



4 July 2024

<https://github.com/EESSI/meetings/wiki>

Agenda



1. Quick introduction by new people
2. EESSI-related meetings and events in last month
3. Progress update per EESSI layer
4. Update on EESSI production repository `software.eessi.io`
5. Update on EESSI test suite + build-and-deploy bot
6. Additional EESSI repositories: `dev.eessi.io`, `riscv.eessi.io`
7. AWS/Azure sponsorship update
8. Upcoming/recent events
9. Q&A

Quick introduction by new people



New people on the call: feel free to introduce yourself!

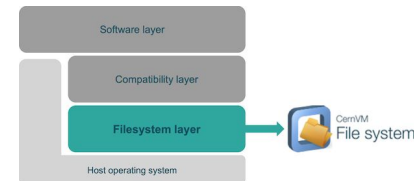
- Who are you, where do you work, on what?
- Why are you interested in the EESSI project?
- Are you planning to actively contribute,
and if so, to which aspect(s) of the project?

EESSI-related meetings & events

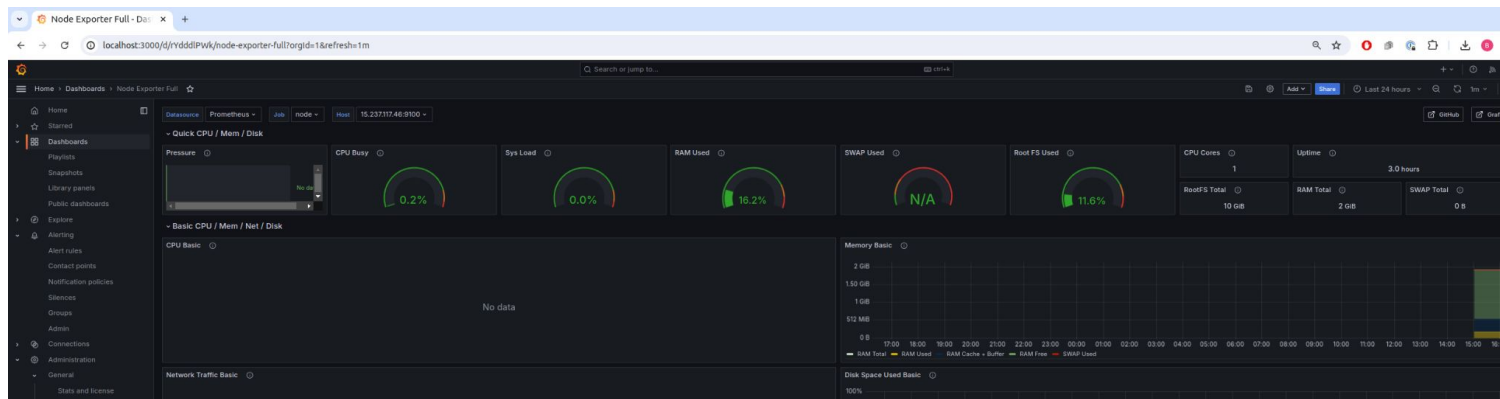


- (10 June'24) CernVM-FS coordination meeting (prepping 2.12.0 release, EESSI updates)
- (11 June'24) MultiXscale WP1+WP5 sync meeting ([notes](#), [notes](#))
- (11 June'24) Sync meeting with Deucalion team on EESSI for A64FX
- (13+27 June'24) EESSI test suite sync meeting ([notes](#))
- (13 June'24) Meeting with AMD on supporting AMD ROCm in EESSI
- (13 June'24) Meeting with Google on integrating EESSI as backend for Ramble
- (14 June'24) Sync meeting on bot support for building for GPUs ([notes](#))
- (14 June'24) Meeting to discuss CVMFS monitoring dashboard ([notes](#))
- (18 June'24) Talk on EESSI at HPC-SIG meeting in Sheffield (UK) - virtual ([more info](#))
- (June'24) Weekly support team sync meetings (*notes are in private wiki on EESSI support portal*)

