



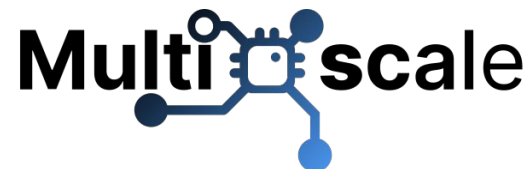
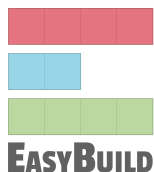
Workflow for
adding additional
software to

E E S S I

EUROPEAN ENVIRONMENT FOR
SCIENTIFIC SOFTWARE INSTALLATIONS

Wed 20 May 2026

Lara Peeters (Ghent University)



Q&A via EESSI Slack

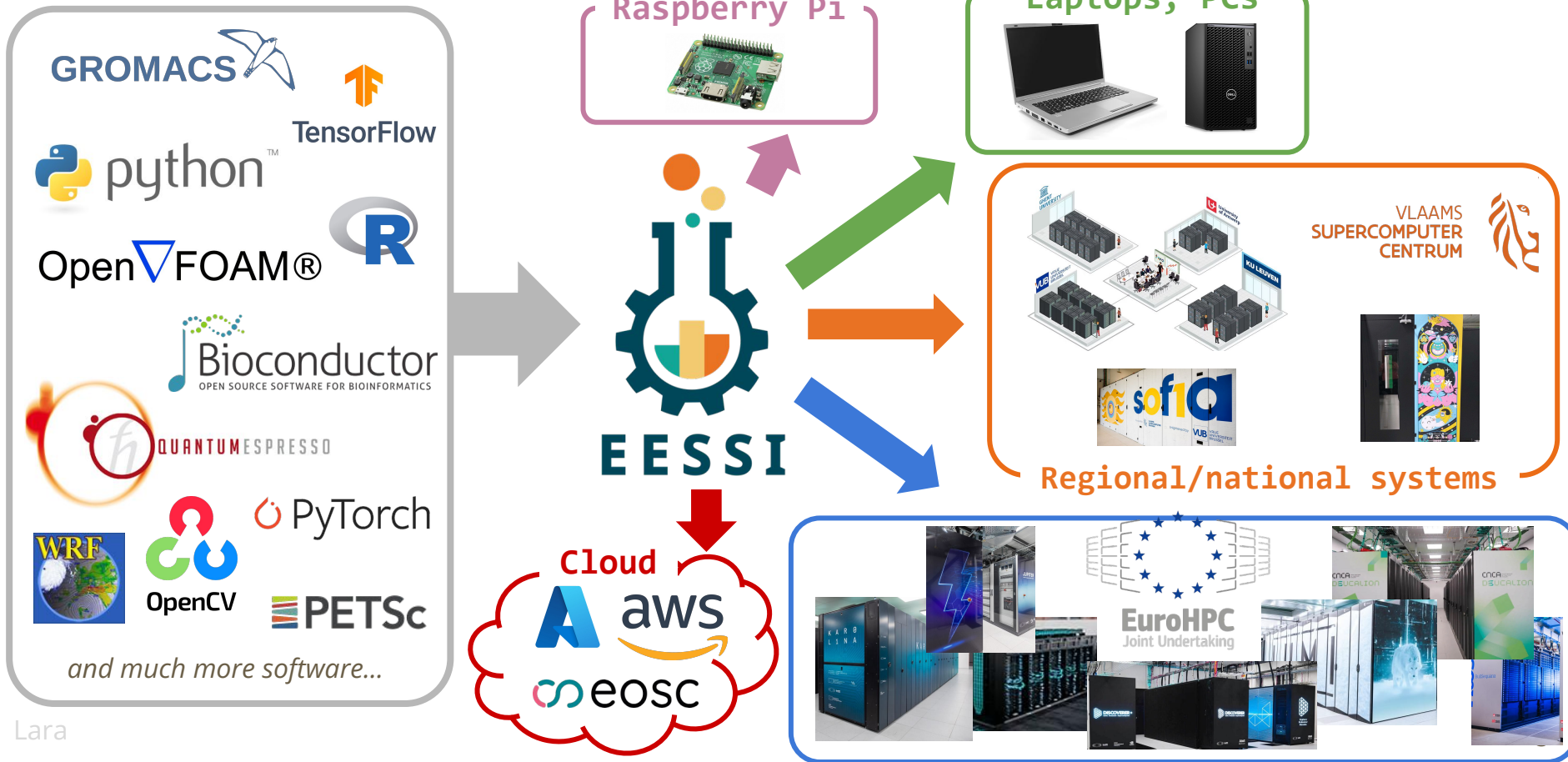
Please join the #cineca-hackathon-may26-org channel in the EESSI Slack for questions and discussion



