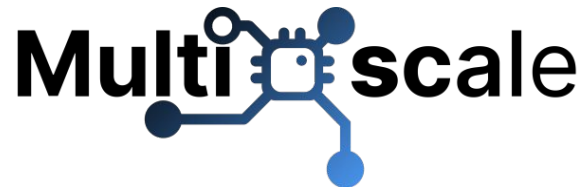
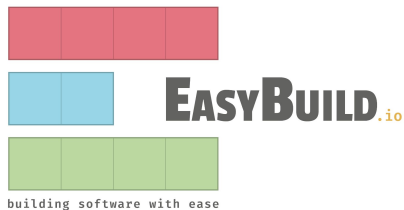


*What if you no longer have to install
a **broad range of scientific software**
from scratch on every laptop, HPC cluster,
or cloud instance you use or maintain,
without compromising on performance?*





Lara Peeters (Ghent University)

EasyBuild + EESSI + Spack tutorial/hackaton - 19 May 2026

Q&A via EESSI Slack



Please join the `#cineca-hackathon-may26-org` channel in the EESSI Slack for questions and discussion

Step 1) **Join the EESSI Slack**, see “Slack channel” link at <https://eessi.io>

Step 2) **Join `#cineca-hackathon-may26-org` channel** in EESSI Slack
(direct link: <https://eessi-hpc.slack.com/archives/C0AAH8CJGTZ>)

Agenda



- 9:00 - 9:15 Welcome
- 9:15 -10:15: quick intro by MaX, CINECA, EBRAINS, ECMWF (no slides required)
- 10:15 - 11:00 EasyBuild [Kenneth]
-
- 11:00-11:30 Coffee break
- **11:30-12:30 EESSI [Lara]**
- 12:30-13:00 Q&A, prep for hands-on

Agenda



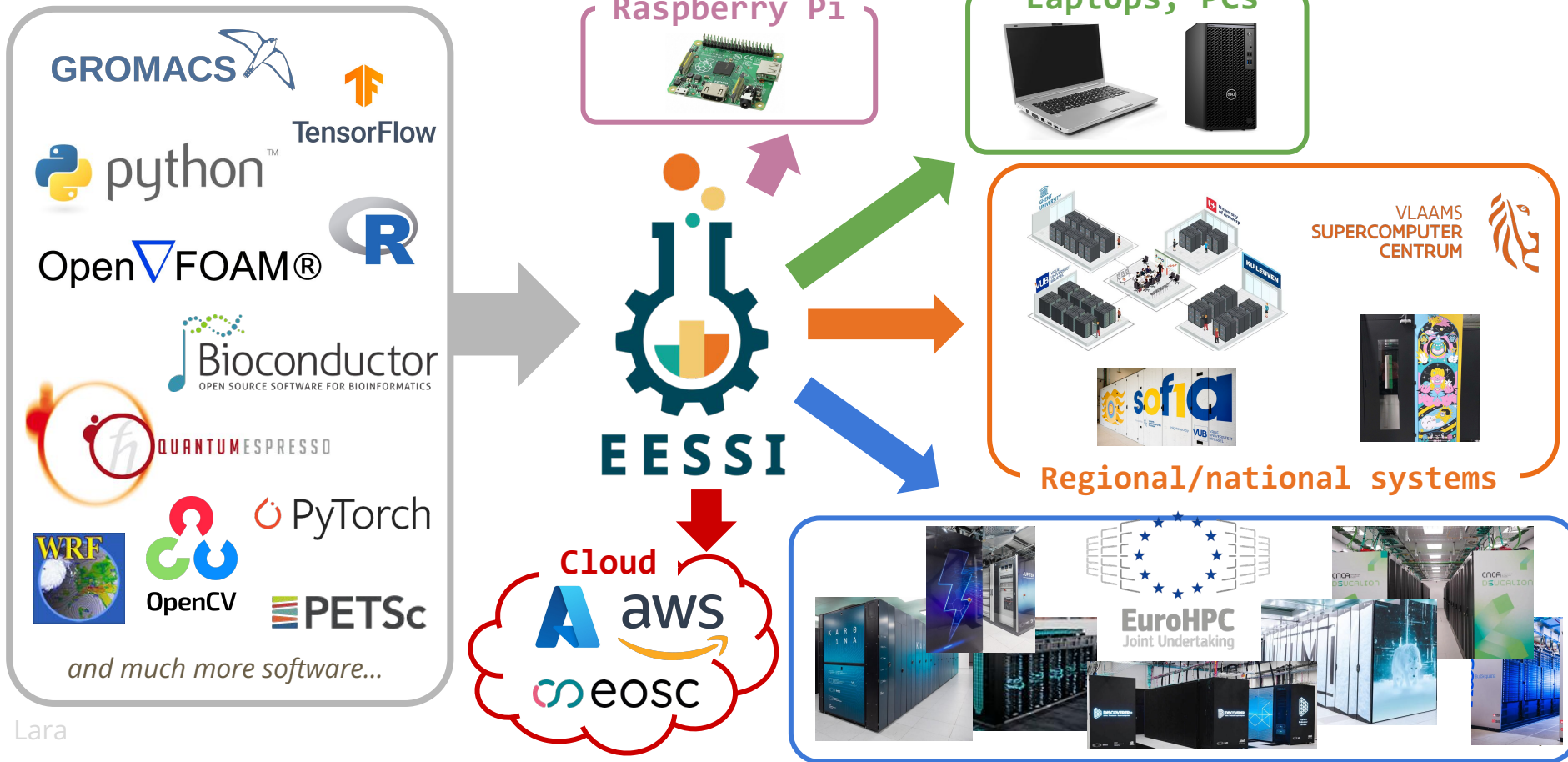
- 13:00 - 14:00 Lunch
- 14:00 - 15:30 Spack (incl. intro to environments + package recipes) [Max+Harmen]
- 15:30-16:00 EFP [Alan]
-
- 16:00-16:30 Coffee Break
- 16:30 - 18:00 Free hands-on (basic usage of EasyBuild, EESSI, Spack, EFP)

Major goals of EESSI



- 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)
- **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 shared software stack for HPC, cloud, and beyond



Demo time!

