

# E E S S I

EUROPEAN ENVIRONMENT FOR  
SCIENTIFIC SOFTWARE INSTALLATIONS



**Birds-of-a-Feather session - SC'24 - Atlanta (US) - 19 Nov 2024**

*Elisabeth Ortega, Helena Vela Beltran, Jordi Blasco (Do IT Now Alliance)*

*Kenneth Hoste & Lara Peeters (Ghent University, Belgium)*

# Get ready for the live poll!



1. Go to the **SC24 website** (<https://sc24.supercomputing.org>)
2.  to the 
3. Go to the page of the **EESSI Birds-of-a-Feather session**  
[sc24.conference-program.com/presentation/?id=bof126&sess=sess657](https://sc24.conference-program.com/presentation/?id=bof126&sess=sess657)
4. Keep an eye on the **Q&A box on the right** to join the interactive poll

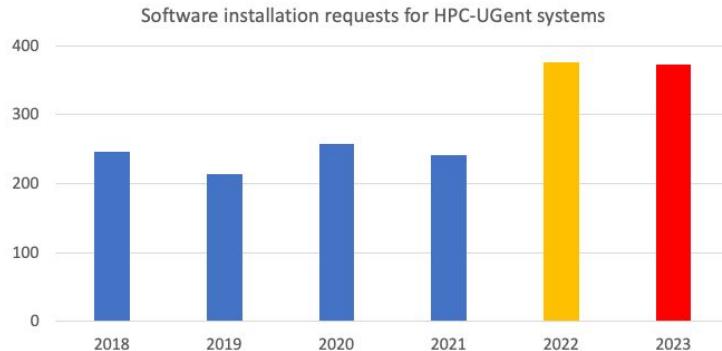
Username or Email Address

Password

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# Landscape of scientific computing is changing

- **Explosion of available scientific software** applications (bioinformatics, AI, ...)
- 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, AWS Graviton, ...),  
RISC-V is coming (soon?)
- Broader adoption of **accelerated computing**, beyond NVIDIA GPUs (AMD, Intel, ...)
- In strong contrast: available (wo)manpower in **HPC support teams** is (still) limited...



# European Environment for Scientific Software Installations

- **Public repository of (optimized!) scientific software *installations***
- **Avoid duplicate work** 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** (incl. WSL & macOS) **and system architecture**
  - From laptops and personal workstations to HPC clusters and cloud
  - Support for different CPUs (AMD, Intel, Arm, RISC-V), interconnects, GPUs, etc.
- **Focus on performance, automation, testing, collaboration**



<https://eessi.io>

<https://eessi.io/docs>



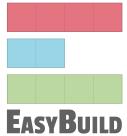
Software layer  
Optimized applications + dependencies

