EESSI

EUROPEAN ENVIRONMENT FOR
SCIENTIFIC SOFTWARE INSTALLATIONS

6 Mar 2025

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

Agenda

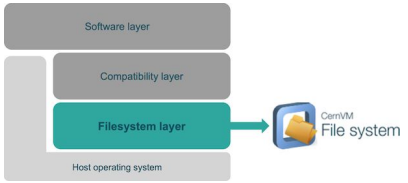
- Quick introduction by new people
- Progress update per EESSI layer
- Update on EESSI production repository `software.eessi.io`
- Update on EESSI test suite, build-and-deploy bot, documentation
- AWS/Azure sponsorship update
- EESSI governance: initial Steering Committee
- Integration of EESSI in EuroHPC Federation Platform (**incl. open position at UGent**)
- Upcoming/recent events
- 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?

Progress update: filesystem layer



- All CernVM-FS servers have been updated to CernVM-FS 2.12.7
- Monitoring showed no noteworthy issues with the infrastructure
  - Few network outages of the Stratum 0 server, which caused no issues
- `cvmfs_shrinkwrap` is now included in the EESSI client container (PR #205)
  - Allows you to export (a part of) the EESSI environment to a SquashFS file
  - See also support issue #90
- Some initial/preparatory work on verifying the signatures of tarballs and metadata files
  - See next slide

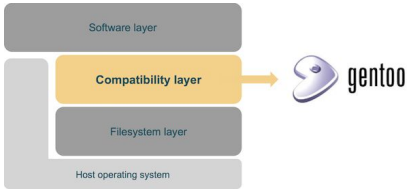
[Bob, Pedro, Kenneth]

Signing and verifying tarballs before ingestion

- Improve security by signing tarballs (and corresponding metadata files) produced by the bot before uploading them to S3 bucket for ingestion on Stratum 0
- Ingestion procedure on Stratum 0 will verify the signatures before ingesting
- Can use GPG or SSH keys
  - For now, use SSH keys, as they're easier to use
  - Every bot uses a different private key
  - Stratum 0 collects the public keys into an authorized signers file
- Hope to have this new procedure tested + required for the new EESSI version (2025.03?)
  - Incl. support for NVIDIA Grace as CPU target

[Lara, Pedro, Helena, Bob, Xin, Kenneth, Caspar…]

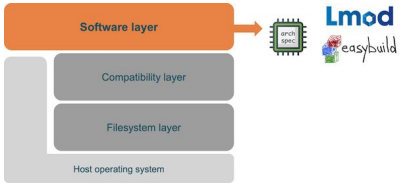
Progress update: compatibility layer



- Progress on compatibility layer of next EESSI version (2025.03?)
  - WIP PR #209 for playbooks & co for compat layer
  - WIP PR #108 for package set
  - Full discussion on new version in support issue #56
  - In short: new toolchains (foss/2024a), latest glibc version, OpenSSL 3.x, `ld.bfd`-only, using EasyBuild 5.0+, version bumps for all components, signed tarballs
  - glibc version 2.41 with significant performance improvements for Arm has been released (Jan'25)
  - Latest test builds for `x86_64`, `aarch64`, `riscv64` were successful 🎉
  - Should be almost ready now
    - Only some small changes (e.g. for `host_injections`) required?

[Bob, Kenneth, Thomas, …]

Progress update: software layer (1/4)



Highlights of recently merged software PRs:

- elfx86exts 0.6.2 (PR #846), DP3 6.2 + EveryBeam 0.6.1 + WSClean 3.5 (PR #877), archspec 0.2.5 (PR #905), OpenCV 4.8.1 (PR #959)

Build entire Sapphire Rapids stack:

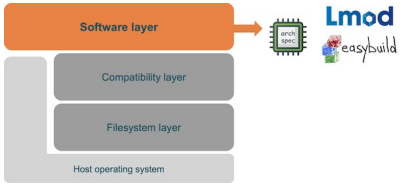
- PRs #921, #923, #925, #926, #927, #928, #929, #930, #931, #932, #933, #934, #935, #936, #938, #939, #940, #941, #942, #943, #944, #945, #946, #947, #950, #952, #953, #954, #955, #956, #960

Rebuilds:

- LAMMPS for `*/generic` targets to make sure that CPU-specific optimizations are disabled (PR #788)
- SciPy-bundle 2023.07 w/ additional patches (PR #866)
- R-bundle-CRAN-2023.12 extensions sync between CPU targets (PR #914)
- rebuild `CUDA/*` module files (PR #919)
- scikit-build-core w/ additional extension (PR #957)
- R-bundle-Bioconductor 3.18 extension sync (PR #958)