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

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
  |   |-- a64fx
  |   |-- nvidia
  |       |-- grace
  |-- x86_64
  |   |-- amd
  |   |   |-- zen2
  |   |   |-- zen3
  |   |   |-- zen4
  |   |   |-- zen5
  |   |-- generic
  |-- intel
  |   |-- haswell
  |   |-- cascadelake
  |   |-- icelake
  |   |-- sapphirerapids
  |   |-- skylake_avx512
  |       |-- modules
  |       |-- software
```

```
$ source /cvmfs/software.eessi.io/versions/2025.06/init/lmod/bash
Modules purged before initialising EESSI
Module for EESSI/2025.06 loaded successfully
```

EESSI has selected x86_64/amd/zen2 as the compatible CPU target for EESSI/2025.06 **Automatically detects CPU microarchitecture**

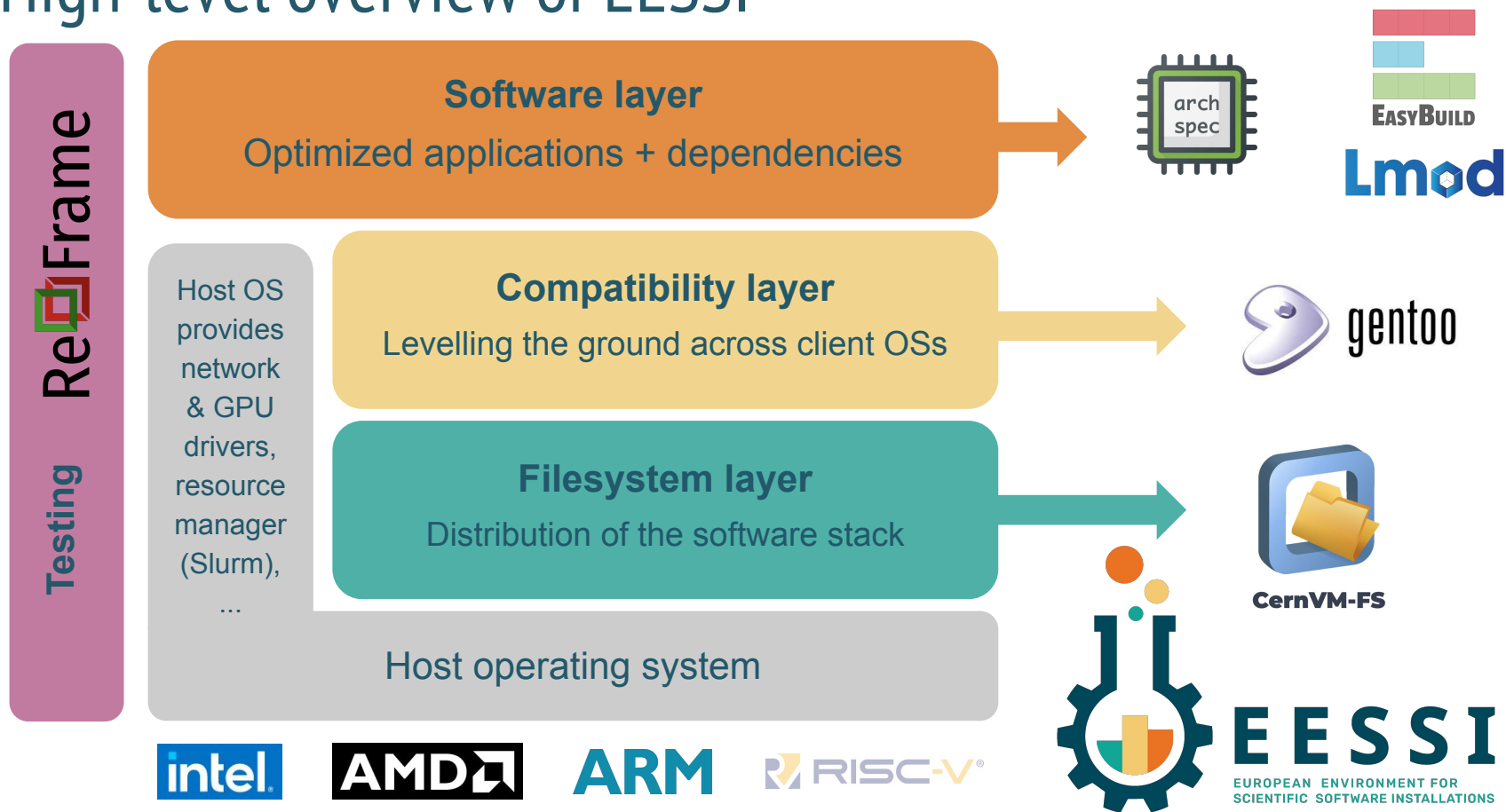
EESSI did not identify an accelerator on the system
(for debug information when loading the EESSI module, set the environment variable EESSI_MODULE_DEBUG_INIT)

```
{EESSI 2023.06} $ module load R/4.5.1-gfbbf-2025a
```

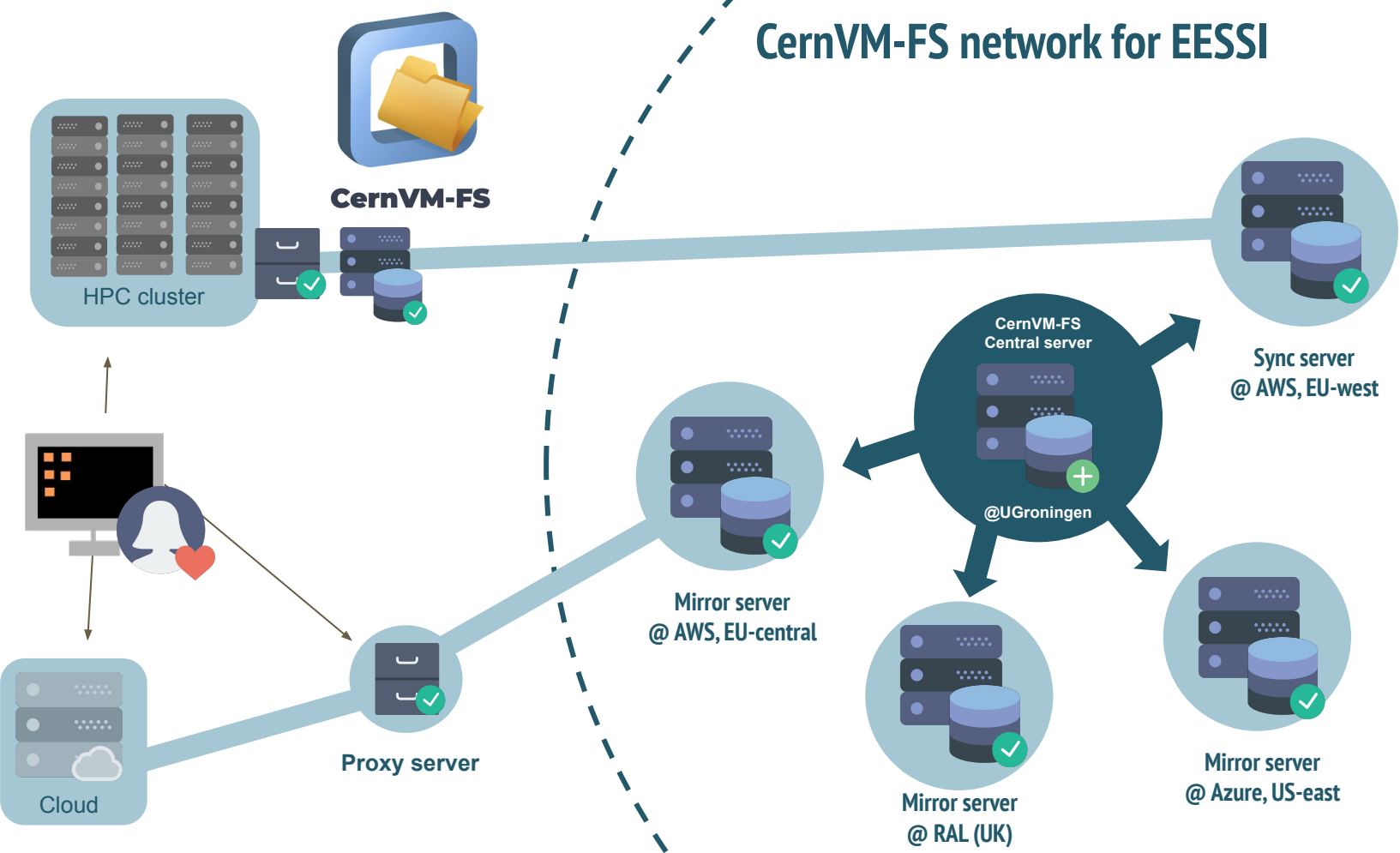
```
{EESSI 2023.06} $ which R
/cvmfs/software.eessi.io/versions/2025.06/software/linux/x86_64/
amd/zen2/software/R/4.5.1-gfbbf-2023a/bin/R
```

