

Streaming Optimised Scientific Software, an Introduction to

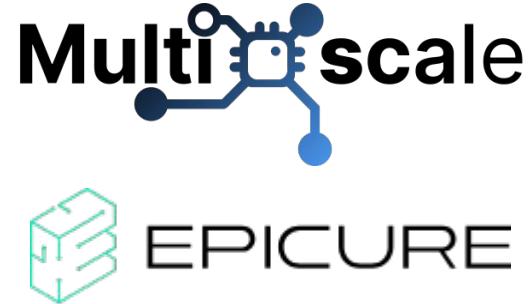
E E S S I

EUROPEAN ENVIRONMENT FOR
SCIENTIFIC SOFTWARE INSTALLATIONS

Kenneth Hoste - Ghent University (BE)

Alan O'Cais - University of Barcelona (ESP) + CECAM

Pedro Santos Neves - University of Groningen (NL)



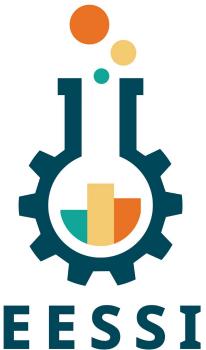
Fri 15 Nov 2024



Agenda



EPICURE



- The **MultiXscale** EuroHPC Centre-of-Excellence in a nutshell
- Motivation for & high-level **introduction to EESSI**
- Hands-on live **demo: getting access** to and **using EESSI**
- More in-depth overview of **layered design** of EESSI
- Overview of **available software + supported hardware**
- Workflow for **contributing** additional software installations to EESSI
- Status on **GPU support** (incl. live demo)
- **Use cases** enabled by EESSI: CI, training, collaboration with developers, ...

Interactive poll/quiz



EPICURE

Join at
slido.com
#4129 0527



EESSI

Help us choose for the hands-on demo...



You can help determine the details of the hands-on demo!

- Which **OS & software** should we use for the demo?
- Which **CPU** should we use for the demo?



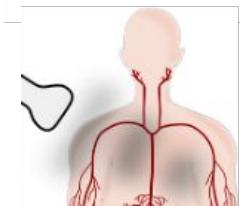
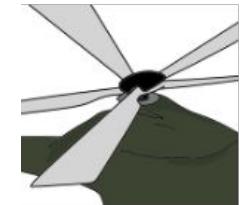
Join at
slido.com
#4129 0527



MultiXscale Centre-of-Excellence in a nutshell

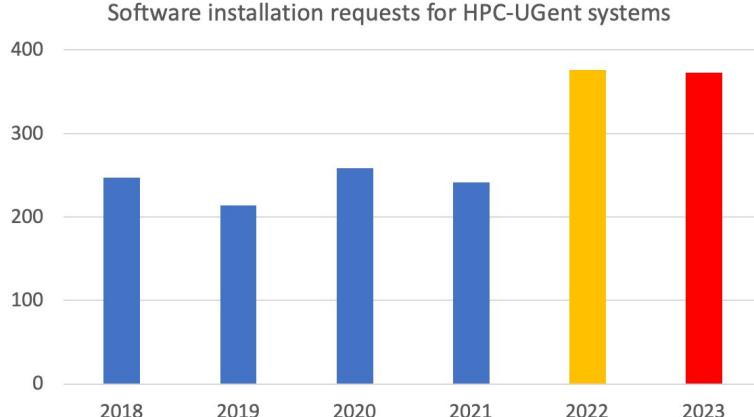


- 4-year project (started in Jan 2023), ~€6M budget
- Collaboration between EESSI and CECAM (total of 16 partners)
 - **EESSI** primarily addresses technical aspects
 - **CECAM** network provides scientific expertise
- Scientific target: multiscale simulations with 3 key use cases
 - Helicopter design and certification for civil transport
 - Battery applications to support the sustainable energy transition
 - Ultrasound for non-invasive diagnostics and biomedical applications
- More info: <https://multixscale.eu>



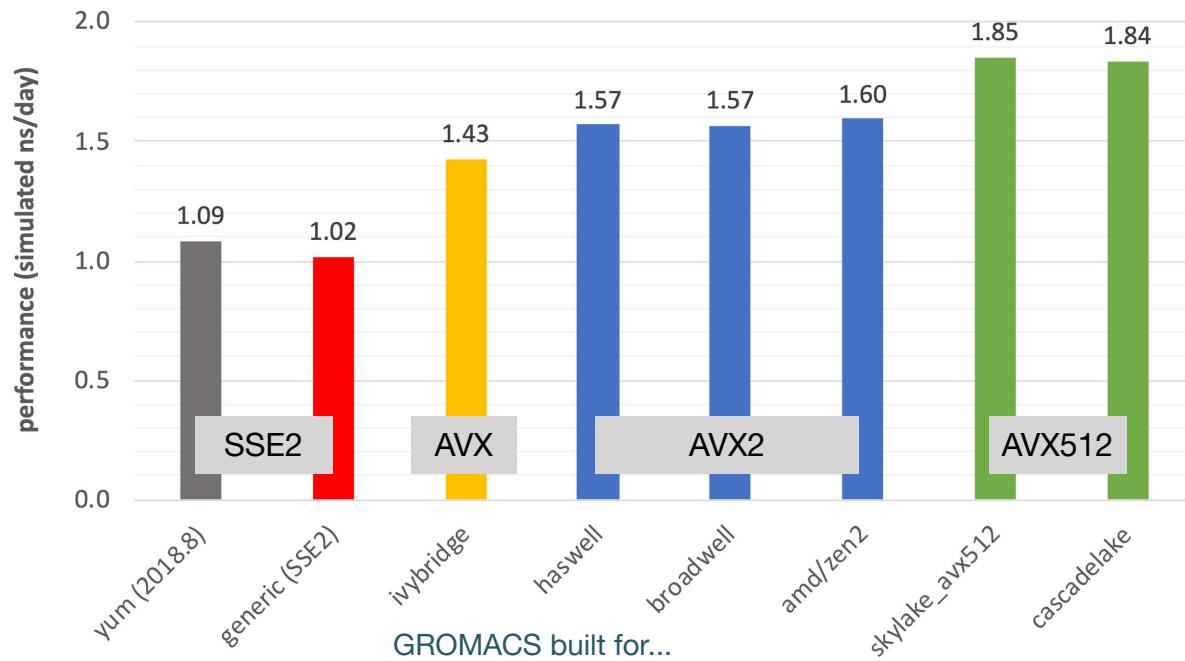
The changing landscape of scientific computing

