



university of
groningen

center for
information technology



E E S S I

EUROPEAN ENVIRONMENT FOR
SCIENTIFIC SOFTWARE INSTALLATIONS

Keeping it Simple, Keeping it

Updates from 2023-2024



Pedro Santos Neves
SURF Advanced Computing User Day
Utrecht 12/12/2024



EuroHPC
Joint Undertaking

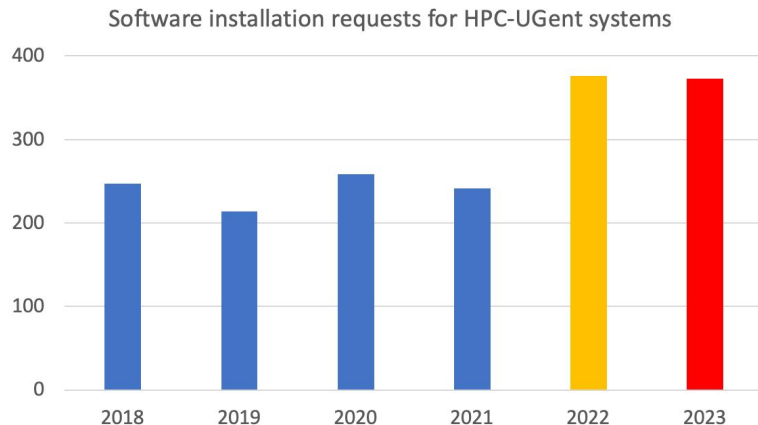
Contents



- Brief introduction to EESSI and MultiXscale
- GPU and RISC-V builds
- Building on top of EESSI - EESSI-extend
- Development repository - dev.eessi.io
- EESSI CI/CD
- Assorted news

The changing landscape of scientific computing

- **Explosion of available scientific software** applications (bioinformatics, AI boom, ...)
- 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](#), [DEUCALION](#)...), RISC-V is coming (soon?)
- In strong contrast: available (wo)manpower in **HPC support teams is (still) limited...**



EESSI in a nutshell



- European Environment for Scientific Software Installations (EESSI)
- **Shared repository of (optimized!) scientific software installations**
- Uniform way of providing software to users, regardless of the system they use!
- Should work on any Linux OS (+ WSL, macOS via Lima) and system architecture
- From laptops and personal workstations to HPC clusters and cloud
- Support for different CPU (micro)architectures, interconnects, GPUs, etc.
- **Focus on performance, automation, testing, collaboration**

<https://eessi.io>

<https://eessi.io/docs>

Try it out!

https://www.eessi.io/docs/getting_access/is_eessi_accessible/

Major goals of EESSI

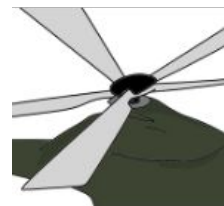


- **Avoid duplicate work** (for researchers, HPC support teams, sysadmins, ...)
 - Tools that automate software installation process (EasyBuild, Spack) are not sufficient anymore
 - Go beyond sharing build recipes => work towards a shared software stack
- Providing a truly **uniform software stack**
 - Use the (exact) same software environment everywhere
 - **Without sacrificing performance** for “mobility of compute” (like is typically done with containers/conda)
- Facilitate HPC training, development of (scientific) software, ...

