



Workflow for
adding additional
software to

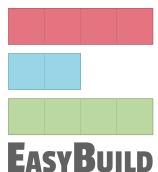
E E S S I

EUROPEAN ENVIRONMENT FOR
SCIENTIFIC SOFTWARE INSTALLATIONS



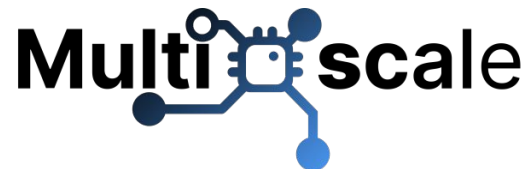
ISC

High Performance

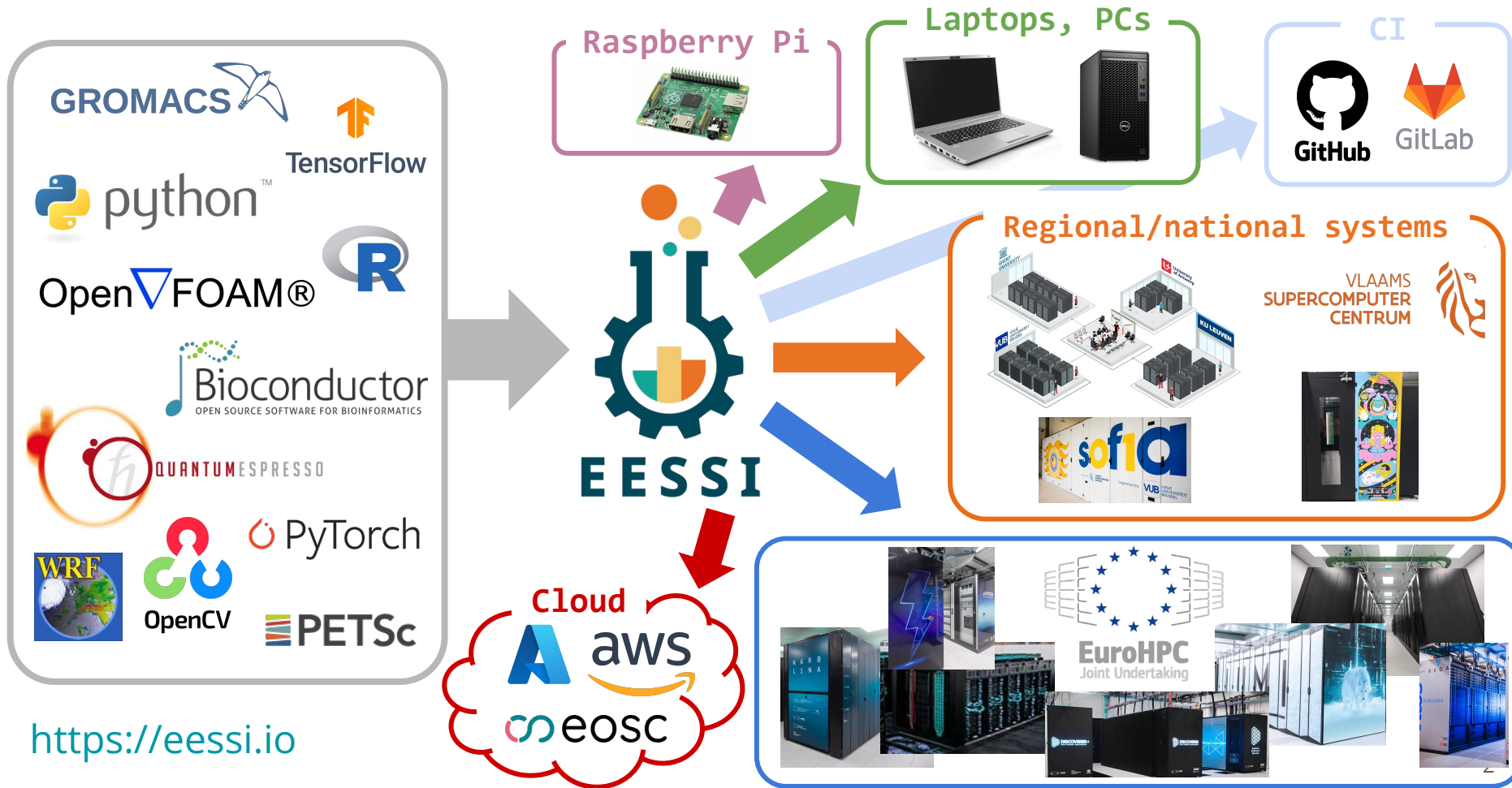


Fri 26 June 2026

Lara Peeters (Ghent University)

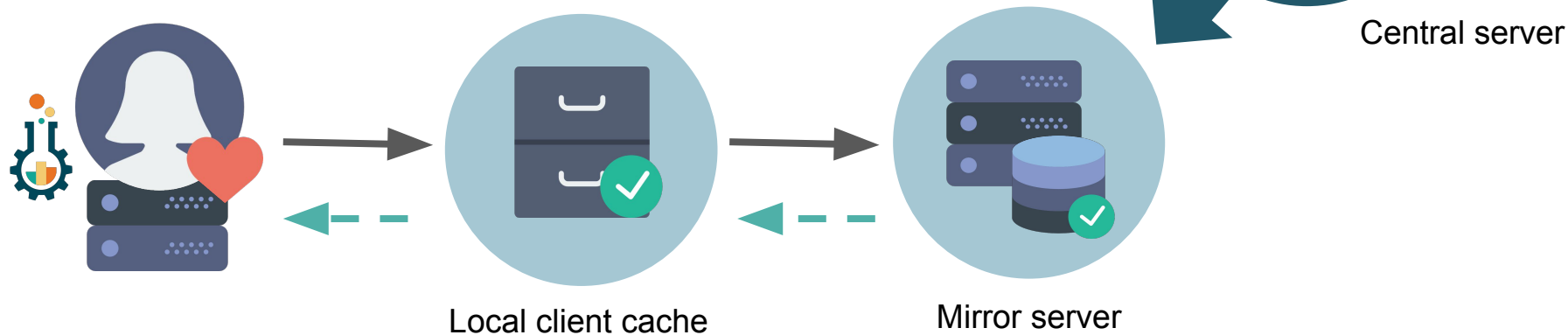


EESSI as shared software stack for HPC, and beyond



Running scientific software in 1, 2, 3

```
source /cvmfs/software.eessi.io/versions/2025.06/init/lmod/bash  
module load GROMACS/2025.4-foss-2025b  
gmx ...
```



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



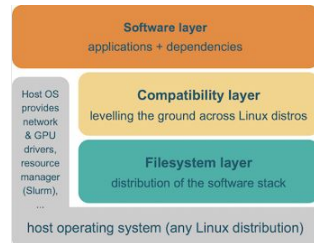
- NVIDIA (CUDA)
 - Different generations of NVIDIA GPUs, based on CUDA Compute Capability (CC), see also <https://developer.nvidia.com/cuda/gpus>
 - In EESSI 2023.06: CC 7.0 (V100, T4), 8.0 (A100 & co, incl. L40), 9.0 (H100/H200)
 - In EESSI 2025.06: CC 7.0, 8.0, 9.0, 10.0 (B100/B200/B300), 12.0 (B10, RTX Pro Blackwell)
 - GPU driver libraries (include `libcuda.so`) must be exposed to EESSI
 - See https://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, included in EasyBuild 5.3.1 (mid June 2026)

