JEDI Portability Across Platforms

Containers, Cloud Computing, and HPC

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Academy website

http://academy.jcsda.org/june2019

- Instructions for accessing AWS
- Activity instructions
- Presentation slides
- Doxygen documentation for fv3-bundle

We will add further content throughout the week

Outline

I) JEDI Portability Overview

- ✦ Unified vision for software development and distribution

II) Container Fundamentals

- ✦ What are they? How do they work?
- ✦ Docker, Charliecloud, and Singularity

III) Using the JEDI Containers

- ✦ How they are built and deployed
- ✦ Mac and Windows (Vagrant)

IV) HPC and Cloud Computing

- ✦ Environment modules
- ✦ Containers in HPC?

V) Summary and Outlook

JEDI Software Dependencies

- **Essential**
  - ✦ Compilers, MPI
  - ✦ CMake
  - ✦ SZIP, ZLIB
  - ✦ LAPACK / MKL, Eigen 3
  - ✦ NetCDF4, HDF5
  - ✦ udunits
  - ✦ Boost (headers only)
  - ✦ ecbuild, eckit, fckit

Common versions among users and developers minimize stack-related debugging

- **Useful**
  - ✦ ODB-API, eccodes
  - ✦ PNETCDF
  - ✦ Parallel IO
  - ✦ nccmp, NCO
  - ✦ Python tools (py-ncepbufr, netcdf4, matplotlib…)
  - ✦ NCEP libs
  - ✦ Debuggers & Profilers (ddt/TotalView, kdbg, valgrind, TAU…)

The JEDI Portability Vision

I want to run JEDI on…

- My Laptop/Workstation/PC

  Development

  - ✦ We provide software containers
  - ✦ Mac & Windows system need to first establish a linux environment (e.g. a Vagrant/VirtualBox virtual machine)

- In the Cloud

  Development

  Applications

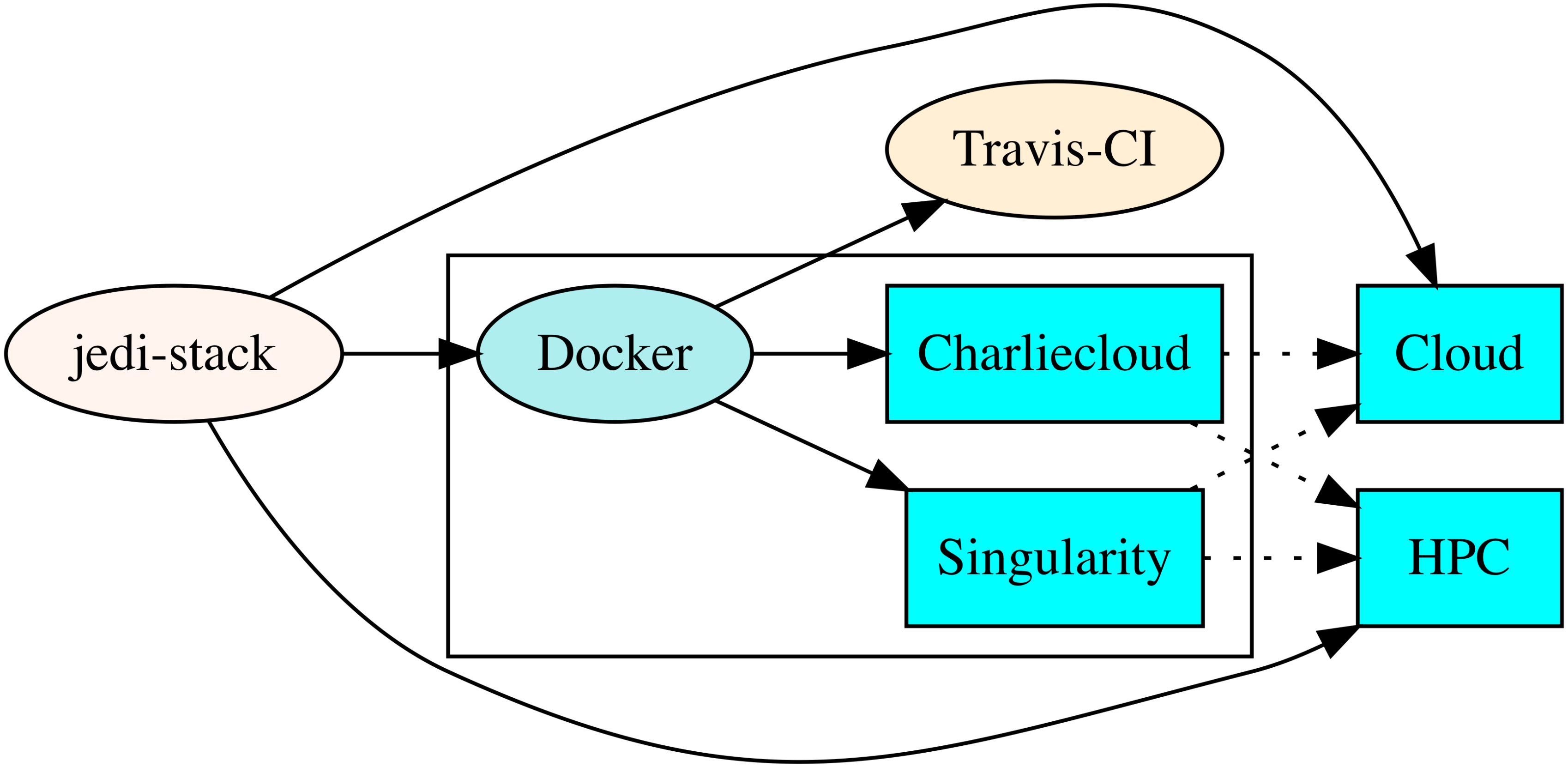
  - ✦ We provide containers, machine images (AMIs)
  - ✦ We provide access via a Web-based Front End (in development)!

- On an HPC System

  Applications

  - ✦ We provide environment modules on selected systems (Theia, Discover, Cheyenne…)
  - ✦ We provide high-performance containers (in development)
  - ✦ We provide access to selected HPC resources and JEDI applications via the web front end (in development)

Unified Build System



Tagged jedi-stack releases can be used to build tagged containers, AMIs, and HPC environment modules, ensuring common software environments across platforms

Part II: Container Fundamentals

Software container (working definition)

A packaged user environment that can be "unpacked" and used across different systems, from laptops to cloud to HPC

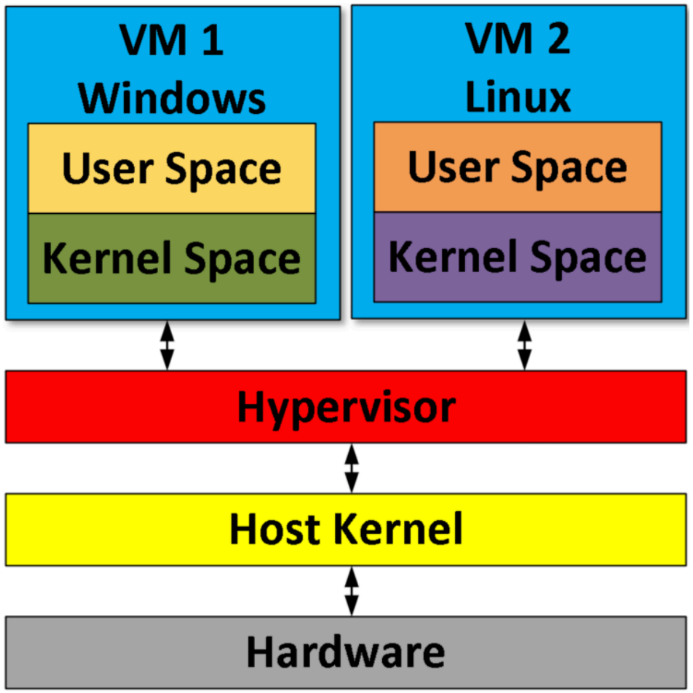
Container Benefits

- BYOE: Bring your own Environment
- Portability
- Reproducibility
  - Version control (git)
- Workflow/Composability
  - Develop on laptops, run on cloud/HPC
  - Get new users up and running quickly

