Streaming Optimised Scientific Software, an Introduction to EESSI

EUROPEAN ENVIRONMENT FOR SCIENTIFIC SOFTWARE INSTALLATIONS

MultiXscale

Thu 27 Mar 2025

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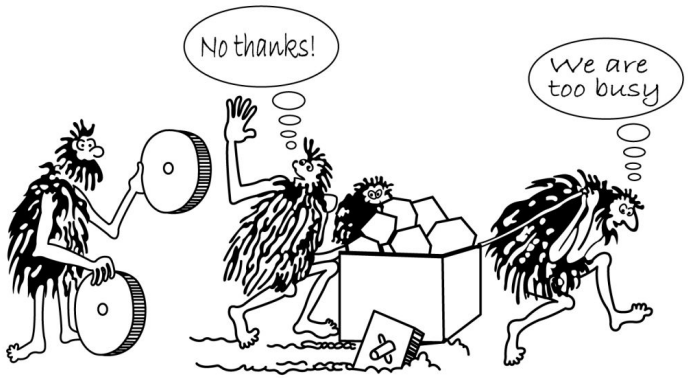
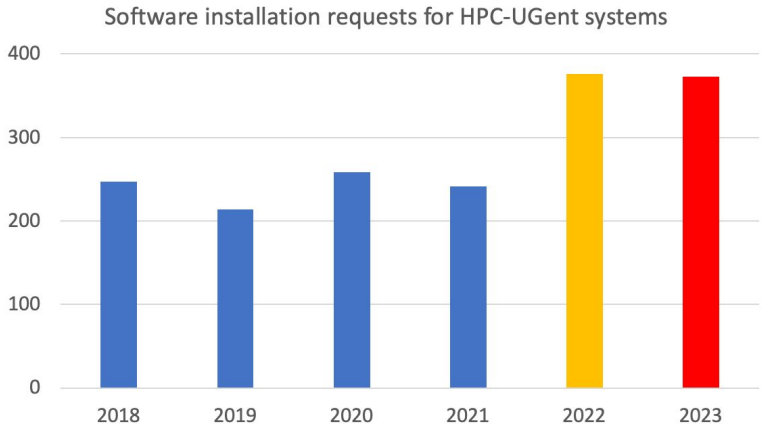
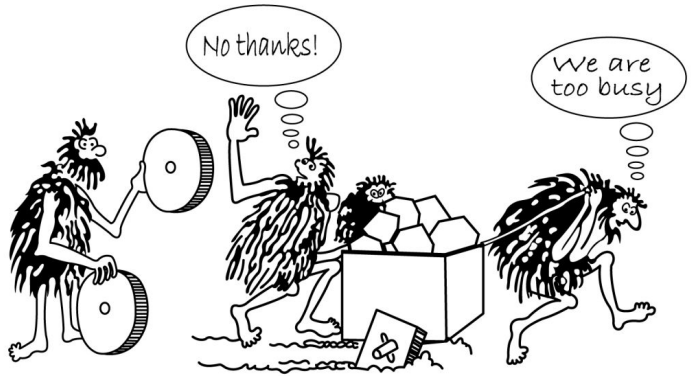


The changing landscape of scientific computing

- **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**…

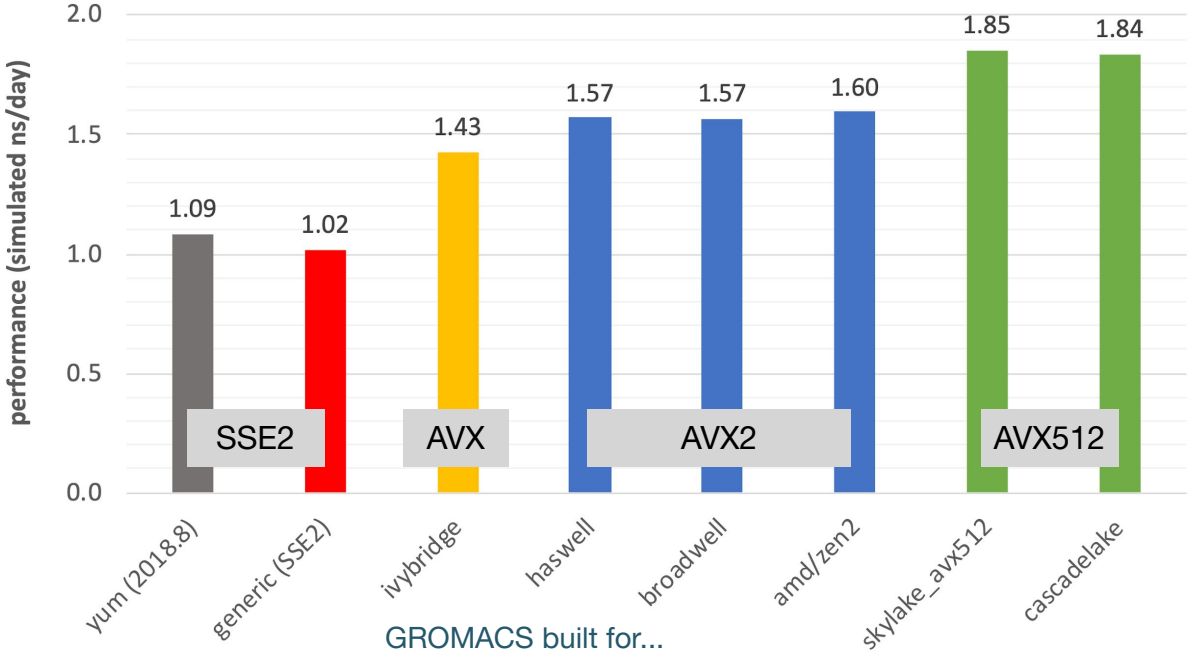




Optimized scientific software installations

- Software should be optimized for the system it will run on (keep the P in HPC!)
- 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**



What if you no longer have to install

*a **broad range of scientific software***

from scratch on every laptop, HPC cluster,

or cloud instance you use or maintain,

without compromising on performance?

Alan

EESSI in a nutshell

- European Environment for Scientific Software Installations (EESSI)
- **Shared repository of (optimized!) scientific software installations**
- Uniform way of providing software to users, regardless of the system they use!
- Should work on any Linux OS (+ WSL, macOS via Lima) and system architecture
- From laptops and personal workstations to HPC clusters and cloud
- Support for different CPU (micro)architectures, interconnects, GPUs, etc.
- **Focus on performance, automation, testing, collaboration**

https://eessi.io

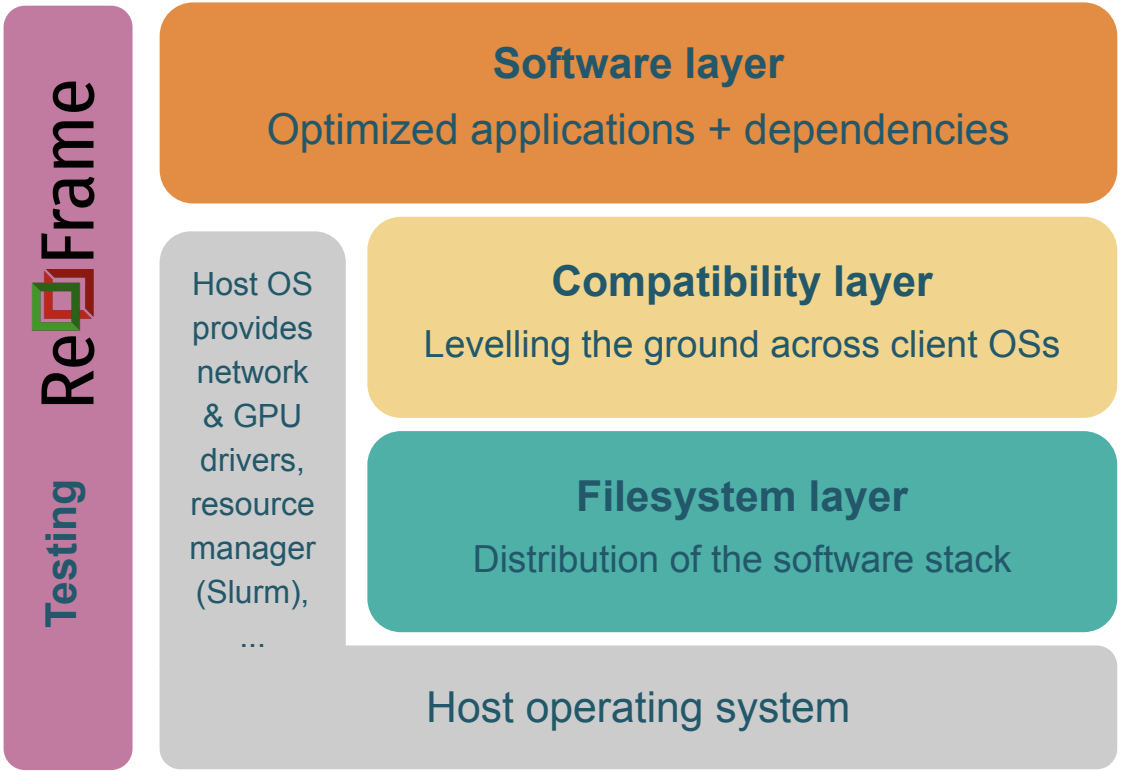
https://eessi.io/docs

Alan

Major goals of EESSI

- **Avoid duplicate work** (for researchers, HPC support teams, sysadmins, …)
  - Tools that automate software installation process (EasyBuild, Spack) are not sufficient anymore
  - 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, …

