EESSI

EUROPEAN ENVIRONMENT FOR SCIENTIFIC SOFTWARE INSTALLATIONS

Multi scale

Extending Arm's Reach by Going EESSI

ISC'24 - Hamburg - 15 May 2024

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whoami

GHENT UNIVERSITY

VLAAMS SUPERCOMPUTER CENTRUM

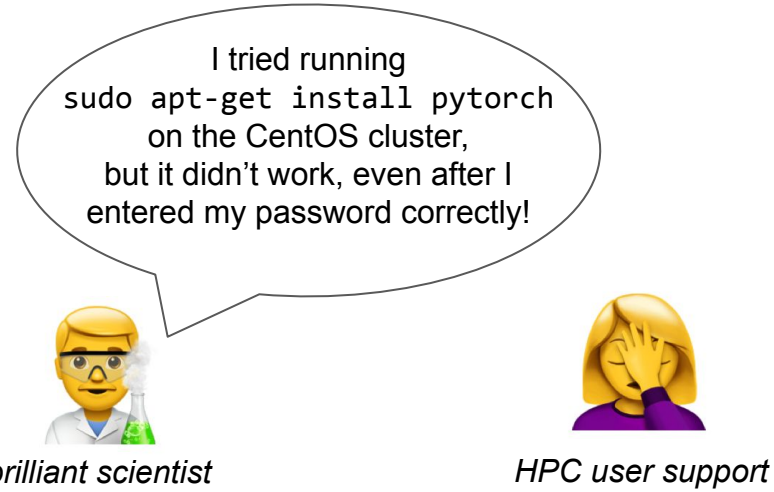
ugent.be/hpc vscentrum.be

Kenneth Hoste: Computer scientist from Belgium

- HPC system administrator + user support at Ghent University since Oct 2010
- BDFL of **EasyBuild** - tool to build & install **scientific software on HPC clusters**
- Active contributor to **EESSI**, partner in MultiXscale EuroHPC CoE
- Fan of open source software (FOSS), beers, and stickers
- "How To Make Package Managers Cry" talk at FOSDEM'18 (if you haven't seen it, you should!)

Scientific software is a different breed

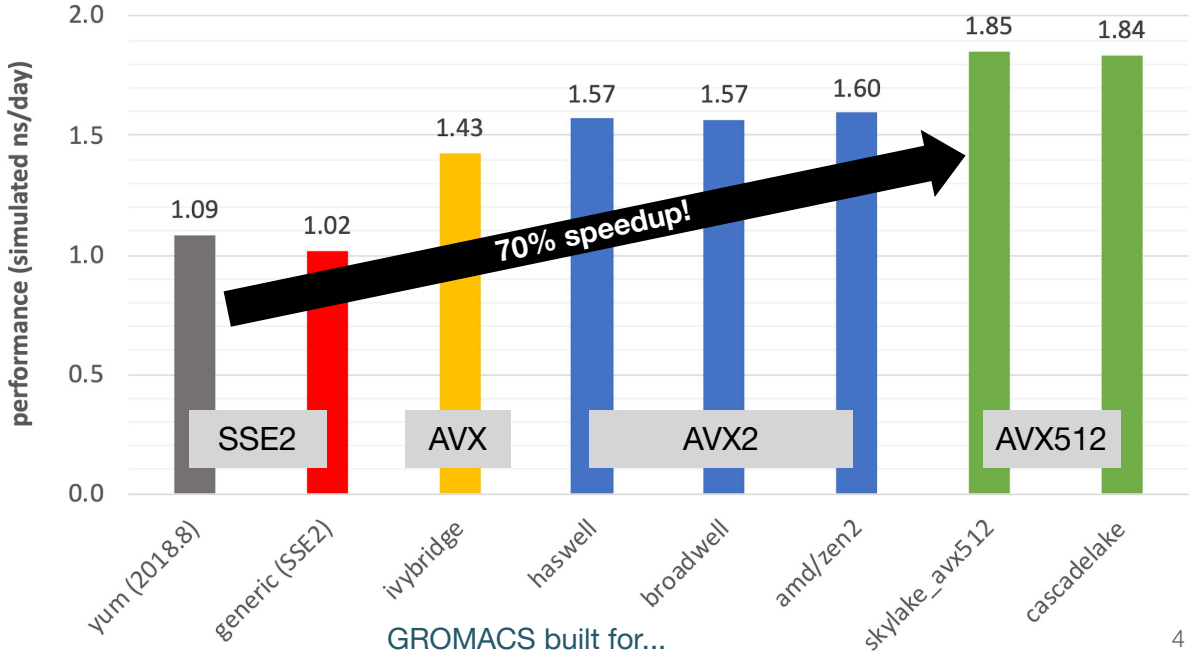
- Scientists may not be trained software engineers (and that's OK)
- They often need help to get the software installed properly (especially on HPC systems)
- **Standard packaging tools do not suffice**, we ~~want~~ need to **build from source**
- Scientific software should be compiled for system on which it will be used (performance!)



