



E E S S I

EUROPEAN ENVIRONMENT FOR
SCIENTIFIC SOFTWARE INSTALLATIONS

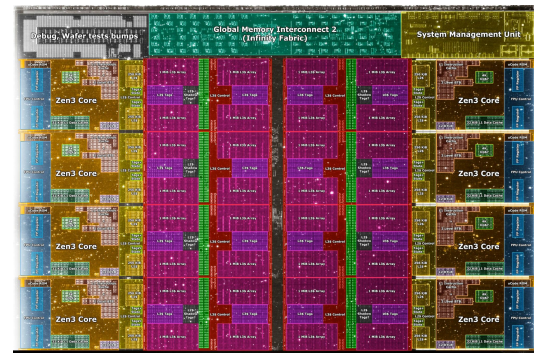
HPC-UGent User meeting | 29 May 2026

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hpc@ugent.be

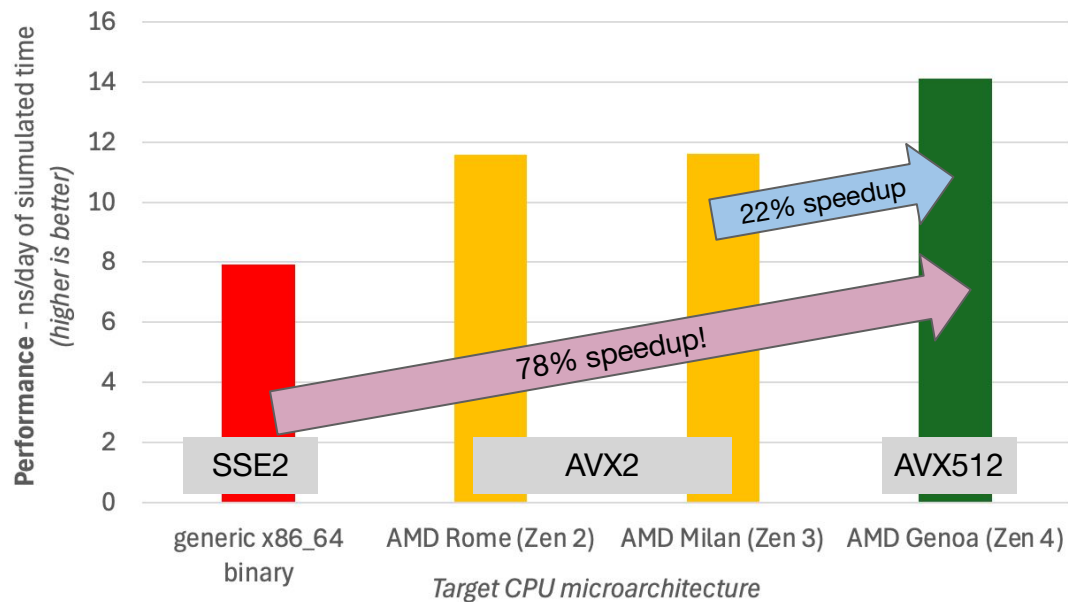
Modern CPUs

- Modern microprocessors support **vector instructions**, a.k.a. SIMD (Single Instruction Multiple Data)
- Like AVX2, AVX-512, AVX10 (AMD, Intel), or SVE (Arm), ...
- Parts of the microprocessor are *dedicated* to running these vector instructions
- If you run binaries that are not using these instructions, you're not using a significant part of what the CPU supports!
- ... and **performance suffers** (potentially a lot)
- Downside: binaries that use vector instructions are less “portable”...



Keeping the P in HPC

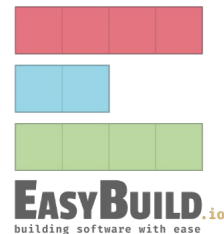
- Software should be **optimized** for (the CPU/GPU of) the system it will be run on
- This implies **building software from source code**, using specific compiler options, ...
- Impact on **software performance** is often *significant* for scientific software!