[Kenneth, Thomas, Richard, Pedro, Bob, Lara, Caspar, Satish, Alan, …]

Progress update: software layer (2/4)

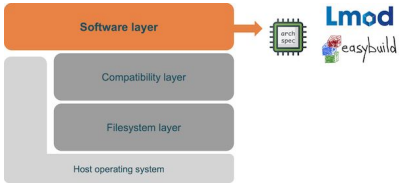


Recent active open PRs + for general improvements:

- Add pre-install hook that raises an error in case `keeppreviousinstall` (used for rebuilds) is set but the installation directory still contains files (PR #881)
- Add dev.eessi.io support including project subdirectories (PR #885)
- Test building on Snellius @ SURF: Zen4/H100 (PR #903)
- Test if non CUDA builds are not added to accelerator path with jax (PR #917)
- Updated `link_nvidia_host_libraries.sh` for better edge case handling (PR #922)
- proof of concept for GitHub action that opens an issue for a PR (PR #937)
- Add a script that can sign a file based on an ssh key (PR #948)
- Add OpenMPI host injection script (PR #963)
- Add new GPU workflow (PR #949)

[Kenneth, Thomas, Richard, Pedro, Bob, Lara, Caspar, Satish, Alan, …]

Progress update: software layer (3/4)

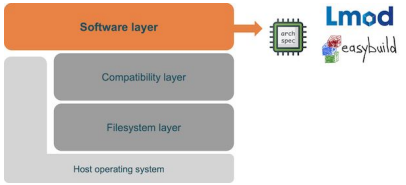


Recently merged general improvement PRs:

- Add support in archdetect for detecting A64FX (PR #608)
- Disable using `x86_64/amd/zen3` installations when `x86_64/amd/zen4` is detected (PR #766)
- Let 2023.06 modulefile redirect RISC-V clients to riscv.eessi.io, add symlink for 20240402 version (PR #840)
- Print `LmodError` when loading GCCcore-12.2.0-based modules on zen4 (PR #841)
- Add support for alternative artefacts checks in check-build.sh (PR #844)
- Make sure `eessi_container.sh` will add `--nv` flag for the test step, when GPUs are available (PR #847)
- Transition CI workflows to Ubuntu 24.04 (PR #849)
- Replace the use of a ReFrame template config file for a manually created one (PR #850)
- Workaround that solves permission issues for rebuilds (PR #871)
- Fix test mapping for OSU test that got renamed in the EESSI test suite (PR #872)
- Generate and hide foss-2022b modules for zen4 (PR #874)
- Make sure the latest release of the test suite is used (#880 + fix) (PR #886)

[Kenneth, Lara, Caspar, Bob, Alan, Thomas …]

Progress update: software layer (3/4)



Recently merged general improvement PRs:

- Improved workaround that solves permission issues for rebuilds (PR #907)
- Fix bug when defining multiple modules in `app.cfg` (PR #908)
- Fix behavior for present but failing `nvidiasmi` (PR #908)
- Make sure that the `TMPDIR` is used as `STORAGE` if it is set (PR #911)
- Add CI to compare stacks, checking for both modules and extensions (PR #913)
- Deploy archdetect spec file that was updated in #889 (PR #913)
- Add Lmod startup hook that prints an error when loading removed/relocated modules (PR #962)

Recently merged GPU improvements and builds:

- Allow Nvidia driver script to set recommendations for `LD_PRELOAD` (PR #754)
- Adjust `SitePackage.lua` for multiple `CUDA/cu*` modules (PR #798)
- Add CUDA toolkits for `zen4_h100` (PR #915)
- rebuild CUDA/* module files (take 2) (PR #919)

[Kenneth, Lara, Caspar, Bob, Alan, Thomas …]

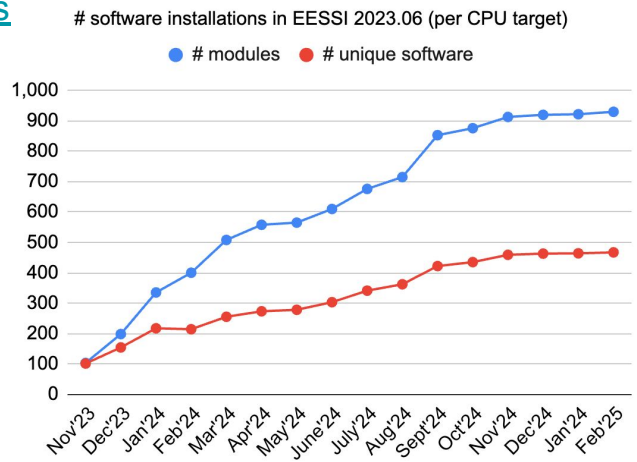
EESSI production repository

eessi.io/docs

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

Version 2023.06 is being populated with software via PRs to software-layer repo + build-and-deploy bot

