I MAKE FOSS

@imakefoss

YouTube

Kenneth Hoste - Monica Ayhens-Madon

whoami

@kehoste @boegel

- Computer scientist from Belgium
- Masters & PhD from Ghent University
- HPC system administrator at UGent since 2010
- User support & training, software installations
- Big fan of FOSS, family, loud music, (good) beer, dad jokes, stickers
- Doesn't like C++, CMake, SCons, Bazel, TensorFlow, OpenFOAM, ...

GHENT UNIVERSITY

Vlaanderen is computing

How I got hooked into FOSS...

FOSDEM

https://fosdem.org

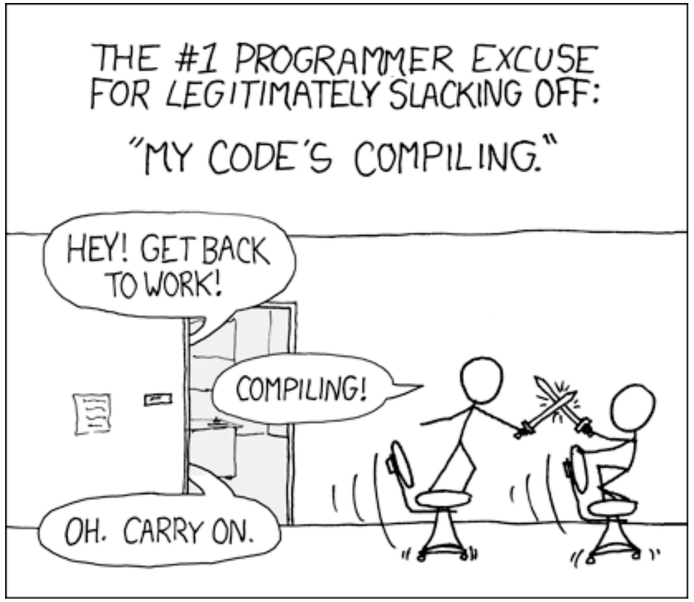
@FOSDEM

Getting Scientific Software Installed

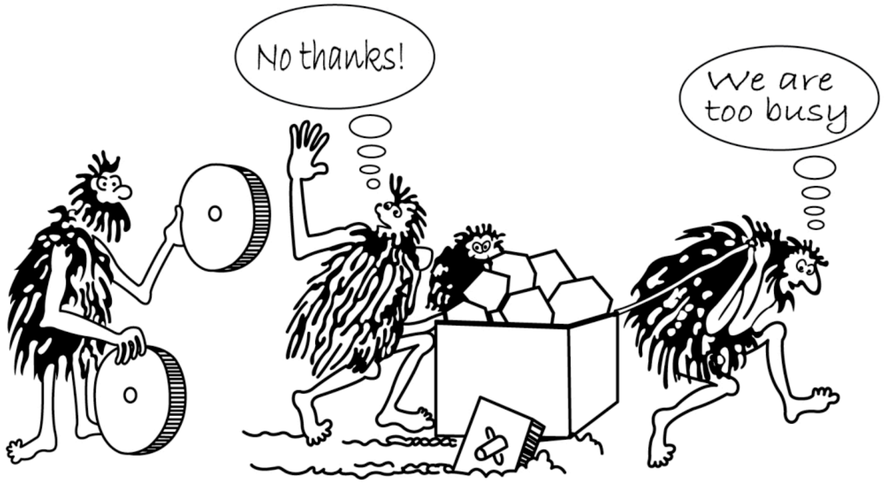
INSTALL.SH

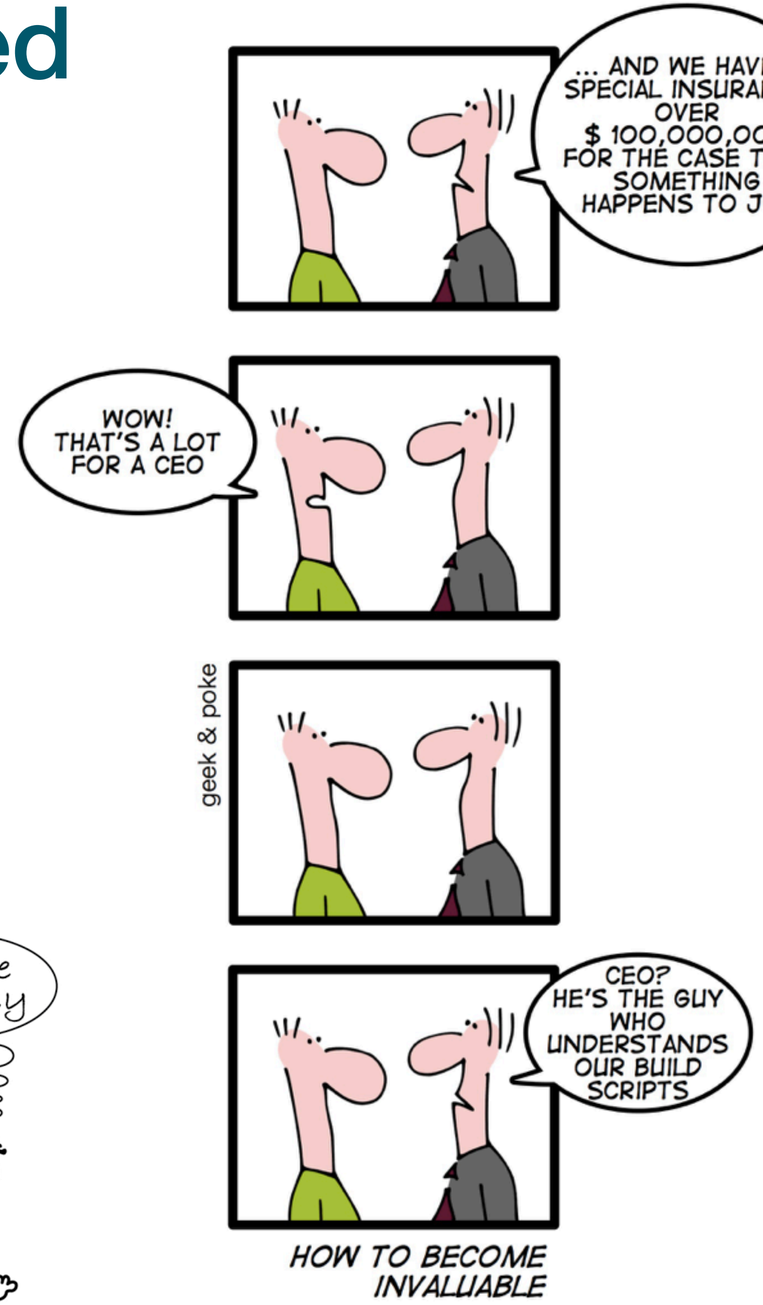
```
#!/bin/bash

pip install "$1" &
easy_install "$1" &
brew install "$1" &
npm install "$1" &
yum install "$1" & dnf install "$1" &
docker run "$1" &
pkg install "$1" &
apt-get install "$1" &
sudo apt-get install "$1" &
steamcmd +app_update "$1" validate &
git clone https://github.com/"$1"/"$1" &
cd "$1";./configure;make;make install &
curl "$1" | bash &
```

