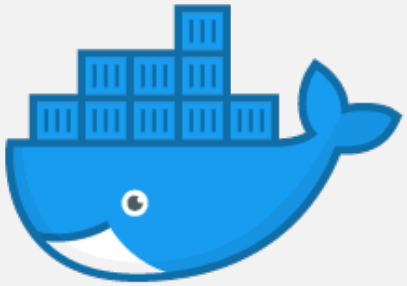

docker

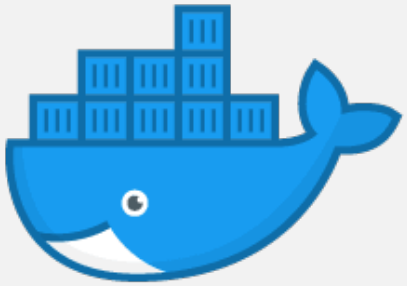


docker



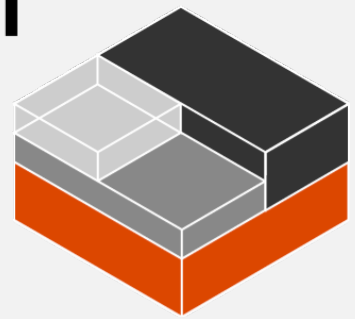
docker

podman

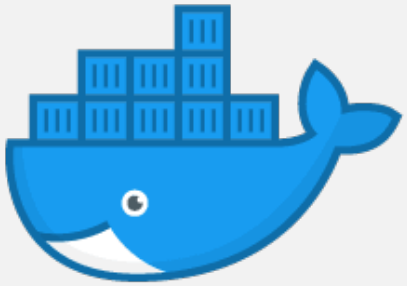


docker

podman



lxd

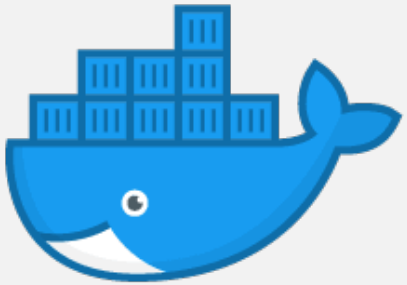


docker

podman

Charliecloud

lxd

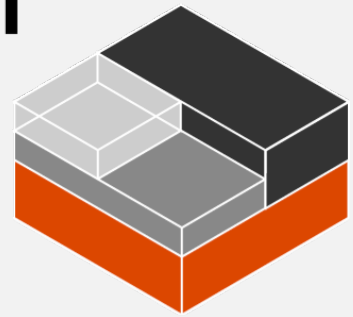


docker

kata
containers

podman

Charliecloud



lxd

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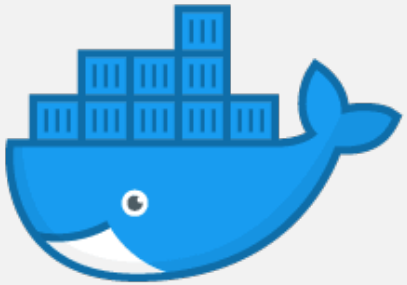

docker

kata containers

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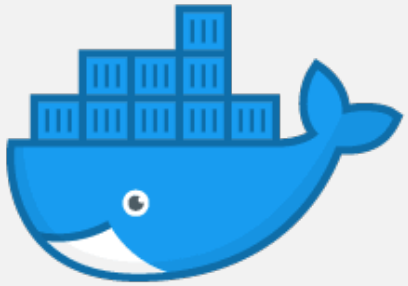
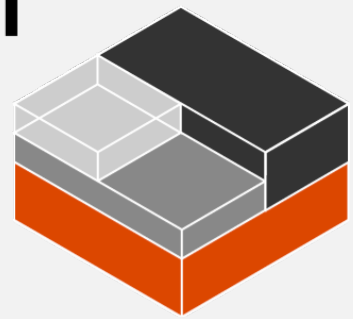


podman



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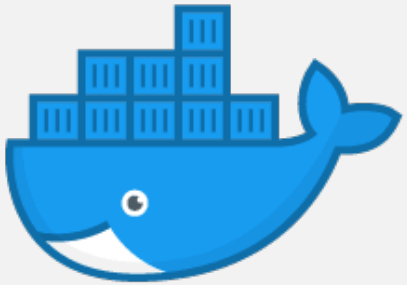

docker

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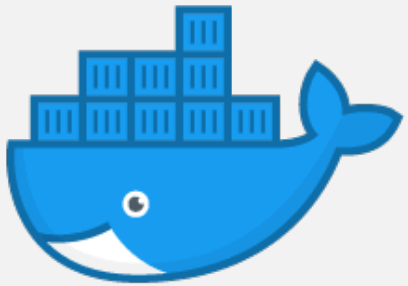