Container Providers

- Docker
- Charliecloud
- Singularity

Containers vs Virtual Machines



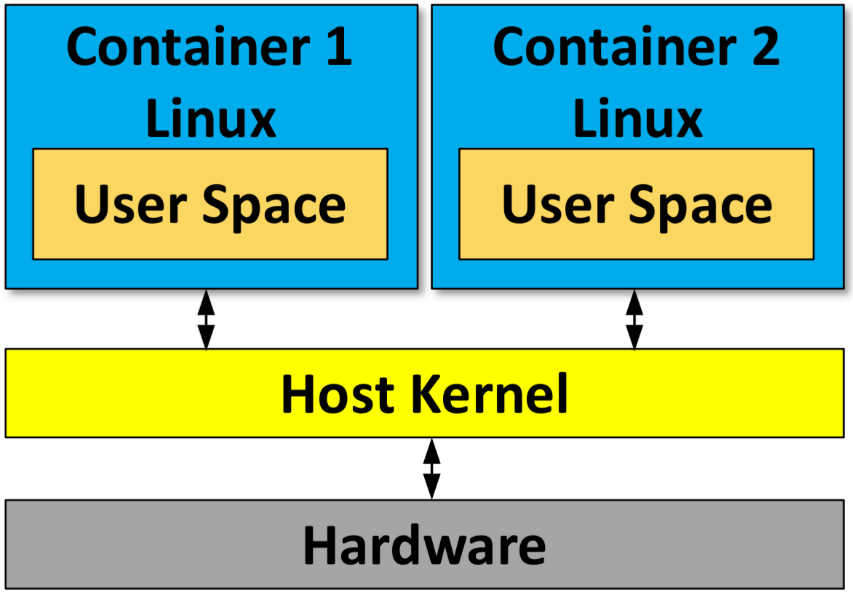
VM 1
Windows
User Space
Kernel Space

VM 2
Linux
User Space
Kernel Space

Hypervisor

Host Kernel

Hardware



Container 1
Linux
User Space

Container 2
Linux
User Space

Host Kernel

Hardware

Containers work with the host system
Including access to your home directory

More lightweight and computationally efficient that a virtual machine

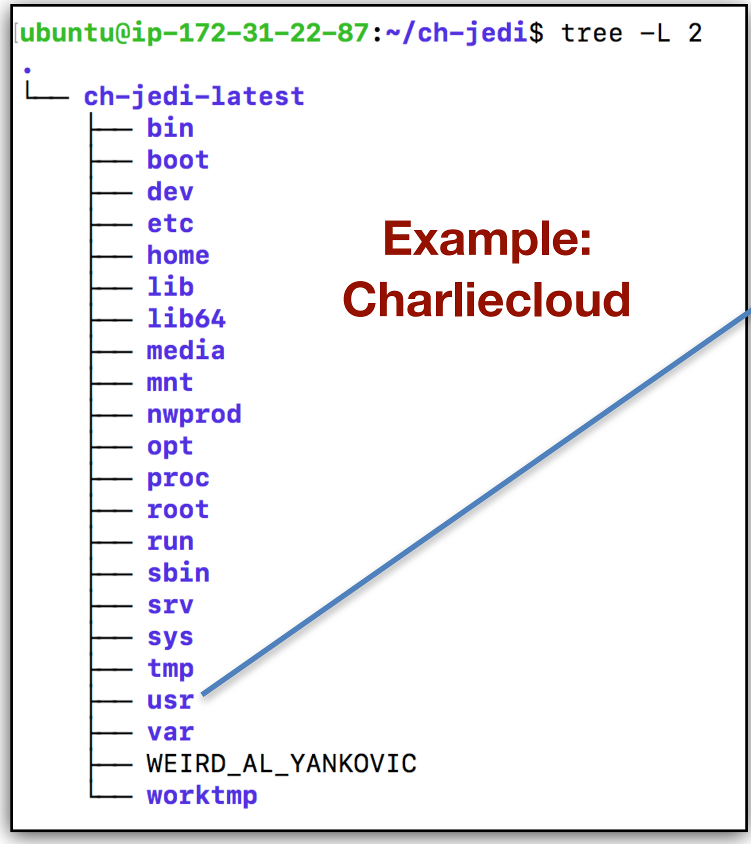
Julio Suarez
arm NEOVERSE

Example: Charliecloud

Containers exploit (linux 3.8)

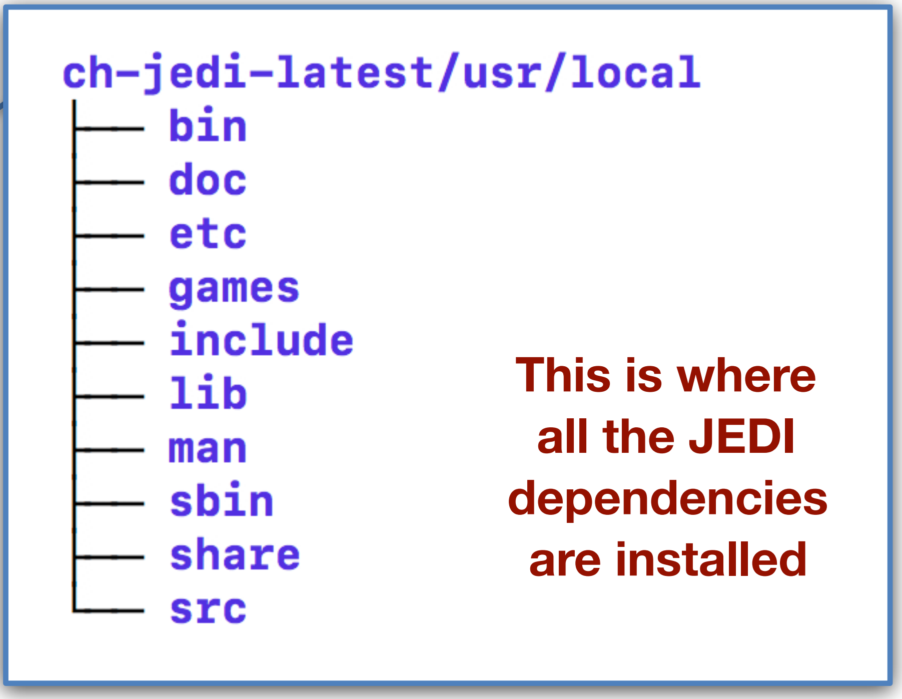
User Namespaces

(..along with other linux features such as cgroups)
to define isolated user environments



```
ubuntu@ip-172-31-22-87:~/ch-jedi$ tree -L 2
.
└── ch-jedi-latest
    ├── bin
    ├── boot
    ├── dev
    ├── etc
    ├── home
    ├── lib
    ├── lib64
    ├── media
    ├── mnt
    ├── nwprod
    ├── opt
    ├── proc
    ├── root
    ├── run
    ├── sbin
    ├── srv
    ├── sys
    ├── tmp
    ├── usr
    ├── var
    ├── WEIRD_AL_YANKOVIC
    └── worktmp
```

