

2 Nov 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) and outlook to new repository (software.eessi.io)
- 5. Documentation
- 6. Infrastructure and monitoring
- 7. EESSI support portal
- 8. AWS/Azure sponsorship update
- 9. Update on MultiXscale EuroHPC project
- 10. Upcoming/recent events
- 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**



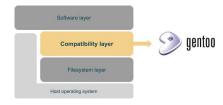
- (10 Oct'23) MultiXscale sync meeting (WP1+WP5) (notes)
- (10 Oct'23) Sync meeting on EESSI support (notes)
- (11 Oct'23) Sync meeting on Magic Castle clusters for EESSI (notes)
- (11 Oct'23) Meeting with SURF visualization team w.r.t. software/test dashboard (notes)
- (12 Oct'23) EESSI/AWS sync meeting (notes)
- (13 Oct'23) Meeting on CVMFS setup for new software.eessi.io repository
   (notes are in a private GitHub repository)
- (19 Oct'23) Sync meeting on EESSI test suite (notes)
- (23 Oct'23) Sync with CernVM-FS developers on Best Practices in HPC tutorial (notes)

# Progress update: filesystem layer



- New Stratum-0 server and Stratum-1 servers for new software.eessi.io repo
  - Ansible playbook + roles are in a private CVMFS repository (under the EESSI organization)
  - Added MFA for CVMFS admin accounts
  - Current plan is to start with two Stratum 1 servers:
     one in AWS (eu-central), one in Azure (us-east)
  - Need proper DNS names for the servers, and then we should be ready to start using the new repository
- PR for updating meta information of CVMFS servers and repositories <a href="https://github.com/EESSI/filesystem-layer/pull/161">https://github.com/EESSI/filesystem-layer/pull/161</a>
- We should improve/rethink the ingestion workflow
  - Approving separate PRs for each CPU target is a bit of a hassle
- CVMFS 2.11.2 was released today
  - https://cvmfs.readthedocs.io/en/2.11/cpt-releasenotes.html

# Progress update: compatibility layer



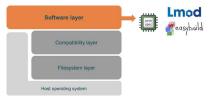
- 2023.06 version is available in EESSI pilot repository (pilot.eessi-hpc.org)
  - Was built with bot (see PR #188)
  - Deployment was still done manually, needs more work to automate (see <u>issue #189</u>)
  - No recent changes here
- Compat layers for software.eessi.io repo have been built (version 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
  - We still need to set up a good mechanism to deal with this

# Progress update: software layer (1/2)



- Incorrect CPU detection by archspec for zen3 (<u>issue #322</u>) and neoverse\_v1 (<u>issue #320</u>)
- Fix for archdetect, so we can use it by default in EESSI init script (open PR #264)
- CI for testing if EESSI stack is available is only checking single architecture (<u>issue #349</u>)
- Use module file to configure EasyBuild to extend EESSI (open <u>PR #371</u>)
- Supporting NVIDIA GPUs (overview <u>issue #375</u>, PRs in progress)
- First radio astronomy software supported (<u>PR 370</u>)
- Remove Lua from filtered dependencies since version is ancient (<u>issue #377</u>)
- EasyStack files not resolving dependencies from linked PR when easyconfig exists in release (<u>issue #378</u>)

# Progress update: software layer (2/2)



- Every now and then, we run into problems that only pop up when building for EESSI
  - Failing tests on aarch64/neoverse\_v1CPU target (which supports SVE vector instructions)
  - Problems specific to use compatibility layer or RPATH linking
  - Very recent Python in compat layer (CMake issue)
- Recently merged EasyBuild PRs relevant to EESSI:
  - Add support for % (sysroot) s template value (<u>framework PR #4359</u>)
  - Use sysroot template in wget easyconfigs to define PKG\_CONFIG\_PATH (<u>easyconfigs PR #19080</u>)
  - Enhance TensorFlow easyblock to avoid -mcpu=native for XNNPACK on aarch64 (<u>easyblock PR #3011</u>)
  - Only set flag --enable-asmjit for PLUMED when installing on x86\_64 (easyconfigs PR #19110)
  - Only add tbb as dependency in LAMMPS easyconfigs when installing on x86\_64 (easyconfigs PR #19000)
  - Make sure Python dependency included for ESPResSo is actually used by specifying -DPYTHON\_EXECUTABLE (easyconfigs PR #18963)
     [Kenneth, Thomas, Richard, Lara, Caspar, Satish, Xin]

