EESSI meeting

3 Aug 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. Contribution policy (proposal)
6. EESSI support portal
7. AWS/Azure sponsorship update
8. Update on MultiXscale EuroHPC project
9. Past & upcoming events
10. Q&A

Quick introduction by new people

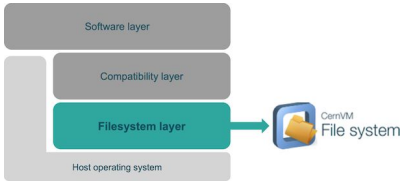
New people on the call: feel free to introduce yourself!

- 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

- *(7 July'23)* Call with CernVM-FS developers on Best Practices in HPC tutorial (notes)
- *(11 July'23)* MultiXscale sync meeting (WP1+WP5) (notes)
- *(13 July'23)* Sync meeting on EESSI test suite (notes)
- *(14 July'23)* Meeting on adding test for ESPResSo to EESSI test suite (notes)
- *(27 July'23)* Sync meeting on EESSI test suite (notes)
- *(1 Aug'23)* Sync meeting on development of build-and-deploy bot (MultiXscale T5.3) (notes)

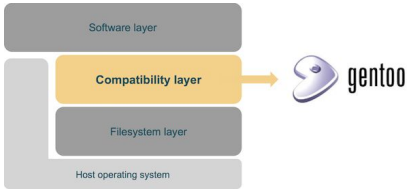
Progress update: filesystem layer



- Github Action for building client packages was fixed (PR #158, cfr. issue #155)
- New Stratum-0 server for EESSI at Univ. of Groningen
  - Plan is to use this for `*.eessi.io` CernVM-FS repositories
  - Hardware is up and running - needs work on RAID, network, firewall cfg, yubikeys (Bob)
  - Determine access rules: who can help administer it?
- Still need to figure out performance issues with Stratum-1 @ RUG (issue #151)

[Bob, Kenneth]

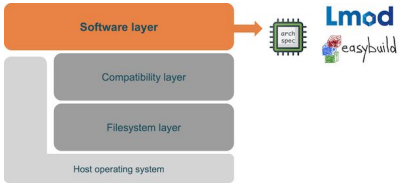
Progress update: compatibility layer



- 2023.06 version is now 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)
- 2023.04 version of compat layer should be removed from pilot repository
  - There will be no software layer on top of 2023.04 compat layer,
    Too many problems with OpenSSL 3.x (see issues #257, #258, #259)

[Bob, Thomas, Kenneth]

Progress update: software layer (1/3)

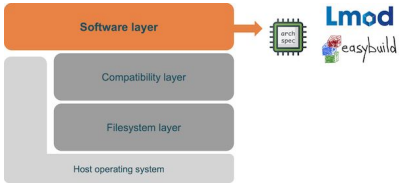


Software layer for EESSI pilot 2023.06 is gradually being populated

- All software installations are performed by the build-and-deploy bot, no exceptions
- EasyBuild v4.7.2 + easystack files are used to specify what should be installed
- Via pull request to software-layer repo + bot instructions, see documented procedure
- Current status:
  - Building + deploying with bot is working well, several more people actively involved now
  - **EasyBuild log for failing builds can be accessed via shared directory on AWS Slurm cluster**
  - Over 160 modules already for all CPU targets (Intel, AMD, Arm):
    - GCC 10.3.0 + 11.2.0 + 11.3.0 + 12.2.0, `foss/{2021a,2021b}` (other versions are WIP)
    - CMake, Python, Qt5, HDF5, LLVM, ELPA, ReFrame, …
    - GROMACS + QuantumESPRESSO + SciPy-bundle with `foss/2021a`

[Kenneth, Thomas, Lara, Caspar, Satish, Xin]

Progress update: software layer (2/3)

