Supporting cutting edge development of LAMMPS with

Helena Vela Beltran - Do IT Now! (Spain)

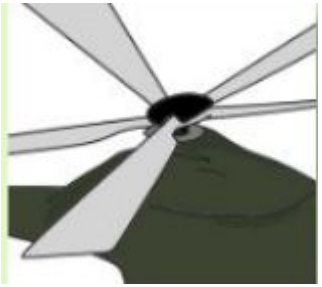
Readiness of HPC Extreme-scale Applications (2nd Edition)

ISC25 - Hamburg - 13/06/25

Multiscale

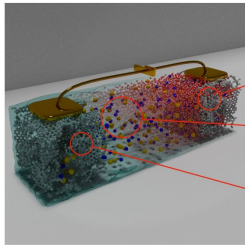
EuroHPC
Joint Undertaking

MultiXScale Centre-of-Excellence in a nutshell



Collaboration between EESSI and CECAM (total of 16 partners)

- EESSI primarily addresses technical aspects
- CECAM network provides scientific expertise



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

MultiXScale targets

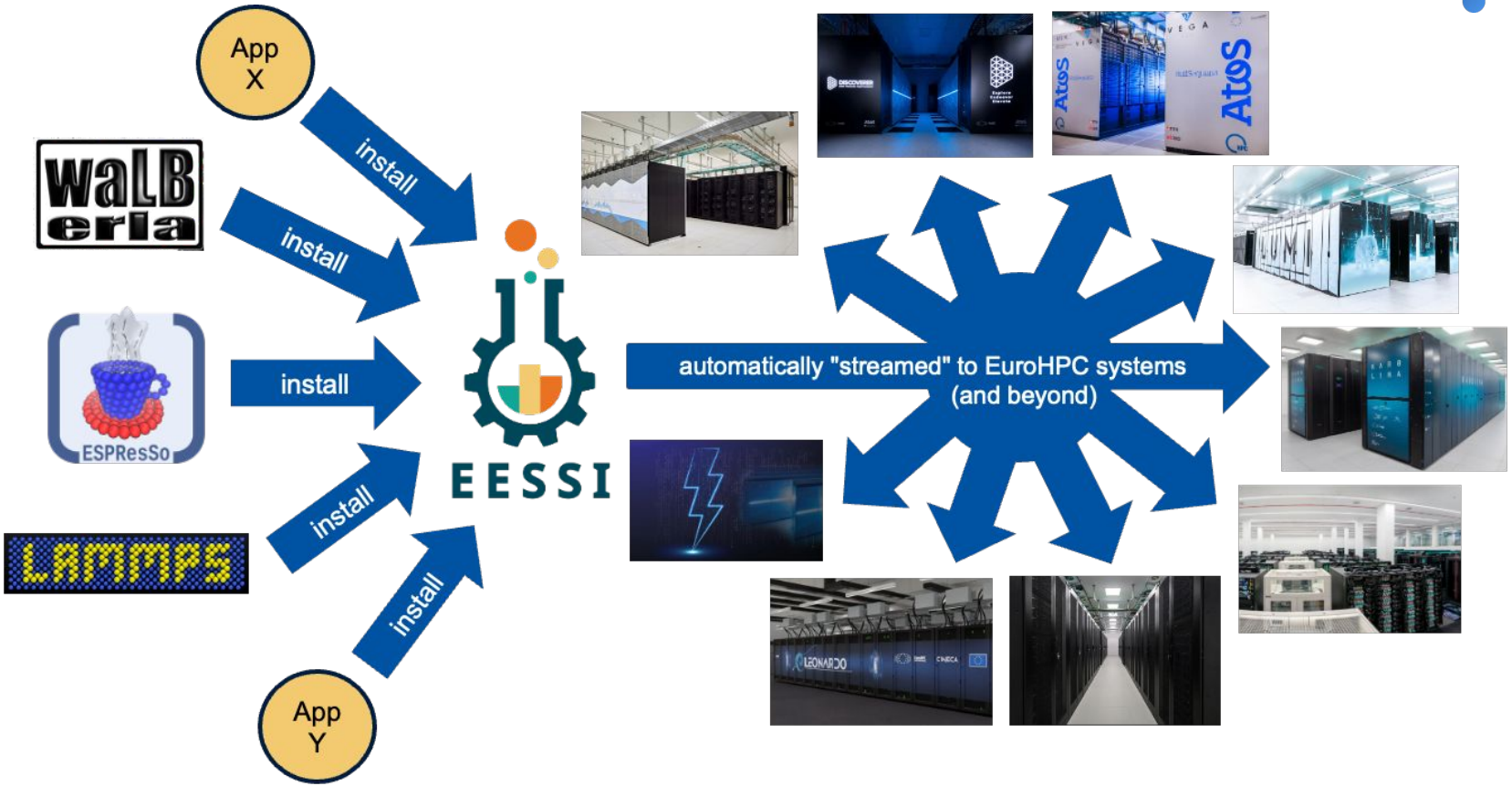
- To improve the
  - **Performance** of those codes on EuroHPC hardware (and beyond)
  - **Portability** of the codes and workflows from laptop to server to cloud to HPC
  - **Productivity** of scientists who develop and/or use open source codes
- Advances the transition towards use of exascale resources for the community

