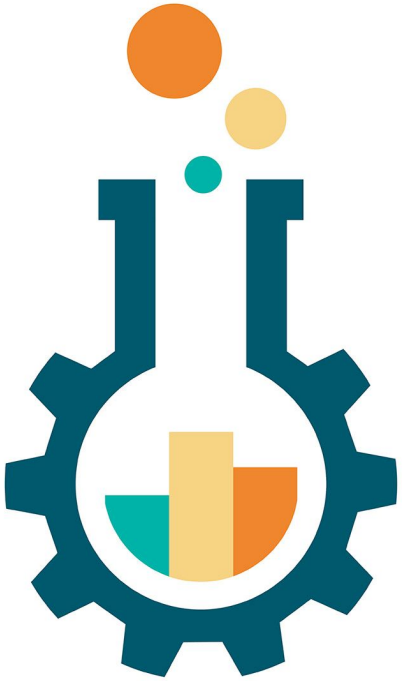
Prepared environment

- This information (and more!) is available at https://hackmd.io/@multixscale/CASTIEL2

- Small AlmaLinux 8 cluster (in the cloud)
  - System will be up until the end of the tutorial (~18:00 CET)

- **You need to create an account!**
  - Signup: https://mokey.cluster.eessi.science/auth/signup
  - Accounts will only be approved for access on the day, so **please record your username/password !**
    - "Reset password" link does **not** work, instead raise any login problem in Slack

- Access via `ssh` or web browser **(pick one and stick to it!)**
  - Shell access: `ssh <username>@cluster.eessi.science`
    - Use login node for hands-on, it has only 16 cores but should be fine to share for small group
  - Via browser: https://cluster.eessi.science
    - Make sure to change default "Time" to 2 hours, increase number of cores to 2 with 6GB RAM



EasyBuild

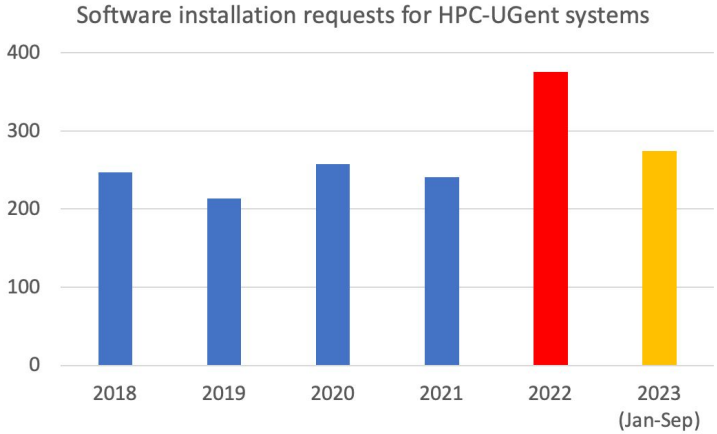
Introduction to EESSI

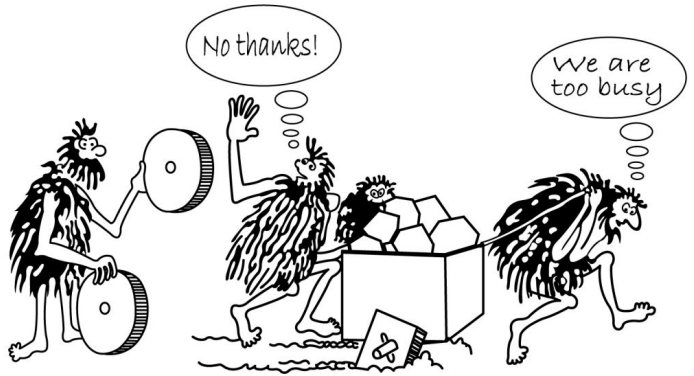
EUROPEAN ENVIRONMENT FOR SCIENTIFIC SOFTWARE INSTALLATIONS

Alan O'Cais
University of Barcelona/CECAM
alan.ocais@cecam.org

The changing landscape of scientific computing

- **Explosion of available scientific software** applications (bioinformatics, AI boom, …)
- Increasing interest in **cloud** for scientific computing (flexibility!)
- **Increasing variety in processor (micro)architectures** beyond Intel & AMD:
  Arm is ~~coming~~ already here (see Fugaku, JUPITER, …), RISC-V is coming (soon?)
- In strong contrast: available (wo)manpower **in HPC support teams is (still) limited**…