https://xkcd.com/303



https://xkcd.com/1654





http://geek-and-poke.com/geekandpoke/2010/5/14/how-to-become-invaluable.html

easybuild in a nutshell

https://easybuilders.github.io/easybuild - https://easybuild.readthedocs.io

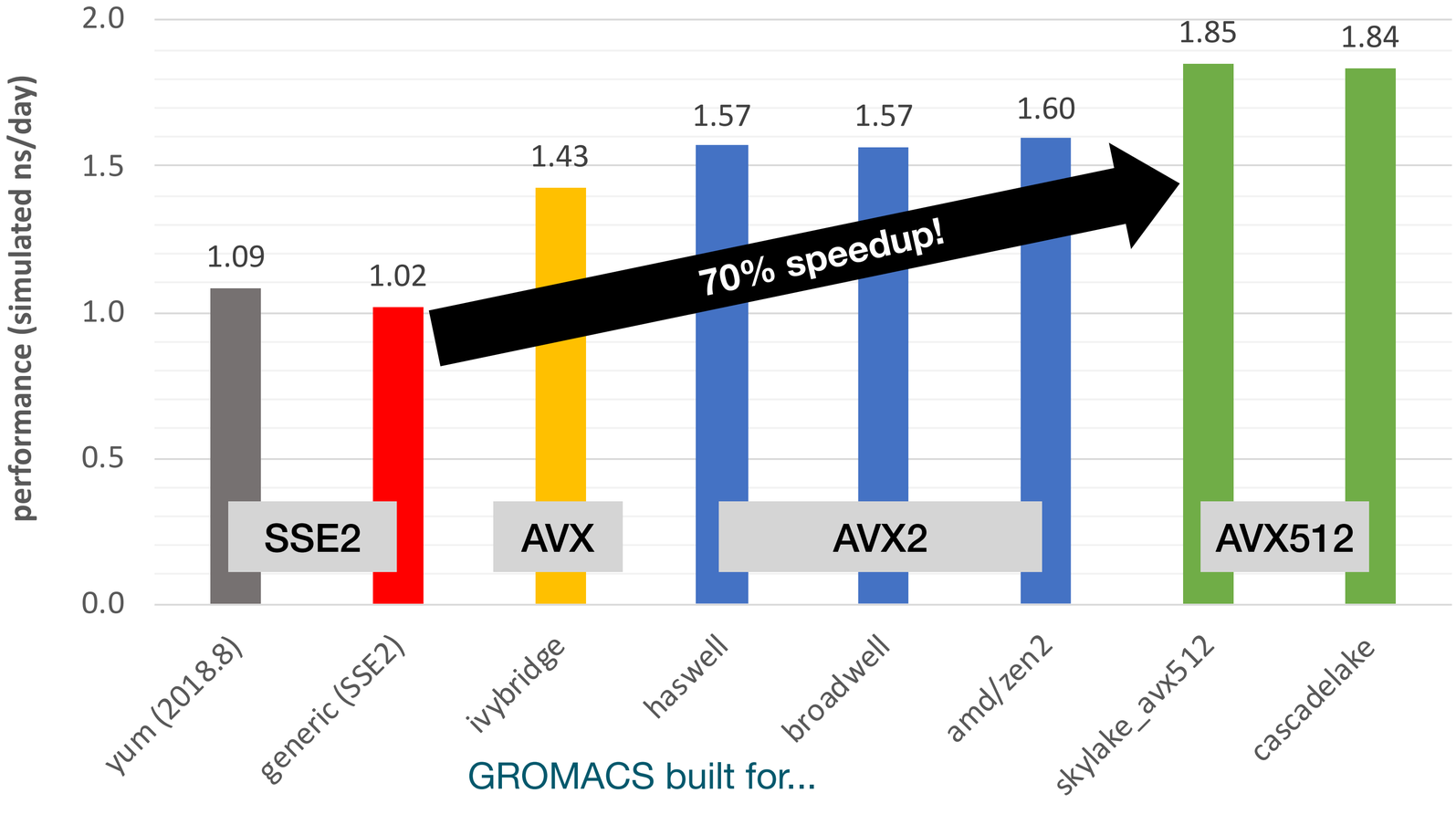
- **framework for installing scientific software** *(built from source when possible)*
- strong focus on Linux & HPC systems (and hence also performance)
- implemented in Python (2.6+ or 3.5+)
- available under GPLv2 license via PyPI + GitHub
- supports different compilers & MPI libraries, x86_64/Arm/POWER, ...
- currently supports over 2000 different software packages (+ extensions)
- welcoming and helpful worldwide community

Keeping the P in HPC

(HPC: High-Performance Computing)

- **Software should be optimised for the system it will run on**
- Impact on performance is often significant for scientific software

- Example: GROMACS
  (PRACE benchmark, Test Case B)
- Metric: (simulated) ns/day,
  higher is better
- Test system: dual-socket
  Intel Xeon Gold 6420
  (Cascade Lake, 2x18 cores)



Installing TensorFlow from source with **one command**...


```
$ eb TensorFlow-2.1.0-fosscuda-2019b-Python-3.7.4.eb
```

Installing TensorFlow from source with **one command**...


```
$ eb TensorFlow-2.1.0-fosscuda-2019b-Python-3.7.4.eb
== temporary log file in case of crash /tmp/eb-GyvPHx/easybuild-U1TkEI.log
== processing EasyBuild easyconfig TensorFlow-2.1.0-fosscuda-2019b-Python-3.7.4.eb
== building and installing TensorFlow/2.1.0-fosscuda-2019b-Python-3.7.4...
== fetching files...
== creating build dir, resetting environment...
== unpacking...
== patching...
== preparing...
== configuring...
== building...
```