Progress update: filesystem layer

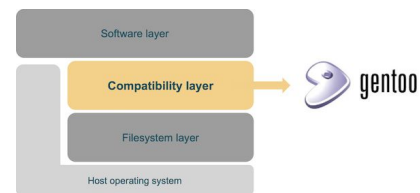


- Small fix for correctly showing the contents of tarballs in staging PRs (PR [#195](#))
- Fix broken Ansible CI on Ubuntu 22.04 (PR [#196](#) and `ansible-cvmfs` PR [#13](#))
- Work on a CVMFS monitoring dashboard has started
 - Grafana + Prometheus
 - Ansible for configuring the monitor host and targets



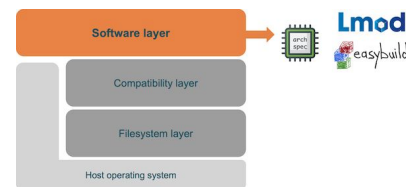
[Bob, Kenneth]

Progress update: compatibility layer



- Use the latest Ubuntu version in CI workflow for running EESSI tests (PR [#206](#))
- Fix broken/ignored ReFrame tests and drop support for pilot repository (PR [#208](#))
- Discussion / ideas for compatibility layer of next EESSI version:
<https://gitlab.com/eessi/support/-/issues/56>

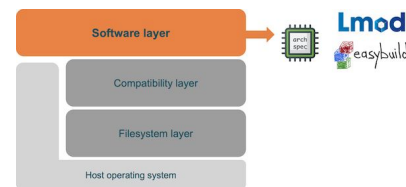
Progress update: software layer (1/3)



Recently merged PRs:

- Additional software: NLTK 3.8.1 ([PR #596](#)), SEPP 4.5.1 ([PR #597](#)), BLAST+ 2.14.1 ([PR #599](#)), Valgrind 3.21.0 & 3.23.0 ([PR #601](#)), OrthoFinder 2.5.5 ([PR #602](#)), EasyBuild 4.9.2 ([PR #604](#)), IPython 8.17.2 ([PR #617](#)), dlb 3.4 ([PR #619](#)), BCFtools 1.18 ([PR #628](#))
- Additional software zen4: ESPResSo 4.2.1 ([PR #598](#)) & 4.2.2 ([PR #609](#)), TensorFlow 2.13.0 ([PR #610](#)), R 4.3.2 ([PR #611](#)), GROMACS 2024.1 ([PR #612](#)), ParaView 4.11.2 ([PR #631](#)), missing installations with foss/2023b ([PR #614](#))
- Additional software A64FX: OpenMPI 4.1.5 ([PR #620](#)), foss/2023a ([PR #622](#)), SciPy-bundle 2023.07 ([PR #624](#)), ESPResSo 4.2.2 ([PR #625](#)), foss/2023b ([PR #626](#))
- Fix emoticon for failing test step ([PR #600](#))
- Add mem per node setting in ReFrame configuration template ([PR #605](#)) & dynamically create ReFrame config with correct amount of memory ([PR #606](#))
- Fix --extra-bind-paths argument in bot/test.sh ([PR #607](#)); use latest Ubuntu in CI workflows ([PR #621](#))

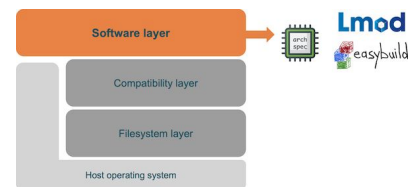
Progress update: software layer (2/3)



Recent active open PRs + issues:

- Additional software: CP2K 2023.1 ([PR #630](#))
- Support for installing GPU builds into a sub-directory ([PR #615](#))
- Enable `eessi_container.sh` to mount several CVMFS repos with individual access mode ([PR #616](#))
 - Useful for `dev.eessi.io` repository
- Support for multiple CVMFS repositories in `eessi_container.sh` ([PR #618](#))
- Workaround to fix broken curl installation ([PR #623](#))

Progress update: software layer (3/3)