## Bot for building + deploying software layer

# Compatibility layer Filesystem layer Host operating system

#### Progress on implementation of build-and-deploy bot

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

- Next bugfix release v0.1.1 soon:
  - PR#217 tool to clean up disk space (removing tarballs of closed/merged PRs)
  - PR#220 omit header lines in squeue output
  - PR#221 add instructions on setting Permissions for GitHub App
  - PR#224 Upgrade bot to be compatible with PyGithub v2.1.1
- Next minor releases:
  - v0.2.0: Support running EESSI test suite after a build, before deploy (PR#222 + PR#366)
  - v0.3.0: Remove code in the deployment function that is specific to <u>EESSI/software-layer</u>

# EESSI pilot repository (1/2)

#### 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 <a href="http://www.eessi.io/docs/software\_layer/cpu\_targets">http://www.eessi.io/docs/software\_layer/cpu\_targets</a>
  - Recently added software installations (for all supported CPU targets):
    - WRF 4.4.1 (<u>PR #336</u>)
    - ESPResSo 4.2.1 (<u>PR #331</u>)
    - EasyBuild 4.8.2 (<u>PR #376</u>)
    - DP3 6.0 and WSClean 3.4 (PR #370)
    - X11 20230603 (<u>PR #364</u>)
    - SciPy-bundle 2022.05 (<u>PR #352</u>)
  - Only increase limit for numerical test failures for OpenBLAS for aarch64/neoverse\_v1 (PR #345)
  - We currently have ~450 software installations per CPU target => 3,600 installations in total!

# EESSI pilot repository (2/2)

#### https://eessi.github.io/docs/pilot

# NOT FOR PRODUCTION USE!



- 2023.06 is being populated via <u>PRs to software-layer repo</u> + build-and-deploy bot
  - TensorFlow (v2.7.1 in <u>PR #321</u>, v2.8.4 in <u>PR #343</u>, v2.11.0 in <u>PR #346</u>, v2.13.0 in <u>PR #347</u>)
    - 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 4.3 (PR <u>#290</u>):
    - Failing/hanging tests on aarch64/neoverse-v1
  - ESPResSo 4.3.2 with foss/2021a (PR <u>#332</u>): some tests time out
  - o matplotlib v3.4.3 with foss/2021b (PR #339): trouble with hardcoded /usr/\* paths used by Pillow dependency
  - LAMMPS 23Jun2022 (<u>PR #360</u>): issues with PLUMED (solved) and ScaFaCoS dependencies
  - TODO:
    - Bioconductor, waLBerla, ...
    - Ensure that Lmod cache update is done correctly, includes \*all\* available modules
    - Come up with a better approach to replace existing software installationsnneth, Bob, Caspar, Lara, Richard, ...]

#### Contribution policy (proposal)

EESSI

- Proposal for contribution policy for adding software to EESSI (docs PR #108)
  - Has been reworked based on feedback (mostly rephrasing, added a version and changelog)
  - o Initial policy can be revised later as needed (policy will be versioned, changelog will be kept)
  - Meeting Nov 7th to discuss last minute updates, then will be published on <u>EESSI docs</u>

#### Summary:

- Only open source software (we should verify this by requiring <u>SPDX license IDs</u>)
- Software must be built by the bot (no manual builds) and support by latest EasyBuild release
- o 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 <u>EESSI test suite</u>

#### **EESSI** test suite

#### Merged pull requests:

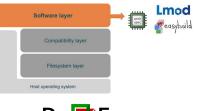
- Add content type of long description + license to setup.cfg (PR #92)
  - Required to publish version 0.1.0 to PyPI

#### Open pull requests:

- Updated CI driving scripts (PR #93)
- Add additional scales 1\_cpn\_2\_nodes and 1\_cpn\_4\_nodes (PR #94)

#### Next steps

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





#### **EESSI** documentation



https://www.eessi.io/docs/ - GitHub repo https://github.com/EESSI/docs

- Documentation has seen several updates throughout 2023
  - Getting access, Using EESSI, Getting support, Test suite, Build-and-deploy bot
- More updates are coming soon
  - PR#108 contribution policy for adding software to EESSI
  - PR#117 Interactive building for debugging
  - PR#118 How to build on top of EESSI
  - PR#119 add new scales (related to test suite)
  - PR#120 Update landing page
- Some parts are a bit outdated and the structure could be improved
  - We are thinking about a doc sprint (dates not set yet)

# Infrastructure + monitoring

http://status.eessi-infra.org



No updates

## Support portal for EESSI (MultiXscale task 5.1)



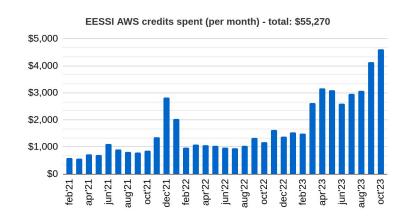
- EESSI support portal set up at <a href="https://gitlab.com/eessi/support">https://gitlab.com/eessi/support</a>
  - Tickets can be created by opening an issue in GitLab, or sending an email to support@eessi.io
  - o Information on support portal and initial support policy now in EESSI docs: <a href="https://eessi.io/docs/support">https://eessi.io/docs/support</a>
  - Support is "reasonable effort" + only for problems with how software was installed in EESSI
  - Proposal for the support rotation in the wiki (<a href="https://gitlab.com/eessi/support/-/wikis/Proposal-for-rotation">https://gitlab.com/eessi/support/-/wikis/Proposal-for-rotation</a>)
- 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
  - Tickets are starting to be opened and are followed up, thanks to the support rotation and the weekly support syncs

