EESSI meeting

2 Mar 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. Usage tracking in EESSI?
5. EESSI documentation update
6. EESSI pilot repository
7. AWS/Azure sponsorship update
8. Update on MultiXscale EuroHPC project + open position at HPC-UGent
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

- (13 Feb'23) Monthly CernVM-FS Coordination Meeting
  - Notes: https://hackmd.io/7otdq5tSRuyIWAJaF7NH6A
  - CernVM Program of Work 2023
    - CernVM-FS 2.11 (2023Q2) will mostly focus on performance improvements for clients
    - CernVM-FS 2.12 (2023Q4) will have improvements for cold caches (prefetching)
  - Next CernVM workshop planned for early 2024
  - Some nice discussions about questions we raised:
    - Ways of tracking usage of a CVMFS repository
    - Replacing existing directories (e.g. compatibility layers) in a more efficient way
    - Setting up a Stratum 1 using another Stratum 1 (instead of using the Stratum 0)
    - Experiences with and different scenarios of using S3-backed Stratum servers
  - Next meeting: Mon 13 Mar’23 - https://indico.cern.ch/category/5485

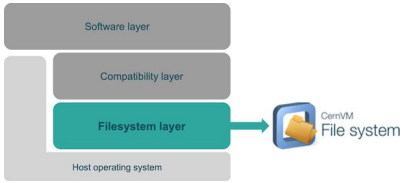
[Kenneth, Bob]

EESSI-related meetings

- *(9 Feb'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-(2023-02-09)
- *(9 Feb'23)* AWS/EESSI sync meeting - cancelled due to miscommunication
  next meeting is scheduled for 9 March'23
- *(14 Feb'23)* MultiXscale sync meeting (monthly - all project partners)
  notes available at https://github.com/multixscale/meetings/wiki/Sync-meeting-2023-02-14
- *(14 Feb'23)* Sync meeting on development of build-and-deploy bot (MultiXscale task 5.3)
  - Attended by Thomas, Kenneth, Bob
  - Notes available at https://github.com/multixscale/meetings/wiki/sync-meetings-bot-T5.3
  - + additional one-on-one sync meetings (Thomas + Kenneth) to discuss/review/merge PRs
- *(17 Feb'23)* Azure/EESSI sync meeting (Azure + Alan/Bob/Ivar)
  notes available at https://github.com/EESSI/meetings/wiki/Azure-meeting-2023-02-17

[Kenneth, Thomas, Bob, Alan]

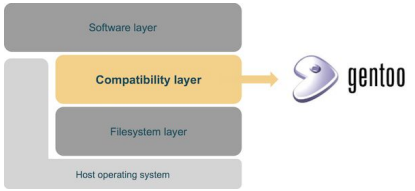
Progress update: filesystem layer



- **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)
- PR #139: Tarball ingestion script can now handle a "scripts" tarball, containing files from https://github.com/EESSI/software-layer/tree/main/scripts

[Bob, Kenneth]

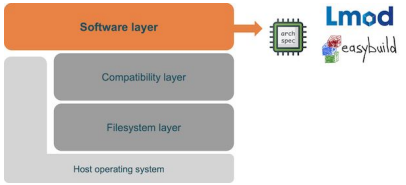
Progress update: compatibility layer



- Preparing a new compatibility layer (2023.03?)
  - Updates for packages (`archspec`, `Lmod`, etc) and new package sets in PR #84 of gentoo-overlay
  - If any packages still need to be added, please let it know as soon as possible!
  - Currently testing the bootstrap with an updated bootstrap script and updated gentoo repository commit
  - Quite some (breaking) changes have been made in Gentoo, causing the bootstrap to fail
    https://bugs.gentoo.org/892876
    https://bugs.gentoo.org/895240
  - Ultimately, we will let the bot do the build using PR #163
- 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)

[Kenneth, Bob, Thomas]