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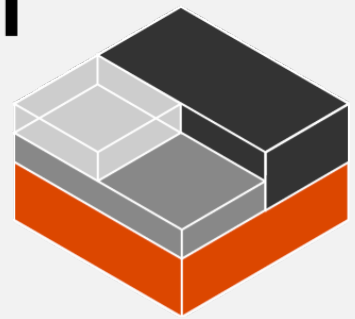

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```
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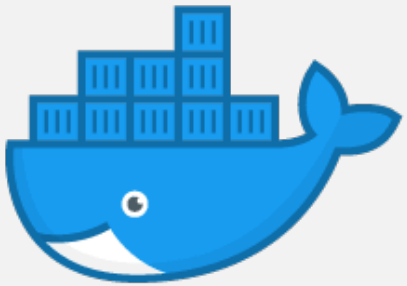

docker

kata containers

podman

Charliecloud

lxd

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kubernetes

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HTCondor

kubernetes

slurm
workload manager

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HTCondor

kubernetes

slurm
workload manager

GRID ENGINE

Popper

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```

HTCondor

kubernetes

slurm
workload manager

GRID ENGINE

Popper

```
$> popper run
```

```
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HTCondor

kubernetes

slurm
workload manager

GRID ENGINE

Popper

```
$> popper run --resman slurm
```

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- id: delete existing jobs
  uses: popperized/bin/sh@master
  args: [rm, -fr, sweep/jobs]

- id: install sweepj2
  uses: popperized/python-actions@master
  args: [pip, install, sweepj2]

- id: generate sweep
  uses: jefftriplett/python-actions@master
  args: [
    "sweepj2",
    "--template", "./sweep/script.j2",
    "--space", "./sweep/space.yml",
    "--output", "./sweep/jobs/",
    "--make-executable"
  ]

- id: run sweep
  uses: popperized/spack@master
  args: [run-parts, ./sweep/jobs]
```