- Barplot shows performance of different GROMACS binaries, **same source code & workload, same hardware & OS**
- GROMACS version 2025.2
Test Case B from PRACE UEABS v2.2
- 1 shinx node: 2x 96-core AMD Zen 4
- Hybrid run on 192 cores in total
48 MPI ranks with 4 OpenMP threads each

EasyBuild in a nutshell

<https://easybuild.io>

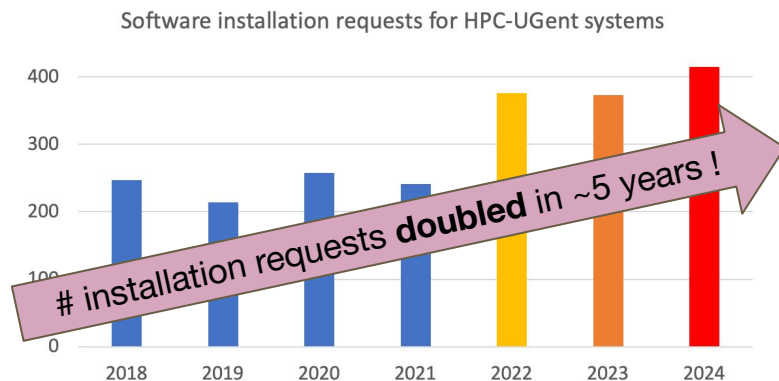


- Tool to install (scientific) software on HPC systems, usually from source code
- Created by HPC-UGent in summer 2009
- Open source software (GPLv2) since Nov 2012
- Easy installation (pip install easybuild), extensive documentation (<https://docs.easybuild.io>)
- Used to manage central software stack on VSC systems + LUMI, JUPITER, Deucalion, ...
- Worldwide community grew around it, used all over Europe + Canada, US, Australia, ...



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 here (see Fugaku, JUPITER, ...), RISC-V is coming (soon?)