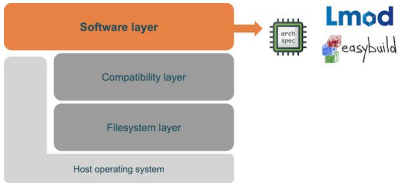


Work-in-progress PRs for adding software:

- WRF v4.3 with `foss/2021a` (PR #290): build fails, update to our hook fixing WRF build on aarch64 is required
- RStudio-Server (PR #299)
  - Failing installation of Xvfb dependency due to use of `cp -a` fixed via hook
  - Installation of R dep fails because `libcurl` from compat layer is too new (8.1.2 vs required 7.x)
- GROMACS v2021.5 with `foss/2021b` (PR #304): installation of SciPy-bundle dependency fails
- SciPy-bundle v2021.10 with `foss/2021b` (PR #306): failing tests for numpy on `aarch64/neoverse_v1`
- `foss/2022b` (PR #309): 344 failing (numerical) tests for OpenBLAS on `aarch64/neoverse_v1`
- `foss/2022a` (PR #310): failing tests for FFTW on `aarch64/neoverse_v1`

[Kenneth, Thomas, Lara, Caspar, Satish, Xin]

Progress update: software layer (3/3)

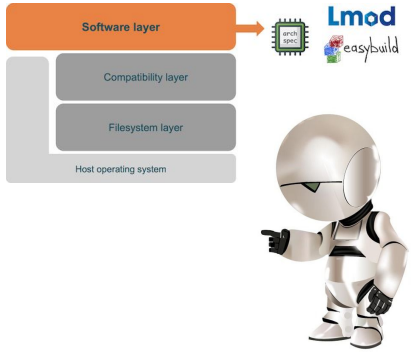


EasyBuild v4.8.0 was released on 7 July 2023

- Easyconfigs for the 2023a update of the `foss` + `intel` common toolchains
- 2 new easyblocks: a generic `PerlBundle` easyblock + a custom easyblock for Rust
- Updated software versions, incl. elastix 5.0.0, GROMACS 2023.1, PyTorch 1.13.1, VTK 9.2.6, ...
- Support for installing 76 new software applications and libraries
- Fixes relevant for EESSI, including:
  - Fix extracting glibc version from output of '`ldd --version`' in Gentoo Linux (relevant for Qt5)
  - Patch CMake's `UnixPaths.cmake` script if `--sysroot` is set
  - Use patch files for Qt5 v5.17.7 to fix compatiblity with glibc 2.34

[Kenneth, Thomas, Lara, Caspar, Satish, Xin]

Bot for building + deploying software layer



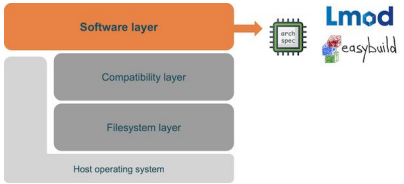
Progress on implementation of build-and-deploy bot

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

- Add support for specifying path to build logs directory (PR #195)
- In conjunction with changes in software layer scripts (PRs #302, #303, #305) to copy build log for failing builds to shared directory

[Thomas, Kenneth, Bob]

EESSI test suite



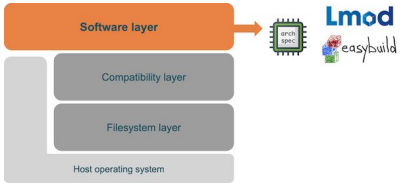
ReFrame

Pull requests:

- TensorFlow test got merged (PR #38)
- Use ReFrame ‘extra’ config option to specify e.g. GPU vendor for test filtering (PR #60)
  - Allows filtering e.g. all tests that are valid for NVIDIA GPUs
- ReFrame config merged for Snellius (SURF PR #66), Vega (EuroHPC, PR #62, PR #76)
  - Ready for review: config for AWS (CitC, PR #53) (CPU autodetect issue resolved)
- Script for daily runs of test suite on Vega (PR #70, PR #71)
- Hyperthreading: currently launching 1 thread per hardware thread. Not always good for performance, but ok for GROMACS & TensorFlow https://github.com/EESSI/test-suite/issues/74 (might revisit later)
- Add test for OSU Microbenchmarks (PR #54, CPU point-to-point works, working on GPU)