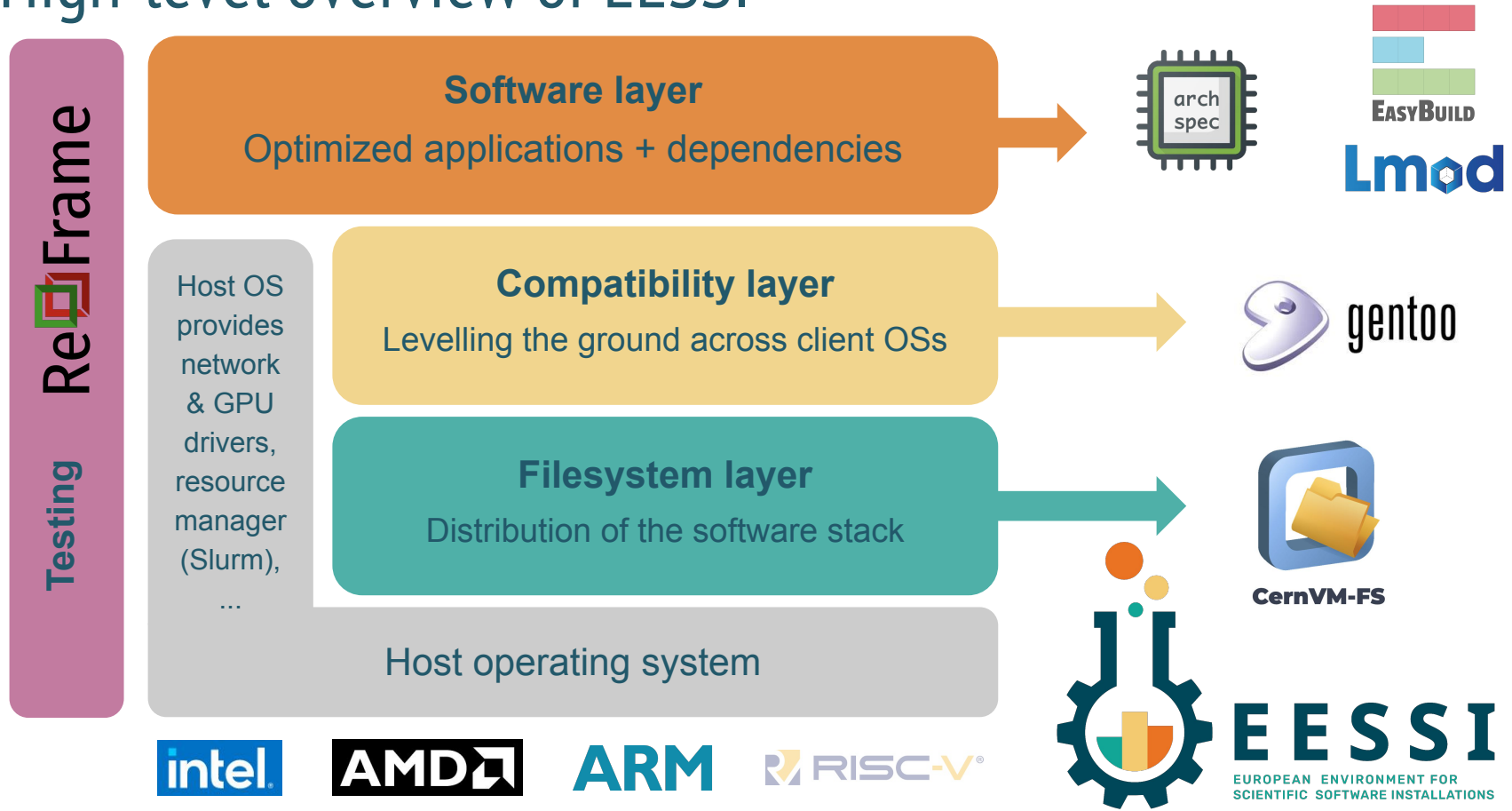
High-level overview of EESSI



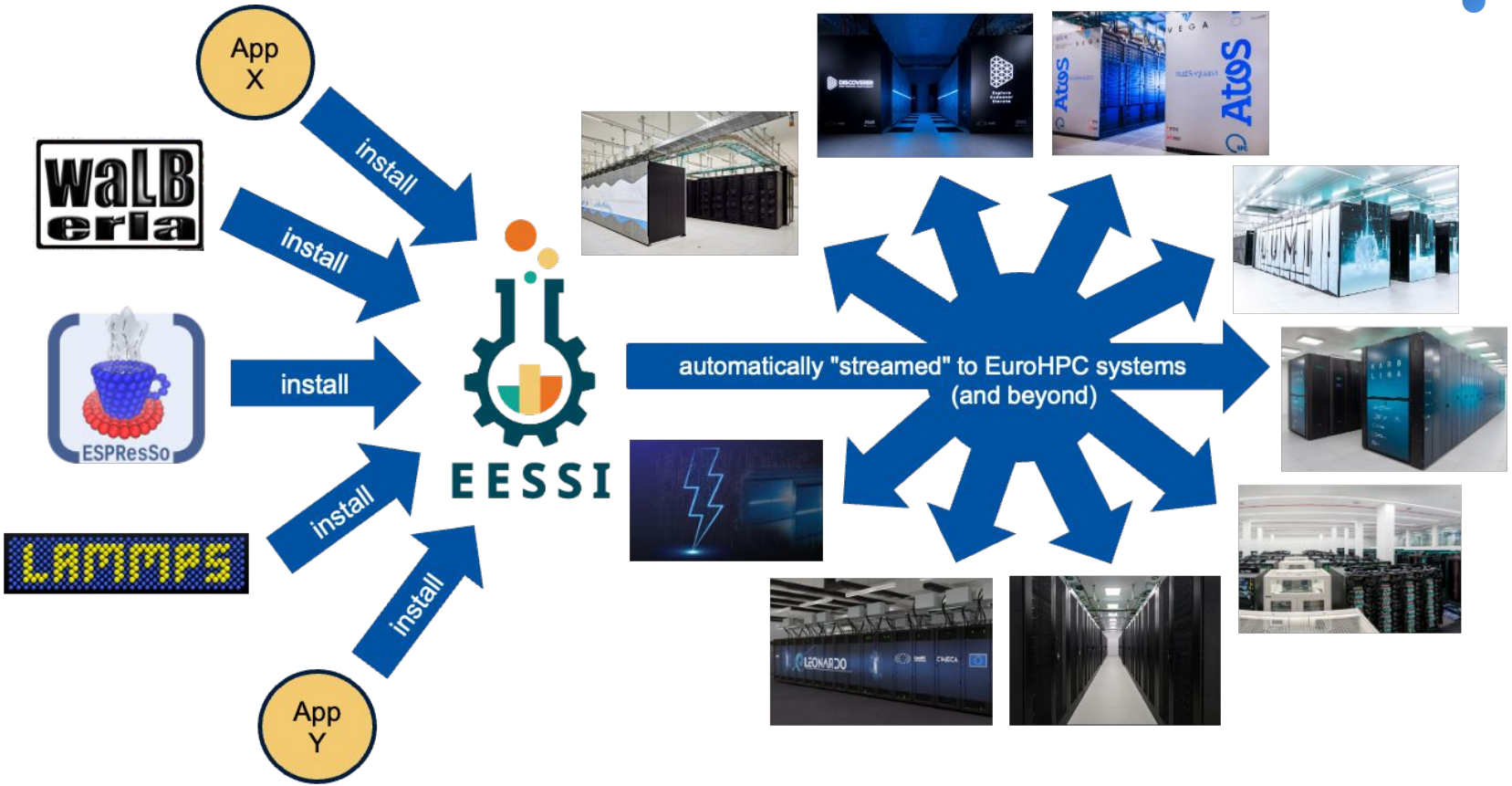
EESSI
EUROPEAN ENVIRONMENT FOR SCIENTIFIC SOFTWARE INSTALLATIONS

Alan

High-level overview of EESSI



EESSI as a shared software stack



Hands-on live demo

Getting access to EESSI

Using EESSI

Kenneth

Native installation of CernVM-FS

```
# Native installation
# Installation commands for RHEL-based distros
# like CentOS, Rocky Linux, Almalinux, Fedora, ...

# install CernVM-FS
sudo yum install -y
https://ecsft.cern.ch/dist/cvmfs/cvmfs-release/cvmfs-release-latest.noarch.rpm
sudo yum install -y cvmfs

# create client configuration file for CernVM-FS
# (no proxy, 10GB local CernVM-FS client cache))
sudo bash -c "echo 'CVMFS_CLIENT_PROFILE="single"' > /etc/cvmfs/default.local"
sudo bash -c "echo 'CVMFS_QUOTA_LIMIT=10000' >> /etc/cvmfs/default.local"

# Make sure that EESSI CernVM-FS repository is accessible
sudo cvmfs_config setup
```

See docs for alternative ways of installing CernVM-FS natively, via a VM on a personal computer
eessi.io/docs/getting_access/eessi_wsl/ - eessi.io/docs/getting_access/eessi_limactl/

Native installation of CernVM-FS on an HPC cluster

- For a single system, it's sufficient to install and configure CernVM-FS client
- For an HPC cluster, a bit more work is needed to:
  - Enhance the reliability of the access to EESSI
  - Improve startup performance of software
- It is recommended to:
  - Have a full copy of the EESSI repositories in your local network, by setting up a private CernVM-FS Stratum-1 "mirror" server
  - Have one or more proxy servers, to offload the Stratum-1 server(s)
- See also https://multixscale.github.io/cvmfs-tutorial-hpc-best-practices

Demo: Using EESSI

eessi.io/docs/using_eessi/eessi_demos

s

```
/cvmfs/software.eessi.io/versions/2023.06/software
`-- linux