Optimized scientific software installations

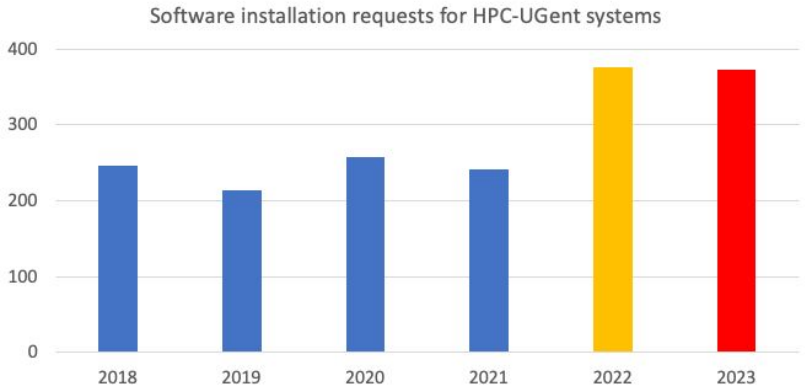
- Software should be optimized for the system it will run on
- Impact on performance is often significant for scientific software

- Example: GROMACS 2020.1 (PRACE benchmark, Test Case B)
- Metric: (simulated) ns/day, higher is better
- Test system: dual-socket Intel Xeon Gold 6420 (Cascade Lake, 2x18 cores)
- **Performance of different GROMACS binaries, on exact same hardware/OS**



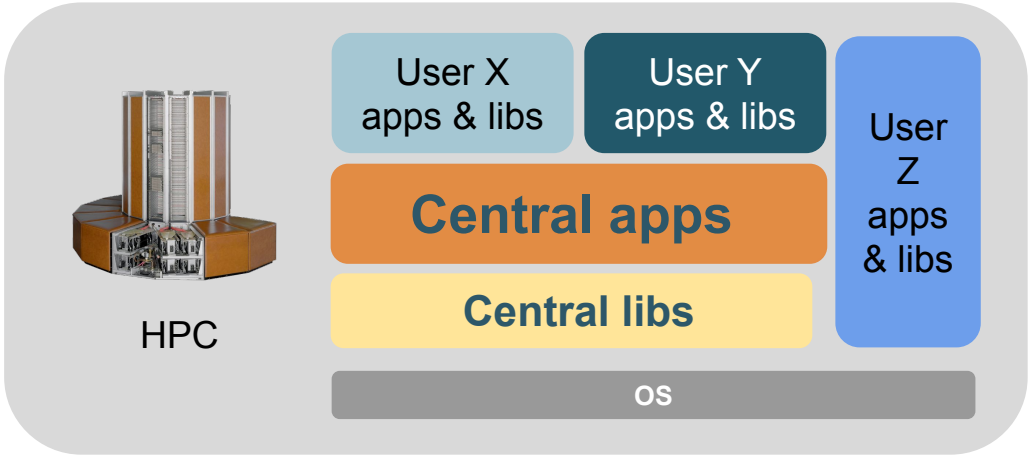
Landscape of scientific computing is changing

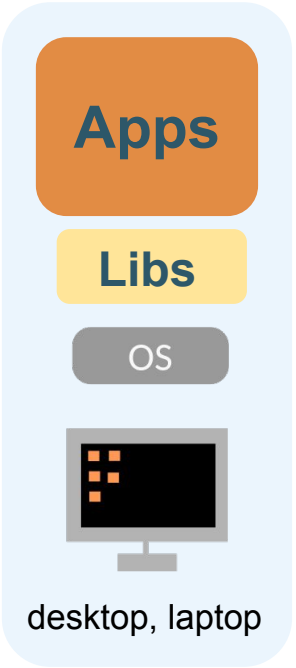
- **Explosion of available scientific software** applications (bioinformatics, AI, …)
- Increasing interest in **cloud** for scientific computing (flexibility!)
- **Increasing variety in processor (micro)architectures** beyond Intel & AMD:
  Arm is ~~coming~~ already here (see Fugaku, JUPITER, …), RISC-V is coming (soon?)
- Broader adoption of **accelerated computing**, beyond NVIDIA GPUs
- In strong contrast: available (wo)manpower **in HPC support teams is (still) limited**…

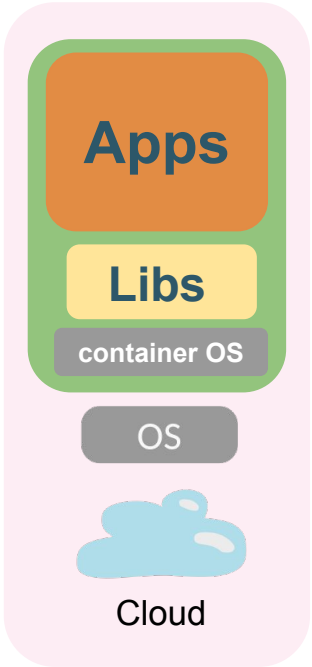


We need to collaborate more…

- **Too much software** for a single support team to handle
- Different systems (CPU, GPU, OS, …) => different problems
- Existing tools (EasyBuild, Spack) are **not sufficient anymore…**
- Lots of **duplicate work** across HPC sites and scientists
- **Diverse software stacks** across different platforms







