EESSI

EUROPEAN ENVIRONMENT FOR SCIENTIFIC SOFTWARE INSTALLATIONS

Birds-of-a-Feather session - ISC'24 - Hamburg - 14 May 2024

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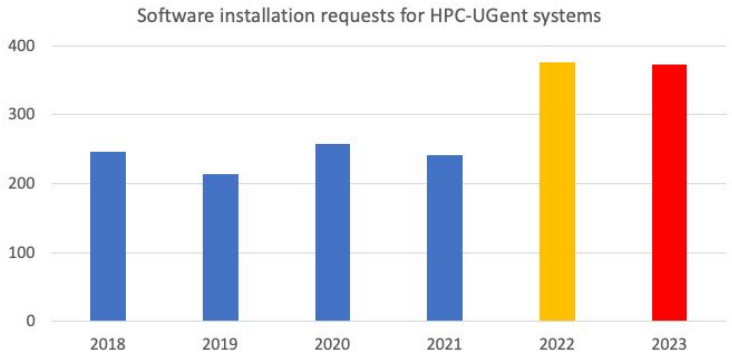
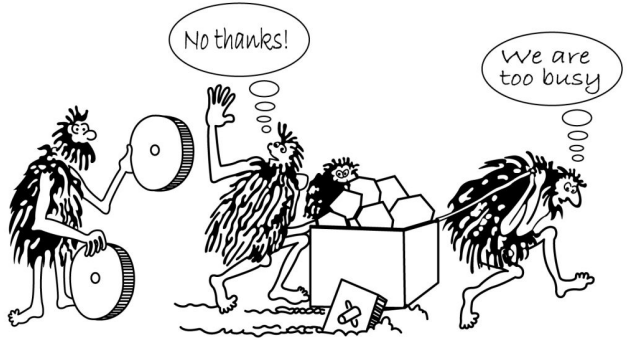
Landscape of scientific computing is changing

- **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) **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**

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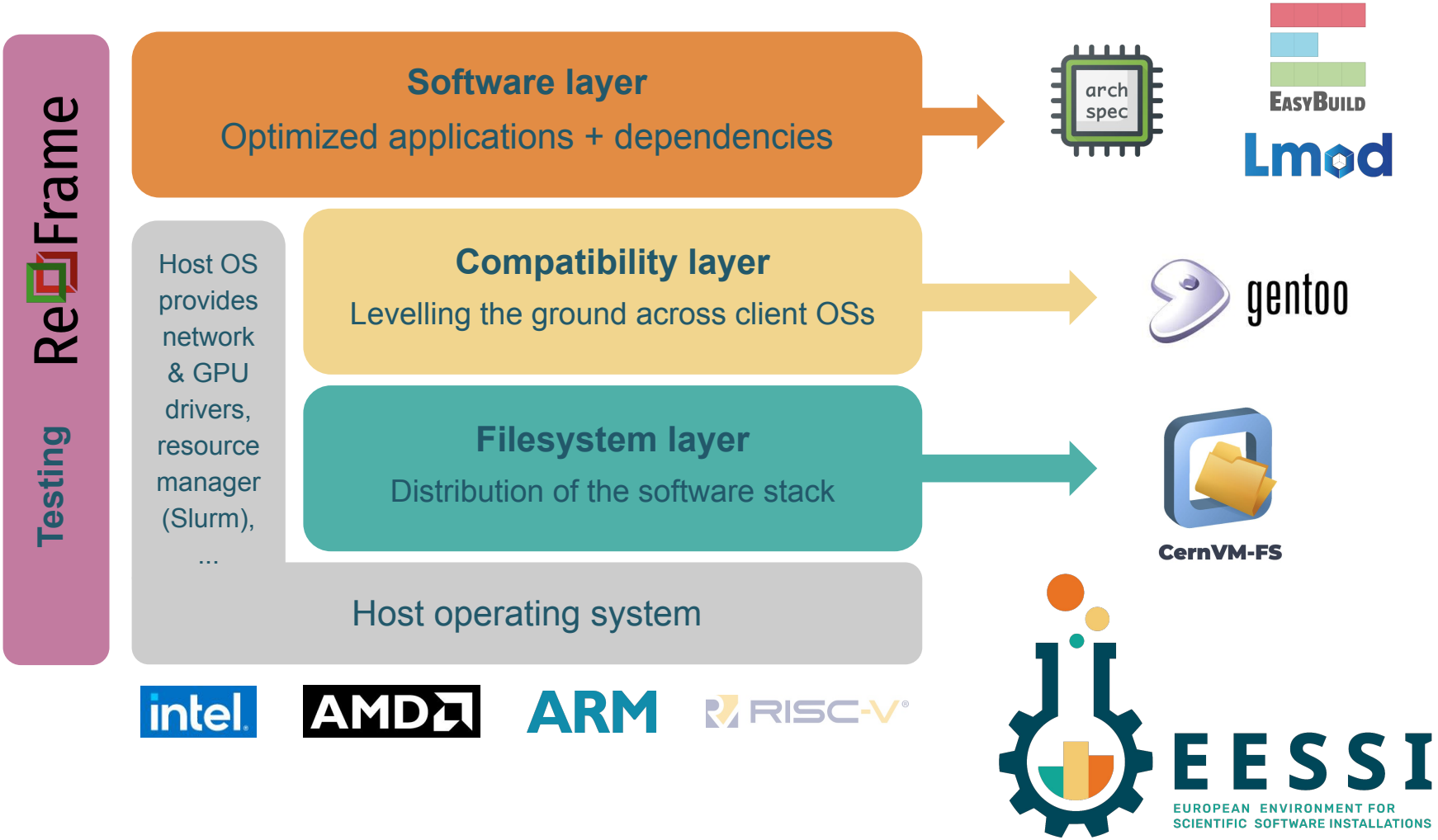
https://eessi.io