Example:
Charliecloud

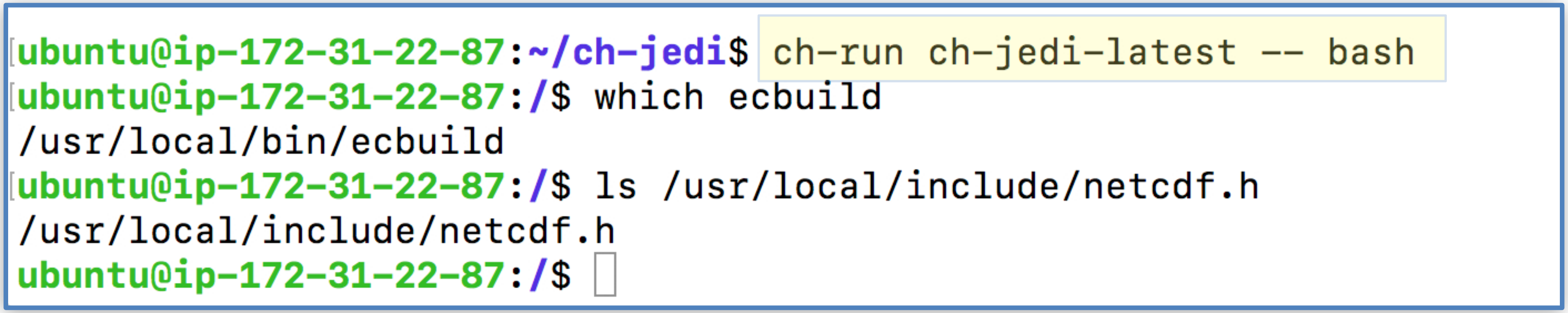


```
ch-jedi-latest/usr/local
├── bin
├── doc
├── etc
├── games
├── include
├── lib
├── man
├── sbin
├── share
└── src
```

This is where all the JEDI dependencies are installed

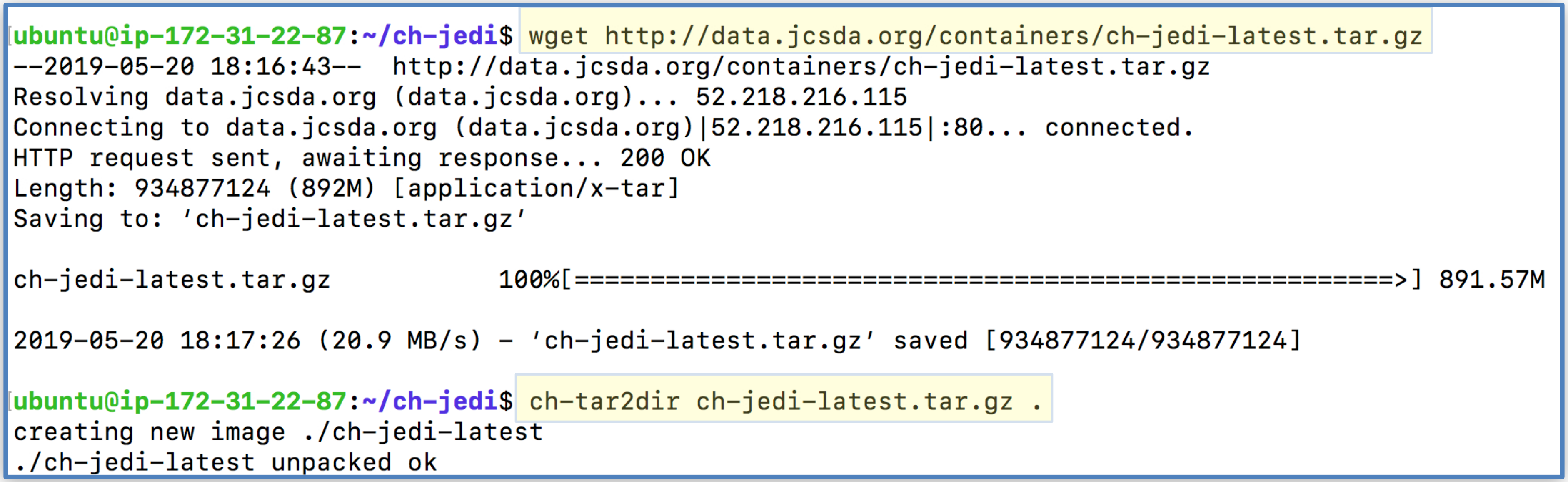
Example: CharlieCloud

A user “enters the container” with a simple command



```
[ubuntu@ip-172-31-22-87:~/ch-jedi$ ch-run ch-jedi-latest -- bash
[ubuntu@ip-172-31-22-87:/$ which ecbuild
/usr/local/bin/ecbuild
[ubuntu@ip-172-31-22-87:/$ ls /usr/local/include/netcdf.h
/usr/local/include/netcdf.h
ubuntu@ip-172-31-22-87:/$ 
```

A user obtains the container by unpacking an image file



```
[ubuntu@ip-172-31-22-87:~/ch-jedi$ wget http://data.jcsda.org/containers/ch-jedi-latest.tar.gz
--2019-05-20 18:16:43--  http://data.jcsda.org/containers/ch-jedi-latest.tar.gz
Resolving data.jcsda.org (data.jcsda.org)... 52.218.216.115
Connecting to data.jcsda.org (data.jcsda.org)|52.218.216.115|:80... connected.
HTTP request sent, awaiting response... 200 OK
Length: 934877124 (892M) [application/x-tar]
Saving to: ‘ch-jedi-latest.tar.gz’

ch-jedi-latest.tar.gz          100%[=======================================================>] 891.57M

2019-05-20 18:17:26 (20.9 MB/s) - ‘ch-jedi-latest.tar.gz’ saved [934877124/934877124]

[ubuntu@ip-172-31-22-87:~/ch-jedi$ ch-tar2dir ch-jedi-latest.tar.gz .
creating new image ./ch-jedi-latest
./ch-jedi-latest unpacked ok
```

Container Technologies

- **Docker**
  - ✦ Main Advantages: industry standard, widely supported, runs on native Mac/Windows OS
  - ✦ Main Disadvantange: Security (root privileges)

- **Charliecloud**
  - ✦ Main Advantages: Simplicity, no need for root privileges
  - ✦ Main Disadvantages: Fewer features than Singularity, Relies on Docker (to build, not to run)

- **Singularity**
  - ✦ Main Advantages: Reproducibility, HPC support
  - ✦ Main Disadvantage: Not available on all HPC systems

Container Technologies

Kurtzer, Sochat & Bauer (2017)

