EESSI meeting

1 June 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
7. Past & upcoming events (HPCKP'23, ISC'23)
8. Q&A

Quick introduction by new people

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

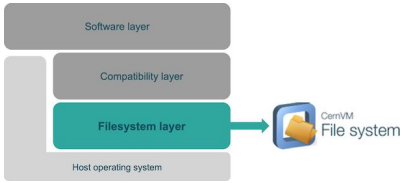
- Who are you, where do you work, on what?
- Why are you interested in the EESSI project?
- Are you planning to actively contribute,
  and if so, to which aspect(s) of the project?

EESSI-related meetings

- *(Mon 8 May'23)* EESSI software layer sync meeting (notes)
- *(Tue 9 May'23)* MultiXscale WP1+WP5 sync meeting (notes)
- *(Thu 11 May'23)* AWS/EESSI sync meeting (notes)
- *(Mon 15 May'23)* CASTIEL2 meeting on pairing MultiXscale with EuroHPC JU system Vega
- *(Tue 16 May'23)* EESSI software layer sync meeting (notes)
- *(Wed 17 May'23)* EESSI test suite sync meeting (notes)
- *(Tue 23 May'23)* build-and-deploy bot sync meeting (notes)
- *(Thu 25 May'23)* MultiXscale T5.1 sync meeting on support portal for EESSI (notes)
- *(Thu 25 May'23)* Meeting with CernVM-FS developers on "Best Practices for CernVM-FS on HPC" tutorial (notes)
- *(Fri 26 May'23)* build-and-deploy bot sync meeting on PR #172
- *(Tue 30 May'23)* recording of AWS HPC Tech Short on EESSI - **resulting YouTube video is expected in a couple of weeks**
- *(Tue 30 May'23)* EESSI software layer sync meeting (notes)
- (Wed 31 May'23) EESSI test suite sync meeting (notes)

[Kenneth, Thomas, Bob, Alan]

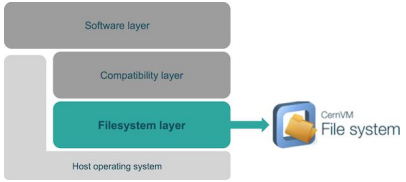
Progress update: filesystem layer (1/2)



- Open pull requests
  - PR#149: Fix tarball content type check
- Ongoing work to enhance ingestion:
  - WIP PR#146: update status of PR comments when ingesting a tarball
  - Restructure S3 bucket: top-level directories (requires change of upload script used by bot)
    - `tarballs` for tarballs
    - `new`, `staged`, `approved`, `rejected`, `ingested`, `unknown` for metadata files
  - Use on-disk `EESSI/staging` repository

[Bob, Kenneth, Thomas]

Progress update: filesystem layer (2/2)



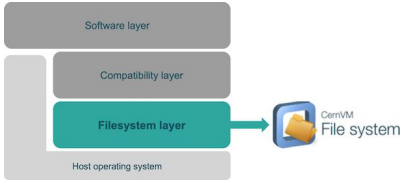
- **Removed pilot version 2021.06 from EESSI repository**
  - 2021.12 pilot version provides everything in 2021.06, and more (+ has updated compat layer)
  - The `2021.06/init/bash` script is still there: it prints a warning and sources `2021.12/init/bash`
    - https://github.com/EESSI/software-layer/tree/main/versions/2021.06/init
  - People who are still using 2021.06 should not see any breakage, only a warning

- TODO: 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)

- Physical server for new Stratum-1 (+ yubikeys) was delivered at RUG, will be set up so it can be used for `eessi.io` (in the next couple of weeks)

[Bob, Kenneth]

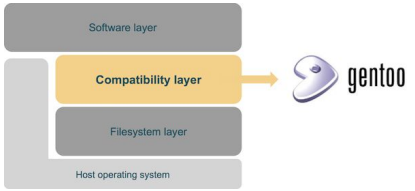
Filesystem layer - performance monitoring



- Observed dramatic performance variation of Stratum-1 server at RUG
  - Running TensorFlow demo could take up to 50min due to this…
  - Extensive testing but no clear source for issue
  - Issue appeared and disappeared seemingly randomly
  - Full discussion in https://github.com/EESSI/filesystem-layer/issues/151
- TODO: we need to start monitoring the performance of our Stratum-1 servers since these are the gateway to EESSI (particularly for new users)
  - Should consider using CDN(s) by default - like Cloudflare (which is free), or Cloudfront (AWS), …
  - For cloud, should be using CDN for the Stratum-1 at that cloud provider (will GeoAPI solve selection problem for us?)
  - Due to our Azure subscription via SURF, we have a special situation where we think we don't pay for outbound traffic… should verify this?