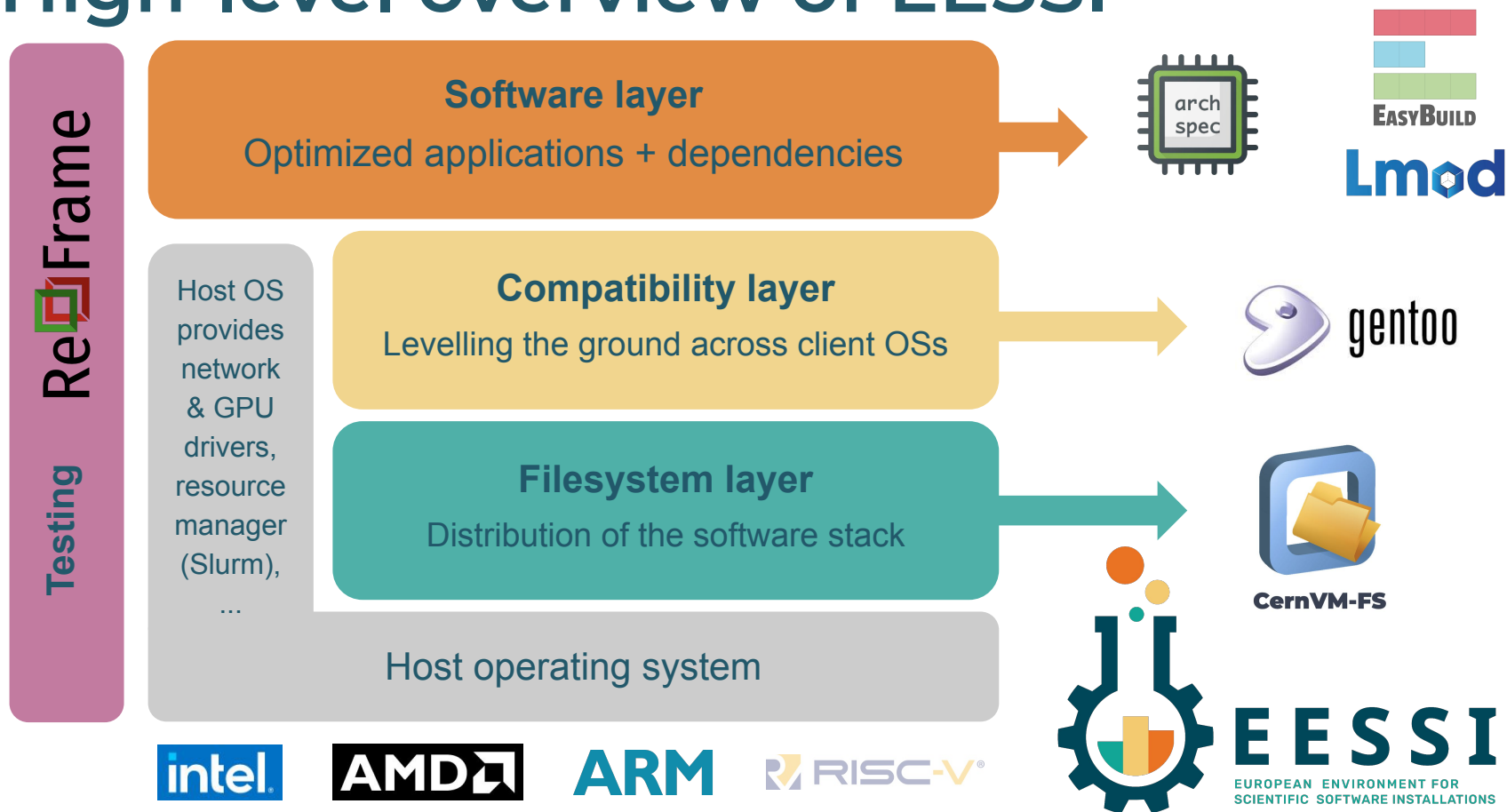
MultiXscale Centre-of-Excellence in a nutshell