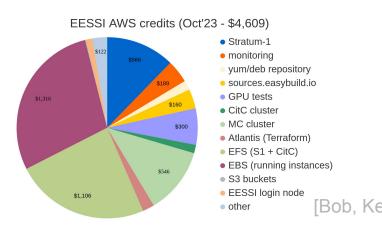
# Sponsored AWS credits

- Ask in #aws-resources Slack channel to get access!
- Currently ~\$24k worth of sponsored credits left (valid until 29 Feb'24)



- o Includes new Stratum 1 servers for eessi.io, new Magic Castle Slurm cluster, GPU support test machine
- ~\$55k 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





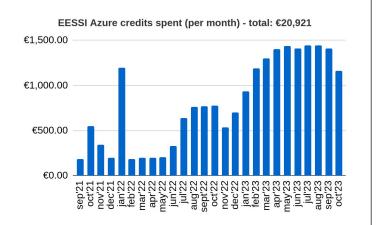


# Sponsored Azure credits





- Sponsored credits (€40,000) are being put to good use!
- Ask in #azure-resources Slack channel to get access!
- In Oct'23: ~€1,163 worth of credits spent
- ~€20.9k 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 <u>Azure Cyclecloud</u> is not used
- Will start over with Magic Castle, same tool as used in AWS (WIP)





Oct'23









www.multixscale.eu

github.com/multixscale

- Introduction to EESSI tutorial (05-12-2023 14:30 16:30)
  - Register at <a href="https://event.ugent.be/registration/event/201863f3-cead-498b-9659-16d98c966eab">https://event.ugent.be/registration/event/201863f3-cead-498b-9659-16d98c966eab</a>
- "Best Practices for CernVM-FS on HPC systems" training event
  - Being developed in <a href="https://github.com/multixscale/cvmfs-tutorial-hpc-best-practices">https://github.com/multixscale/cvmfs-tutorial-hpc-best-practices</a>
  - In collaboration with CernVM-FS developers & experts
  - Mon 4th Dec'23 fully virtual event (registration will be open soon)
- CI/CD collaboration via CASTIEL2
  - Still not clear what demands will come from this
  - Funding call expected from EuroHPC in this space
- Relevant deliverables due end of 2023
  - D1.1: Report on shared software stack prototype
  - D1.2: Plan for design of a portable test suite
  - o D5.1: Community contribution policy and GitHub App
  - o D5.2: Support portal for EESSI

# EESSI @ PackagingCon'23

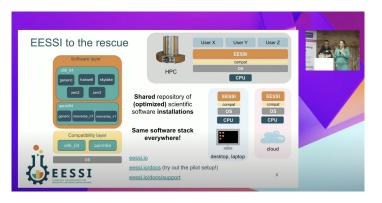




- 26-28 Oct'23 in Berlin (Germany) <a href="https://packaging-con.org">https://packaging-con.org</a>
- Talk on EESSI by Lara & Kenneth (<a href="https://cfp.packaging-con.org/2023/talk/9WAN3N">https://cfp.packaging-con.org/2023/talk/9WAN3N</a>)
   "Streaming optimized scientific software installations on any Linux distro with EESSI"
- Really well received, broad interest incl. by people from IBM Research & NVIDIA







# EESSI @ Supercomputing'23?





- 12-17 Nov'23 in Denver (US) <a href="https://sc23.supercomputing.org">https://sc23.supercomputing.org</a>
- Who is planning to attend? (confirmed: Alan, Henk-Jan, HPCNow!)
- Planned activities:
  - Magic Castle tutorial (Alan)
  - Booth talks @ Microsoft
    - Alan will ask this week
  - MultiXscale presence in EuroHPC boot?
    - Video only
    - No swag... but if we bring some stickers maybe they will not complain?

# EESSI @ SURF Advanced Computing User Day



- 7 Dec'23 in Amsterdam <a href="https://www.surf.nl/en/agenda/advanced-computing-user-day">https://www.surf.nl/en/agenda/advanced-computing-user-day</a>
- 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 submitted by Bob:
   One scientific software stack for all systems, that's EESSI
  - Accepted! 🎉
  - Track 1: The power of High-Performance Computing