- **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?*



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>



Major goals of EESI

- **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

Testing ReFrame

Host OS provides network & GPU drivers, resource manager (Slurm), ...

Host operating system

Software layer

Optimized applications + dependencies

Compatibility layer

Levelling the ground across client OSs

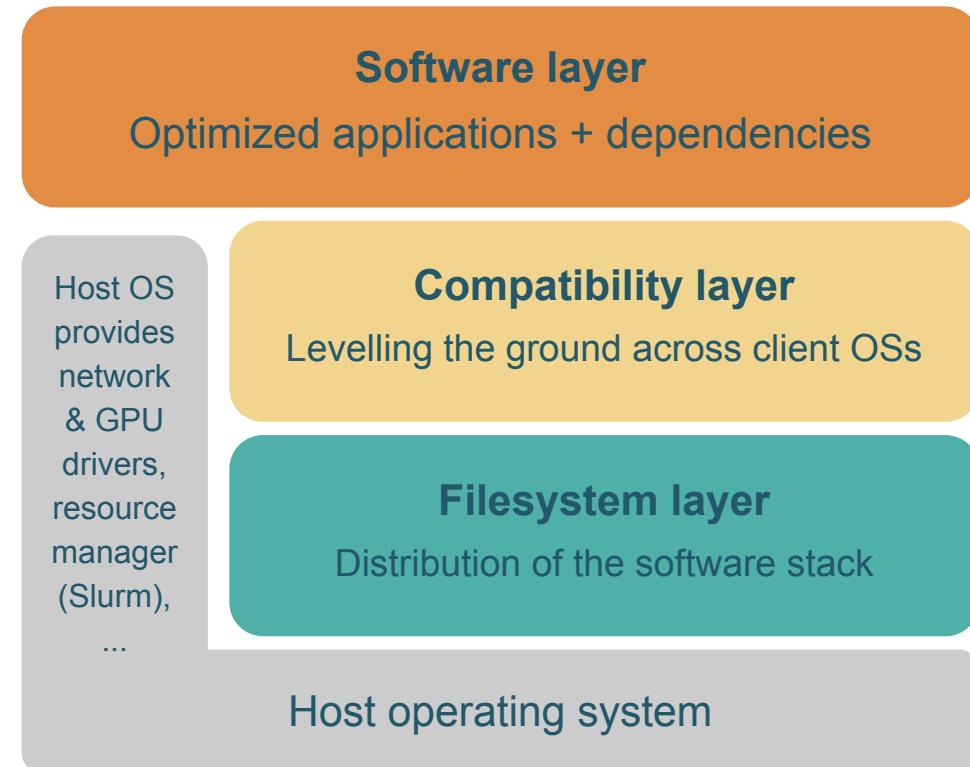
Filesystem layer

Distribution of the software stack



High-level overview of EESSI

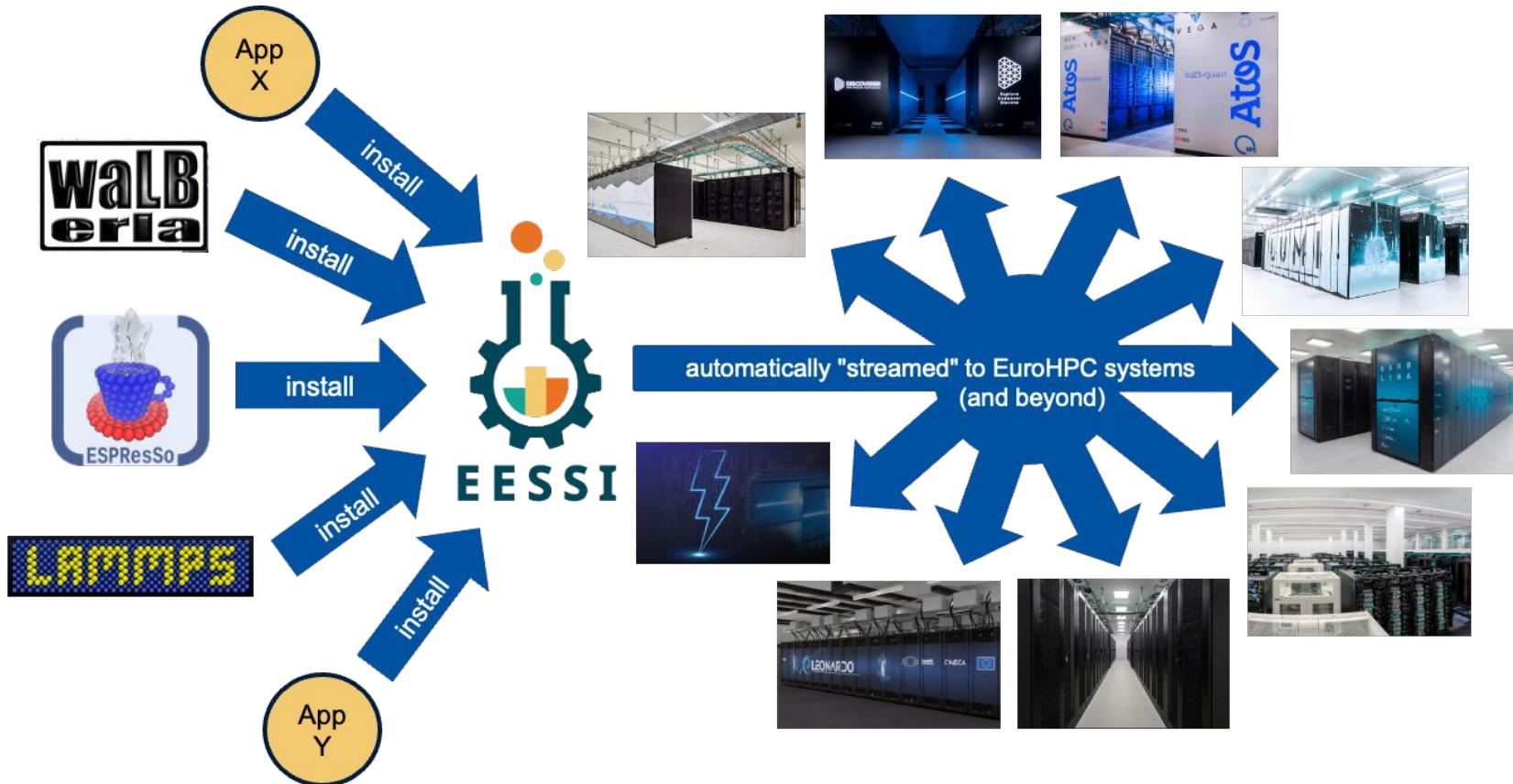
Testing ReFrame



EESSI
EUROPEAN ENVIRONMENT FOR
SCIENTIFIC SOFTWARE INSTALLATIONS



EESI as a shared software stack

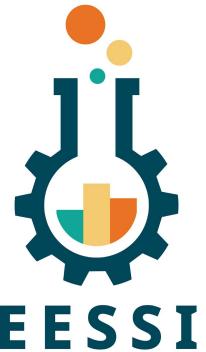


Join the quiz!

Question 1: What does the first 'E' in EESSI stand for?

- Everywhere
- Efficient
- European
- Enabling
- EESSI-is-not-EasyBuild

Join at
slido.com
#4129 0527



Join the quiz!

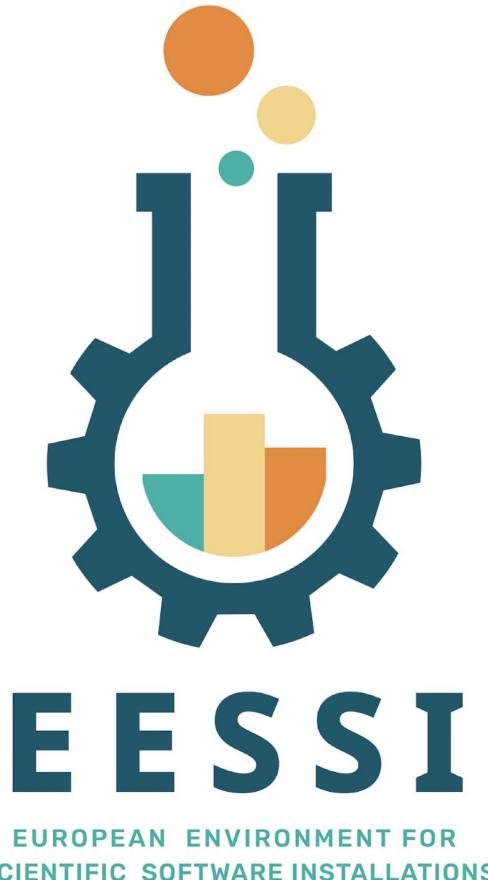


Question 2: What does EESSI provide?