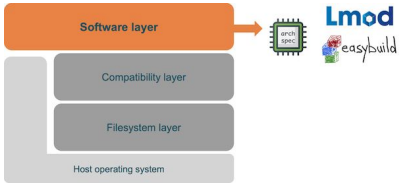
Progress update: software layer



- `eessi_container.sh` script was enhanced (see PR #232)
  - Support for `-l`/`--list-repo` option
  - Be aware of HTTP(S) proxy configuration
  - Keep/reuse copy of container image from previous run when using `--resume`
  - Pass `$EESSI_SOFTWARE_SUBDIR_OVERRIDE` into container (if set)
- Bug in experimental support for easystack files in EasyBuild was fixed (see easybuild-framework PR #4213)
- Next steps:
  - Add `bot/build.sh` script that uses `eessi_container.sh` (PR #233)
    - Replaces EESSI-specific Slurm job script currently used by bot (see also bot PR #155)
  - 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`)

[Kenneth, Thomas]

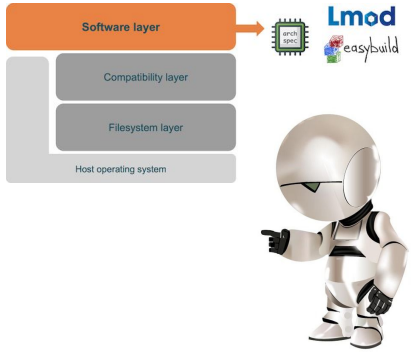
Progress update: software layer



- GPU support
  - 2 main PRs, lot's of tidying up going on
    - One that installs CUDA runtime and CUDA software in software layer (PR #212)
    - Another then installs the compat libraries and checks CUDA is working (PR #235)
  - Difficult/tedious to test things without merging PR #212 first
  - Arch specific guards not in place (and don't know what they should be)
  - Hope to have both in review-able shape by tomorrow
  - Approach to GPUs does not seem to work in containers
    - May need to add a way to directly use the system drivers
      - Add an "Am I in a container" check?
    - Should be able to copy that from Apptainer?
  - Will require follow-up Lmod hook PR for UI

[Alan, Kenneth]

Bot for building + deploying software layer



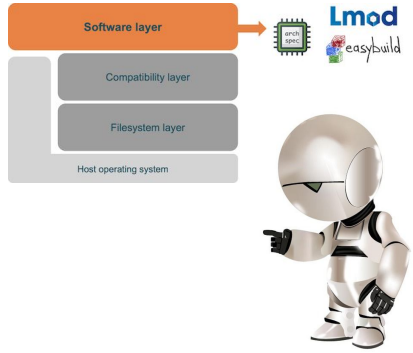
Progress on implementation of build-and-deploy bot

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

- Feb'23
  - PRs: 1 merged - 1+1+2 open (ready+draft+stalled) PRs
  - issues: 2 closed - 56 still open (+2 vs Jan'23)
    - PR #153 fix bug in determining running job
    - draft PR #155 support for `bot/build.sh`
    - outdated PR #85 resubmit a build job locally
    - hackathon PR #127 status overview for PR
- Major rewrite of interface between bot and software-layer (~ 2000 LoC incl comments)
  - work-in-progress in PR #155
  - using `bot/build.sh` and `eessi_container.sh` (EESSI/software-layer PRs #215, #216, #232, #233)
  - in use for ~ 2-3 weeks within NESSI project by 5 software builders (see next slide)

[Thomas, Kenneth]

Bot for building + deploying software layer



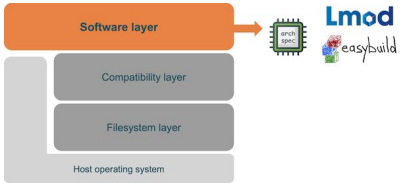
Progress on *use* of build-and-deploy bot in NESSI project

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

- Feb'23
  - NESSI: workshop to introduce project members to using the bot
    - demo & hands-on (~ 2.5 hours)
    - how to create a PR to the software layer (using NESSI/2022.11pilot)
    - using `bot:build` label to trigger build jobs being submitted
  - NESSI: use of the bot
    - building for 5 `x86_64` architectures across 4 clusters
    - ~ 20 PRs ongoing, 6 PRs finished and ingested
    - revealed bug in rewritten bot (lack of support for arch `generic`) => not sure if `EASYBUILD_OPTARCH=GENERIC` always works as intended
    - also documentation to simplify work for project members

[Thomas, Kenneth]

EESSI test suite



- See https://github.com/EESSI/test-suite
- Current status:
  - GROMACS test in place (CPU + GPU)
- First goal is to come up with a good example of a *portable* test (across variety of systems)
- Current work-in-progress (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`)
  - Should fix a bunch of issues: #7, #8, #10, #13, #14, #15, #19
- Also looking into proper packaging of EESSI test suite, to support `pip install`'ing it (PR #17)

[Caspar, Sam, Satish, Kenneth]

Usage “tracking” in EESSI?

