



Join the live poll!

[menti.com](https://www.menti.com)

6200 2126



# E E S S I

EUROPEAN ENVIRONMENT FOR  
SCIENTIFIC SOFTWARE INSTALLATIONS



**Birds-of-a-Feather session - ISC'26 - Hamburg - 25 June 2026**

<https://eessi.io> | <https://eessi.io/docs> | <https://github.com/EESSI>

[support@eessi.io](mailto:support@eessi.io)

# Agenda for this Birds-of-a-Feather session



## **Part 1: Presentation (~15min)**

- Quick introduction to EESSI
- Quick live demo of EESSI user experience
- Recent developments in EESSI

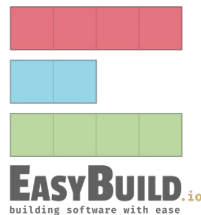
## **Part 2: Live poll, discussion, Q&A (~45min)**

- We expect your active participation!
- Join poll via <https://menti.com>  
(laptop, smartphone),  
use 6200 2126 as code



# EasyBuild in a nutshell

<https://easybuild.io>



- Tool to install (scientific) software on HPC systems, usually from source code
- Created by HPC team at Ghent University (Belgium) in summer 2009
- Open source software (GPLv2) since Nov 2012 (during SC'12)
- `pip install easybuild`, extensive documentation ([docs.easybuild.io](https://docs.easybuild.io))
- Used to manage central software stack on various systems, incl. LUMI, JUPITER, ...
- Worldwide community grew around it, used all over Europe, Canada, US, Australia, ...



*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 set of ready-to-use (optimized!) scientific software installations**
- Goal: **avoid duplicate work** across by collaborating on a shared software stack
- **Uniform software environment**, regardless of the system you 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**



**E E S S I**  
EUROPEAN ENVIRONMENT FOR  
SCIENTIFIC SOFTWARE INSTALLATIONS

<https://eessi.io>

*inspired by the  
ComputeCanada software stack*

# EESSI is powered by open source software



gentoo linux™

## Compatibility layer

Abstraction from the  
host operating system



CernVM-FS

## Filesystem Layer

Global distribution of  
software installations  
(on-demand streaming)