- Recipes to install software from source
- Pre-built software packages to install
- Optimized installations of software
- Documentation with best practices for using software

Join at slido.com #4129 0527





Hands-on live demo

Getting access to EESSI

Using EESSI

Demo scenario



Starting from an “empty” virtual machine in AWS cloud

- No CernVM-FS installed yet, so EESSI not available yet, but only takes 2 min...
- Requires admin rights (`sudo` to install and configure CernVM-FS)
- Set up EESSI environment by sourcing init script
- Running EESSI demo script
- **OS:** see poll result
- **Software application used in demo:** see poll result
- **CPU architecture:** see poll result



Demo: Accessing EESSI via 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
```

Alternative ways of accessing EESSI are available, via a container image, via cvmfsexec, ...
eessi.io/docs/getting_access/native_installation - eessi.io/docs/getting_access/eessi_container



CernVM-FS

Demo: Using EESSI

eessi.io/docs/using_eessi/eessi_demos



```
/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
```

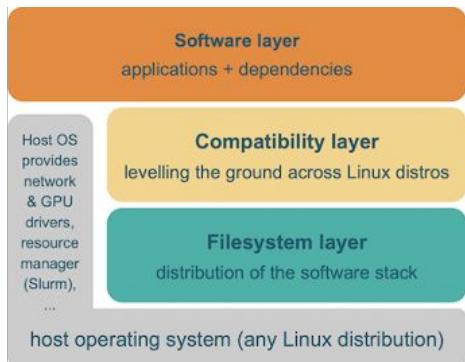
```
$ source /cvmfs/software.eessi.io/versions/2023.06/init/bash
Found EESSI pilot repo @
/cvmfs/software.eessi.io/versions/2023.06!
archdetect says x86_64/amd/zen3
Using x86_64/amd/zen3 as software subdirectory
...
Environment set up to use EESSI pilot software stack, have fun!