Step 1) **Join the EESSI Slack**, see “Slack channel” link at <https://eessi.io>

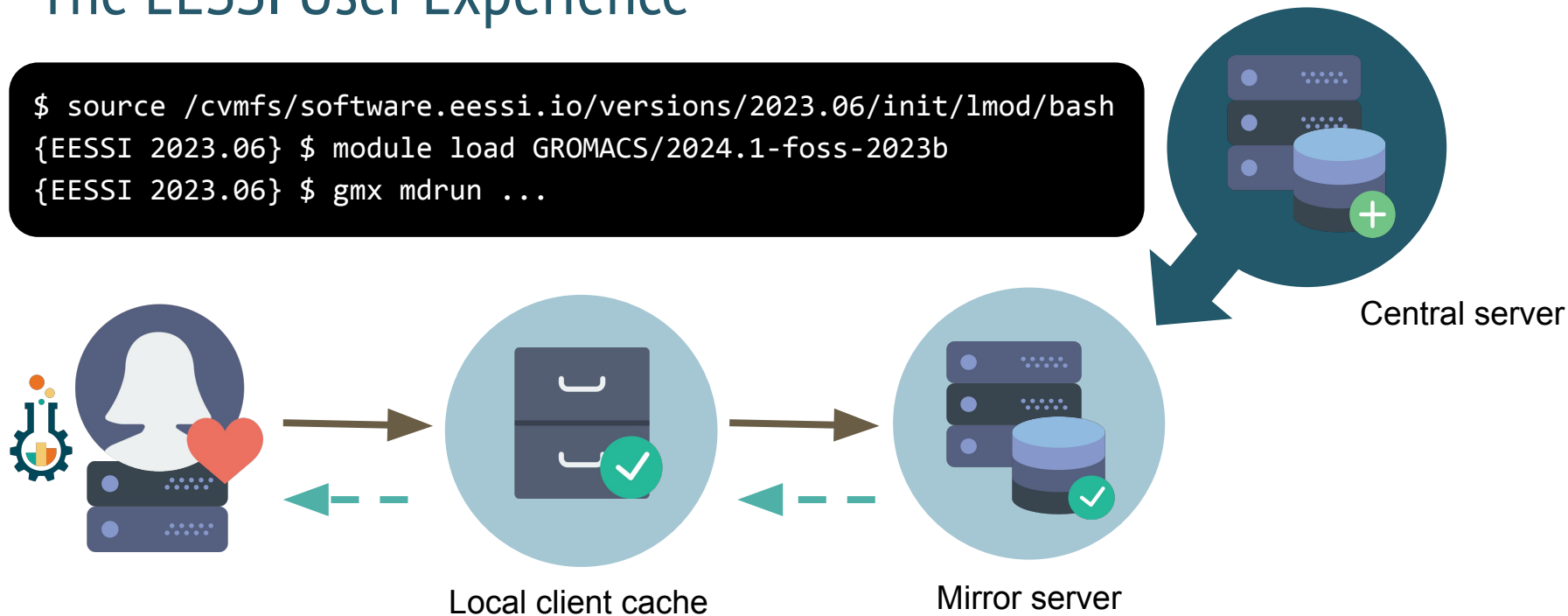
Step 2) **Join** [#cineca-hackathon-may26-org](https://eessi-hpc.slack.com/archives/C0AAH8CJGTZ) **channel** in EESSI Slack
(direct link: <https://eessi-hpc.slack.com/archives/C0AAH8CJGTZ>)