```
{EESSI 2023.06} $ R --version
R version 4.5.1
```

High-level overview of EESSI



CernVM-FS network for EESSI



New releases and developments

New releases and repositories

software.eessi.io

2023.06

- Default one since June 2023
- **1189** software installed (total: 16,681)
- **6151** unique packages
- foss/(2022b+23a+23b) -> GCC 12.4 ↓

dev.eessi.io

- Developer repository
- More about it later :)

2025.06

- Already available but ongoing effort to add more software
- **775** software installed (total: 11,821)
- **414** unique packages
- foss/(2024a+25a+25b) -> GCC 13.3 ↑

Overview of available software



Currently more than 2,000 software installations available per supported CPU target
via `software.eessi.io` CernVM-FS repository, increasing every week

- 15 supported CPU targets (x86_64 + Arm) + RISC-V actively being explored
- **~750 different software packages** + another ~3,000 extensions (Python packages, R libraries, ...)
- ~30,000 software installations in total
- Including GROMACS, LAMMPS, OpenFOAM, PyTorch, R, QuantumESPRESSO, TensorFlow, WRF, ...
- EESSI 2023.06 provides software built with `foss/2023a` and `foss/2023b` toolchains
- EESSI 2025.06 provides software built with `foss/2024a`, `foss/2025a`, `foss/2025b` toolchains

Overview of available software

An up-to-date overview of available software is available in the EESSI documentation:

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

Software available in EESSI

Overview of software available in [EESSI's production repository](https://www.eessi.io) [software.eessi.io](https://www.eessi.io).

752 unique software projects (+ 3007 unique extensions)

name:GROMACS

GROMACS

[\(more details\)](#)

<https://www.gromacs.org>

GROMACS is a versatile package to perform molecular dynamics, i.e. simulate the Newtonian equations of motion for systems with hundreds to millions of particles. This is a CPU only build, containing both MPI and threadMPI binaries for both single and double precision. It also contains the gmxml extension for the single precision MPI build.

Available in EESSI versions: [2023.06](#) [2025.06](#)

Supported CPU families: [AMD](#) [Intel](#) [Arm](#)

Supported GPU families: [NVIDIA](#)



GROMACS

GROMACS is a versatile package to perform molecular dynamics, i.e. simulate the Newtonian equations of motion for systems with hundreds to millions of particles.

This is a GPU enabled build, containing both MPI and threadMPI binaries.

It also contains the gmxml extension for the single precision MPI build.

homepage: <https://www.gromacs.org>

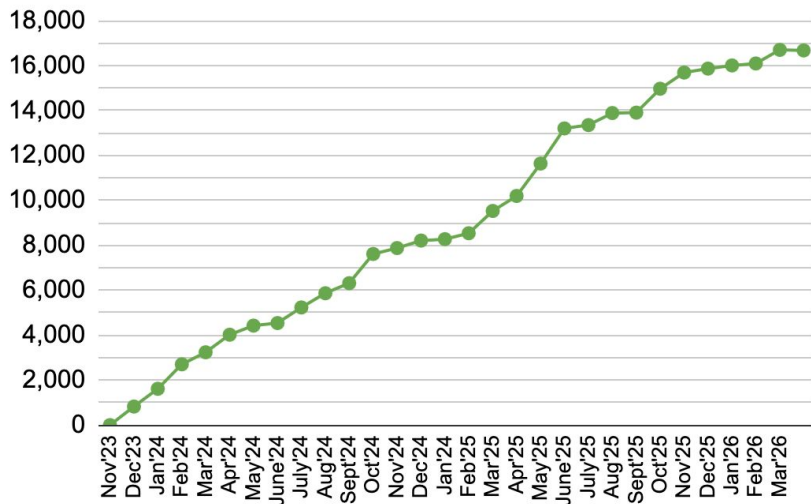