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

Compatibility layer  
Levelling the ground across client OSs

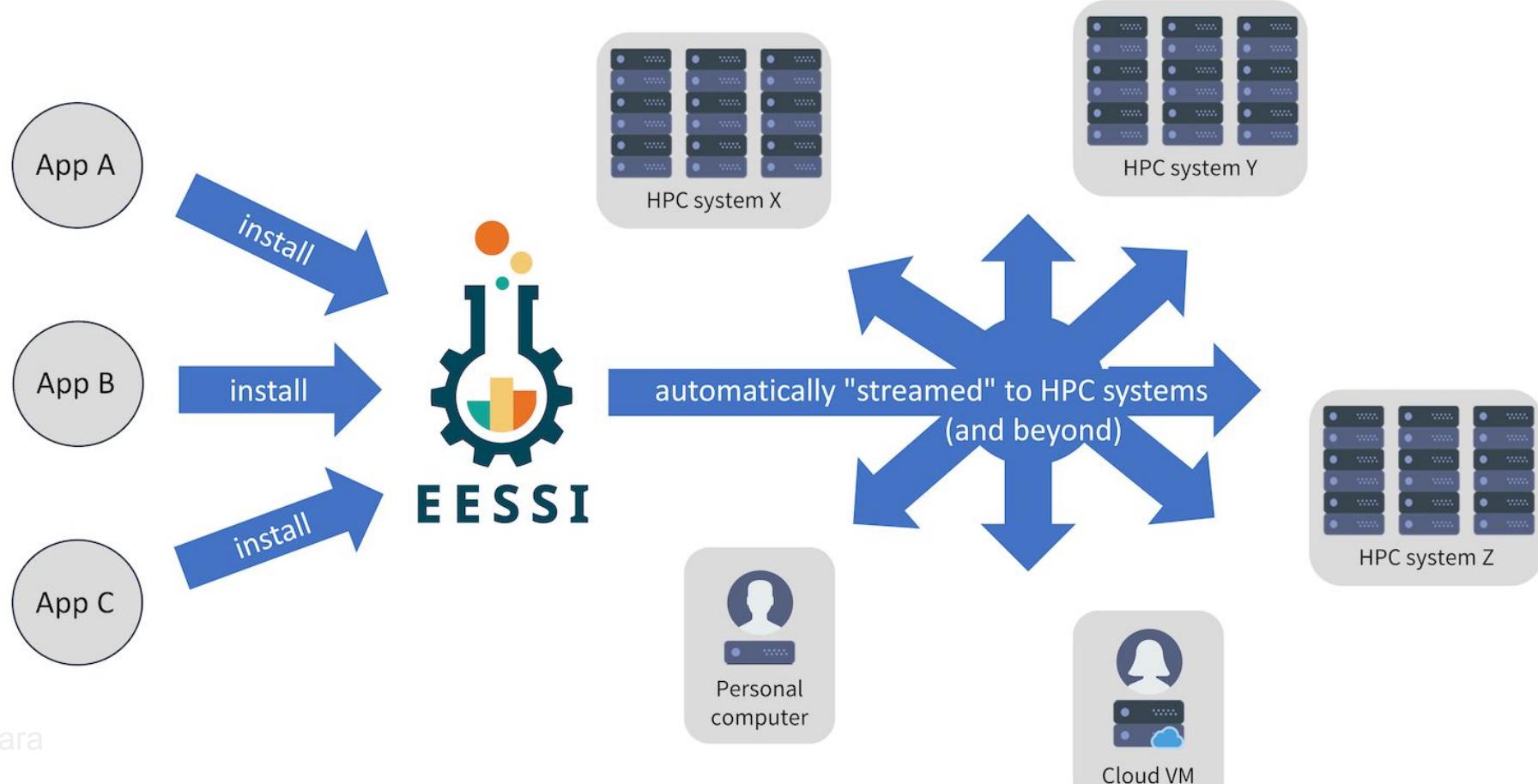
Filesystem layer  
Distribution of the software stack

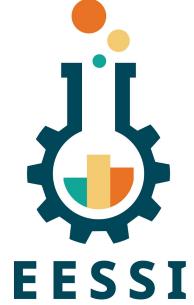
Host operating system



**ESSI**  
EUROPEAN ENVIRONMENT FOR  
SCIENTIFIC SOFTWARE INSTALLATIONS

# EESSI as a shared software stack





# Getting access to EESSI

- Native installation of CernVM-FS (*requires admin privileges*)  
[eessi.io/docs/getting\\_access/native\\_installation](https://eessi.io/docs/getting_access/native_installation)
- Using a container (via Apptainer)  
[eessi.io/docs/getting\\_access/eessi\\_container](https://eessi.io/docs/getting_access/eessi_container)
- Via cvmfsexec  
[github.com/cvmfs/cvmfsexec](https://github.com/cvmfs/cvmfsexec)

**To check whether you have access to EESSI:**

```
ls /cvmfs/software.eessi.io
```

# Accessing EESSI via CernVM-FS (demo)



```
# 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"

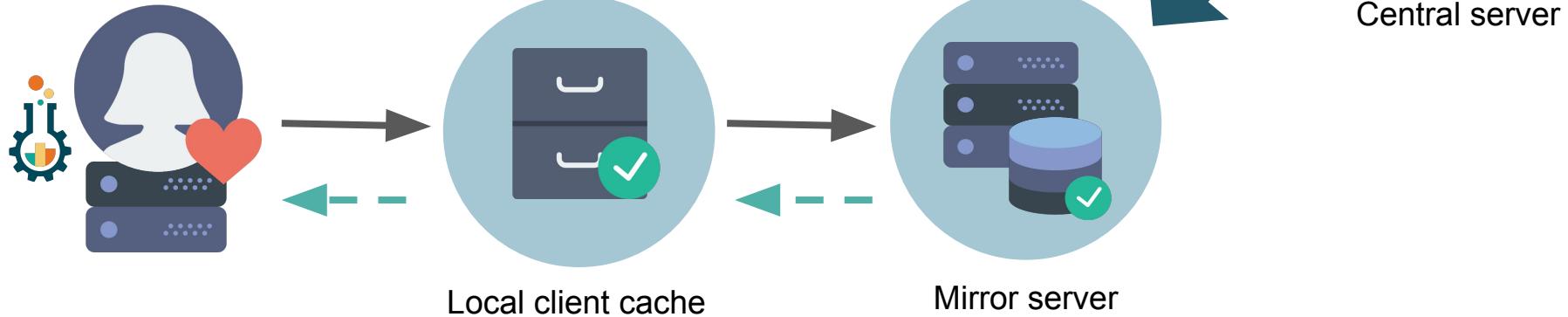
# Make sure that EESSI CernVM-FS repository is accessible
sudo cvmfs_config setup
```