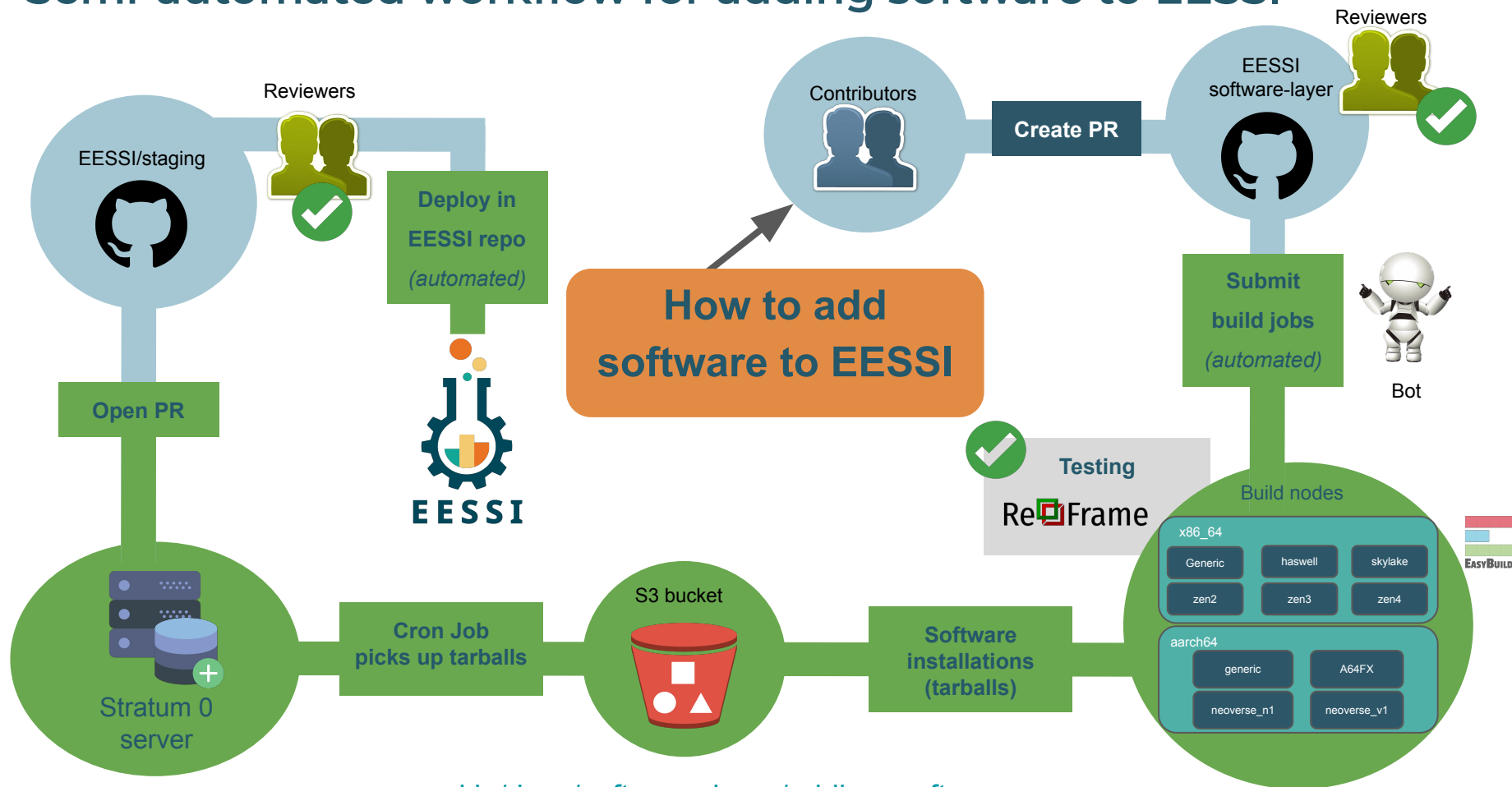
- 4-year project (started in Jan 2023), ~€6M budget
- Collaboration between EESSI and CECAM (total of 16 partners)
 - **EESSI** primarily addresses technical aspects
 - **CECAM** network provides scientific expertise
- Scientific target: multiscale simulations with 3 key use cases
 - Helicopter design and certification for civil transport
 - Battery applications to support the sustainable energy transition
 - Ultrasound for non-invasive diagnostics and biomedical applications
- More info: <https://multixscale.eu>