[Bob, Kenneth, Alan]

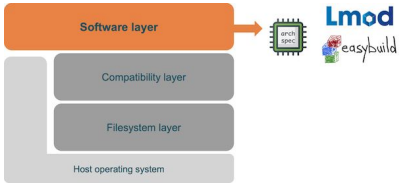
Progress update: compatibility layer



- **Tarballs for new compatibility layer (2023.04, `aarch64` and `x86_64`) have been ingested**
  - Goal of automating building + deploying compat layer with bot was not reached (yet)
  - Used for testing build of first software packages for software layer
- Updated the GitHub Action that tests the compatibility layer (PR #183)
  - Removed 2021.06
  - Fixed the path to new versions (which are now under a `versions` subdirectory)
  - Added 2021.12
  - TODO: add 2023.04
- Alexander has set up a CI for testing the Gentoo Prefix bootstrap
  - https://github.com/APN-Pucky/gentoo-prefix-tester
  - We should set up custom GitHub runners to work around the default time limits (and have some more resources)

[Bob, Thomas, Kenneth]

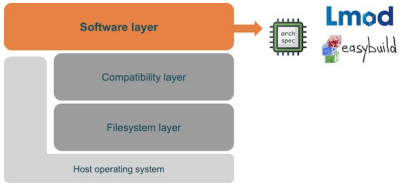
Progress update: software layer



- Merged PRs:
  - Add replacement init script for removed 2021.06 pilot version (PRs #246 + #249)
  - Don't print warning when unknown targets are found during init (PR #248)
  - Implement post-prepare hook for GCCcore to also have a wrapper in place with system type prefix like 'x86_64-pc-linux-gnu' (PR #251)
  - Update rpath injection hook for 'versions' subdir (PR #254)
- Open PRs:
  - Improve check_missing_installations.sh (PR #244)
  - First version of bot/check-result.sh script (WIP PR #241)
  - Flesh out load_easybuild_module.sh script (WIP PR #255)

[Kenneth, Alan, Thomas]

Progress update: software layer

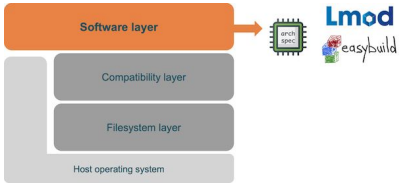


Action plan for 2023.04 software layer (see also meeting notes)

- Configure **build-and-deploy bots** in AWS + Azure - CPU targets like 2021.12 pilot, except `ppc64le`
- Start new install script for 2023.04 software layer - **using easystack files**
- Install EasyBuild 4.7.2 (with dedicated script, cfr. PR #255)
- Install GCC(core) base compilers: 9.3.0 (?), 10.2.0, 10.3.0, 11.2.0, 11.3.0, 12.2.0, 12.3.0, 13.1.0
- Install foss toolchains: 2020a (?), 2020b, 2021a, 2021b, 2022a, 2022b
- Install supporting tools & libraries with different GCC(core) versions: Perl, Python, CMake, Rust, …
- Install software: GROMACS, OpenFOAM, TensorFlow, R + Bioconductor, WRF, ESPResSo, …
- Aim to be on-par with EESSI pilot 2021.12 in terms of available software (with reasonable effort)
- Start extending set of provided software - through contributor workflow that lets bot build & deploy

[Kenneth, Alan, Thomas]

EasyBuild v4.7.2 release

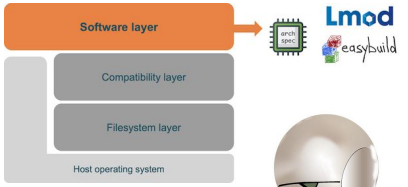


- Fix for GCC easyblock to build on top of EESSI compat layer (PR #2921)
- Add make 4.3 as build dependency for recent OpenBLAS versions
- New generic easyblocks for controlled installation of Rust software:

  `Cargo` + `CargoPythonPackage`
- Custom RPATH sanity check for Go software
- Easyconfigs for GCC 12.3.0 + 13.1.0, ESPResSo (MultiXscale), ColabFold, Bioconductor v3.16, …
- Detailed release notes available at https://docs.easybuild.io/release-notes