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**

EESSI

EUROPEAN ENVIRONMENT FOR SCIENTIFIC SOFTWARE INSTALLATIONS

https://eessi.io

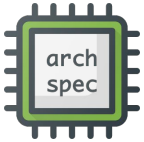
https://eessi.io/docs

ReFrame

Testing

Software layer

Optimized applications + dependencies



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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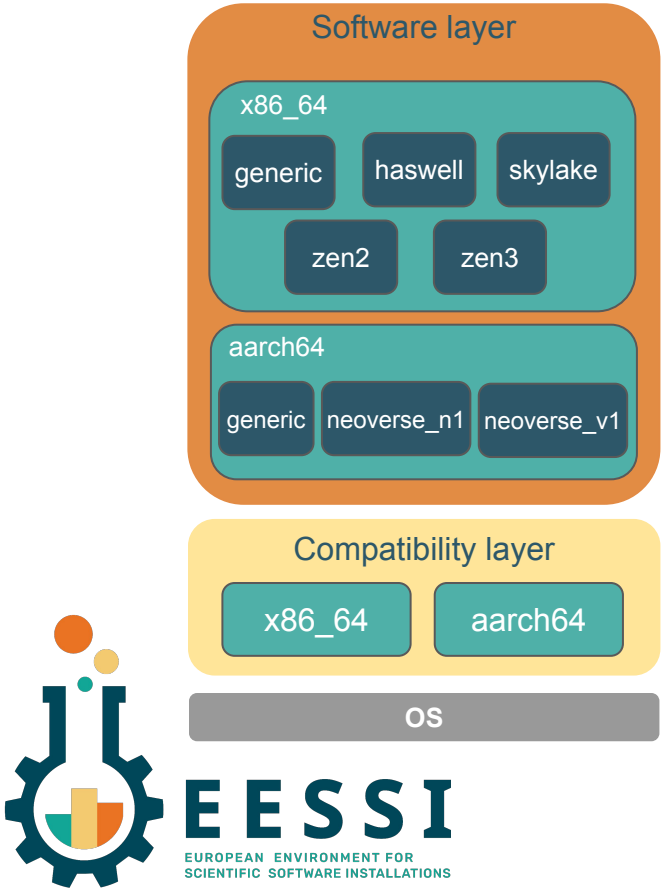
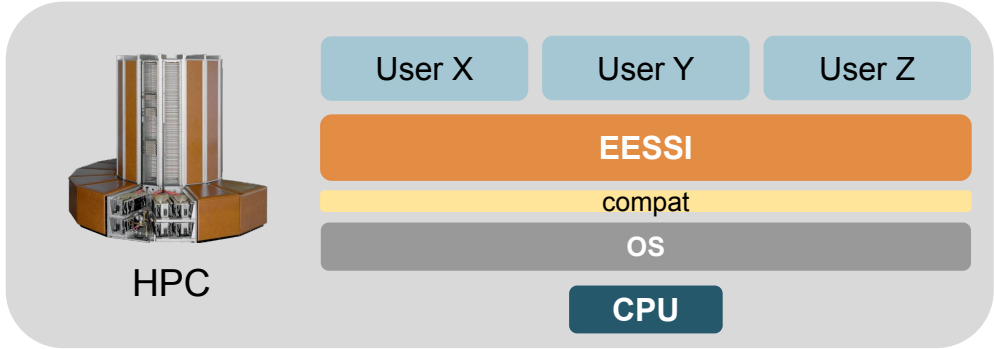
EUROPEAN ENVIRONMENT FOR SCIENTIFIC SOFTWARE INSTALLATIONS

EESSI to the rescue!





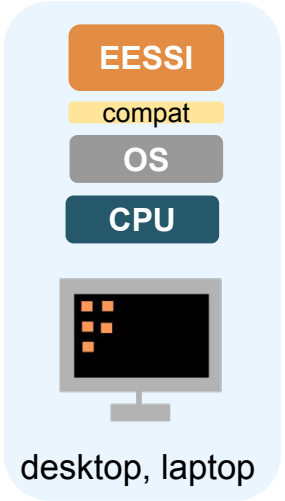
Shared repository of **(optimized)** scientific software **installations**

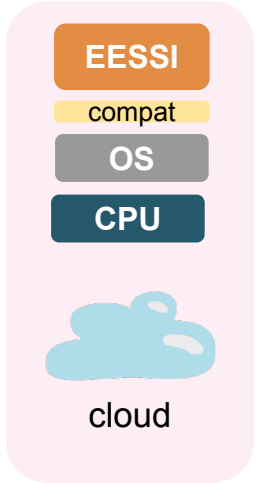
Same software stack everywhere!

eessi.io

eessi.io/docs

eessi.io/docs/support





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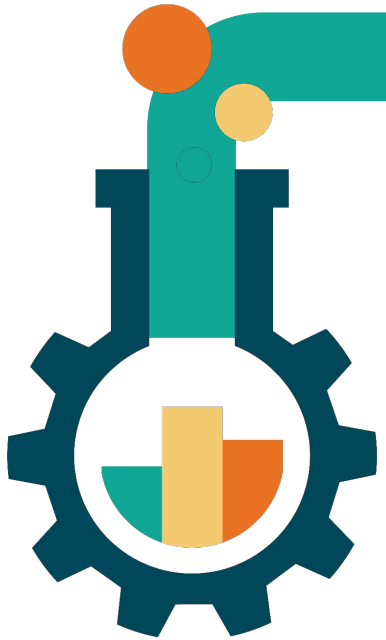
EESSI ingredients: filesystem layer



