



EESSI meeting

6 Apr 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
5. AWS/Azure sponsorship update
6. Update on MultiXscale EuroHPC project (incl. kickoff meeting)
7. Upcoming events
8. Q&A

Quick introduction by new people



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

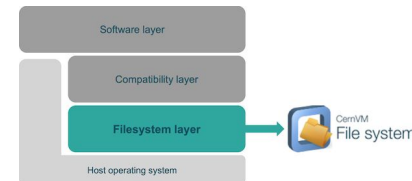
- Who are you, where do you work, on what?
- Why are you interested in the EESSI project?
- Are you planning to actively contribute,
and if so, to which aspect(s) of the project?

EESSI-related meetings



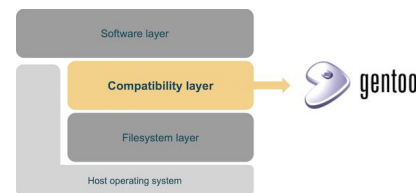
- (9 Mar'23) AWS/EESSI monthly sync meeting (every 2nd Thursday of the month)
notes available at <https://github.com/EESSI/meetings/wiki/AWS-meeting-2023-03-09>
- (10 Mar'23) Sync meeting on EESSI test suite (MultiXscale task 1.3)
notes available at [https://github.com/EESSI/meetings/wiki/Sync-meeting-on-EESSI-test-suite-\(2023-03-10\)](https://github.com/EESSI/meetings/wiki/Sync-meeting-on-EESSI-test-suite-(2023-03-10))
- (10 Mar'23) EESSI/Australian BioCommons BYOD meeting
 - Attended by Kenneth, Alan
 - Notes available at [https://github.com/EESSI/meetings/wiki/Meeting-with-BioCommons-\(2023-03-10\)](https://github.com/EESSI/meetings/wiki/Meeting-with-BioCommons-(2023-03-10))
- (14 Mar'23) MultiXscale virtual sync meeting (monthly - all project partners)
notes available at <https://github.com/multixscale/meetings/wiki/Sync-meeting-2023-03-14>
- (30 Mar'23) Sync meeting on EESSI test suite (MultiXscale task 1.3)
notes available at [https://github.com/EESSI/meetings/wiki/Sync-meeting-on-EESSI-test-suite-\(2023-03-30\)](https://github.com/EESSI/meetings/wiki/Sync-meeting-on-EESSI-test-suite-(2023-03-30))
- (Mar'23) Azure/EESSI sync meeting cancelled, meeting timing was too hard (Friday afternoon)
next meeting planned for Mon 17 April 2023

Progress update: filesystem layer



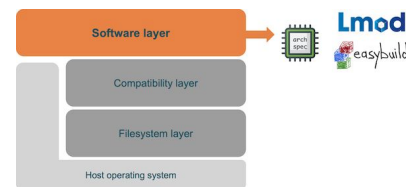
- No updates since last month
- **Planning to remove 2021.06 pilot version in EESSI repository**
 - 2021.12 pilot version provides everything in 2021.06, and more (+ has updated compat layer)
 - Hugo raised some concern about this via the EESSI mailing list (on 9 Jan '23)
 - Current proposal:
 - Remove `/cvmfs/pilot.eessi-hpc.org(/versions)/2021.06`
 - Make `2021.06/init/bash` print a warning + source `2021.12/init/bash`
 - => People who are still using 2021.06 should not see any breakage, only a warning
- We should try the `-d` (delete) option of `cvmfs_server ingest` again for replacing directories (e.g. the entire compat layer) instead of manually extracting the new tarball, also to prevent the weird permission issues that we saw last month (see [issue #143](#))

Progress update: compatibility layer



- Preparing a new compatibility layer (2023.04)
 - Updates/new packages (`archspec`, `Lmod`, `direnv`, etc) and new overlay in [PR #90 of gentoo-overlay](#)
 - **If any packages still need to be added, please let us know as soon as possible!**
 - Updated bootstrap script works with gentoo repository commit (March 13), *trying to use more recent one*
 - Commit [3a38f9b](#) introduces a circular dependency (CMake)
 - Quite some (breaking) changes have been made in Gentoo, causing the bootstrap to fail
 - Failing bootstrap on arm64 (<https://bugs.gentoo.org/892876>) => using Bob's suggested workaround
 - Problem with binutils during bootstrap <https://bugs.gentoo.org/895240> => SOLVED
 - We plan to prune the compatibility layer by removing build tools, editors, and other tools - see issue [#172](#)
 - Merged PRs [#163](#) + [#166](#)-[#169](#), opened [#PR #170](#) & [PR #171](#) with the goal to let bot build compatibility layer
- Bart Oldeman (the Alliance, Canada) made us aware that the changes in Gentoo (see [gentoo PR #28851](#)) may affect the way EasyBuild should build GCC/Clang ([see GCC easyblock in EasyBuild](#))