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

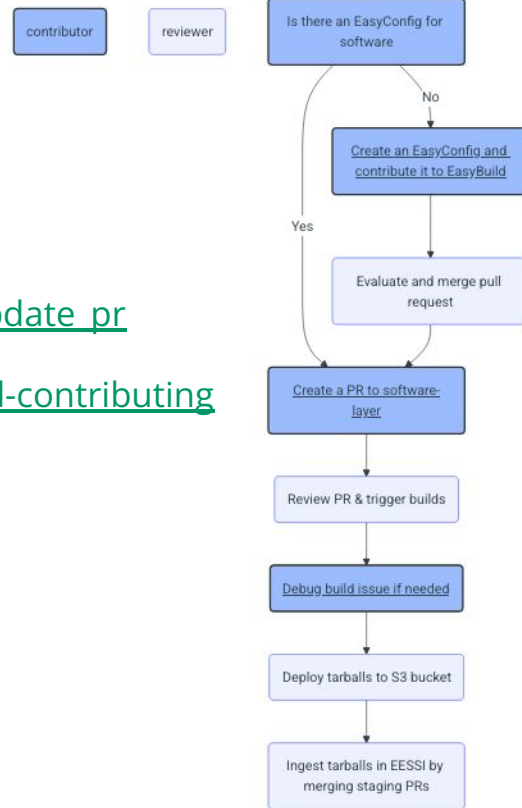


- **Test locally first**, using `EESSI-extend`
 - Can be on multiple CPU targets or families, but not strictly required
- Always **use latest EasyBuild release** (see `module avail EasyBuild` in EESSI)
- Pull request to EESSI can be opened while `easyconfig` PR to EasyBuild is still open, but *deployment* 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

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-ebuild-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



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

Check EasyBuild for software you want



develop easybuild-easyconfigs / easybuild / easyconfigs / s / scikit-image

Q scikit-image Add file History

Micket Archive foss-2021b 541253e · 2 months ago History

Name	Last commit message	Last commit date
..		
scikit-image-0.18.1_fix-README-cache-perms.patch	add patch for scikit-image 0.18.1 to avoid 'Permission denied' error ...	5 years ago
scikit-image-0.19.3-foss-2022a.eb	clean up easyconfigs that explicitly set use_pip, `sanity_pip_check...	3 years ago
scikit-image-0.21.0-foss-2022b.eb	clean up easyconfigs that explicitly set use_pip, `sanity_pip_check...	3 years ago
scikit-image-0.22.0-foss-2023a.eb	don't enable download_dep_fail, use_pip, sanity_pip_check in recent e...	2 years ago
scikit-image-0.24.0-foss-2023b.eb	clean up easyconfigs that explicitly set use_pip, `sanity_pip_check...	last year
scikit-image-0.25.0-foss-2024a.eb	Remove download_dep_fail, use_pip, sanity_pip_check = True	last year
scikit-image-0.25.0-foss-2025a.eb	adding easyconfigs: scikit-image-0.25.0-foss-2025a.eb, imageio-2.37.0...	7 months ago
scikit-image-0.25.0-foss-2025b.eb		

```
(eb_job_doduo_RHEL9) [vsc46128@gligar11 ~]$ eb -S scikit-image
== found valid index for /kyukon/data/gent/vo/000/gvo00002/vsc46128/easybuild/eb_job_doduo_RHEL9/easybuild/easyconfigs, so using it...
CFGS1=/kyukon/data/gent/vo/000/gvo00002/vsc46128/easybuild/eb_job_doduo_RHEL9/easybuild/easyconfigs/s/scikit-image
* $CFGS1/scikit-image-0.18.1_fix-README-cache-perms.patch
* $CFGS1/scikit-image-0.19.3-foss-2022a.eb
* $CFGS1/scikit-image-0.21.0-foss-2022b.eb
* $CFGS1/scikit-image-0.22.0-foss-2023a.eb
* $CFGS1/scikit-image-0.24.0-foss-2023b.eb
* $CFGS1/scikit-image-0.25.0-foss-2024a.eb
* $CFGS1/scikit-image-0.25.0-foss-2025a.eb
* $CFGS1/scikit-image-0.25.0-foss-2025b.eb
(eb_job_doduo_RHEL9) [vsc46128@gligar11 ~]$
```

