



E E S S I

EUROPEAN ENVIRONMENT FOR
SCIENTIFIC SOFTWARE INSTALLATIONS

5 Oct 2023

<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 (incl. build-and-deploy bot + test suite)
4. EESSI pilot repository (2023.06)
5. Outlook to new EESSI repository (`software.eessi.io`)
6. EESSI support portal
7. AWS/Azure sponsorship update
8. Update on MultiXscale EuroHPC project
9. Upcoming events
10. Q&A

Quick introduction by new people



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

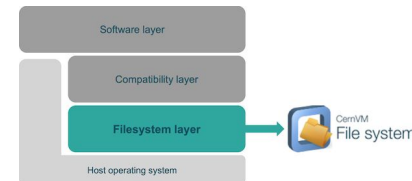
- Who are you, where do you work, on what?
- Why are you interested in the EESSI project?
- Are you planning to actively contribute,
and if so, to which aspect(s) of the project?

EESSI-related meetings



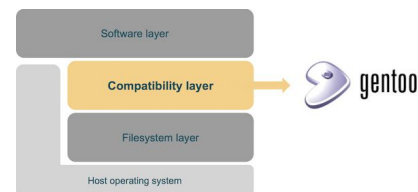
- (12 Sept'23) MultiXscale sync meeting (WP1+WP5) ([notes](#))
- (14 Sept'23) EESSI/AWS sync meeting (no notes?)
- (18 Sept'23) EESSI/Azure sync meeting ([notes](#))
- Sync meetings on building software for EESSI 2023.06 (notes: [12 Sept](#), [20 Sept](#), [26 Sept](#), [3 Oct](#))
- Sync meetings on EESSI test suite (notes: [20 Sept](#), [4 Oct](#))
- Sync meetings on Magic Castle clusters for EESSI (notes: [21 Sept](#), [26 Sept](#), [4 Oct](#))
- (25 Sept'23) Sync with CernVM-FS developers on Best Practices in HPC tutorial ([notes](#))
- (26 Sept'23) Sync meeting on EESSI support portal ([notes](#))
- (2 Oct'23) CernVM-FS coordination meeting ([notes](#))

Progress update: filesystem layer



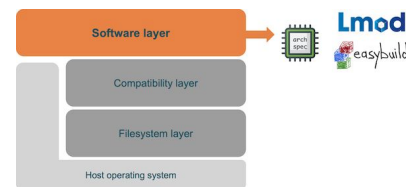
- New Stratum-0 server for EESSI at Univ. of Groningen
 - More or less ready, except for giving more people access
 - Created a new `software.eessi.io` repository
 - Tested with three (temporary) Stratum 1 servers in AWS and Azure: one uses S3 storage
 - WIP [PR#160](#): contains the new (temporary) configuration, see build artifacts for client packages
- How do we want to set up the entire CVMFS infrastructure for the new repository?
 - Meeting to discuss this next week
- Still need to figure out performance issues with Stratum-1 @ RUG ([issue #151](#))
- Automated ingestion is having (performance) issues due to the increasing number of tarballs
 - Hitting a GitHub API rate limit
 - Some quick improvements have been made, but it hasn't fully solved the issue

Progress update: compatibility layer



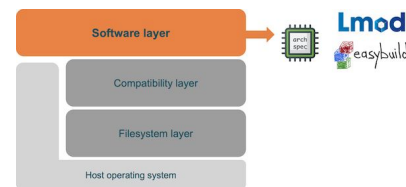
- 2023.06 version is available in EESSI pilot repository (`pilot.eessi-hpc.org`)
 - Was built with bot (see [PR #188](#))
 - Deployment was still done manually, needs more work to automate (see [issue #189](#))
 - No recent changes here
- **2023.04 version of compat layer has been removed from pilot repository**
 - Only consisted of compat layer (incl. OpenSSL 3.x) - no software layer was in place
- Compat layers for `software.eessi.io` repo have been built (version 2023.06) ([PR #191](#))
 - Basically same setup as in EESSI pilot 2023.06, but with repo under `eessi.io`
 - May be a nice opportunity to also let bot take care of deployment (not just building it)
- Quite a lot of Gentoo security (GLSA) notifications recently
 - How much do we care about these, since everything is running in user space anyway?

