EESSI

EUROPEAN ENVIRONMENT FOR SCIENTIFIC SOFTWARE INSTALLATIONS

6 June 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. Using EESSI on macOS
8. AWS/Azure sponsorship update
9. Upcoming/recent events: ISC'24
10. Q&A

Quick introduction by new people

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

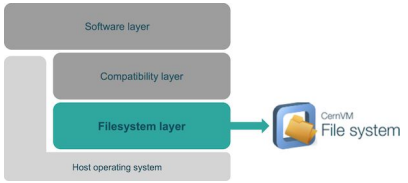
- Who are you, where do you work, on what?
- Why are you interested in the EESSI project?
- Are you planning to actively contribute,
  and if so, to which aspect(s) of the project?

EESSI-related meetings & events

- *(3+23 May'24)* EESSI test suite sync meeting (notes, notes)
- *(3 May'24)* Meeting to discuss public dashboard (notes)
- *(13 May'24)* CernVM-FS coordination meeting (preparing a 2.12 feature release)
- *(14 May'24)* MultiXscale WP1+WP5 sync meeting (notes)
- *(24 May'24)* dev.eessi.io discussion (notes)
- *(27 May'24)* sync meeting on GPU support (notes)
- *(May'24)* Weekly support team sync meetings *(notes are in private wiki on EESSI support portal)*

[Bob, Kenneth]

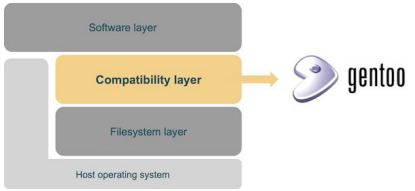
Progress update: filesystem layer



- The playbooks in the filesystem-layer GitHub repo are now using our fork of ansible-cvmfs role (PR #179)
  - Includes a bunch of fixes and additional features that we need, e.g. S3 support
- Fixed DNS name of the EESSI Stratums in the Squid proxy configuration template (PR #189)

[Bob, Kenneth]

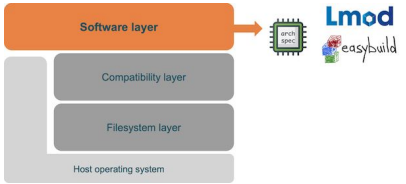
Progress update: compatibility layer



- 2023.06 version in EESSI pilot repository (`pilot.eessi-hpc.org`)
  - No recent changes here, **EESSI pilot repository is no longer actively maintained!**
  - The initialization scripts now make this clear (PR #551)
    - Print a deprecation message
    - Automatically use `software.eessi.io` if available
    - Stick to `pilot.eessi-hpc.org` otherwise, or if `$EESSI_FORCE_PILOT` is set
  - We will/should remove the `pilot.eessi-hpc.org` repository at some point…

[Bob, Kenneth, Thomas, …]

Progress update: software layer (1/3)

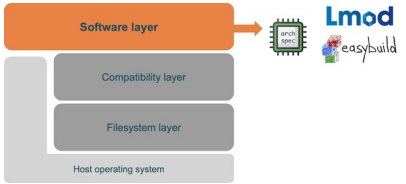


Recently merged PRs:

- Additional software: ESPResSo 4.2.2 (PR #584), ipympl 0.9.3 (PR #587), GATK 4.5.0.0 (PR #588), ParaView 5.11.1 + deps (PR #590), WhatsHap 2.2 + deps (PR #592), ASE (PR #595), Java 17.0.6 (PR #588)
- Easyconfig that can extend EESSI (PR #371)
- Add support for detecting zen4 in archdetect (PR #451)
- Initial installations for `x86_64/amd/zen4` CPU target: foss/2023a (PR #565), foss/2023b (PR #566)
- Ship matches for name stubs of allowlist for CUDA (PR #559)
- Show Lmod warning/message when ESPResSo v4.2.1 is loaded (PRs #560 + #589)
- Use `x86_64/amd/zen3` with Zen4 until optimized software is available (PR #569 + #573)
- Fix CI: Rebuild GROMACS, and fix check for missing installations after updates upstream to libfabric (PR #576)
- Automatically redirect RISC-V users to riscv.eessi.io + initial RISC-V support for archdetect (PR #583)

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

Progress update: software layer (2/3)