- In strong contrast: available (wo)manpower in **HPC support teams is (still) limited**
- Software installation tools like EasyBuild and Spack are **no longer sufficient...**



*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?*



European Environment for Scientific Software Installations

- **Shared repository of (optimized!) scientific software installations**
- Avoid duplicate work across 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 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**
- Development effort funded through **MultiXscale** EuroHPC Centre-of-Excellence
- Base for Federated Software Stack of **EuroHPC Federation Platform**



E E S S I
EUROPEAN ENVIRONMENT FOR
SCIENTIFIC SOFTWARE INSTALLATIONS

<https://eessi.io>

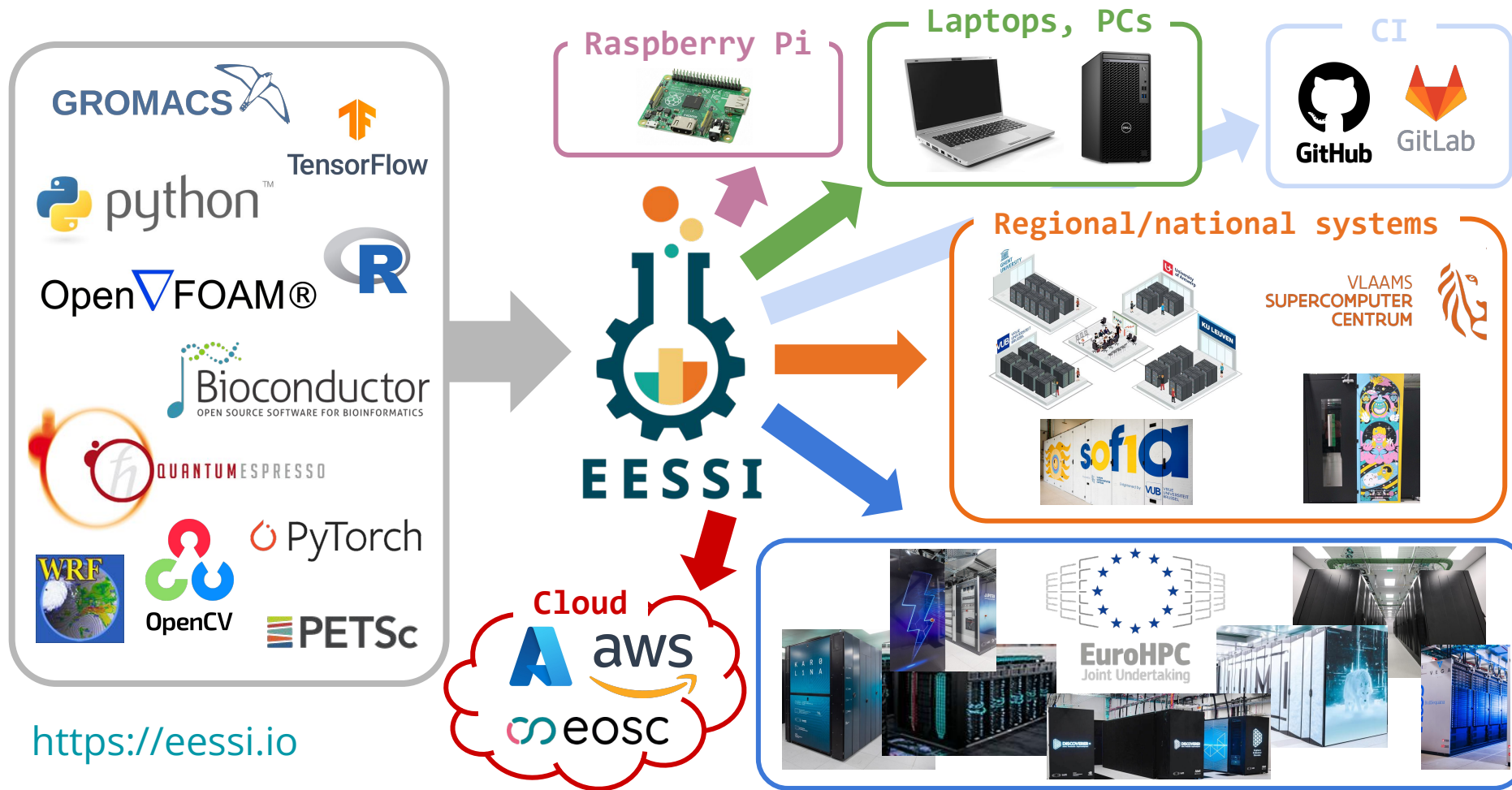
*inspired by the
ComputeCanada software stack*