Progress update: software layer (1/3)



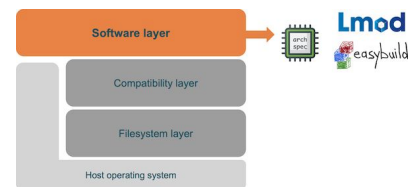
- Incorrect CPU detection by archspec for zen3 ([issue #322](#)) and neoverse_v1 ([issue #320](#))
- Fix for archdetect, so we can use it by default in EESSI init script (open [PR #264](#))
- Script to more easily inspect a build job - ready to test/review/merge (open [PR #317](#))
- YAML file to keep track of known issues in EESSI pilot 2023.06 (PRs [#340](#) + [#353](#))
 - For now just to have a record of known issues, can later be used to generate overview of available software
- Determine easystack files to process via PR patch file (PRs [#351](#) + [#354](#))
 - To help avoid hitting GitHub rate limit quickly due to use of `eb --*from-pr`
- Use easybuild/sources subdirectory in shared filesystem path as EasyBuild source path (PRs [#337](#) + [#342](#))
- CI for testing if EESSI stack is available is only checking single architecture ([issue #349](#))
- Bot configuration files have been moved to (private) [EESSI/bot-configs repo](#) ([PR #356](#))

Progress update: software layer (2/3)



- Every now and then, we run into problems that only pop up when building for EESSI
 - Failing tests on `aarch64/neoverse_v1` CPU target (which supports SVE vector instructions)
 - Problems specific to use compatibility layer or RPATH linking
- Recently merged EasyBuild PRs relevant to EESSI:
 - Only use `-DCMAKE_SKIP_RPATH=ON` for CMake < 3.5.0 ([easyblocks PR #3012](#))
 - Add patch for MPFR 4.1.0 to fix failing `tsprintf` test with `glibc` >= 2.37 ([easyconfigs PR #18746](#))
 - Add patch for OpenBLAS 0.3.23 to fix hanging tests ([easyconfigs PR #18790](#))
 - Fix permission issues when copying `xvfb-run` script in Xvfb easyconfigs ([easyconfigs PR #18834](#))
 - Fix issue with detection of NeoverseV1 CPU architecture in OpenBLAS v0.3.20 ([easyconfigs PR #18870](#))
 - Avoid use of hardcoded paths for Pillow with `--disable-platform-guessing` ([easyconfigs PR #18881](#))

Progress update: software layer (3/3)



New Slurm clusters being set up using [Magic Castle](#)

- Actively developed/supported neutral tool to spin up “throwaway” Slurm clusters
- Significantly more mature than Cluster-in-the-Cloud, supports both AWS + Azure (& more)
- Configuration stored in [EESSI/magic-castle-clusters](#) (private repo, contains sensitive data)
- All figured out on AWS, test cluster in place, doing final checks...
- Will migrate build-and-deploy bot from CitC cluster in AWS to Magic Castle cluster in AWS soon...
- Will also look into spinning up a Magic Castle cluster in Azure (for building, testing, ...)

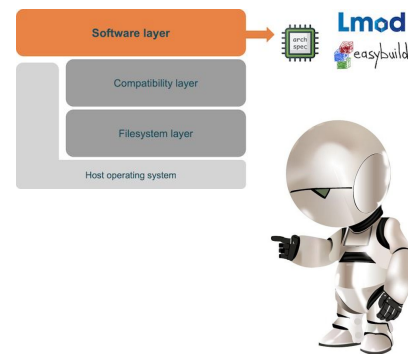
See also [Magic Castle tutorial at SC'23](#) in Denver (Nov'23)!