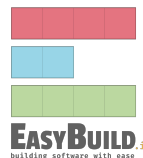
ReFrame

Regression  
testing  
of software



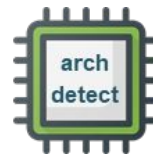
E E S S I

EUROPEAN ENVIRONMENT FOR  
SCIENTIFIC SOFTWARE INSTALLATIONS



**Optimized** software  
installations for specific  
CPU microarchitectures

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

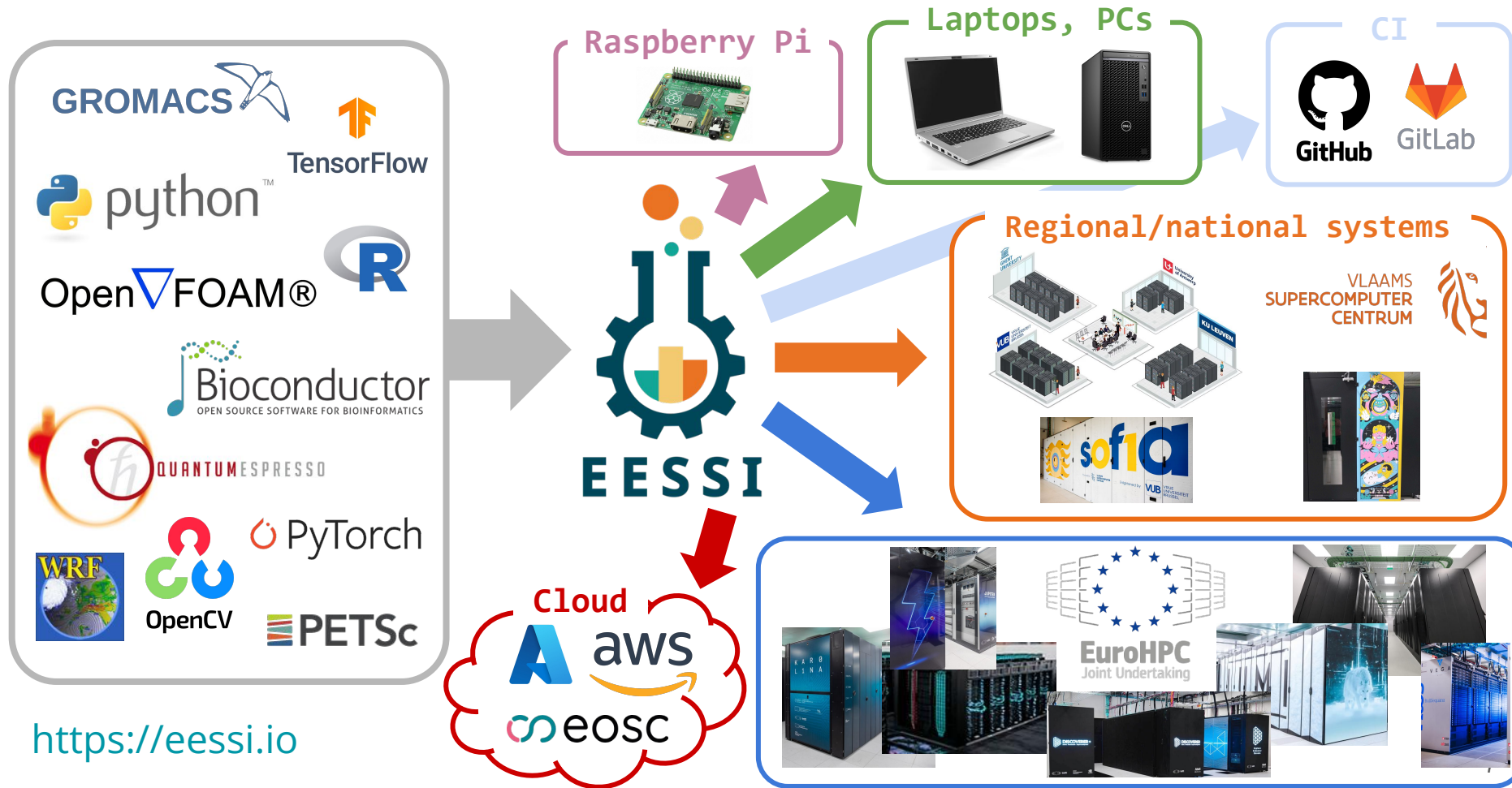


Automatic selection of  
best suited part of  
software stack for  
CPU microarchitectures



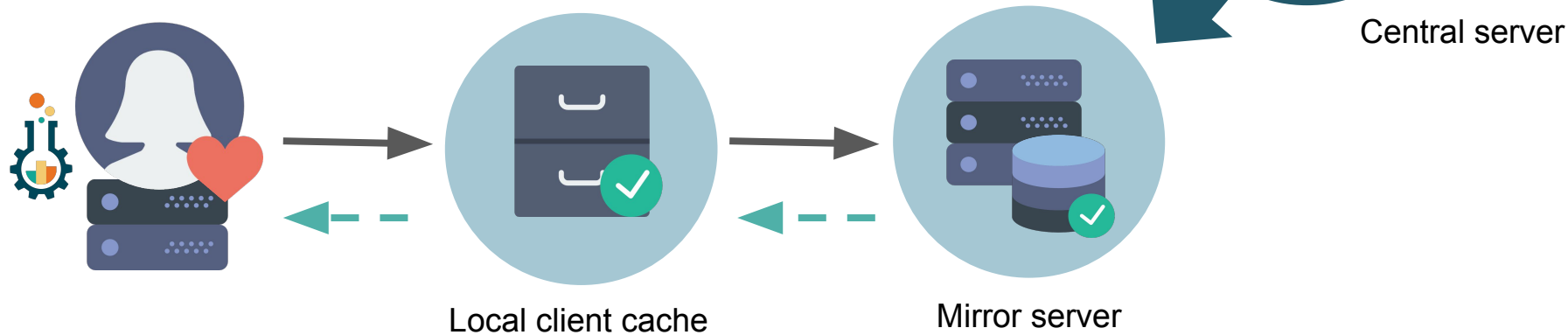
Magic Castle  
to create (ephemeral)  
clusters in the cloud