High-level overview of EESSI



Semi-automated workflow for adding software to EESSI

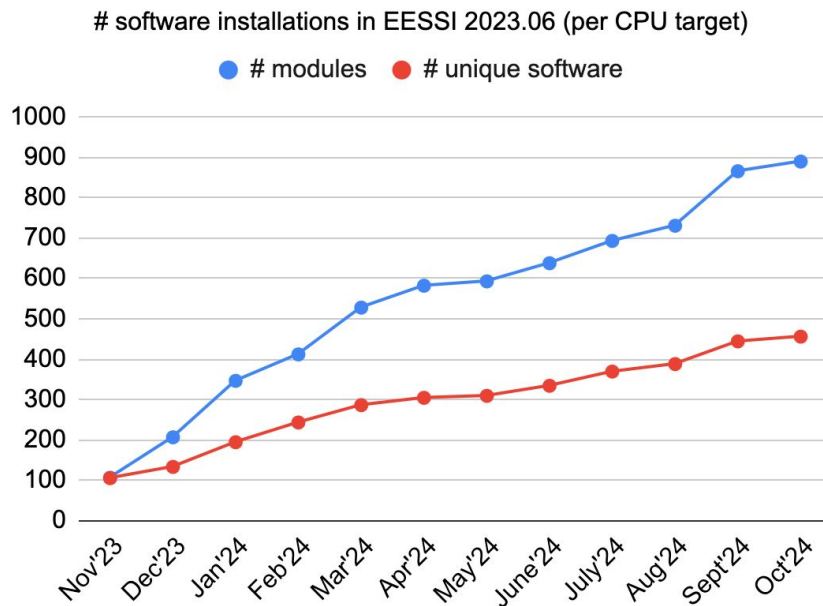


Overview of available software



Currently ~900 software software installations available
per CPU target via 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
- Using recent compiler toolchains: currently focusing on `foss/2023a` and `foss/2023b`



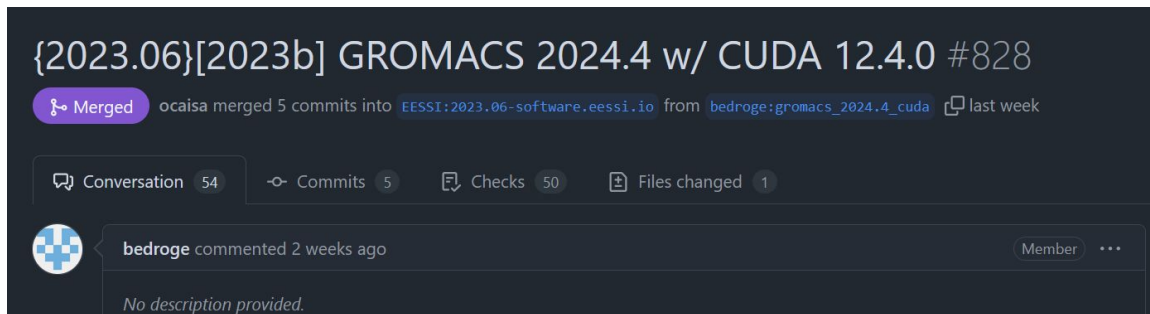


Highlights from 2023/2024

GPU and RISC-V support



- riscv.eessi.io repository with generic builds
 - Compatibility layer + some software (GROMACS, R, etc)
 - Work in progress, but already accessible!
 - <https://www.eessi.io/docs/repositories/riscv.eessi.io/>
- First GPU builds of scientific software on AMD Rome (zen2) with NVIDIA CC 8.0 (A100) - Systems are quite heterogeneous





Building on top of EESSI - EESSI-extend

- **EESSI-extend module**
 - Simple way expand user or site's software stack
 - **module load EESSI-extend/2023.06-easybuild**
 - Automatically build against compatibility layer
 - Other EESSI modules picked up as dependencies
- **Can install in:**
 - User space - **\$EESSI_USER_INSTALL**
 - Shared project directory - **\$EESSI_PROJECT_INSTALL**
 - Restricted directories by sysadmins - **\$EESSI_SITE_INSTALL**

https://www.eessi.io/docs/using_eessi/building_on_eessi/



Building on top of EESSI - EESSI-extend

- **`$EESSI_SITE_INSTALL`**
 - HPC site managers can set `$EESSI_SITE_SOFTWARE_PATH` where software built on top of EESSI will be installed
 - Available to all users
- **`$EESSI_PROJECT_INSTALL`**
 - A directory shared by some users in `$EESSI_PROJECT_INSTALL`
- **`$EESSI_USER_INSTALL`**
 - Default if envvar is not set on loading
 - Let end-users build their software on top of EESSI for themselves