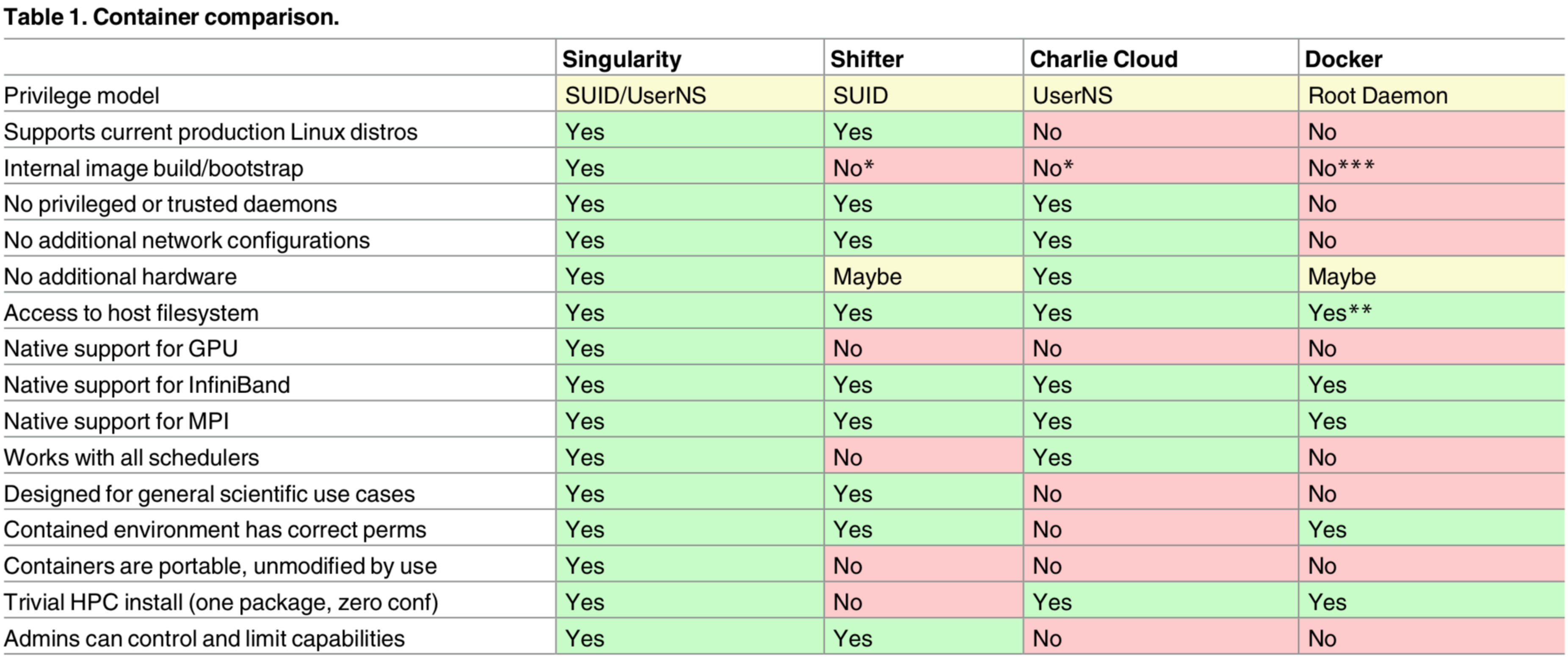


Table 1. Container comparison.

	Singularity	Shifter	Charlie Cloud	Docker
Privilege model	SUID/UserNS	SUID	UserNS	Root Daemon
Supports current production Linux distros	Yes	Yes	No	No
Internal image build/bootstrap	Yes	No*	No*	No***
No privileged or trusted daemons	Yes	Yes	Yes	No
No additional network configurations	Yes	Yes	Yes	No
No additional hardware	Yes	Maybe	Yes	Maybe
Access to host filesystem	Yes	Yes	Yes	Yes**
Native support for GPU	Yes	No	No	No
Native support for InfiniBand	Yes	Yes	Yes	Yes
Native support for MPI	Yes	Yes	Yes	Yes
Works with all schedulers	Yes	No	Yes	No
Designed for general scientific use cases	Yes	Yes	No	No
Contained environment has correct perms	Yes	Yes	No	Yes
Containers are portable, unmodified by use	Yes	No	No	No
Trivial HPC install (one package, zero conf)	Yes	No	Yes	Yes
Admins can control and limit capabilities	Yes	Yes	No	No

This is why we will continue to support all three (Docker, Singularity, Charliecloud)

Container Types

- ## Development Containers
  - ✦Include dependencies as compiled binaries
  - ✦Include compilers
  - ✦JEDI code pulled from GitHub repos and built in container

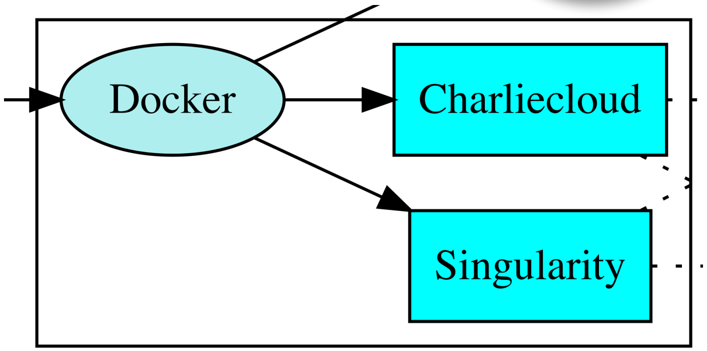
- ## Application Containers
  - ✦Include dependencies as compiled binaries
  - ✦Runtime libraries only (no compilers)
  - ✦Include compiled (binary) releases of JEDI code
  - ✦Optimized for high performance

Each Distributed as Singularity and Charliecloud image files

Each tagged with release numbers to ensure consistent user environments

Part III: Using the JEDI Containers

The JEDI Docker image is built in two steps



- **docker_base**
  - ✦ Bootstrap from ubuntu 16.04
  - ✦ Installs compilers, MPI libraries
  - ✦ Leverages NVIDIA's HPC container maker to optimize MPI configuration (e.g. Mellanox drivers for infiniband)
    https://github.com/NVIDIA/hpc-container-maker

- **docker**
  - ✦ Bootstraps from docker_base
  - ✦ Build and installs jedi-stack