{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
```

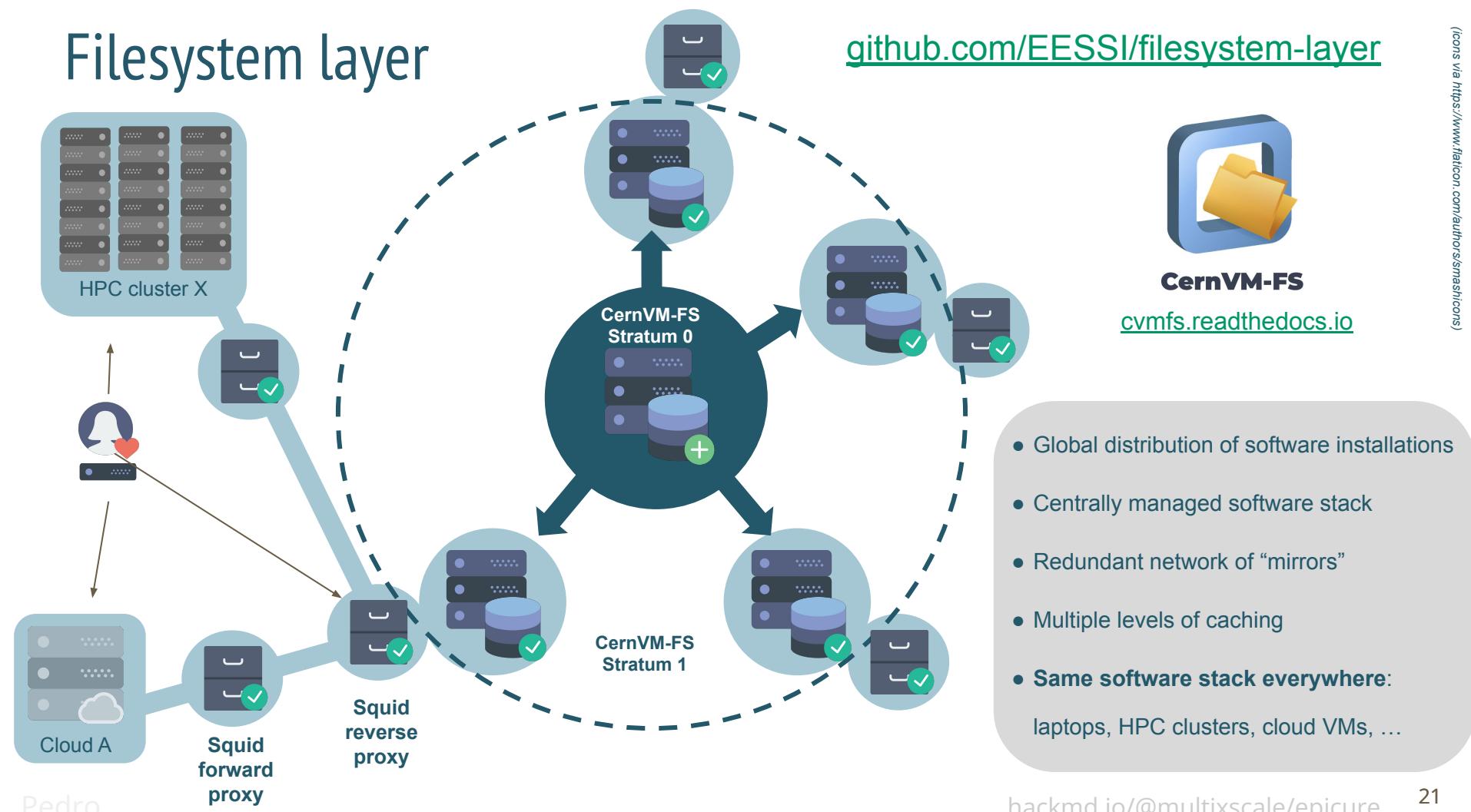
How does EESSI work?



- 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

Filesystem layer

github.com/EESSI/filesystem-layer

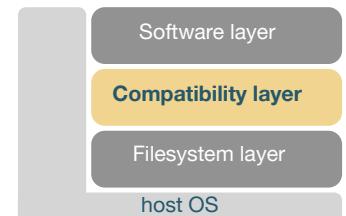


Compatibility layer

github.com/EESSI/compatibility-layer

- 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`



Software layer

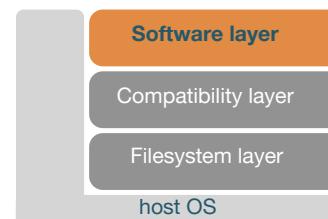
github.com/EESSI/software-layer



- 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
 **EASYBUILD.io**

Lmod



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

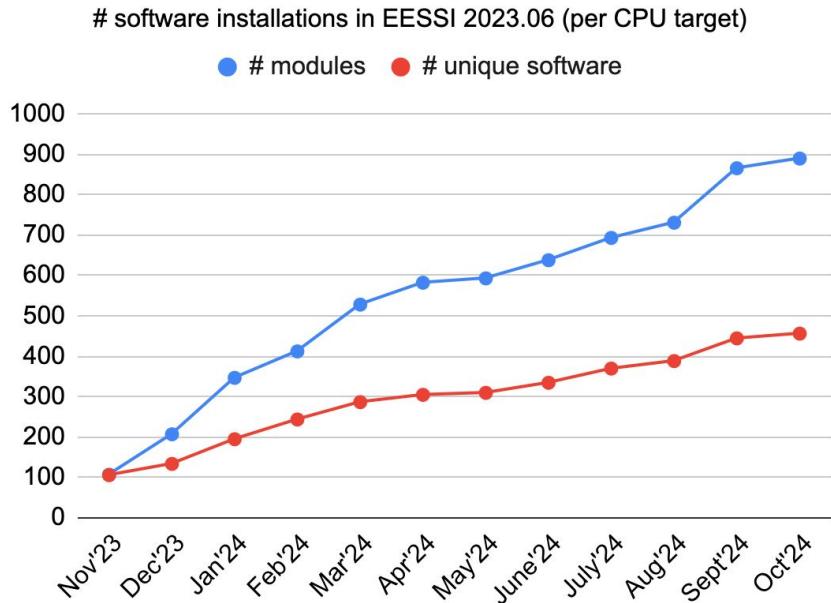


Overview of available software



Currently ~900 software installations available
per CPU target via software.eessi.io CernVM-FS repository;
increasing every day

- Over 450 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](https://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, coming soon)
 - Also works on laptops, in virtual machines in the cloud, on Raspberry Pi boards, etc.
- Different accelerators: **NVIDIA GPUs** (today) + **AMD GPUs** (soon)