Development repository - dev.eessi.io

- Let developers deploy and test their pre-production code
- Similar CernVM-FS repository:
 - `/cvmfs/dev.eessi.io/version/project`
 - Similar infrastructure:
 - GitHub repository to track builds
 - CI on PRs
 - Bot instance that builds, runs tests, ingests software (semi-)automatically

dev.eessi.io - Key differences

software.eessi.io

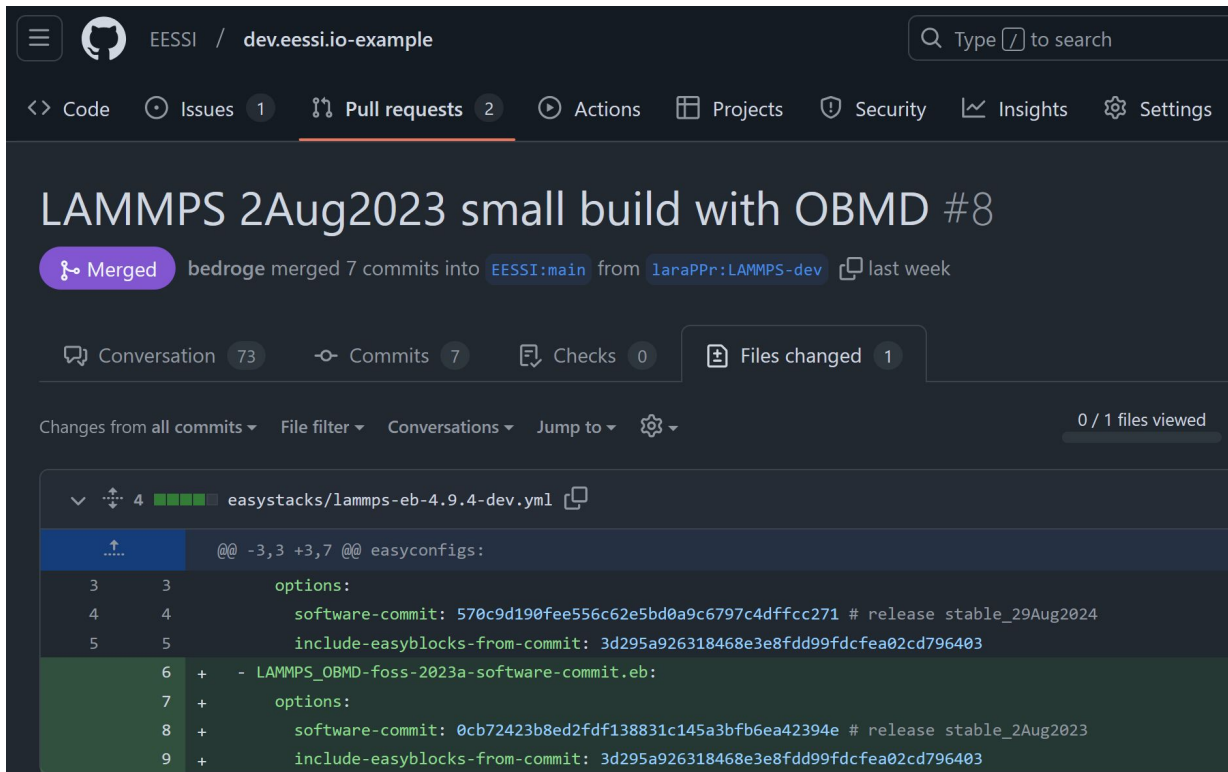
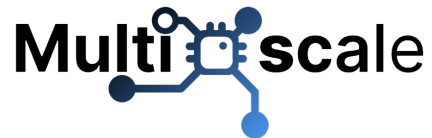
- Permanent installations
- Only install releases
- Builds for all CPU architectures
- `/cvmfs/software.eessi.io/version/`

dev.eessi.io

- Temporary installations
- Can install from commits
- Can skip some CPU targets
- dev.eessi.io built on top of software.eessi.io
- Subdirectories per project
- `/cvmfs/dev.eessi.io/version/project`



dev.eessi.io-example



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

Leveraging EESSI in CI environments



- EESSI can be used in CI environments like:
 - GitHub: github.com/marketplace/actions/eessi
 - GitLab: gitlab.com/explore/catalog/eessi/gitlab-eessi
- EESSI can provide:
 - Different compilers to test your software with
 - Required dependencies for your software
 - Additional tools like ReFrame, performance analysis tools, ...
- **Other than CernVM-FS to get access to EESSI, no software installations required!**
 - Everything that is actually needed is pulled in on-demand by CernVM-FS
- Significantly facilitates also running CI tests in other contexts (laptop, HPC, ...)