[Caspar, Sam, Satish, Kenneth]

EESSI test suite



ReFrame

Meetings

- Met with ESPResSo developer, got a test case for ESPResSo (used in MultiXscale)
  - To do: deploy ESPResSo in EESSI & turn test case into ReFrame test
- Regular sync meeting (13 july, 27 july)

[Caspar, Sam, Satish, Kenneth]

EESSI pilot repository

NOT FOR PRODUCTION USE!

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

- 2021.12 version is “frozen”, no more changes planned there, but it's still the default ("`latest`") version
- 2023.06 is being populated (via build-and-deploy bot)
  - Compatibility layer: in place for `aarch64` + `x86_64` (`ppc64le` no longer supported)
  - Software layer:
    - Targets: `aarch64/generic`, **`aarch64/neoverse_n1`**, **`aarch64/neoverse_v1`**, `x86_64/generic`, `x86_64/amd/zen2`, `x86_64/amd/zen3`, `x86_64/intel/haswell`, `x86_64/intel/skylake_avx512`
    - Aiming to have same software available as in 2021.12 version:
      GROMACS, OpenFOAM, TensorFlow + Horovod, R + Bioconductor, QuantumESPRESSO, WRF, …
    - Also expanding with more software (for MultiXscale): ESPResSo, waLBerla, LAMMPS, …
  - TODO / work-in-progress:
    - Ensure that Lmod cache update is done correctly, includes *all* available modules

[Kenneth]

Contribution policy (proposal)

- **Proposal** for contribution policy for adding software to EESSI (docs PR #108)
  - Preview available here - will be reworked based on feedback - **more feedback welcome!**
  - Initial policy - can be revised later as needed
- Summary:
  - Only open source software (we should verify this by requiring SPDX license IDs)
  - Software must be built by the bot (no manual builds)
  - Software must be supported by latest EasyBuild release (can be relaxed later);

    `--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

[Kenneth, Bob]

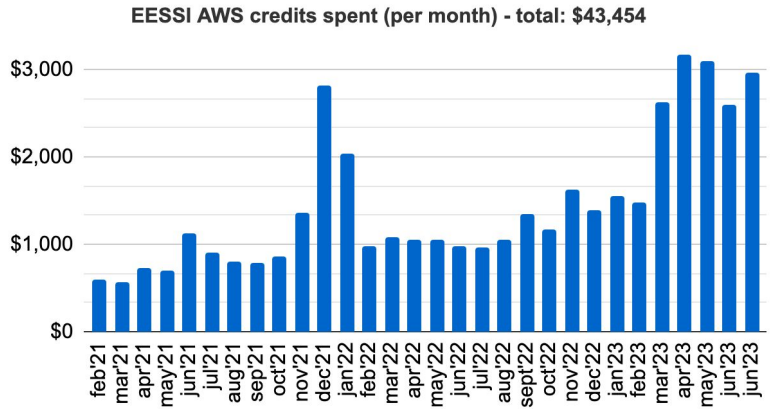
Support portal for EESSI (MultiXscale task 5.1)