# EESSI as shared software stack for HPC, and beyond



# Running scientific software in 1, 2, 3

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



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

# Example: Running GROMACS with EESSI

```
#!/bin/bash
```

```
eessi-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 xzf 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)
```

```
gmx mdrun -s ion_channel.tpr -maxh 0.50 -nsteps 1000 -g logfile
```

# Example: Running GROMACS with 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
```



```
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
```

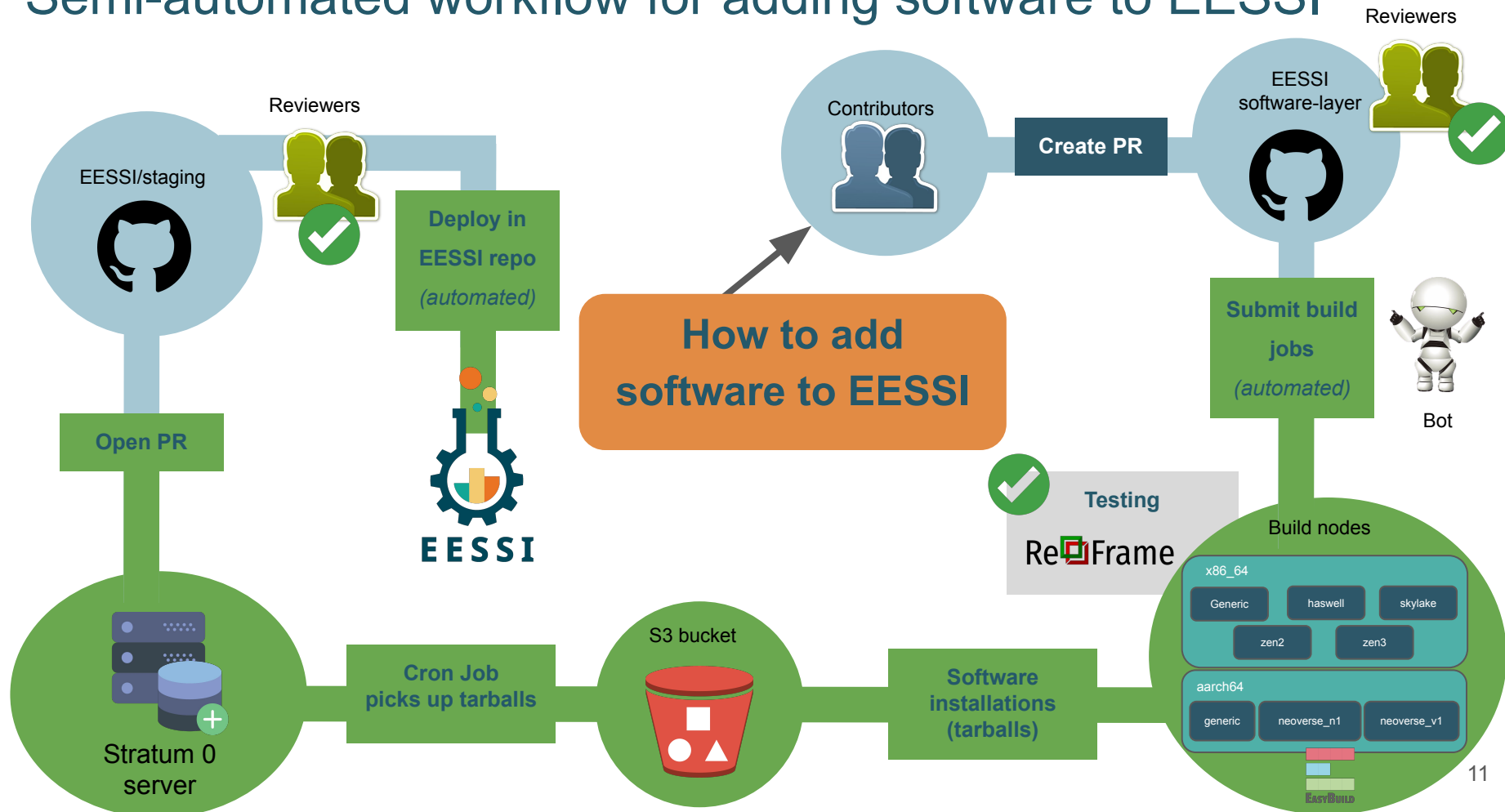
```
deucalion $ cat slurm-7654321.out
```