EESSI
EUROPEAN ENVIRONMENT FOR SCIENTIFIC SOFTWARE INSTALLATIONS

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, …

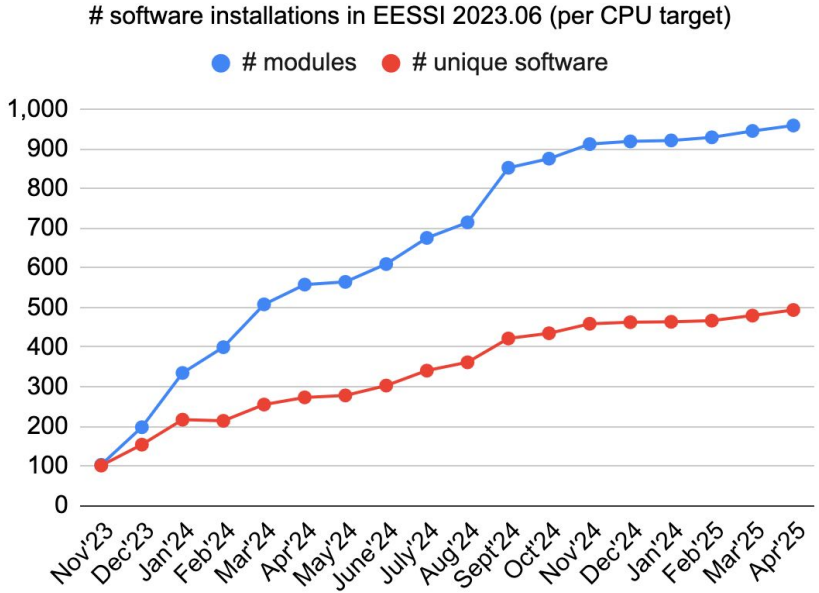
EESSI as a shared software stack



Overview of available software

Currently ~960 software installations available per CPU target via software.eessi.io CernVM-FS repository; increasing every week

- Almost 500 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
- Using recent compiler toolchains: currently focusing on `foss/2023a` and `foss/2023b`