Progress update: software layer



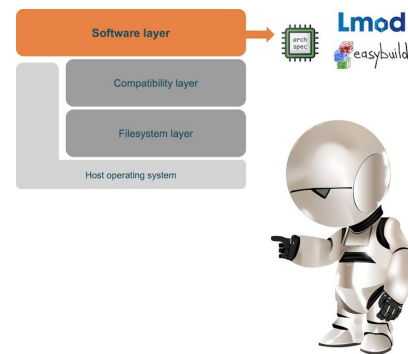
- `bot/build.sh` using `eessi_container.sh` ([PR #233](#))
 - `bot/build.sh` is run by EESSI bot ... think of a standard interface to build any software (layer)
- Stored configuration for production bot ([PR #240](#))
 - Moves EESSI software-layer specifics from bot to EESSI/software-layer repo
- Opened PRs for smaller issues
 - Fix check for missing installations ([PR #237](#)), needed when using EasyBuild v4.7.0 or newer
 - Restore `$*PATHs` only after last run of pip installed eb ([PR #238](#)), installation fails for a new software directory
 - Only tar new software directories ([PR #239](#)), previously existing packages could leak into a tarball
- Next steps:
 - Move towards using `easystack` files (when building a new pilot version?)
 - Figure out “Permission denied” problems with `eessi_container.sh` tests ([WIP PR #227](#))
 - Fix “Illegal instruction” problem when installing OpenFOAM for `aarch64/graviton2` ([PR#195](#))
 - Fix remaining build issues for 2021.12 software layer for Ampere Altra (Azure)
 - Get EasyBuild PRs related to EESSI merged (so we limit use of `--from-pr`)

Bot for building + deploying software layer

Progress on implementation of build-and-deploy bot

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

- Mar'23
 - [PRs](#): 5 merged - 1+1+3 open (ready & tested + draft + stalled) PRs
 - [issues](#): 1 closed - 61 still open (+6 in Mar'23)
- On-going work to implement more flexible way of interacting with bot via comments
 - Support acting on comments such as
 - `bot: build architecture:intel`
 - `bot: build instance:AWS repository:eessi-2023.04`
 - Bot then only submits jobs that match the spec/filter
 - Other commands possible: `help`, `showconfig`, ...
 - Almost working, see last comments in [trz42/software-layer test PR60](#)

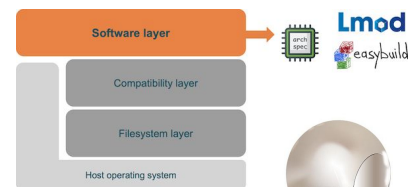


Bot for building + deploying software layer

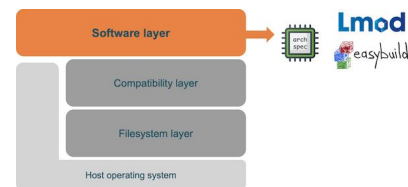
Progress on *use* of build-and-deploy bot in NESSI project

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

- March'23:
 - Building for 5 x86_64 + 1 aarch64 CPU architectures across 4 clusters (AWS + 3 in Norway)
 - 14 PRs ongoing, 24 PRs finished and ingested
 - Significant effort to rebuild stacks for `generic` architectures
 - Work resulted in discovering several issues in `software-layer` and `eessi-bot-software-layer`
 - Having a test (suite) available before ingesting would be very welcome!
 - Started wiki page for [troubleshooting](#)
- Goals for April/May'23:
 - Include all EESSI pilot software in NESSI stack 2022.11
 - Add software available on local clusters to NESSI stack 2022.11
 - Start building new stack for {E,N}ESSI/2023.04



EESSI test suite



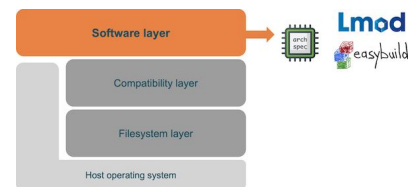
ReFrame

See <https://github.com/EESSI/test-suite> (recent meeting notes [here](#))