```
...
```

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



# Semi-automated workflow for adding software to EESSI

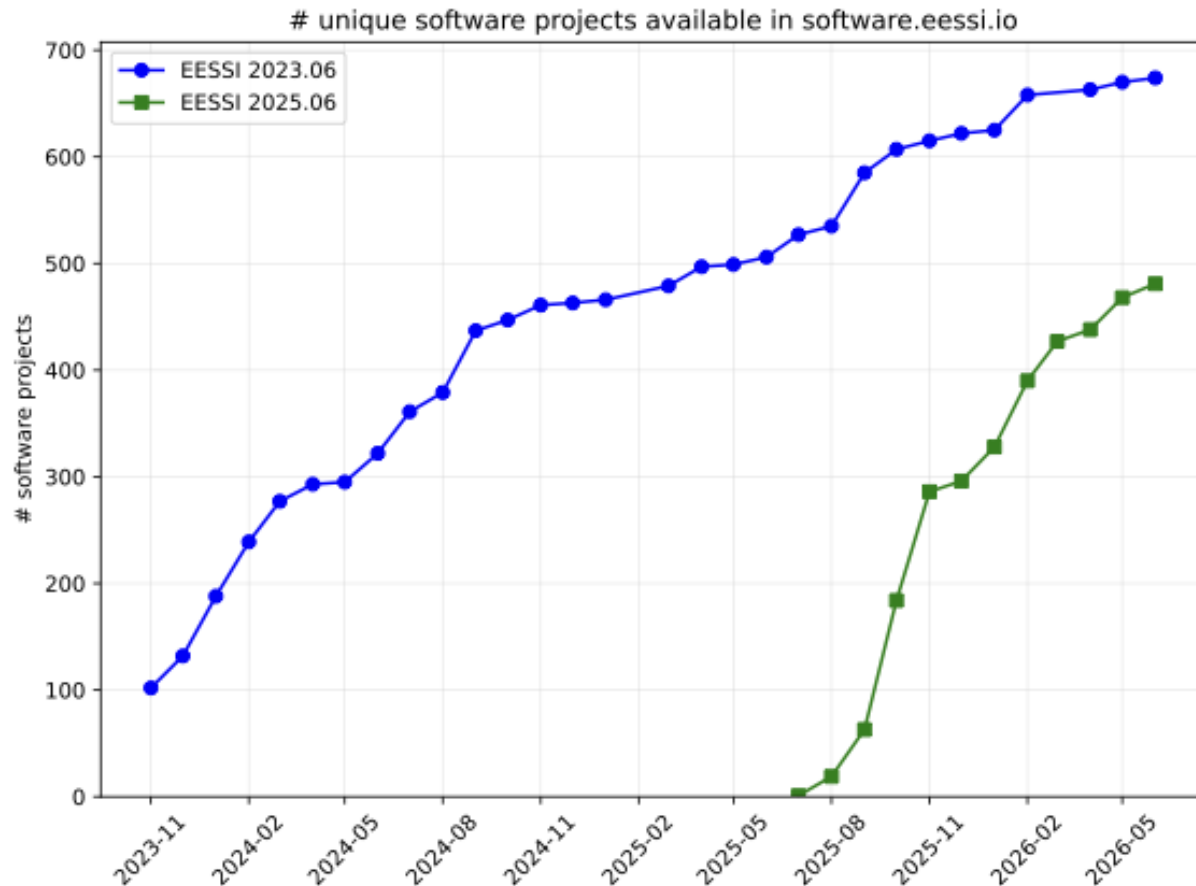


# Recent developments in a nutshell



- **AMD Zen 5** (Turin) recently added as supported CPU targets, now 15 in total
- Growing set of available software: **over 750 unique software projects** (+ ~3,000 extensions), totaling ~30,000 software installations, see [eessi.io/docs/available\\_software](https://eessi.io/docs/available_software)
- **NVIDIA GPUs** fully supported, [eessi.io/docs/gpu](https://eessi.io/docs/gpu)
- **Work-in-progress**: support for AMD GPUs (ROCm ecosystem) & RISC-V CPUs
- **Regression testing** on various systems using [EESSI test suite](https://eessi.io/docs/test_suite), see [dashboard.eessi.io](https://dashboard.eessi.io)
- User-friendly **EESSI CLI** tool is in the works, install it with `pip install eessi`
- **EESSI is available on all EuroHPC supercomputers** now, as the base for the Federated Software Catalog of the EuroHPC Federation Platform

# Set of available software is growing steadily...



# Overview of available software

An up-to-date overview of available software

is available in the EESSI documentation:

[https://eessi.io/docs/available\\_software](https://eessi.io/docs/available_software)

## Software available in EESSI

Overview of software available in EESSI's production repository [software.eessi.io](https://software.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 gmxapi 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 gmxapi 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<br>Arm: a64fx, neoverse_n1, neoverse_v1, nvidia/grace<br>AMD: zen2, zen3, zen4<br>Intel: haswell, skylake_avx512, sapphirerapids, icelake, cascadelake | (none)                   | 2025.06       | GROMACS/2025.4-foss-2025b  |
| 2025.2          | generic: aarch64, x86_64<br>Arm: a64fx, neoverse_n1, neoverse_v1, nvidia/grace<br>AMD: zen2, zen3, zen4<br>Intel: haswell, skylake_avx512, sapphirerapids, icelake, cascadelake | (none)                   | 2025.06       | GROMACS/2025.2-foss-2025a  |
| 2024.4          | generic: aarch64, x86_64<br>Arm: neoverse_n1,                                                                                                                                   | NVIDIA: cc70, cc80, cc90 | 2023.06       | GROMACS/2024.4-foss-2023b- |



# Leveraging EESSI in CI environment

Using EESSI in GitHub Actions is trivial (and works *really* well):