https://eessi.io/docs


ReFrame
Testing
Software layer
Optimized applications + dependencies
arch spec
EasyBuild
Lmod
Compatibility layer
Levelling the ground across client OSs
gentoo
Filesystem layer
Distribution of the software stack
CernVM-FS
Host OS provides network & GPU drivers, resource manager (Slurm), ...
Host operating system
intel
AMD
ARM
RISC-V
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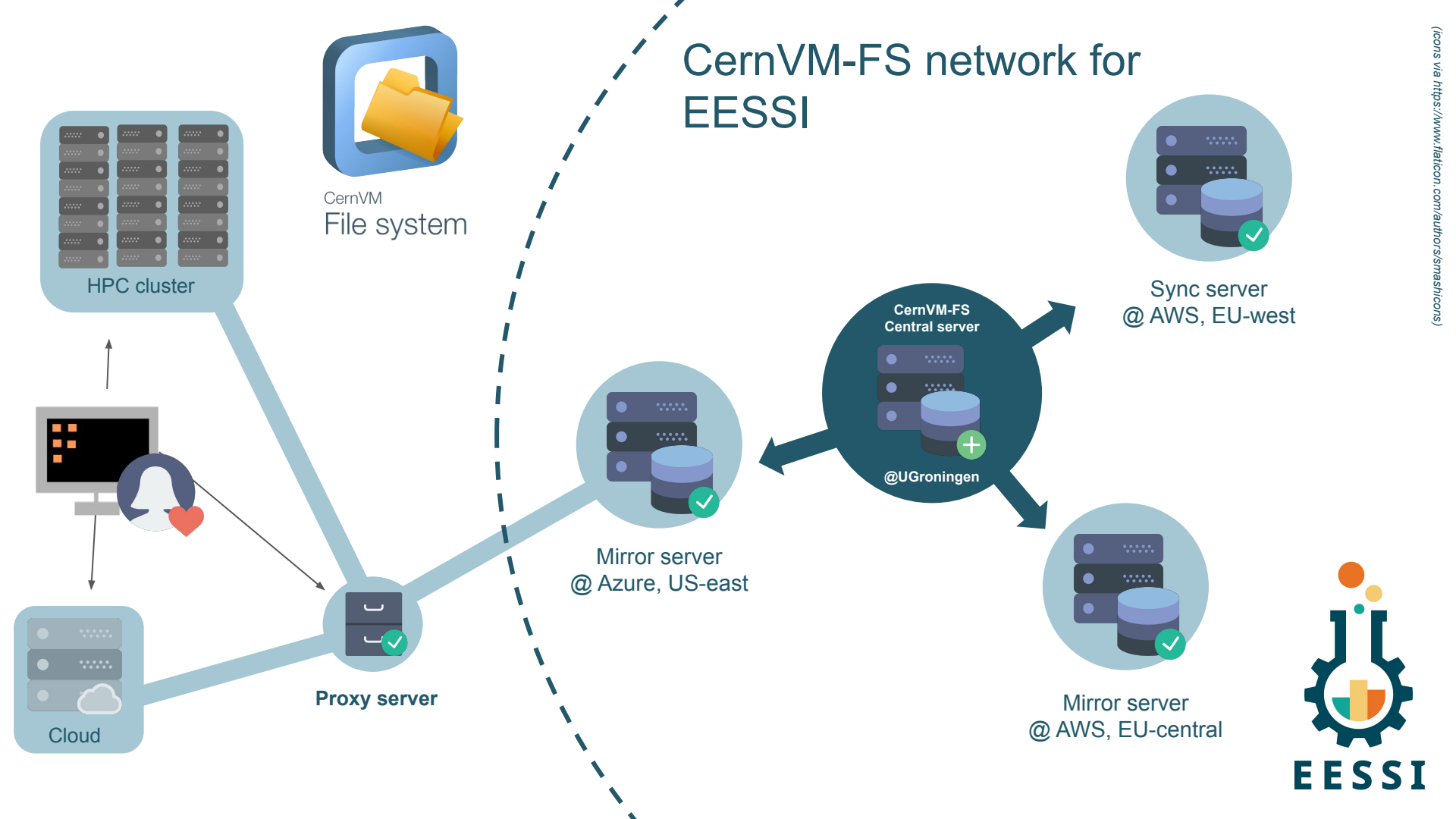
CernVM-FS network for EESSI



(icons via https://www.flaticon.com/authors/smashicons)

Tutorial “Best Practices for CernVM-FS in HPC”

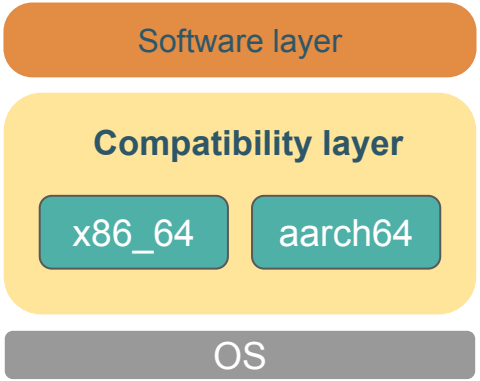
- https://multixscale.github.io/cvmfs-tutorial-hpc-best-practices
- Held online on 4 Dec 2023 (~3 hours), **recorded & available on YouTube**
- Over 200 registrations, ~125 attending the meeting
- Lecture + hands-on demos
- Topics:
  - Introduction to CernVM-FS + EESSI
  - Configuring CernVM-FS: client, Stratum 1 mirror server, proxy server
  - Troubleshooting problems
  - Benchmarking of start-up performance