Available installations

GROMACS version	Supported CPU targets	Supported GPU targets	EESSI version	Module
2025.4	generic: aarch64, x86_64 Arm : a64fx, neoverse_n1, neoverse_v1, nvidia/grace AMD : zen2, zen3, zen4 Intel : haswell, skylake_avx512, sapphirerapids, icelake, cascadelake	(none)	2025.06	GROMACS/2025.4-foss-2025b
2025.2	generic: aarch64, x86_64 Arm : a64fx, neoverse_n1, neoverse_v1, nvidia/grace AMD : zen2, zen3, zen4 Intel : haswell, skylake_avx512, sapphirerapids, icelake, cascadelake	(none)	2025.06	GROMACS/2025.2-foss-2025a
2024.4	generic: aarch64, x86_64 Arm : neoverse_n1,	NVIDIA : cc70, cc80, cc90	2023.06	GROMACS/2024.4-foss-2023b-

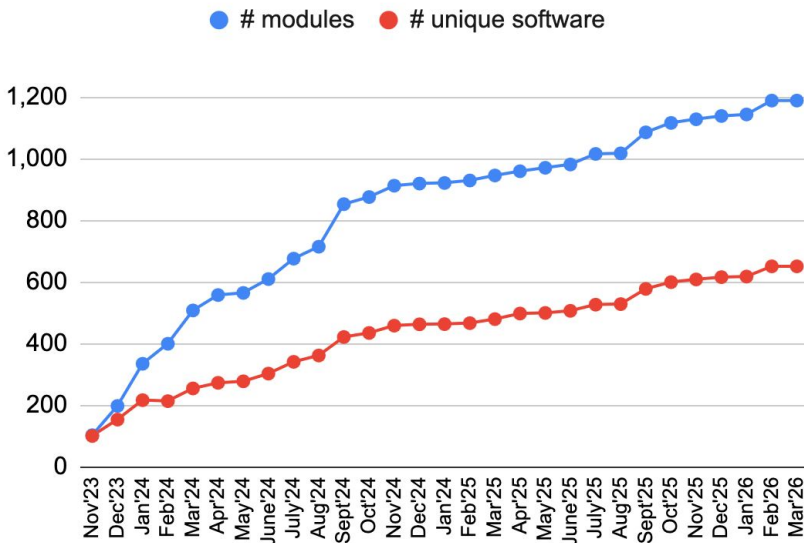
New software evolution (2023.06)



software installations in EESSI 2023.06 (total)



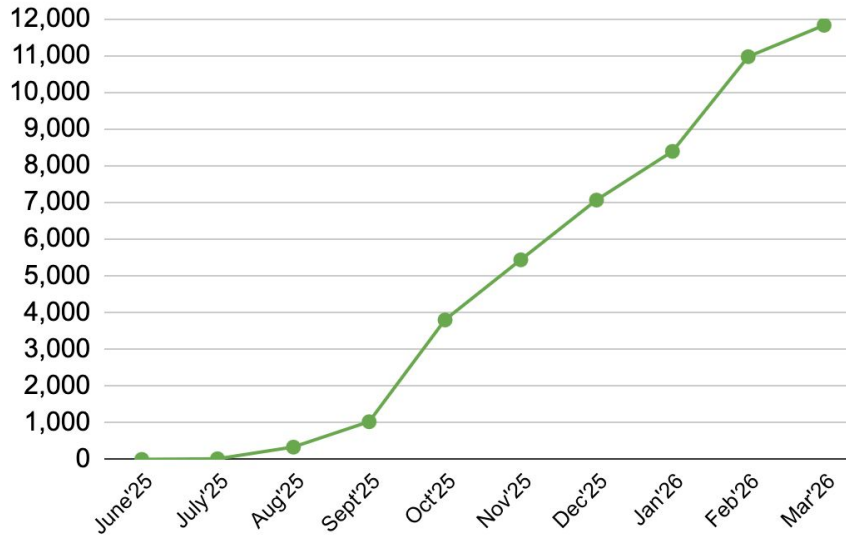
software installations in EESSI 2023.06 (per CPU target)



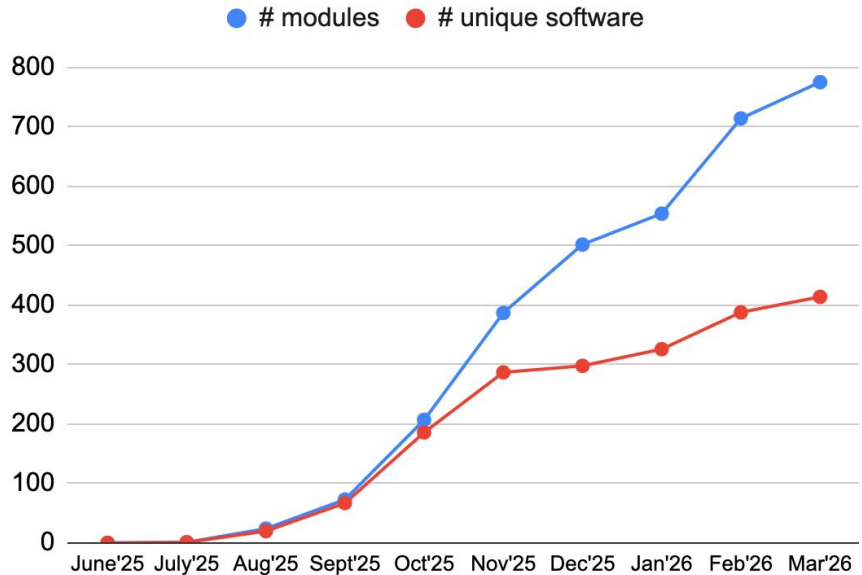
New software evolution (2025.06)



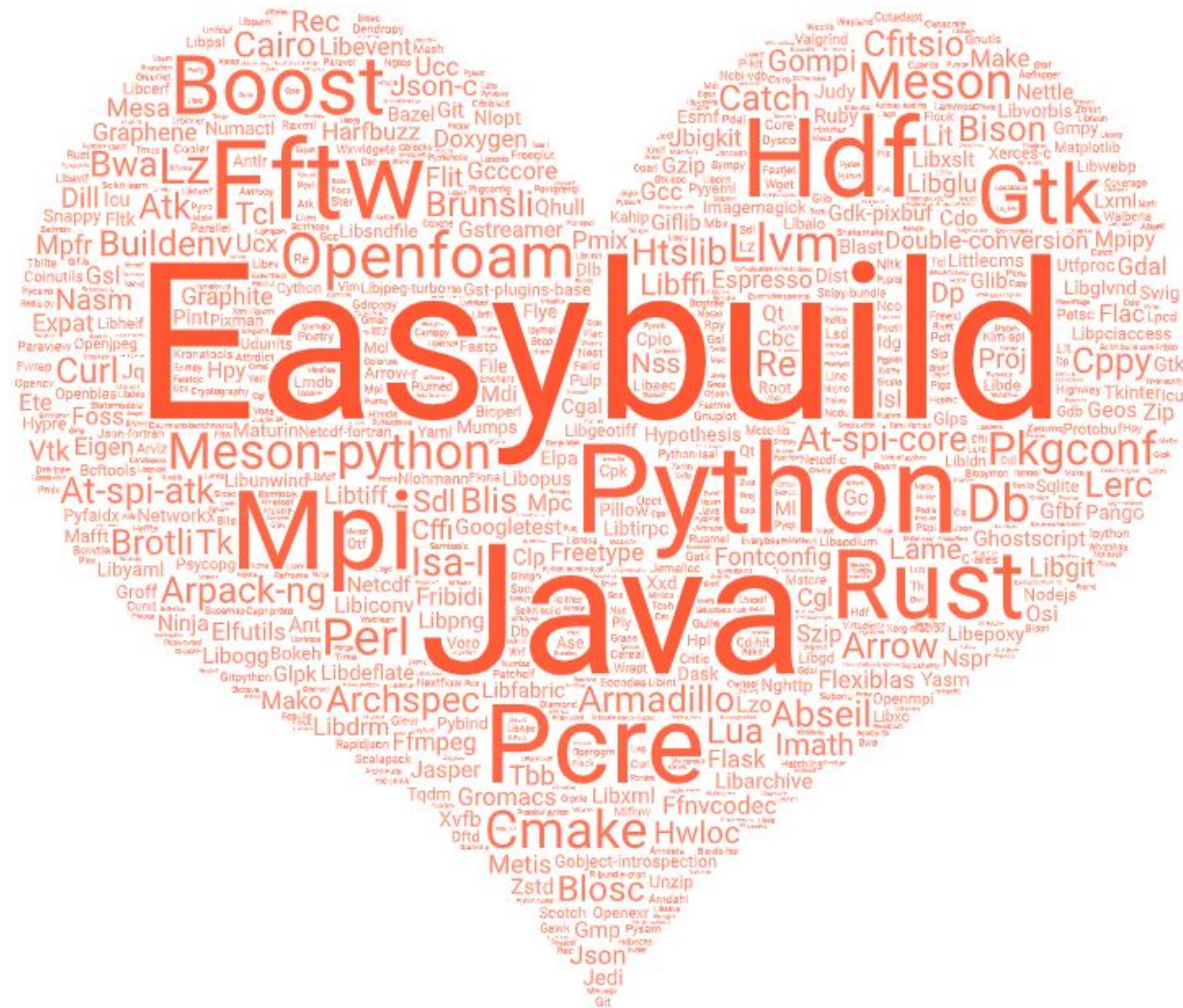
software installations in EESSI 2025.06 (total)



software installations in EESSI 2025.06 (per CPU target)



Wordcloud - software available in EESSI



Supported CPU targets

https://eessi.io/docs/software_layer/cpu_targets



- AMD, Intel (`x86_64`)
 - 5 generations of Intel CPUs: Haswell, Skylake, Cascade Lake, Ice Lake, Sapphire Rapids
 - 4 generations of AMD CPUs: Zen2 (Rome), Zen 3 (Milan), Zen4 (Genoa), Zen5 (Turin)
- Arm (`aarch64`)
 - 4 different microarchitectures: Fujitsu A64FX, NVIDIA Grace, Neoverse N1 + V1
- Plus a generic fallback for both `x86_64` and `aarch64`
- RISC-V CPUs are work-in-progress
 - Exploration ongoing via RISC-V-specific subdirectory of `dev.eessi.io` repository

Supported GPU targets

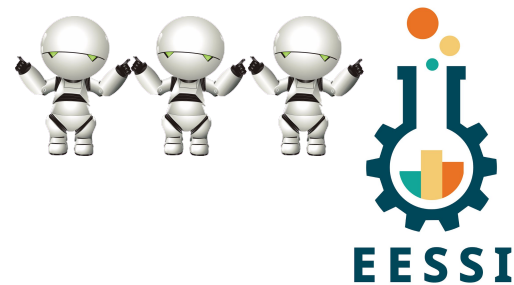
https://eessi.io/docs/software_layer/gpu_targets



- NVIDIA (CUDA)
 - Different generations of NVIDIA GPUs, based on CUDA Compute Capability (CC), see also <https://developer.nvidia.com/cuda/gpus>
 - In EESSI 2023.06: CC 7.0 (V100, T4), 8.0 (A100 & co, incl. L40), 9.0 (H100/H200)
 - In EESSI 2025.06: CC 7.0, 8.0, 9.0, 10.0 (B100/B200/B300), 12.0 (B10, RTX PRO Blackwell)
 - GPU driver libraries (include `libcuda.so`) must be exposed to EESSI
 - See https://www.eessi.io/docs/site_specific_config/gpu
- AMD (ROCm)
 - Work-in-progress, initial support included in EasyBuild 5.3.0 (mid April 2026)
 - PR for easyconfigs for ROCm 6.4.1 merged, will be included in next EasyBuild release

See also *NVIDIA + AMD GPU support in EESSI* talk @ EUM'26 ([slides](#), [recording](#))

Automated procedure via EESSI build-deploy bots