```
name: ubuntu_gromacs
on: [push, pull_request]
jobs:
  build:
    runs-on: ubuntu-latest
    steps:
      - uses: actions/checkout@v2
      - uses: eessi/github-action-eessi@v3
        with:
          eessi_stack_version: '2023.06'
      - name: Test EESSI
        run: |
          module load TensorFlow/2.13.0-foss-2023a
          python test_with_tensorflow.py
    shell: bash
```

[github.com/EESSI/github-action-eessi](https://github.com/EESSI/github-action-eessi)



# EESSI in the EuroHPC Federation Platform



**EuroHPC**  
Joint Undertaking

## Federation Platform

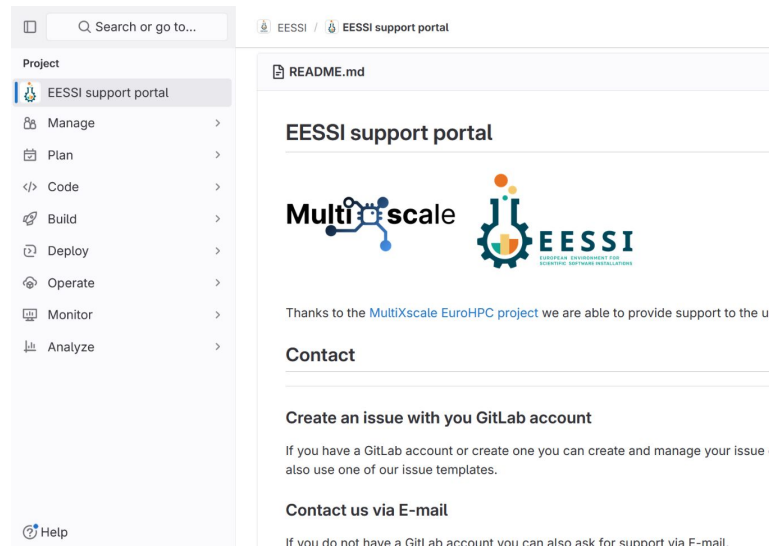
- Ghent University was invited into the consortium led by CSC.fi that is currently developing the **EuroHPC Federation Platform (EFP)**
- EFP is a “one-stop shop” for people to access & use EuroHPC systems
- For entire EuroHPC ecosystem: supercomputers, AI factories, quantum computers
- **EESSI is being integrated into EFP as base for the Federated Software Stack (FSC)**
- First version of EFP became operational in April 2026, with FSC available in beta mode
- Recordings of first EFP webinar series available via <https://my-eurohpc.eu/training>
- Detailed presentation of EFP FSC: <https://youtu.be/ISsLJkUpUT0>

# Getting support for EESSI



[eessi.io/docs/support](https://eessi.io/docs/support)

- Via GitLab, or via email: [support@eessi.io](mailto: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 

# Acknowledgements



Co-funded by  
the European Union



**EuroHPC**  
Joint Undertaking