EESSI compatibility layer

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

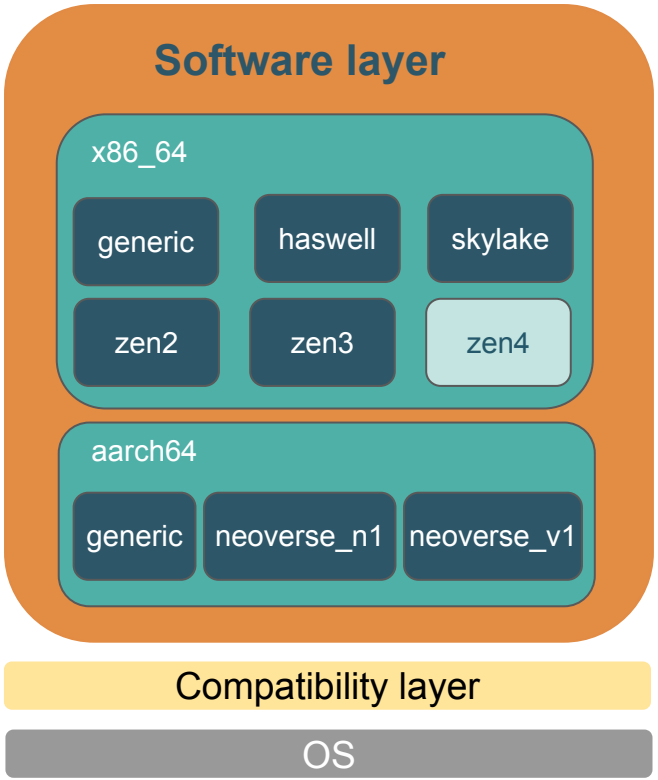
```
$ ls /cvmfs/software.eessi.io/versions/2023.06/compat/linux/aarch64/
bin  etc  lib  lib64  opt  reprod  run  sbin  stage1.log  stage2.log
stage3.log  startprefix  tmp  usr  var
```



Software layer

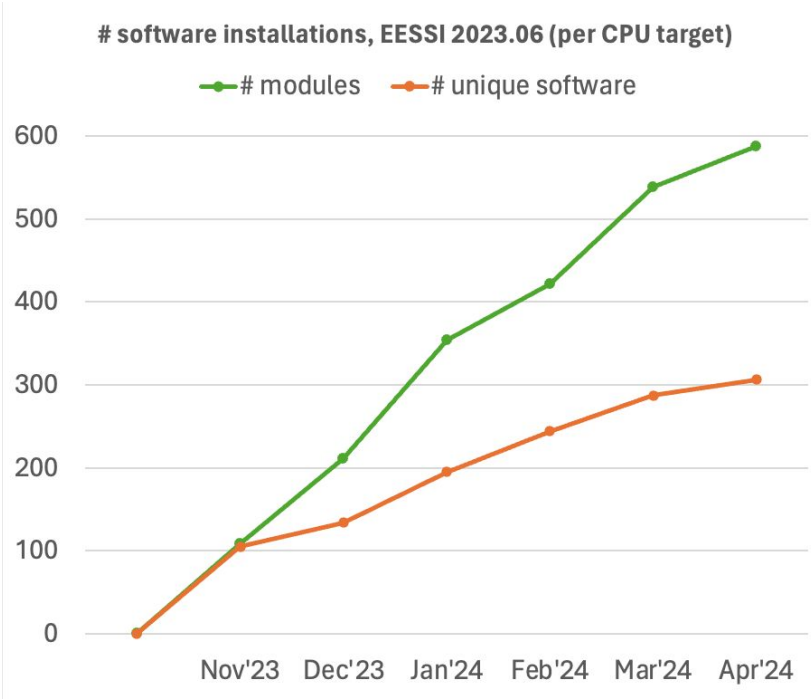
github.com/EESSI/software-layer

- 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)
- **Best subset of software installations for host CPU Is automatically selected**



Overview of installed software

- Currently ~600 software software installations available per CPU target, increasing every day
  - Including ESPResSo, GROMACS, LAMMPS, OpenFOAM, PyTorch, R, QuantumESPRESSO, TensorFlow, WRF
  - eessi.io/docs/available_software (coming soon!)
- using recent compiler toolchains: currently focusing on foss/2023a and foss/2023b