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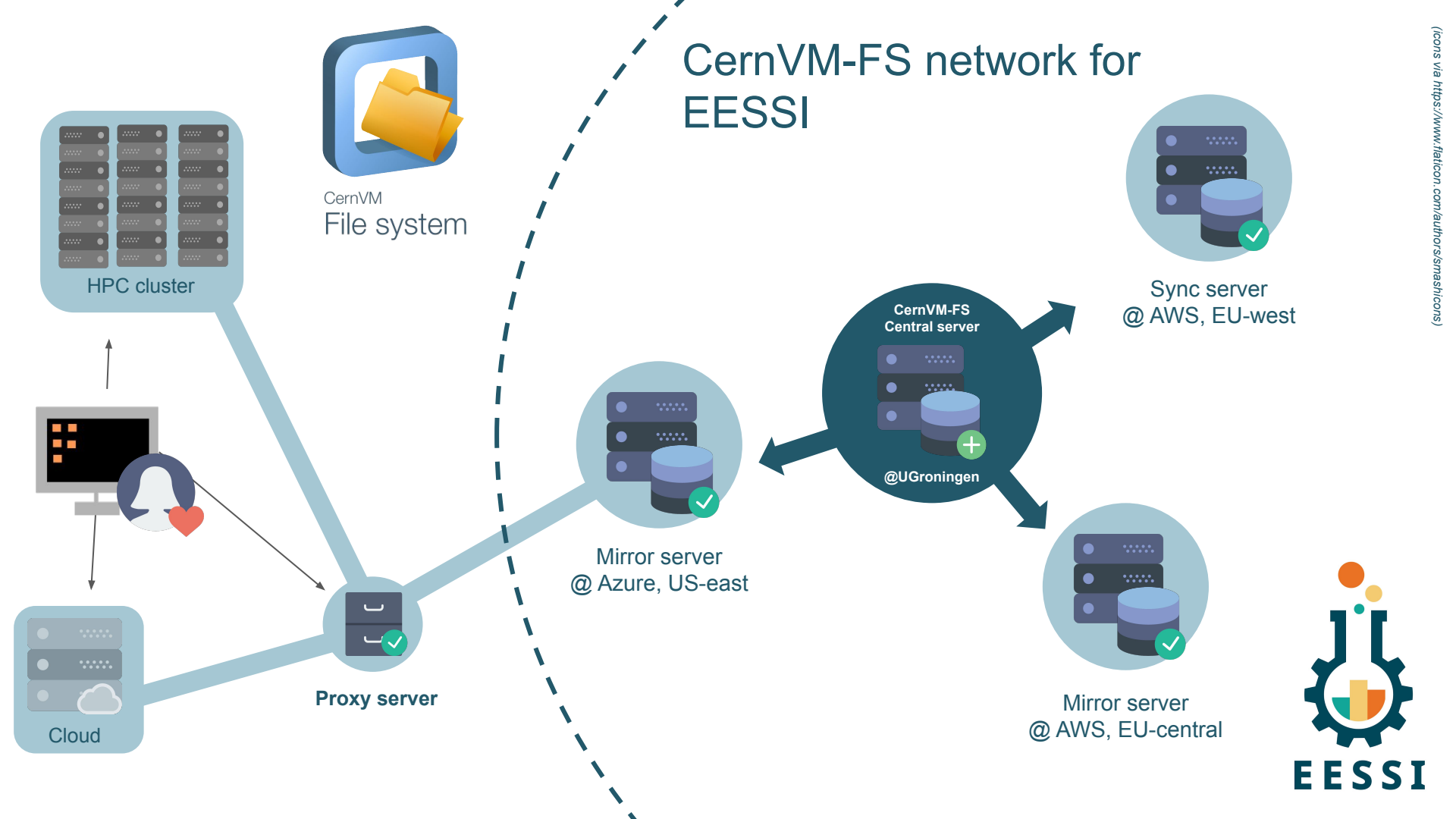
CernVM File system

Global distribution of software installations

https://cernvm.cern.ch/fs

Read-only network filesystem
"Streaming Scientific Software"

CernVM-FS network for EESSI

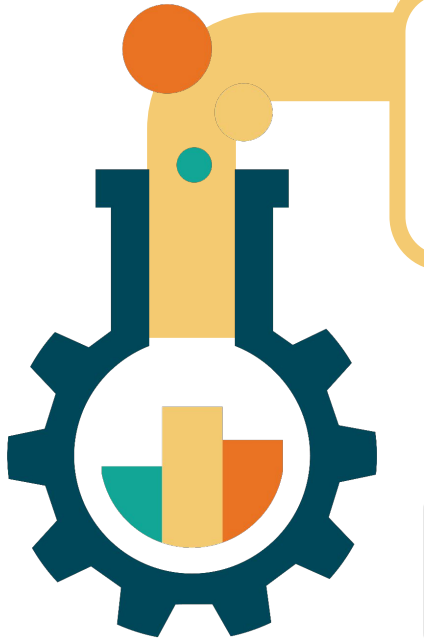


(icons via https://www.flaticon.com/authors/smashicons)

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 ingredients: compatibility layer



gentoo linux™

Abstraction away from host operating system

Similar to container images

"Containers without the containing"

CernVM File system

Global distribution of software installations

EESSI

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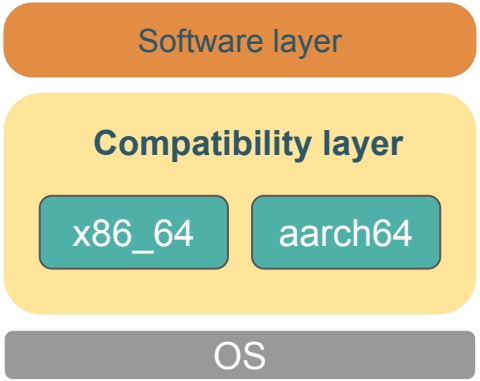
EESSI compatibility layer