    |-- aarch64
    |   |-- generic
    |   |-- neoverse_n1
    |   `-- neoverse_v1
    `-- x86_64
        |-- amd
        |   |-- zen2
        |   `-- zen3
        |-- generic
        `-- intel
            |-- haswell
            `-- skylake_avx512
                |-- modules
                `-- software
```

```
$ source /cvmfs/software.eessi.io/versions/2023.06/init/bash
Found EESSI pilot repo @
/cvmfs/software.eessi.io/versions/2023.06!
archdetect says x86_64/amd/zen3
Using x86_64/amd/zen3 as software subdirectory
...
Environment set up to use EESSI pilot software stack, have fun!

{EESSI 2023.06} $ module load R/4.3.2-gfbf-2023a

{EESSI 2023.06} $ which R
/cvmfs/software.eessi.io/versions/2023.06/software/linux/x86_64/
amd/zen3/software/R/4.3.2-gfbf-2023a/bin/R

{EESSI 2023.06} $ R --version
R version 4.3.2
```

Demo: Running LAMMPS in a Slurm job script

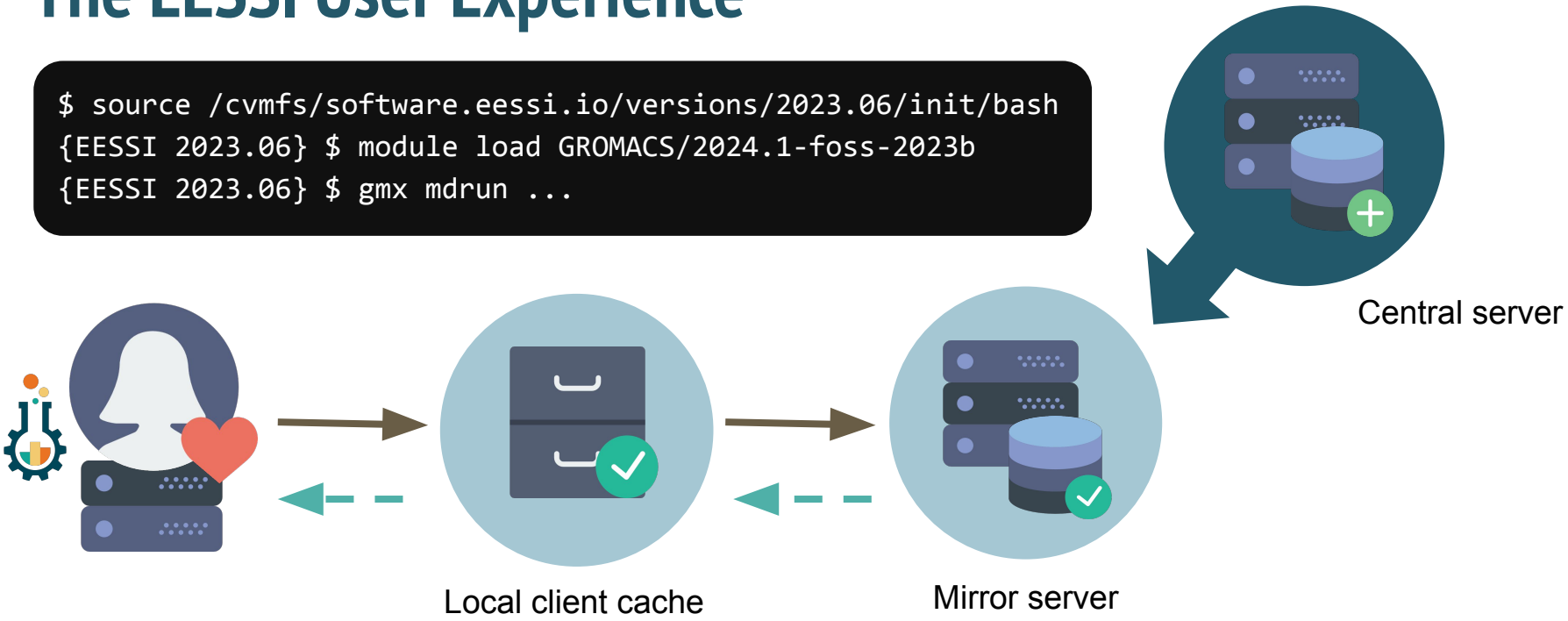

```
#!/bin/bash
# EESSI_demo.sh script
#SBATCH --job-name="EESSI_Demo_LAMMPS_lj"
#SBATCH --ntasks=4
#SBATCH --ntasks-per-node=4
#SBATCH --cpus-per-task=1
#SBATCH --output=EESSI_demo.out
#SBATCH --error=EESSI_demo.err
#SBATCH --time=0:30:0
#SBATCH --partition=cpu_rome

source /cvmfs/software.eessi.io/versions/2023.06/init/bash
module load LAMMPS/29Aug2024-foss-2023b-kokkos
mkdir /tmp/$USER && cd /tmp/$USER
curl -o in.lj https://raw.githubusercontent.com/lammps/lammps/refs/heads/develop/bench/in.lj
export OMP_NUM_THREADS=1
mpirun -np 4 lmp -in in.lj
rm -r /tmp/$USER
```

EESSI

CernVM-FS

The EESSI User Experience

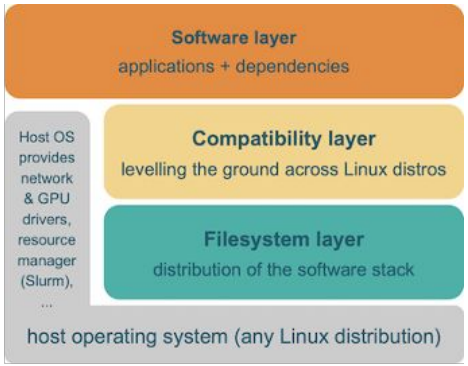
```
$ source /cvmfs/software.eessi.io/versions/2023.06/init/bash
{EESSI 2023.06} $ module load GROMACS/2024.1-foss-2023b
{EESSI 2023.06} $ gmx mdrun ...
```



EESSI provides **on-demand streaming**

of (scientific) software (like music, TV-series, …)

How does EESSI work?