Getting access to EESSI

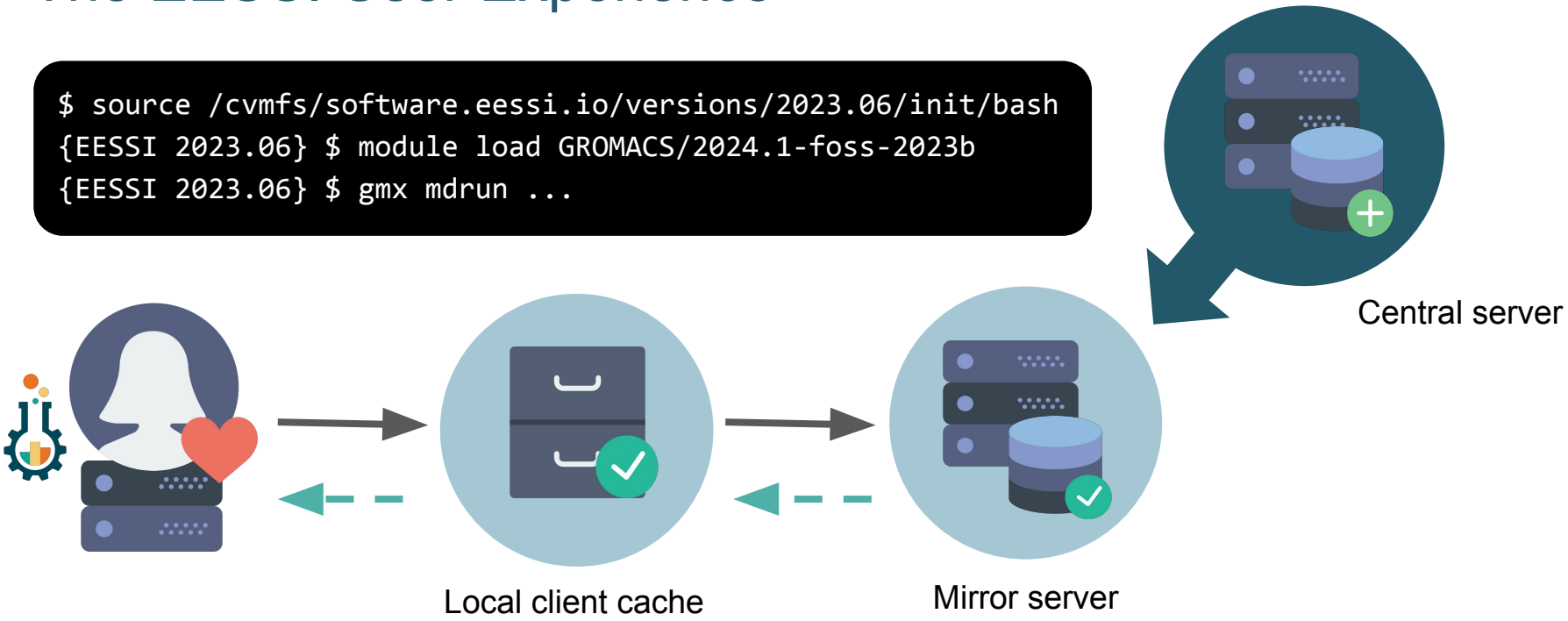
- Native installation of CernVM-FS *(requires admin privileges)*
  eessi.io/docs/getting_access/native_installation
- Using a container (via Apptainer)
  eessi.io/docs/getting_access/eessi_container
- Via cvmfsexec
  github.com/cvmfs/cvmfsexec

To check whether you have access to EESSI:

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

The EESSI User Experience

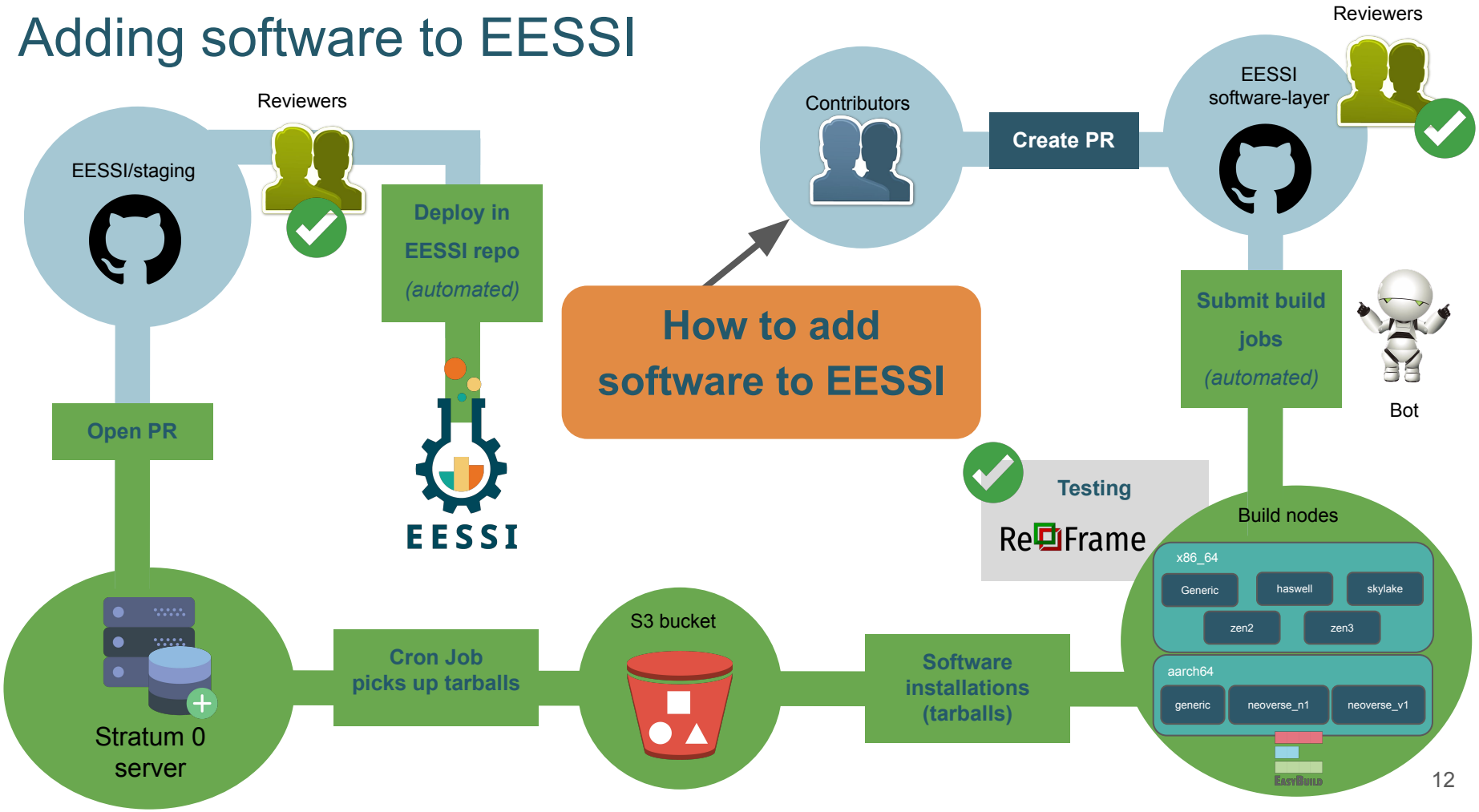
```
$ source /cvmfs/software.eessi.io/versions/2023.06/init/bash
{EESSI 2023.06} $ module load GROMACS/2024.1-foss-2023b
{EESSI 2023.06} $ gmx mdrun ...
```