Test easyconfig locally first with EESSI-extend



```
$ source /cvmfs/software.eessi.io/versions/2025.06/init/lmod/bash
EESSI has selected x86_64/amd/zen2 as the compatible CPU target for EESSI/2025.06
{EESSI 2025.06} $ module load EESSI-extend/2025.06-easybuild
{EESSI 2025.06} $ eb scikit-image-0.25.0-foss-2024a.eb
```

```
== 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 ~]$
```

Contributing software to EESSI



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



{2025.06}[foss/2024a] scikit-image 0.25.0 #1504

Open

[bedroge](#) merged 2 commits into [EESSI:main](#) from [laraPPr:scikit-image](#) on May 20

Conversation 17

Commits 2

Checks 59

Files changed 1



All commits ▾

Filter files...



▼ easystack/software.eessi.io/2025....

eessi-2025.06-eb-5.3.0-2024a.yml

▼ easystack/software.eessi.io/2025.06/eessi-2025.06-eb-5.3.0-2024a.yml

... @@ -1,2 +1,4 @@

1 1 easyconfigs:

2 2 - Siesta-5.4.2-foss-2024a.eb

3 + - scikit-image-0.25.0-foss-2024a.eb

4 +

Builders and deployers engaging with the bot





laraPPr commented on [May 20](#)

Member Author ...

bot: build repo:eessi.io-2025.06-software instance:eessi-bot-mc-aws for:arch=aarch64/neoverse_n1





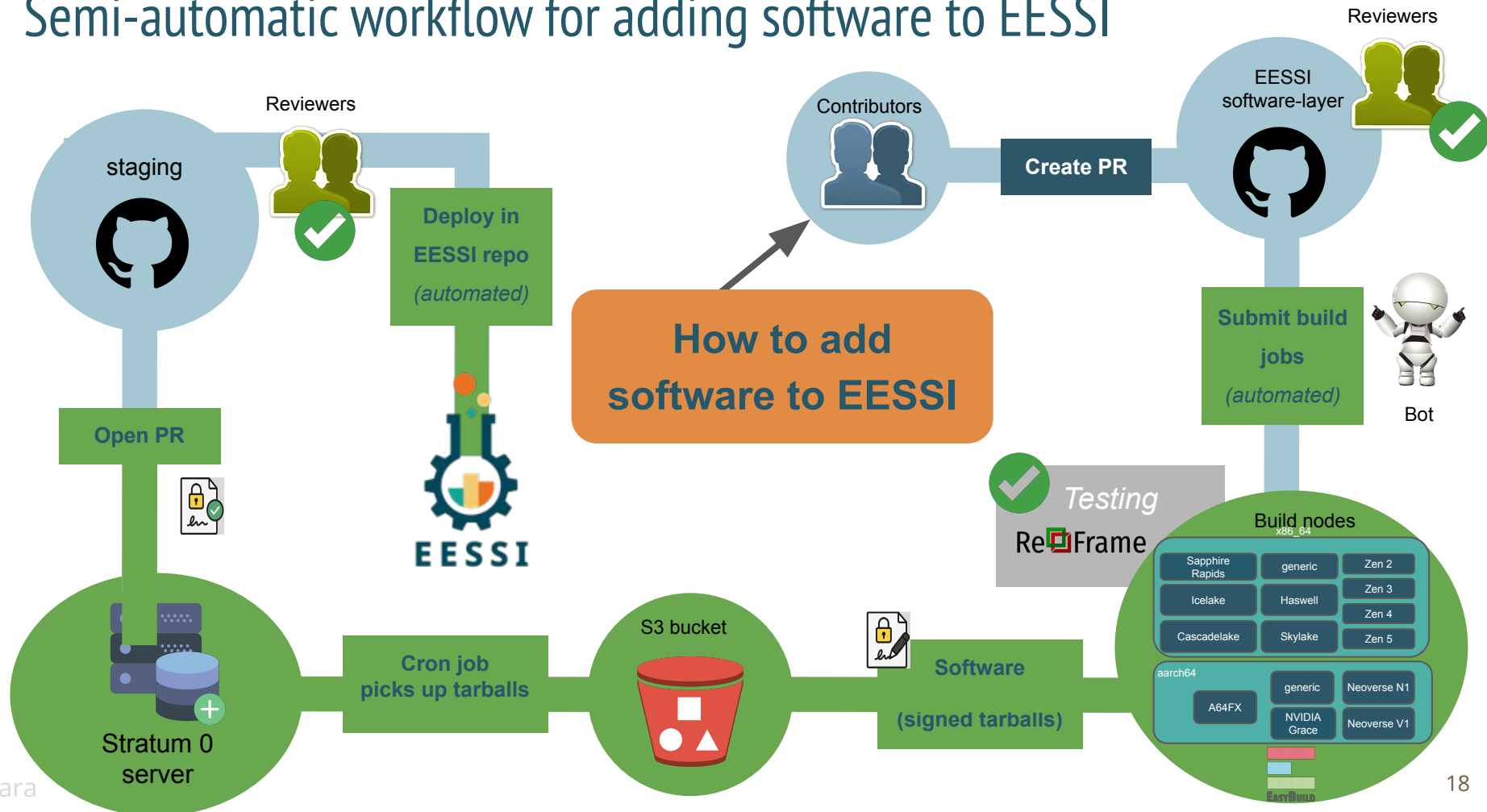
eessi-bot-aws Bot commented on [May 20](#) • edited ...