Merged PRs in past month:

- GROMACS test improvements ([PR #11](#)):
 - Use `features` in ReFrame to only generate GPU tests when it make sense (instead of skipping them)
 - Make GROMACS test more configurable on command line (with `--setvar`)
 - Fixes issues: [#7](#), [#8](#), [#10](#), [#13](#), [#14](#), [#15](#), [#19](#)
 - Code cleanup ([PR #22](#))
- Make EESSI test suite installable with `pip` ([PR #17](#))

EESSI test suite



ReFrame

Planned work:

- GROMACS
 - Move logic *not* specific to GROMACS test into general hooks ([PR #26](#))
 - Add support for custom executable options ([PR #23](#))
- Add test for TensorFlow ([PR #2](#))
 - Using as much as possible same structure & hooks as GROMACS test
- Add test for OSU Micro-Benchmarks ([#29](#))
 - Low level test to check e.g. functionality of communication libraries
 - See if hooks developed for high level tests (GROMACS) generalize for low level tests
- Rethink namespaces ([#25](#))
 - Now: `eessi_utils.hooks` , probably want something like `eessi.testing.hooks`

EESSI pilot repository

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

**NOT FOR
PRODUCTION USE!**



- 2021.06: considered “end of life”: **will soon be removed**
- Current status for 2021.12 (default version)
 - Compatibility layer: in place for `aarch64` / `ppc64le` / `x86_64` (security updates are in place!)
 - Software layer:
 - Software installations included in 2021.06 also in place for 2021.12, incl.
GROMACS, OpenFOAM, TensorFlow + Horovod, R + Bioconductor, QuantumESPRESSO
 - Additional software (vs 2021.06): SciPy-bundle with foss/2021a, WRF, Nextflow,
OSU Micro-Benchmarks, R 4.1.0, OpenFOAM v9 (missing for `aarch64/graviton2`)
 - Targets: `aarch64/generic`, `aarch64/graviton2`, `aarch64/graviton3`, **`aarch64/ampere`**
(partial),
`ppc64le/generic` (partial), `ppc64le/power9le` (partial), `x86_64/generic`, `x86_64/amd/zen2`,
`x86_64/amd/zen3`, `x86_64/intel/haswell`, `x86_64/intel/skylake_avx512`
 - TODO / work-in-progress:
 - Bot to automate workflow of adding software to EESSI (to avoid losing time doing it manually)
 - Ensure that Lmod cache update is done correctly, includes **all** available modules
 - Complete installing software-layer optimized for Azure's Ampere Altra (Arm) CPUs

Outlook to next pilot version (2023.04)

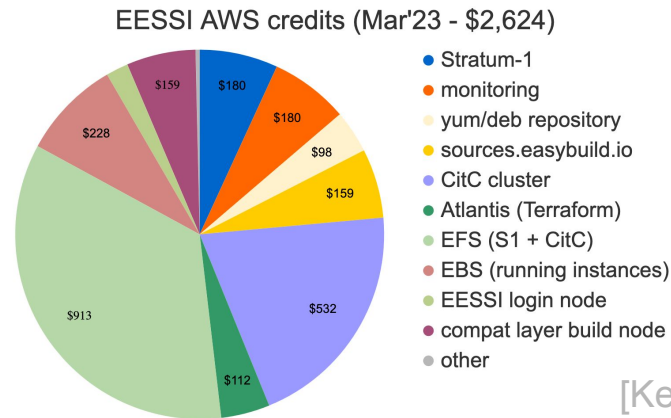
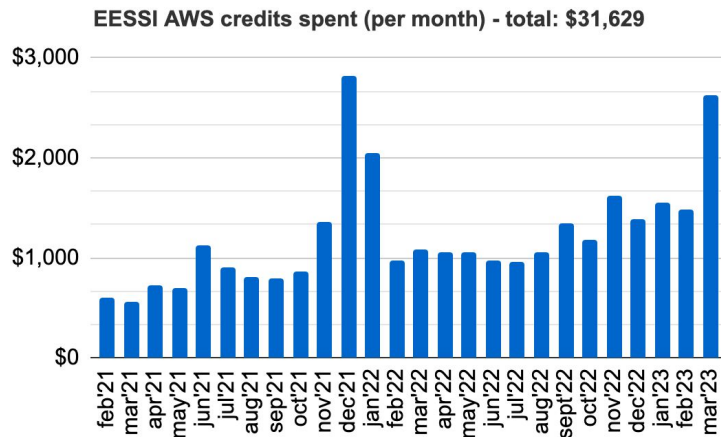