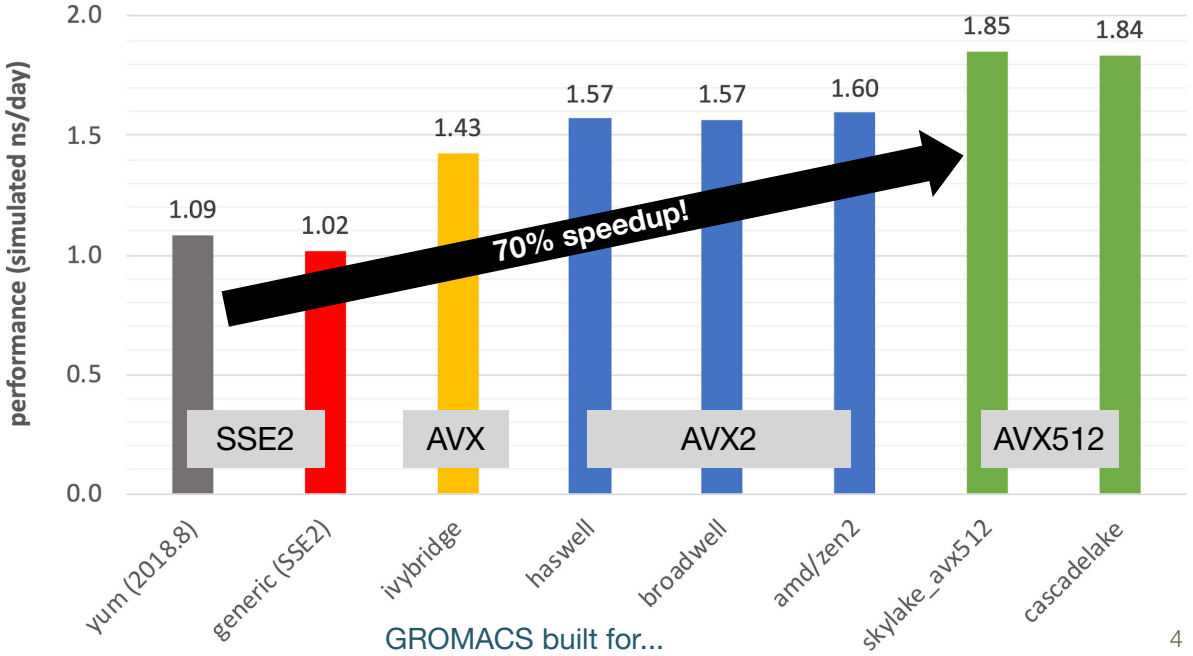




Optimized scientific software installations

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

- Example: GROMACS 2020.1 (PRACE benchmark, Test Case B)
- Metric: (simulated) ns/day, higher is better
- Test system: dual-socket Intel Xeon Gold 6420 (Cascade Lake, 2x18 cores)
- **Performance of different GROMACS binaries, on exact same hardware/OS**



EESSI in a nutshell

- *European Environment for Scientific Software Installations (EESSI)*
- **Shared repository of (optimized!) scientific software *installations***
- Avoid duplicate work across (HPC) sites by collaborating on a shared software stack
- Uniform way of providing software to users, regardless of the system they use!
- Should work on any Linux OS (+ WSL, and possibly macOS) and system architecture
  - From laptops and personal workstations to HPC clusters and cloud
  - Support for different CPUs, interconnects, GPUs, etc.
- **Focus on performance, automation, testing, collaboration**