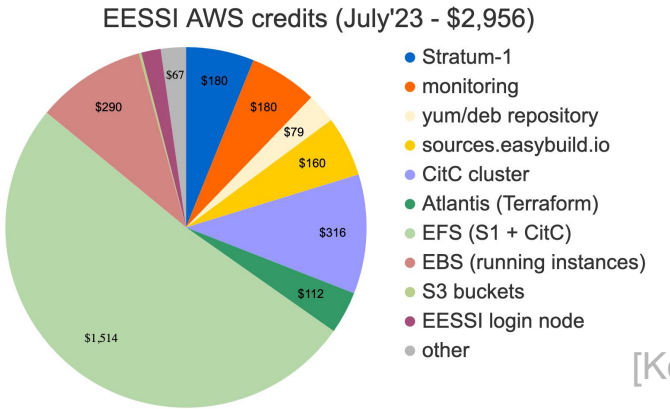
- **EESSI support portal** set-up at https://gitlab.com/eessi/support
  - Labels for issues are updated
  - Repository updated (templates for issues, replies, …)
  - Wiki updated (internal docs for EESSI support team members)
- **TODO**
  - Define initial level of support for EESSI (what is supported, what is not, …)
  - Set up and document support portal
    - Messages sent to support@eessi.io should result in issue being opened
    - Update the EESSI documentation (add page on “Getting support”)
  - Create form or templates for reporting problems
    - Update repository
  - Set up support rotation among MultiXscale partners involved in task 5.4

[Lara, Kenneth, Alan, …]

Sponsored AWS credits

- Ask in #aws-resources Slack channel to get access!
- Currently ~$10.3k worth of sponsored credits left (valid until Nov'23)
- ~$2,956 "spent" in July'23 on Stratum-1, monitoring, sources.easybuild.io, **Slurm cluster (build bot)**
- ~$43.5k 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**
- Growing large cost for Elastic File System (EFS) service - mostly due to huge tarballs created by the bot?
- Monthly sync meetings with Brendan/Angel/Matt/Francesco (AWS) every 2nd Thursday of the month



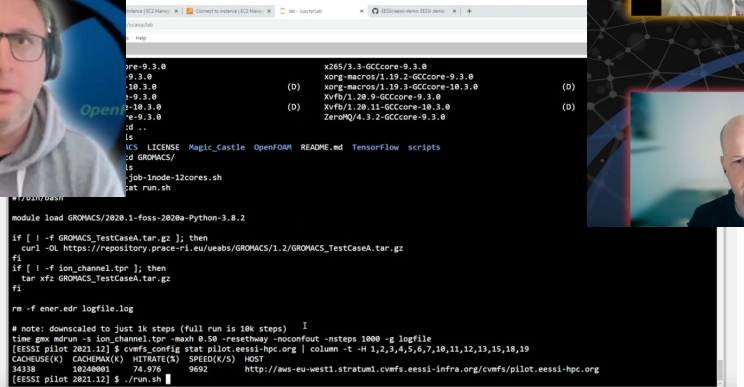


[Kenneth]

AWS HPC Tech Short on EESSI

- 8-min YouTube video introducing EESSI (by Alan + Kenneth)
- **"Making scientific software EESSI - and fast"**
- Was published on 15 June 2023
- Spins EESSI as "streaming scientific software", includes quick demo starting from scratch
- https://day1hpc.com/post/making-scientific-software-eessi-and-fast