EESSI as shared software stack for HPC, cloud, and beyond



The EESSI User Experience

```
$ source /cvmfs/software.eessi.io/versions/2023.06/init/lmod/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, ...)

Overview of available software

An up-to-date overview of available software is available in the EESSI documentation:

https://www.eessi.io/docs/available_software

Software available in EESSI

Overview of software available in [EESSI's production repository](https://www.eessi.io) [software.eessi.io](https://www.eessi.io).

752 unique software projects (+ 3007 unique extensions)

name:GROMACS

GROMACS

[\(more details\)](#)

<https://www.gromacs.org>

GROMACS is a versatile package to perform molecular dynamics, i.e. simulate the Newtonian equations of motion for systems with hundreds to millions of particles. This is a CPU only build, containing both MPI and threadMPI binaries for both single and double precision. It also contains the gmxml extension for the single precision MPI build.

Available in EESSI versions: [2023.06](#) [2025.06](#)

Supported CPU families: [AMD](#) [Intel](#) [Arm](#)

Supported GPU families: [NVIDIA](#)



GROMACS

GROMACS is a versatile package to perform molecular dynamics, i.e. simulate the Newtonian equations of motion for systems with hundreds to millions of particles.

This is a GPU enabled build, containing both MPI and threadMPI binaries.

It also contains the gmxml extension for the single precision MPI build.

homepage: <https://www.gromacs.org>

Available installations

GROMACS version	Supported CPU targets	Supported GPU targets	EESSI version	Module
2025.4	generic: aarch64, x86_64 Arm : a64fx, neoverse_n1, neoverse_v1, nvidia/grace AMD : zen2, zen3, zen4 Intel : haswell, skylake_avx512, sapphirerapids, icelake, cascadelake	(none)	2025.06	GROMACS/2025.4-foss-2025b
2025.2	generic: aarch64, x86_64 Arm : a64fx, neoverse_n1, neoverse_v1, nvidia/grace AMD : zen2, zen3, zen4 Intel : haswell, skylake_avx512, sapphirerapids, icelake, cascadelake	(none)	2025.06	GROMACS/2025.2-foss-2025a
2024.4	generic: aarch64, x86_64 Arm : neoverse_n1,	NVIDIA : cc70, cc80, cc90	2023.06	GROMACS/2024.4-foss-2023b-

Supported CPU targets

https://eessi.io/docs/software_layer/cpu_targets



- AMD, Intel (`x86_64`)
 - 5 generations of Intel CPUs: Haswell, Skylake, Cascade Lake, Ice Lake, Sapphire Rapids
 - 4 generations of AMD CPUs: Zen2 (Rome), Zen 3 (Milan), Zen4 (Genoa), Zen5 (Turin)
- Arm (`aarch64`)
 - 4 different microarchitectures: Fujitsu A64FX, NVIDIA Grace, Neoverse N1 + V1
- Plus a generic fallback for both `x86_64` and `aarch64`
- RISC-V CPUs are work-in-progress
 - Exploration ongoing via RISC-V-specific subdirectory of `dev.eessi.io` repository

Supported GPU targets

https://eessi.io/docs/software_layer/gpu_targets



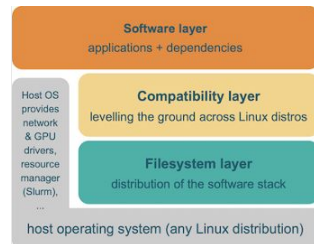
- NVIDIA (CUDA)
 - Different generations of NVIDIA GPUs, based on CUDA Compute Capability (CC), see also <https://developer.nvidia.com/cuda/gpus>
 - In EESSI 2023.06: CC 7.0 (V100, T4), 8.0 (A100 & co, incl. L40), 9.0 (H100/H200)
 - In EESSI 2025.06: CC 7.0, 8.0, 9.0, 10.0 (B100/B200/B300), 12.0 (B10, RTX PRO Blackwell)