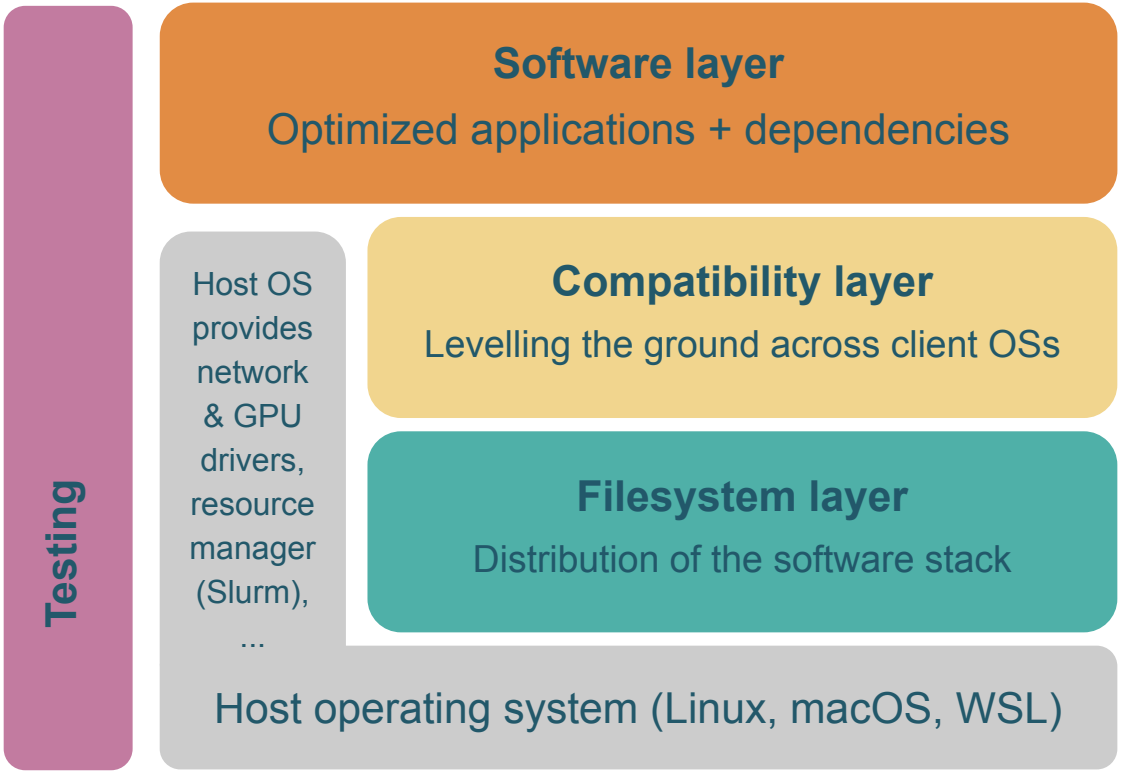
https://www.eessi.io

https://www.eessi.io/docs/

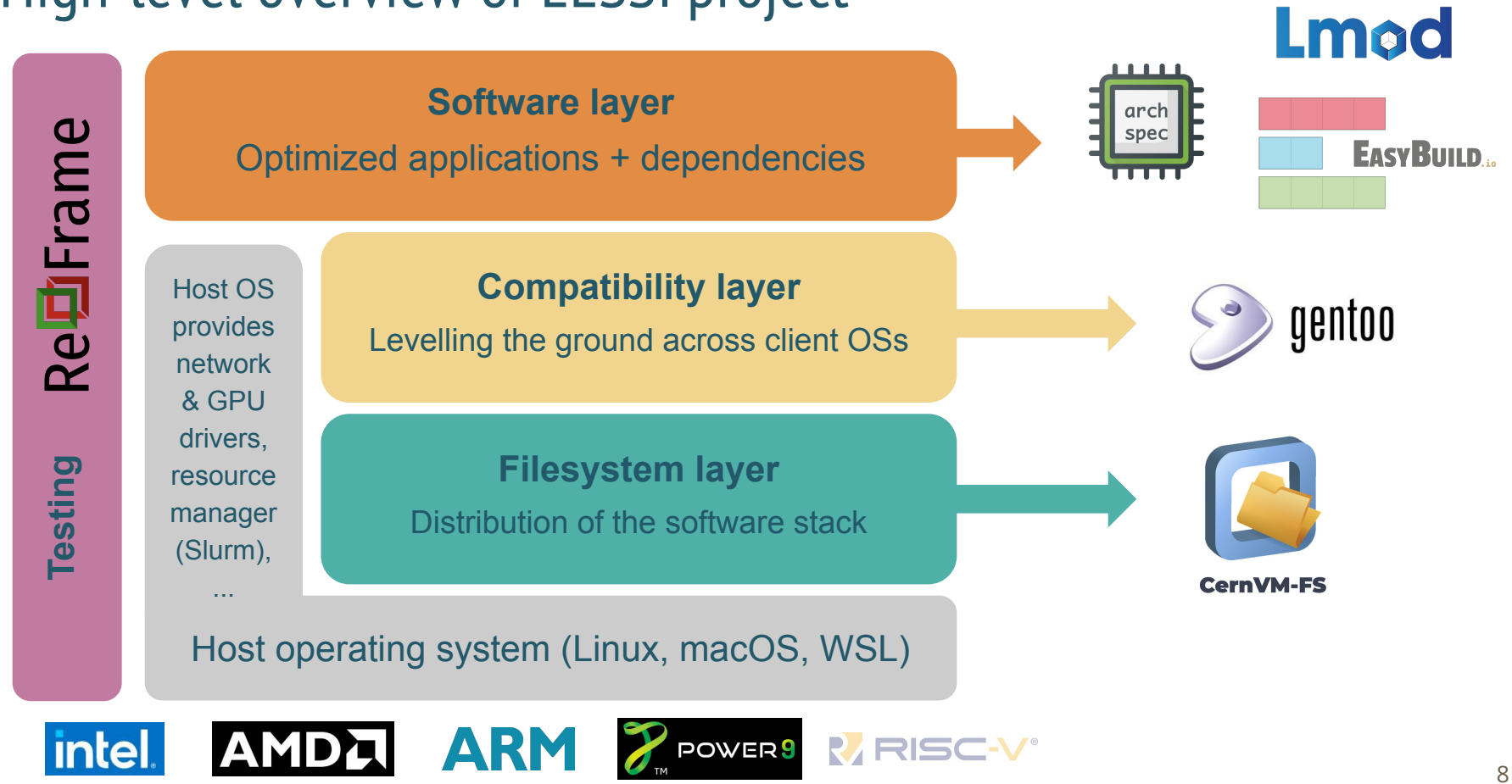
Major goals of EESSI

- **Avoid duplicate work** (for researchers, HPC support teams, …)
  - Tools that automate software installation process (EasyBuild, Spack) are not sufficient
  - Go beyond sharing build recipes => work towards a shared software stack
- Providing a truly **uniform software stack**
  - Use the (exact) same software environment everywhere
  - Without sacrificing performance for “mobility of compute” (like is typically done with containers/conda)
- Facilitate HPC training, development of (scientific) software, …

High-level overview of EESSI project



High-level overview of EESSI project



High-level overview of EESSI project

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DEMO

Demo scenario

- Demo: Using an “empty” **Amazon Linux 2023** VM in AWS (**Arm Graviton2**)
  - No CernVM-FS installed, EESSI not available yet, but only takes 2 min.
  - Requires admin rights (`sudo` to install extra packages)
  - Set up EESSI environment by sourcing init script
  - Running EESSI demo script from

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

Demo: Amazon Linux 2023 Arm VM in AWS (1/2)

- We needed to: https://github.com/EESSI/eessi-demo
  - Install CernVM-FS packages
  - Install EESSI CernVM-FS configuration (`cvmfs-eessi-config*` package)
  - Set up minimal client configuration in `/etc/cvmfs/default.local`
- For production usage (especially large-scale), you should also:
  - Use a squid proxy, next to a local client cache (better start-up performance)
  - Set up your own Stratum-1 mirror server (protection against network disconnects)
  - Also recommended to “be a good citizen” in the EESSI CernVM-FS network

Demo: Amazon Linux 2023 Arm VM in AWS (2/2)

- Once CernVM-FS + EESSI configuration is installed, you're good to go!
- Set up EESSI environment by sourcing the init script, load modules, run.

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

```
$ ls /cvmfs/pilot.eessi-hpc.org
host_injections latest versions

$ source /cvmfs/pilot.eessi-hpc.org/latest/init/bash
...
Environment set up to use EESSI pilot software stack, have fun!

$ module avail GROMACS TensorFlow OpenFOAM Bioconductor

------ /cvmfs/pilot.eessi-hpc.org/versions/2021.12/software/linux/aarch64/graviton2/modules/all -------

      GROMACS/2020.1-foss-2020a-Python-3.8.2       OpenFOAM/9-foss-2021a                      (D)
      GROMACS/2020.4-foss-2020a-Python-3.8.2 (D)   R-bundle-Bioconductor/3.11-foss-2020a-R-4.0.0
      OpenFOAM/v2006-foss-2020a                    TensorFlow/2.3.1-foss-2020a-Python-3.8.2
      OpenFOAM/8-foss-2020a
```

Demo: Amazon Linux 2023 Arm VM in AWS (2/2)

- Once CernVM-FS + EESSI configuration is installed, you're good to go!