Alternative ways of accessing EESSI are available, via a container image, via cvmfsexec, ...

[eessi.io/docs/getting\\_access/native\\_installation](https://eessi.io/docs/getting_access/native_installation) - [eessi.io/docs/getting\\_access/eessi\\_container](https://eessi.io/docs/getting_access/eessi_container)

# 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, ...)

# Using EESSI (demo)

[eessi.io/docs/using\\_eessi/eessi\\_demos](https://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

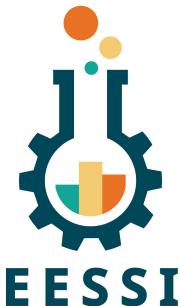
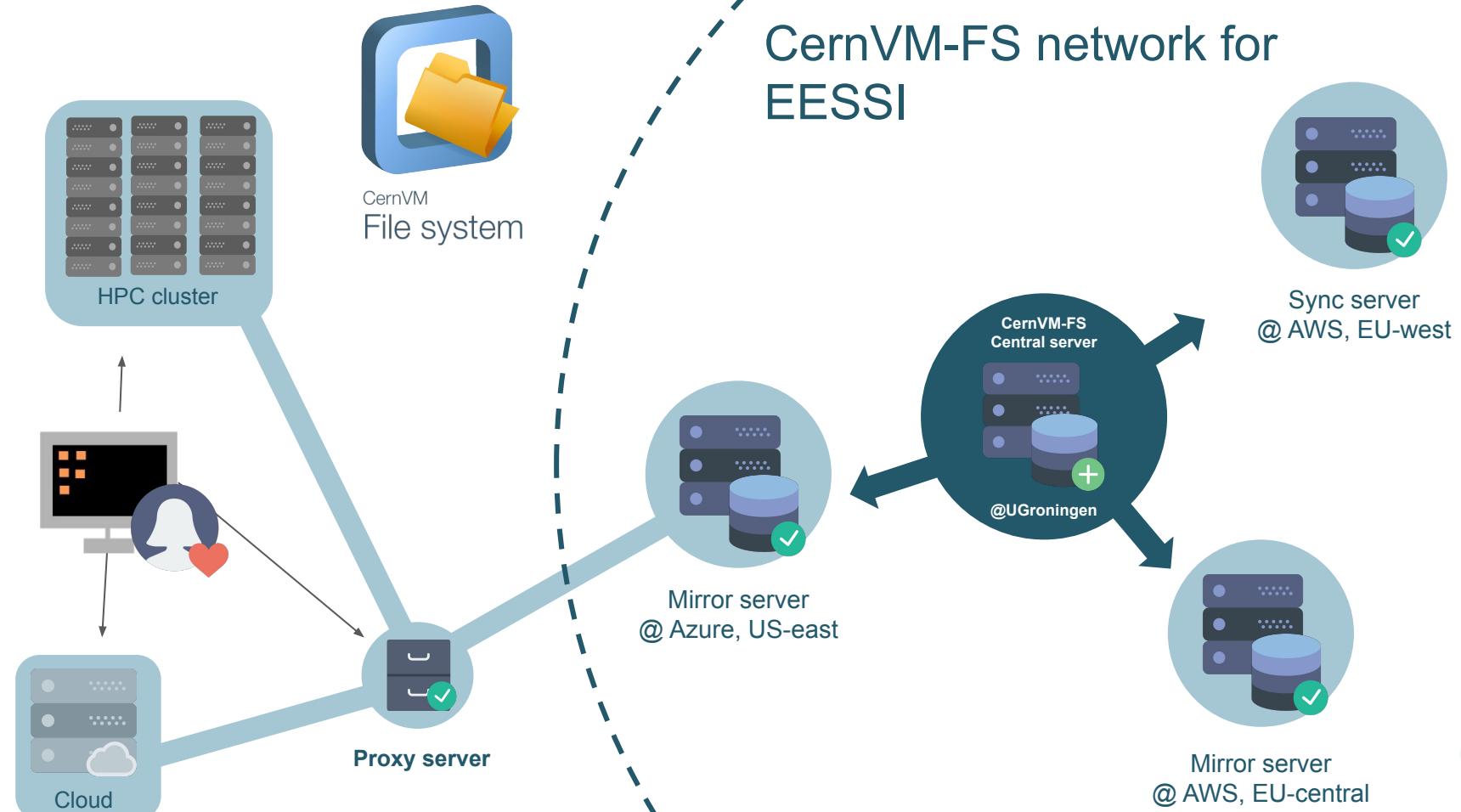
{EESSI 2023.06} $ R --version
R version 4.3.2
```

# 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

# CernVM-FS network for EESSI



# Tutorial “Best Practices for CernVM-FS in HPC”



- [multixscale.github.io/cvmfs-tutorial-hpc-best-practices](https://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



# EESSI compatibility layer

[github.com/EESSI/compatibility-layer](https://github.com/EESSI/compatibility-layer)



- “Containers without the containing”
- Minimal collection of tools and libraries (incl. glibc, bash, Python, Lmod, ...)
- Built from source per CPU family (x86\_64, aarch64, ...) with [Gentoo Prefix](#)
- Installations included in software layer only link to compat layer (RPATH)
- Ensures compatibility with any client system running Linux

