EESSI

EUROPEAN ENVIRONMENT FOR SCIENTIFIC SOFTWARE INSTALLATIONS

11 Jan 2024

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. Update on EESSI production repository `software.eessi.io`
5. Update on support for NVIDIA GPUs in EESSI
6. Update on EESSI test suite
7. Support for EESSI
8. AWS/Azure sponsorship update
9. Update on MultiXscale EuroHPC project
10. Upcoming/recent events: EuroHPC User Day 2023 + ISC'24
11. Q&A

Quick introduction by new people

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

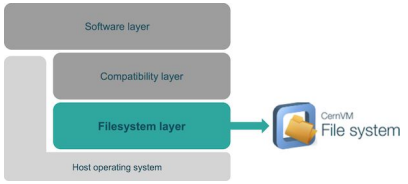
- Who are you, where do you work, on what?
- Why are you interested in the EESSI project?
- Are you planning to actively contribute,
  and if so, to which aspect(s) of the project?

EESSI-related meetings

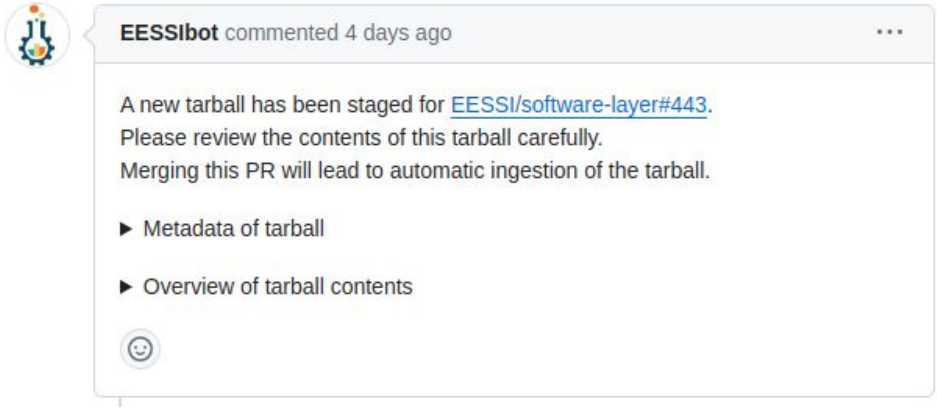
- *(11 Dec'23)* CernVM-FS coordination meeting (notes - CERN (guest) account required)
- *(12 Dec'23)* Sync meeting EESSI - SKA (notes)
- *(18 Dec'23)* Sync meeting with Azure (notes)
- *(20 Dec'23)* Sync meeting on GPU support (notes)
- *(Dec'23)* Sync meetings on MultiXscale deliverables *(notes are private to MultiXscale project partners)*
- *(Dec'23)* Weekly support team sync meetings *(notes are in private wiki on EESSI support portal)*

[Bob, Kenneth]

Progress update: filesystem layer



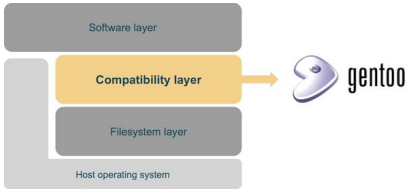
- Staging PRs now include a link to the software layer PR that triggered the build: PR #170



- Add `strace` to our containers, useful for debugging issues: PR #171

[Bob, Kenneth]

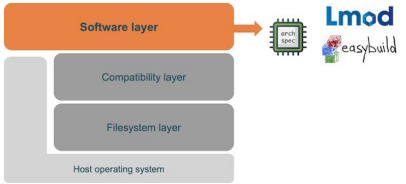
Progress update: compatibility layer



- 2023.06 version for `software.eessi.io` (see PR#191)
  - ~30 recent Gentoo Linux Security Advisories, see https://security.gentoo.org/glsa
    - Our installation is not affected, so no updates required
    - Procedure to check security advisories that affect EESSI should be documented/automated…
- 2023.06 version in EESSI pilot repository (`pilot.eessi-hpc.org`)
  - No recent changes here
  - We should apply some older updates (see PR#193) to the pilot too
  - **EESSI pilot repository is no longer actively maintained!**
  - Initialization script should make this (very) clear, and suggest to use `software.eessi.io` instead…