Production version is **`software.eessi.io`** :

`source /cvmfs/software.eessi.io/versions/2023.06/init/bash`

(but doesn't work with all demo examples yet)

```
OpenFOAM/v2006-foss-2020a
OpenFOAM/8-foss-2020a
TensorFlow/2.3.1-foss-2020a-Python-3.8.2
```

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Hands-on 1: Running a demo

Hands-on scenario

- On provided infrastructure (**AlmaLinux 8**)
  - EESSI CernVM-FS repository readily available and configured
  - Nodes are pretty low-spec (16 cores, Skylake), front-end has 16 cores...but the examples are also not very demanding
  - Run an EESSI demo script after:

```
git clone https://github.com/EESSI/eessi-demo
```

Try out EESSI yourself using Apptainer!

- Only Apptainer (or Singularity) is required to run the EESSI client container
- **Should work on any Linux distribution**, on Intel/AMD/Arm CPUs
- Detailed instructions available at https://www.eessi.io/docs/pilot

```
$ apptainer shell --fusemount ...
...
Apptainer> ls /cvmfs/software.eessi.io/
host_injections  README.eessi  versions

Apptainer> source /cvmfs/software.eessi.io/versions/2023.06/init/bash

Found EESSI repo @ /cvmfs/software.eessi.io/versions/2023.06!
archdetect says x86_64/generic
Using x86_64/generic as software subdirectory.
Using /cvmfs/software.eessi.io/versions/2023.06/software/linux/x86_64/generic/modules/all as the directory to be
added to MODULEPATH.
Found Lmod configuration file at
/cvmfs/software.eessi.io/versions/2023.06/software/linux/x86_64/generic/.lmod/lmodrc.lua
Initializing Lmod...
Prepending /cvmfs/software.eessi.io/versions/2023.06/software/linux/x86_64/generic/modules/all to $MODULEPATH...
Environment set up to use EESSI (2023.06), have fun!
```

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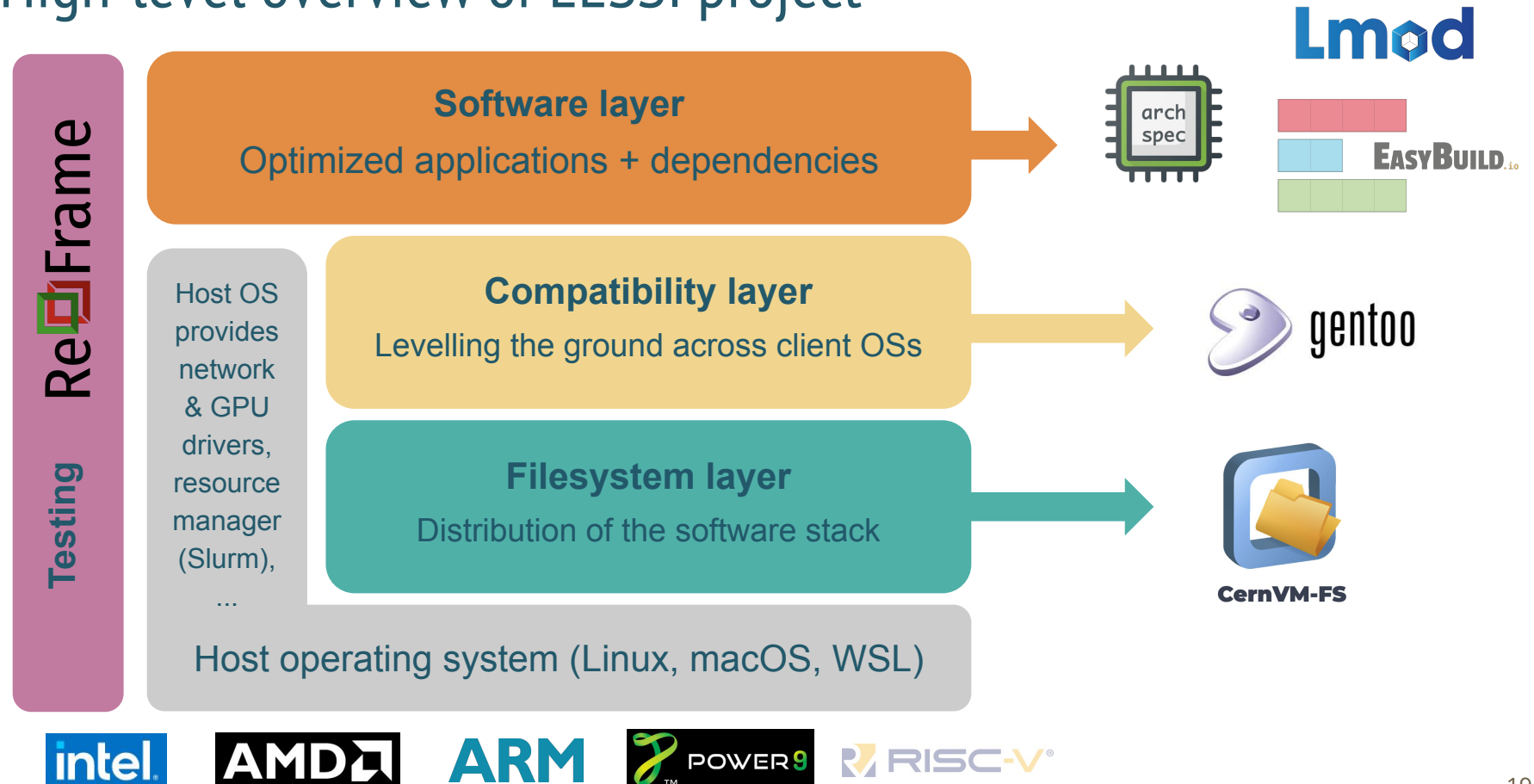
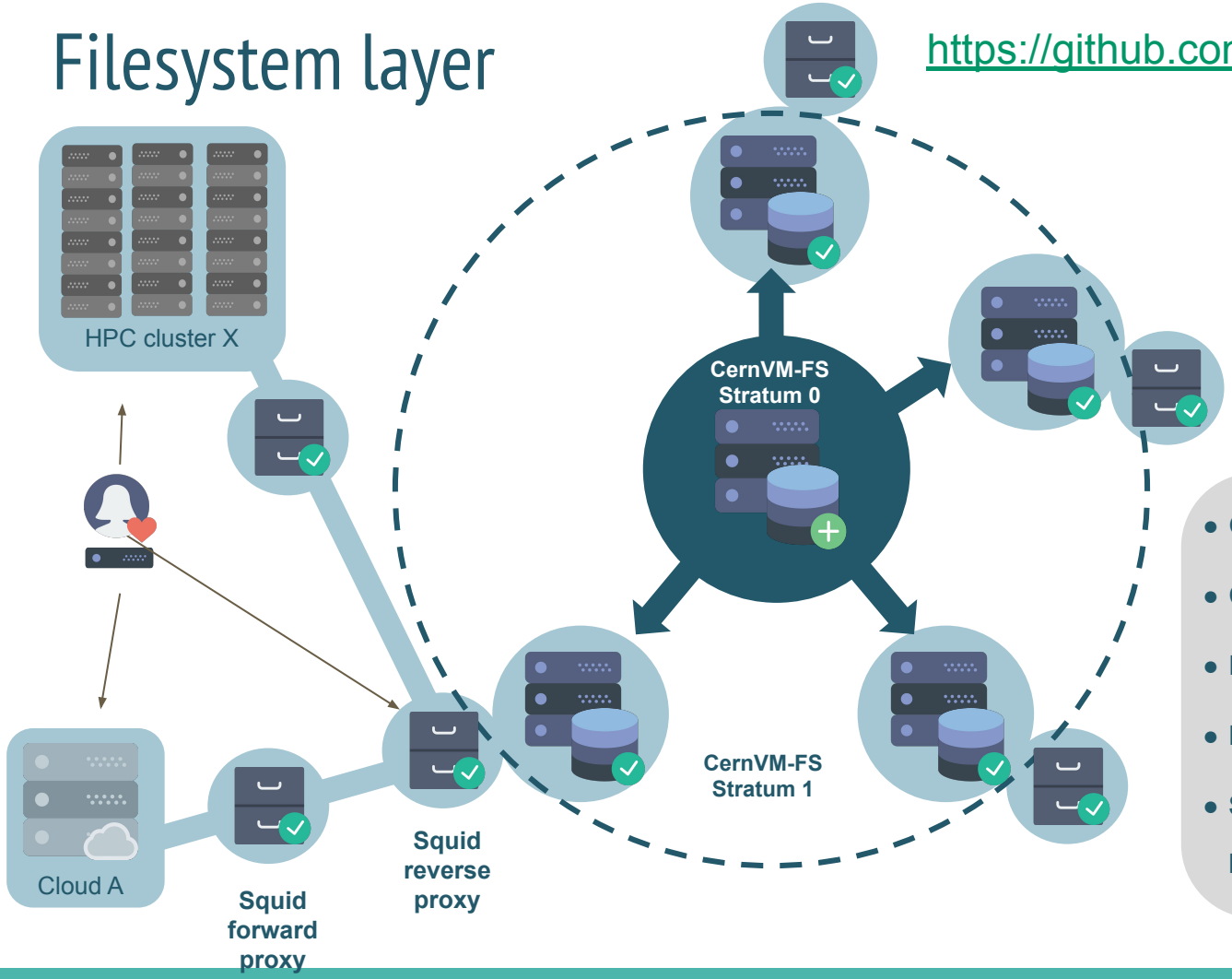
How exactly does it work?