HTCondor

kubernetes

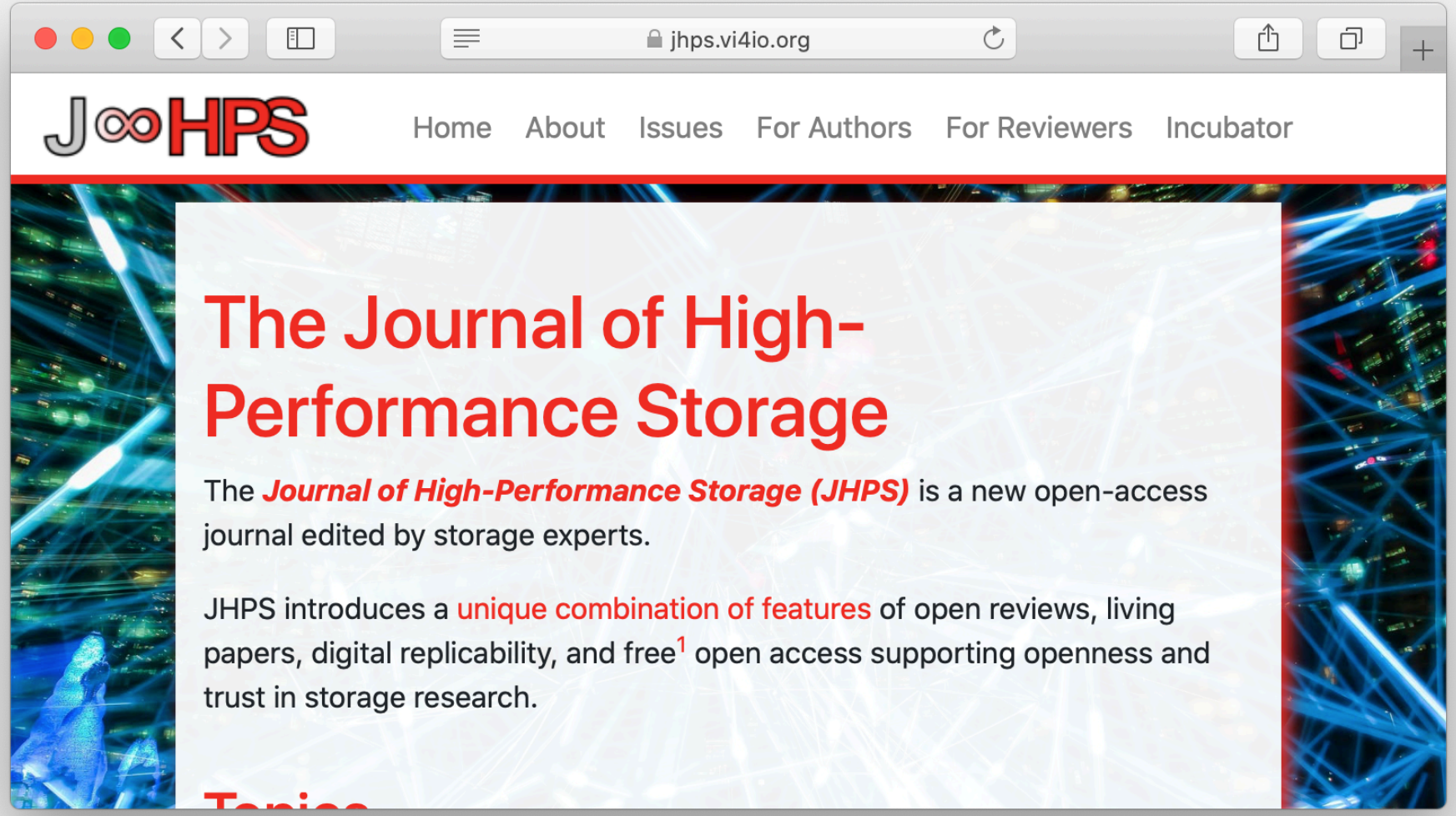
slurm
workload manager

GRID ENGINE

Take away

- The container-native paradigm improves reproducibility aspects of experimentation workflows.
- But, as always, there's no free lunch: working under this new paradigm comes with its associated problems
- Popper addresses these in a holistic and user-friendly way

Popper as an alternative for minimizing overheads in the peer-review process of journal and conference submissions



reproducibility.acm.org

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Reproducibility and Replicability

Fostering a diverse and inclusive community around the issues of reproducibility and replicability of computational research.

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Mission

Foster a broad and inclusive intellectual community around the issues of reproducibility of computational research. Attain SIG status within ACM.

Activities

The EIG proposes two working groups, one to focus on conference planning and execution activities, and the other to coordinate discussions and efforts regarding reproducibility (best/better) practices.

Events

Extreme Scale Multi-Physics Simulations of the Tsunamigenic 2004 Sumatra Megathrust Earthquake

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ABSTRACT

We present a high-resolution simulation of the 2004 Sumatra-Andaman earthquake, including non-linear frictional failure on a megathrust-splay fault system. Our method exploits unstructured meshes capturing the complicated geometries in subduction zones that are crucial to understand large earthquakes and tsunami generation. These up-to-date largest and longest dynamic rupture simulations enable analysis of dynamic source effects on the seafloor displacements.

To tackle the extreme size of this scenario an end-to-end optimization of the simulation code SeisSol was necessary. We implemented a new cache-aware wave propagation scheme and optimized the dynamic rupture kernels using code generation. We established a novel clustered local-time-stepping scheme for dynamic rupture. In total, we achieved a speed-up of 13.6 compared to the previous implementation. For the Sumatra scenario with 221 million elements this reduced the time-to-solution to 13.9 hours on 86,016 Haswell cores. Furthermore, we used asynchronous output to overlap I/O and compute time.

CCS CONCEPTS

• **Applied computing → Earth and atmospheric sciences**;

KEYWORDS

ADER-DG; earthquake simulation; tsunami coupling; dynamic rupture; petascale performance; hybrid parallelization; local time stepping; asynchronous output

ACM Reference format:
Carsten Uphoff, Sebastian Rettenberger, Michael Bader, Elizabeth H. Madden, Thomas Ulrich, Stephanie Wollherr, and Alice-Agnes Gabriel. 2017. Extreme Scale Multi-Physics Simulations of the Tsunamigenic 2004 Sumatra Megathrust Earthquake. In *Proceedings of SC17, Denver, CO, USA, November 12–17, 2017,* 16 pages.
DOI: 10.1145/3126908.3126948

1 INTRODUCTION

"Megathrust" earthquakes in subduction zones, caused by oceanic lithosphere sliding into the mantle beneath an overriding tectonic plate, have released most of the seismic energy over the last century. No other type of tectonic activity is known to produce earthquakes that exceed moment magnitudes M_w of 9 and trigger teletsunamis traveling whole oceans.