EESSI provides **on-demand streaming**

of (scientific) software (like music, TV-series, …)

Adding software to EESSI



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:
  - 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 libs)
- In EESSI, we provide scripts to deal with both these problems:
  - 1) **`link_nvidia_host_libraries.sh`** to link GPU driver libraries "into" EESSI (requires write access to `/cvmfs/software.eessi.io/host_injections` variant symlink)
  - 2) **`install_cuda_host_injections.sh`** installs full CUDA to subdirectory of `/cvmfs/software.eessi.io/host_injections`

Software testing is an important part of EESSI

We encountered failing tests in GROMACS test suite when installing it in EESSI

- See https://gitlab.com/eessi/support/-/issues/47
- Filesystem race when running tests concurrently (GROMACS PR #4066)
- **Bug in 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!
  - WIP fix in https://gitlab.com/gromacs/gromacs/-/merge_requests/4299
  - Will be fixed in upcoming GROMACS release (2024.2?)

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
```

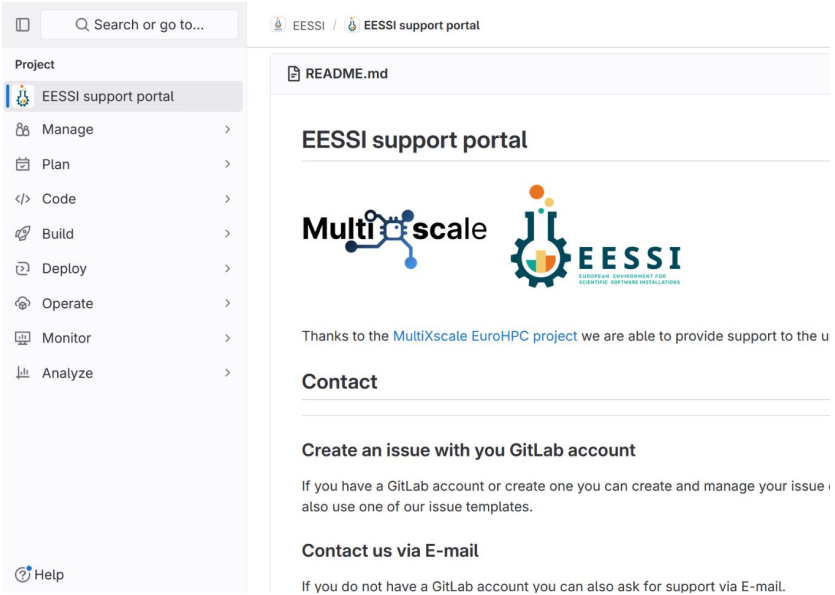
github.com/EESSI/github-action-eessi

Getting support for EESSI

GitLab

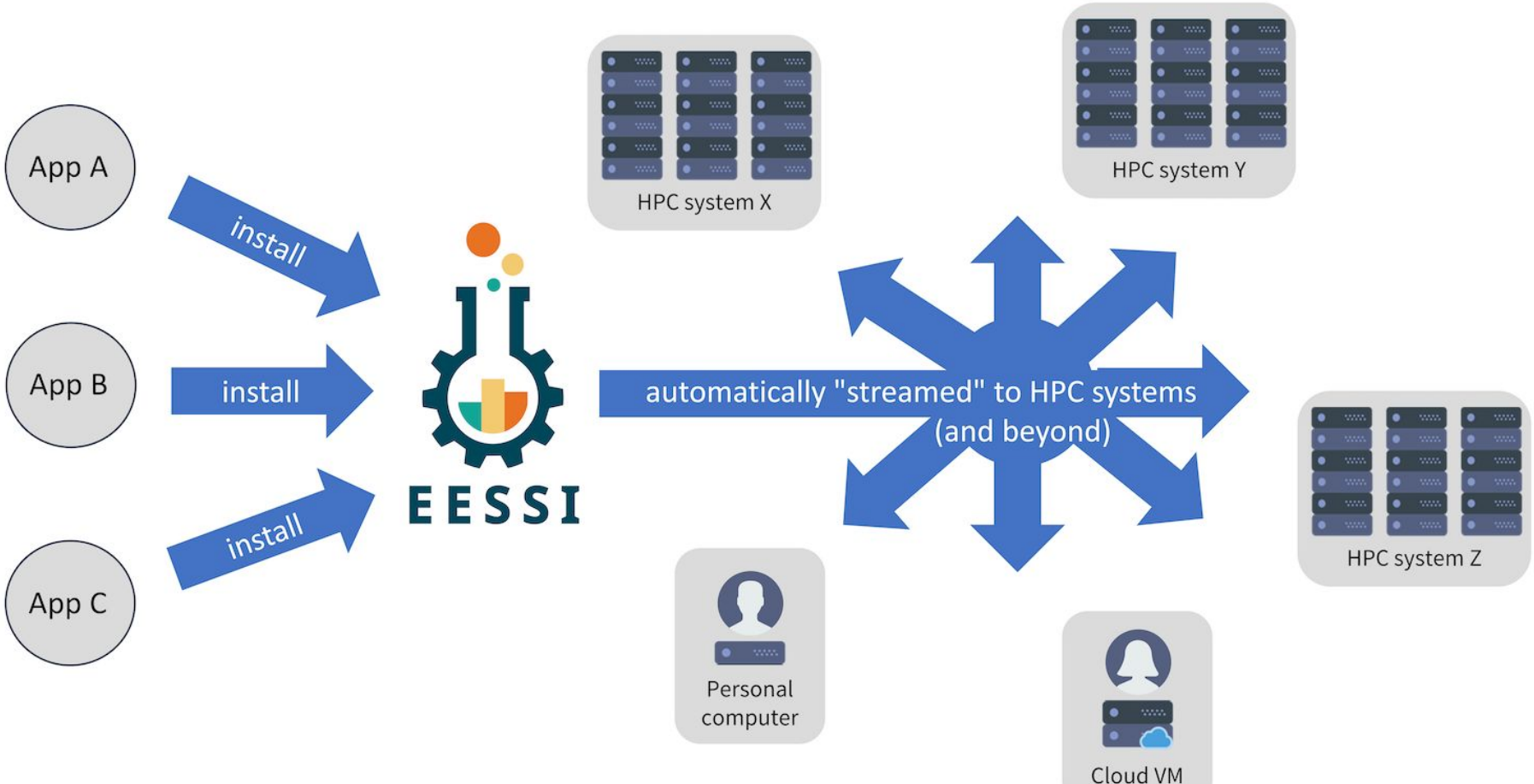
gitlab.com/eessi/support

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



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

EESSI as a shared software stack



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!**

EESSI

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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 - eessi.io/docs/getting_access/eessi_container

Using EESSI (demo)

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
```