[Kenneth]

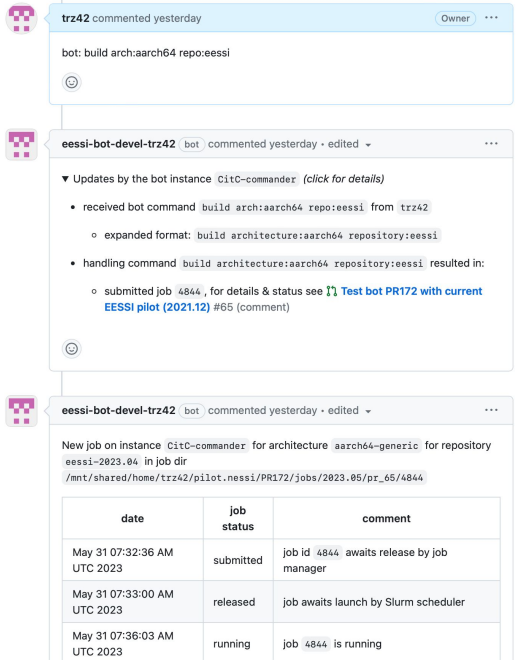
Bot for building + deploying software layer



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

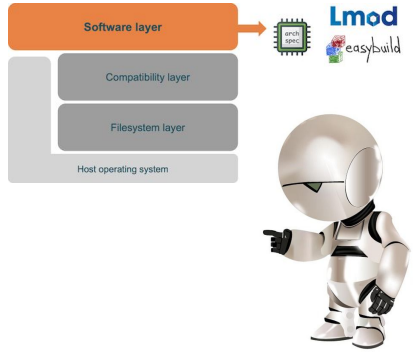
https://github.com/EEESI/eessi-bot-software-layer

- May'23
  - PRs: 3 merged - 4+1 open (ready + draft) PRs
  - issues: 2 closed, 1 created, 60 still open (-1 in May'23)
- PR #172 (ready to merge): send commands to bot
- WIP PR #174: move job result checking to target repository
- PR #178: replay a GitHub event locally
- PR #181: added default comments
- PR #182: add comment id to metadata uploaded to S3



[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

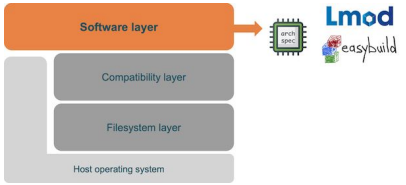
- May'23:
  - Building for 5 `x86_64` + 1 `aarch64` CPU architectures across 3/4 clusters (AWS CitC + 2/3 in Norway)
  - 25 PRs ongoing, 29 PRs finished and ingested
    - 20 PRs for NESSI/2023.04
      - foss/2021a: toolchain (80%), open PRs: Qt5, SciPy, GROMACS, TensorFlo, QuantumE..
      - foss/2022a & foss/2022b: compilers built
  - Continuing work on wiki page for troubleshooting
- Goals for June'23:
  - Add EESSI pilot software to NESSI/2022.11 & add software from local clusters
  - Continue building new stack for NESSI/2023.04
  - Test enhancements: `bot/check-result.sh`

[Thomas]

EESSI test suite

github.com/EESSI/test-suite

recent meeting notes here



ReFrame

Merged PRs for “blueprint” GROMACS test:

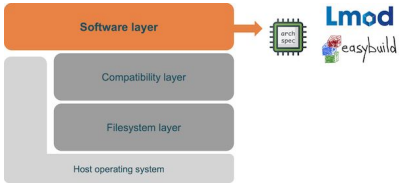
- Extend scales (2_core, 1_node, 1_4_node (quarter node), etc.) + add constants (PR #28)
- Add more comments, docs to the gromacs test (PR #42)
- Use smallest input (Crambin) as CI test for GROMACS (PR #46)

[Caspar, Sam, Satish, Kenneth]

EESSI test suite

github.com/EESSI/test-suite

recent meeting notes here



ReFrame

Merged PRs for “blueprint” GROMACS test:

- Add test for TensorFlow (PR #38)
  - Created ReFrame test for TensorFlow, based on `tf.distribute`
  - TODO: figure out how to do proper binding in a portable way
- Add test for OSU Microbenchmarks (no PR yet, CPU pt to pt works, working on GPU)
- Example ReFrame configuration file for VSC Tier-1 system *Hortense* (PR #24)
- Github Action workflow to run EESSI test suite in dry-run (PR #44)
- Namespace refactor to `eessi.testsuite.*` (WIP PR #45)
- Expanded developer instructions (PR #36)

Future work

- Look into support for hierarchical module naming scheme, for collaboration with The Alliance (#32)
- Start running EESSI test suite at regular interval in AWS and/or Azure

[Caspar, Sam, Satish, Kenneth]

EESSI pilot repository

NOT FOR PRODUCTION USE!