Major goals of EESSI

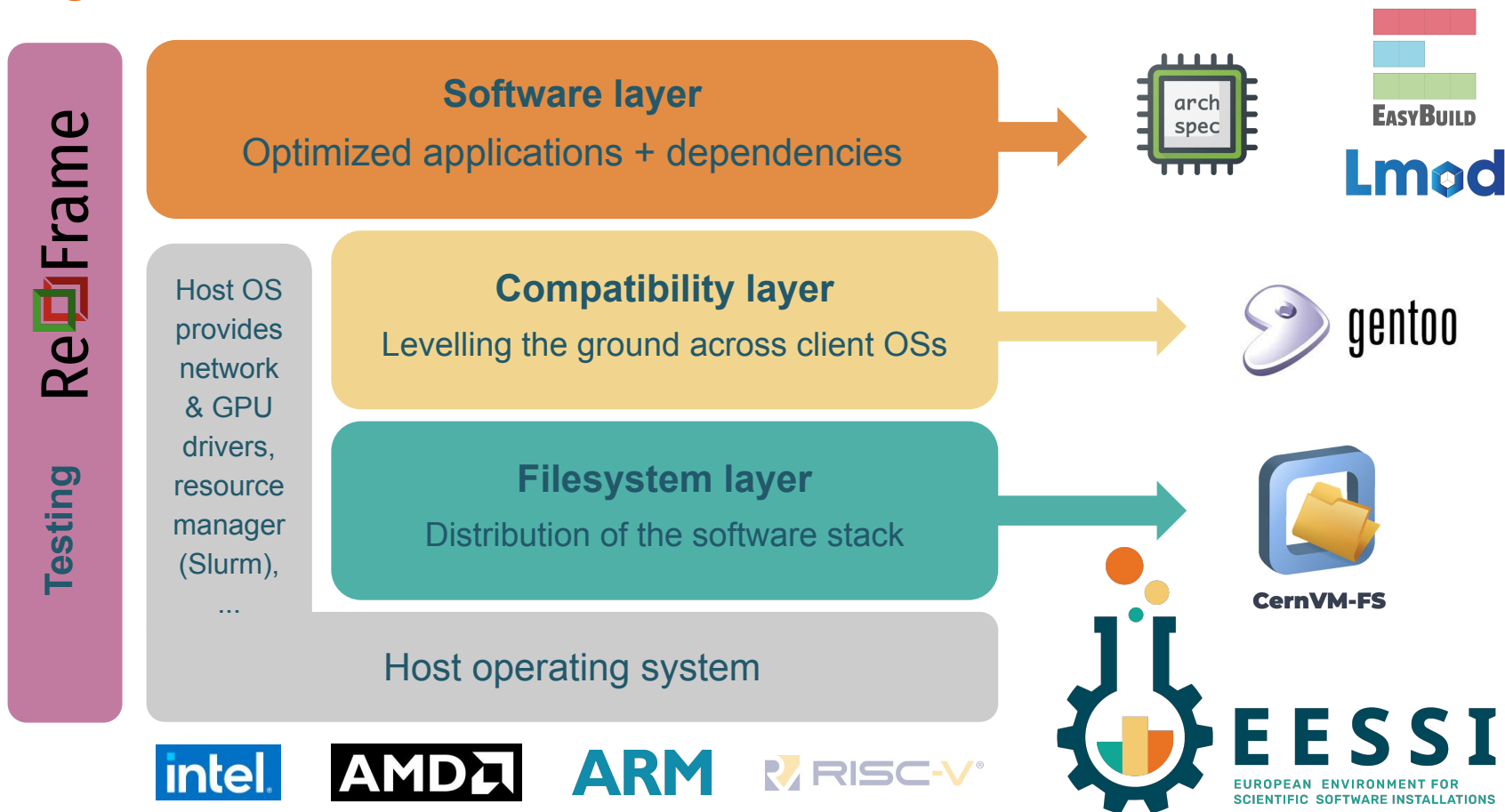


- Providing a truly **uniform software stack**, across a broad variety of systems
 - Have access to the (exact) same software environment everywhere
 - Across HPC, cloud, laptop, Continuous Integration environments, ...
 - **Without sacrificing performance** for “mobility of compute”
(like is typically done with containers or Conda)
- **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
- **Facilitate** HPC training, development of (scientific) software, ...

EESSI as a shared software stack for HPC, cloud, and beyond



High-level overview of EESSI



EESSI is powered by FOSS



gentoo linux™

Compatibility layer

Abstraction from the
host operating system



CernVM-FS

Filesystem Layer

Global distribution of
software installations
(on-demand streaming)

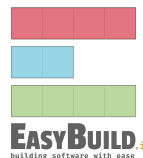
ReFrame

Regression
testing
of software



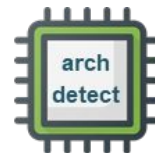
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Optimized software
installations for specific
CPU microarchitectures

Intuitive user interface:
module avail,
module load, ...



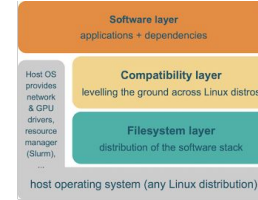
Automatic selection of
best suited part of
software stack for
CPU microarchitectures