Installing TensorFlow from source with **one command**...


```
$ eb TensorFlow-2.1.0-fosscuda-2019b-Python-3.7.4.eb
== temporary log file in case of crash /tmp/eb-GyvPHx/easybuild-U1TkEI.log
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== fetching files...
== creating build dir, resetting environment...
== unpacking...
== patching...
== preparing...
== configuring...
== building...
== testing...
== installing...
== taking care of extensions...
== postprocessing...
== sanity checking...
== cleaning up...
== creating module...
== permissions...
== packaging...
== COMPLETED: Installation ended successfully
== Results of the build can be found in the log file /software/TensorFlow/2.1.0-...
== Build succeeded for 1 out of 1
== Temporary log file(s) /tmp/eb-GyvPHx/easybuild-U1TkEI.log* have been removed.
== Temporary directory /tmp/eb-GyvPHx has been removed.
```

EESSI in a nutshell

EESSI

- **European Environment for Scientific Software Installations**
  (EESSI, pronounced as "easy")
- Collaboration between different partners in HPC community
- Goal: **building a common scientific software stack**
  for HPC systems & beyond (cloud, workstations, ...)

https://eessi-hpc.org

https://github.com/eessi

https://eessi.github.io/docs/pilot

@eessi_hpc

Scope & goals

EESSI

- **Shared repository of scientific software installations**
- Collaborate, avoid duplicate work across HPC sites
- **Uniform way of providing software to researchers**
- Offer broad platform support (Linux, macOS, Windows)
- **Targets: laptops, personal workstations, HPC clusters, and the cloud**
- Support for different CPUs, interconnects, GPUs, etc.
- Focus on **performance**, automation, testing, tuning

http://www.thecomicstrips.com/subject/The-Collaboration-Comic-Strips.php

EESSI is powered by FOSS

CernVM-FS

- Software distribution service
- Scalable, read-only
- Mount filesystem over HTTP

https://cernvm.cern.ch/fs

gentoo

- Linux distribution, installs from source
- Prefix project: install packages in <prefix>
- Supports x86_64, Arm, ... & Linux, macOS

https://wiki.gentoo.org/wiki/Project:Prefix

easybuild

- Installation tool for scientific software
- Optimises for build host (by default)
- Supports over 2,000 software pkgs

https://easybuilders.github.io/easybuild

Lmod

- Environment modules tool (written in Lua)
- Intuitive access to software installations
- Multiple software versions side-by-side

https://lmod.readthedocs.io

- Python library
- Detect CPU family
- Compare CPUs (compatibility)