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

- 2021.06: **removed** (no changes in May'23)
- 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

[Kenneth]

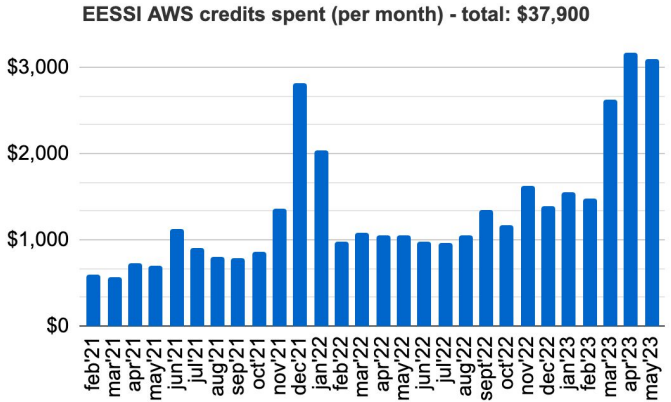
Outlook to next pilot version (2023.04)

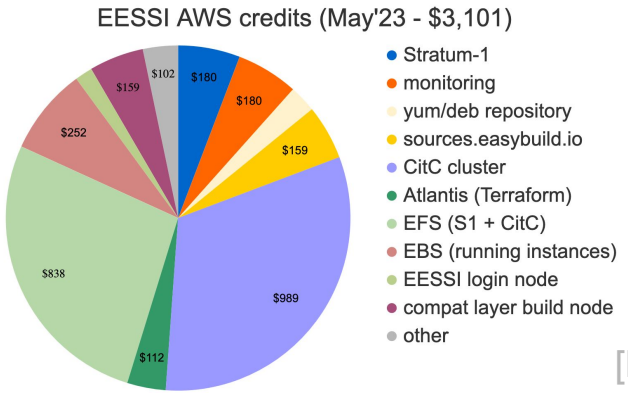
- Small changes to compatibility layer: updated Lmod, **less packages installed**, …
- Include enhancements/changes that are necessary for CUDA GPU support
- **Will get rid of ugly install script, switch to driven by easystack files**
- **Build software layer via bot, no more manual deployments!**
- 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) - when available
- **Effort is ongoing: actively looking into building software layer for 2023.04 pilot version**
- Will use EasyBuild v4.7.2 for 2023.04 software layer

[Bob, Thomas, Kenneth]

Sponsored AWS credits

- Ask in #aws-resources Slack channel to get access!
- Currently ~$18k worth of sponsored credits left ($15k valid until Nov'23)
- ~$3,102 "spent" in May'23 on Stratum-1, monitoring, sources.easybuild.io, **Slurm cluster (build bot)**
- Cost for EFS (shared FS for Stratum-1 + Slurm cluster) was cut in half compared to Apr'23 ($1,554 to $838)
- ~$37,900 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 in NESSI project**
- Monthly sync meetings with Brendan/Angel/Matt/Francesco (AWS) every 2nd Thursday of the month





[Kenneth]

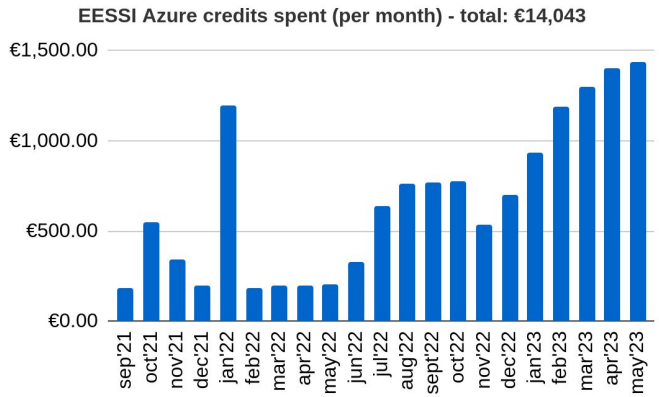
Issues arising from prep work for tech short