Magic Castle
to create (ephemeral)
clusters in the cloud

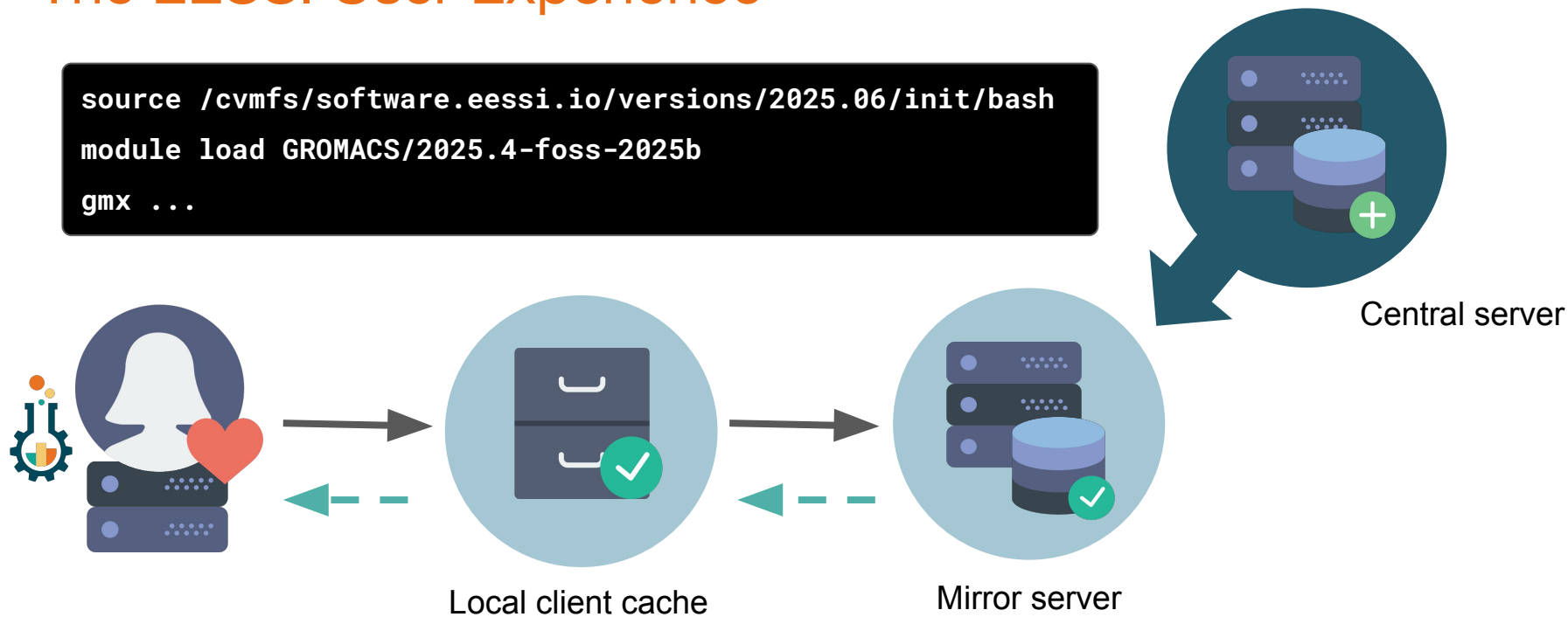
How does EESSI work?

- 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 + GPU generations
 - **Ready-to-use**: no explicit installation or updating required
- Initialization script **auto-detects** CPU + GPU of the system



The EESSI User Experience

```
source /cvmfs/software.eessi.io/versions/2025.06/init/bash  
module load GROMACS/2025.4-foss-2025b  
gmx ...
```



EESSI provides **on-demand streaming**
of (scientific) software (like music, TV-series, ...)

Hands-on demo: Using EESSI

```
source /cvmfs/software.eessi.io/versions/2025.06/init/bash
```

```
Found EESSI repo @ /cvmfs/software.eessi.io/versions/2025.06!
```

```
archdetect says x86_64/amd/zen3
```

```
archdetect found supported accelerator for CPU target x86_64/amd/zen3: accel/nvidia/cc80
```

```
Using x86_64/amd/zen3 as software subdirectory.
```

```
Using /cvmfs/software.eessi.io/versions/2025.06/software/linux/x86_64/amd/zen3/modules/all
```

```
Using ...
```

```
...
```

```
Environment set up EESSI (2025.06), have fun!
```

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

```
cd eessi-demo/GROMACS
```

```
./run.sh
```

See also https://eessi.io/docs/using_eessi/eessi_demos

Script for running GROMACS with ~~ease~~ EESSI

```
#!/bin/basheessi-demo.sh  
  
source /cvmfs/software.eessi.io/versions/2025.06/init/lmod/bash  
module load GROMACS/2025.4-foss-2025b  
  
# download input file + unpack (only if it's missing)  
if [ ! -f ion_channel.tpr ]; then  
    curl -OL https://repository.prace-ri.eu/ueabs/GROMACS/1.2/GROMACS_TestCaseA.tar.gz  
    tar xfz GROMACS_TestCaseA.tar.gz  
fi  
  
# cleanup, to force new run  
rm -f ener.edr logfile.log  
  
# run GROMACS (downscaled to 1k steps instead of full run with 10k steps)  
gmxd mdrun -s ion_channel.tpr -maxh 0.50 -nsteps 1000 -g logfile
```

Running GROMACS with ~~ease~~ EESSI

```
macbook-pro $ lima shell eessi
```

```
lima $ ls /cvmfs/software.eessi.io  
host_injections  init  
README.eessi  versions
```

```
lima $ ./eessi-demo.sh
```

```
...
```