Key differences

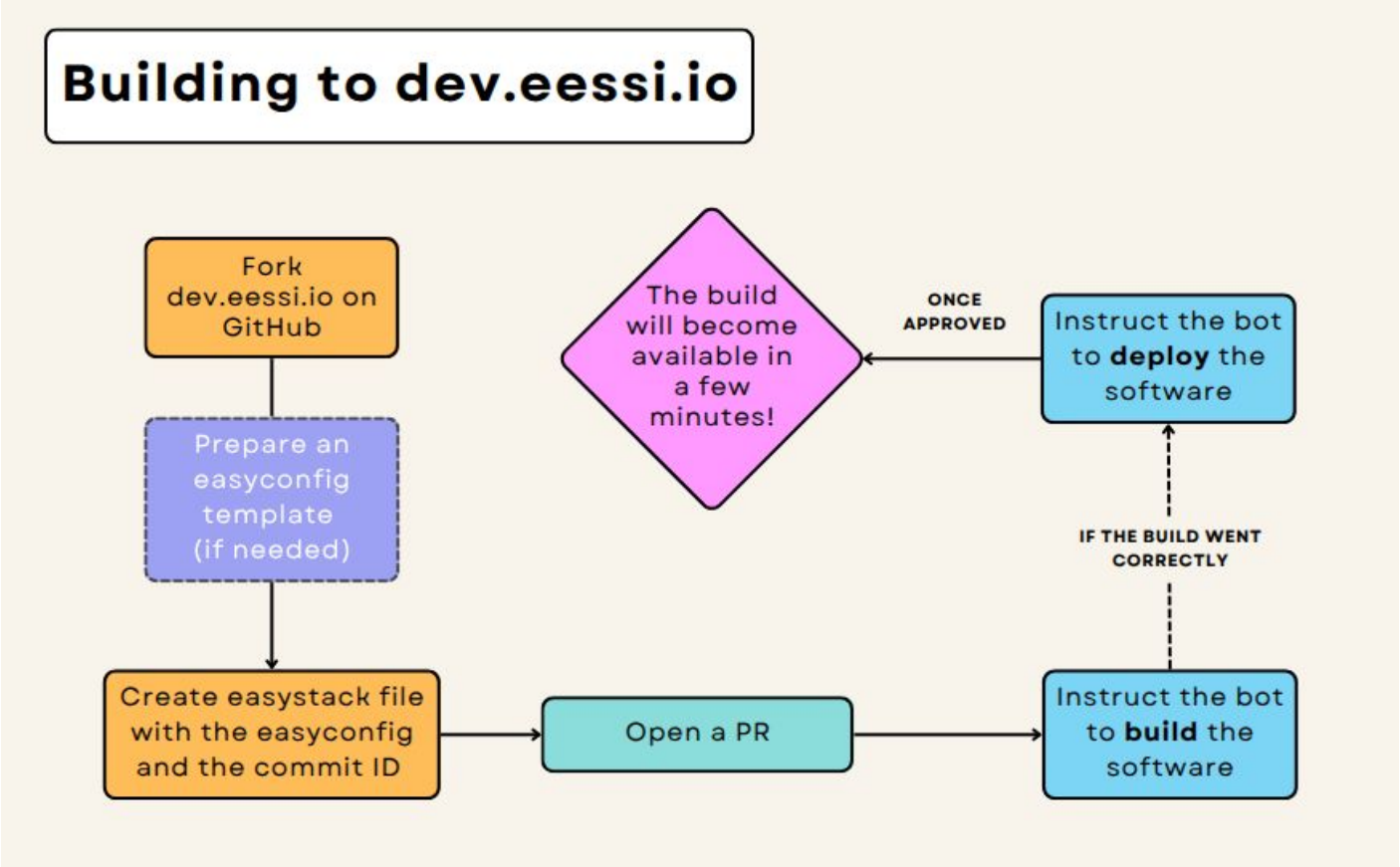
software.eessi.io (production)

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

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/

The developers workflow



Example: Running LAMMPS in a Slurm job script with dev.eessi.io


```
#!/bin/bash
#SBATCH --job-name="EESSI_Demo_LAMMPS_lj"
#SBATCH --ntasks=4
#SBATCH --ntasks-per-node=4
#SBATCH --cpus-per-task=1
#SBATCH --output=EESSI_demo.out
#SBATCH --error=EESSI_demo.err
#SBATCH --time=0:30:0
#SBATCH --partition=cpu_rome

# CPU microarchitecture is automatically detected by EESSI init script
source /cvmfs/software.eessi.io/versions/2023.06/init/bash
module use /cvmfs/dev.eessi.io/versions/2023.06/software/linux/x86_64/amd/zen2/modules/all
module load LAMMPS/570c9d190fee556c62e5bd0a9c6797c4dffcc271-foss-2023a-kokkos-dev_OBMD
mkdir /tmp/$USER && cd /tmp/$USER
curl -o in.lj https://raw.githubusercontent.com/lammps/lammps/refs/heads/develop/bench/in.lj
export OMP_NUM_THREADS=1
mpirun -np 4 lmp -in in.lj
rm -r /tmp/$USER
```

Supporting the development of the coupling of:

EESSI

\+ Additional libraries for LAMMPS

Developers said :D

" So far the EESSI infrastructure has helped me in two ways. Firstly it allows me to utilize many of the required modules to actually compile and run both of the simulation codes on any machine (either a laptop or an HPC), which really accelerates the workflow to develop the actual code without dealing with the installation or compilation of the needed software. Secondly we have already used the EESSI repository to use our extended LAMMPS code in a hackathon this winter, which went really smoothly. This allowed the participants to directly use our software by just a couple of lines "

"The value dev.eessi.io brings to us and EESSI is really in the help of bringing our patch to users."