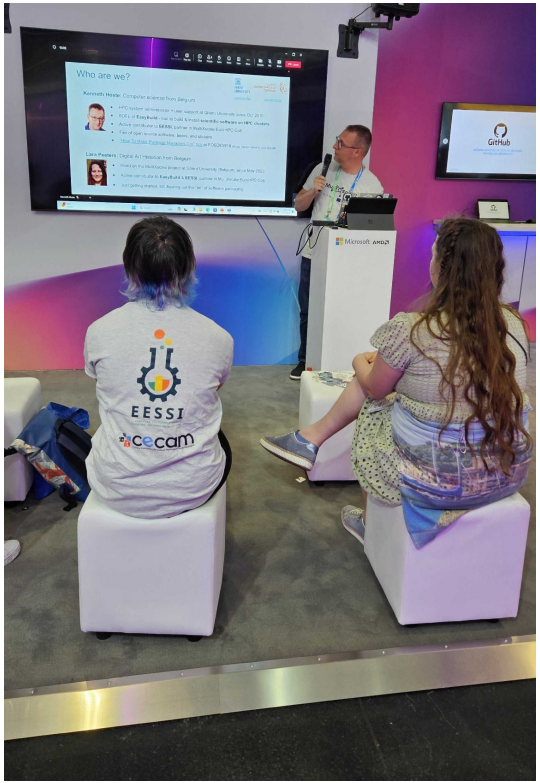
Learn more about EESSI at ISC'24

EESSI demo session

- Azure booth (F30)
- Tue 14 May (today!), 14:00-18:00

1-hour presentation on EESSI

- Azure booth (F30)
- Wed 15 May, 13:00-14:00



Acknowledgements

- 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.

Website: eessi.io

GitHub: github.com/eessi

Documentation: eessi.io/docs

YouTube channel: youtube.com/@eessi_community

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

EESSI support portal: gitlab.com/eessi/support

Monthly online meetings (first Thursday, 2pm CEST)

Join our mailing list & Slack channel

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www.menti.com

Enter the code

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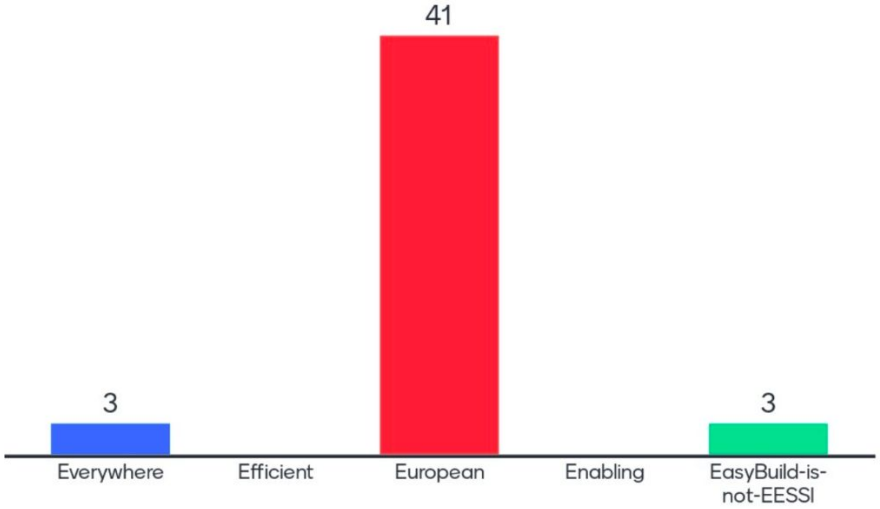
What does the first 'E' in EESSI stand for?