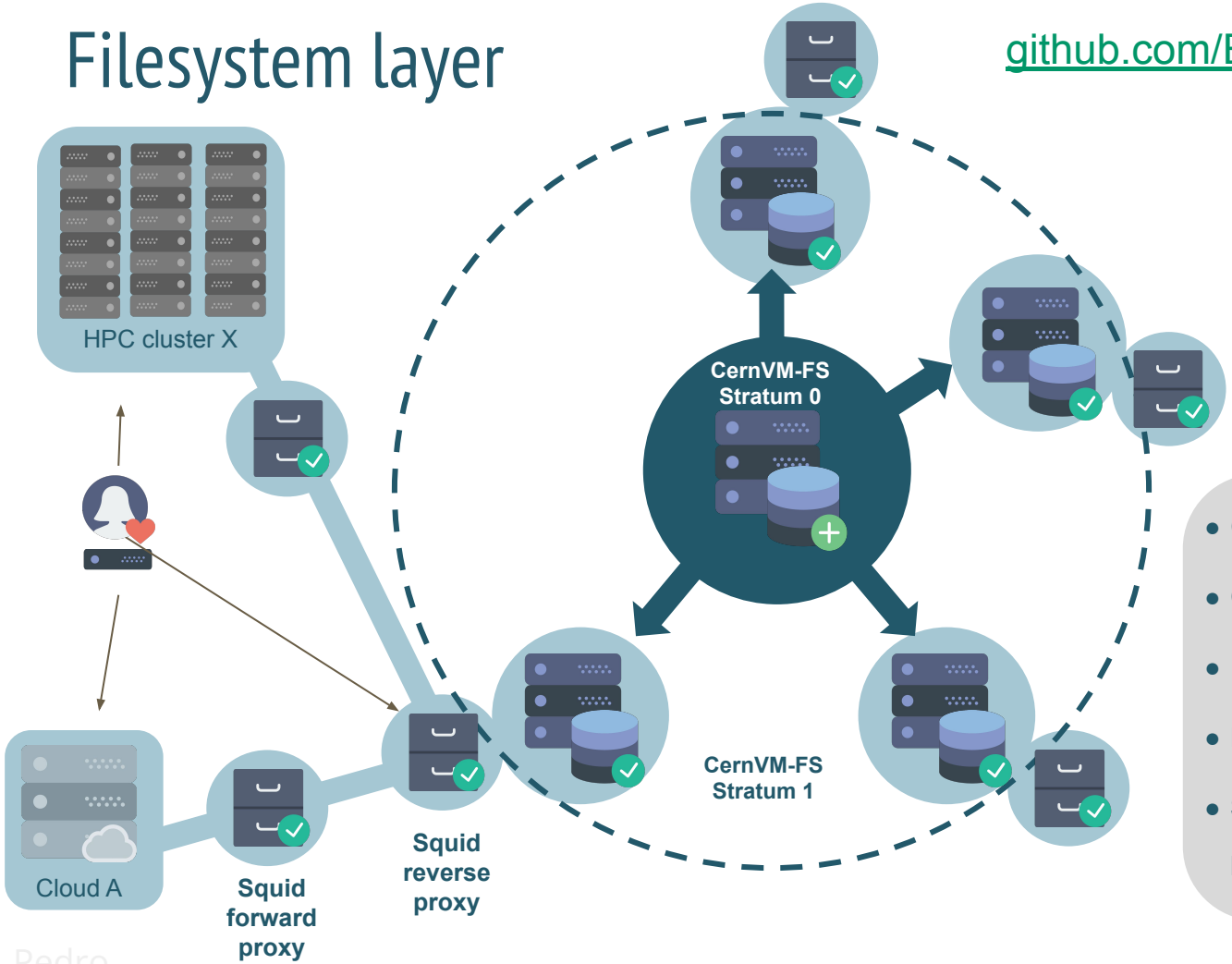
- Software installations included in EESSI are:
  - Automatically **“streamed in” on demand** (via CernVM-FS)
  - Built to be **independent of the host operating system**

    “Containers without the containing”
  - **Optimized** for specific CPU generations + specific GPU types
- Initialization script **auto-detects** CPU + GPU of the system

Pedro

Filesystem layer

github.com/EESSI/filesystem-layer



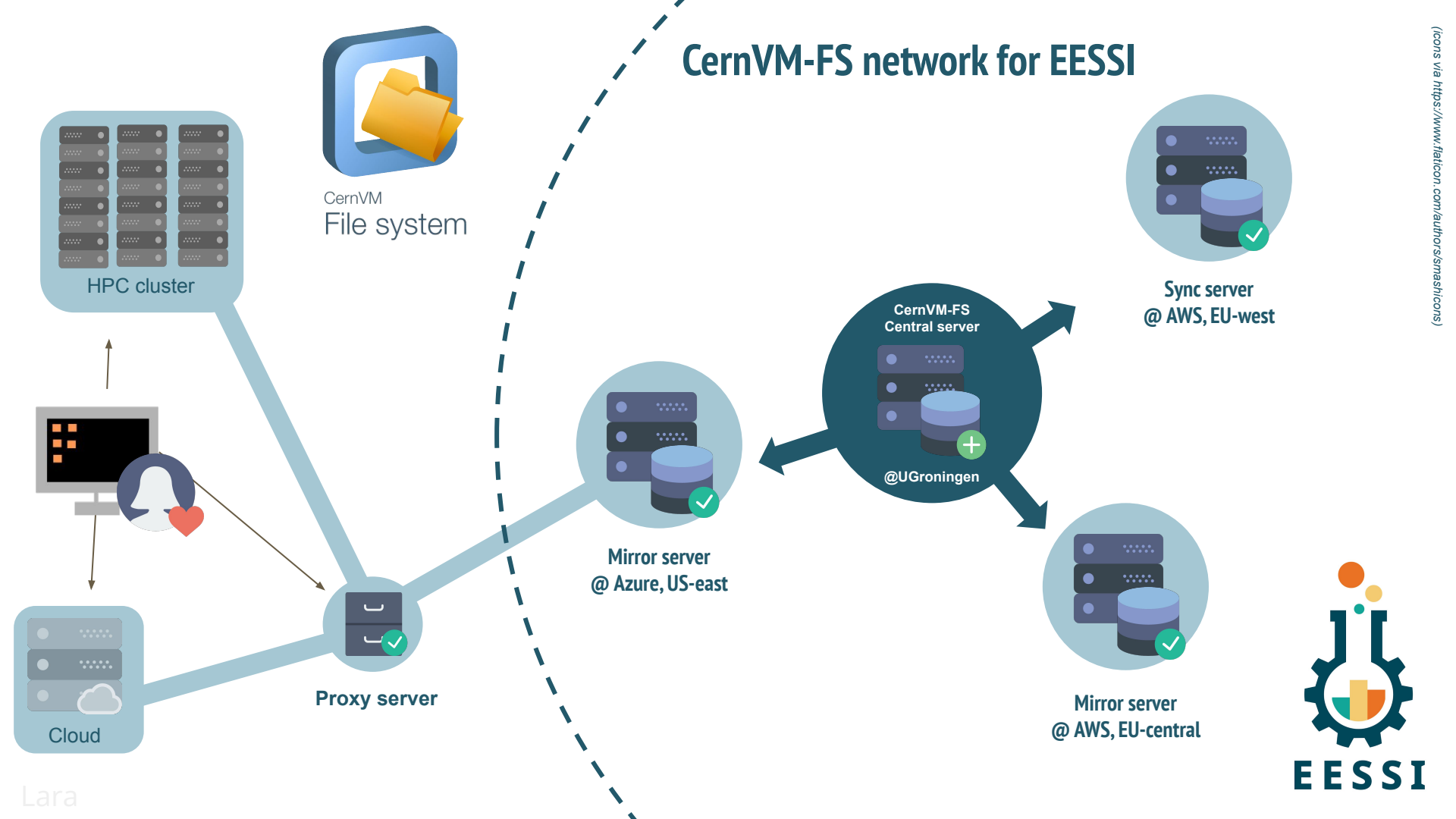
CernVM-FS

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)

CernVM-FS network for EESSI



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

Lara

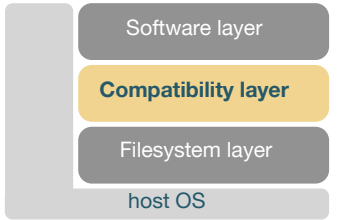
Compatibility layer

github.com/EESSI/compatibility-layer

EESSI

- Gentoo Prefix installation (in `/cvmfs/.../compat/<os>/<arch>/`)
- **Set of Linux 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 distributions)
- 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 gentoo