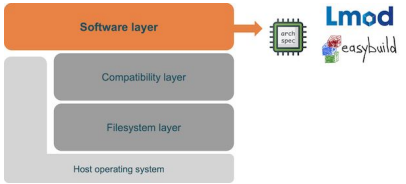


Recent active open PRs + issues:

- Additional software: Extrae (PR #554), QuantumESPRESSO 7.3 (PR #504), Qt6 (PR #534), OpenFOAM v2312 (PR #563), Paraver (PR #570), PyTorch-bundle (PR #585)
- Add possibility to ignore certain hooks on local modules (PR #530)
- Enable mounting previous overlay-upper read-only (PR #550)
- Use `--from-commit` instead of `--from-pr` (PR #558)
  - Requires bug fix in EasyBuild, see framework issue #4540
- Only run OSU test for now in test step (PR #571)
- Use directory of called script as base dir for other scripts (PR #580)
- SciPy-bundle for x86_64/amd/zen4 CPU target: PRs #593 + #594

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

Progress update: software layer (3/3)



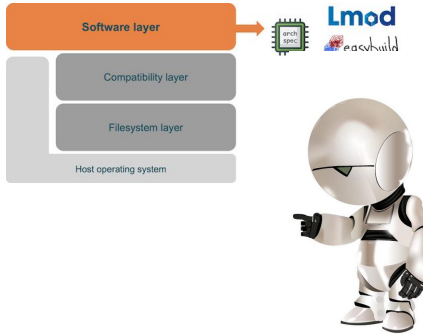
Adding GPU-software:

- Open PRs (work in progress): cuDNN (PR #581), PyTorch w/ CUDA (PR #586)
- Discussion/plan on supporting GPUs/accelerators (Issue #59)
- Build non-optimised fallback for supported CPU families (ARM, x86) which will work on all GPUs
    - Lowest non-deprecated CUDA compute capability (believed to be 6.0)
- Build a finite set of build that are specific to CPU + CUDA compute capability
    - Example installation path for EasyBuild would be (to be set via hook):

`software/x86_64/generic/accel/nvidia/cc60` (generic CPU + NVIDIA P100 or newer)
`software/x86_64/amd/zen2/{software,modules/all}` # CPU (current installation path)
`software/x86_64/amd/zen2/accel/nvidia/cc80/{software,modules/all}` # A100 (Vega)
`software/x86_64/amd/zen2/accel/nvidia/cc80` (Vega: AMD Rome + A100 - compute capability 8.0)
`software/x86_64/amd/zen3/accel/amd/gfx90a` (LUMI: AMD Milan + MI250X - LLVM target gfx90a)

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

Bot for building + deploying software layer

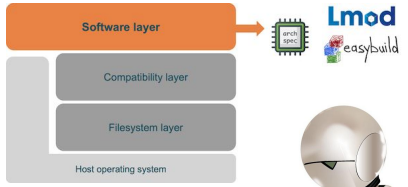


https://github.com/EESSI/eessi-bot-software-layer

- May'24
  - New release v0.5.0: more concise display of build targets, repo-agnostic deployment, improved handling of string constants, verification of bot configuration
- Ongoing work
  - 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 12,000 Slurm jobs have been submitted on AWS Slurm cluster (bot + test suite)

[Thomas, Bob, Kenneth, Lara, Pedro]

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:linux/x86_64/amd/zen3`
  - Submit job to zen3 node *AND* to set value of `$EESSI_SOFTWARE_SUBDIR_OVERRIDE`
- Extend this to build for compute capabilities (CC) and to submit to nodes w/out GPUs

  `arch:zen3+cc80` -> arch value defines install directory and requests CUDA CC

  `node:zen3+cc80` -> node value ensures job is submitted to node with zen3 CPU and cc80 GPU

  `bot: build arch:zen3+cc80 node:zen3+cc80` -> software tests that require a GPU could run

  `bot: build arch:zen3+cc80 node:zen3` -> software tests that require a GPU could NOT run

  Maybe use `target` instead of `architecture`?