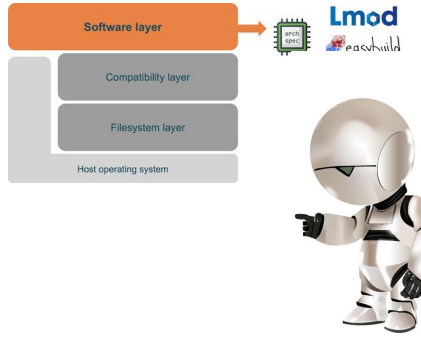
- **10** supported CPU targets: see eessi.io/docs/software_layer/cpu_targets
- **AMD Zen4 (Genoa)** + **Intel Sapphire Rapids** now also fully supported
- Optimized builds for A64FX (Deucalion) is still work-in-progress
- Initial support for NVIDIA GPUs is in place, see eessi.io/docs/gpu
- **Currently: 930 software installations per CPU target**
  (+10 in Jan+Feb'25)
  - 467 different software projects (+4),
    9,453 software installations (across 10+1 CPU targets, +1,176)



- Current focus:
  - Adding more (CUDA) software, processing incoming contributions, fixing broken builds/test suites, …
  - Complete set of installations for A64FX

[Kenneth, Bob, Alan, Caspar, Lara, Thomas, Richard, Pedro,, …]

Bot for building + deploying software layer



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

- January-February'25
  - PR #292: Bot only reports moving to trash_bin when relevant
  - PR #293: Added information in README.md on how to create a ReFrame configuration file for the software-layer test step
  - PR #297: First attempt at enabling two ways to submit/receive jobs -> submitted job into the future (2095)
  - PR #298: Fix for the docs
  - PR #299: Set the local_tmp that is configured for a site as tmpdir
  - PR #302: Add setting for a script to customize build environment
- Ongoing work
  - Installing bot on clusters with support for GPUs: UGent, SURF, JSC
  - Signing tarballs and metadata files: bot PR303 & software-layer PR948
- Side note: almost 50,000 Slurm jobs have been submitted on AWS Slurm cluster (bot + test suite)

[Thomas, Bob, Kenneth, Lara, Pedro]

EESSI documentation

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

Improvements to the EESSI documentation: ~17 merged PRs (+ 10 updates to software overview)

Highlights:

- Make EESSI more FAIR by adding schema.org metadata to the software overview pages (PR #385)
  - Related issue with more information: issue #383
  - Example: search.google.com/test/rich-results/result?id=KE5D95wqXROwc64wqTWQPw
- Add Zen 4 and Sapphire Rapids to supported CPUs and software overview pages (PR #306 + #376)
  - eessi.io/docs/available_software/overview
  - eessi.io/docs/software_layer/cpu_targets
- Blog post about integrating EESSI into the EuroHPC Federation Platform (PR #380)
- Added slides of SURF ACUD2024 talk and EPICURE Arm hackathon

[Lara, Pedro, Helena, Bob, Xin, Kenneth, Caspar…]

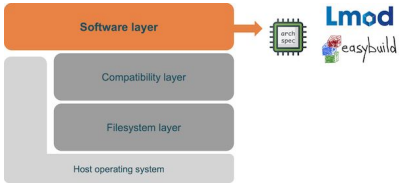
EESSI documentation

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

- Auto-updates to overview of available software: eessi.io/docs/available_software/overview
- Several new entries to the overview of systems where EESSI is known to be available: eessi.io/docs/systems
  - **If you know about additional systems where EESSI is available, let us know!**
- EESSI blog: eessi.io/docs/blog

[Lara, Pedro, Helena, Bob, Xin, Kenneth, Caspar…]

EESSI test suite



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

ReFrame

Highlights

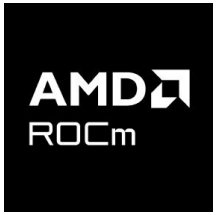
- Implemented the `eessi_mixin` for the existing tests
  (see PRs for QuantumESPRESSO , PyTorch , TensorFllow, OSU + PR #246 with bug fix)
- Add hook for `exact_memory` (#214, #245)
- Update and Bug fixes of the CI (#227, #220, #225, #226, #227, #247)
- New release 0.5.0 and 0.5.1, see github.com/EESSI/test-suite/releases