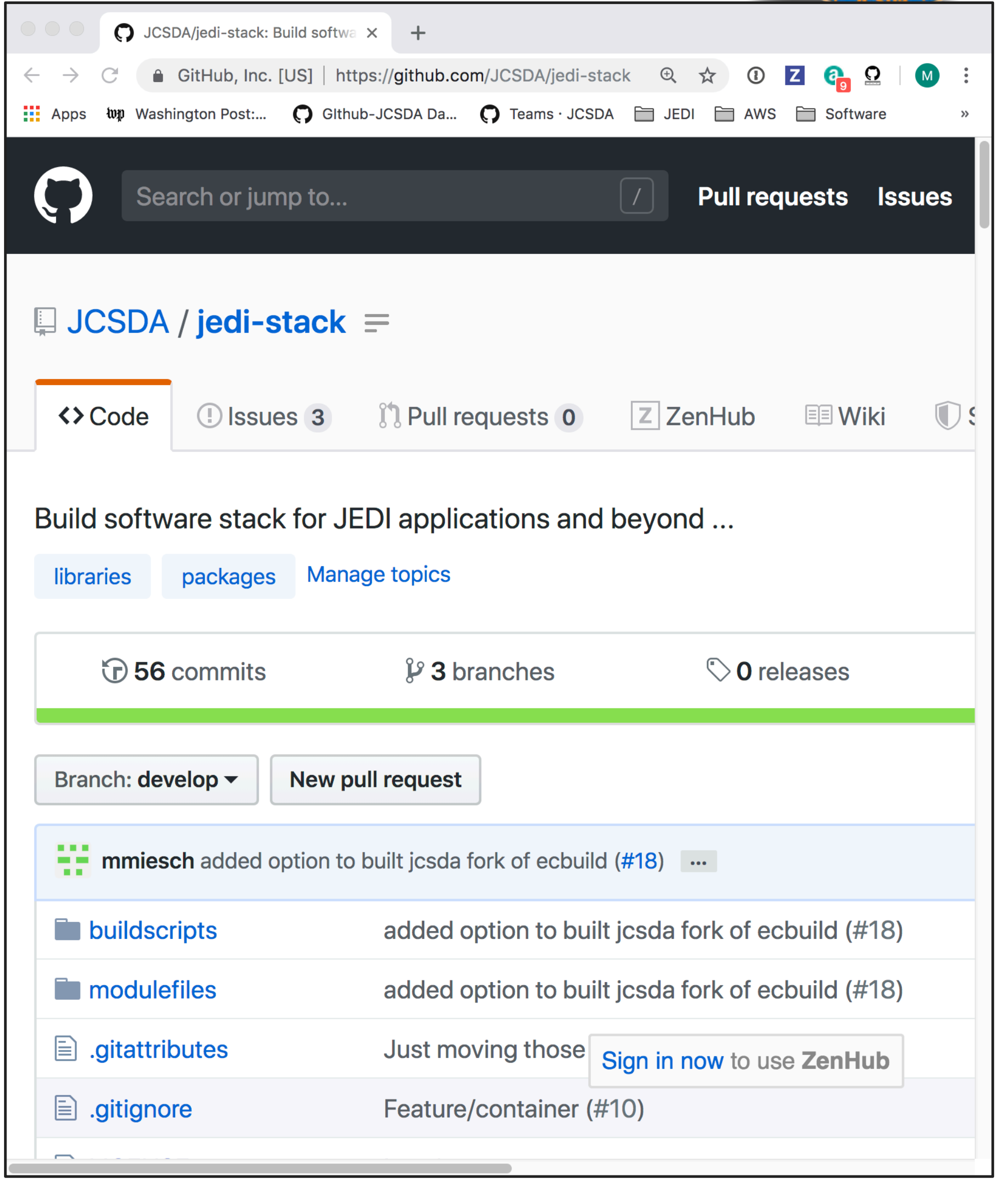
JEDI Stack

Jedi-stack is a public repo

Installs customizable hierarchy of environment modules for different compiler/mpi combinations

Tested on AWS, Cheyenne, Mac OS (so far)

No modules in containers
Libs installed in /usr/local
Separate container for each compiler/MPI combo



Build software stack for JEDI applications and beyond ...

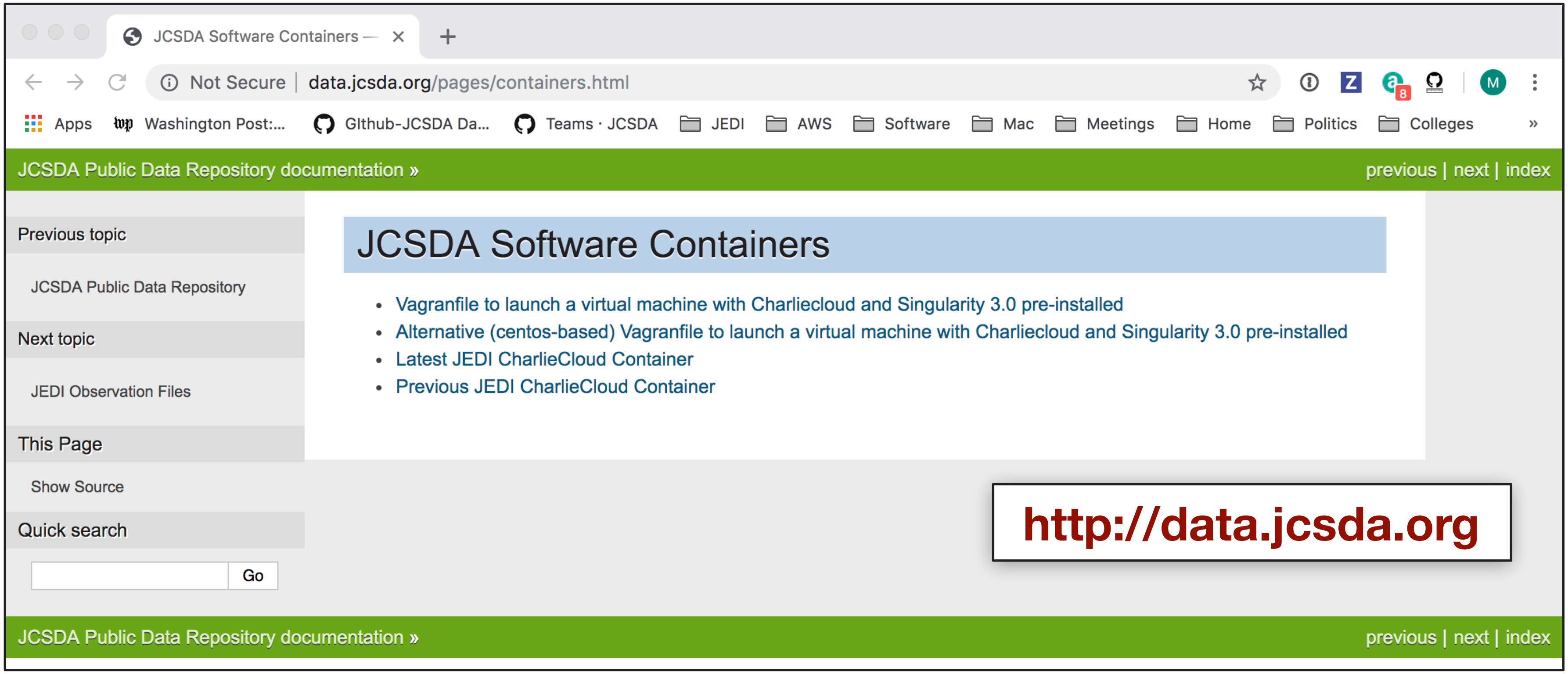
mmiesch added option to built jcsda fork of ecbuild (#18) ...

buildscripts	added option to built jcsda fork of ecbuild (#18)
modulefiles	added option to built jcsda fork of ecbuild (#18)
.gitattributes	Just moving those
.gitignore	Feature/container (#10)

Sign in now to use ZenHub

How to get the JEDI Charliecloud container

JCSDA Public Data Repository



JCSDA Software Containers

- Vagranfile to launch a virtual machine with Charliecloud and Singularity 3.0 pre-installed
- Alternative (centos-based) Vagranfile to launch a virtual machine with Charliecloud and Singularity 3.0 pre-installed
- Latest JEDI CharlieCloud Container
- Previous JEDI CharlieCloud Container