 - GPU driver libraries (include `libcuda.so`) must be exposed to EESSI
 - See https://www.eessi.io/docs/site_specific_config/gpu
- AMD (ROCm)
 - Work-in-progress, initial support included in EasyBuild 5.3.0 (mid April 2026)
 - PR for easyconfigs for ROCm 6.4.1 merged, will be included in next EasyBuild release

See also *NVIDIA + AMD GPU support in EESSI* talk @ EUM'26 ([slides](#), [recording](#))

The trick behind the EESSI software layer

Software installations only link to **libraries from compatibility layer or other installations in software layer**, *not* from host (Linux) operating system.

- Because of this, these software installations work on any Linux distribution
- This is ensured via *RPATH linking*
- Build tools (like CMake) need to be made aware of alternative system root (sysroot)
- Some exceptions need to be made: GPU driver libraries must be provided by host OS
- “Containers without the containing”



Contributing software to EESSI



To contribute additional software to EESSI, the following must be taken into account:

- An easyconfig file must be available in EasyBuild to install the software
 - Either in the latest EasyBuild release, or in a (merged) pull request to EasyBuild
- A pull request must be opened to the `EESSI/software-layer` repository
- The EESSI contribution policy must be followed
 - See https://eessi.io/docs/adding_software/contribution_policy
 - Must be redistributable software (like open source), must work on all CPU targets, must be built by EESSI bot, should be recent software version and use recent toolchain, ...



Contributing software to EESSI, step-by-step

1. Find or create a (working) **easyconfig file** to install the software
2. **Test it in the EESSI build environment** (using `EESSI-extend`)
3. **Contribute it to EasyBuild** (if it hasn't been yet)
4. Open a **pull request** to the `EESSI/software-layer` repository
5. See if installation works on **all supported CPU targets**
 - Somebody from the EESSI “builders” team will trigger bot to do test builds
6. When that all checks out, the software installations will be **deployed to EESSI**

Recommendations for contributing software to EESSI

- **Test locally first**, using `EESSI-extend`
 - Can be on multiple CPU targets or families, but not strictly required
- Always **use latest EasyBuild release** (see `module avail EasyBuild` in EESSI)
- Pull request to EESSI can be opened while `easyconfig` PR to EasyBuild is still open, but *deployment* to EESSI can only be done when EasyBuild PR has been *merged*
- Work with EESSI “builders” team to resolve any problems that may pop up
 - Via comments in pull requests
 - Via EESSI Slack (see `#software-layer` or `#support` channels), see link @ eessi.io

Recommendations for contributing software to EESSI

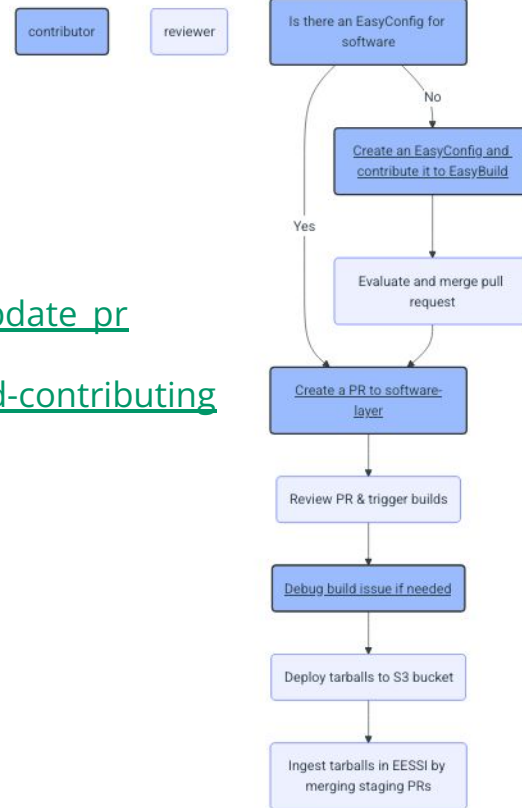


```
== COMPLETED: Installation ended successfully (took 5 mins 52 secs)
== Results of the build can be found in the log file(s)
/home/ec2-user/eessi/versions/2025.06/software/linux/aarch64/neoverse_n1/software/scikit-image/0.25.0-foss-2024a/easyb
uild/easybuild-scikit-image-0.25.0-20260519.160252.log.bz2
== Running post-easyblock hook...