```
$ ls /cvmfs/software.eessi.io/versions/2023.06/compat/linux/aarch64/
bin  etc  lib  lib64  opt  reprod  run  sbin  stage1.log  stage2.log
stage3.log  startprefix  tmp  usr  var
```

Software layer

Compatibility layer

x86\_64

aarch64

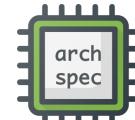
OS

# Software layer

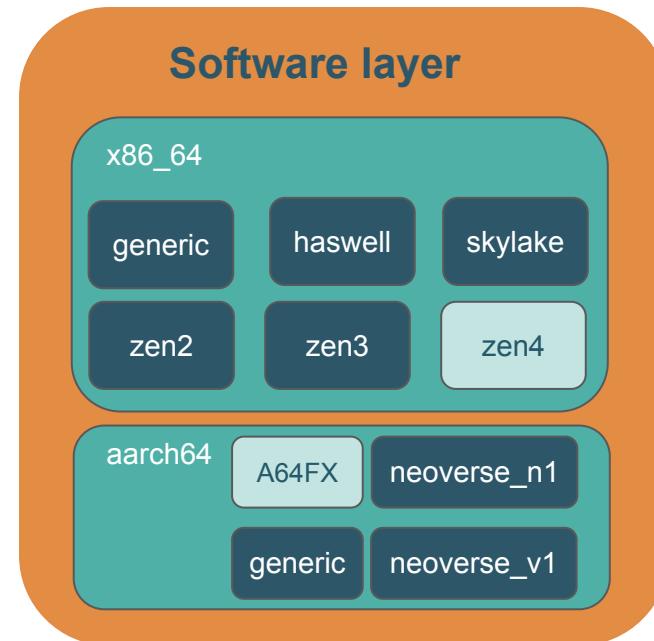
[github.com/EESSI/software-layer](https://github.com/EESSI/software-layer)



Lmod



- Installations of scientific software applications
- **Optimized for specific CPU targets**
- Works on any client system running Linux, since we only link to libraries in compat layer
- Built using [EasyBuild](#)
- Environment modules as user interface (via [Lmod](#))
- Detection of host CPU via [archspec](#) (Python) or archdetect (bash)
- Magic Castle to manage our (build)clusters in the cloud
- **Best subset of software installations for host CPU is automatically selected**



Compatibility layer

OS

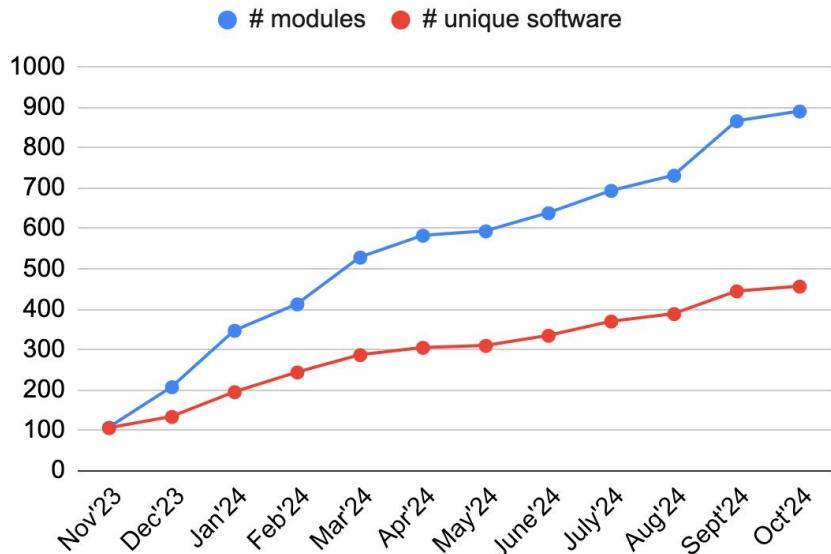
# Overview of installed software

Currently ~900 software installations available

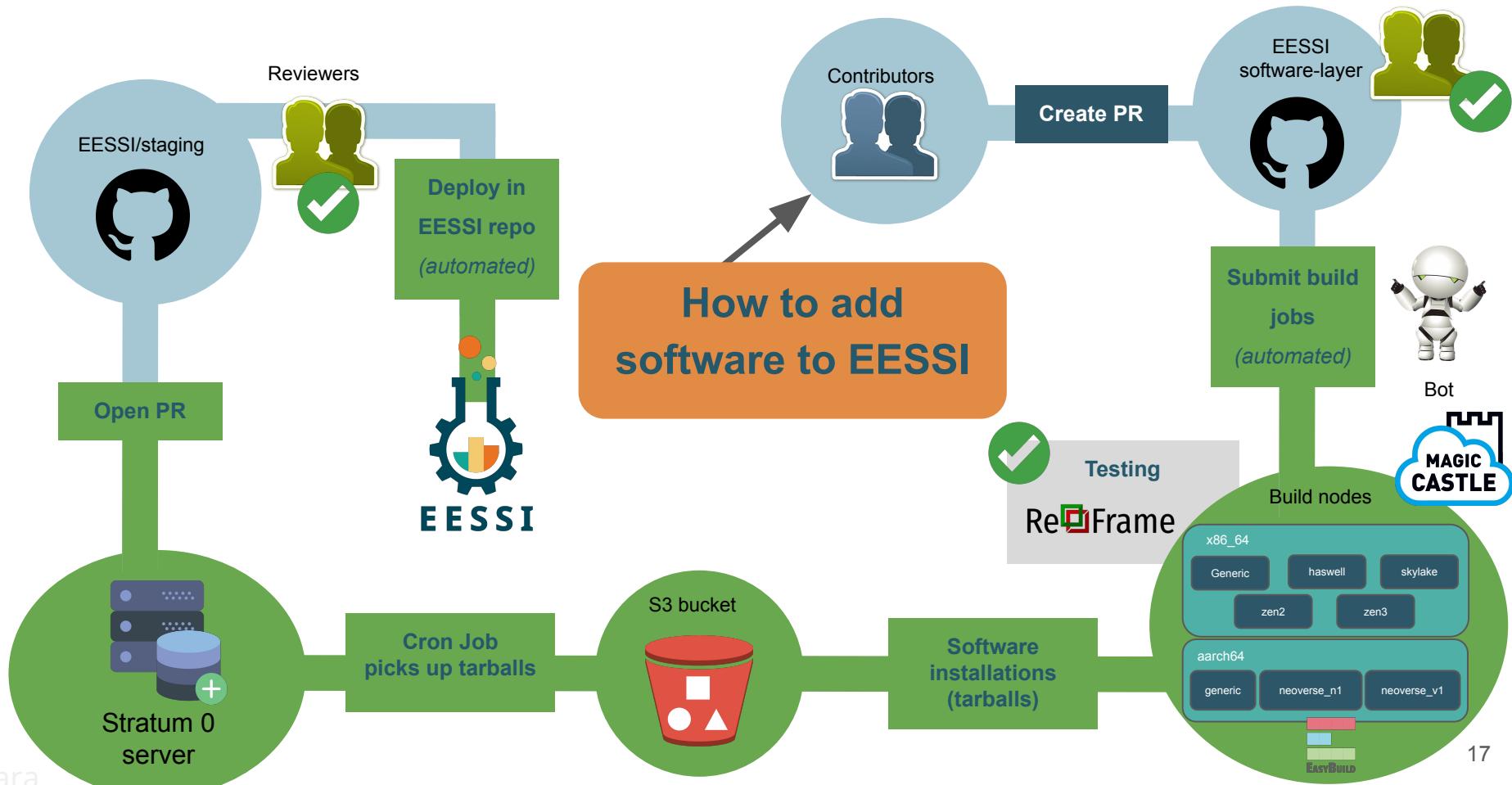
per CPU target via [software.eessi.io](https://software.eessi.io) CernVM-FS repository;  
increasing every day

- 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`

# software installations in EESSI 2023.06 (per CPU target)



# Semi-automated workflow for adding software to EESSI



# NVIDIA GPU support in EESSI



- CUDA software is in place in EESSI version 2023.06
- Two 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...
- We provide **scripts to deal with both problems**, see documentation: [eessi.io/docs/gpu](https://eessi.io/docs/gpu)
- **Available CUDA software in EESSI:** ESPResSo, LAMMPS, NCCL, OSU Micro-Benchmarks
- Currently only for systems with **AMD Rome (Zen2) CPU + NVIDIA A100 GPU** (CUDA cc 8.0)
- More CPU/GPU combos + software coming soon: GROMACS, PyTorch, TensorFlow, AlphaFold

# Software testing is an important part of EESSI

- EESSI test suite: [eessi.io/docs/test-suite](https://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!



# Leveraging EESSI in CI environment

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