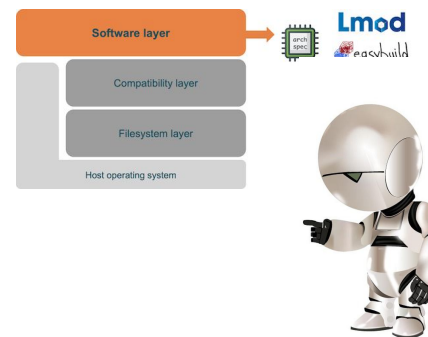


Additional CPU targets

- **AMD Genoa (zen4)**
 - ~50% done (298 modules in place, vs 644 for fully supported CPU targets)
 - Trouble with Highway, see [PR #627](#), required for R-bundle-Bioconductor 3.18 ([PR #613](#))
- **Intel Sapphire Rapids**
 - New build cluster in AWS is set up incl. Sapphire Rapids partition, need to configure bot
- **Arm A64FX** (mainly for EuroHPC system Deucalion)
 - 119 modules in place (~18% done), incl. ESPResSo
 - Requires work in archdetect, see ([PR #608](#))
 - [Blog post](#) available on ESPResSo on Vega/Karolina/Deucalion via EESSI

Bot for building + deploying software layer

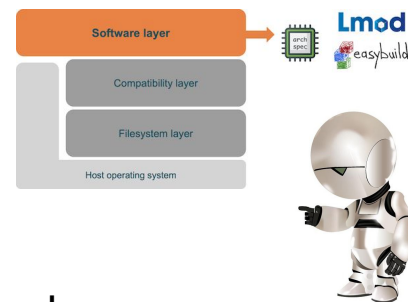
<https://github.com/EESSI/eessi-bot-software-layer>



- June'24
 - Bot instance started on Deucalion for `aarch64/a64fx`
- Ongoing work
 - Add setting to give all jobs a unique name [PR#273](#)
 - Automatic cleanup of shared disk storage when PR has been merged [PR#271](#)
 - Enabling GPU builds (next slide)
 - Revisit software-layer [PR#267](#): cleanup of local tmp disk storage on compute nodes
 - Improve deployment (ingestion efficiency, single approval PR, flexible tasks)
- Side note: over 13,000 Slurm jobs have been submitted on AWS Slurm cluster (bot + test suite)

Bot for building + deploying software layer

<https://github.com/EESSI/eessi-bot-software-layer>



Enabling GPU builds: changes/additions to `bot: build ...` commands

- Traditional command syntax `bot: build architecture:x86_64/amd/zen3`
 - Submit job to zen3 node *AND* to set value of `$EESSI_SOFTWARE_SUBDIR_OVERRIDE`
- Extend this to build for accelerators by using an additional parameter: `accel:nvidia/cc80`
 - This will install the software to a subdirectory of the corresponding CPU target
- Initially, only build on CPU nodes. Can be extended later on by actually using GPU nodes.
 - Not all combinations of CPU+GPU are available
 - Control build node type with an additional parameter, e.g. `"node:"`

EESSI production repository

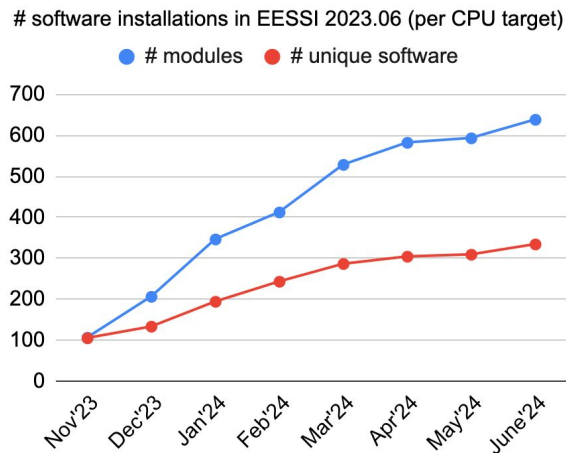
eessi.io/docs



`software.eessi.io` is the **production-ready EESSI repository**

Version 2023.06 is now being populated with software via [PRs to software-layer repo](#) + build-and-deploy bot