Bot for building + deploying software layer

Progress on implementation of build-and-deploy bot

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

- **First release v0.1.0** (29 September 2023) - see [v0.1.0 release in GitHub](#)
 - Total stats for v0.1.0: 82 merged PRs, 48 closed issues
 - Possibly some bugfix release(s) 0.1.x before next minor release (0.2.0)
 - [PR#220](#) omit header lines in `squeue` output
- Next minor release: v0.2.0
 - Support running EESSI test suite after a build, before deploy
 - Remove code in the deployment function that is specific to [EESSI/software-layer](#)
 - Tool to clean up disk space (removing tarballs of closed/merged PRs) [PR#217](#)



EESSI pilot repository (1/3)

<https://www.eessi.io/docs/pilot>

**NOT FOR
PRODUCTION USE!**



- 2021.12 version is “frozen”, no more changes planned there, but it's still the default ("latest") version
- 2023.06 is being populated via [PRs to software-layer repo](#) + build-and-deploy bot
 - Supported CPU targets: see http://www.eessi.io/docs/software_layer/cpu_targets
 - Recently added software installations (for all supported CPU targets):
 - R 4.1.0 with foss/2021a ([PR #328](#)) + R 4.2.0 with foss/2021b ([PR #335](#))
 - GDAL v3.3.0 with foss/2021b ([PR #329](#)) + OpenFoam v2112 with foss/2021b ([PR #330](#))
 - EasyBuild v4.8.1 + re-install Java/11 with it ([PR #333](#)) + ReFrame 4.3.3 ([PR #338](#))
 - foss/2022a ([PR #310](#)) + [issue #325](#) (flaky tests for FFTW.MPI on neoverse_v1)
 - foss/2023a ([PR #334](#))
 - BAMM ([PR #350](#))
 - Only increase limit for numerical test failures for OpenBLAS for aarch64/neoverse_v1 ([PR #345](#))
 - **We currently have 375 software installations per CPU target => 3,000 installations in total !**

EESSI pilot repository (2/3)

<https://eessi.github.io/docs/pilot>

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- 2023.06 is being populated via [PRs to software-layer repo](#) + build-and-deploy bot
 - TensorFlow (v2.7.1 in [PR #321](#), v2.8.4 in [PR #343](#), v2.11.0 in [PR #346](#), v2.13.0 in [PR #347](#))
 - Failing tests on `aarch64/*` with v2.7.1 probably too to properly support running on Arm?
 - Build problems with newer versions on aarch64 due to passing `-mcpu=native` to XNNPACK (fixed w/ patch)
 - More build problems on aarch64 due use of outdated Eigen library (fix is WIP...)
 - WRF (PRs [#290](#) + [#336](#)):
 - hook updated to support recent WRF versions
 - [fix in CMakeMake easyblock](#) available to fix problems with netCDF tests due to RPATH
 - ESPResSo (PRs [#331](#) + [#332](#)): wrong Python is being used, need to add more CMake options?
 - matplotlib v3.4.3 with foss/2021b ([PR #339](#)): trouble with hardcoded `/usr/*` paths used by Pillow dependency
 - SciPy-bundle 2022.05 with foss/2022a ([PR #352](#)): built, deploying...
 - TODO:
 - Bioconductor, waLBerla, LAMMPS, ...
 - Ensure that Lmod cache update is done correctly, includes `*all*` available modules
 - Come up with a better approach to replace existing software installations

EESSI pilot repository (3/3)

<https://eessi.github.io/docs/pilot>

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Policy to deal with limited number of failing tests that only occur on a particular CPU target