```
name: ubuntu_gromacs
on: [push, pull_request]          github.com/EESSI/github-action-eessi
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
```



# EESSI in a nutshell

- **On-demand streaming of optimized scientific software installations**
- **Works on any Linux distribution** thanks to EESSI compat layer
- **Uniform software stack** across various systems: laptop, HPC, cloud, ...
- Community-oriented: **let's tackle the challenges we see together!**



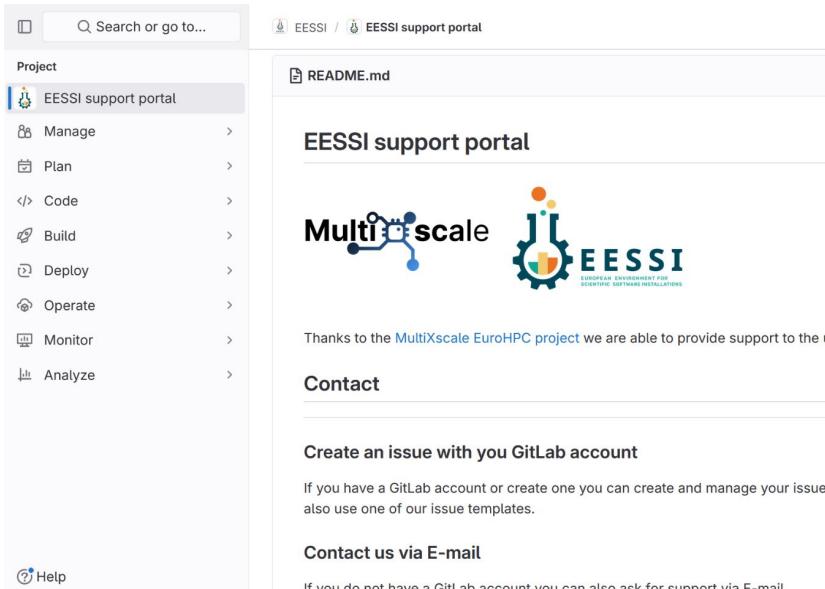
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# Getting support for EESSI



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



The screenshot shows the GitLab interface for the EESSI support portal. On the left is a sidebar with project management options: Manage, Plan, Code, Build, Deploy, Operate, Monitor, and Analyze. The main area displays the README.md file, which includes the MultiXscale and EESSI logos, a thank you message for the MultiXscale EuroHPC project, a contact section, and instructions for creating an issue on GitLab. It also mentions that users can ask for support via email if they do not have a GitLab account.

Project

EESSI support portal

- Manage >
- Plan >
- Code >
- Build >
- Deploy >
- Operate >
- Monitor >
- Analyze >

Help

EESSI / EESSI support portal

README.md

## EESSI support portal

Thanks to the [MultiXscale EuroHPC project](#) we are able to provide support to the u

### Contact

Create an issue with your GitLab account

If you have a GitLab account or create one you can create and manage your issue also use one of our issue templates.

### Contact us via E-mail

If you do not have a GitLab account you can also ask for support via E-mail.

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

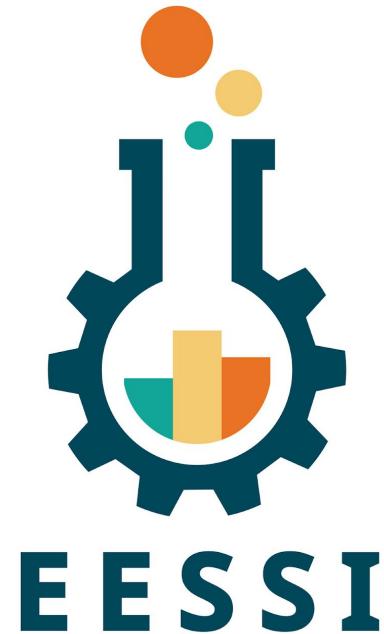
# EESI got nominated for an HPCWire award...



- “*Best HPC Programming Tool or Technology*” category
- See also our blog post on this:  
[eessi.io/docs/blog/2024/09/20/hpcwire-readers-choice-awards-2024](https://eessi.io/docs/blog/2024/09/20/hpcwire-readers-choice-awards-2024)
- Winner was decided by popular vote...