	(ns/day)	(hour/ns)
Performance:	2.215	10.834



```
$ ssh slurm-cluster-aws
```



```
aws $ P=aarch64-neoverse-v1-node
```

```
aws $ sbatch -p $P -c 8 eessi-demo.sh  
113508
```

```
aws $ cat slurm-113508.out
```

```
...
```

	(ns/day)	(hour/ns)
Performance:	7.758	3.094

```
$ ssh tier1.hpc.ugent.be
```

VLAAMS
SUPERCOMPUTER
CENTRUM



```
vsc $ qsub -l nodes=1:ppn=16 eessi-demo.sh  
13001403
```

```
vsc $ cat eessi-demo.sh.*13001403
```

```
...
```

	(ns/day)	(hour/ns)
Performance:	20.802	1.154

```
$ ssh login.deucalion.macc.fccn.pt
```

```
deucalion $ sbatch -p normal-arm eessi-demo.sh  
Submitted batch job 7654321
```

```
deucalion $ cat slurm-7654321.out
```

```
...
```

	(ns/day)	(hour/ns)
Performance:	8.960	2.678



Getting access to EESSI (native via CernVM-FS)



```
# Native installation of EESSI using CernVM-FS, requires admin privileges
# Installation commands are for RHEL-based distros
# Like CentOS, Rocky Linux, AlmaLinux, Fedora, ...

# Install CernVM-FS to get access to CernVM-FS repositories (incl. EESSI)
sudo yum install -y
    https://ecsft.cern.ch/dist/cvmfs/cvmfs-release/cvmfs-release-latend.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"

# Complete setup of CernVM-FS
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

Available software in EESSI



~2,000 software installations available per supported CPU target

via `software.eessi.io` CernVM-FS repository, increasing every week

- **15 supported CPU targets** (AMD, Intel, Arm, RISC-V is WIP)
see https://eessi.io/docs/software_layer/cpu_targets

- **~750 different software packages**,
plus ~3,000 extensions (Python packages, R libraries)

- ~30,000 software installations in total (+ extensions)

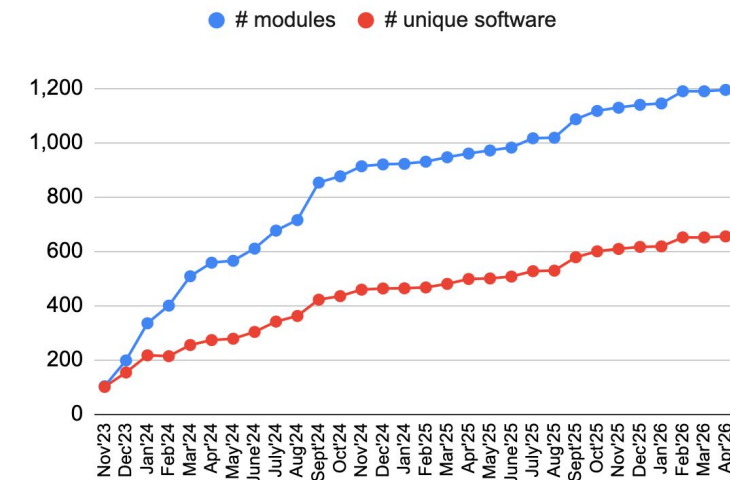
- Including ESPResSo, GROMACS, LAMMPS, OpenFOAM, PyTorch, R, QuantumESPRESSO, TensorFlow, waLBerla, WRF, ...