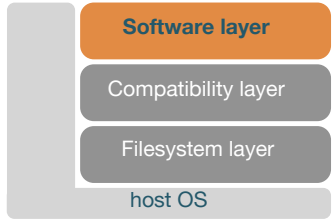
Pedro

Software layer

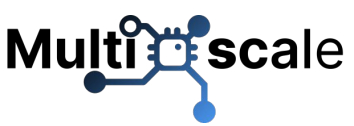
github.com/EESSI/software-layer

- Provides **installations of scientific software** applications & libraries (incl. deps)
- Optimized for specific CPU microarchitectures (AMD Zen3, ...)
  - Separate subdirectory/tree for each (in `/cvmfs/.../software/...`)
- Support for specific generation of **(NVIDIA) GPUs** via `/accel/` subdirectories
- **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 archdetect

powered by



Current status of EESSI



- Production CernVM-FS repository **`software.eessi.io`** available since Nov'23
- Ansible playbooks, scripts, docs available at https://github.com/eessi
- CernVM-FS: Stratum 0 @ Univ. of Groningen + two Stratum 1 servers in AWS + Azure
- Target CPU microarchitecturs (see also https://eessi.io/docs/software_layer/cpu_targets):

  `{aarch64,x86_64}/generic`

  `intel/{haswell, skylake_avx512}, amd/{zen2,zen3,zen4},`

  `aarch64/{neoverse_n1,neoverse_v1,a64fx}`

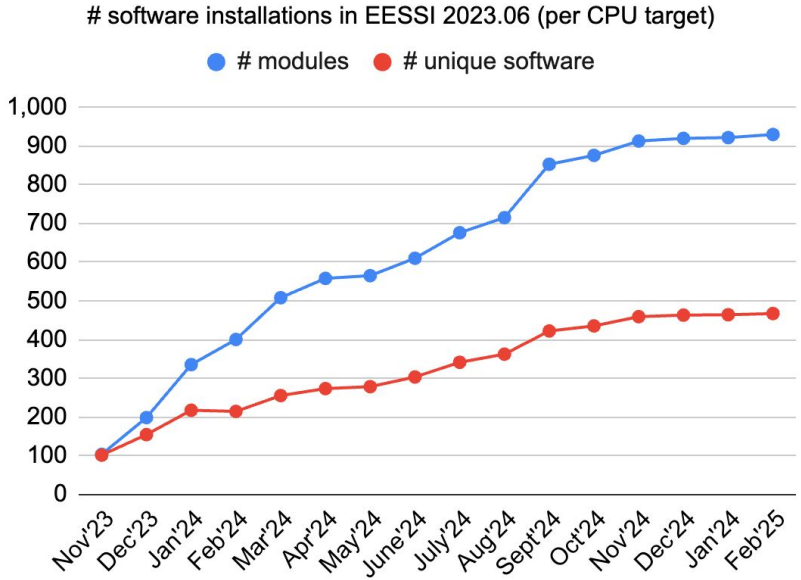
- **NVIDIA GPU support in place**, limited set of GPU software installed

- **Supported by Azure and AWS**: sponsored credits to develop necessary infrastructure

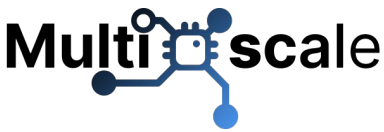
Overview of available software

Currently ~940 software installations available per CPU target via software.eessi.io CernVM-FS repository; increasing every day

- Over 467 different software packages
- Excl. extensions: Python packages, R libraries
- Including ESPResSo, GROMACS, LAMMPS, OpenFOAM, PyTorch, R, QuantumESPRESSO, TensorFlow, waLBerla, WRF, …
- eessi.io/docs/available_software/overview
- Using recent compiler toolchains: currently focusing on `foss/2023a` and `foss/2023b`

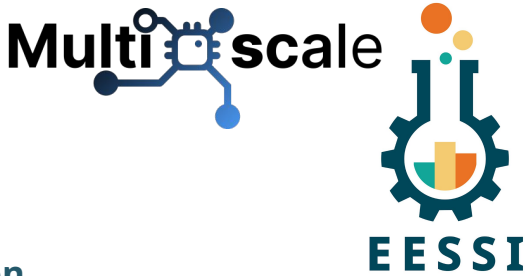


Supported system architectures



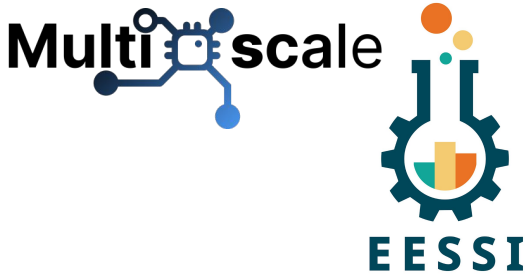
- Different generations of `x86_64` (Intel, AMD) and Arm 64-bit CPUs; RISC-V is WIP
  - Including A64FX (Deucalion, WIP) & NVIDIA Grace (JUPITER, WIP)
  - Also works on laptops, in virtual machines in the cloud, on Raspberry Pi boards, etc.
- Different accelerators: **NVIDIA GPUs** (today) + **AMD GPUs** (soon)
  - Available combination: AMD Rome (Zen2) + NVIDIA A100 (cc80), AMD Milan (zen3) + NVIDIA A100 (cc80) and AMD Genoa (zen4) + NVIDIA H100 (cc90) only software installations for AMD Rome (Zen2) + NVIDIA A100 are available
- **Various interconnects** like Infiniband, via “fat” MPI libraries
  - Support for injecting a vendor-provided MPI library is available
- Goal is to support system architecture of **all** (current & future) **EuroHPC systems**

On which systems is EESSI already available?



- EuroHPC JU systems:
  - Native installation (via CernVM-FS) on **Vega** + **Karolina + Deucalion**
  - Semi native installation (via rsync) on **MareNostrum5**
  - EESSI can be used via `cvmfsexec` tool on Deucalion, Discoverer, MeluXina (see blog post)
  - Native installation on **MeluXina**, **Lumi** is a work-in-progress
  - JSC has expressed significant interest to make EESSI available on **JUPITER**
- EESSI is already available on various other European systems (and beyond)
  - Snellius @ SURF, EMBL, Univ. of Stuttgart, VSC sites in Belgium, Sigma2 in Norway, etc.
- **Overview of (known) systems that have EESSI available at eessi.io/docs/systems**

NVIDIA GPU support in EESSI



- Initial support for CUDA software is in place in EESSI version 2023.06
- Detailed documentation available at eessi.io/docs/gpu
- Problems we had to deal with:

    1) We don't know where the **NVIDIA GPU driver libraries** are in host OS…

    2) We **can not redistribute the full CUDA installation** due to EULA, only runtime libraries…