 - For now, 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?



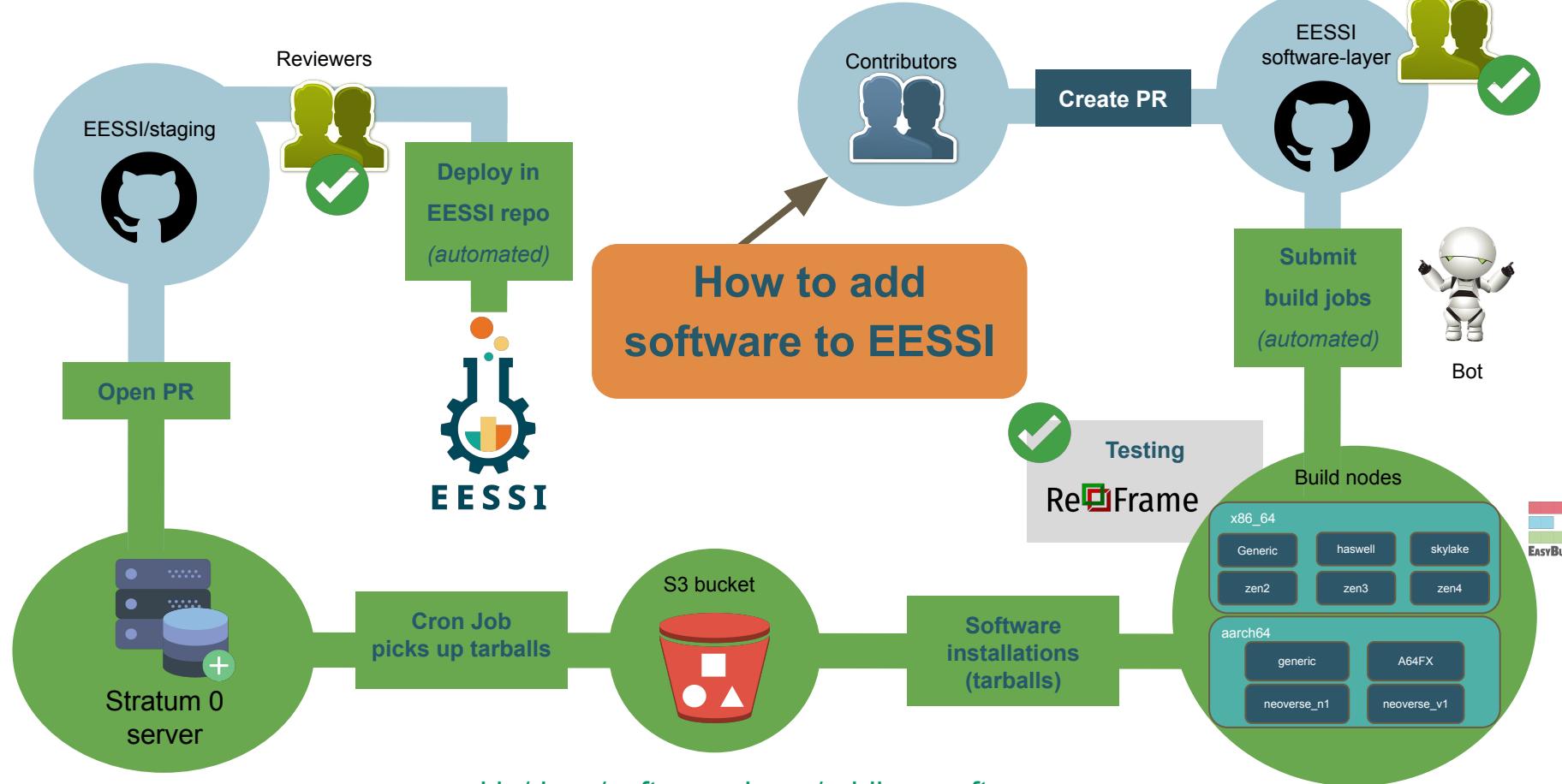
- EuroHPC JU systems:
 - Native installation (via CernVM-FS) on **Vega** + **Karolina**
 - EESSI can be used via `cvmfsexec` tool on Deucalion, Discoverer, MeluXina ([see blog post](#))
 - Native installation on **MeluXina**, **Deucalion**, **MareNostrum5** is a work-in-progress
 - JSC has expressed 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**

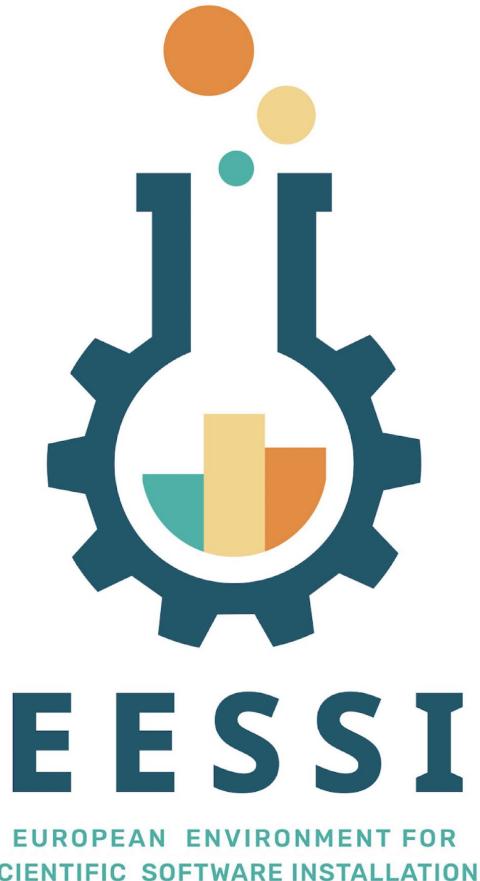
NVIDIA GPU support in EESSI



- 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
- Currently only for systems with **AMD Rome** (Zen2) CPU + **NVIDIA A100** GPU (CUDA compute capability 8.0)
- More CPU/GPU combos and software (GROMACS, PyTorch, TensorFlow, AlphaFold) coming soon...

Semi-automated workflow for adding software to EESSI





Hands-on live demo

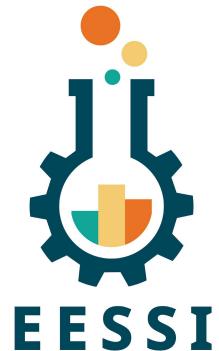
NVIDIA GPU support in EESSI

Contributing software to EESSI

Join the quiz!

Question 3: Which CPU architectures does EESSI support?

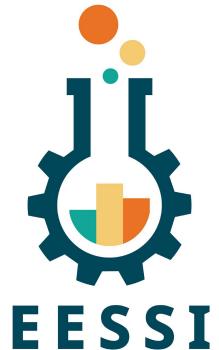
- Intel + AMD (x86_64)
- Arm 64-bit (aarch64)
- RISC-V