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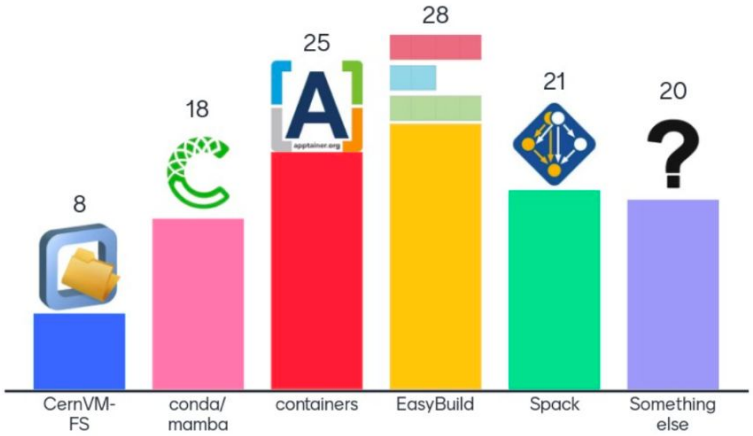
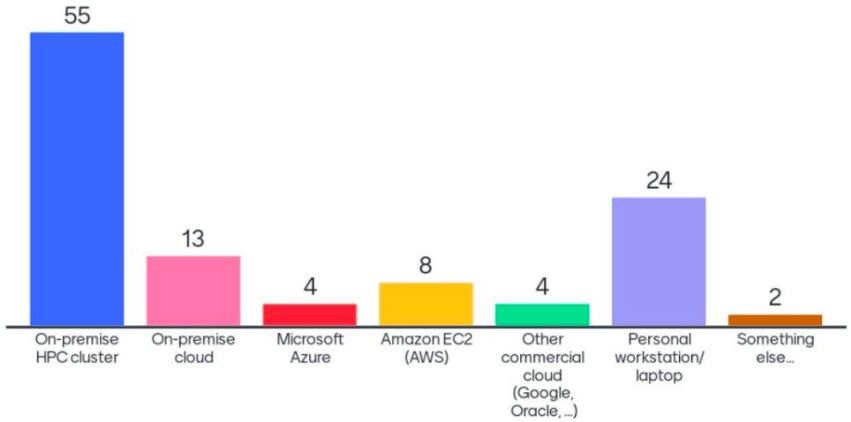
Live poll + discussion

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



Live poll + discussion

Which systems do you use for running scientific workloads?



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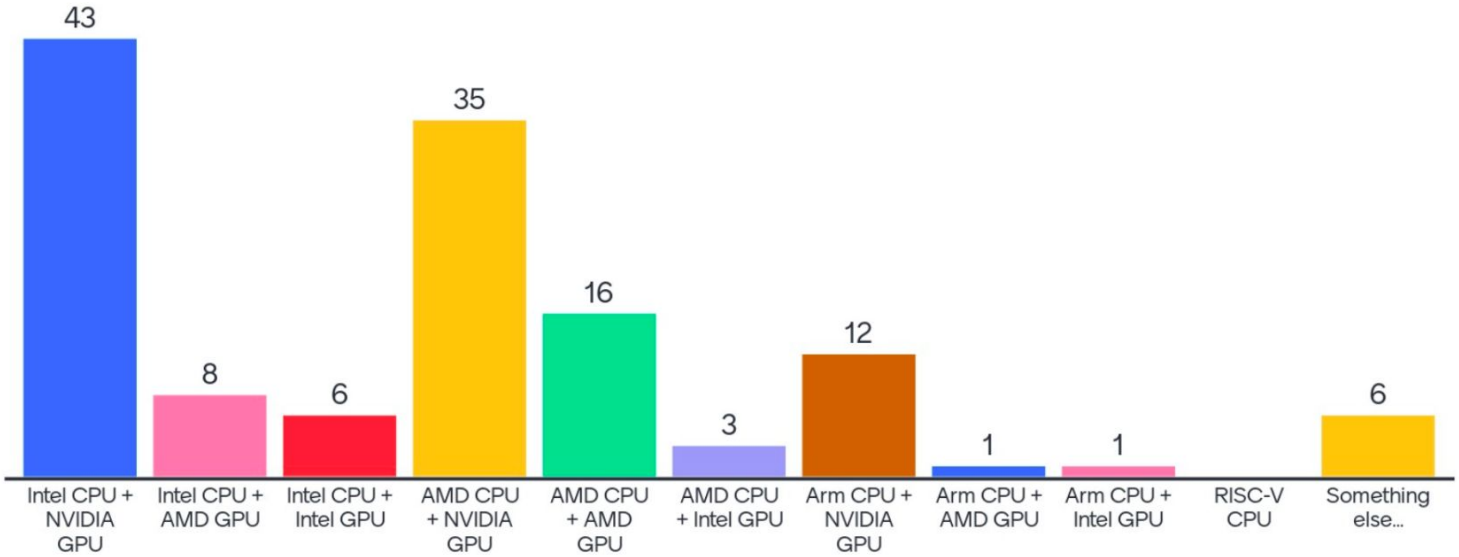
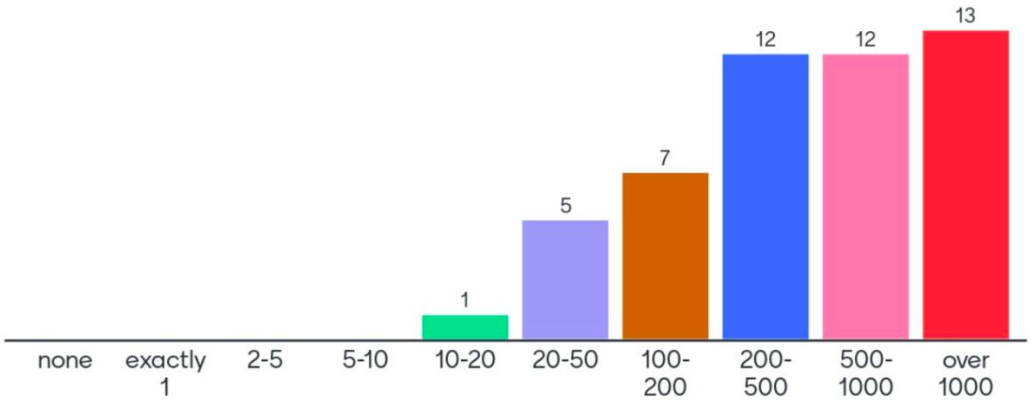
Live poll + discussion