Planned

- API documentation
- Engage more users and contributors to the test-suite
  - Planned hand-on session during EUM'25 for users to create configs on their system(s)

[Caspar, Sam, Satish, Kenneth, Lara]

Adding support for AMD GPUs (ROCm)

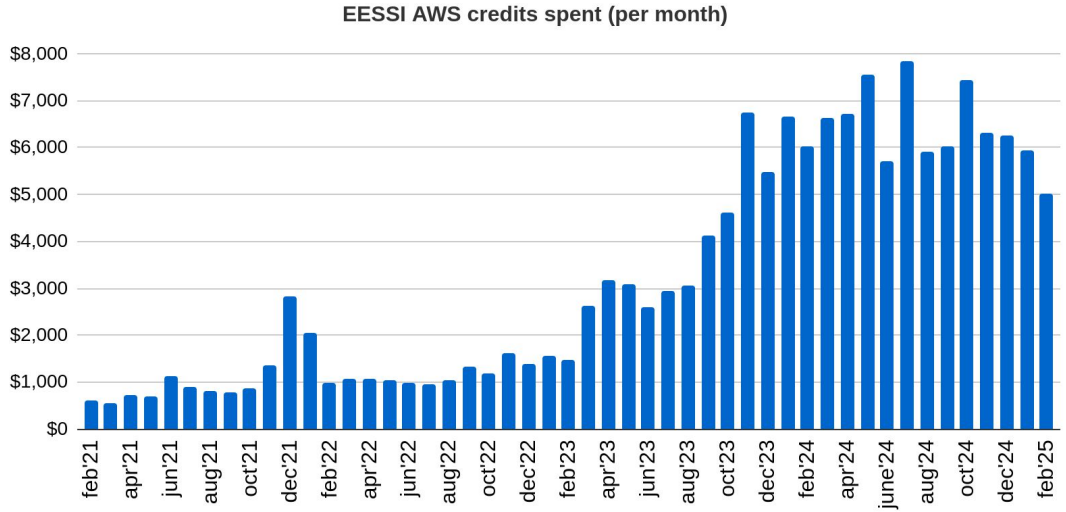


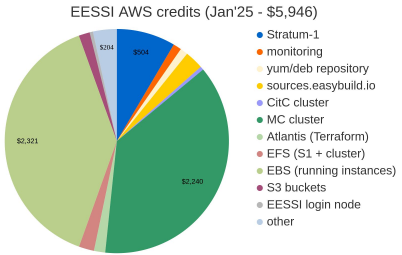
- Work on adding support for AMD GPUs has started
- Gitlab ticket with a lot of information, discussion, and feedback
  - https://gitlab.com/eessi/support/-/issues/71
- First trying to get the ROCm stack installed with EasyBuild
  - Current easyconfigs and the ones in open PRs are very outdated
  - Lots of things have been changed in the meantime
  - Some initial draft versions at https://github.com/bedroge/eb-rocm
- Recent sync meeting about the current status and short-term plans
  - https://github.com/EESSI/meetings/wiki/Sync-meeting-on-EESSI-ROCm-support-(2025-02-21)

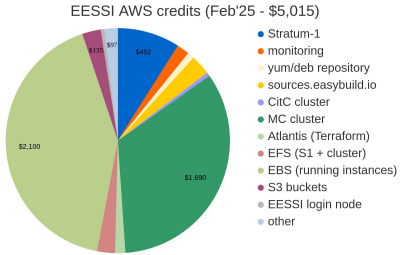
[Bob]

Sponsored AWS credits

- Ask in #aws-resources Slack channel to get access!
- ~$5,946 + $5,015 “spent” in Jan'25 + Feb'25 on Stratum-1 servers, monitoring, demos, sources.easybuild.io, debugging (build) issues, Slurm clusters (build bot), building for Sapphire Rapids, …
- **Bulk of consumed credits due to EESSI build-and-deploy bot**
- Regular sync meetings with AWS - more sponsored credits have been provided for coming months