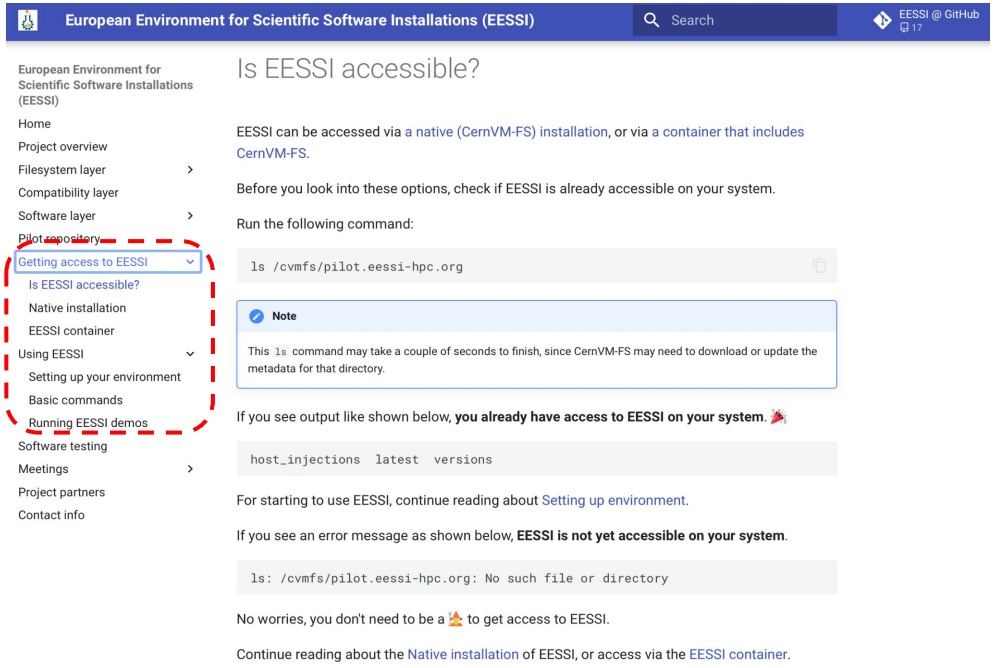
(this is not in place yet, just an idea, polling for feedback)

- We currently have no idea how often the EESSI (pilot) repository is used…
- Difficult to track due to EESSI being a publicly accessible CernVM-FS repository (HTTP traffic)
  - (private) mirror servers (Stratum-1), proxy cache, client cache, etc.
- An interesting suggestion was made during last CernVM-FS coordination meeting
  - **Automatically trigger sending of a UDP packet to a “counting server”** (see expcounter utility)
  - Could be done in EESSI init script, but maybe (also) somewhere in compat layer (Lmod?)
  - UDP packet could include useful (anonymous) info (EESSI version, OS, CPU arch, in CI or not, …)
  - We should definitely provide an easy way to opt out (`$EESSI_NO_TRACKING`?)
  - Data collection must be very light-weight (only harvest environment variables?)
  - Won’t be perfect, but better than being totally oblivious?
  - Would help with motivating need for more sponsored credits from AWS/Azure
  - **Any objections/concerns about this?**

[Kenneth]

EESSI documentation update

- Two new sections: *Getting access to EESSI* and *Using EESSI*
  - Step-by-step guides
  - Examples
  - Use of `eessi_container.sh`
  - Running demos
- Feedback welcome!
- See https://eessi.github.io/docs



[Kenneth, Thomas]

EESSI pilot repository

NOT FOR PRODUCTION USE!