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
```



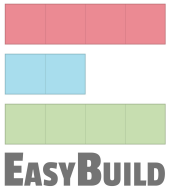
EESSI ingredients: software layer

Abstraction away from host operating system

Global distribution of software installations

EESSI

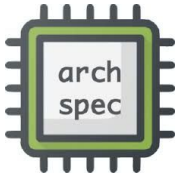
EUROPEAN ENVIRONMENT FOR SCIENTIFIC SOFTWARE INSTALLATIONS



Optimized software installations for specific CPU microarchitectures

Intuitive user interface

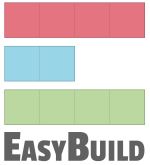
```
module avail,
module load, ...
```



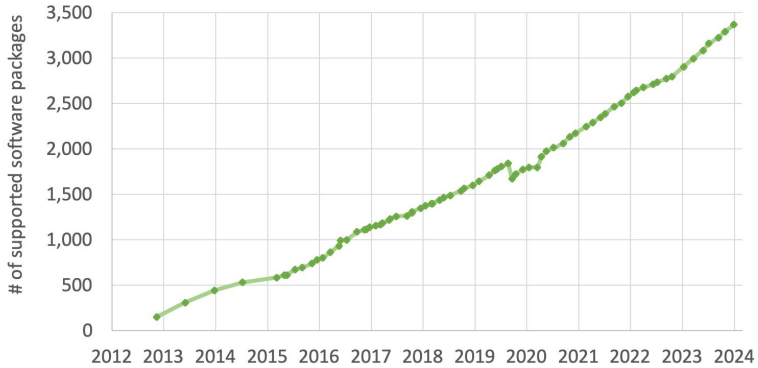
Automatic selection of best suited part of software stack for host CPU microarchitecture

EasyBuild (in a nutshell)

https://easybuild.io



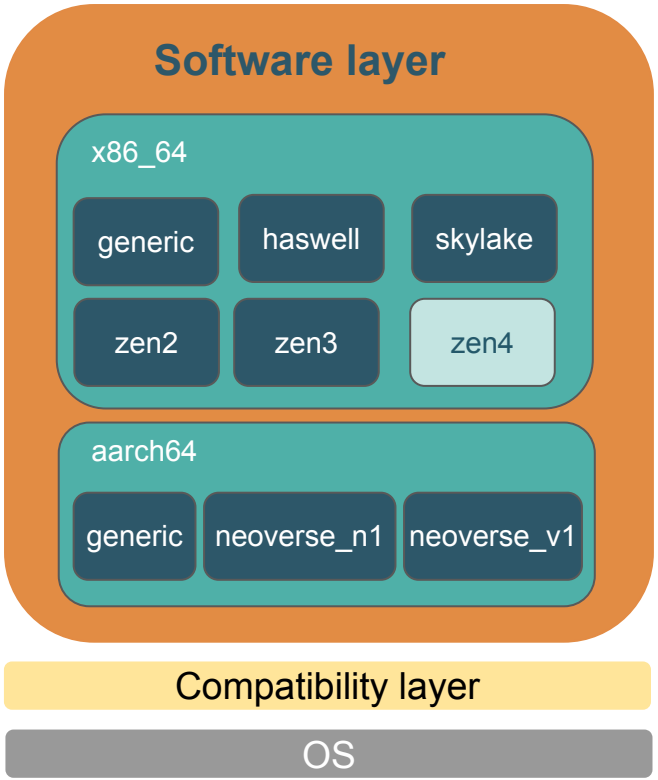
- EasyBuild is a tool to make **installing (scientific) software on HPC systems** easier
- **Building from source** + optimizing for specific CPU is strongly preferred (performance!)
- Created in 2009 by HPC-UGent team, open source (GPLv2) since 2012
- Now a **world-wide community** (> 400 unique contributors, close to 3,000 PRs per year)
- ~3,500 different software projects supported (excl. versions) + ~2,000 “extensions”



Software layer

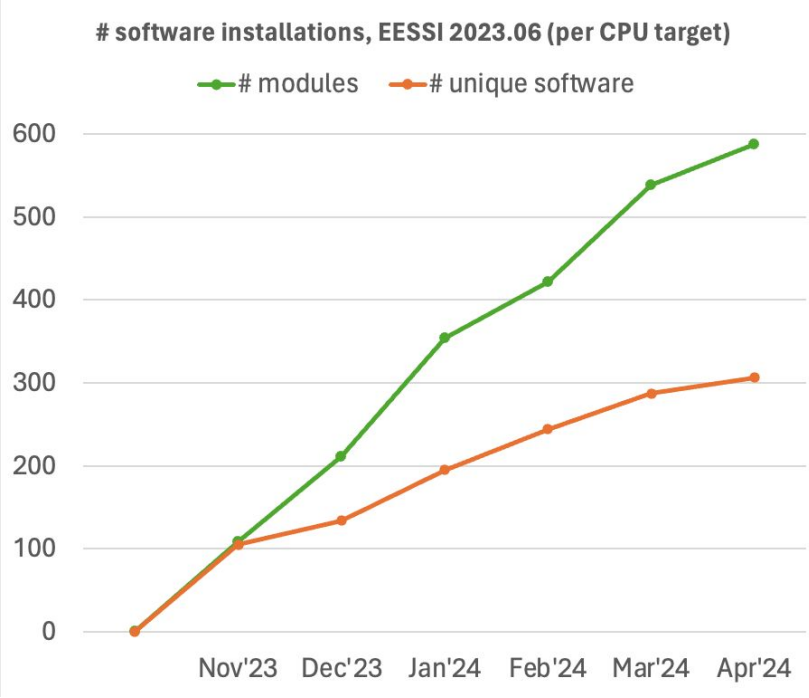
github.com/EESSI/software-layer

- 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

- ~600 software software installations available per CPU target, and increasing every day
  - Including ESPResSo, GROMACS, LAMMPS, OpenFOAM, PyTorch, R, QuantumESPRESSO, TensorFlow, WRF
  - eessi.io/docs/available_software (coming soon!)
- Includes (**but is not limited to!**) applications specific to the MultiXscale CoE
- Focus on recent compiler toolchains: currently targeting 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
```