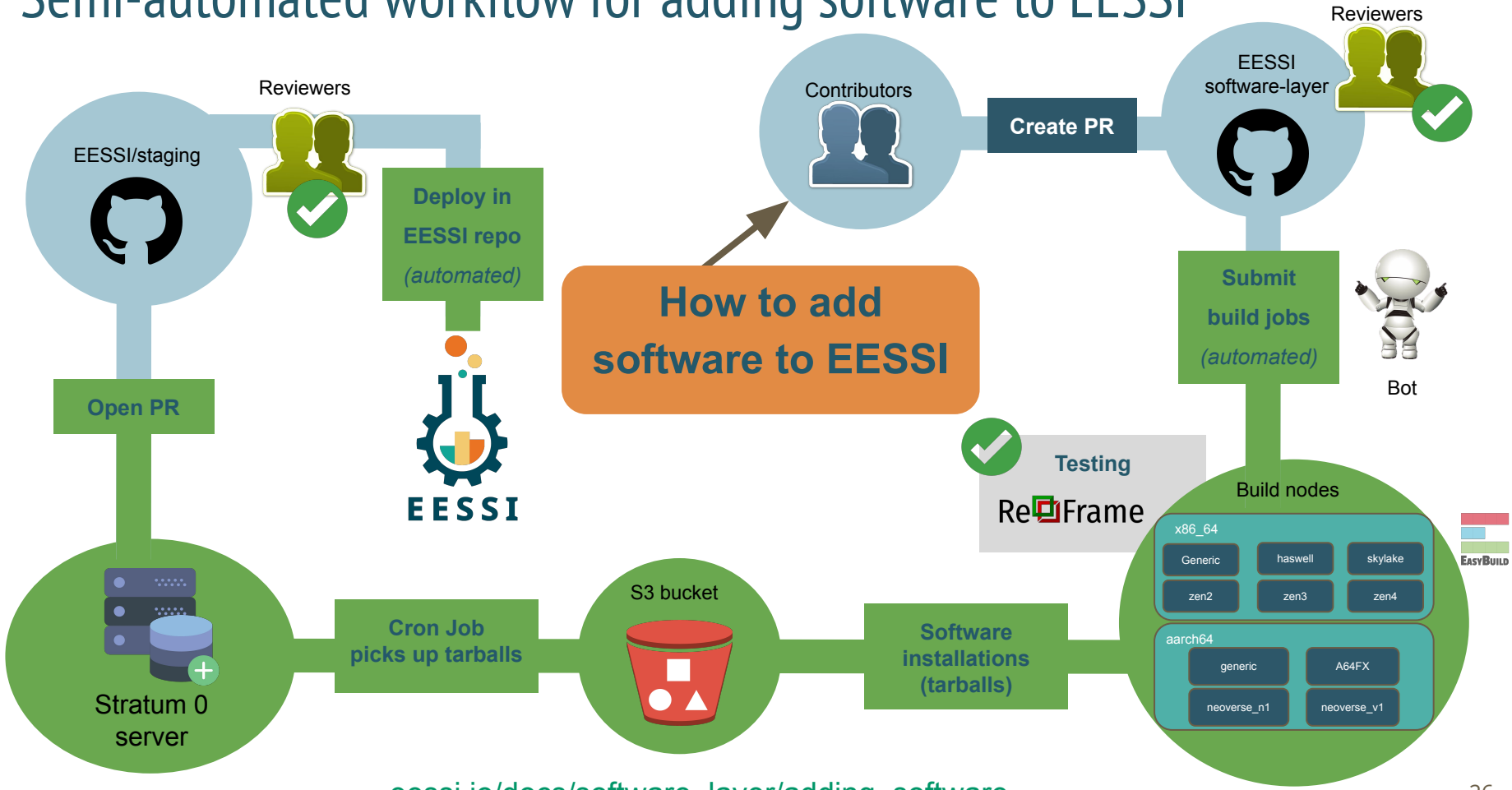
- In EESSI, we provide scripts to deal with both these problems:

    1) `link_nvidia_host_libraries.sh` script to link GPU driver libraries provided by OS "into" EESSI; (requires write access to (target of) `/cvmfs/software.eessi.io/host_injections`)

    2) `install_cuda_host_injections.sh` script to **install full CUDA installation** to subdirectory of (target of) `/cvmfs/software.eessi.io/host_injections` (and unbreak symlinks in CUDA in EESSI)

- **Available CUDA software in EESSI:** CUDA-Samples, ESPResSo, LAMMPS, NCCL, OSU Micro-Benchmarks
- More CPU/GPU combos and software (GROMACS, PyTorch, TensorFlow, AlphaFold) coming soon…

Semi-automated workflow for adding software to EESSI



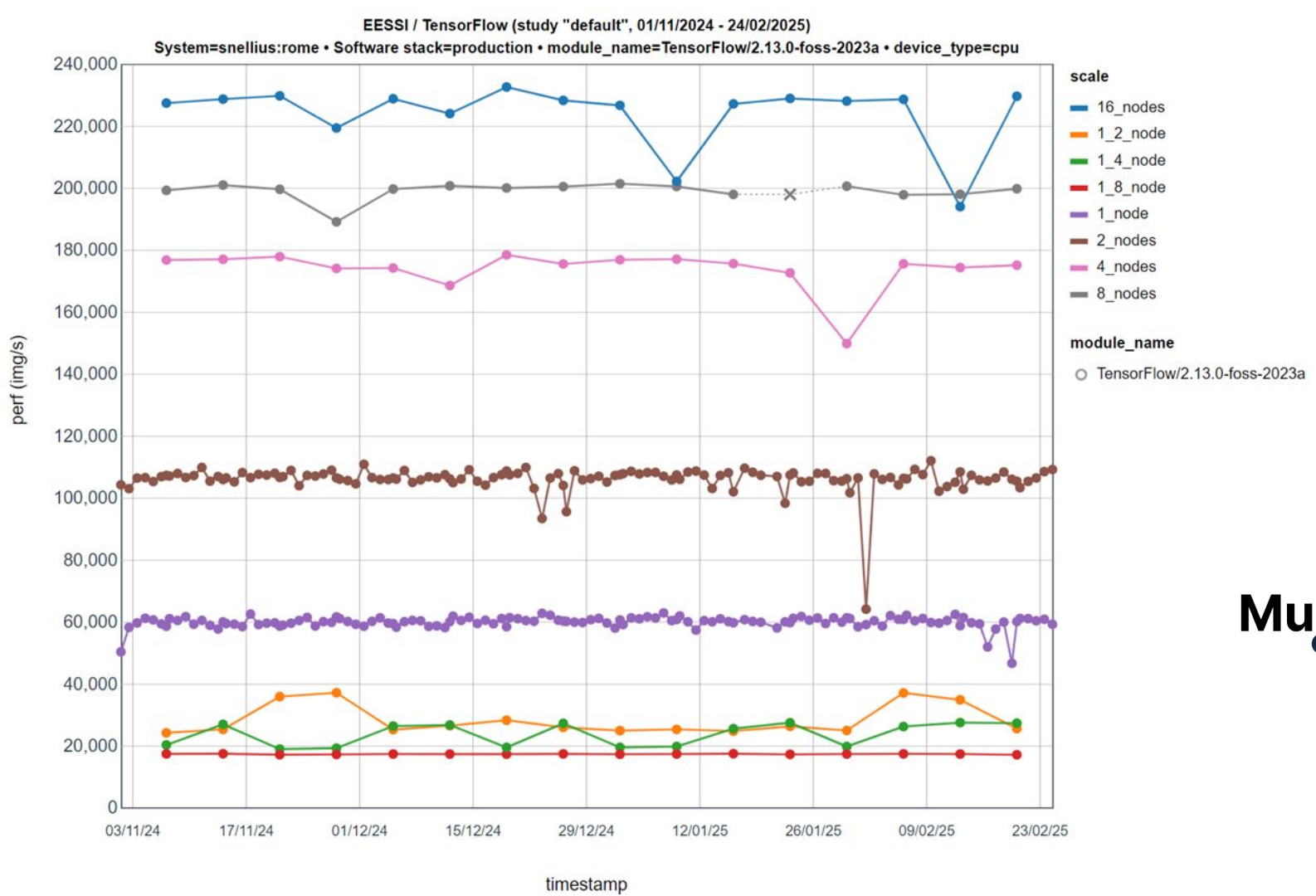
eessi.io/docs/software_layer/adding_software

Software testing is an important part of EESSI

- EESSI test suite: eessi.io/docs/test-suite
  - Collection of *portable* tests for software available in EESSI
  - Periodically (daily/weekly) on about 6 different systems
  - Running of selected (single node) tests when building new Software for EESSI (before deployment)
  - Can also be used for other software stacks than the EESSI software stack