- All of the above!



Join at slido.com #4129 0527



Join the quiz!



Question 4: How many software *installations* does EESSI provide today, in total?

- A handful
- About 100
- Close to 1,000
- Over 8,000

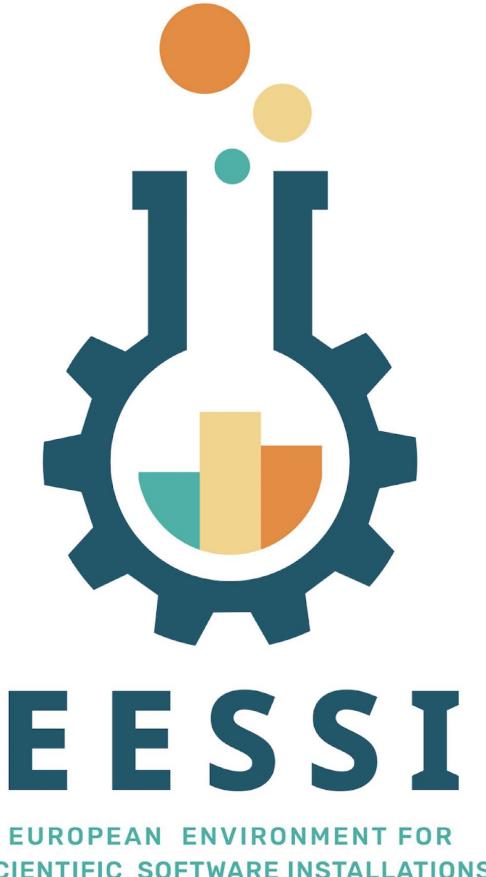
Join at slido.com #4129 0527





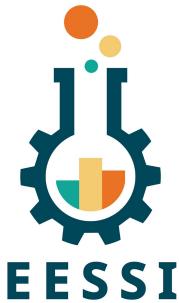
Software testing is an important part of EESSI

- EESSI test suite: eessi.io/docs/test-suite
 - Collection of *portable* tests for software available in EESSI
- 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 use cases

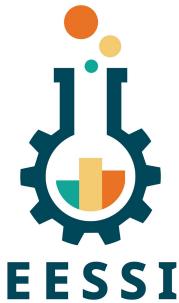
Use cases enabled by EESSI



- 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



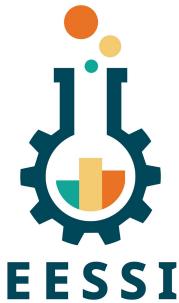
- Portable workflows are significantly easier when relying on EESSI
- They often involve running a broad set of tools, which all need to be available
- Workflows definitions (Snakemake, Nextflow,...) can leverage (or be included in) EESSI
- You can ship your execution environment inside your git repository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

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:

```
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



build
Succeeded 2 minutes ago in 1m 1s

Q Search logs ⚙

- > Set up job 2s
- > Run actions/checkout@v2 0s
- > Run eessi/github-action-eessi@main 52s
- ▽ Test EESSI 5s

```
1 ▼ Run module load GROMACS
2 module load GROMACS
3 gmx --version
4 shell: /usr/bin/bash --noprofile --norc -e -o pipefail {0}
5 env:
6 EESSI_SILENT: 1
7 BASH_ENV: /cvmfs/pilot.eessi-hpc.org/versions/2021.06/init/bash
8
9          :- GROMACS - gmx, 2020.4-MODIFIED (-:
10
11         GROMACS is written by:
12         Emile Apol      Rossen Apostolov    Paul Bauer      Herman J.C. Berendsen
13         Par Bjelkmar   Christian Blau     Viacheslav Boilnykh   Kevin Boyd
14         Aldert van Buuren Rudi van Drunen   Anton Feenstra   Alan Gray
15         Gerrit Groenhof Anca Hamararu    Vincent Hindriksen M. Eric Irrgang
16         Aleksei Iupinov Christoph Junghans Joe Jordan    Dimitrios Karkoulis
17         Peter Kasson      Jiri Kraus      Carsten Kutzner  Per Larsson
18         Justin A. Lemkul Viveca Lindahl   Magnus Lundborg Erik Marklund
19         Pascal Merz      Pieter Meulenhoff Teemu Murtola   Szilard Pall
20         Sander Pronk     Roland Schulz   Michael Shirts Alexey Shvetsov
21         Alfons Sijbers   Peter Tielemans Jon Vincent   Teemu Virolainen
22         Christian Wennberg Maarten Wolf   Artem Zhmurov
23
24         and the project leaders:
```

<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



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, ...

Support for installing, using, contributing to EESSI



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, ...)

The screenshot shows the EESSI support portal interface on a GitLab page. The left sidebar lists project management tasks: Manage, Plan, Code, Build, Deploy, Operate, Monitor, and Analyze. The main content area displays the README.md file for the EESSI support portal. It includes the MultiXscale logo, the EESSI logo, and a message of thanks to the MultiXscale project. It also provides contact information and links to create an issue with a GitLab account or contact via email.