http://data.jcsda.org

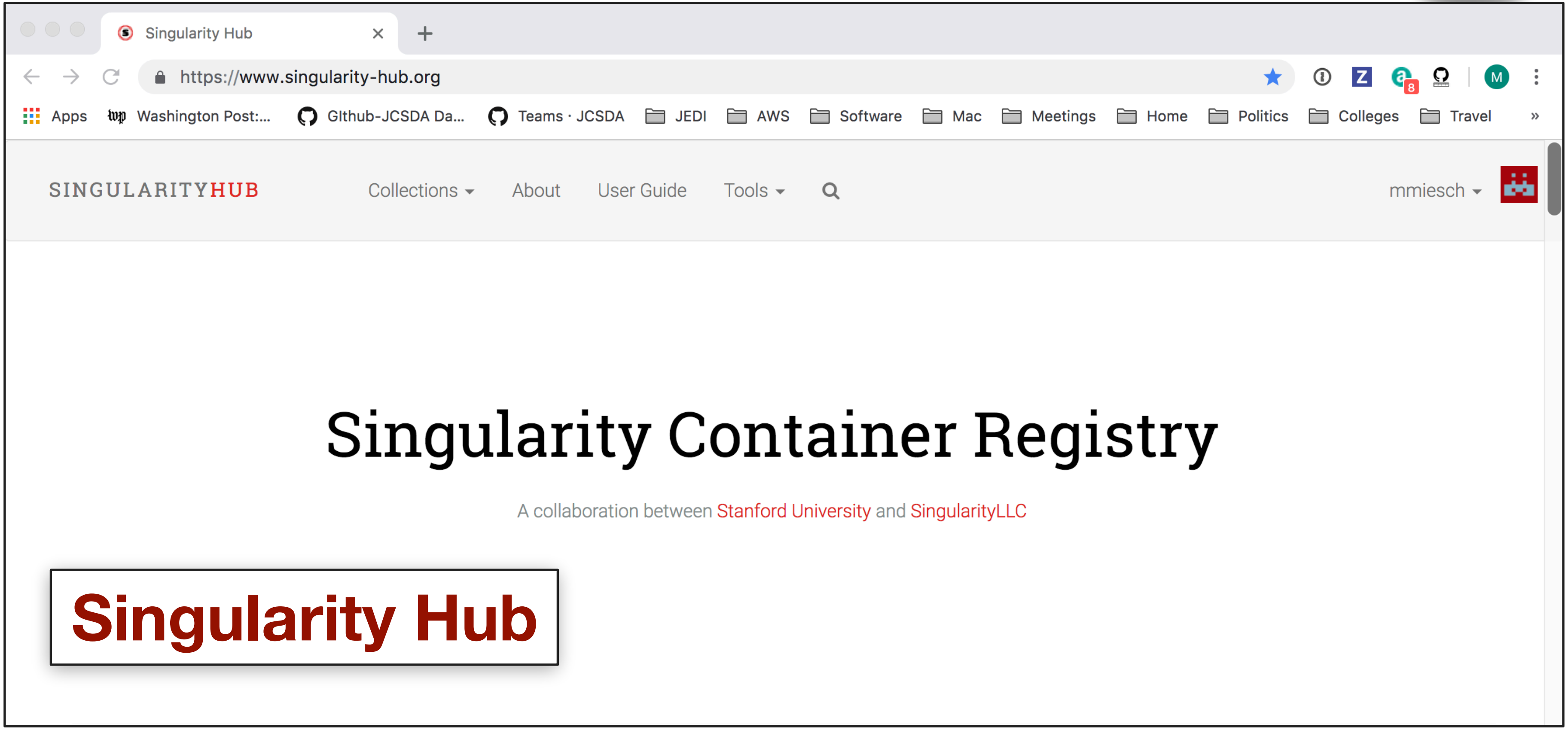
```
wget http://data.jcsda.org/containers/ch-jedi-latest.tar.gz
ch-tar2dir ch-jedi-latest.tar.gz
ch-run ch-jedi-latest — bash
```

How to install Charliecloud

```
mkdir ~/build
cd ~/build
git clone --recursive https://github.com/hpc/charliecloud.git
cd charliecloud
make
make install PREFIX=$HOME/charliecloud
```

You can install this yourself in your home directory
Even if you do not have root privileges
No need to rely on system administrators

How to get the JEDI Singularity Container



Singularity Container Registry

A collaboration between Stanford University and SingularityLLC

Singularity Hub

```
singularity pull shub://JCSDA/singularity
singularity shell -e singularity_latest.simf
```

Root privileges required to install but not to run Singularity

Using the Containers on a Mac

Mac OS does not currently support the linux user namespaces and other features that many container technologies rely on

So, to run Singularity or Charliecloud on a Mac you have to first create a linux environment by means of a virtual machine (VM)

Vagrant (HashiCorp) provides a convenient interface to Oracle's Virtualbox VM platform

```
brew cask install virtualbox
brew cask install vagrant
brew cask install vagrant-manager
```

Similar actions needed on a Windows Machine

HashiCorp Vagrant

JEDI Vagrantfile

We provide a Vagrant configuration file that is provisioned with both Singularity and Charliecloud

```
wget http://data.jcsda.org/containers/Vagrantfile
vagrant up
vagrant ssh
```

For much more information on how to use Vagrant, Singularity, and Charliecloud, see the JEDI Documentation

https://jointcenterforsatellitedataassimilation-jedi-docs.readthedocs-hosted.com

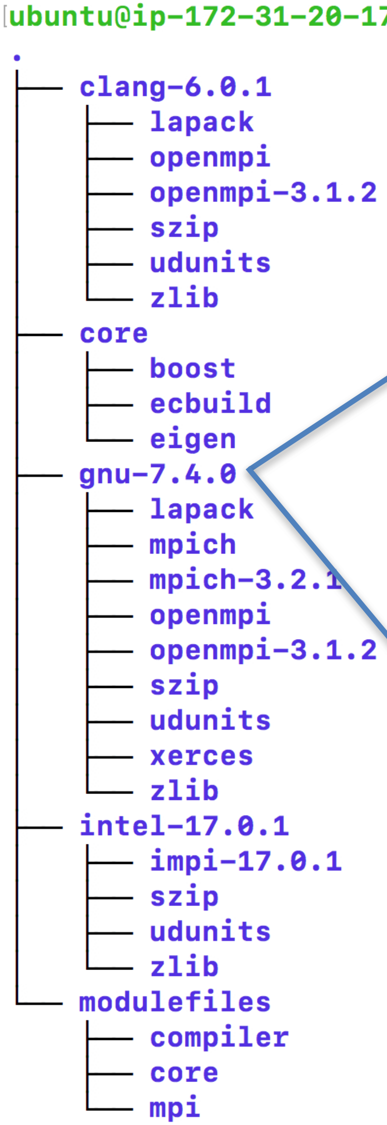
Part IV: HPC and Cloud Computing

- ## Containers in HPC?
  - An attractive option, particularly for new JEDI users
  - Need to access native compilers, MPI for peak performance

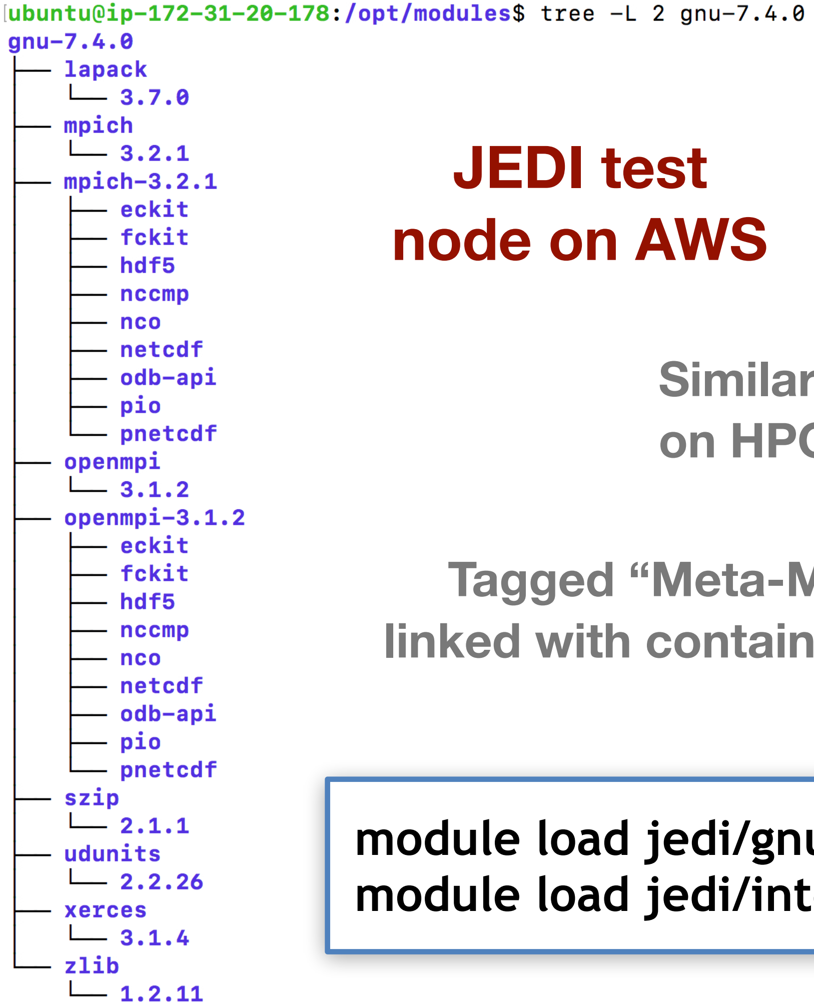
- ## Containers in the Cloud?
  - Can be an attractive option but often unnecessary with the availability of machine images (e.g. AMIs)