High-level overview of EESSI project



Filesystem layer

https://github.com/EESSI/filesystem-layer



CernVM-FS

https://cvmfs.readthedocs.io

- Global distribution of software installations
- Centrally managed software stack
- Redundant network of “mirrors”
- Multiple levels of caching
- **Same software stack everywhere**:
  laptops, HPC clusters, cloud VMs, …

(icons via https://www.flaticon.com/authors/smashicons)

Compatibility layer

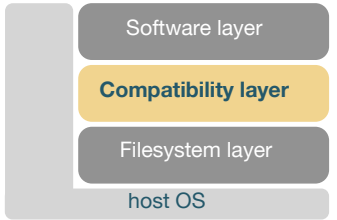
https://github.com/EESSI/compatibility-layer

- **Gentoo Prefix** installation (in `/cvmfs/.../compat/<os>/<arch>/`)
- Set of tools & libraries installed in non-standard location
- Limited to low-level stuff, incl. glibc (no Linux kernel or drivers)
  - Similar to the OS layer in container images
- Only targets a supported processor **family** (`aarch64`, `x86_64`, `riscv64`)
- **Levels the ground for different client operating systems** (Linux distros, later also macOS?)
- Currently in production repository:

  `/cvmfs/software.eessi.io/versions/2023.06/compat/linux/aarch64`

  `/cvmfs/software.eessi.io/versions/2023.06/compat/linux/x86_64`

powered by



Software layer

https://github.com/EESSI/software-layer

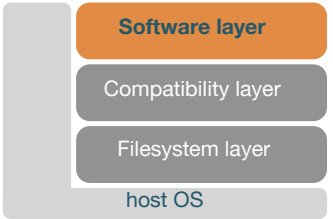
- Provides scientific software applications, libraries, and dependencies
- **Optimized for specific CPU microarchitectures** (Intel Haswell, ...)
  - Separate subdirectory/tree for each (in `/cvmfs/.../software/...`)
- **Leverages libraries** (like glibc) **from compatibility layer** (not from host OS)
- Installed with EasyBuild, incl. environment module files
- Lmod environment modules tool is used to access installations
- **Best subdirectory for host is selected automatically** via archspec (`archdetect` in production version)