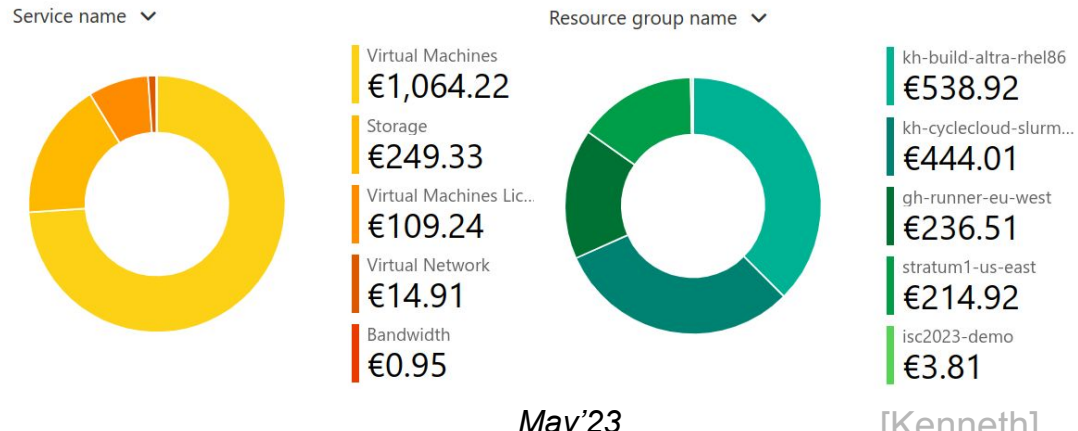
- Amazon Linux support added to demo repo installation scripts directory (PRs #19, #20, #21, #23)
- Location of Stratum-1 relative to instance has massive impact on performance
  - No surprise, but GeoAPI is really just “poor man’s CDN” (quote from CVMFS developers)
  - GeoAPI is a weak link if Stratum-1 performance is uneven/unpredictable
- EESSI works with EFA and ParallelCluster with trivial changes to cluster config yaml file
  - Major issue for AWS is that we are using our own libfabric… and that will never be supported
    - This use case could not be included in HPC Tech Short recording…
  - Able to `$LD_PRELOAD` the necessary libs
    - Observed improvement in latency for OSU benchmarks
    - Observed major performance drop in examples (GROMACS)… needs further investigation
- Examples fail on low memory machines, and error/segfault in some configurations
  - Has nothing to do with EESSI, but everyone will come asking us (general problem)

[Alan]

Sponsored Azure credits

- Sponsored credits (€40,000) are being put to good use!
- **Ask in #azure-resources Slack channel to get access!**
- In May'23: ~€1,439 worth of credits spent
- ~€14,043 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…)





May'23

[Kenneth]

www.multixscale.eu github.com/multixscale

- CI/CD collaboration with Deucalion (Portugal) via CASTIEL2
  - Deucalion not available until Q3, using Vega (Slovenia)
  - **EESSI already available on Vega**
- Two training events planned this year
  - Hybrid EESSI introductory user training event at HPCKP'23 meeting - DONE
  - "Best Practices for CernVM-FS on HPC systems"
    - In collaboration with CernVM-FS developers & experts
    - Date to be determined, likely Sept-Oct'23 - most likely fully virtual
    - Initial discussion with CermVM-FS developers has taken place, outline done
- Support portal for EESSI is a deliverable in MultiXscale due by end of 2023
  - Still evaluating/comparing alternatives like GitHub, GitLab, JIRA, etc. (meeting notes)
  - Decision soon

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

- hpckp.org/annual-meeting
- 17-18 May 2023 - Barcelona, Spain.
- **2-hour EESSI tutorial** Thu 18 May (afternoon)
    - Video recording of the session available soon in HPCKP webpage
- Would be nice to get feedback
    - We should prepare a questionnaire for this
- Alans experience:
    - Need to fine tune training material and decide useful order
    - Be careful not to get too deep into technical details
    - Need to integrate hands-on throughout material
    - Created new content: https://github.com/EESSI/eessi-nextflow-example

[Alan]

- EESSI was “present” at ISC’23 in Hamburg (21-25 May 2023)
- By Elisabeth (HPCNow!)
- MultiXscale poster + EESSI Talk/demo at EuroHPC booth
- Talk/demo on EESSI + MultiXscale at Azure booth
- Picture was featured in social media posts by EuroHPC JU

[Elisabeth]