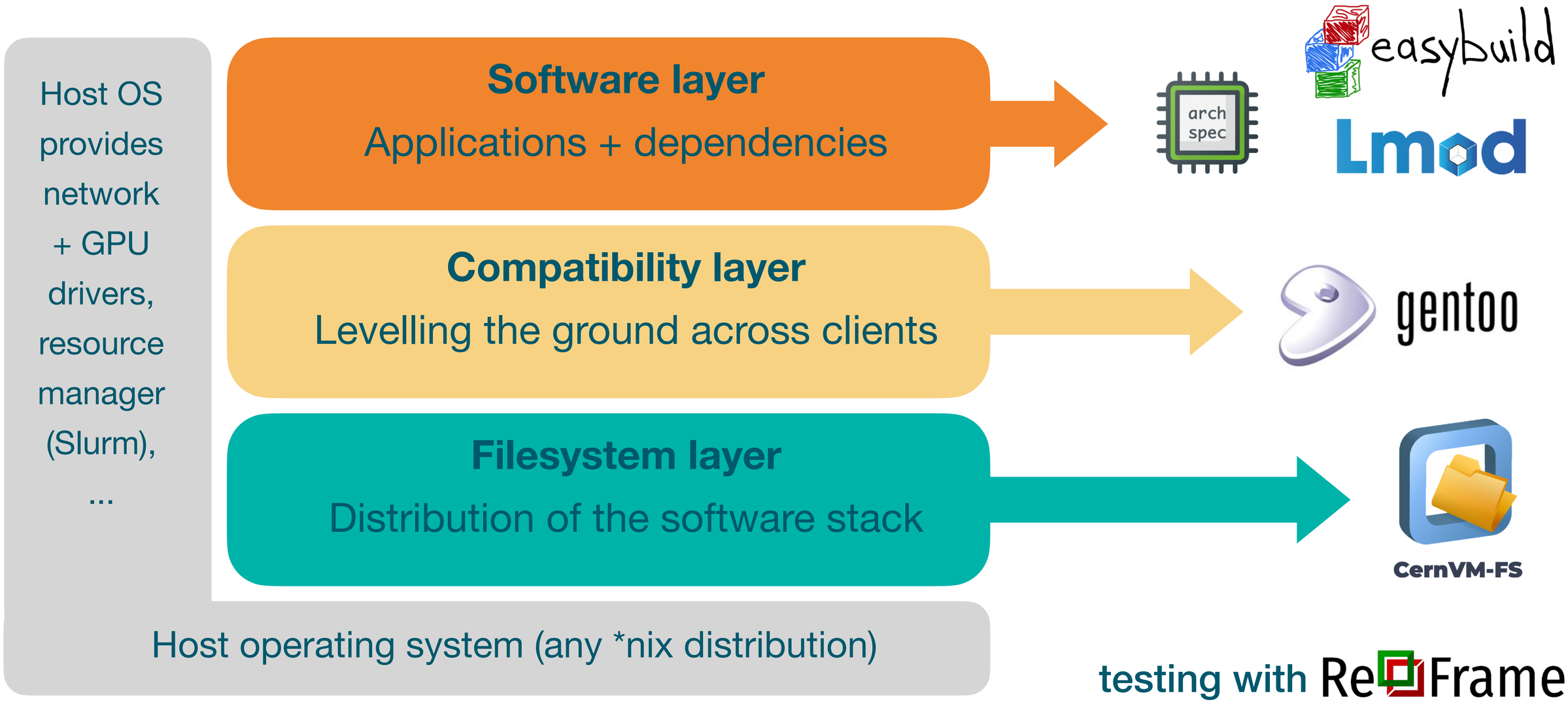
https://github.com/archspec

ReFrame

- regression testing framework for HPC
- tests are implemented in Python

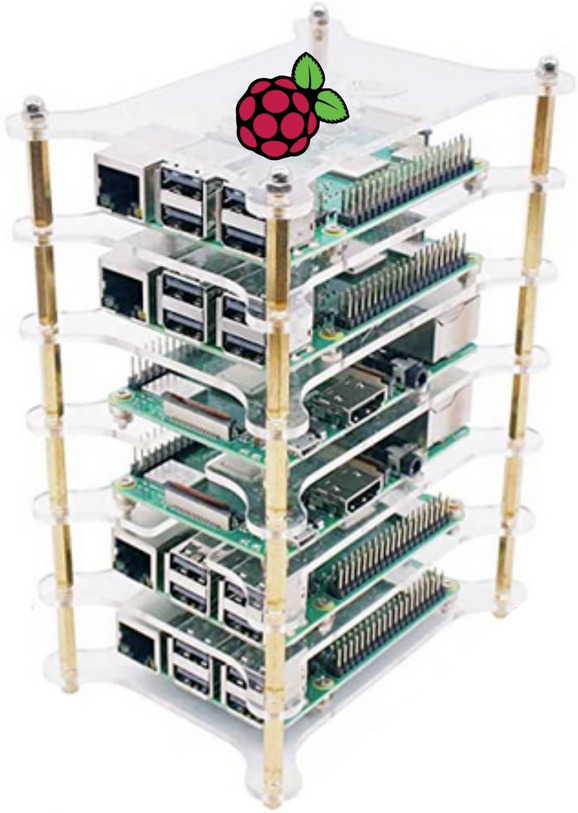
https://reframe-hpc.readthedocs.io

High-level overview of EESSI project



Demo time!

https://github.com/boegel/eessi-demo



EESSI

EUROPEAN ENVIRONMENT FOR
SCIENTIFIC SOFTWARE INSTALLATIONS

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@kehoste (Twitter)

Website: https://www.eessi-hpc.org

Join our mailing list & Slack channel

https://www.eessi-hpc.org/join

Documentation: https://eessi.github.io/docs

GitHub: https://github.com/eessi

Twitter: @eessi_hpc

EESSI

EUROPEAN ENVIRONMENT FOR
SCIENTIFIC SOFTWARE INSTALLATIONS

SORSE

International Series of Online Research Software Events

https://sorse.github.io

EESSI software demo

Wed Nov 25th 2020 - 3pm UTC

https://sorse.github.io/programme/software-demos/event-028