- ## Environment Modules
  - Greater flexibility for testing and optimization
    - JEDI Test Node on AWS
  - Maximum Performance (built from native compiler/mpi modules)
  - Maintained on selected HPC systems (Theia, Discover, Cheyenne…)

Environment modules



```
[ubuntu@ip-172-31-20-178:/opt/modules$ tree -L 2
.
├── clang-6.0.1
│   ├── lapack
│   ├── openmpi
│   ├── openmpi-3.1.2
│   ├── szip
│   ├── udunits
│   └── zlib
├── core
│   ├── boost
│   ├── ecbuild
│   └── eigen
├── gnu-7.4.0
│   ├── lapack
│   ├── mpich
│   ├── mpich-3.2.1
│   ├── openmpi
│   ├── openmpi-3.1.2
│   ├── szip
│   ├── udunits
│   ├── xerces
│   └── zlib
├── intel-17.0.1
│   ├── impi-17.0.1
│   ├── szip
│   ├── udunits
│   └── zlib
└── modulefiles
    ├── compiler
    ├── core
    └── mpi
```



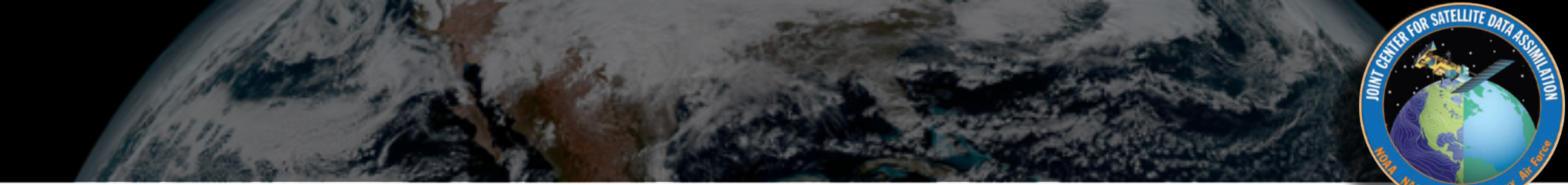
```
[ubuntu@ip-172-31-20-178:/opt/modules$ tree -L 2 gnu-7.4.0
gnu-7.4.0
├── lapack
│   └── 3.7.0
├── mpich
│   └── 3.2.1
├── mpich-3.2.1
│   ├── eckit
│   ├── fckit
│   ├── hdf5
│   ├── nccmp
│   ├── nco
│   ├── netcdf
│   ├── odb-api
│   ├── pio
│   └── pnetcdf
├── openmpi
│   └── 3.1.2
├── openmpi-3.1.2
│   ├── eckit
│   ├── fckit
│   ├── hdf5
│   ├── nccmp
│   ├── nco
│   ├── netcdf
│   ├── odb-api
│   ├── pio
│   └── pnetcdf
├── szip
│   └── 2.1.1
├── udunits
│   └── 2.2.26
├── xerces
│   └── 3.1.4
└── zlib
    └── 1.2.11
```

JEDI test node on AWS

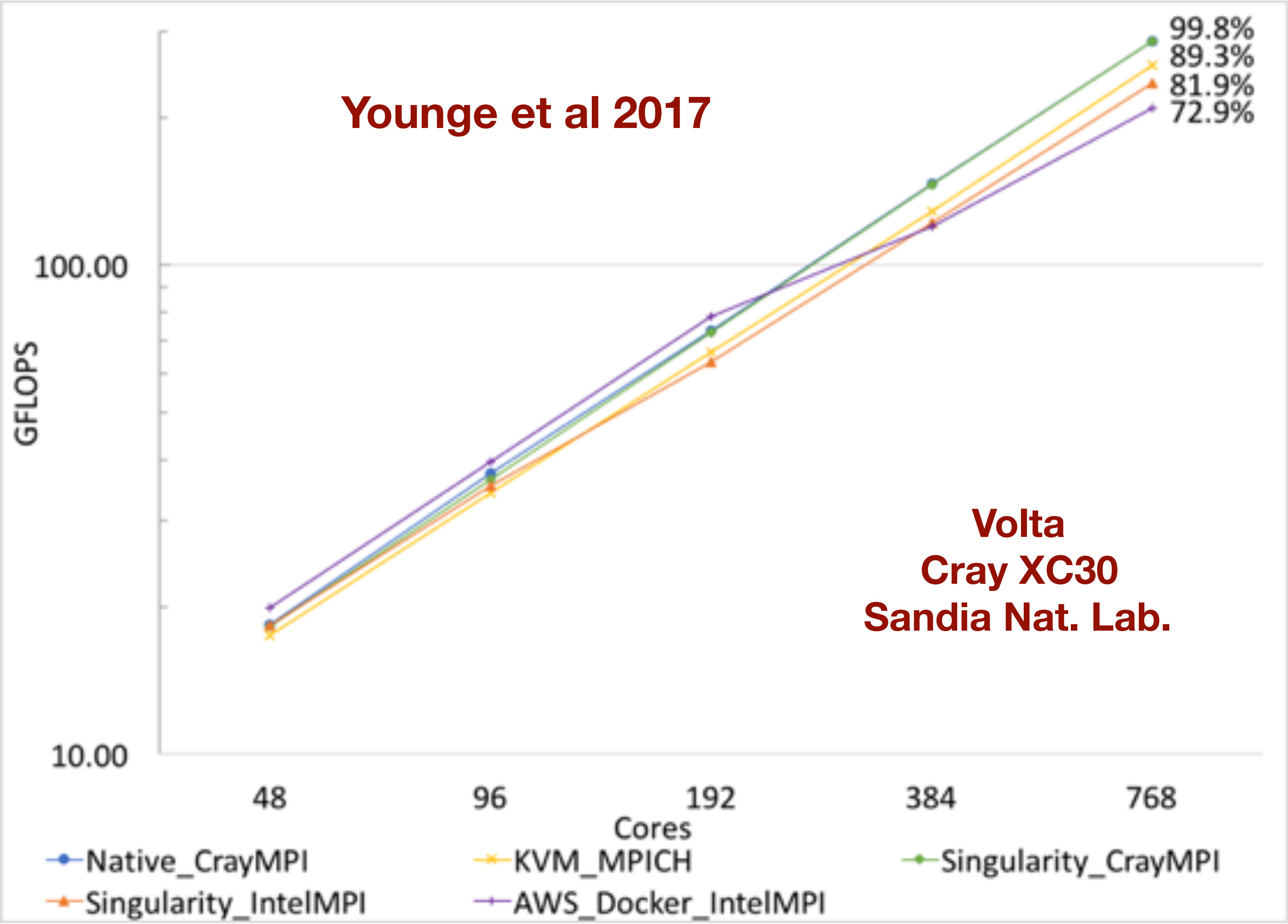
Similar structure on HPC systems

Tagged “Meta-Modules” linked with container releases

```
module load jedi/gnu-openmpi
module load jedi/intel-impi
```



Containers can achieve near-native performance (negligible overhead) but only if you tap into the native MPI libraries



Younge et al 2017

Volta
Cray XC30
Sandia Nat. Lab.