Leveraging EESSI in CI environments



We have an EESSI GitHub Action that provides EESSI+direnv:

See it in action in the `github-eessi-action` repository:

github.com/EESSI/github-action-eessi

github.com/EESSI/github-action-eessi/blob/main/.github/workflows/tensorflow-usage.yml

```
name: ubuntu_tensorflow
on: [push, pull_request]
jobs:
```

```
  build:
```

```
    runs-on: ubuntu-latest
```

```
    steps:
```

```
      - uses: actions/checkout@v3
```

```
      - uses: eessi/github-action-eessi@v3
```

```
      with:
```

```
        eessi_stack_version: '2023.06'
```

```
      - name: Test EESSI
```

```
        shell: bash
```

```
        run: |
```

```
          module load TensorFlow
```

```
          python -c 'import tensorflow; print(tensorflow.__version__)'
```



Leveraging EESSI GitHub Action



```
build
succeeded 2 minutes ago in 1m 1s

> ✓ Set up job 2s
> ✓ Run actions/checkout@v2 0s
> ✓ Run eessi/github-action-eessi@main 52s
▼ ✓ Test EESSI 5s

1 ▼ Run module load GROMACS
2 module load GROMACS
3 gmx --version
4 shell: /usr/bin/bash --noprofile --norc -e -o pipefail {0}
5 env:
6   EESSI_SILENT: 1
7   BASH_ENV: /cvmfs/pilot.eessi-hpc.org/versions/2021.06/init/bash
8
9   :~) GROMACS - gmx, 2020.4-MODIFIED (~:
10
11      GROMACS is written by:
12      Emile Apol      Rossen Apostolov      Paul Bauer      Herman J.C. Berendsen
13      Par Bjelkmar    Christian Blau    Viacheslav Bolnykh    Kevin Boyd
14      Aldert van Buuren  Rudi van Drunen  Anton Feenstra      Alan Gray
15      Gerrit Groenhof  Anca Hamuraru    Vincent Hindriksen    M. Eric Irrgang
16      Aleksei Iupinov  Christoph Junghans  Joe Jordan      Dimitrios Karkoulis
17      Peter Kasson     Jiri Kraus        Carsten Kutzner      Per Larsson
18      Justin A. Lemkul  Viveca Lindahl    Magnus Lundborg      Erik Marklund
19      Pascal Merz       Pieter Meulenhoff  Teemu Murtola        Szilard Pall
20      Sander Pronk      Roland Schulz      Michael Shirts      Alexey Shvetsov
21      Alfons Sijbers    Peter Tieleman     Jon Vincent          Teemu Virolainen
22      Christian Wennberg  Maarten Wolf      Artem Zhmurov
23      and the project leaders:
```



<https://github.com/EESSI/github-action-eessi/actions/runs/11183032689/job/31090668500>

Leveraging EESSI GitLab Component



```
include:
  - component: $CI_SERVER_FQDN/eessi/gitlab-eessi/eessi@1.0.5
build:
  stage: build
  artifacts:
    paths:
      - msx_map.png
  script:
    # Create directory for personal R library
    - mkdir $CI_BUILDS_DIR/R
    - export R_LIBS_USER=$CI_BUILDS_DIR/R
    # Load the R module from EESSI
    - module load R-bundle-CRAN/2023.12-foss-2023a
    # Install eessirmaps, the rnatrualearth dep and create the plot
    - R -e "install.packages('rnatrualearthdata', repos = 'https://cran.rstudio.com/');
remotes::install_gitlab('neves-p/eessirmaps', upgrade = FALSE);
eessirmaps::multixscale_map(); ggplot2::ggsave('msx_map.png', bg = 'white')"
```