[Thomas, Bob, Kenneth]

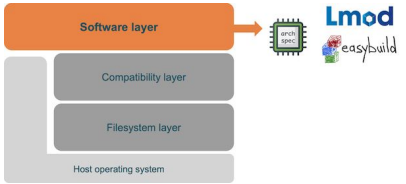
Progress update: software layer



- Recently merged PRs:
  - Add JSON file + Python script to keep track of software licenses (PR #400)
  - NVIDIA GPU support (PR #410, PR #434, PR #437)
  - More software: `foss/2022b` (PR #416), LHAPDF (PR #417), LoopTools (PR #423), R 4.3.2 (PR #426), Boost (PR #430), netCDF (PR #431), FFmpeg (PR #432), Qt5 (PR #422), ALL (PR #439), EasyBuild v4.9.0 (PR #440) `foss/2023b` (PR #442), SciPy-bundle w/ `foss/2023a` (PR #443)
  - Prepend EESSI version to `$PS1` instead of overwriting `$PS1` (PR #411)
  - Fix permission denied when echoing to `/dev/stdout` (PR #415)
  - Get rid of “pilot” (PR #420)
  - Fix check for missing installations in CI (PR #433)

[Kenneth, Thomas, Richard, Lara, Caspar, Satish, Xin, Alan, …]

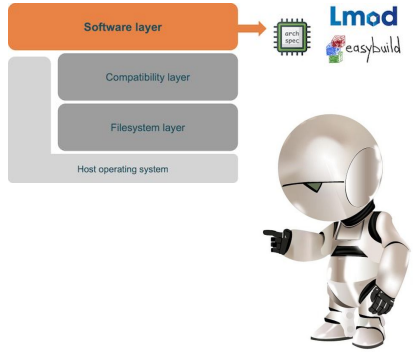
Progress update: software layer



- Recent open PRs:
  - More software: GROMACS (PR #401), OpenFOAM v10 (PR #404), Rivet 3.1.7 (PR #418), GDAL (PR #419), waLBerla (PR #424), CDO (PR #427), R-bundle-CRAN (PR #428), BWA (PR #429), QuantumESPRESSO (PR #436), PyTorch v2.1.2 (PR #444), OpenFOAM v11 (PR #446), SciPy-bundle w/ `foss/2022b` (PR #448)
  - Add support for zen4 / AMD Genoa to archdetect (PR #447)

[Kenneth, Thomas, Richard, Lara, Caspar, Satish, Xin, Alan, …]

Bot for building + deploying software layer



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

- No updates in December'23
- Bot is running smoothly
- Slurm cluster on which bot is running was updated, local disk on login node is now 50GB
- Currently looking into improvements to the deployment procedure
  - Bundling of multiple tarballs into a single staging PR
  - Efficiency of the deployment
  - Removing code specific to deployments for `EESSI/software-layer` repo
- Open meeting to discuss future developments (priorities for 2024)
  - Fri 12 Jan 2024, 09:00 CET (ask Thomas for connection details)

[Thomas, Kenneth, Bob]

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
  - Supported CPU targets: see http://www.eessi.io/docs/software_layer/cpu_targets
  - **NVIDIA GPU support has been added** 🎉, see: https://www.eessi.io/docs/gpu and dedicated slide
  - **We currently have ~270 software installations per CPU target** (+160 compared to last month)
    - 139 different software projects, ~2,150 software installations (across 8 CPU targets)
  - Current focus:
    - Adding software relevant for MultiXscale project
    - Processing incoming contributions to add more software
    - Fix failing installations in EESSI build environment, failing tests on `aarch64/neoverse_v1`, etc.
  - Starting to consider also providing optimized software installations of AMD Genoa (Zen4)

[Kenneth, Bob, Alan, Caspar, Lara, Thomas, Richard, Pedro, Xin, …]