A particularly devastating example is the M_w 9.1 2004 Sumatra-Andaman Earthquake and Indian Ocean Tsunami. The Sumatra earthquake ruptured the greatest fault length of any recorded earthquake and triggered a series of tsunamis, killing up to 280,000 people in 14 countries, and even displaced Earth's North Pole by 2.5 cm.

For the coming decades, there is no realistic hope to reliably predict earthquakes, such that the method of choice to mitigate earthquake- and tsunami-related damage to our societies is to forecast seafloor displacement and strong ground motions for likely earthquake scenarios. Dynamic rupture simulations combine non-linear frictional failure and seismic wave propagation in a multi-physics manner to produce physics-based forecasts [e.g. 5, 20, 30, 38, 65] and provide insight into the poorly understood fundamental processes of earthquake faulting [e.g. 2, 4, 29, 32, 33, 68].

A correct representation of subduction zone complexity is crucial, but, in concurrence with the giant spatial extent and temporal duration to be resolved, extremely challenging from a numerical point of view. Simulations must capture slip and seismic waves occurring for hundreds of seconds along hundreds of kilometers but at the same time resolve the meter-scale physical processes taking place at the rupture tip of the earthquake source.

A recent rise of 3D HPC earthquake simulation software [e.g. 18, 43, 48, 49, 72, 75, 76] allows for the simulation of various aspects of earthquake scenarios and enables researchers to answer geophysical questions complicated by the lack of sufficiently dense

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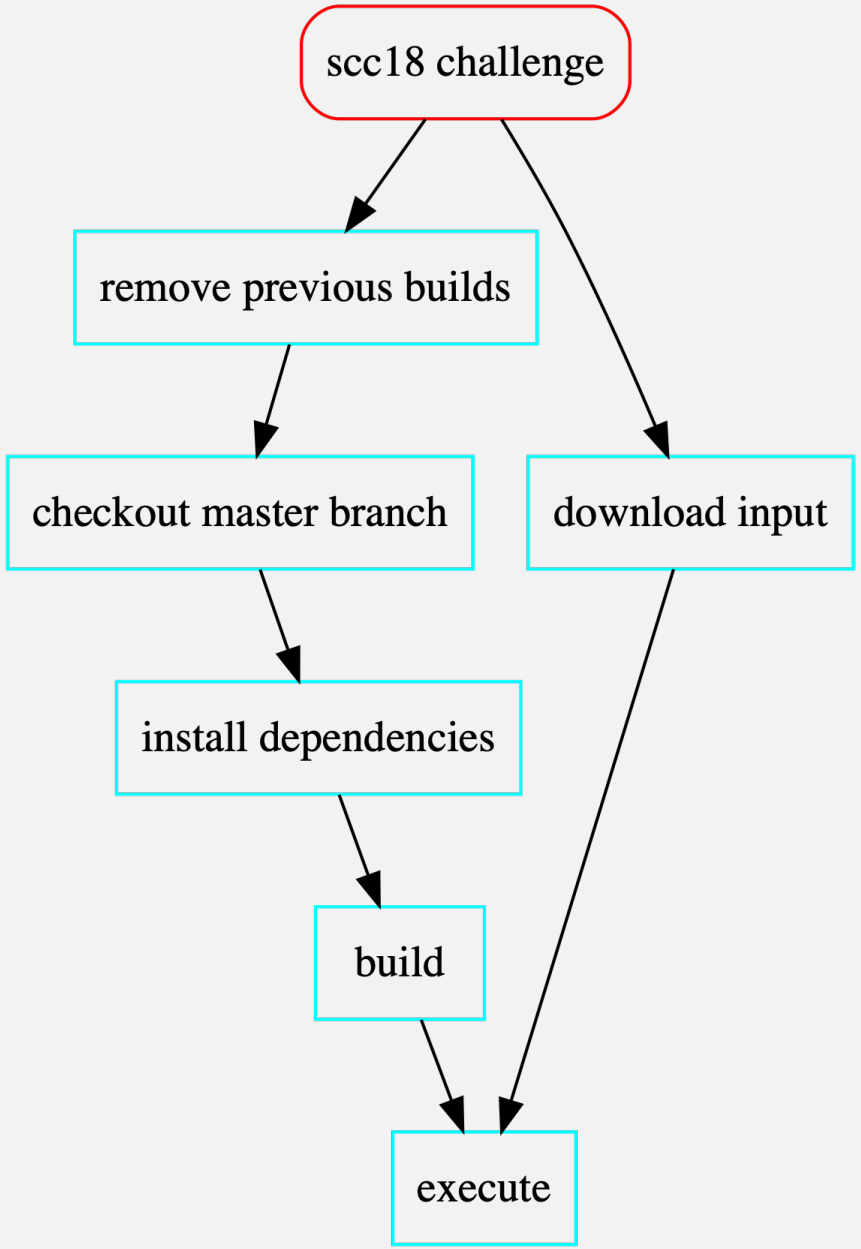