- Software installations deployed in EESSI are built by the EESSI build-deploy bots (using EasyBuild), see also <https://eessi.io/docs/bot>
- Semi-automatic installation procedure (human in the loop)
- Via pull request to [E E S S I / s o f t w a r e - l a y e r](#) repository
- Contributors do not need access to all CPU targets supported by EESSI

Build-test-deploy bot

- Build/Deploy/Ingest Strategy - Fully automatic or with human in the loop
- Interaction model: Plain CI, external CLI, GitHub App, ...
 - GitHub App / scripts that understand(s) structured commands in PR comments, labels, and merge/close
- Whole CI infrastructure underneath:
 - GitHub runners, self-hosted runners → HPC clusters (on-prem/Cloud), each running its own bot instance
- Bot only defines interface, repo owners define the actual build & test logic

<https://eessi.io/docs/bot>



ocaisa commented [last week](#)

Memt

bot: build repo:eessi.io-2025.06-software instance:eessi-bot-mc-aws for:arch=x86_64/amd/zen3
bot: build repo:eessi.io-2025.06-software instance:eessi-bot-mc-aws for:arch=x86_64/amd/zen4
bot: build repo:eessi.io-2025.06-software instance:eessi-bot-mc-aws for:arch=x86_64/intel/skylake_avx512
bot: build repo:eessi.io-2025.06-software instance:eessi-bot-mc-aws for:arch=x86_64/intel/haswell
bot: build repo:eessi.io-2025.06-software instance:eessi-bot-mc-aws for:arch=x86_64/intel/icelake
bot: build repo:eessi.io-2025.06-software instance:eessi-bot-mc-aws for:arch=x86_64/intel/cascadelake
bot: build repo:eessi.io-2025.06-software instance:eessi-bot-mc-aws for:arch=x86_64/intel/sapphirerapids
bot: build repo:eessi.io-2025.06-software instance:eessi-bot-mc-aws for:arch=x86_64/generic
bot: build repo:eessi.io-2025.06-software instance:eessi-bot-mc-aws for:arch=aarch64/generic
bot: build repo:eessi.io-2025.06-software instance:eessi-bot-mc-aws for:arch=aarch64/neoverse_n1
bot: build repo:eessi.io-2025.06-software instance:eessi-bot-mc-aws for:arch=aarch64/neoverse_v1



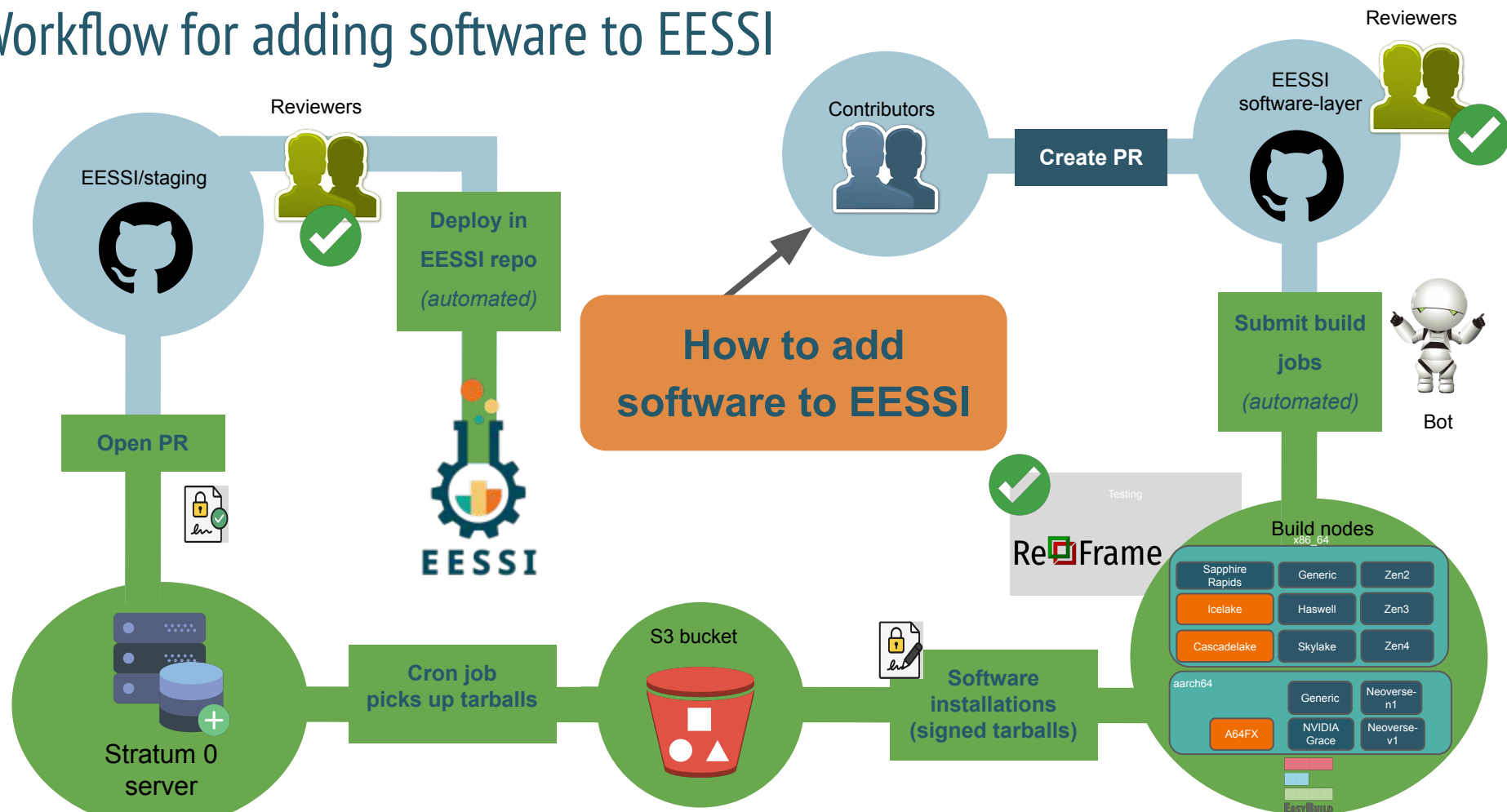
eessi-bot-aws bot commented [last week](#) • edited ▾

New job on instance `eessi-bot-mc-aws` for repository `eessi.io-2025.06-software`
Building on: `amd-zen3`
Building for: `x86_64/amd/zen3`
Job dir: `/project/def-users/SHARED/jobs/2026.01/pr_1357/122018`

date	job status	comment
Jan 15 11:22:04 UTC 2026	submitted	job id <code>122018</code> awaits release by job manager
Jan 15 11:23:02 UTC 2026	released	job awaits launch by Slurm scheduler
Jan 15 11:38:24 UTC 2026	running	job <code>122018</code> is running
Jan 15 13:32:50 UTC 2026	finished	► 😊 SUCCESS (click triangle for details)