- Assess whether failing tests really seem to signal a serious problem
 - Very small number of (additional) failing tests => probably not a reason to block installation
 - Only for a specific CPU target: `neoverse_v1` is Arm 64-bit with SVE vector instructions support
- Put workaround in place to ignore failing tests (yet retain test suite result in EasyBuild installation log)
 - Should be relatively easy to do via the custom EasyBuild hooks we use ([eb_hooks.py](#))
- **Open tracker issue** in [EESSI/software-layer repo](#) that provides all details + allows following up
- **Report the problem upstream**, try and get feedback to assess severity of the problems + how to fix
- Examples: OpenBLAS, FFTW, numpy on `aarch64/neoverse_v1` (issues [#314](#), [#318](#), [#325](#), [#344](#))
- TODO: Properly document this policy, should probably be part of contribution policy ([docs PR #108](#))

Contribution policy (proposal)



- **Proposal** for contribution policy for adding software to EESSI ([docs PR #108](#))
 - Preview available [here](#) - will be reworked based on feedback
 - **Final request for feedback**, contribution policy will be added to EESSI docs mid Oct'23
 - Initial policy - can be revised later as needed (policy will be versioned, changelog will be kept)
- Summary:
 - Only open source software (we should verify this by requiring [SPDX license IDs](#))
 - Software must be built by the bot (no manual builds) and support by latest EasyBuild release
 - `eb --from-pr` and `--include-easyblocks-from-pr` should only be used for *merged* PRs
 - A compiler toolchain still supported by latest EasyBuild release must be used
 - Ideally all software is installed for all supported CPU targets (exceptions allowed)
 - Recent software versions and toolchains should be preferred
 - There should be a way of testing the installations - ideally via the [EESSI test suite](#)
- Policy being applied when limited number of tests fail for a specific CPU target will be included
- We should create a checklist for PRs that to `software-layer` repo that must be used

EESSI test suite

Merged pull requests:

- Update example configurations for Hortense (PR [#88](#)) and Snellius (PR [#84](#))
- Cleanup of README file (point to docs) (PR [#90](#))
- Release notes for v0.1.0 (PR [#91](#))

Open pull requests:

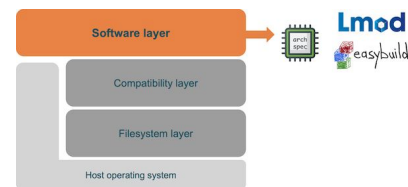
- OSU point-to-point + collective tests (CPU and GPU) ([PR #54](#)), ready for testing!

Other:

- **Version 0.1.0 has been released!** (see [GitHub](#) + [PyPI](#))
- **Documentation on installing, configuring, using test suite available at eessi.io/docs/test-suite**

Next steps

- Add more tests (ESPReso, OpenFOAM, `eb --sanity-check-only`, ...)



ReFrame

Infrastructure + monitoring

<http://status.eessi-infra.org>



- Our [Atlantis](#) setup seems to be broken :(
 - Expired keys, DNS issues
 - Terje has quickly looked into it, but is currently on vacation
 - Useful to have it back for setting up the servers and DNS records (and S3 buckets) for the new `eessi.io` repository
- In order to use Terje's [Github authorized keys](#) functionality, we need a Github token that provides access to the EESSI Github teams
 - Use a bot account for this? Probably needs to be part of the EESSI organization.
 - Nice mechanism for easily giving certain Github team members access to servers

Support portal for EESSI (MultiXscale task 5.1)