EESSI Documentation

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

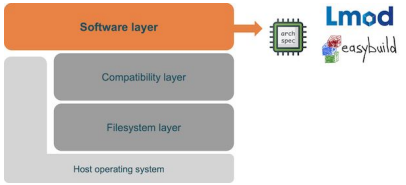
Improvements to the EESSI documentation

- Clarify procedure to open a PR (#135): https://www.eessi.io/docs/adding_software/opening_pr
- Overview of recent talks on EESSI (PR #137): https://www.eessi.io/docs/talks
- Document support for GPUs (PR #138): https://www.eessi.io/docs/gpu
- Make support portal easier to find (PR #130)
- A couple of open PRs: see https://github.com/EESSI/docs/pulls

Planned: auto-updated overview of available software in EESSI

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

EESSI NVIDIA GPU support

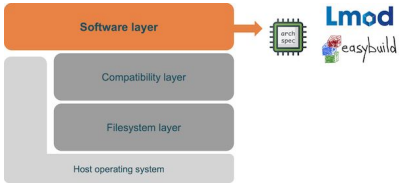


Initial support for NVIDIA GPUs is now in place in EESSI version 2023.06!

- Does not work out of the box, some minor action is required (by someone with sysadmin rights)
- See documentation at https://www.eessi.io/docs/gpu
- To give GPU software included in EESSI access to your GPU,
  we need to expose the system GPU driver
  => via `link_nvidia_host_libraries.sh` script that uses `host_injections` variant symlink
- To build GPU software on top of EESSI, a full installation of CUDA is required
  (EESSI only includes CUDA runtime libraries, which can be re-distributed)
  => via `install_cuda_host_injections.sh` script,
  which uses EasyBuild to install CUDA in `/cvmfs/software.eessi.io/host_injections` path

[Alan, Caspar, Kenneth]

EESSI test suite



ReFrame

Merged pull requests:

- Add hook to assign tasks per node (PR #97 + PR #98)
- Fix for example configuration file for VSC Tier-1 Hortense (PR #99)

Open pull requests:

- OSU-Microbenchmark test: point-to-point + collections, incl. GPU support (PR #54)

Next steps

- Add more tests (ESPResSo, CUDA samples, EasyBuild sanity check, …)
- Make GROMACS skip test if too many cores for given test case

MultiXscale deliverable D1.2 *Plan for design of a portable test suite* (available via multixscale.eu/deliverables)

[Caspar, Sam, Satish, Kenneth, Lara]

Support for EESSI (MultiXscale task 5.4)

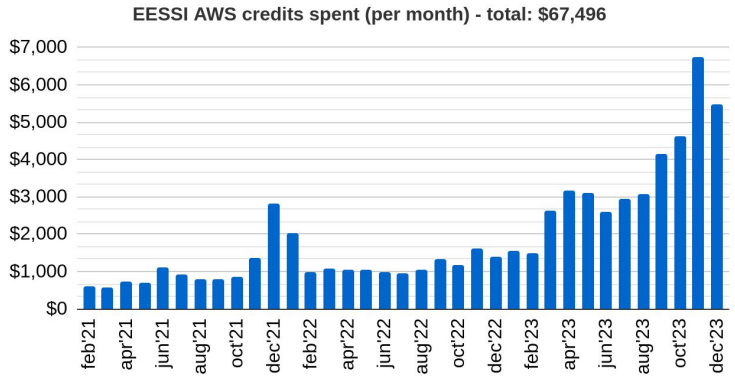
- EESSI support portal: gitlab.com/eessi/support
  - Support requests can be created by:
    - Opening an **issue in GitLab**
    - Sending an **email** to `support@eessi.io`
  - Issues in support portal can be public or private (only visible to reporter + support team)
  - **Information on support portal and support policy => https://eessi.io/docs/support**
  - Support is “reasonable effort” + only for problems with how software was installed in EESSI