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



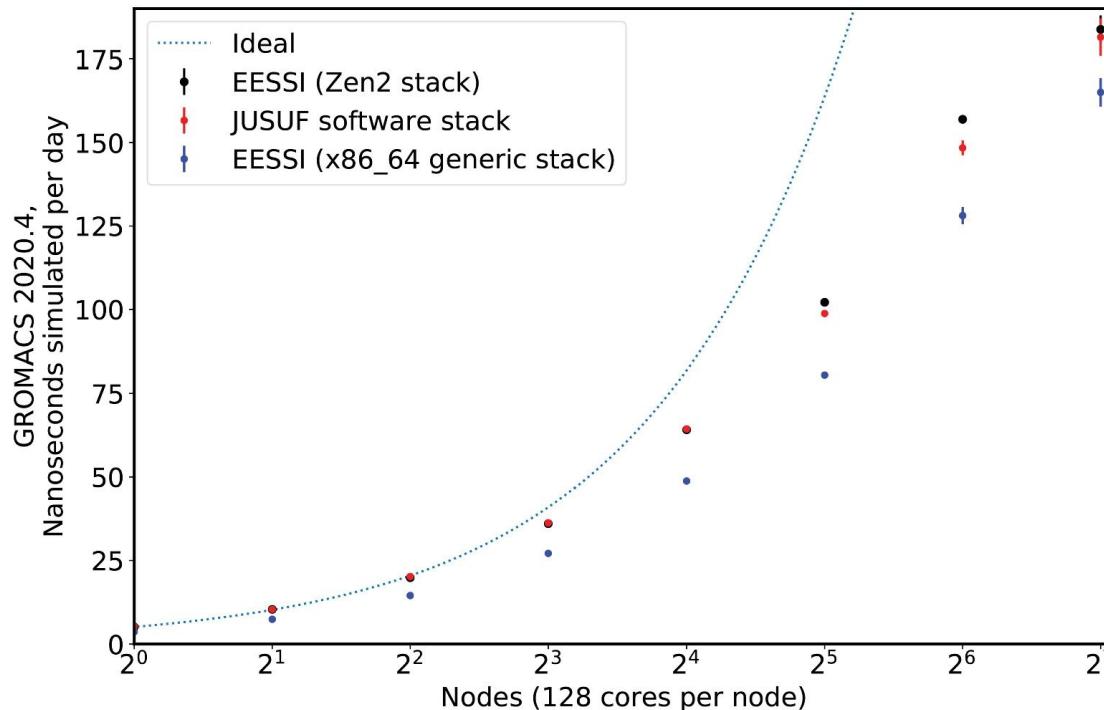
hackmd.io/@multixscale/epicure

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...**





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)

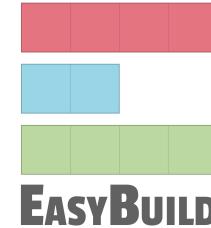
EESSI at Supercomputing'24



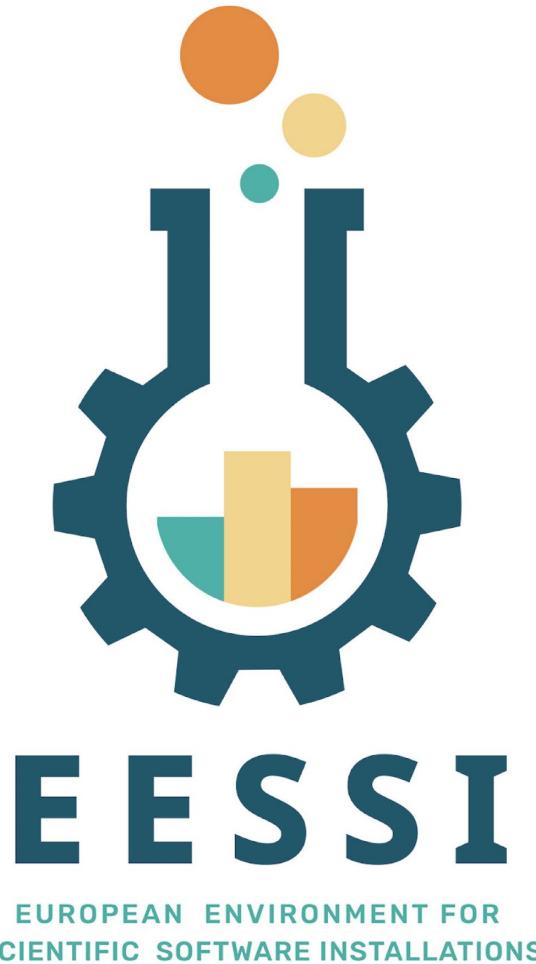
- 17-22 Nov 2024 in Atlanta, Georgia (US)
- <https://sc24.supercomputing.org>
- **Birds-of-a-Feather session on EESSI:** Tue 19 Nov 12:15-13:15 EST
- **Presentation at Microsoft Azure booth** at SC'24 exhibit
(Wed 20 Nov 14:40-15:00 EST)
- **Free stickers** for everyone who bumps into us
EESSI, EasyBuild, CernVM-FS, ...
- + Some nice news about EESSI
which we can not disclose yet...



EPICURE webinar: Introduction to EasyBuild



- **Fri 13 Dec 2024, 14:00-15:30 CET** (mark your calendars!)
- Introductory tutorial on EasyBuild
 - What is EasyBuild?
 - Installation + configuration of EasyBuild
 - Terminology
 - Basic usage: installing software with EasyBuild
 - Troubleshooting failing installations
 - Writing easyconfigs (build recipes for EasyBuild)
 - Advanced topics: using hooks to customize EasyBuild, implementing easyblocks, ...
- Will also briefly cover how you can install software on top of ESSI
- **Registration will be open soon, see EPICURE website!**



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)

Multiscale



Co-funded by
the European Union



Web page: multixscale.eu

Facebook: [MultiXscale](#)

Twitter: [@MultiXscale](#)

LinkedIn: [MultiXscale](#)



UNIVERSITAT DE
BARCELONA



SORBONNE
UNIVERSITÉ