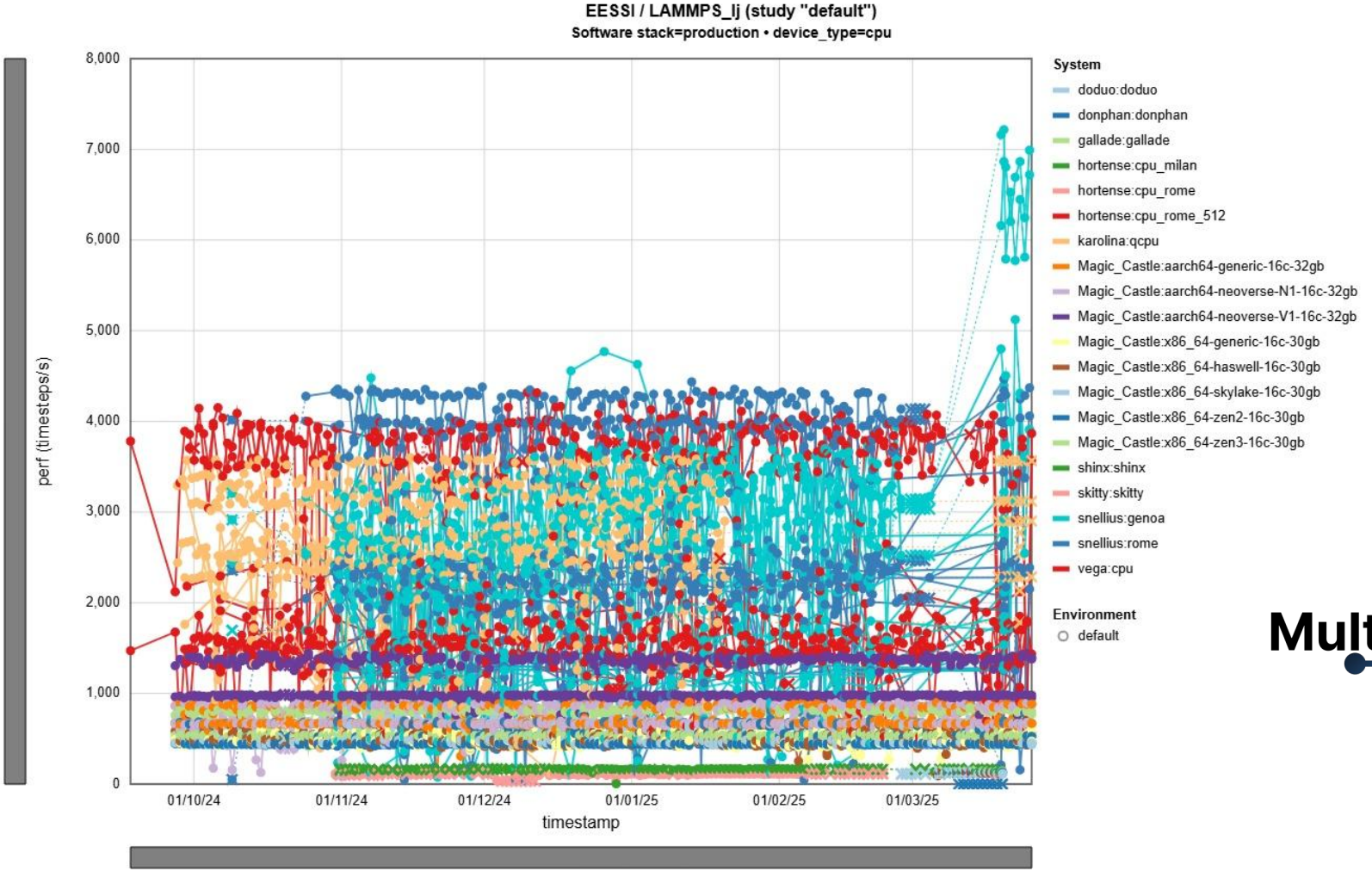
Software testing is an important part of EESSI

- Example: failing tests in GROMACS test suite when installing it in EESSI
  - See https://gitlab.com/eessi/support/-/issues/47
  - Filesystem race in GROMACS test suite when running tests concurrently
  - **Bug in Arm SVE support**, leading to (very) wrong results for several tests
    - See https://gitlab.com/gromacs/gromacs/-/issues/5057
    - Works fine on A64FX (512-bit SVE), but problem on Graviton 3 + NVIDIA Grace!



EESSI

Multi scale



EESSI

Multi scale

EESSI test suite

- 13:50-14:10 Hands-on: run the test suite yourself
- ideally: be ready to login to your own HPC
    - If your system is very full, maybe try to reserve one (ideally CPU) node
- Alternative: local laptop with module env
- You'll need one of the following modules
    - Torchvision, Pytorch-bundle, TensorFlow, LAMMPS, EspresSo, QuantumEspresso, CP2K, Gromacs, Metalwalls, OSU
    - If you don't have any: install OSU with EasyBuild - it's the fastest install

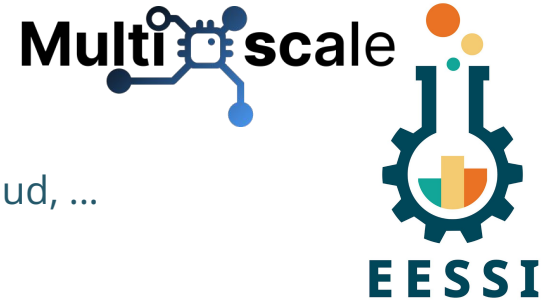
EESSI use cases

Use cases enabled by EESSI

- A **uniform software stack** across HPC clusters, clouds, 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

EESSI as a uniform software stack



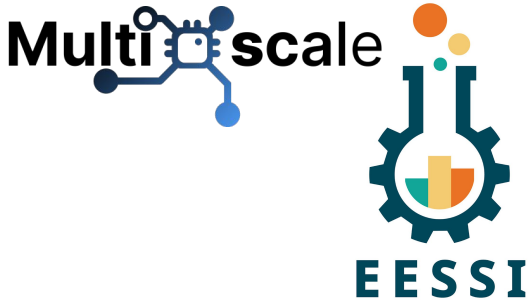
- Main goal: **same software everywhere**: laptop, server, HPC, cloud, …
- Wide variety of systems supported
  - CPUs: `x86_64` (Intel, AMD), `aarch64` (Arm), `riscv64` (work-in-progress…)
  - OS: any Linux distribution, on Windows via WSL, on macOS via Lima
  - High-speed interconnects (Infiniband), 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!

Alan

Leveraging EESSI in CI environments



- EESSI can be used in CI environments like:
  - GitHub: github.com/marketplace/actions/eessi
  - GitLab: gitlab.com/explore/catalog/eessi/gitlab-eessi
- EESSI 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 to get access to EESSI, 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 environments

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

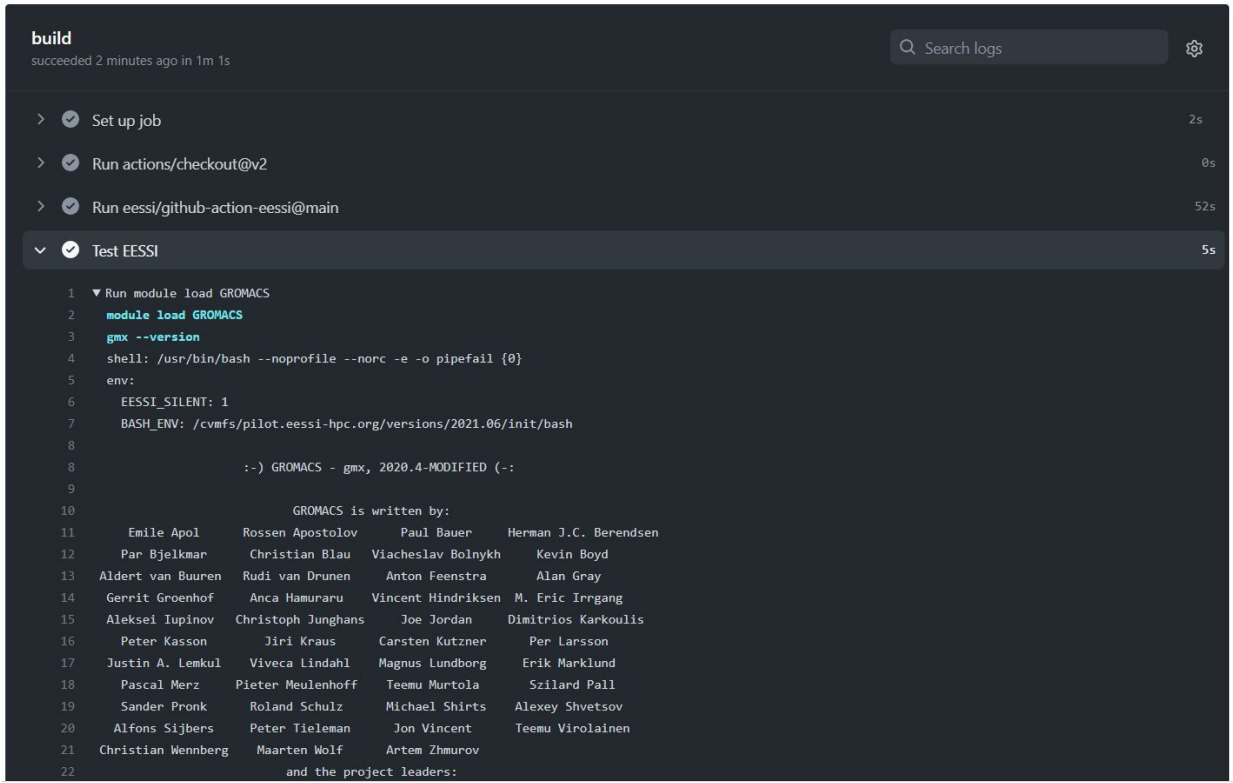
See it in action in the `github-eessi-action` repository:

github.com/EESSI/github-action-eessi

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

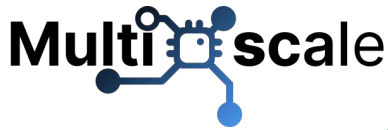
```yaml
name: ubuntu_tensorflow
on: [push, pull_request]
jobs:
 build:
   runs-on: ubuntu-latest
   steps:
   - uses: actions/checkout@v3
   - uses: eessi/github-action-eessi@v3
     with:
       eessi_stack_version: '2023.06'
   - name: Test EESSI
     shell: bash
     run: |
       module load TensorFlow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

Leveraging EESSI GitHub Action



https://github.com/EESSI/github-action-eessi/actions/runs/11183032689/job/31090668500

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**
  - Simple process once you have cloud credits:
    - Create cluster 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 some of the build-and-deploy “bots”
  - There are also commercial alternatives that can/do 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

Alan

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, …

Deployment of test-release of Scientific Software with EESSI

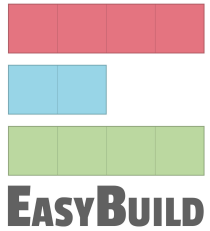
- **Dev.eessi.io**
  - Available on Vega
  - https://eessi.io/docs/repositories/dev.eessi.io
  - More information Coming soon

```
/cvmfs/dev.eessi.io/versions/2023.06/software
`-- linux
    `-- x86_64
        |-- amd
        |   |-- zen2
                |-- modules
                    |-- all
                        |-- Espresso
                        |   |-- 4.2.2-foss-2023a-2ba17de6096933275abec0550981d9122e4e5f28.lua
                        |-- Gromacs
                        |   |-- 2024.3-foss-2023b-d0f934abfd1394621c40858a2c2dd9123451df4e.lua
                        |-- LAMMPS
                        |   |-- 570c9d190fee556c62e5bd0a9c6797c4dffcc271-foss-2023a-kokkos-dev_OBMD.lua
                        |-- ...
```

EESSI won an HPCWire Reader's Choice award!

EESSI

Webinar series: Different aspects of EESSI



5 Mondays in a row May-June 2025 (subject to change)

- **CernVM-FS for HPC sites**
- **Introduction to EESSI webinar/tutorial**
- **Using EESSI as the base for a system stack webinar**
- **Introduction to EasyBuild**
- **EESSI for CI/CD webinar/tutorial**

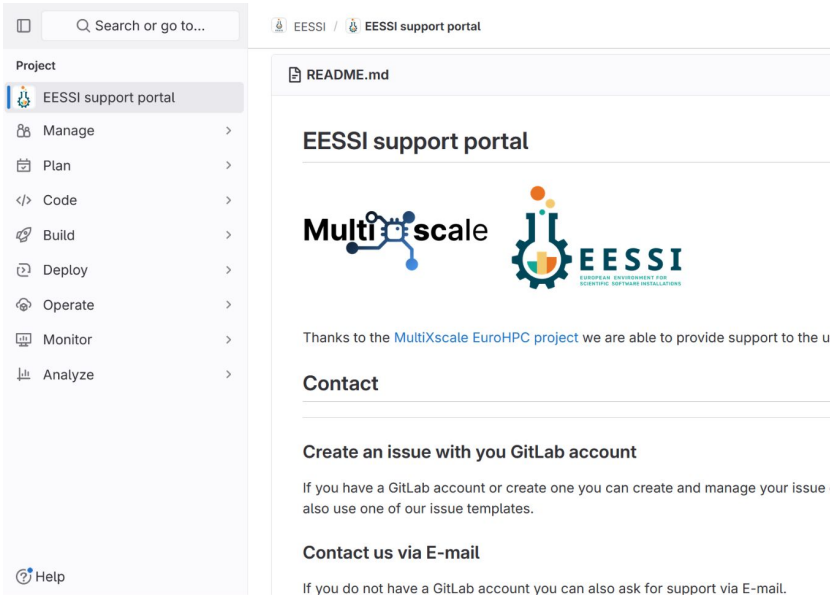
More details will be announced soon

Support for installing, using, contributing to EESSI

GitLab

eessi.io/docs/support

- Via GitLab, or via email: `support@eessi.io`
- Report problems
- Ask questions
- Request additional software
- Get help with contributing to EESSI
- Suggest enhancements, additional features, ...
- Confidential tickets possible (security issues, ...)



Dedicated support team, thanks to EuroHPC Centre-of-Excellence Multiscale

Tutorial *"Best Practices for CernVM-FS in HPC"*

- multixscale.github.io/cvmfs-tutorial-hpc-best-practices
- Held online on 4 Dec 2023 (~3 hours), recorded & available on YouTube
- Over 200 registrations, ~125 attending the meeting
- Lecture + hands-on demos
- Topics:
  - Introduction to CernVM-FS + EESSI
  - Configuring CernVM-FS: client, Stratum 1 mirror server, proxy server
  - Troubleshooting problems
  - Benchmarking of start-up performance w/ TensorFlow
- **We are planning to organise this again soon…**

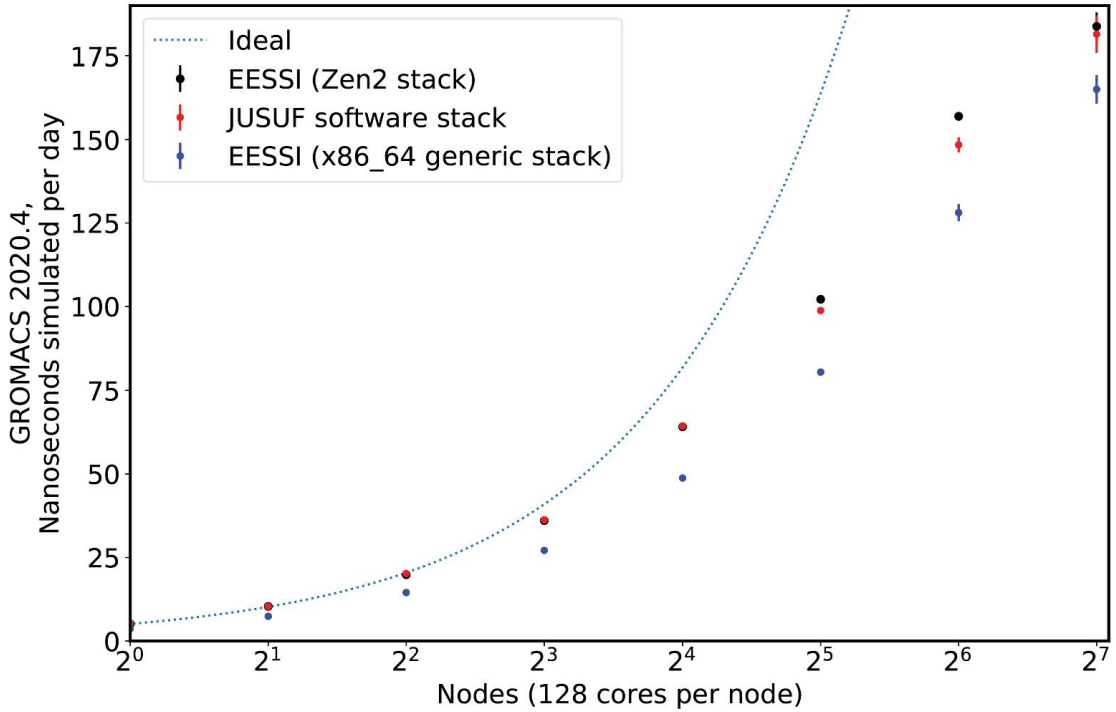
CernVM-FS

EESSI

Kenneth

EESSI paper (open access, Feb'22)

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)

Kenneth

Website: eessi.io

GitHub: github.com/eessi

Documentation: eessi.io/docs

Blog: eessi.io/docs/blog

Join the EESSI Slack

YouTube channel: youtube.com/@eessi_community

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

EESSI support portal: gitlab.com/eessi/support

Bi-monthly online meetings (1st Thu, odd months, 2pm CE(S)T)

Kenneth

MultiXscale

Co-funded by the European Union

EuroHPC Joint Undertaking

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Twitter: @MultiXscale

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