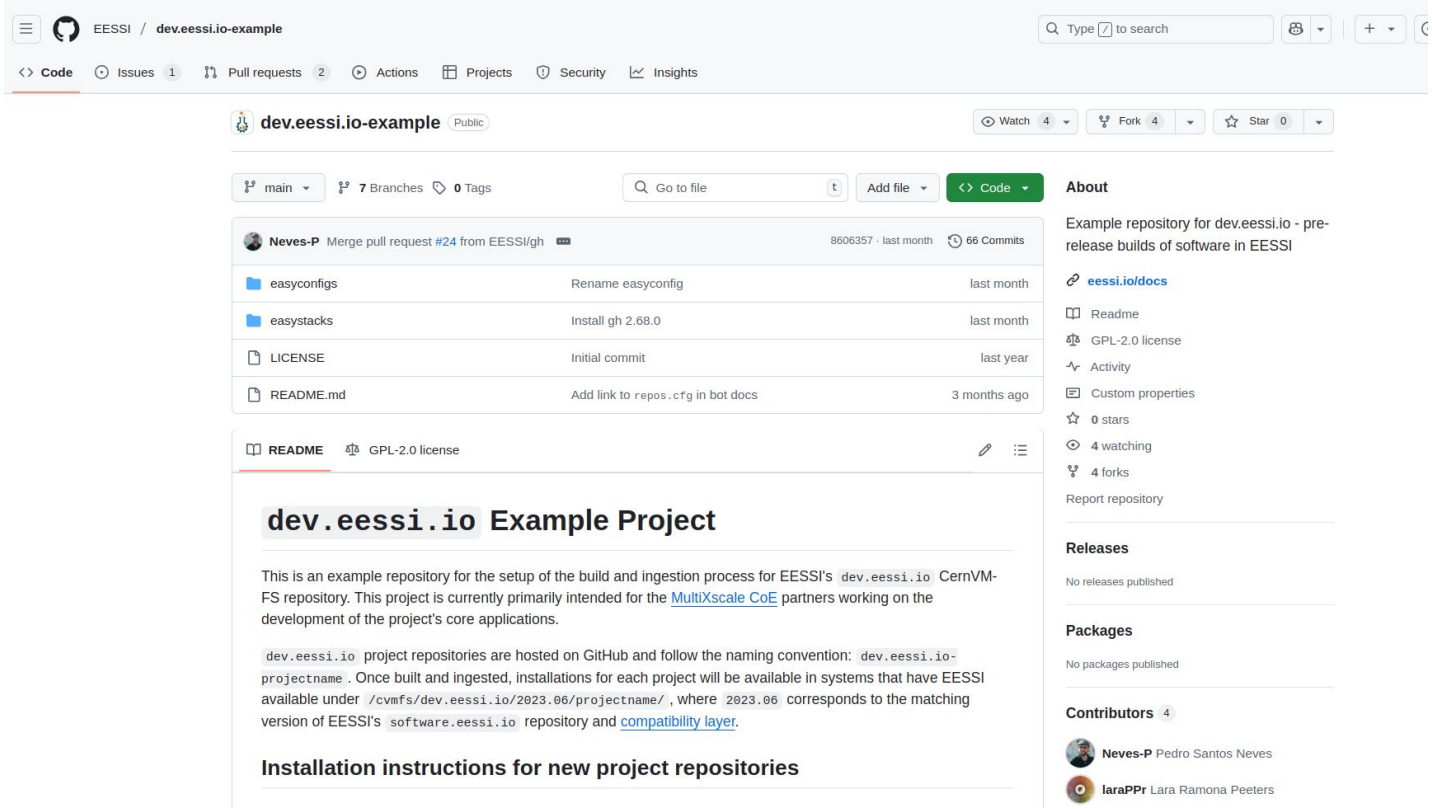
Multiscale

And what about exascale?

EESSI (and therefore dev.eessi.io) will be available on JUPITER!