- Funded by the European Union. This work has received funding from the European High Performance Computing Joint Undertaking (JU) and countries participating in the project under grant agreement No 101093169.



- Thanks to Amazon Web Services (AWS) and Microsoft Azure for generously sponsoring the EESSI project with funds, cloud credits, feedback, and guidance.





Website: [eessi.io](https://eessi.io)

GitHub: [github.com/EESSI](https://github.com/EESSI)

Documentation: [eessi.io/docs](https://eessi.io/docs)

Blog: [eessi.io/docs/blog](https://eessi.io/docs/blog)

Getting support: [eessi.io/docs/support](https://eessi.io/docs/support)

**[Join](#) the EESSI Slack** (see link on EESSI website)

YouTube channel: [youtube.com/@eessi\\_community](https://youtube.com/@eessi_community)

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

EESSI support portal: [gitlab.com/eessi/support](https://gitlab.com/eessi/support)

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

Live poll, discussion, Q&A

Go to

[www.menti.com](https://www.menti.com)

enter the code

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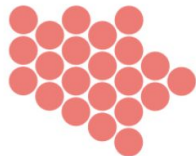


# Live poll, discussion, Q&A

Which tool(s) do you use for "installing" scientific software?



17 conda /  
mamba



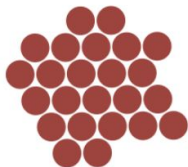
22 containers



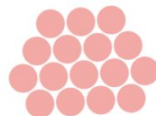
28 EasyBuild



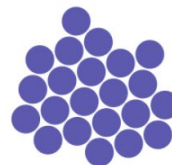
1 Nix/Guix



24 Spack



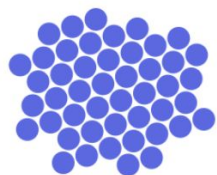
16 EESSI



22 something else

# Live poll, discussion, Q&A

Which platform(s) do you use for running scientific workloads?