HPC containers promising, but currently not “plug and play”

Cloud Computing at JCSDA (currently)

- **JEDI Testing/Optimization**
  - ✦ CI with multiple compiler/mpi combinations
  - ✦ Scalable configurations for Parallel applications
- **JEDI Training**
  - ✦ Compute nodes for JEDI Academy
- **NWP with FV3-GFS**
  - ✦ 10-day forecast at operational resolution on AWS
    - Pre-oerational configuration
    - c5.18xlarge nodes (36 cores, 144 GiB, 25 Gbps)
    - 10-day forecast in 74 min (7.4 min/day) on 48 nodes (1536 cores)
    - 125 min (12.5 min/day) on 27 nodes (768 cores)
- **…And more**
  - ✦ Machine learning
  - ✦ FSOI
  - ✦ Data Repository

New technology should improve performance further!
FSx, EFA

Performance Estimates

Preliminary comparison (in core hours) of a moderate fv3-jedi application run on 216 cores on AWS and Discover

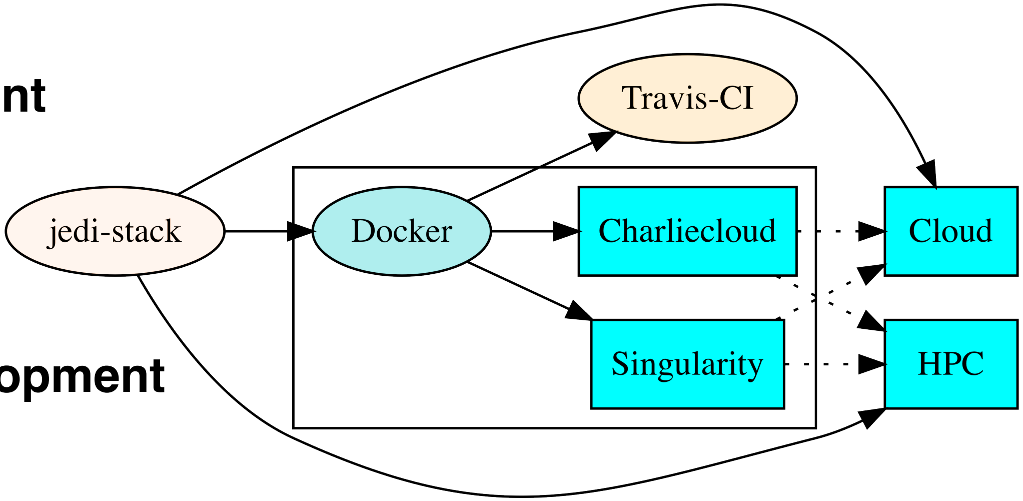
	AWS (6 c5n.18xlarge nodes)	Discover
bumpparameters_loc_geos	1.7	26
bumpparameters_cor_geos	11	39
hyb-3dvar_geos	8.8	7.7

Cheyenne	Native	Charliecloud
FV3-bundle unit tests	808.19 s	808.52 s

Summary and Outlook

I want to run JEDI on...

- My Laptop/Workstation/PC
  - ✦ Singularity/Charliecloud/Vagrant
- In the Cloud
  - ✦ Containers, AMIs (+?)
  - ✦ Web-based Front End in development
- On an HPC System
  - ✦ Environment modules on selected systems (Theia, Discover, Cheyenne…)
  - ✦ High-performance containers
  - ✦ Web-based Front End in development

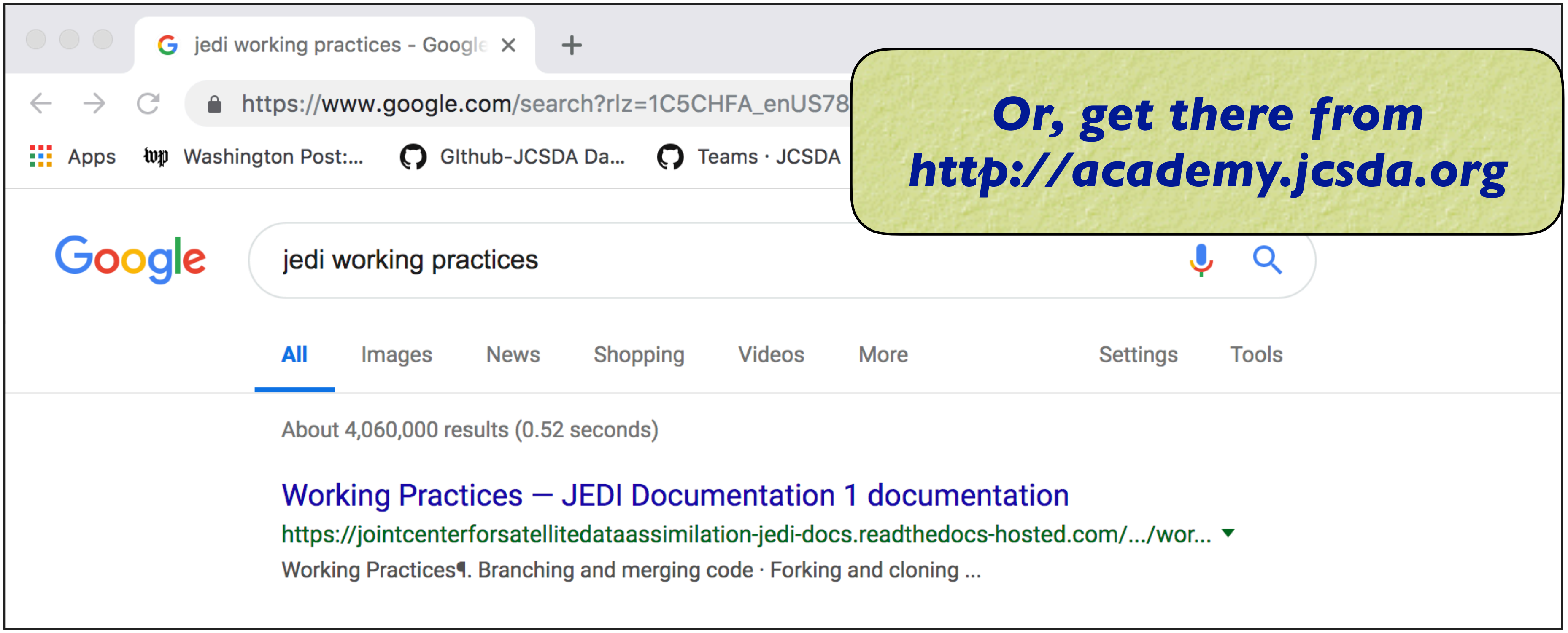


Unified, module-based build system with tagged releases

Summary and Outlook

ReadtheDocs!

https://jointcenterforsatellitedataassimilation-jedi-docs.readthedocs-hosted.com



jedi working practices

About 4,060,000 results (0.52 seconds)

Working Practices — JEDI Documentation 1 documentation

https://jointcenterforsatellitedataassimilation-jedi-docs.readthedocs-hosted.com/.../wor...

Working Practices¶. Branching and merging code · Forking and cloning ...

Or, get there from http://academy.jcsda.org