EESSI

powered by

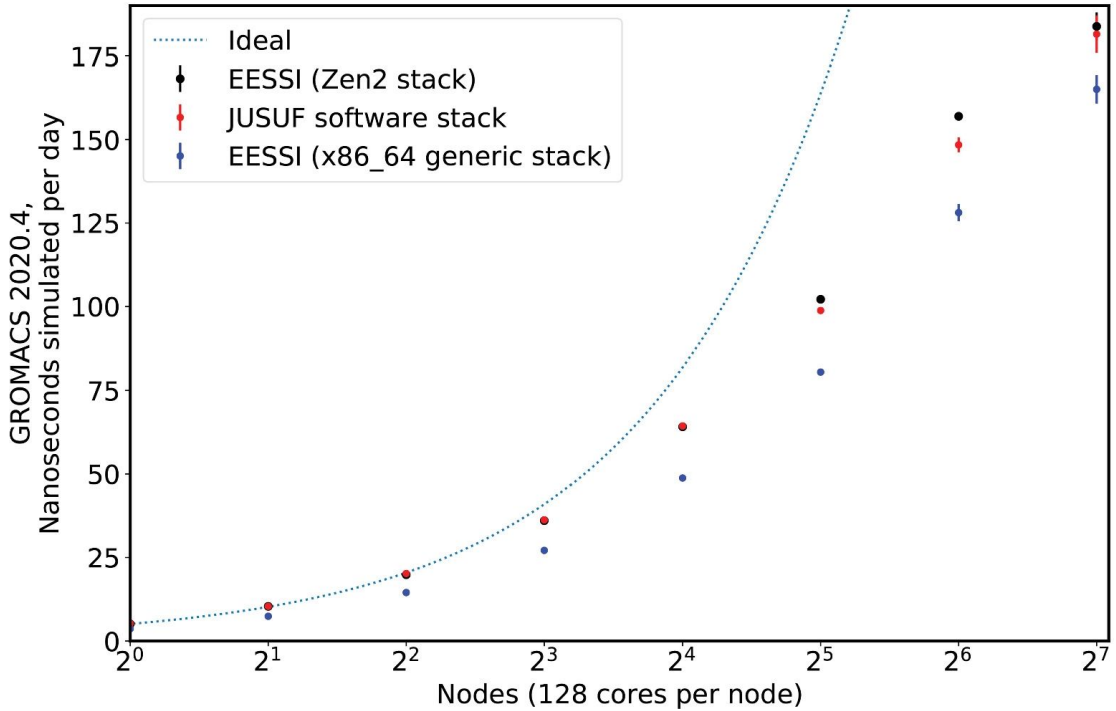
EasyBuild

Lmod



EESSI paper (open access)

doi.org/10.1002/spe.3075



Paper includes proof-of-concept performance evaluation compared to system software stack, performed at JUSUF @ JSC using GROMACS 2020.4, up to 16,384 cores (CPU-only)

Current status of EESSI

- **Production repository `software.eessi.io` has been released!**
- Ansible playbooks, scripts, docs at `https://github.com/eessi`
- CernVM-FS: Stratum 0 @ Univ. of Groningen + two Stratum 1 servers
- Software (CPU-only): Bioconductor, GROMACS, OpenFOAM, R, TensorFlow, ...
- Hardware targets:
  - `{aarch64,x86_64}/generic`
  - `intel/{haswell,skylake_avx512}, amd/{zen2,zen3}, aarch64/{neoverse_n1,neoverse_v1)`
- NVIDIA GPU support verified and under code review
- Supported by Azure and AWS: sponsored credits to develop necessary infrastructure

Microsoft Azure

aws

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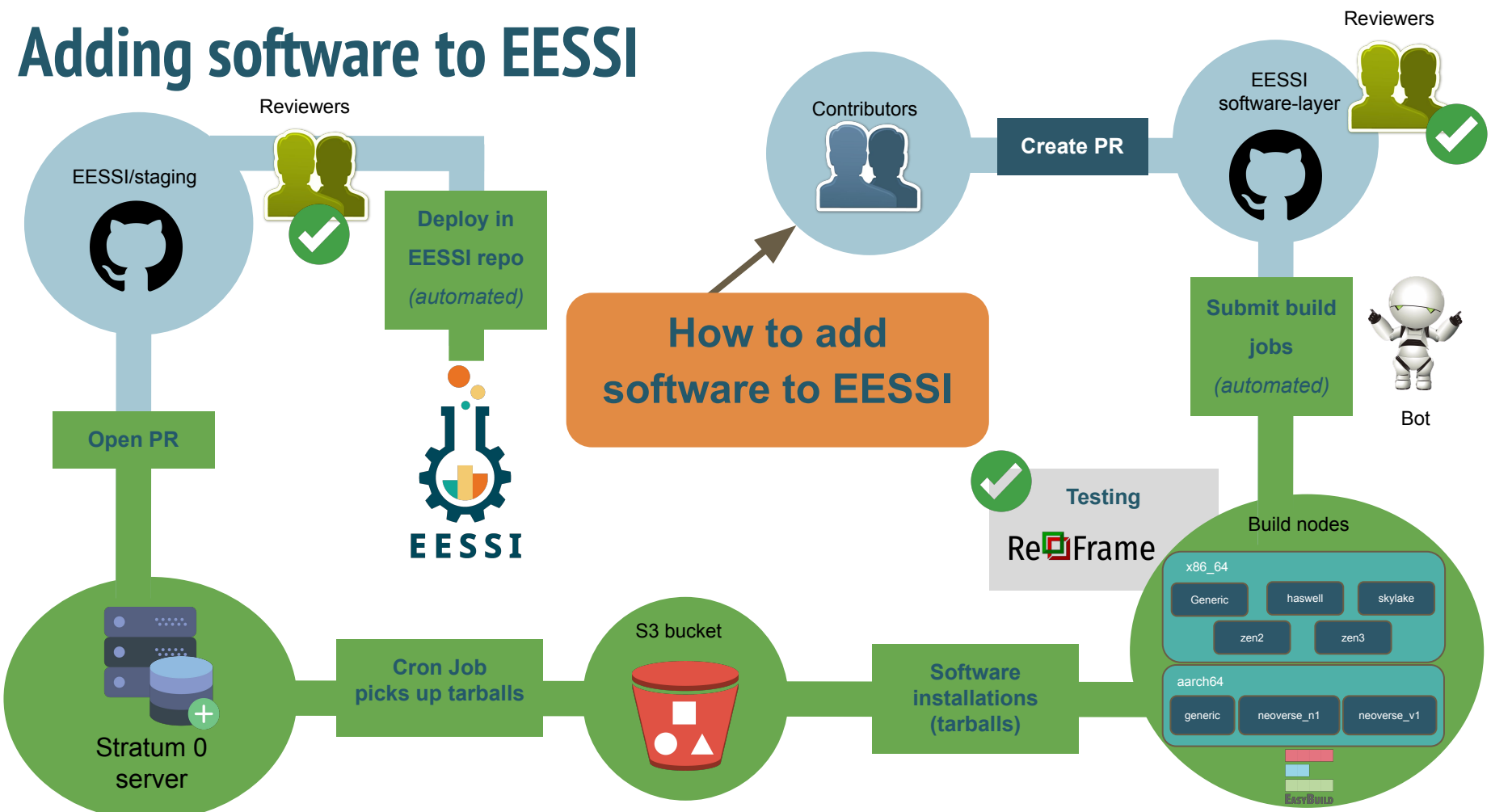
What about adding the software I care about?