- The work is done, we just need the machine to be in production!
- GRACE Hopper software stack available in EESSI

Take a look by yourself



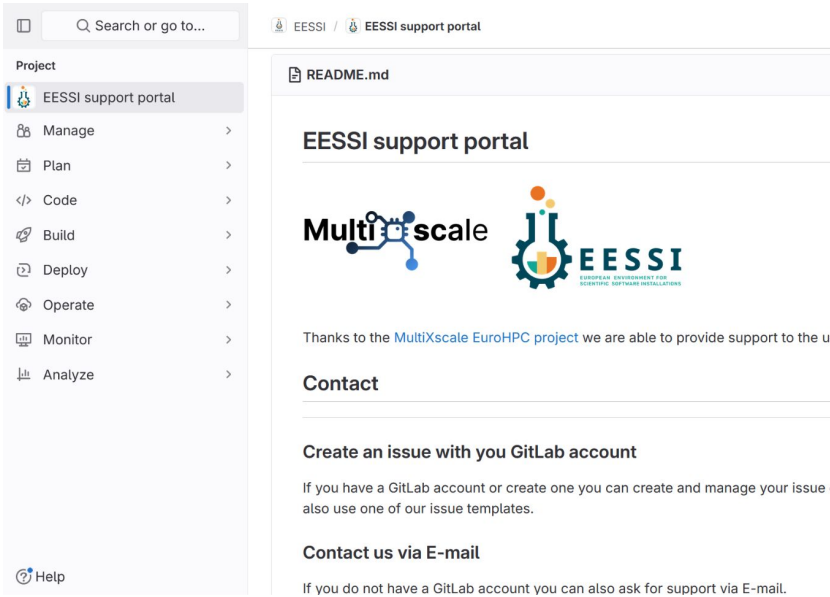
https://github.com/EESSI/dev.eessi.io-example

Support for installing, using, contributing to EESSI

GitLab

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 Multiscale

Richard

The dev.eessi.io tiger team + LAMMPS developers :)

- *Lara Peeters (@laraPPr)*
- *Kenneth Hoste (@boegel)*
- *Alan O'Cais (@ocaisa)*
- *Pedro Santos (@neves-p)*
- *Bob Dröge (@bedroge)*
- *Richard Topouchian (@Richard-T)*
- *Thomas Röblitz (@trz42)*
- *Tilen Potisk (NIC)*
- *Rodrigo Bartolomeu (JSC)*
- *Yannic Kitten (JSC)*

Website: eessi.io

GitHub: github.com/eessi

Documentation: eessi.io/docs

Blog: eessi.io/docs/blog

Join the EESSI Slack

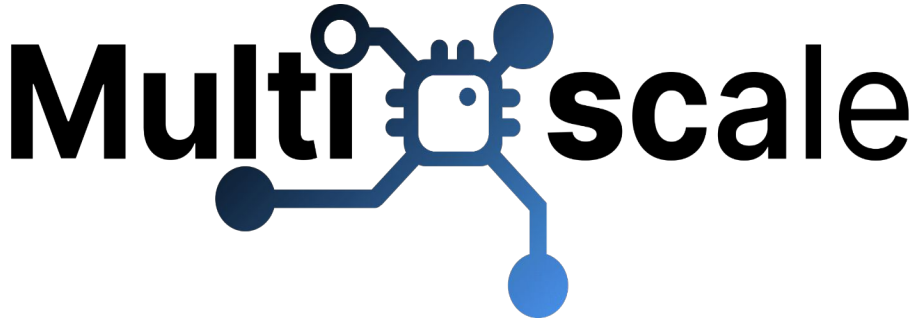
YouTube channel: youtube.com/@eessi_community

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)

Richard



Co-funded by the European Union

EuroHPC Joint Undertaking

Web page: multixscale.eu

Facebook: MultiXscale

Twitter: @MultiXscale

LinkedIn: MultiXscale

BlueSky: MultiXscale

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 Centro Nacional de Supercomputación

LEONARDO

iit ISTITUTO ITALIANO DI TECNOLOGIA

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.

Webinar series: Different aspects of EESSI

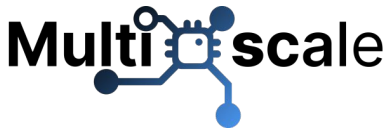
5 Mondays in a row May-June 2025

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

Watch the live recordings!→

Collaboration with software developers + experts

- A central software stack by/for the community opens new doors…
- We can **work with software developers/experts** to verify the installation
  - Check how installation is configured and built
  - Help to verify whether software is functional for different use cases
  - Show us how to do extensive testing of their software
  - Evaluate performance of the software, enable performance monitoring
  - *"Approved by developers"* stamp for major applications included in EESSI
- Relieve software developers from burden of getting their software installed
  - Remove need to provide pre-built binary packages?
- Developers can also leverage EESSI themselves: dependencies, CI, …



Richard