Jan 15 13:32:50 UTC 2026	test result	► 😊 SUCCESS (click triangle for details)



Workflow for adding software to EESSI



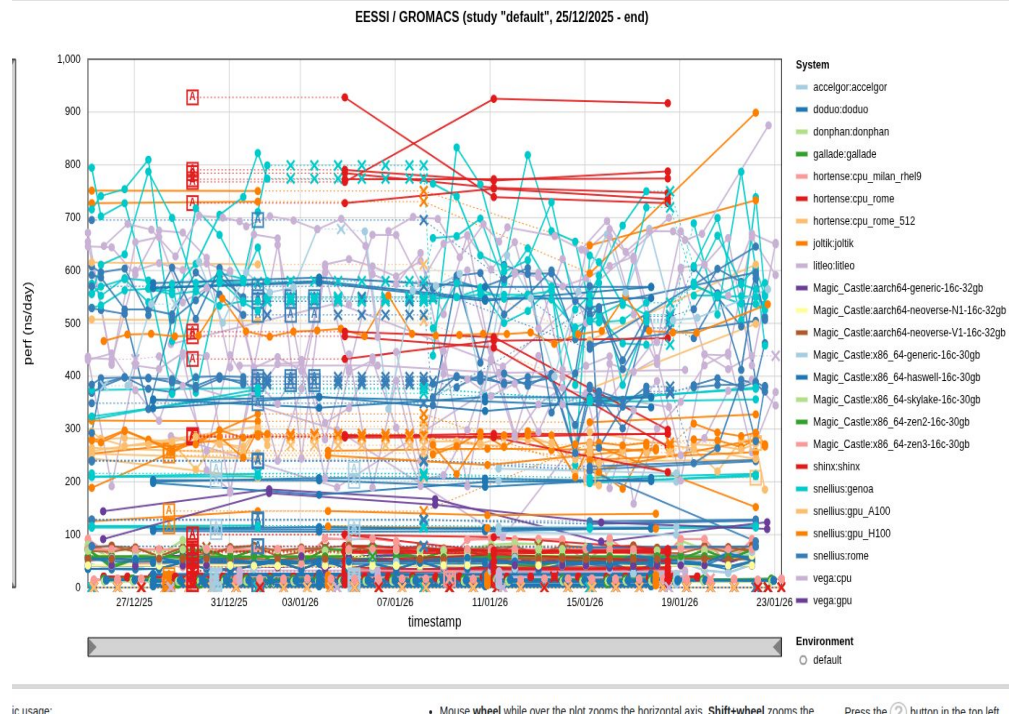
Software testing is an important part of EESSI



- Smoke test: sanity check commands are run by EasyBuild to check that installed software is not horribly broken while using EasyBuild
- Regression testing via EESSI test suite: eessi.io/docs/test-suite
 - Collection of portable tests for software available in EESSI
 - Running on selected (single node) tests when building new software for EESSI (before deployment)
 - Periodically (daily/weekly) on about multiple different systems
 - Can also be used for other software stacks (that are built with EasyBuild)
 - Periodic runs of EESSI test suite help to catch performance regressions

EESSI dashboard

- Centralized interface for visualizing results generated by the EESSI test suite. It supports a range of use cases, including:
 - System monitoring, providing insight into the health and stability of platforms where EESSI is deployed
 - Cross-system performance comparison
 - Aids in regression source identification
- Open to publish data from other systems, contact: support@eessi.io



Building on top of EESSI improvements



With EasyBuild

- Just module load `EESSI-extend!`

Wrapper module to set up all the environment for you

Without Automated build tools

- Load `buildenv` module
- Procedure is documented
- Most cases untested and undocumented, we appreciate feedback!

Manually building software on top of EESSI (without EasyBuild)

Warning

Even with the help of the `buildenv` module, this documentation is intended for "experts" in the runtime linker and its behaviour, and most cases are untested. Any feedback on this topic is highly appreciated.

Building and running software on top of EESSI without EasyBuild is now more straightforward thanks to the freshly developed `buildenv` module.

EESSI uses a [compatibility layer](#) to ensure that it takes as few libraries from the host as possible. Starting an EESSI prefix shell before building and loading any of the `buildenv` modules (one per `foss` toolchain), this is the safest way to make sure all libraries will point to the required locations in the compatibility layer and do not leak in from the host operating system. A step by step:

With Spack...? 🤔

<https://www.eessi.io/docs/blog/2026/02/05/Spack-on-top-of-EESSI-best-of-both-worlds>

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

software.eessi.io (production)

- Permanent installations
- Only install releases
- Builds for all CPU architectures
- `/cvmfs/software.eessi.io/version/`