# EESSI won an HPCWire Reader's Choice award!

*Thank you  
for voting  
for us!*



# Learn more about EESSI at SC'24



Short presentation on EESSI on exhibit floor

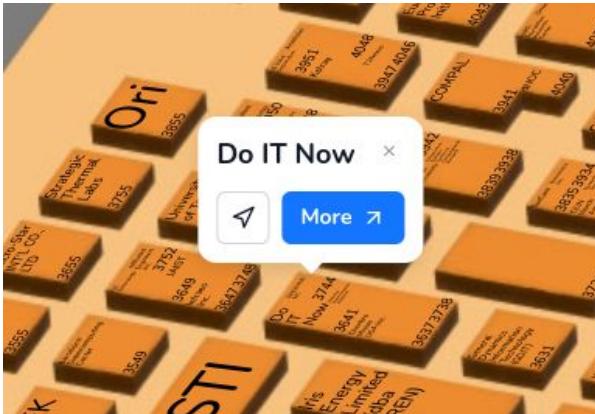
- Microsoft Azure booth
- Wed 20 Nov'24, 14:40-15:00



# Get a live demo on EESSI at the DoltNow booth



- Booth #3641
- Ask for Kenneth, Lara, or Helena!
- Win a Raspberry Pi 5 4GB starter kit!



# Join the EESSI community in Slack!



- **Win a Raspberry Pi 5 4GB starter kit!**
- Join the #sc24 channel in the EESSI Slack (if you haven't yet)
  - See link via <https://eessi.io>
- Say “Hello from SC24 in Atlanta, I want to win a Raspberry Pi!”
- We will draw a lucky winner...
- Prize will be handed out Wed 4.30pm  
at DoItNow booth (#3641)



# EESI tutorial at HiPEAC 2025 (Barcelona, Jan'25)



- [hipeac.net/2025/barcelona](https://hipeac.net/2025/barcelona)
- EESI tutorial: Wed 22 Jan 2025 14:00-17:30
- MultiXscale presentation in Women@HPC session

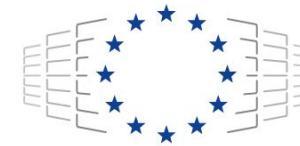


Join us in Barcelona for #HiPEAC25 >

# Acknowledgements

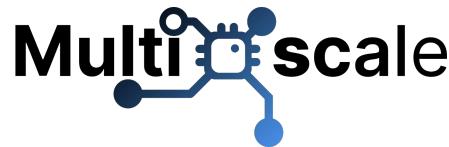


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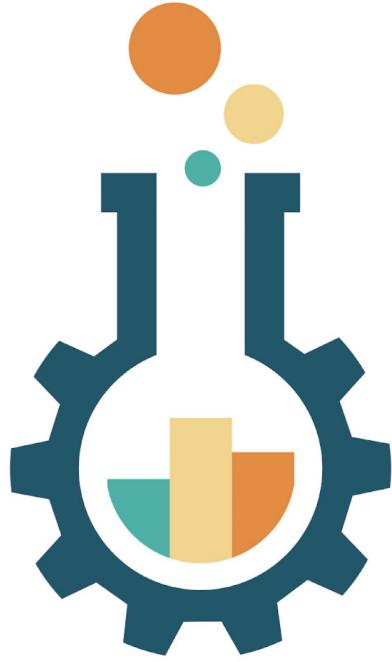
EuroHPC  
Joint Undertaking

- 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 cloud credits, feedback, and guidance.





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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)

[Join](#) the EESSI Slack

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)

# Get ready for the live poll!



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4. Keep an eye on the **Q&A box on the right** to join the interactive poll

# Live poll + discussion



## 1) What does the first 'E' in EESSI stand for?

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

# Live poll + discussion



2) Which tool(s) do you use for "installing" software on the HPC systems you use? (multiple choice)

- CernVM-FS
- Conda/mamba
- Containers (Apptainer, Singularity, ...)
- EasyBuild
- EESSI
- Spack
- Something else...

# Live poll + discussion



## 3) Which systems do you use for running scientific workloads? (multiple choice)

- On-premise HPC cluster