47 On-premise HPC cluster



9 On-premise cloud



6 Amazon EC2 (AWS)



6 Microsoft Azure



4 Other commercial cloud (Google, Oracle, ...)



25 Personal workstation/laptop



3 Single-Board Computer (SBC), like Raspberry Pi



5 Something else

# Live poll, discussion, Q&A



## Which hardware platform (s) do you use or manage?



36 CPU only (intel or AMD)



10 Arm CPU only



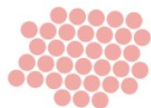
37 Intel CPU + NVIDIA GPU



5 Intel CPU + AMD GPU



6 Intel CPU + Intel GPU



35 AMD CPU + NVIDIA GPU



15 AMD CPU + AMD GPU



1 AMD CPU + Intel GPU



15 Arm CPU + NVIDIA GPU



1 Arm CPU + AMD GPU



2 RISC-V CPU

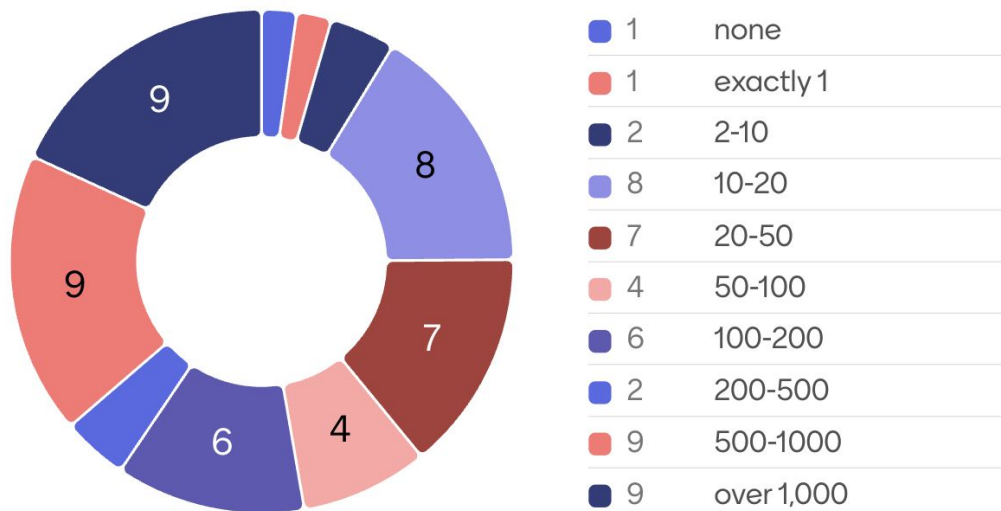


5 something else



# Live poll, discussion, Q&A

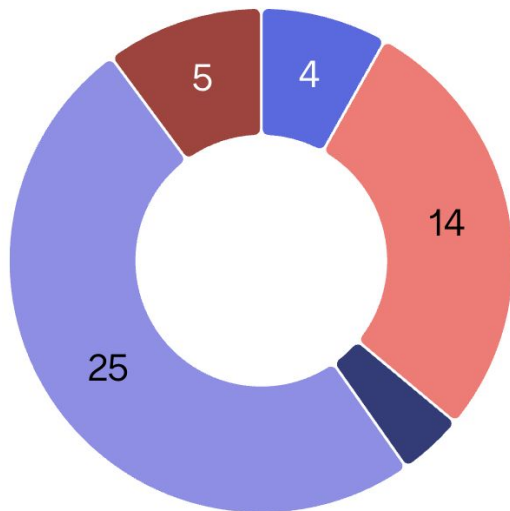
How many different software applications, tools, and libraries do you use or provide for running scientific workloads?



# Live poll, discussion, Q&A



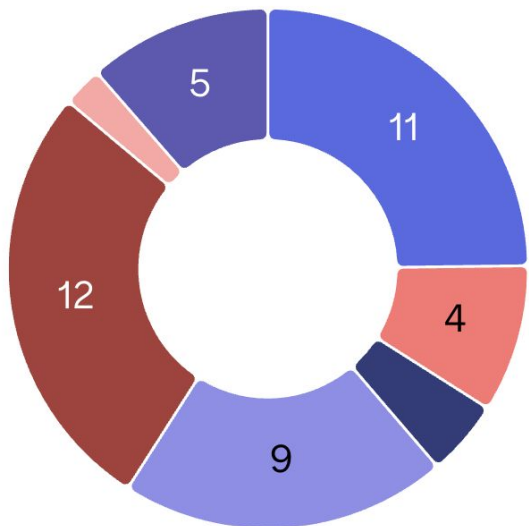
How much time does it take to install the scientific software you are using or need to provide?



- 4 It's all I do ! I wish I had time for something else
- 14 I don't spend much time on it, but my colleague does
- 2 I'm waiting for days or weeks until the software I requested is available
- 25 Not that bad, say hours, because I use good tooling that alleviates the pain
- 5 I just snap my fingers and it's there. It's EESSI

# Live poll, discussion, Q&A

How long would it take you to get an optimized installation of GROMACS ready to run?

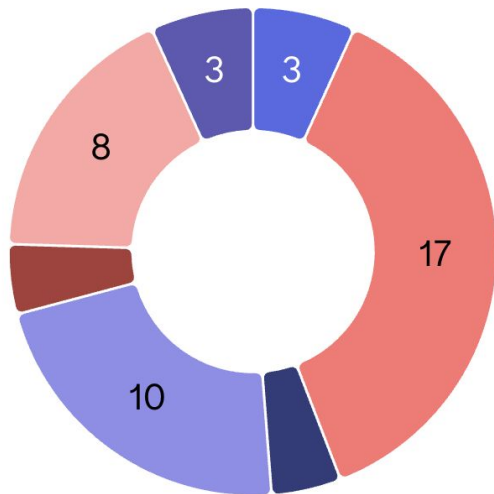