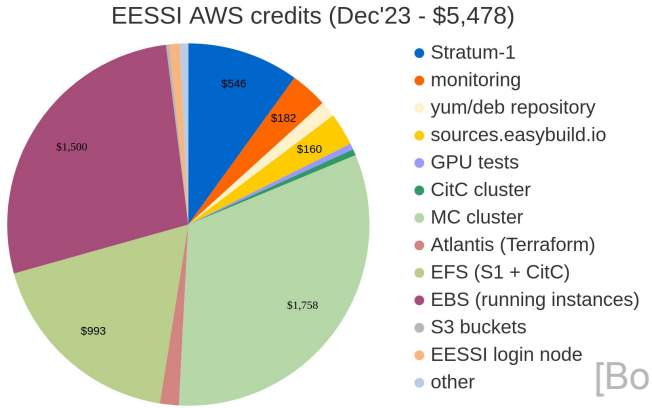
- Support rotation (in scope of MultiXscale Task 5.4)
  - A MultiXscale project partner is primarily responsible for support for 2 consecutive weeks
  - Weekly regular support sync meetings between MultiXscale project partners
  - Since Jan’24: ~1 FTE dedicated for support effort (across all project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

[Lara, Kenneth, …]

Sponsored AWS credits

- Ask in #aws-resources Slack channel to get access!
- Got another batch of $30k of sponsored credits
- Currently ~$41.2k worth of sponsored credits left ($11.2k valid until 29 Feb'24, $30k valid until 31 Dec'24)
- ~$5,478 "spent" in Dec'23 on Stratum-1 servers, monitoring, sources.easybuild.io, **Slurm clusters (build bot)**
  - Includes new Stratum 1 servers for eessi.io, new Magic Castle Slurm cluster, GPU support test machine
- **Increase in consumed credits due to extensive activity with build-and-deploy bot**
- Monthly sync meetings with Brendan/Angel/Matt/Francesco (AWS) every 2nd Thursday of the month

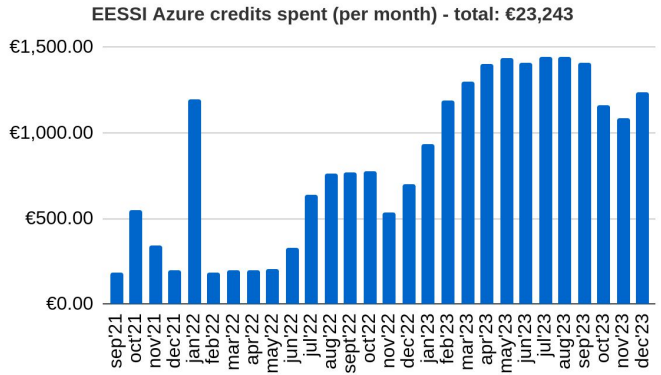


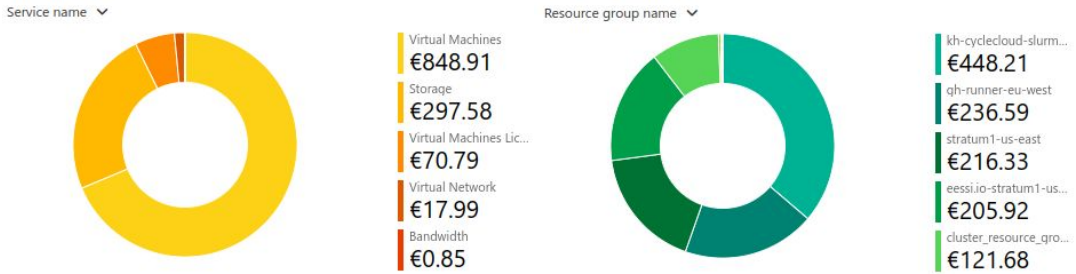


[Bob, Kenneth]

Sponsored Azure credits

- Sponsored credits (€40,000)
- Ask in #azure-resources Slack channel to get access!
- In Dec'23: ~€1,236 worth of credits spent
- Used for: Stratum-1 mirror servers, GitHub Runners, heterogeneous Slurm cluster (with Cyclecloud)
- Current Slurm cluster using Azure Cyclecloud is not used
- Currently trying to set up a Magic Castle cluster, same tool as used in AWS, figuring out which node images to use (ideally Rocky Linux, or similar)