- 8 supported CPU targets: see eessi.io/docs/software_layer/cpu_targets
- 3 more CPU targets being added: zen4, sapphirerapids, a64fx
- Initial support for NVIDIA GPUs is in place, see eessi.io/docs/gpu
- **Currently: 638 software installations per CPU target**
(+46 compared to last EESSI update meeting)
 - 334 different software projects (+35),
5,522 software installations (across 8+3 CPU targets, +695)
- Current focus:
 - Providing optimized software installations for AMD Genoa (Zen4) + Intel Sapphire Rapids + A64FX
 - Adding more software, processing incoming contributions, fixing broken builds/test suites



EESSI documentation



eessi.io/docs - GitHub repo github.com/EESSI/docs

Improvements to the EESSI documentation: ~20 closed PRs

- Update known issue about lmod hook in host-injection ([PR #183](#))
- How to do site-specific configuration, deploy Lmod hooks, etc ([PR #188](#))
- **Docs running EESSI from a virtual machine (via Lima on macOS, WSL on Windows)** ([PR #201](#))
- Run workflow to update overview of available software every 4 hours (PRs [#203](#) + [#204](#) + [#205](#))
- Update link to available software in repository page (PR [#202](#))
- Updates for software overview (PRs [#200](#), [#206](#), [#208](#), [#211](#), [#213](#), [#220](#))
- Exclude a64fx from overview of available software for now ([PR #216](#))
- Add new available tests to documentation ([PR #217](#))
- **Add blog post on Portable test run of ESPResSo on EuroHPC systems via EESSI** ([PR #218](#))

EESSI documentation



eessi.io/docs - GitHub repo github.com/EESSI/docs

Overview of available software in EESSI (`software.eessi.io`, version 2023.06)

- High-level overview: https://www.eessi.io/docs/available_software/overview
- Separate page per supported software project with more details,
see for example https://www.eessi.io/docs/available_software/detail/OpenFOAM
- Does not include CPU targets yet for which installations are incomplete (zen4, a64fx, ...)
- Semi-automatically updated as more software gets added
 - PR is opened automatically by GitHub Actions workflow if update is needed
 - Overview in documentation is updated when PR is merged

EESSI documentation

eessi.io/docs - GitHub repo github.com/EESSI/docs



Improvements to the EESSI documentation - open PRs:

- How to build on top of EESSI without EB ([PR #175](#))
- Add zen4 to software overview (draft) ([PR #185](#))

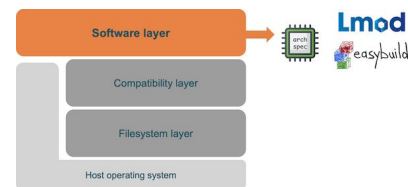
EESSI test suite

eessi.io/docs/test-suite - github.com/EESSI/test-suite

3 releases: [v0.3.0](#), [v0.3.1](#), [v0.3.2](#)

Merged pull requests:

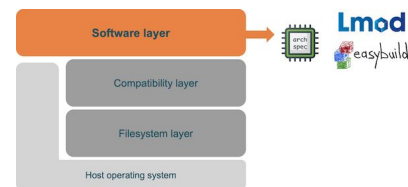
- Update config AWS MC cluster to use `software.eessi.io` ([PR #126](#))
- Test for QuantumESPRESSO (pw.x) ([PR #128](#))
- Tests for ESPResSo: P3M + Lennard-Jones (PRs [#144](#), [#155](#), [#158](#), [#160](#))
- Use compact process binding for GROMACS ([PR #139](#))
- Use `software.eessi.io` repo in CI ([PR #146](#))
- Use MiB units for memory per node (PRs [#151](#), [#152](#), [#153](#))
- Change behavior for `assign_tasks_per_compute_unit` on hyperthreading-enabled systems ([PR #160](#))
- Add config for Deucalion ([PR #162](#))



ReFrame

EESSI test suite

eessi.io/docs/test-suite - github.com/EESSI/test-suite



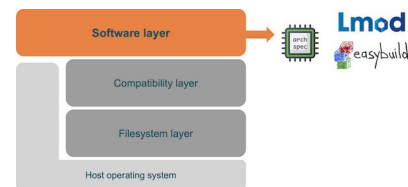
ReFrame

Open pull requests:

- Test for PyTorch ([PR #130](#))
- Test for LAMMPS, depends on hook from CP2K PR ([PR #131](#))
- Test for CP2K, depends on hook from QuantumEspresso (now merged) ([PR #133](#))
- Test for mpi4py (WIP), simple test, will serve as example for documentation on how to write tests for the EESSI test suite ([PR #149](#))

EESSI as backend in Ramble

<https://googlecloudplatform.github.io/ramble>



- Ramble is tool to easily run experiments for software applications
- Spack was used as “package manager” backend
 - To (build and) install software before running tests with it
- Very interesting use case for EESSI
 - No need to install anything if EESSI repo is mounted & software is available in EESSI !
- Meeting on 13 June'24 with lead developer after quick chat at Google booth @ ISC'24
- Major enhancement to re-design package manager support was already happening ([PR #535](#))
- Pull request in Ramble has been opened to add EESSI as “package manager” backend, see <https://github.com/GoogleCloudPlatform/ramble/pull/551>

EESSI RISC-V repository

[eessi.io/docs/repositories/
riscv.eessi.io/](https://eessi.io/docs/repositories/riscv.eessi.io/)



`riscv.eessi.io` is the **development repository for a RISC-V software stack**

- Same client config: if you can access `software.eessi.io`, you can also access `riscv.eessi.io`
- Version 20240402 is currently being worked on
 - Compat layer has been modified to fix user id resolving issues (see [issue #32](#) in EESSI support portal)
 - Sourcing the init script of `software.eessi.io` will automatically redirect you to `riscv.eessi.io`
 - Fixes for failing numpy tests have been added to the easyconfig (PR [#20847](#))
 - ESPResSo 4.2.2 has been installed with foss/2023b 🎉 (PR [#20878](#))
 - ReFrame 4.3.3 has been installed, after applying a fix for its PyYAML dependency (PR [#20879](#))
 - Extrae 4.2.0 was successfully built (not ingested yet) on RISC-V (PR [#20690](#))

EESSI development repository



`dev.eessi.io` is the **development repository for EESSI**

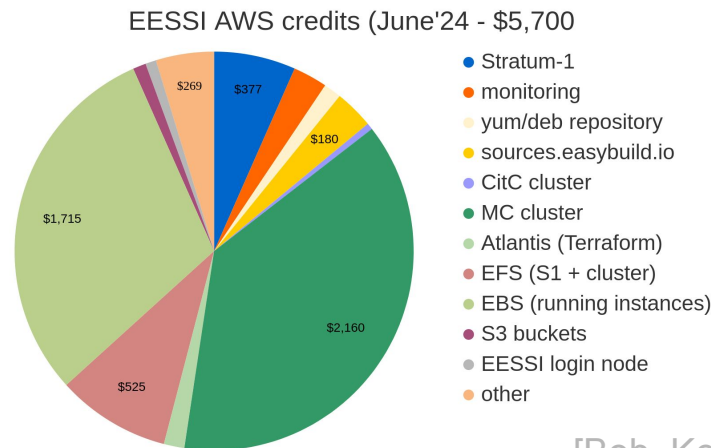
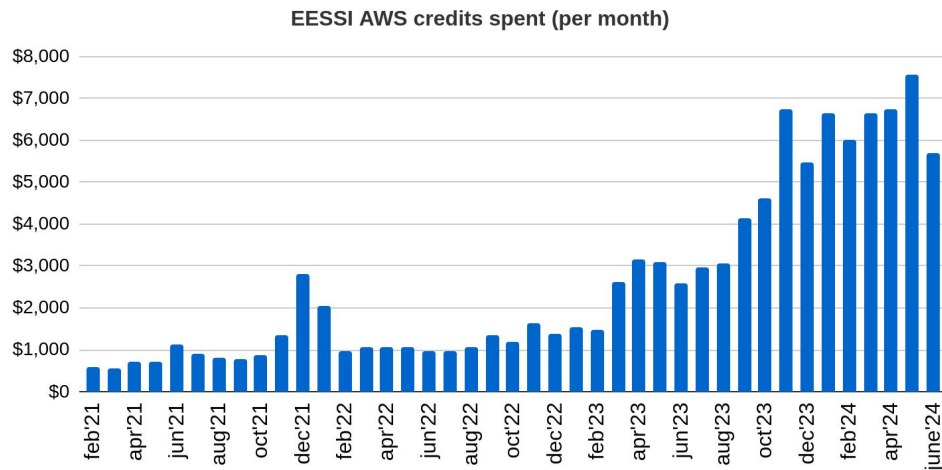
Allows developers to make pre-release versions available, facilitate testing across various systems, avoid rebuilding pre-release versions... progress in support portal [#61](#)