  One could add specifiers like `cpu` and `gpu` to value parts, e.g., `arch:cpu-zen3+gpu-cc80`

[Thomas, Alan]

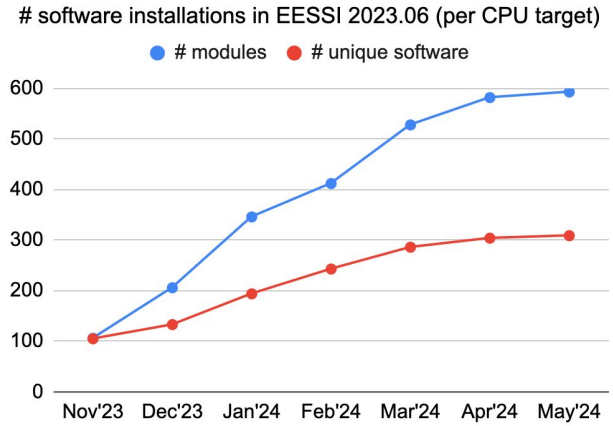
EESSI production repository

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
- Initial support for NVIDIA GPUs is in place, see eessi.io/docs/gpu
- **Currently: 593 software installations per CPU target**
  (+11 compared to last EESSI update meeting)
  - 309 different software projects (+5),
    4,827 software installations (across 8+1 CPU targets, +152)
- Current focus:
  - Providing optimized software installations for AMD Genoa (Zen4) + Intel Sapphire Rapids
  - Adding more software, processing incoming contributions, fixing broken builds/test suites



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

EESSI documentation

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

Improvements to the EESSI documentation - 27 closed PRs!

- How to setup private Stratum 1 (PR #157)
- How to debug test step (PR #158)
- How to rebuild software (PR #170)
- Known issues (PR #172)

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

EESSI documentation

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

Improvements to the EESSI documentation - 27 closed PRs!

- Add blog post on ISC'24 (PR #178)
- CI improvements (PR #180, #181, #187, #196)
- Add overview of available software (PR #161, #162, #163, #184, #186, #189, #190, #192, #193, #194, #195, #197, #199)
- Several expansions / improvements to existing docs (PR #173, #176, #177, #182)

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

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
- GitHub Actions workflow in place to keep this automatically updated as more software gets added (not running automatically yet, but will soon)

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

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)
- Update known issues (PR #183)
- Add zen4 to software overview (draft) (PR #185)
- How to do site-specific configuration, deploy Lmod hooks, etc (PR #188)

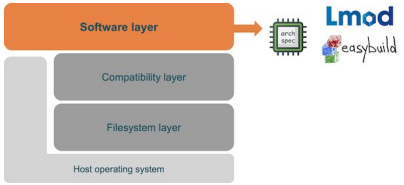
[Lara, Pedro, Helena, Bob, Xin, Kenneth, Caspar…]

EESSI website

- https://www.eessi-hpc.org now auto-redirects to https://eessi.io
- Outdated non-maintained old website is now gone (was top search result in Google & co)
- eessi-hpc.org domain is owned by Univ. of Groningen (was Dell)

[Bob, Henk-Jan, Alan, Kenneth]

EESSI test suite



ReFrame

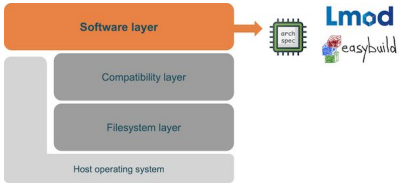
eessi.io/docs/test-suite - github.com/EESSI/test-suite

Merged pull requests:

- Test for QuantumEspresso (PR #128)
- Fixed process binding hook + applied to GROMACS (PR #139)
- Renamed two scales, for easier tag selection (PR #140)
- Set `$SRUN_CPUS_PER_TASK` to avoid issues with certain SLURM versions (PR #141)
- Fix MPI issues for daily runs on Karolina (PR #142)
- Reduce OSU iteration count for faster test to keep runtime reasonable on slower networks (PR #143)
- Use `software.eessi.io` for CI (PR #146)
- Fix some forgotten version updates for 0.2.0 release and release instructions (PR #147, PR #148)

[Caspar, Sam, Satish, Kenneth, Lara]

EESSI test suite



ReFrame

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

Open pull requests:

- Test for PyTorch, ready for review (PR #130)
- Test for ESPResSo, ready for review (PR #144)
- 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)

[Caspar, Sam, Satish, Kenneth, Lara]