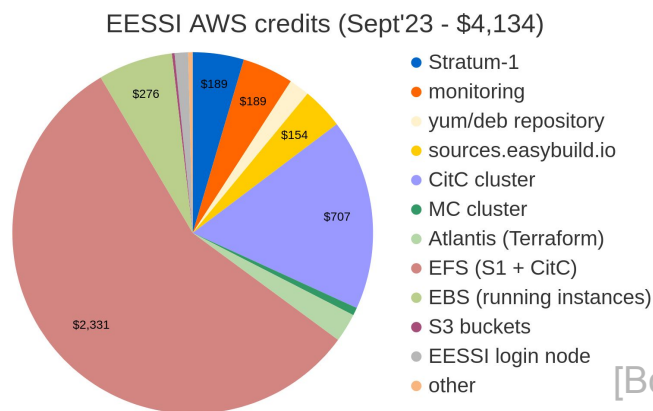
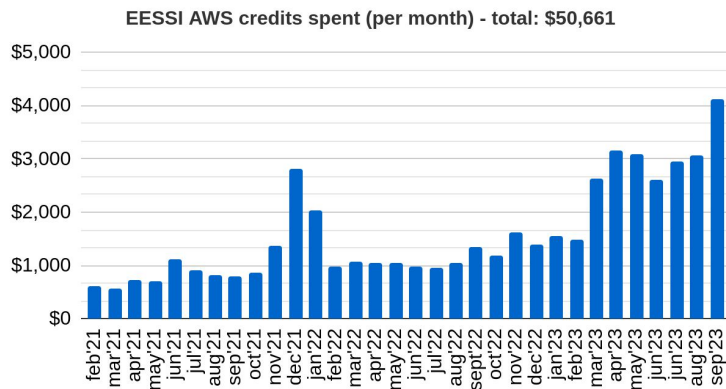


- EESSI support portal set up at <https://gitlab.com/eessi/support>
 - **Tickets can be created by opening an issue in GitLab, or sending an email to `support@eessi.io`**
 - Labels for issues are updated (<https://gitlab.com/eessi/support/-/labels>)
 - Repository updated (templates for issues, replies, ...)
 - Wiki updated (not public, internal docs for EESSI support team members)
 - **Information on support portal and initial support policy now in EESSI docs: <https://eessi.io/docs/support>**
 - Support is “reasonable effort” + only for problems with how software was installed in EESSI
 - Proposal for the support rotation in the wiki (<https://gitlab.com/eessi/support/-/wikis/Proposal-for-rotation>)
- Next steps:
 - 1 Oct - 22 Dec’23 (experimental) support rotation between the MultiXscale partners
 - A MultiXscale partner is “first-line” for incoming support requests for 2 weeks
 - Weekly regular support sync or hand-over meetings

Sponsored AWS credits



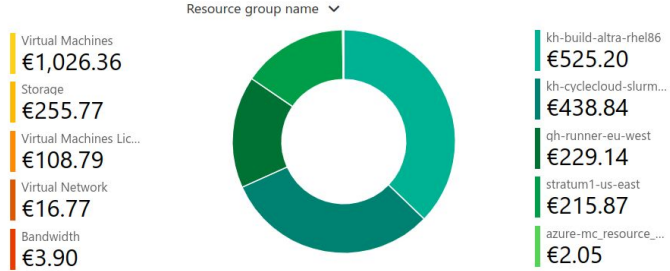
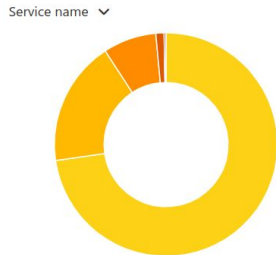
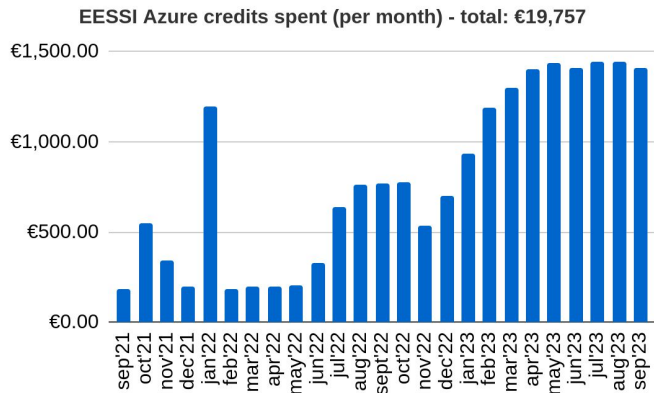
- Ask in #aws-resources Slack channel to get access!
- **Got another batch of \$25k**, currently ~\$28k worth of sponsored credits left (valid until 29 Feb'24)
- ~\$4,134 “spent” in Sept'23 on Stratum-1 servers, monitoring, sources.easybuild.io, **Slurm clusters (build bot)**
 - Includes new Stratum 1 servers for eessi.io, and new Magic Castle Slurm cluster
- ~\$50.5k worth of credits spent in total so far (since Feb'21), all covered by sponsored credits
- **Increase in consumed credits due to extensive activity with build-and-deploy bot**
- Large cost for shared fs (TBs) due to huge tarballs created by the bot (was ~\$90/day, now back to ~\$35/day)
- Monthly sync meetings with Brendan/Angel/Matt/Francesco (AWS) every 2nd Thursday of the month