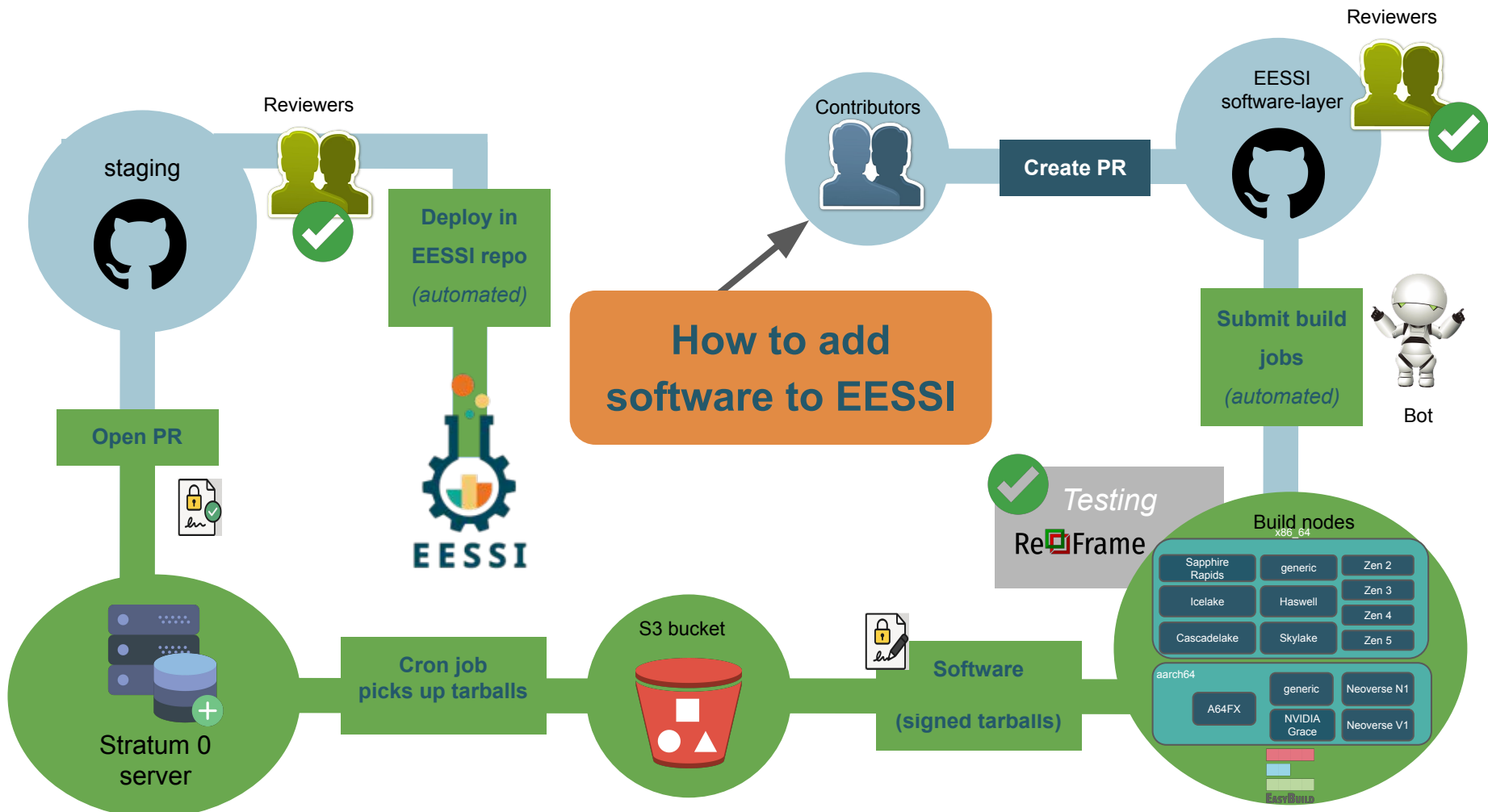
New job on instance `eessi-bot-mc-aws` for repository `eessi.io-2025.06-software`
Building on: `neoverse_n1`
Building for: `aarch64/neoverse_n1`
Job dir: `/project/def-users/SHARED/jobs/2026.05/pr_1504/158723`