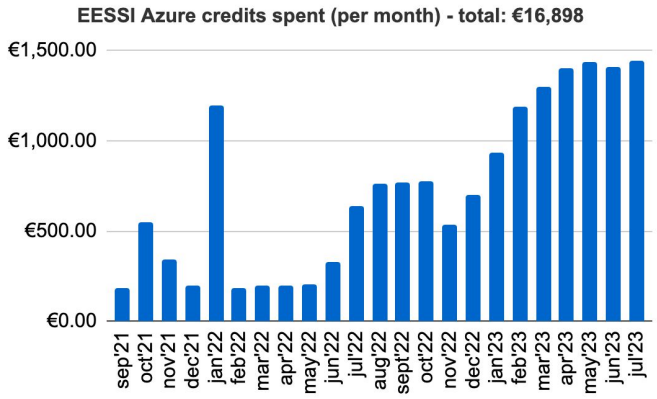
https://youtu.be/Fzv4ieil1jo

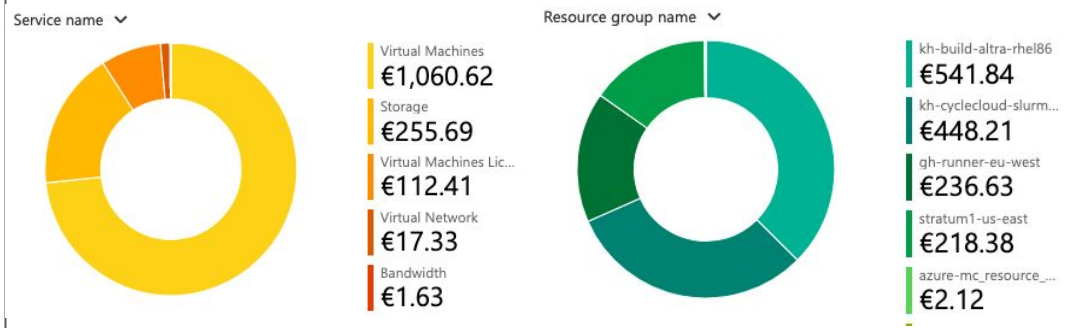


[Kenneth, Alan]

Sponsored Azure credits

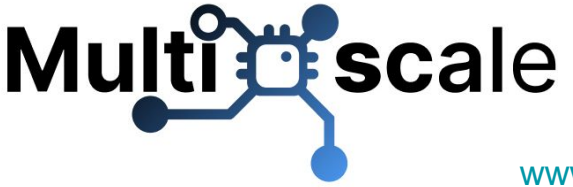
- Sponsored credits (€40,000) are being put to good use!
- **Ask in #azure-resources Slack channel to get access!**
- In July'23: ~€1,447 worth of credits spent
- ~€17k worth of (sponsored) credits spent in total (since Sept'21)
- Used for: Stratum-1, GitHub Runners, heterogeneous Slurm cluster, Ampere Altra build node
- Virtual Slurm cluster in Azure
    - Current setup using Azure Cyclecloud is WIP - may start over with Magic Castle instead





July'23

[Kenneth]



EuroHPC
Joint Undertaking

EESSI

www.multixscale.eu github.com/multixscale

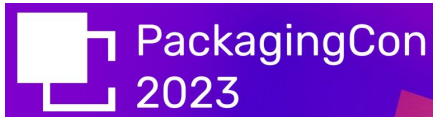
- CI/CD collaboration with Deucalion (Portugal) via CASTIEL2
  - Pathway to making EESSI available on different EuroHPC JU systems
  - **EESSI already available on Vega (Slovenia)**
  - Discussion with Karolina (Czech Republic) + Meluxina (Luxembourg) ongoing
  - Deucalion (Portugal) not available until Q3

- “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 (end of 2023?) - most likely fully virtual event

- 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

[Alan, Kenneth, Lara, Bob, Thomas, Caspar, Satish, Elisabeth, …]

EESSI @ PackagingCon'23?



- 26-28 Oct'23 in Berlin (Germany), hybrid event - https://packaging-con.org
- Conference on "package management" (in broad sense)
- Considering to submit a talk on EESSI, maybe also EasyBuild (Kenneth)
- Submission deadline is Sun 6 Aug'23
    - Talk proposal, basically only title + short abstract, so lightweight submission
- Speakers can be hybrid, but pre-recording talk may be required for remote speakers…

[Kenneth]

EESSI @ Supercomputing'23?

- 12-17 Nov'23 in Denver (US) - https://sc23.supercomputing.org
- Who is planning to attend? (confirmed: Alan, HPCNow!)
- Planned activities:
  - Magic Castle tutorial accepted (Alan)
  - WIP: submission on EESSI for HPC User Support Tools (HUST) workshop (Alan)
  - Booth talks @ Microsoft + AWS?
  - MultiXscale presence in EuroHPC booth?

[Alan, Kenneth]