Dec'23

[Bob, Kenneth]

www.multixscale.eu github.com/multixscale

- MultiXscale deliverables (due end of 2023) are now available via multixscale.eu/deliverables
  - D1.1: Report on shared software stack prototype (EESSI)
  - D1.2: Plan for design of a portable test suite (see also eessi.io/docs/test-suite)
  - D5.1: Community contribution policy and GitHub App (see also eessi.io/docs/bot)
  - D5.2: Support portal for EESSI (see also eessi.io/docs/support)
- CernVM-FS + EESSI is mentioned explicitly in EuroHPC CASTIEL2 deliverable D5.8 on “CI/CD platform”
- MultiXscale project partners are currently preparing progress report + project review meeting (mid Feb’24)
- **Please follow the MultiXscale project on the various social media channels!**

  YouTube: youtube.com/@MultiXscale

  Twitter/X: twitter.com/multixscale

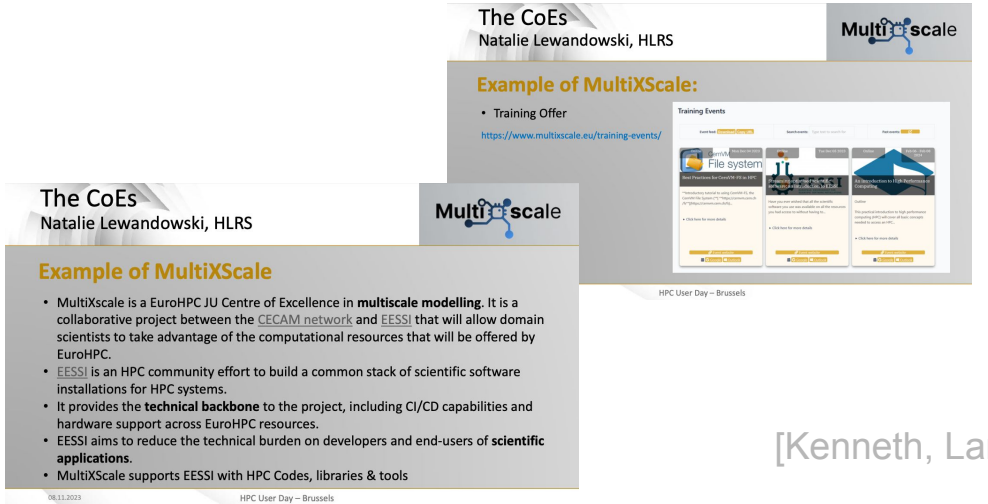
  Facebook: facebook.com/people/MultiXscale/100090773041074

  LinkedIn: linkedin.com/company/multixscale

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

1st EuroHPC User Day 2023

- 11 Dec'23 in Brussels (Belgium)
  https://eurohpc-ju.europa.eu/news-events/events/eurohpc-user-day-2023-12-11_en
- **MultiXscale + EESSI got an explicit mention** during talk on EuroHPC NCCs and CoEs
- Quotes: *"Outstanding example", "fits very well into our overall strategy"*
- Recording available at https://webcast.ec.europa.eu/eurohpc-ju-user-day-2023-12-11 (see ~11:37:30)



[Kenneth, Lara]

EESSI @ ISC'24

- 12-16 May 2024 in Hamburg (Germany) - https://www.isc-hpc.com

- **3 tutorial proposals submitted** (deadline was 18 Dec'23)
  - *Magic Castle: Terraforming the Cloud to Teach HPC* (EESSI as software stack)
    by Félix-Antoine Fortin (Magic Castle lead developer) + Alan & Kenneth
  - *Efficient Software Distribution for HPC: an Introduction to CernVM-FS* (EESSI as example repo)
    by Kenneth, Lara, Alan, Bob (EESSI) + Laura, Valentin, Jakob (CernVM-FS development team)
  - *Streaming Optimised Scientific Software: an Introduction to EESSI* (user-facing tutorial)
    by Sebastian Achilles (JSC) + Kenneth & Alan

- **Proposal for Birds-of-a-Feather session "EESSI Community BoF" submitted** (deadline was 10 Jan'24)

- Acceptance notifications expected by 9 Feb'24 (tutorials) and 14 Feb'24 (BoF)

[Kenneth, Alan, Lara, Bob]