date	job status	comment
May 20 07:22:31 UTC 2026	submitted	job id <code>158723</code> awaits release by job manager
May 20 07:23:28 UTC 2026	released	job awaits launch by Slurm scheduler
May 20 07:28:31 UTC 2026	running	job <code>158723</code> is running
May 20 07:55:12 UTC 2026	finished	▶ 🎉 SUCCESS (click triangle for details)
May 20 07:55:12 UTC 2026	test result	▶ 🎉 SUCCESS (click triangle for details)
May 20 09:31:34 UTC 2026	uploaded	transfer of <code>eessi-2025.06-software-linux-aarch64-neoverse_n1-17792633590.tar.zst</code> to S3 bucket succeeded



Semi-automatic workflow for adding software to EESSI

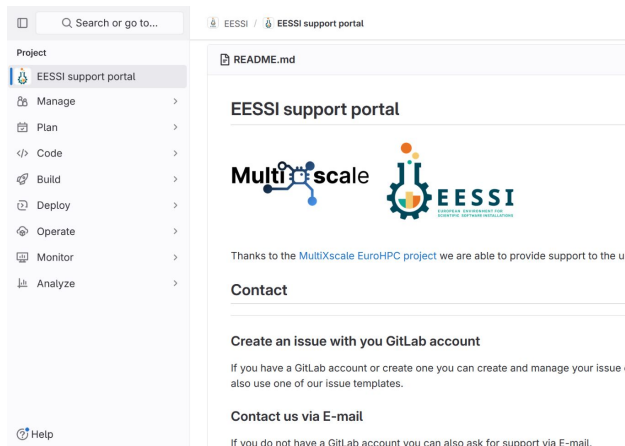




Support for installing, using, contributing to EESSI

- 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



Acknowledgements



Co-funded by
the European Union



EuroHPC
Joint Undertaking

- 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 1010193169
- Thanks to Amazon Web Services (AWS) and Microsoft Azure for generously sponsoring the EESSI project with funds, cloud credits, feedback, and guidance.





Website: eessi.io

GitHub: github.com/EESSI

Documentation: eessi.io/docs

Blog: eessi.io/docs/blog

Getting support: eessi.io/docs/support

[Join](#) the EESSI Slack (see link on EESSI website)

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)