- See overview @ https://eessi.io/docs/available_software

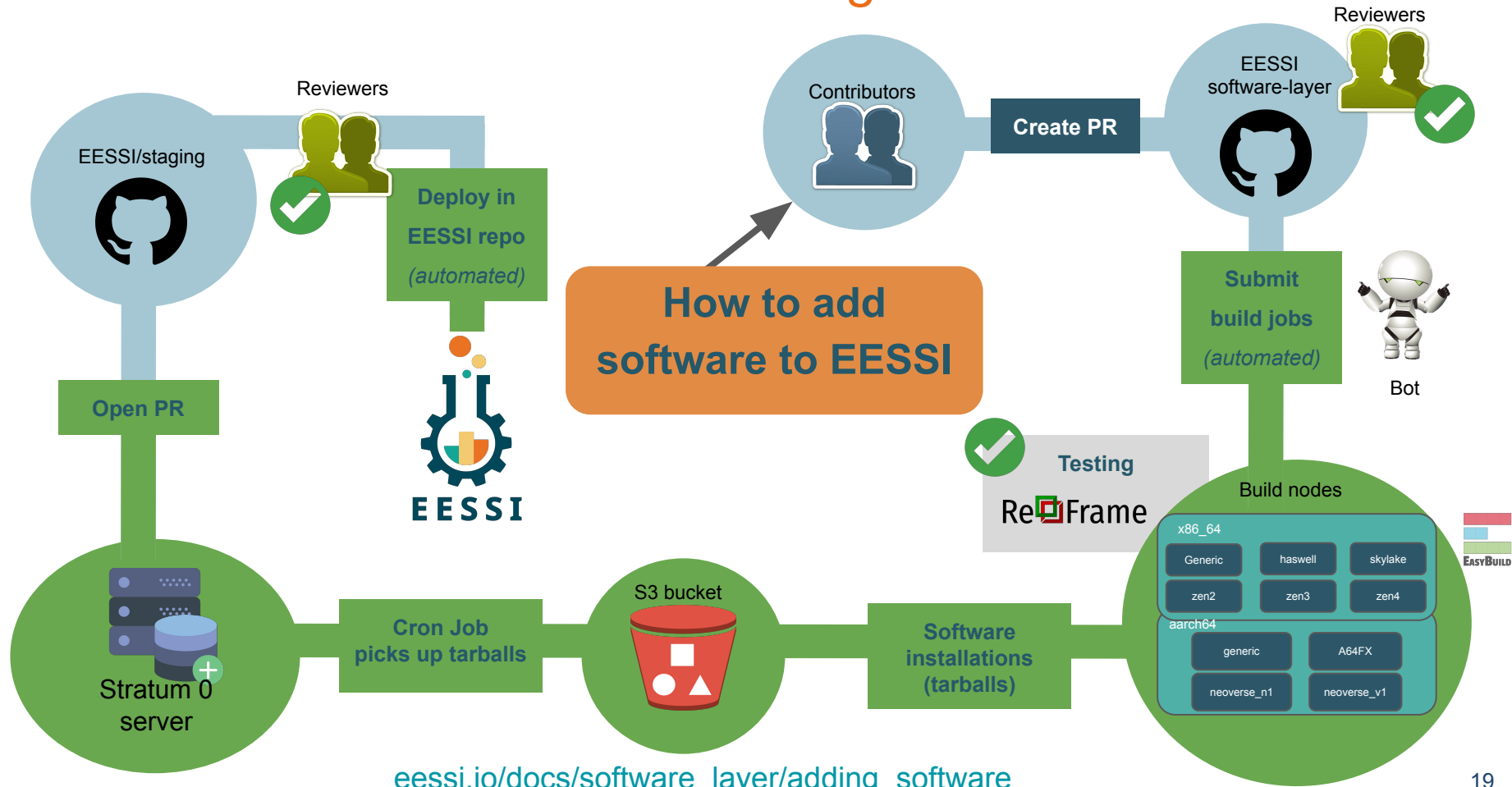
- EESSI version 2023.06: using `foss/2023a` and `foss/2023b` toolchains

- EESSI version 2025.06: using `foss/2024a`, `foss/2025a`, and `foss/2025b` toolchains

software installations in EESSI 2023.06 (per CPU target)



Semi-automated workflow for adding software to EESSI



Building software on top of EESSI



- You can use the software available in EESSI to **resolve dependencies** of the software you need
- To install software with EasyBuild on top of EESSI, first load the **EESSI-extend** module to correctly configure EasyBuild
- To “manually” install software on top of EESSI (by running `gcc`, `make`, etc.), first load the **buildenv** module
- See also https://eessi.io/docs/using_eessi/building_on_eessi
- Using Spack to install software on top of EESSI is also possible, see blog post on proof-of-concept implementation: <https://eessi.io/docs/blog/2026/02/05/Spack-on-top-of-EESSI-best-of-both-worlds>

On which systems is EESSI available today?



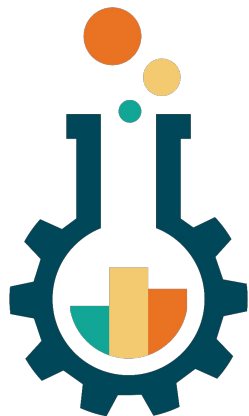
- On supercomputers in Flanders (Vlaams Supercomputer Centrum, VSC):
 - **Available today on Tier-2 at UGent, VUB, KUL + Tier-1 Hortense** (+ sofia soon)
 - Tier-1 cloud: can deploy it yourself and have access to a full software stack in minutes
- On **various systems throughout Europe** (and beyond)
 - **EuroHPC JU systems** incl. Vega, Karolina, MareNostrum 5, Deucalion, Discoverer, LUMI, ...
 - Snellius @ SURF, EMBL, Univ. of Stuttgart, Sigma2 & Olivia in Norway, etc.
- EESSI can be used in virtual machine in European Open Science Cloud (EOSC),
see also <https://www.eessi.io/docs/blog/2025/10/22/eosc>
- Overview of (known) systems that have EESSI available at <https://eessi.io/docs/systems>