Adding software to EESSI



eessi.io/docs/software_layer/adding_software

EESSI use cases

Overview of use cases enabled by EESSI

- A uniform software stack across HPC clusters, clouds, servers, and laptops
- Enable portable workflows
- Can be leveraged in continuous integration (CI) environments
- Significantly facilitates setting up infrastructure for HPC training
- Enhanced collaboration with software developers and application experts

Also discussed in our open-access paper, available via [doi.org/10.1002/spe.3075](doi.org/10.1002/spe.3075)

EESSI provides a uniform software stack

- Main goal: **same software everywhere**: laptop, server, HPC, cloud, …
- Wide variety of systems supported
  - CPUs: `x86_64` (Intel, AMD), `aarch64` (Arm), `riscv64` (soon…)
  - OS: any Linux distribution, Windows via WSL, macOS should be possible too
  - High-speed interconnects (Infiniband), GPUs, etc.
- **Without compromising on software performance**
  - Optimized software installations for specific CPU microarchitectures + auto-detection
  - Large contrast with generic binaries often used in containers
- Facilitates migrating from laptop to HPC, cloud bursting, …

EESSI enables portable workflows

- Portable workflows are significantly easier when relying on EESSI
- They often involve running a broad set of tools, which all need to be available
- Workflows definitions (Snakemake, Nextflow,…) can leverage (or be included in) EESSI
- You can ship your execution environment *inside* your git repository using `direnv`
    - If your users have EESSI and `direnv`, then can start running your workflow after cloning!

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Hands-on 2: Shipping a workflow

Hands-on scenario

- On provided infrastructure (AlmaLinux 8)
  - EESSI is available but `direnv` is not
- Clone a workflow that leverages EESSI
  - `git clone https://github.com/EESSI/eessi-nextflow-example`
- Workflow is trivial so can be run via shell
  - Enter repository: `cd eessi-nextflow-example`
  - Setup `direnv`: `source ./.install_direnv.sh`
  - Allow `direnv` in dir: `direnv allow`
  - Run the workflow: `./hello_plus_version.nf`

Leveraging EESSI in CI environments

- EESSI can be used in CI environments like Jenkins, GitHub Actions, …
- We can provide:
  - Different compilers to test your software with
  - Required dependencies for your software
  - Additional tools like ReFrame, performance analysis tools,…
- Other than CernVM-FS, no software installations required
  - Everything that is actually needed is pulled in on-demand by CernVM-FS
- Significantly facilitates also running CI tests in other contexts (laptop, HPC, …)

Leveraging EESSI in CI environment

We have an EESSI GitHub Action that provides EESSI+`direnv`:

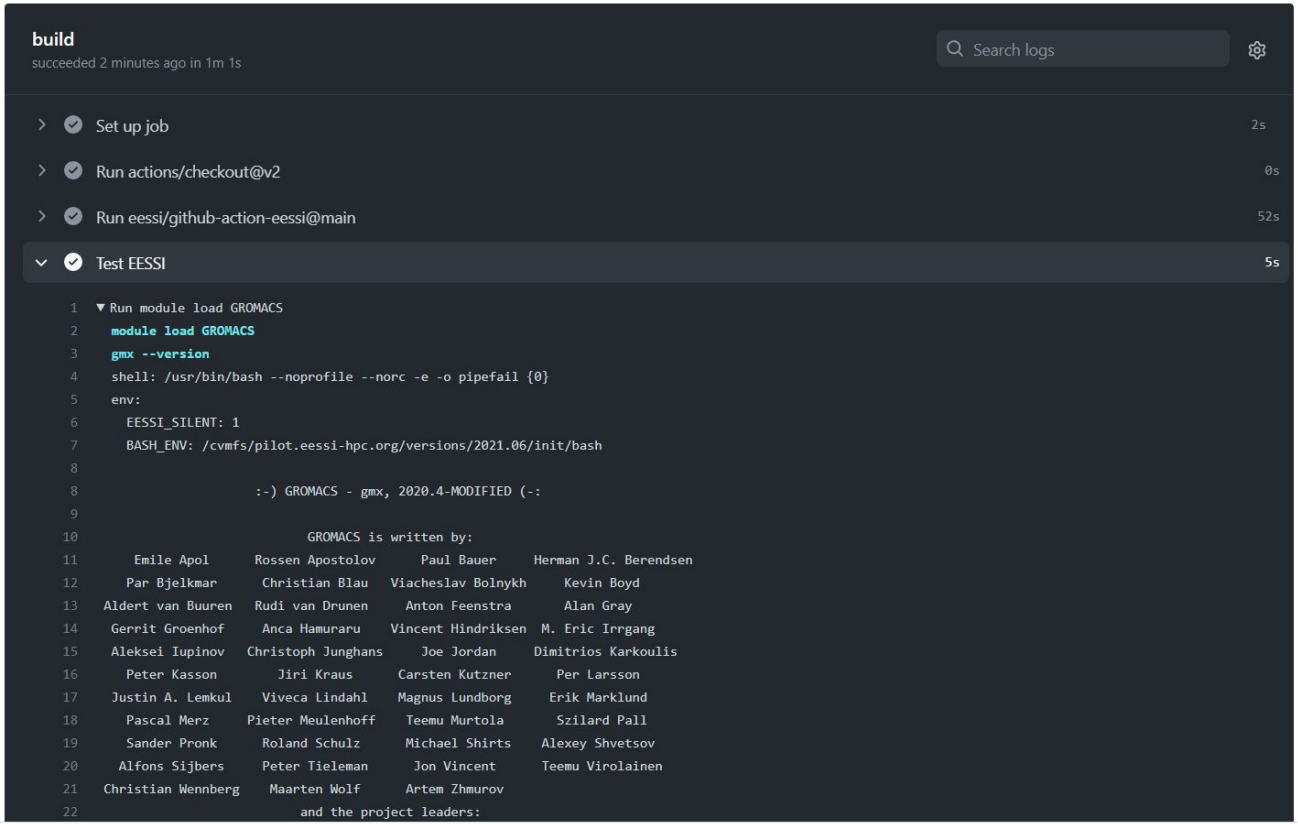
See it in action in the `github-essi-action` repository:

github.com/EESSI/github-action-eessi

github.com/EESSI/github-action-eessi/blob/main/.github/workflows/gromacs-usage.yml

```yaml
name: ubuntu_tensorflow
on: [push, pull_request]
jobs:
 build:
   runs-on: ubuntu-latest
   steps:
   - uses: actions/checkout@v3
   - uses: eessi/github-action-eessi@v3
     with:
       eessi_stack_version: '2023.06'
   - name: Test EESSI
     shell: bash
     run: |
       module load TensorFlow
       python -c 'import tensorflow; print(tensorflow.__version__)'
```

Leveraging EESSI GitHub Action



https://github.com/EESSI/github-action-eessi/actions/runs/3044539257/jobs/4905040409

Facilitate HPC training

- EESSI can significantly reduce effort required to set up infrastructure for HPC training sessions (introductory, software-specific, …)
- Setting up a throwaway Slurm cluster in the cloud is easy via Magic Castle
  - Used Magic Castle today:
    - Cluster was created by editing a single file
    - Automatically configured within 20 minutes
    - Includes support for GPU and fast interconnects (infiniband, EFA)
  - EESSI project uses Magic Castle for the build-and-deploy “bot”
  - There are also commercial alternatives that can/will support EESSI (Azure/AWS)
- EESSI can provide (scientific) software that is required for the training
- Attendees can easily set up the *same* software environment later on their own system(s) by leveraging EESSI

Collaboration with software developers + experts

- A central software stack by/for the community opens new doors…
- We can work with software developers/experts to verify the installation
  - Check how installation is configured and built
  - Help to verify whether software is functional for different use cases
  - Show us how to do extensive testing of their software
  - Evaluate performance of the software, enable performance monitoring
  - **“Approved by developers” stamp for major applications included in EESSI**
- Relieve software developers from burden of getting their software installed
  - Remove need to provide pre-built binary packages?
- Developers can also leverage EESSI themselves: dependencies, CI, …

EESSI

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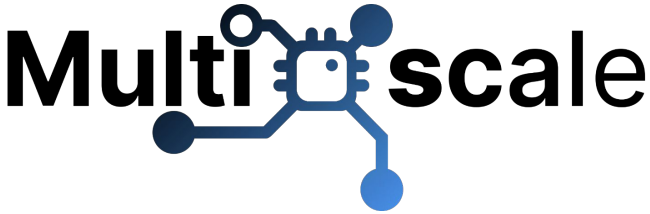
Who pays for this?

The MultiXscale EuroHPC Project



- EuroHPC Centre of Excellence
  - 4 year project, started Q1 2023
- Budget of ~6M EUR (50% EU funding, 50% national funding)
  - Roughly 50% of funding for EESSI-related activities
- Collaboration between EESSI and CECAM (total of 16 partners)
  - EESSI primarily addresses technical aspects
  - CECAM network provides scientific expertise
- Scientific target are multiscale simulations with 3 key use cases
  - Helicopter design and certification for civil transport
  - Battery applications to support the sustainable energy transition
  - Ultrasound for non-invasive diagnostics and biomedical applications
- https://www.multixscale.eu

Website: eessi.io

GitHub: github.com/eessi

Documentation: eessi.io/docs

YouTube channel: youtube.com/@eessi_community

Paper (open access): doi.org/10.1002/spe.3075

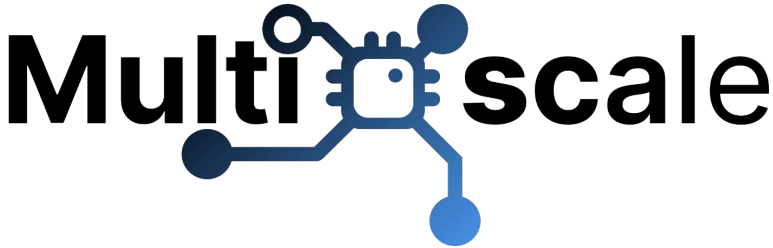
EESSI support portal: gitlab.com/eessi/support

Monthly online meetings (first Thursday, 2pm CEST)

eessi.io/docs/meetings/2022-09-amsterdam

Join our mailing list & Slack channel

Feedback request!



https://form.typeform.com/to/qaXPPdc3

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