- Completed tasks: CernVM-FS repository setup, GitHub repository, S3 bucket for ingestion
- Work in progress: Script to auto-generate easyconfig from a commit, changes in `eessi_container.sh` ([PR #618](#))
- To do: add functionality to software-layer scripts, create new bot instance, setup slurm build cluster on Azure, setup private GitHub repository for bot configuration

Sponsored AWS credits



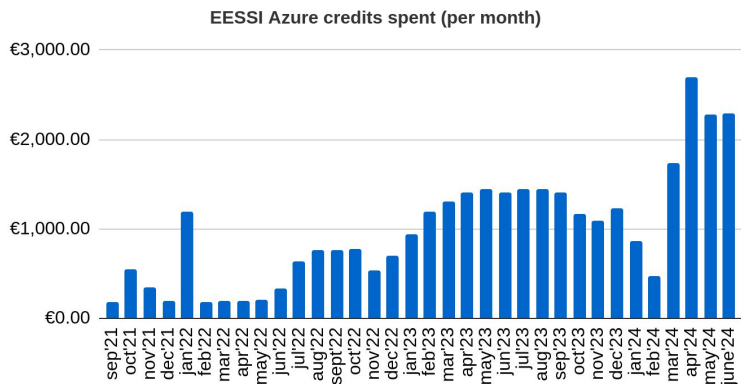
- Ask in #aws-resources Slack channel to get access!
- ~\$5,700 “spent” in June’24 on Stratum-1 servers, monitoring, sources.easybuild.io, debugging (build) issues, demos, **Slurm clusters (build bot)**, testing on Sapphire Rapids, ...
- **Bulk of consumed credits due to EESSI build-and-deploy bot**
- Small decrease thanks to cleaning up EFS for old Slurm cluster (still not entirely finished)
- ~Monthly sync meetings with AWS



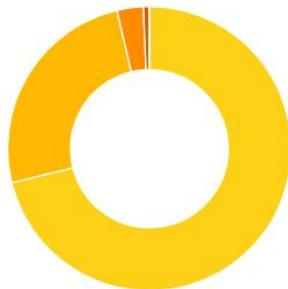
Sponsored Azure credits



- Ask in #azure-resources Slack channel to get access!
- In June: ~€2,288 worth of credits spent
- Used for: **Slurm cluster for bot (Zen4)**, Stratum-1 mirror servers, GitHub Runners
- Slurm cluster with Magic Castle in place for EESSI build-deploy bot



Service name ▾



Resource group name ▾



June'24

[Bob, Kenneth]

Upcoming events

- CernVM Workshop 2024: 16-18 Sept 2024 @ CERN (Geneva)
<https://indico.cern.ch/event/1347727/overview>
 - Talk on EESSI submitted by Thomas
- EuroHPC User Day 2024: 22+23 Oct 2024 in Amsterdam,
https://eurohpc-ju.europa.eu/news-events/events/eurohpc-user-day-2024-2024-10-22_en
 - We plan to have a strong presence at this event...



Next EESSI update meeting

- **There will be no update meeting on Thu 1 Aug 2024** (summer break)
- Next EESSI update meeting on Thu 5 Sept 2024, 12:00 UTC (14:00 CEST)