```
/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
          -- ...
```

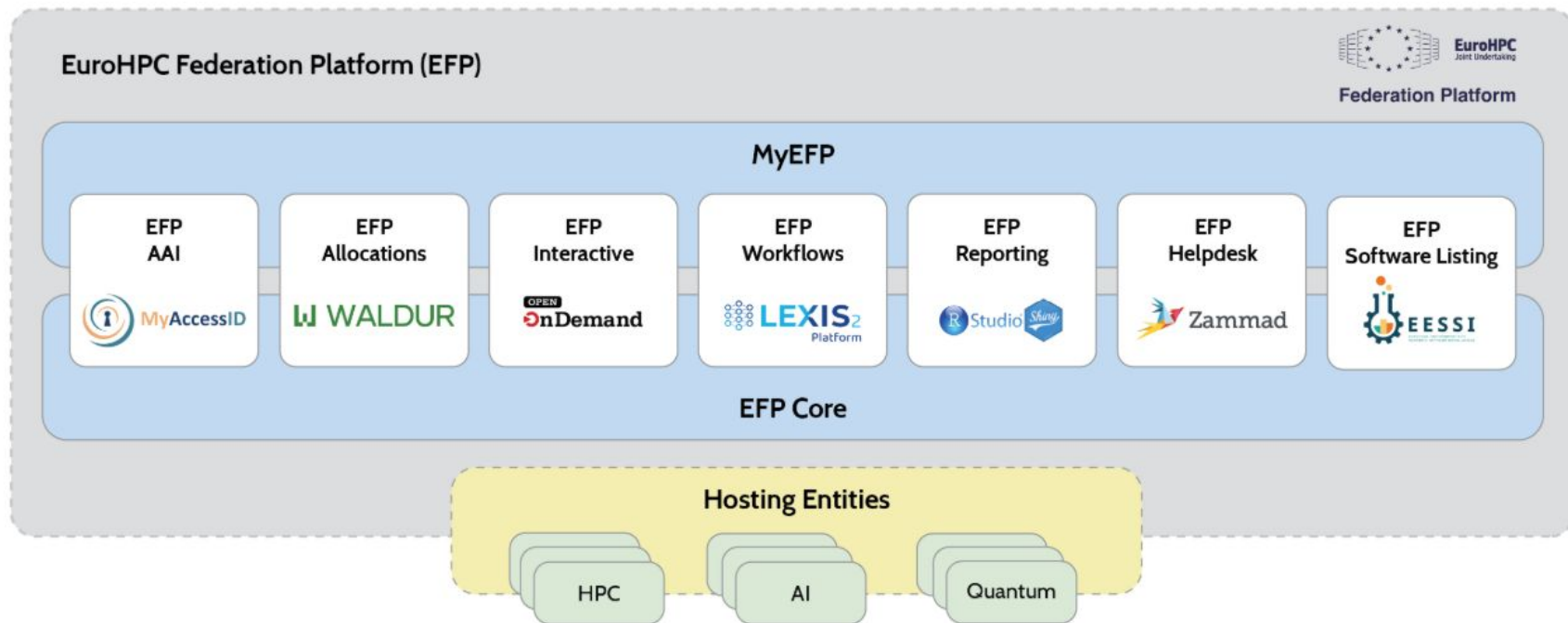
dev.eessi.io

- Temporary installations
- Can install from commits
- Patches can be added
- Can skip some CPU targets
- dev.eessi.io built on top of software.eessi.io
- Subdirectories per project
- `/cvmfs/dev.eessi.io/project/version/`

Currently only available for codes
within the MultiXscale project!

Further integrations

European Federation Platform (EFP)



<https://my-eurohpc.eu>

European Open Science Cloud (EOSC)



October 22, 2025 · 5 min read

EESSI available on EOSC EU Node



EESSI has recently been working together with the [European Open Science Cloud \(EOSC\)](#) to provide easy access to EESSI for those using EOSC compute resources.

A first implementation of EESSI support is now available as the [EESSI Compute Node tool in the EOSC EU Node Tools Hub](#).

[Continue reading](#)

Tools Hub

The place to find, create, publish and run tools.

[About Tools Hub](#)

+ Create

Search

Q Search

All Tools

My Tools

Favourites

Deployments

Alan O'Cais

EESSI Compute Node

Deploy a compute node with an extra HD disk, EESSI (<https://eessi.github.io/docs>) installed, getting the IP and SSH credentials to access via ssh.

Status: Published



Deploy

<https://eessi.io/docs/blog/2025/10/22/eosc/>

Open OnDemand (OOD)

- Web Desktop Based application
- Modules field to select software needed by the user
- Selected modules unwritable field to check the selected ones
- Search mechanism to find specific modules

Home / My Interactive Sessions / EESSI General App

Interactive Apps

Desktops

- Classiq
- Desktop XFCE-GNOME
- Desktop w.Container

GUIs

- Avogadro2
- DIA
- MATLAB
- ParaView
- VMD

Script Execution

- Cnes App
- Pandoc App
- Script launcher (DEMO)

Servers

- Code Server
- Jupyter Notebook
- Jupyter Notebook EESSI

Test

- API test
- EESSI General App**

EESSI General App

This app will launch a Desktop on one node with the modules of EESSI loaded. You will be able to interact with it through a VNC session.

Desktop Environment

gnome

Account

example_account_2

Number of hours

1

Module list

Module Filter

- ☐ Abseil/20230125.2-GCCcore-12.2.0
- ☐ HDF/4.2.15-GCCcore-12.2.0
- ☐ OpenJPEG/2.5.0-GCCcore-13.2.0
- ☐ Abseil/20230125.3-GCCcore-12.3.0
- ☐ HDF/4.2.16-2-GCCcore-12.3.0
- ☐ OpenMPI/4.1.4-GCC-12.2.0

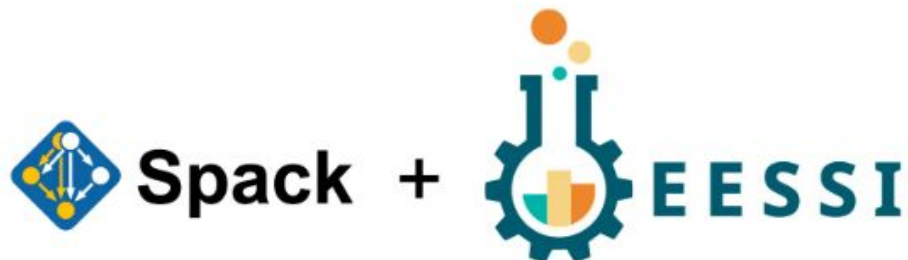
Selected Modules

Launch

* The EESSI General App session data for this session can be accessed under the [data root directory](#).



Using Spack on top of EESSI: A Proof of Concept



EESSI provides a rich set of software installations, which were built and installed using [EasyBuild](#).

Can we convince [Spack](#) to reuse software installed in EESSI, and by doing so make EESSI more attractive to those of you who prefer using Spack over EasyBuild?

Several people have expressed interest in exposing the software installations provided by EESSI to Spack, so they can be used as dependencies when building and installing software with Spack.

<https://eessi.io/docs/blog/2026/02/05/Spack-on-top-of-EESSI-best-of-both-worlds>