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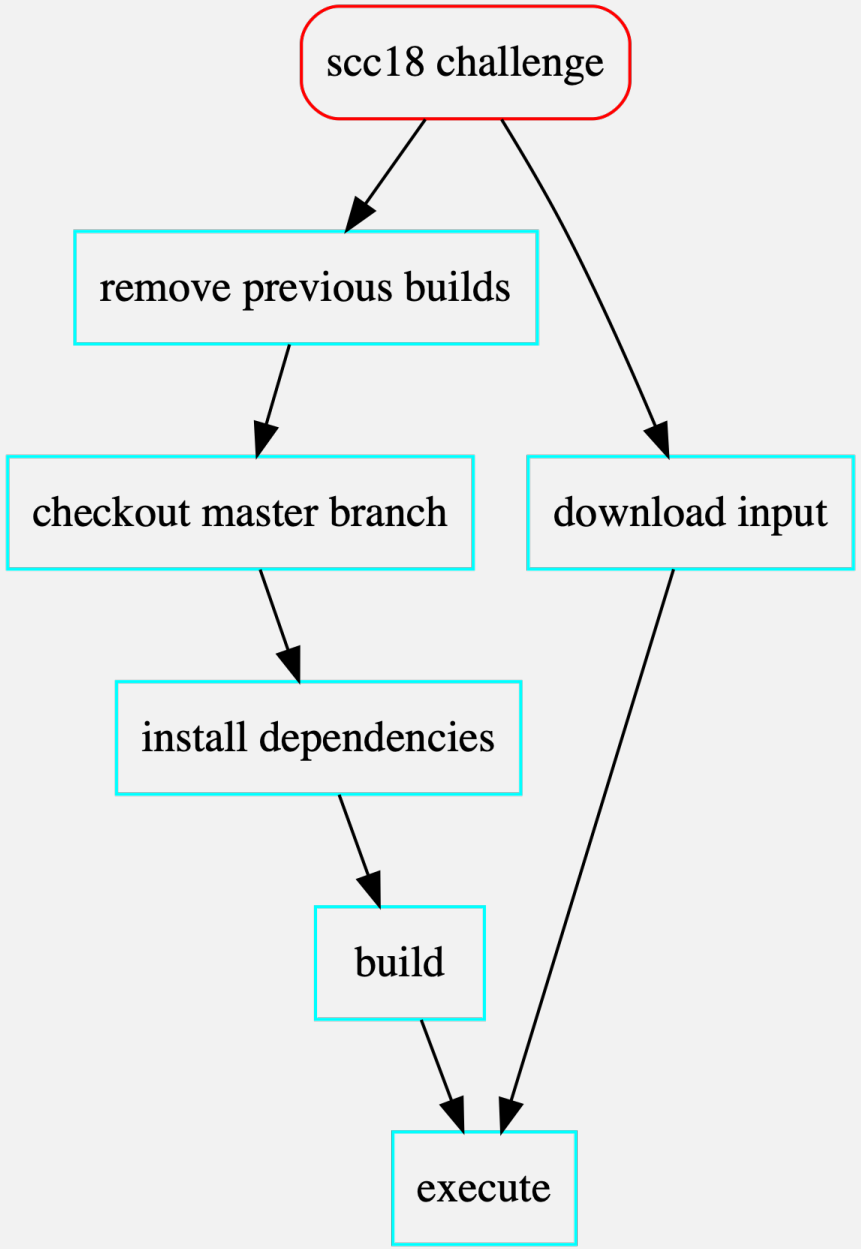

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SCC18: https://github.com/getpopper/seissol-workflows
SCC19: https://github.com/getpopper/normalmodes-workflows

Thanks!

github.com/getpopper/popper