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

Using EESSI

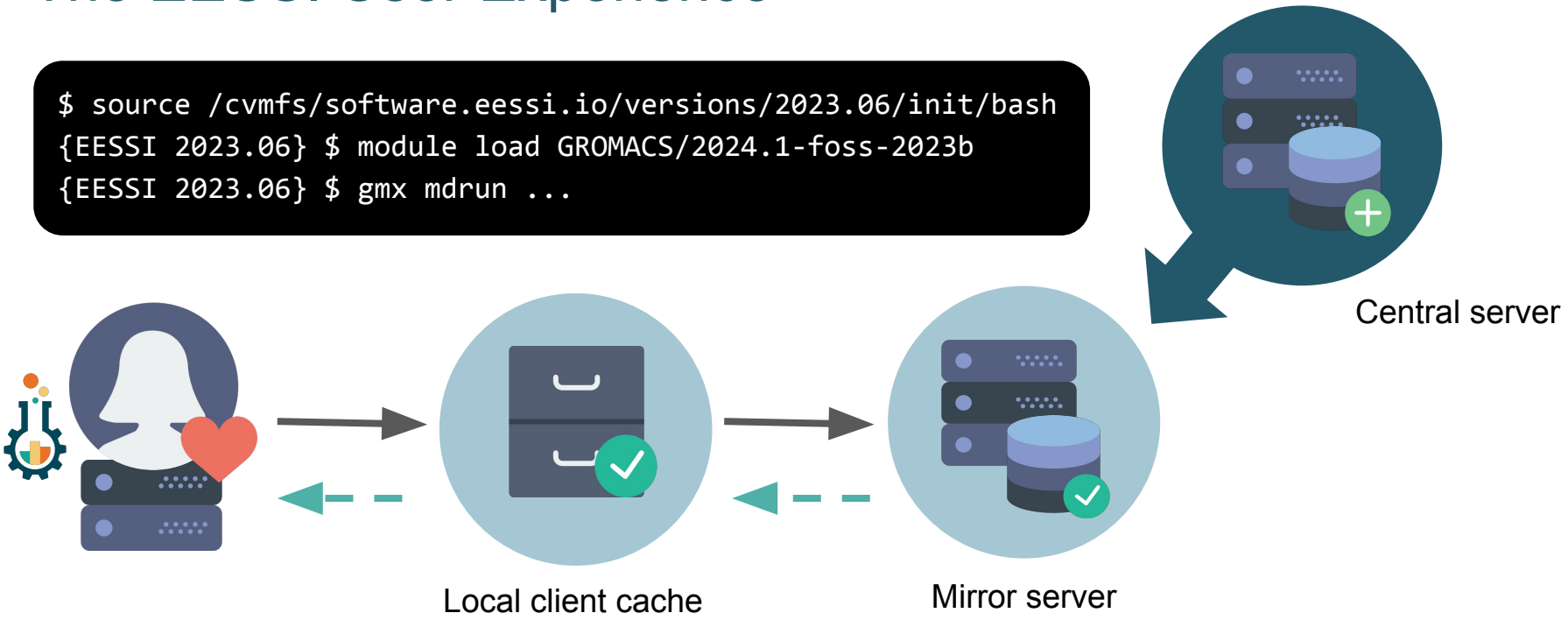
eessi.io/docs/using_eessi/eessi_demos

```
/cvmfs/software.eessi.io/versions/2023.06/software
`-- linux
    |-- aarch64
    |   |-- generic
    |   |-- neoverse_n1
    |   `-- neoverse_v1
    |       |-- modules
    |       `-- software
    `-- x86_64
        |-- amd
        |   |-- zen2
        |   |-- zen3
        |   `-- zen4
        |-- generic
        `-- intel
            |-- haswell
            `-- skylake_avx512
```

```
$ source /cvmfs/software.eessi.io/versions/2023.06/init/bash
Found EESSI pilot repo @
/cvmfs/software.eessi.io/versions/2023.06!
archdetect says aarch64/neoverse_v1
Using aarch64/neoverse_v1 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/aarch64
/neoverse_v1/software/R/4.3.2-gfbf-2023a/bin/R

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

The EESSI User Experience

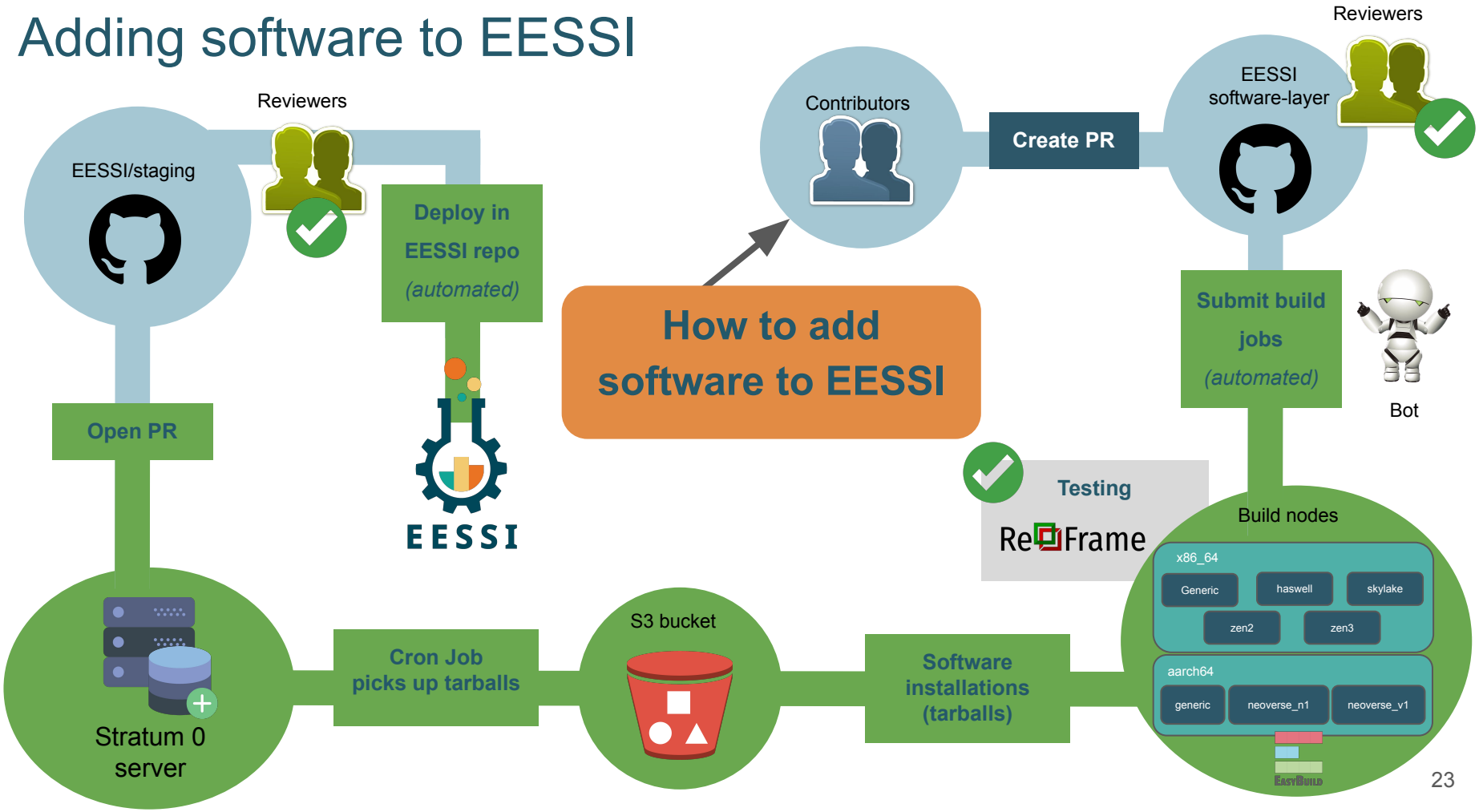
```
$ source /cvmfs/software.eessi.io/versions/2023.06/init/bash
{EESSI 2023.06} $ module load GROMACS/2024.1-foss-2023b
{EESSI 2023.06} $ gmx mdrun ...
```



EESSI provides **on-demand streaming**

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

Adding software to EESSI



EESSI test suite

ReFrame

eessi.io/docs/test-suite

EESSI

- Ensure quality of the software installations provided by EESSI
