

2 May 2024

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

Agenda

J'L

- 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. EESSI RISC-V repository riscv.eessi.io
- 7. EESSI support portal
- 8. AWS/Azure sponsorship update
- 9. Update on MultiXscale EuroHPC project
- 10. Upcoming/recent events: EasyBuild User Meeting 2024 + ISC'24
- 11. 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



- (9 Apr) MultiXscale WP1+WP5 sync meeting (notes)
- (15 Apr'24) Azure/EESSI sync meeting (notes)
- (18 Apr'24) MultiXscale general meeting (scientific + technical work packages) (no public notes)
- (18 Apr'24) EESSI test suite sync meeting (notes)
- (22 Apr'24) CernVM-FS coordination meeting (mostly about patch release 2.11.3)
- (Apr'24) Weekly support team sync meetings (notes are in private wiki on EESSI support portal)

Progress update: filesystem layer



- Stratum 1 servers using the Geo API need to update to CernVM-FS 2.11.3 as soon as possible
 - The GeoAPI has changed, and otherwise database updates fail (as of May 1st)
 - Done for the EESSI Stratum 1 servers (both for the pilot and production repositories)
- Add software build container based on Debian Sid, which has support for RISC-V (PR #132)
- Added a dev.eessi.io repository, which is now available (PR #188)
 - Still need to set up workflows and policies for this repository
- Kenneth ordered a bunch of CernVM-FS stickers (after syncing up with CernVM-FS team)
 - Hopefully will be shipped in time for ISC'24...



Progress update: compatibility layer



- Install nss-pam-ldapd and sssd in compat layer with custom USE flags
 (open PR #199 + gentoo-overlay PR #99)
 - Only installs the clients, and communicates with the host daemons; no need for host symlinks anymore
 - Should solve LDAP / user ID resolving issues, see https://gitlab.com/eessi/support/-/issues/32
 - This has now been deployed to the production repo (software.eessi.io) too
- New RISC-V compatibility layer (PR #204) available at /cvmfs/riscv.eessi.io/versions/20240402
- 2023.06 version in EESSI pilot repository (pilot.eessi-hpc.org)
 - No recent changes here, EESSI pilot repository is no longer actively maintained!
 - Make this clear in the initialization scripts (open <u>PR #551</u>)
 - 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

Progress update: software layer (1/3)



Recently merged PRs:

- Additional software: EasyBuild v4.9.1 (<u>PR #537</u>), ELPA 2023.05.001 (<u>PR #508</u>), GROMACS (<u>PR #499</u>), Highway (PRs #529 + #532), libxc 6.2.2 (<u>PR #508</u>), Modflow 6.4.4 + deps (<u>PR #522</u>), ncdu (<u>PR #542</u>)
 R-bundle-Bioconductor v3.16 (<u>PR #526</u>) + v3.18 (<u>PR #533</u>), R-bundle-CRAN 2023.12 (<u>PR #428</u>), SAMtools (<u>PR #553</u>)
- Add fix for permissions set on Lmod SitePackage (PR #538)
- Fix archdetect: ensure we use instructions introduced with ARM v8.2 for Neoverse N1 (PR #540)
- Make sure software directory that corresponds to \$EESSI_SOFTWARE_SUBDIR_OVERRIDE exists (PR #543)
- Rebuild hatchling 1.18.0, Python 3.11.*, Python-bundle-PyPI-2023.* to solve setuptools_scm issue (PR #546)
- Update demo scripts for Bioconductor and GROMACS (PRs #33 + #35)
- Remove build_container.sh script (replaced by more capable eessi_container.sh) (PR #544)

Progress update: software layer (2/3)



GROMACS success story:

- Failing tests on aarch64/neoverse_v1 blocked inclusion in EESSI 2023.06 for a while
- Problem was reported upstream: https://gitlab.com/gromacs/gromacs/-/issues/5057
- GROMACS developers confirmed bug in SVE support (seems like it was only tested on A64FX, 512-bit SVE)
- Workaround for GROMACS 2024.1 installed for aarch64/neoverse_v1:
 disable use of SVE by configuring GROMACS with -DGMX_SIMD=ARM_NEON_ASIMD
- Nice example of potential in collaborating with developers for software being added to EESSI

Progress update: software layer (3/3)



Recent active open PRs + issues:

- Additional software: Extrae (<u>PR #554</u>), QuantumESPRESSO 7.3 (<u>PR #504</u>), Qt6 (<u>PR #534</u>)
- Easyconfig that can extend EESSI (PR #371)
- Script to determine license for software being included in EESSI (PR #457)
- Make EESSI compatible with archspec 0.2.3+ (PR #485)
- Add possibility to ignore certain hooks on local modules (<u>PR #530</u>)
- Enable mounting previous overlay-upper read-only (PR #550)
- Start installing software for amd/zen4 CPU target: EasyBuild v4.9.1 (PRs #547 + #548)
- Update init scripts for pilot repo to print deprecation warning & use software.eessi.io (PR #551)
- Use --from-commit instead of --from-pr for installations done with EasyBuild v4.9.1 (PR #558)

Bot for building + deploying software layer



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

- April'24
 - Open <u>PR#266</u> rework of how string constants are used
 & check at start that app.cfg contains all needed settings
 - Setup and test of bot on Azure (building for zen4)
- Ongoing work
 - Automatic cleanup of shared disk storage when PR has been merged
 - Revisit software-layer <u>PR#267</u>: cleanup of local tmp disk storage on compute nodes
 - Improve deployment (ingestion efficiency, single approval PR, flexible tasks)
- Side note: over 10,000 Slurm jobs have been submitted on AWS Slurm cluster (bot + test suite)

EESSI production repository

eessi.io/docs



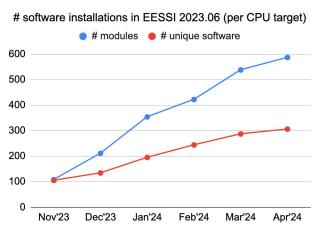
software.eessi.io is the production-ready EESSI repository

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 <u>eessi.io/docs/gpu</u>
- Currently: 587 software installations per CPU target (+54 compared to last EESSI update meeting)
 - 306 different software projects (+19),
 ~4,711 software installations (across 8 CPU targets, +516)



- Providing optimized software installations for AMD Genoa systems (Zen4)
- Adding more software, processing incoming contributions, fixing broken builds/test suites



EESSI documentation

<u>eessi.io/docs</u> - GitHub repo <u>github.com/EESSI/docs</u>

Improvements to the EESSI documentation - open PRs:

- Add overview of available software (<u>PR #161</u>, <u>PR #162</u>, <u>PR #163</u>)
- Add instructions on how to rebuild software (PR #170)
- Add known issues (<u>PR #172</u>)
- Update outdated page on build nodes (<u>PR #173</u>)
- Adding documentation on how to build and run on top of EESSI without EB (PR #175)

EESSI test suite

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

Merged pull requests:

Prevent running scorecards CI on forks (PR #134)

Open pull requests:

- Test for QuantumEspresso (PR #128)
- Test for PyTorch (PR #130)
- Test for LAMMPS (<u>PR #131</u>)
- Test for CP2K (<u>PR #133</u>)

WIP (no PR yet):

- Test for OpenFOAM
- Test for ESPResSo





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 will be removed soon, version 20240402 is currently being worked on
 - Compat layer in /cvmfs/riscv.eessi.io/versions/20240402/compat/linux/riscv64/
 - There are init scripts, but they don't support RISC-V yet; you have to override variables yourself
 - Working towards getting the foss/2023b toolchain installed
 - 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)
 - Issues solved so far: GCC (fixed multiarch support in PR #20035), FFTW (disabled quad precision in PR #3314), UCX (RISC-V support backported in PR #20428; use regular configure script in PR #20429), UCC (RISC-V support backported in PR #20432)
 - Open issue: no RISC-V support in BLIS 0.9.0 (though there is on the main branch)

Support for EESSI (MultiXscale task 5.4)



EESSI support portal: gitlab.com/eessi/support

- Support requests can be created via issue in GitLab, or sending an email to support@eessi.io
- Issues in support portal can be public or private (only visible to reporter + support team)
- Information on support portal and support policy => <u>eessi.io/docs/support</u>
- Support is "reasonable effort" + only for problems with how software was installed in EESSI
- 3 issues opened + 4 closed in last month (some of which are by support team to track ongoing tasks)