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

- 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 (partial!)**
    - Targets: `aarch64/generic`, `aarch64/graviton2`, `aarch64/graviton3`, `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

[Kenneth]

Outlook to next pilot version (2023.x)

- Small changes to compatibility layer: updated Lmod, more tools, …
- 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 ongoing:**

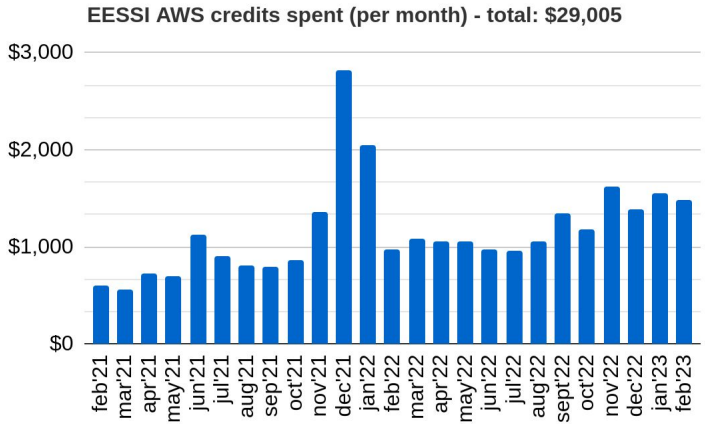
  EESSI/gentoo-overlay PR #87 merged (updated packages + package sets)

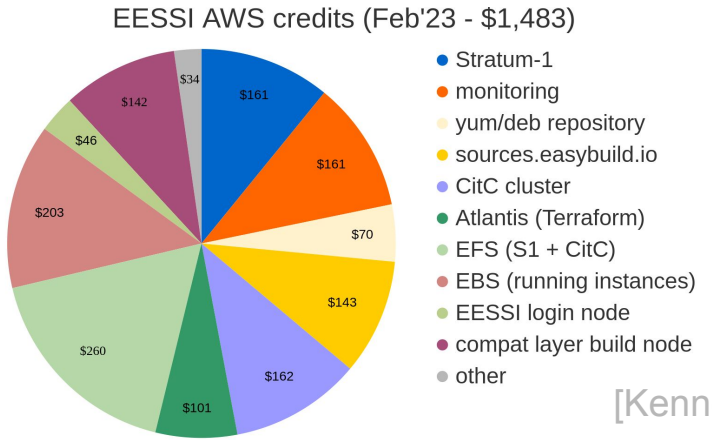
  WIP PRs for new version of compat layer: PR #160 + PR #163 (trouble with Gentoo Prefix bootstrap)

[Kenneth]

Sponsored AWS credits

- **Ask in #aws-resources Slack channel to get access!**
- Monthly sync meetings with Brendan/Angel/Matt (AWS) every 2nd Thursday of the month
- **Extra batch of $10,000 worth of credits provided for 2023Q1 (valid until end of March'23)**
- Currently still ~$9,766 worth of sponsored credits left
- ~$1,483 "spent" in Feb'23 on Stratum-1, monitoring, sources.easybuild.io, Slurm cluster (incl. build bot)
- ~$29,005 worth of credits spent in total so far (since Feb'21), all covered by sponsored credits