- A suite of **portable tests** for scientific software, using ReFrame
- Version 0.2.0 includes tests for GROMACS, TensorFlow, OSU Micro Benchmarks
- WIP: tests for LAMMPS, QuantumESPRESSO, CP2K, OpenFOAM, ESPResSo, PyTorch
- See also MultiXscale deliverable D1.2 “**Plan for the design of a portable test suite**” https://zenodo.org/records/10451718

Problems we have found through software testing (1/2)

Hang/crash in Open MPI's `smcuda` Byte Transport Layer (BTL) component

- See https://gitlab.com/eessi/support/-/issues/41
- Upstream issue: https://github.com/open-mpi/ompi/issues/12270
- Causes hanging or failing tests for FFTW, OpenFOAM, ESPResSo, …
- Only happens on Arm Neoverse V1 (AWS Graviton 3)
- Fixed by Luke Robinson (AWS), see https://github.com/open-mpi/ompi/pull/12338
- Fix will be included in upcoming Open MPI release (v4.1.7+)
- Patch already applied in Open MPI installations included in EESSI 2023.06

Problems we have found through software testing (2/2)

Failing tests in GROMACS test suite

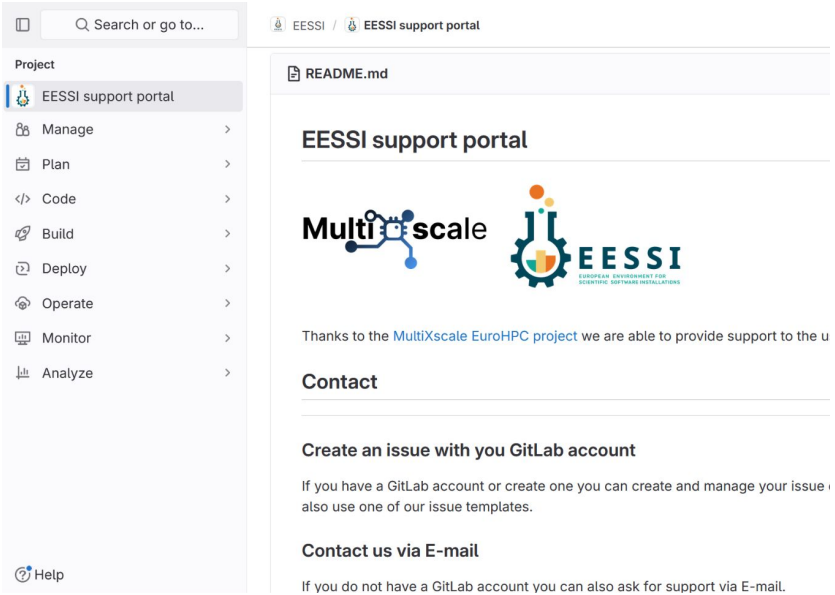
- See https://gitlab.com/eessi/support/-/issues/47
- Filesystem race when running tests concurrently (GROMACS PR #4066)
- **Bug in SVE support, leading to (very) wrong results for several tests**
  - See https://gitlab.com/gromacs/gromacs/-/issues/5057
  - Works fine on A64FX (512-bit SVE), but **problem on Neoverse V1 (256-bit SVE)**