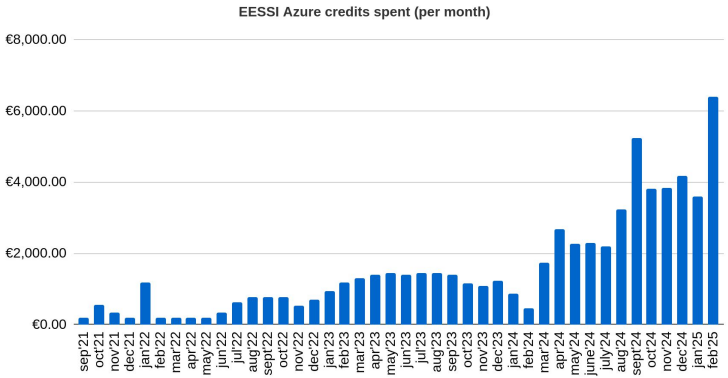


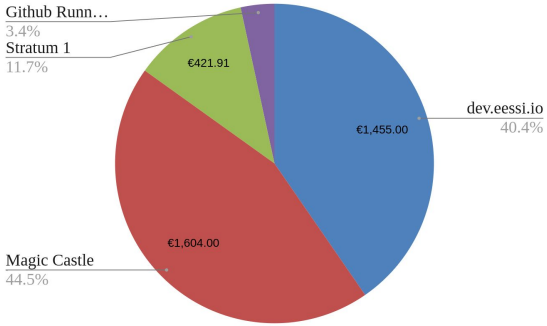


[Kenneth, Bob]

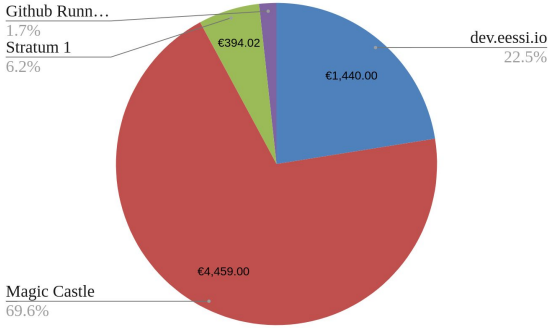
Sponsored Azure credits

- Ask in #azure-resources Slack channel to get access!
- In Jan+Feb'25: €3,604+€6,405 worth of credits spent
- Used for: **Slurm cluster for bot (Zen4)**, Stratum-1 mirror servers, GitHub Runners, GPU nodes, …
- Ongoing discussions to extend sponsored credits into 2025





Jan'25 (€3,604)



Feb'25 (€6,405

[Kenneth, Bob]

EESSI Governance - (interim) Steering Committee

- (interim) Steering Committee https://eessi.io/docs/governance
  - Kenneth/Lara, Alan/Davide, Bob/Henk-Jan, Caspar/Satish, Thomas/Terje
- 2nd meeting of interim Steering Committee for EESSI was held 11 Feb 2025
- Mostly continued discussion on setting up governance for EESSI
- To be continued in next meeting (1 April 2025),
  discussing governance proposal that is currently being drafted

Integration of EESSI in EuroHPC Federation Platform

- Consortium was selected to implement the EuroHPC Federation Platform (EFP), a “one-stop shop” to facilitate usage of EuroHPC systems
- 5-year project (2025-2029)
- Consortium led by CSC.fi, Ghent University as one of the partners
- EESSI will be integrated into EFP as part of the Federated Software Stack component
  - Important to note: EESSI itself (and its development) is **not** funded by EFP
  - Ways of funding EESSI beyond MultiXscale (2023-2026) are being actively explored…
- **Blog post with more details published on 10 Feb 2025:** https://www.eessi.io/docs/blog/2025/02/10/integration-efp
- **Open position in Ghent University to work on this** (applications due by 23 March 2025) https://jobs.ugent.be/job-invite/28366

[Kenneth, Lara]

Upcoming webinars/presentations on EESSI

- **10th EasyBuild User Meeting** 2025: 25-27 March in Jülich (Germany) - https://easybuild.io/eum25
  - All (50) seats taken for in-person attendance
  - Remote attendance still possible (via Zoom), but you need to register!
  - Day 3 will be focused on EESSI
    - Talks on EESSI, MultiXscale, dev.eessi.io, EESSI test suite, NVIDIA GPU support, …
    - Also related talks: EuroHPC Federation Platform, CernVM-FS, Lmod, …
- Proposal for both EESSI tutorial and Birds-of-a-Feather session at ISC'25 were rejected :(

Frequency of EESSI update meeting

- EESSI update meetings are **bi-monthly**
- First Thursday of the month at 14:00 CE(S)T, only in odd months
  - iCalendar URL for calendar integration
- Next meetings:
  - Thu ~~1 May~~ **8** May 2025 14:00 CEST (12:00 UTC)
  - Thu 3 July 2025 14:00 CEST (12:00 UTC)
  - Thu 4 Sept 2025 14:00 CEST (12:00 UTC)