- On-premise cloud
- Microsoft Azure
- Amazon EC2 (AWS)
- Other commercial cloud (Google, Oracle, ...)
- Personal workstation/laptop
- Quantum computer
- Raspberry Pi
- Something else...

# Live poll + discussion



## 4) Which hardware platforms do you use and/or manage? (multiple choice)

- Intel CPU (no GPU)
- Intel CPU + NVIDIA GPU
- Intel CPU + AMD GPU
- Intel CPU + Intel GPU
- AMD CPU (no GPU)
- AMD CPU + NVIDIA GPU
- AMD CPU + AMD GPU
- AMD CPU + Intel GPU
- Arm CPU (no GPU)
- Arm CPU + NVIDIA GPU
- Arm CPU + AMD GPU
- Arm CPU + Intel GPU
- RISC-V CPU
- Something else...

# Live poll + discussion



## 5) How many different software applications, tools, and libraries do you use and/or provide for running scientific workloads? (pick one)

- None
- Exactly 1
- 2-5
- 5-10
- 10-20
- 20-50
- 50-100
- 100-200
- 200-500
- 500-1000
- Over 1000

# Live poll + discussion



## 6) To what extent do you typically test the software you install/use? (pick one)

- Not at all (YOLO)
- Only basic tests (does it run)
- Using software test suite, but ignoring failing tests
- Using test suite, trying to fix failing tests
- Using test suite, must fix failing tests
- Using test suite, but also running additional tests
- Something else...

# Live poll + discussion



## 7) Are you interested in using EESSI for your work?

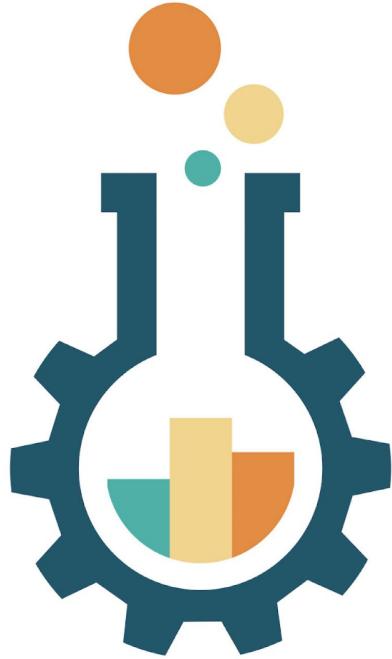
- I'm already using it!
- Yes, definitely interested
- Maybe, I need more convincing
- No, not really
- I have no idea, which BoF is this again?

# Live poll + discussion



## 8) How did you like the SC'24 EESSI Birds-of-a-Feather?

- Very disappointed
- Was expecting better
- Neutral
- Good
- Fan-tas-tic!



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[Join](#) the EESSI Slack

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)

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# Multiscale



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# BACKUP

# SLIDES

# Live poll + discussion (via Mentimeter, **BACKUP**)



Go to

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

Enter the code

6931 2281



Or use QR code