  - WIP fix in https://gitlab.com/gromacs/gromacs/-/merge_requests/4299
  - Will be fixed in upcoming GROMACS release (2024.2?)
  - Workaround for GROMACS 2024.1 in EESSI: use `-DGMX_SIMD=ARM_NEON_ASIMD`

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

Multiscale

www.multixscale.eu

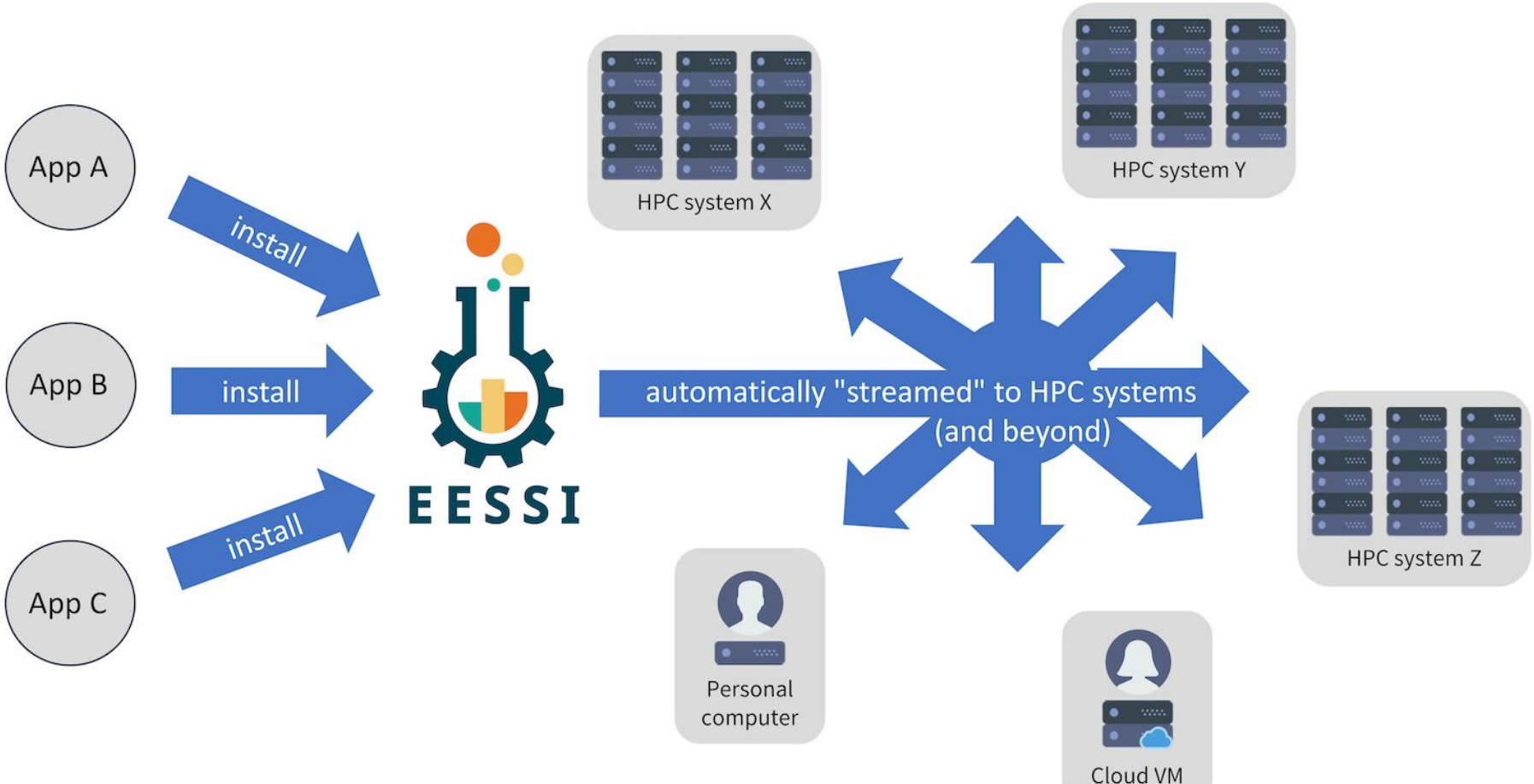
EuroHPC Joint Undertaking

- EuroHPC Centre of Excellence: 4 year project (2023-2026), €6M budget (50% for EESSI)
- Collaboration between EESSI and CECAM: total of 16 partners (academic + industry)
- EESSI focuses on technical aspects: providing a shared stack of scientific software
- Scientific target: multiscale simulations with 3 key use cases
  - Helicopter design and certification for civil transport
  - Battery applications to support the sustainable energy transition
  - Ultrasound for non-invasive diagnostics and biomedical applications

Kemijski inštitut · Universitat de Barcelona · Universität Stuttgart · Universitas Bergensis · Sorbonne Université · Université de Toulouse · Consiglio Nazionale delle Ricerche · Max-Planck-Gesellschaft · HPC Now! · University of Groningen · SURF · Jülich Forschungszentrum · Ghent University · BSC Barcelona Supercomputing Center · Leonardo · iit Istituto Italiano di Tecnologia

The role of EESSI in 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!**

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