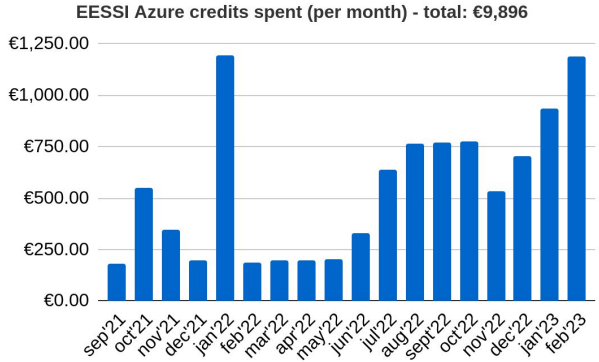




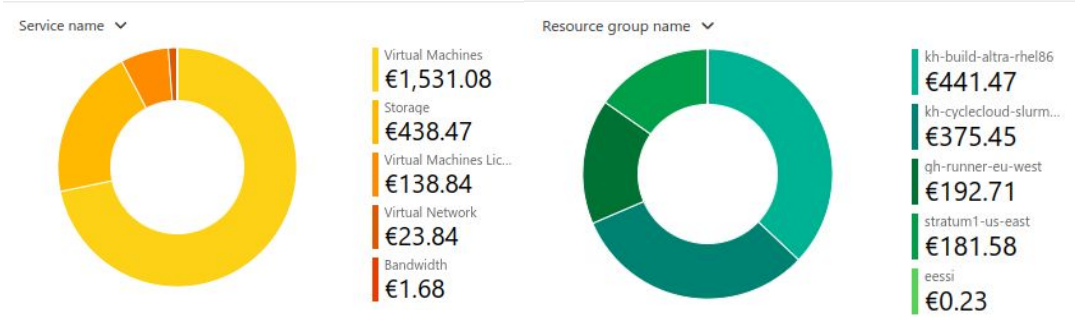
[Kenneth, Bob]

Sponsored Azure credits

- Sponsored credits (€40,000) are being put to good use!
- **Ask in #azure-resources Slack channel to get access!**
- In Feb: ~€1,192 worth of credits spent
- ~€9,896 worth of (sponsored) credits spent in total (since Sept'21)
- Used for: Stratum-1, GitHub Runners, heterogeneous Slurm cluster, Ampere Altra build node
- **New: 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…)

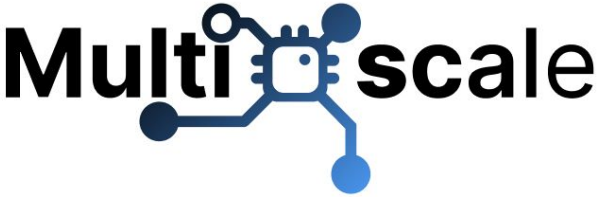


Overview of spent credits per month



Feb'23

[Kenneth]



EuroHPC
Joint Undertaking

- Project started on 1 Jan 2023 - **Official kickoff meeting 23-24 March 2023 (Ljubljana)**
- Effort is ongoing, cfr. progress on build-and-deploy bot, GPU support, test suite
- Will collaborate with CASTIEL2 (which means NCCs and other CoEs)
  - Required to have CI/CD on EuroHPC platforms
  - Jacamar CI (ECP) seems like a likely approach (also used by Spack for build cache)
  - Spack CI setup with (un)trusted builds can be an inspiration?
  - May be opportunity to spread EESSI awareness
- MultiXscale website (still) coming soon…
- Overview of tasks for work packages 1+5 (most relevant for EESSI) in project board in multixscale GitHub org (work-in-progress)

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

Open position at HPC-UGent (MultiXscale CoE)

- The HPC team at Ghent University (Belgium) currently has an open position
- In the context of the MultiXscale EuroHPC Centre-of-Excellence
- **Tasks include actively contributing to EESSI to make it more mature**
- More information via https://www.ugent.be/hpc/en/news-events/news/job-multixscale
- **Deadline for submission is Sun 6 March 2023**

[Kenneth]

Upcoming events

- EuroHPC Summit, @ Gothenburg (Mon-Thu 20-23 March 2023)
  - www.eurohpcsummit.eu
- EuroHPC MultiXscale CoE kickoff meeting @ Ljubljana (Thu-Fri 23-24 March 2023)
- EasyBuild User Meeting @ London (Mon-Wed 24-26 April 2023)
  - easybuild.io/eum23
  - Will include a presentation on current status of EESSI (speaker TBD)
- BioHackathon Europe @ Barcelona (30 Oct - 3 Nov 2023)
  - biohackathon-europe.org - call for project proposals is open (deadline 10 April)

[Kenneth]

Upcoming events: HPCKP

- Website: hpckp.org/annual-meeting
- When: 17-18 May 2023
- Where: Barcelona
- Important Deadlines:
  - 7th April: Abstract submission deadline for presentations
  - 14th April: Confirm accepted presentations
  - 5th May: Presentations submission deadline
  - 12th May: Registration deadline

[Elisabeth/Danilo]