- Small changes to compatibility layer: updated Lmod, **less packages installed**, ...
- Include enhancements/changes that are necessary for CUDA GPU support
- Work towards getting rid of ugly install script, aim for easystack-only (if possible)
- **Ideally build/deploy compat + software layer via bot, no more manual deployments!**
- Initially include same software installations as in 2021.12, then **gradually expand**
- Also install software with more recent toolchains + more applications
- Stop wasting time with supporting POWER (ppc64le) - start considering RISC-V
- Alpha/beta for production EESSI repository
- Switch to `eessi.io` domain + new Stratum 0 (dedicated hardware, yubikey) - if available
- **Effort is ongoing** (Bob, Thomas, ...), **compatibility layer should be in place soon...**
- Hopefully using EasyBuild v4.7.2 (to be released soon - mid April'23) for software layer...

Sponsored AWS credits



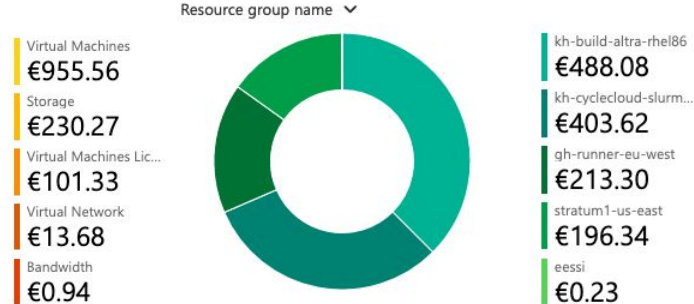
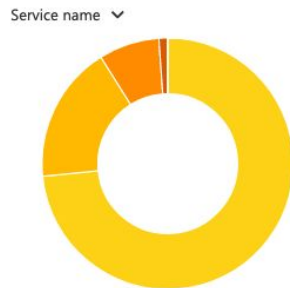
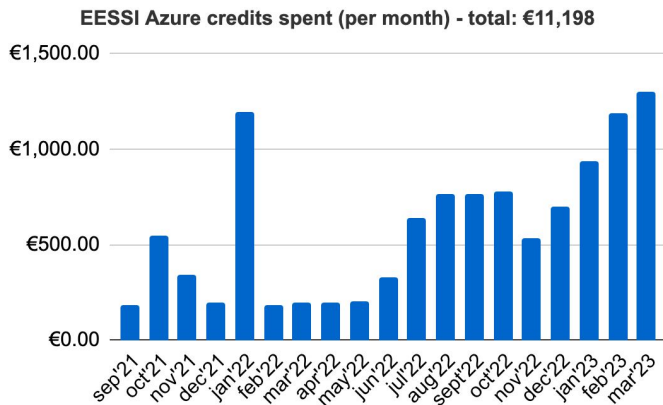
- Ask in #aws-resources Slack channel to get access!
- Currently still ~\$7,131 worth of sponsored credits left (valid until Sept'23)
- ~\$2,624 “spent” in Mar'23 on Stratum-1, monitoring, sources.easybuild.io, **Slurm cluster (build bot)**
- ~\$31,629 worth of credits spent in total so far (since Feb'21), all covered by sponsored credits
- **Increase in consumed credits due to extensive activity with build bot by NESSI partners**
- 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 Mar'23: ~€1,301 worth of credits spent
- ~€11,198 worth of (sponsored) credits spent in total (since Sept'21)
- Used for: Stratum-1, GitHub Runners, heterogeneous Slurm cluster, Ampere Altra build node
- **Virtual Slurm cluster in Azure (set up using [Azure Cyclecloud](#)) - more info [here](#)**
 - Work-in-progress: properly set up partitions for different CPU types (to the extent that's possible...)



Mar'23

[Kenneth]

- **Official kickoff meeting 23-24 March 2023 (Ljubljana)**
 - We made the Slovenian national news: <https://vimeo.com/810503122>
- MultiXscale website is up: <https://www.multixscale.eu>
- Twitter account is active: [@MultiXscale](https://twitter.com/MultiXscale)
- Two training events planned this year
 - Hybrid EESSI user training event at HPCKP meeting (physical)
 - Admin training for CernVM-FS and EESSI, date TBD, most likely virtual
- Will collaborate with CASTIEL2 (which means NCCs and other CoEs)
 - Required to have CI/CD on EuroHPC platforms
 - [Spack CI setup](#) with (un)trusted builds can be an inspiration?
 - May be an opportunity to spread EESSI awareness in EuroHPC landscape...
- Support portal for EESSI is a deliverable in MultiXscale due by end of 2023