- 11 What's a GROMACS, does it bite?
- 4 Totally depends on the support team that will install it for me
- 2 I'll just follow the installation instructions, so should be very smooth, I hope?
- 9 I know GROMACS uses standard tools like cmake & make, so how hard can it be?!
- 12 I'm using an installation tool like EasyBuild or Spack, so it's mostly waiting for the installation to complete
- 1 I found a 12GB container image that provides GROMACS, I'll just blindly trust that
- 5 It's matter of minutes or even seconds, since I'm using EESSI

# Live poll, discussion, Q&A



To what extent do you typically **test** the software you install / use?



- 3 Not at all (YOLO)
- 17 Only basic tests (does it run?)
- 2 Using test suite, but ignoring failing tests
- 10 Using test suite, trying to fix failing tests
- 2 Using test suite, must fix failing tests
- 8 Using test suite which must pass, also additional tests
- 3 Something else

# Live poll, discussion, Q&A



Do you know if the software installations you're using have been tested?

44 / 67

I have no idea

2

Probably not

2

I guess someone tested it... Right? RIGHT?

13

I think so, but I'm not sure

6

Pretty sure it was tested

13

100% sure it was tested extensively

8

20%

40%

60%

80%

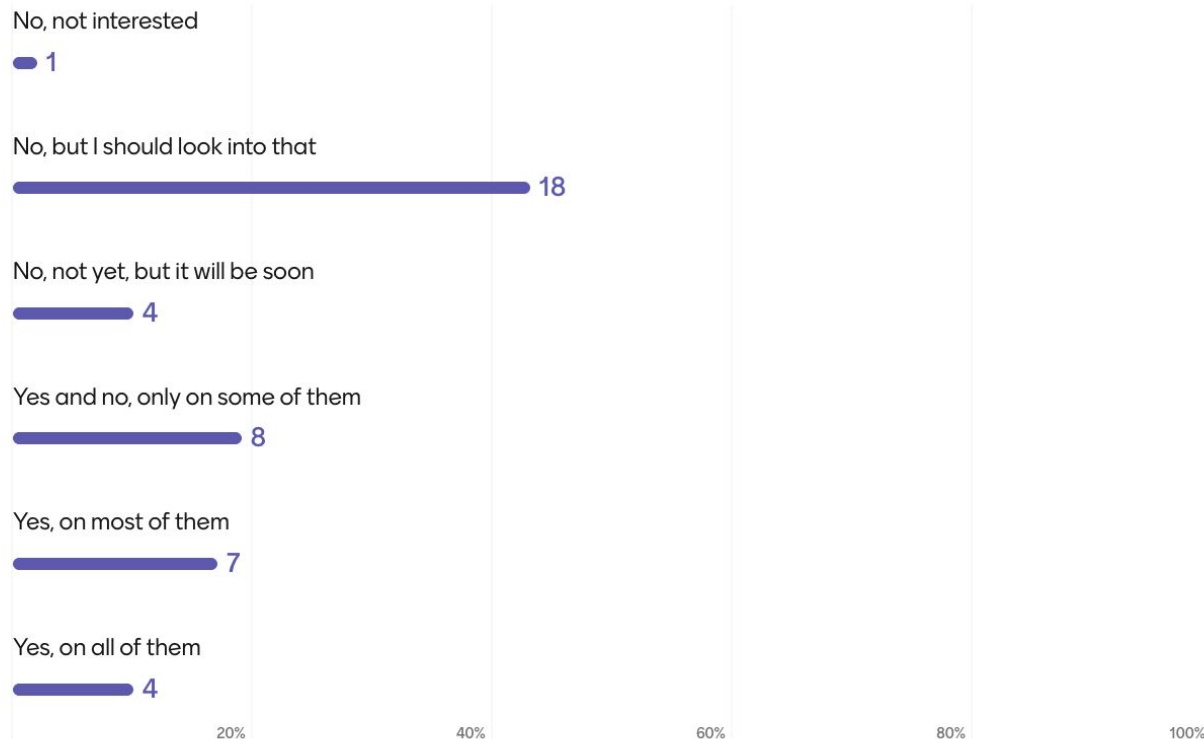
100%

# Live poll, discussion, Q&A



Is EESSI already available on the systems you are using/managing?

42 / 67



# Live poll, discussion, Q&A



How did you like this ISC'26 EESSI BoF session?

49 / 67

Give us a score between 1 (very disappointed) and 10 (Fan-tas-tic!)