EESSI RISC-V repository

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 20240307 has been removed, version 20240402 is currently being worked on
  - Compat layer in `/cvmfs/riscv.eessi.io/versions/20240402/compat/linux/riscv64/`
  - Sourcing the init script of `software.eessi.io` will automatically redirect you to `riscv.eessi.io`
  - The `foss/2023b` toolchain has been installed, and some additional software on top
    - R 4.3.3, GROMACS 2024.1, OSU-Micro-Benchmarks 7.2, etc
    - See notes in https://github.com/EESSI/software-layer/issues/552 and `#risc-v` Slack channel
    - Only doing generic builds for now (EB support added in framework PR #4489)
    - EasyBuild's upcoming `foss/2024a` toolchain should fully support RISC-V out of the box, no components with backported RISC-V support anymore

[Bob, Julian]

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…

- `dev.eessi.io` CernVM-FS repository is available, along with (private) GitHub repository
- Discussion with EESSI maintainers and MultiXscale software developers on 24 May (notes)
  - Obtain needs and requirements from the scientific side, plan next steps
  - Initial goal: be able to build `ESPResSo` from a specific commit and then deploy it semi-automatically to `dev.eessi.io`
- Next steps (progress in support portal #61):
  - Setup Slurm cluster
  - Set up private config repository
  - Adjust scripting / bot build container

[Pedro, Bob, Alan, Kenneth, ..]

Using EESSI on macOS (via Lima)

- A support question came in about using EESSI on macOS (using a container): https://gitlab.com/eessi/support/-/issues/70
- Alan found out that Lima can be used to run Apptainer on macOS
  - It will run a small Linux VM
  - Somewhat similar to WSL on Windows
- You can actually create custom Lima template files (see examples) for the VM to be created
  - Example for one that includes a native CVMFS installation can be found in Bob's comment in the issue, removing the need for Apptainer
- Lara is working on adding this to the EESSI documentation

[Alan, Kenneth, Bob, Lara]

Using EESSI on macOS (via Lima)

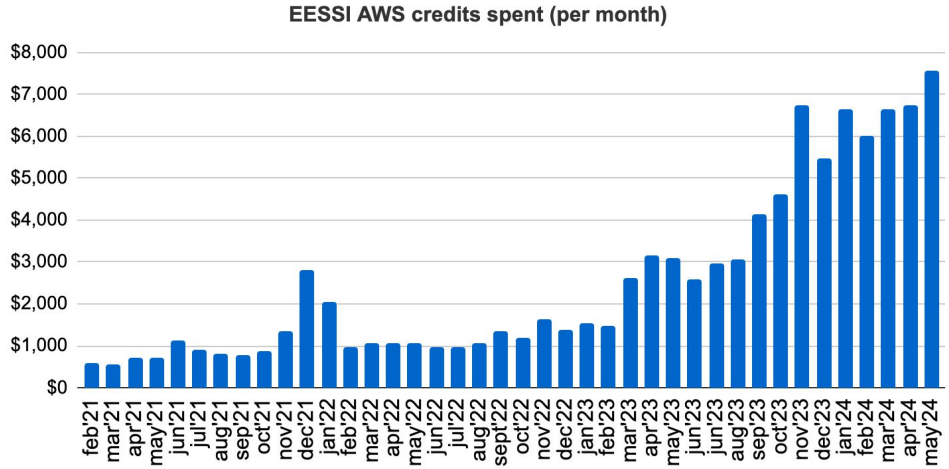
- Install Lima: **`brew install lima`**
- Create VM: **`limactl create --name=eessi eessi.yaml`**
- Start VM: **`limactl start eessi`**
- Open shell in VM: **`limactl shell eessi`**
- Access & use EESSI:

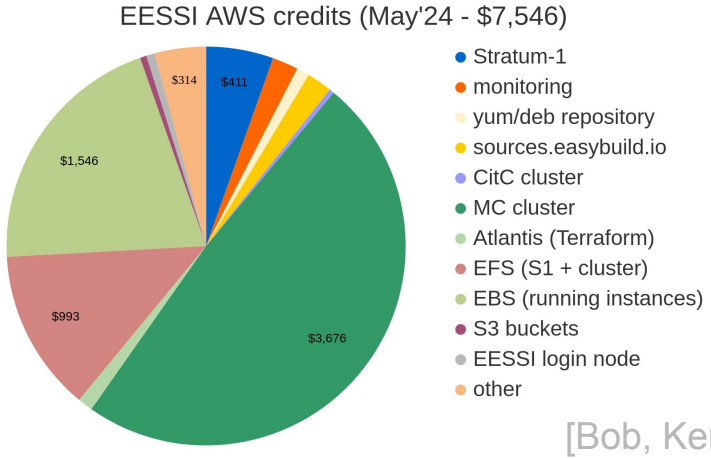
```
kehoste@lima-eessi $ source /cvmfs/software.eessi.io/versions/2023.06/init/bash
Found EESSI repo @ /cvmfs/software.eessi.io/versions/2023.06!
archdetect says aarch64/neoverse_n1
Using aarch64/neoverse_n1 as software subdirectory.
…
Environment set up to use EESSI (2023.06), have fun!
```

[Alan, Kenneth, Bob, Lara]

Sponsored AWS credits

- Ask in #aws-resources Slack channel to get access!
- ~$7,546 “spent” in May’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**
- Frequent sync meetings with Brendan/Angel/Matt/Francesco (AWS)

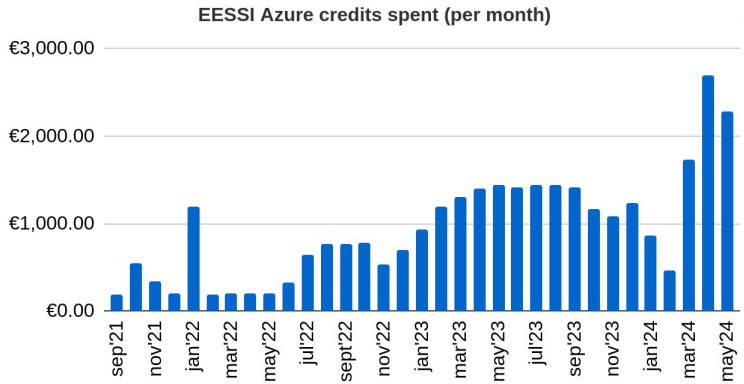


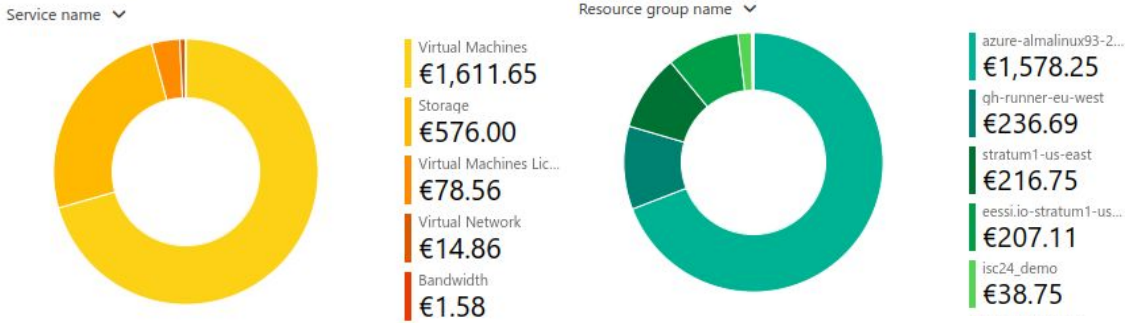


[Bob, Kenneth]

Sponsored Azure credits

- Ask in #azure-resources Slack channel to get access!
- In May: ~€2,283 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





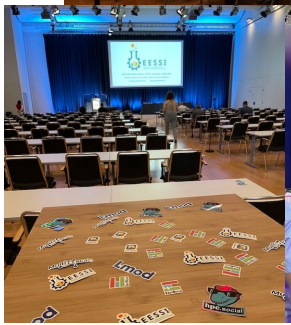
May'24

[Bob, Kenneth]

EESSI @ ISC'24

- 12-16 May 2024 in Hamburg (Germany) - isc-hpc.com

- EESSI was part of official program:
  - Birds-of-a-Feather session
  - 3 workshops: RISC-V, Arm, POP CoE
- Also present at ISC exhibit:
  - Azure booth (two 1h talks + 4h demo session)
  - MultiXscale talk at EuroHPC booth



- Detailed report available at https://www.eessi.io/docs/blog/2024/05/17/isc24

[Kenneth, Lara, Julián, Elisabeth, …]