https://www.eessi.io/docs/using_eessi/eessi_in_ci/



Leveraging EESSI GitLab Component



```
1 Running with gitlab-runner 17.4.0-pre.110.g27400594 (27400594)
2   on blue-5.saas-linux-small-amd64.runners-manager.gitlab.com/default -AzERasQ, system ID: s_4cb09cee29e2
3   ✓ Preparing the "docker+machine" executor 00:20
4   Using Docker executor with image ruby:3.1 ...
5   Pulling docker image ruby:3.1 ...
6   Using docker image sha256:12bc18a740469918b597219b1033d2fd4a60594a8ada2ec29383f64e39e8df0b for ruby:3.1 with digest ruby@sha256:b7fe909968d1e473c5448ee255875bdb65c67df0efe28
   a0991f97a91ce2e71e7 ...
7   ✓ Preparing environment 00:05
8   Running on runner--azerasq-project-61564283-concurrent-0 via runner-azerasq-s-l-s-amd64-1728602156-92403c92...
9   ✓ Getting source from Git repository 00:02
10  Fetching changes with git depth set to 20...
11  Initialized empty Git repository in /builds/neves-p/eessirmaps/.git/
12  Created fresh repository.
13  Checking out 39d2b04b as detached HEAD (ref is main)...
14  Skipping Git submodules setup
15  $ git remote set-url origin "${CI_REPOSITORY_URL}"
16  ✓ Downloading artifacts 00:01
17  ✓ Executing "step_script" stage of the job script 01:45
18  Using docker image sha256:12bc18a740469918b597219b1033d2fd4a60594a8ada2ec29383f64e39e8df0b for ruby:3.1 with digest ruby@sha256:b7fe909968d1e473c5448ee255875bdb65c67df0efe28
   a0991f97a91ce2e71e7 ...
19  Environment set up to use EESSI (2023.06), have fun!
20  $ mkdir $CI_BUILDS_DIR/R
21  $ export R_LIBS_USER=$CI_BUILDS_DIR/R
22  $ module load R-bundle-CRAN/2023.12-foss-2023a
23  $ R -e "install.packages('rnatuarearthdata', repos = 'https://cran.rstudio.com/'); remotes::install_gitlab('neves-p/eessirmaps', upgrade = FALSE); eessirmaps::multixscale_m
   ap(); ggplot2::ggsave('msx_map.png', bg = 'white')"
24  R version 4.3.2 (2023-10-31) -- "Eye Holes"
25  Copyright (C) 2023 The R Foundation for Statistical Computing
26  Platform: x86_64-pc-linux-gnu (64-bit)
```



<https://gitlab.com/neves-p/eessirmaps/-/jobs/8057216299>

HPCwire Readers Choice Award

- EESSI wins HPCwire Readers' Choice Award in the [Best HPC Programming Tool or Technology category](#)
- Award presented at SC 24 conference in Atlanta





E E S S I

EUROPEAN ENVIRONMENT FOR
SCIENTIFIC SOFTWARE INSTALLATIONS

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)

MultiXscale

Web page: multixscale.eu

Facebook: [MultiXscale](https://www.facebook.com/MultiXscale)

Twitter: [@MultiXscale](https://twitter.com/MultiXscale)

LinkedIn: [MultiXscale](https://www.linkedin.com/company/multixscale)



Co-funded by
the European Union



EuroHPC
Joint Undertaking



UNIVERSITAT DE
BARCELONA



Universität
Stuttgart



SORBONNE
UNIVERSITÉ



Université
de Toulouse



Consiglio Nazionale
delle Ricerche

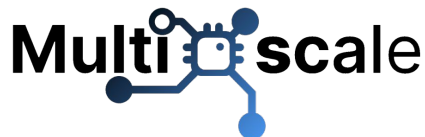


MAX-PLANCK-GESELLSCHAFT



ISTITUTO ITALIANO
DI TECNOLOGIA

Thank you for listening! Questions?



Funded by the European Union, the European High Performance Computing Joint Undertaking (JU) and countries participating in the project under grant agreement No 101093169.



EuroHPC
Joint Undertaking ²⁵