Trainings & dissemination

EESSI Happy Hours



EESSI Happy Hour sessions

provided by [EuroHPC CoE MultiXscale](#)

Come join us
every Monday!!!!!!



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?

The European Environment for Scientific Software Installations [EESSI](#) comes to the rescue!

Join us for EESSI Happy Hour, an informal, weekly online session to explore and discuss key EESSI topics and updates with the community.

Each series will focus on a specific main topic over several sessions, giving participants the opportunity to ask questions, get hands-on guidance, and share experiences.

 **Where?** Online, via Zoom ([click here to join!](#))

 **When?** Mondays, 14:00-15:00 CE(S)T

 **Who should join?** Everyone interested in EESSI.

Older sessions
available in YouTube
[https://www.youtube.com/
@eessi_community](https://www.youtube.com/@eessi_community)

Webinars series (2025)

- Introduction to EESSI
- Introduction to CernVM-FS
- Introduction to EasyBuild
- EESSI for CI/CD
- Using EESSI as the base for a system stack

<https://eessi.io/docs/training-events/2025/webinar-series-2025Q2/>



The screenshot shows a YouTube video player interface. At the top, there is a banner for a webinar titled "Streaming Optimised Scientific Software, an Introduction to EESSI" on Monday, 5 May 2025. The banner includes the EESSI logo, the MultiScale logo, and a cartoon illustration of people working on computers. Below the banner, the video title "EESSI webinar series (May-June 2025)" is displayed, followed by the text "by EESSI". Below this, it says "Playlist • 5 videos • 72 views" and provides the URL "https://eessi.io/docs/training/2025/webinar-series-2025Q2". At the bottom of the player, there is a "Play all" button and icons for bookmarks, share, and more options.

Webinars series - spring 2026



- Introduction to EESSI (27 April 2026)
- Building software on top of EESSI + contributing to EESSI (4 May 2026)
- Using EESSI for Continuous Integration (11 May 2026)
- Introduction to CernVM-FS (18 May 2026)
- Using EESSI as a base for a central software stack (1 June 2026)

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

Hackathons, and other events



Copenhagen, EuroHPC User days 2025

Spotify podcast!↓



HPCKP 2025, Bcn



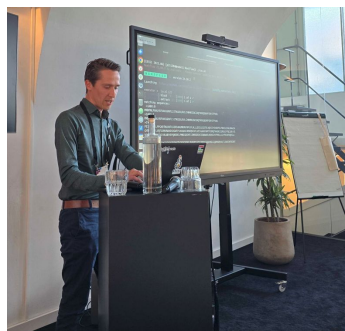
ISC 2025, Hamburg



HIPEAC 2025, Bcn



RSE Days Belgium 2025



SURF Research days 2025



SC 2024, Atlanta



EasyBuild User Meeting 2025, JSC
And much more to come!

EESSI won an HPCWire Reader's Choice award!



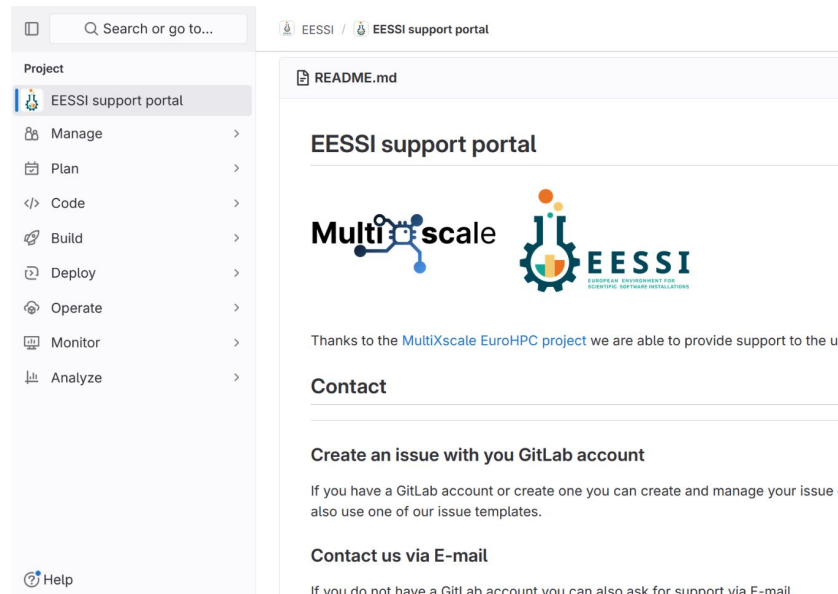
eessi.io/docs/blog/2024/11/18/hpcwire-readers-choice-awards-2024-for-eessi

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, ...)



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





E E S S I

EUROPEAN ENVIRONMENT FOR
SCIENTIFIC SOFTWARE INSTALLATIONS

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)

MultiXscale



Co-funded by
the European Union



EuroHPC
Joint Undertaking

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)

BlueSky: [MultiXscale](https://bsky.app/profile/multixscale)



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