Webinar series: Different aspects of EESSI

<https://eessi.io/docs/training-events/2026/webinar-series-2026Q2>

- Introduction to EESSI (*recorded*)
- Building software on top of + contributing to EESSI (*recorded*)
- Using EESSI for Continuous Integration (*recorded*)
- Introduction to CernVM-FS (*recorded*)
- Using EESSI as a base for a central software stack (*Mon 1 June'26*)

Slides + recordings available



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EESSI in EuroHPC Federation Platform



EuroHPC
Joint Undertaking

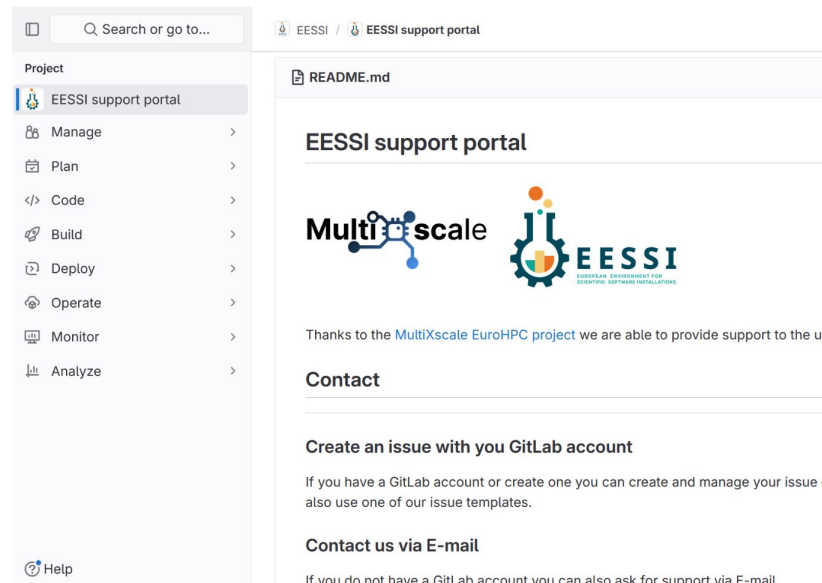
Federation Platform

- Ghent University was invited into the consortium led by CSC.fi that is currently developing the EuroHPC Federation Platform (EFP)
- EFP will be “one-stop shop” for people to access & use EuroHPC systems
- For entire EuroHPC ecosystem: supercomputers, AI factories, quantum
- **UGent is integrating EESSI into EFP as base for the Federated Software Stack**
- First version of EFP became operational in April 2026
- All new EuroHPC projects are onboarded through EFP
- More info via <https://my-eurohpc.eu> , see also [recorded talk from EUM'26](#)
- EFP webinar series ongoing, recordings available: <https://my-eurohpc.eu/training>



Support for installing, using, contributing to EESSI

- 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



HPCWire Reader's Choice award for EESSI



eessi.io/docs/blog/2024/11/18/hpcwire-readers-choice-awards-2024-for-eessi



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)

[EESSI Happy Hour](#): Mondays 2pm CE(S)T

MultiXscale

Web page: multixscale.eu

Facebook: [MultiXscale](https://www.facebook.com/MultiXscale)

Twitter: [@MultiXscale](https://twitter.com/MultiXscale)

LinkedIn: [MultiXscale](https://www.linkedin.com/company/multixscale)



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