- Poster at EuroHPC Summit (20-23 March 2023 in Göteborg, Sweden)
- See <https://www.multixscale.eu/wp-content/uploads/2023/03/32-Poster-MultiXscale.pdf>

EuroHPC Centre of Excellence
Presented by Alan O'Caas (University of Barcelona), Thomas Rößler (University of Bergen)*

OBJECTIVES	OUTCOMES
Scientific <ul style="list-style-type: none"> Increase performance, productivity and portability of the Three P's across the entire spectrum of scientific activities in the domain of multiscale simulation Facilitate the use cases of applied and industrial applications <ul style="list-style-type: none"> Industrial design and verification for car transport Energy applications to support the transition to a green economy Utilisation for non-invasive diagnostics and biomedical applications Technical <ul style="list-style-type: none"> Focus on performance, automation, testing, collaboration Application and system design for multiscale challenges Facilitate technical transfer on domain scenarios Streamlining of multiscale simulation workflow and services such as EESSI Facilitate workflows and portable technologies 	<ul style="list-style-type: none"> Project workflow running on open ecosystem Domestic growth in the number of applications supported by the shared software stack (EESSI) - European commitment for scientific software innovation Automated adoption of EESSI ecosystem services among the community Increasing HPC chain capacity supporting the shared software stack (EESSI) Cloud provision supporting the EESSI stack in cloud environments Large number of developments using our 0 tools Training portal with our training courses and additional training content Adoption of Multiscale software and workflows in the industrial community

ACHIEVEMENTS

- EESSI A merged, production-quality, multiplatform, optimised scientific software stack
- Working proof of concept from <https://www.multixscale.eu>
- Available analysis, service, data in <https://data.multixscale.eu>
- Concrete EU Member @ lists of Gaseous & Free State-3 series
- Software (Python) Backend: GROMACS, OpenMM, A, TensorFlow, ...
- Hardware targets
 - Intel(R) Xeon(R) Platinum 8448C
 - Intel(R) Xeon(R) Platinum 8448C
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 - Intel(R) Xeon(R) Platinum 8448C
- Supported by EESSI and HPC sponsored credits to develop necessary infrastructure

Try EESSI for yourself!

EESSI: Design

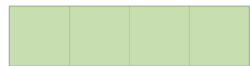
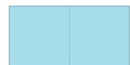
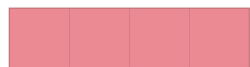
User software contribution workflow to EESSI

MILESTONES

Partners

- Designed by Alan
- Presented by Thomas (with support from Elisabeth)

Upcoming events



EASYBUILD

EasyBuild User Meeting @ London (Mon-Wed 24-26 April 2023)

- easybuild.io/eum23
- Will include a presentation on current status of EESSI (by Caspar)
- **Registering for attending remotely (via Zoom) is still possible!**

- BioHackathon Europe @ Barcelona (30 Oct - 3 Nov 2023)

- biohackathon-europe.org
- Call for project proposals is open (deadline 10 April)
- Sébastien is taking care of submission for EESSI
- On-site attendance by Sébastien, Alan, Elisabeth, Danilo, ...
- Project leads: Sébastien Moretti, Alan O'Cais, Danilo Gonzalez



Upcoming events:

- Website: hpckp.org/annual-meeting
- 17-18 May 2023 - Barcelona, Spain
- Registration is free!
- Important deadlines:
 - 7 April: Abstract submission deadline for presentations
 - 14 April: Confirmation of accepted presentations
 - 5 May: Presentations submission deadline
 - 12 May: Registration deadline
- Travel + hotel expenses for speakers from EU will be covered by HPCKP organisation
- **2h EESSI tutorial will be part of HPCKP'23 program**

Upcoming events:



ISC

High Performance
The HPC Event.

- ISC'23 website: <https://www.isc-hpc.com>
- When: 21-25 May 2023
- Where: Hamburg, Germany
- EasyBuild tutorial was submitted, but not accepted
 - We should submit an EESSI-focused tutorial for ISC'24?
- No EESSI activity as part of official ISC program
- Talk/demo on EESSI + MultiXscale at Azure booth by Elisabeth (HPCNow!)
- Maybe also involvement in AWS presence at ISC'23 (interview on exhibit floor?)
- There will be EESSI swag at Do It Now booth