== Build succeeded for 5 out of 5 (total: 10 mins 13 secs)
== Summary:
* [SUCCESS] imageio/2.36.1-gfbf-2024a
* [SUCCESS] bokeh/3.6.0-gfbf-2024a
* [SUCCESS] dask/2024.9.1-gfbf-2024a
* [SUCCESS] PyWavelets/1.8.0-foss-2024a
* [SUCCESS] scikit-image/0.25.0-foss-2024a
== Temporary log file(s) /tmp/eb-13zsn0gu/easybuild-m2i6ku9x.log* have been removed.
== Temporary directory /tmp/eb-13zsn0gu has been removed.
{EESSI/2025.06} [ec2-user@ip-172-31-32-214 ~]$
```

Detailed guidelines for contributing software to EESSI

- See https://eessi.io/docs/adding_software/overview
- Documentation for contributing to EasyBuild:
 - https://docs.easybuild.io/contributing/#contributing_easyconfigs
 - https://docs.easybuild.io/integration-with-github/#github_new_update_pr
 - <https://tutorial.easybuild.io/2023-eb-eessi-uk-workshop/easybuild-contributing>
- Step-by-step instructions for opening PR to EESSI:
https://www.eessi.io/docs/adding_software/opening_pr



Contributing software to EESSI, hands-on



Hands-on demo (EESSI 2025.06): contributing scikit-image with `foss/2024a`

If test installation of `scikit-image-0.25.0-foss-2024a.eb` is OK,
we can open PR to `EESSI/software-layer` repository:

1. Add entry to `easystacks/software.eessi.io/2025.06/eessi-2025.06-eb-5.3.0-2024a.yml`
2. Open pull request to `EESSI/software-layer` repository
3. Check if installation works on all CPU targets + get it deployed...

Contributing software to EESSI, hands-on

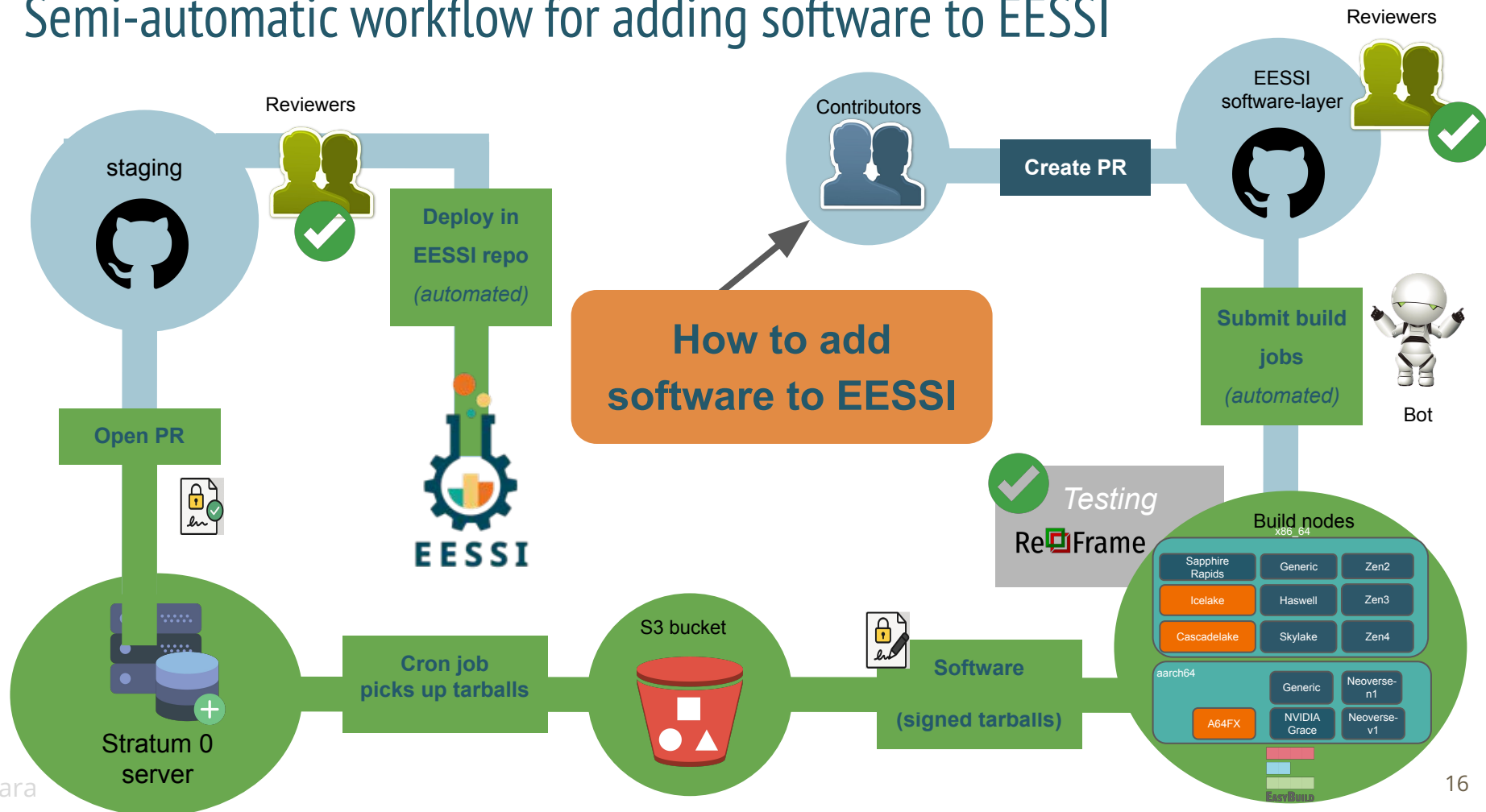


Hands-on demo (EESSI 2025.06): contributing latest scikit-bio (0.7.2) with `foss/2024a`

If test installation of `scikit-image-0.25.0-foss-2024a.eb` from easyconfig PR is OK,
we can open PR to `EESSI/software-layer` repository:

1. Add entry to `easystacks/software.eessi.io/2025.06/eessi-2025.06-eb-5.3.0-2024a.yml`
2. **Use `from-commit` option** to let EasyBuild use easyconfig file(s) from easyconfigs pull request
3. Open pull request to `EESSI/software-layer` repository
4. Check if installation works on all CPU targets
5. Make sure that easyconfig PR gets merged, and then deployment in EESSI can be done

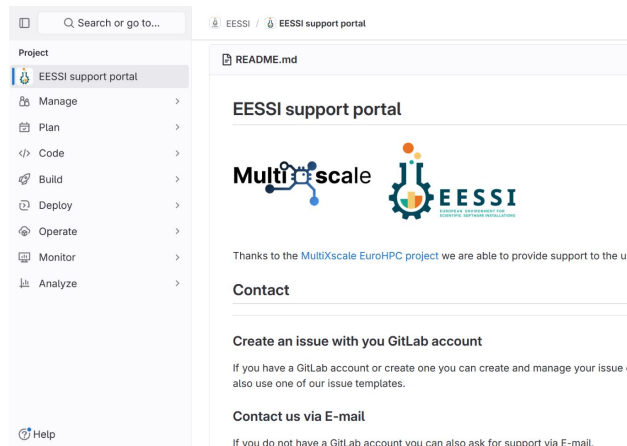
Semi-automatic workflow for adding software to EESSI



Support for installing, using, contributing to EESSI

- 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, ...)

eessi.io/docs/support



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