Sponsored Azure credits



- Sponsored credits (€40,000) are being put to good use!
- **Ask in #azure-resources Slack channel to get access!**
- In Sept'23: ~€1,412 worth of credits spent
- ~€19.8k worth of (sponsored) credits spent in total (since Sept'21)
- Used for: Stratum-1, GitHub Runners, heterogeneous Slurm cluster, Ampere Altra build node
- Current Slurm cluster using [Azure Cyclecloud](#) is not used
- Will start over with Magic Castle, same tool as used in AWS (WIP)

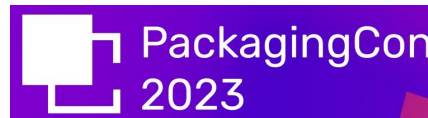


Sept'23

[Bob, Kenneth]

- Presentation by Alan to NCCs about MultiXscale training program (which has EESSI focus)
 - Full tutorial requested, which will be given on the 5th of December
- “Best Practices for CernVM-FS on HPC systems” training event
 - Being developed in <https://github.com/multixscale/cvmfs-tutorial-hpc-best-practices>
 - In collaboration with CernVM-FS developers & experts
 - Date to be determined (tentative Mon 4th Dec'23) - most likely fully virtual event
- CI/CD collaboration via CASTIEL2
 - Still not clear what demands will come from this
 - Deucalion and Meluxina have expressed reservations (due to CernVM-FS primarily)
- Relevant deliverables due end of 2023
 - D1.1: Report on shared software stack prototype
 - D1.2: Plan for design of a portable test suite
 - D5.1: Community contribution policy and GitHub App
 - D5.2 : Support portal for EESSI

EESSI @ PackagingCon'23



- 26-28 Oct'23 in Berlin (Germany), hybrid event - <https://packaging-con.org>
- Conference on software package management (in broad sense)
- Talk submitted on EESSI by Lara & Kenneth - **was accepted** \o/
“Streaming optimized scientific software installations on any Linux distro with EESSI”
- **Scheduled for Fri 27 Oct'23 at 16:45 CEST**
- Nice opportunity to present EESSI, CernVM-FS, MultiXscale to broad audience people with extensive experience in software packaging and installation

EESSI @ Supercomputing'23?



- 12-17 Nov'23 in Denver (US) - <https://sc23.supercomputing.org>
- Who is planning to attend? (confirmed: Alan, Henk-Jan, HPCNow!)
- Planned activities:
 - Magic Castle tutorial accepted (Alan)
 - Submission on EESSI for HPC User Support Tools (HUST) workshop was rejected :(
 - Booth talks @ Microsoft + AWS?
 - No lightning talks this year at AWS booth, but Azure should be possible?
 - MultiXscale presence in EuroHPC booth?
 - Video only (work in progress by HPCNow!)
 - No swag... but if we bring some stickers maybe they will not complain?

EESSI @ SURF Advanced Computing User Day?



- 7 Dec'23 in Amsterdam - <https://www.surf.nl/en/agenda/advanced-computing-user-day>
- Explore trends and connect with other peers in HPC, AI, Machine Learning, Quantum and Data Science on December 7 at Royal Tropical Institute, Amsterdam. Admission is free of charge.
- Proposal for talk in the "*European initiatives on High Performance Computing*" theme submitted by Bob: *One scientific software stack for all systems, that's EESSI*
 - Decision expected by Oct 12



[Bob]