Which hardware platforms do you use and/or manage?



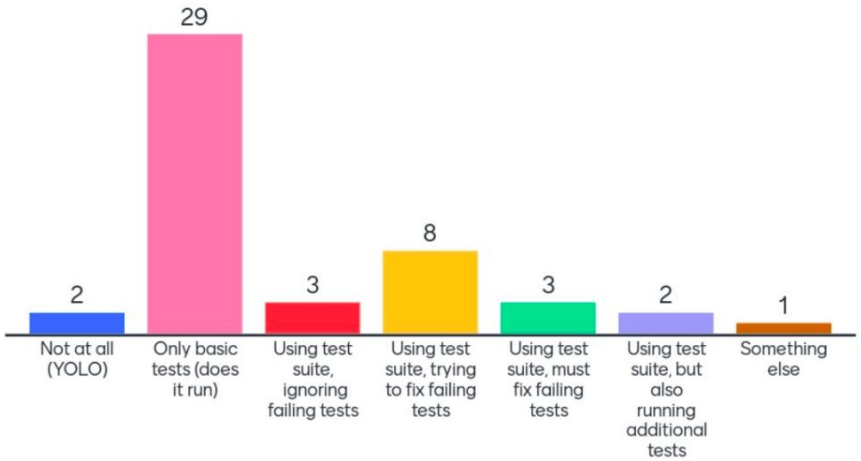
Live poll + discussion

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



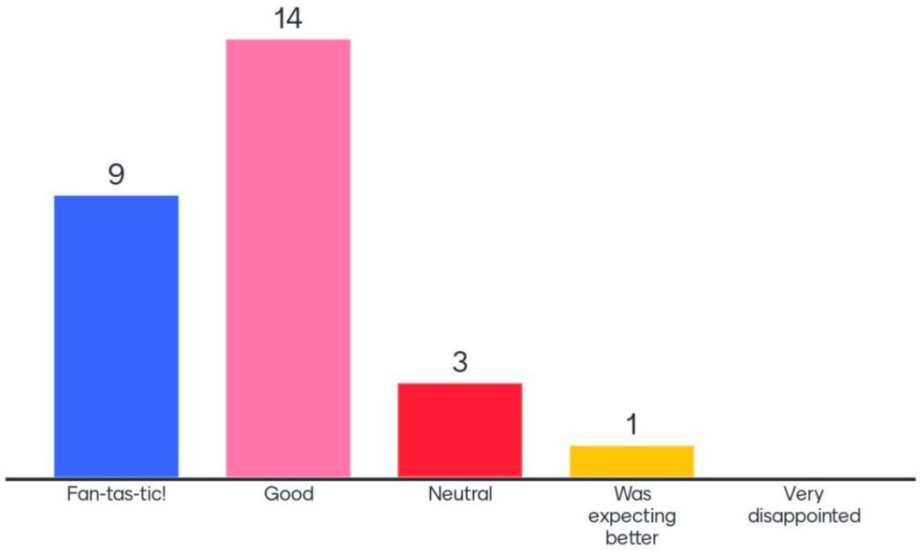
Live poll + discussion

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



Live poll + discussion

How did you like the ISC'24 EESSI Birds-of-a-Feather?



Live poll + discussion - Q&A (1/2)

- In which cases should I absolutely not consider using EESSI?
- What about reproducibility? (Same results in 3 years)
- Do I now have to track Gentoo CVEs, as well as host OS CVEs?
- How can we collaborate with the E4S project?
- Do you track popularity?
- Who are the reviewers? - (sustainability + level of trust)
- Are you working together with OHPC at all? They also test their stuff…
- Is this gnu- or gcc-centric ? (Intel, Portland, amd, etc)
- Is there really a need for containers when using EESSI?

Live poll + discussion - Q&A (2/2)

- Remark: In testing this now: aws-eu-central-s1.eessi.science seems to show up on a fortinet DNS block list (for anybody having problems in testing)
- Where are the binaries physically installed? Any specific network requirement are needed for mounting the FS? Are any performance hits expected? Compared to the local Spack-installed modules
- Will there be any tests on software quality (e.g. tests) and requirements in support from software developers?
- Why only exposing modules to users ?
  Looks like a long path to add something not already available .
- What about python dependencies?