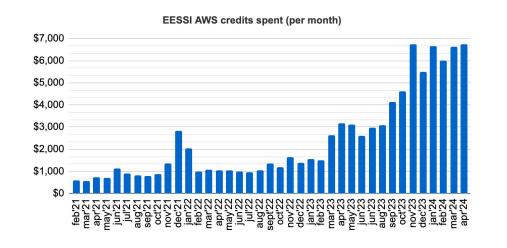
Support rotation (in scope of MultiXscale Task 5.4)

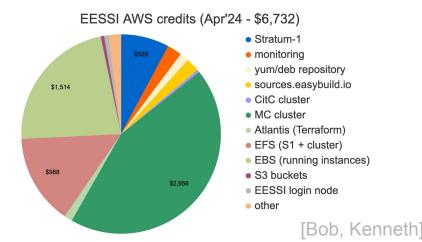
- A MultiXscale project partner is primarily responsible for support for 2 consecutive weeks
- Weekly regular support sync meetings between MultiXscale project partners
- Since Jan'24: ~1 FTE dedicated for support effort (across all project partners)
- Project partners involved in Task 5.4: UGent (lead), SURF, UGroningen, UBarcelona, UBergen, HPCNow!

Sponsored AWS credits



- Ask in #aws-resources Slack channel to get access!
- ~\$6,730 "spent" in Apr'24 on Stratum-1 servers, monitoring, sources.easybuild.io,
 debugging (build) issues, demos, Slurm clusters (build bot)
- Bulk of consumed credits due to EESSI build-and-deploy bot
- Frequent sync meetings with Brendan/Angel/Matt/Francesco (AWS)





Sponsored Azure credits





azure-almalinux93-2...

eessi.io-stratum1-us...

gh-runner-eu-west

€2,079.21

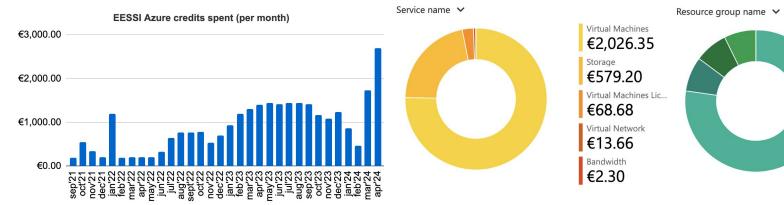
stratum1-us-east

€212.16

€202.95

€195.38

- Ask in #azure-resources Slack channel to get access!
- In Apr: ~€2,690 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



Mar'24

[Bob, Kenneth]

eessi

€0.25









www.multixscale.eu

github.com/multixscale

- MultiXscale deliverables (2023): <u>multixscale.eu/deliverables</u>
- Pairing up of people from technical WPs with developers from scientific WPs
 - Explore how EESSI can be helpful to them
 - Including deployment of "development" versions of the software they work on,
 via new dev.eessi.io CernVM-FS repository
- POP CoE has reached out to us to see if installing their performance analysis tools available in EESSI makes sense (it does)



EasyBuild User Meeting 2024





- Tue-Thu 23-25 April 2024 @ Umeå University (Sweden) <u>easybuild.io/eum24</u>
- Yearly meeting, focus on EasyBuild & related projects
- Slides + recording of all talks available via https://easybuild.io/eum24/#program
- 3rd day was focused on EESSI:
 - Intro to EESSI + overview of current status
 - Contributing to EESSI
 - Hands-on session
 - Beyond the basics: EESSI test suite + GPU support in EESSI

EasyBuild User Meeting 2024













EESSI @ ISC'24





- 12-16 May 2024 in Hamburg (Germany) <u>isc-hpc.com</u>
- (Mon 17:30-18:30) Talk on EESSI at Azure booth
- (Tue 09:00) **Birds-of-a-Feather session "EESSI Community BoF"** (Kenneth + Lara)
- (Tue 14:00-18:00) EESSI demo session at Azure booth
- (Wed 14:45-15:15) MultiXscale talk at EuroHPC booth
- (Thu) Talk at RISC-V workshop (Julián): "Preparing to Hit the Ground Running: Adding RISC-V support to EESSI" (Julián)
- (Thu) Talk at AHUG workshop (Kenneth): "Extending Arms reach by going EESSI"
- (Thu) Talk at POP workshop on MultiXscale & EESSI (Lara)
- Expected involvement in EuroHPC + Azure booth at ISC'24 exhibit (Kenneth, Lara, Elisabeth, ...)
- We may/should also organise some kind of social event...