EESSI meeting

4 May 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 + auth)
4. EESSI pilot repository
5. AWS/Azure sponsorship update
6. Update on MultiXscale EuroHPC project
7. Past & upcoming events (EUM’23, HPCKP’23, ISC’23)
8. Q&A

Quick introduction by new people

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

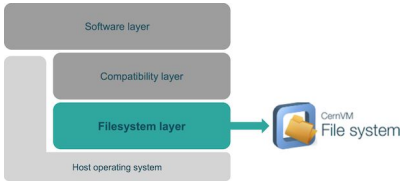
- Who are you, where do you work, on what?
- Why are you interested in the EESSI project?
- Are you planning to actively contribute,
  and if so, to which aspect(s) of the project?

EESSI-related meetings

- *(11 + 25 Apr'23)* Sync meeting on build-and-deploy bot (MultiXscale task 5.3)
  notes available at github.com/multixscale/meetings/wiki/sync-meetings-bot-T5.3
- *(11 Apr'23)* MultiXscale virtual sync meeting (every 2nd Tuesday of the month - all project partners)
  notes available at github.com/multixscale/meetings/wiki/Sync-meeting-2023-04-11
- *(11 Apr'23)* Sync meeting on EESSI compat layer
  notes available at https://github.com/EESSI/meetings/wiki/Sync-meeting-on-EESSI-compat-layer-(2023-04-11)
- *(13 Apr'23)* AWS/EESSI monthly sync meeting (every 2nd Thursday of the month)
  notes available at github.com/EESSI/meetings/wiki/AWS-meeting-2023-04-13
- *(14 Apr'23)* Tutorial for GitHub project board used for MultiXscale planning
  notes available at github.com/multixscale/meetings/wiki/Project-planning-with-Github-project-board---tutorial-meeting
- *(17 Apr'23)* Azure/EESSI monthly sync meeting (every 3rd Monday of the month)
  notes available at github.com/EESSI/meetings/wiki/Azure-meeting-2023-04-17
- *(17 Apr'23)* CernVM-FS coordination meeting
  notes at https://hackmd.io/7otdq5tSRuyIWAJaF7NH6A
- *(20 Apr'23)* Sync meeting on EESSI test suite (MultiXscale task 1.3)
  notes available at github.com/EESSI/meetings/wiki/Sync-meeting-on-EESSI-test-suite-(2023-04-20)

[Kenneth, Thomas, Bob, Alan]

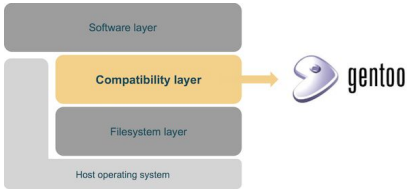
Progress update: filesystem layer



- PR #90 for a script that automates ingestion of tarballs into EESSI repo has been merged
- Other than that, 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)

[Bob, Kenneth]

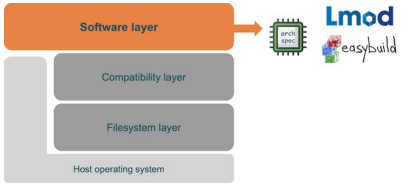
Progress update: compatibility layer



- Bootstrap issue on `ppc64le` while building `dev-python/flit_core`
- PR for missing `arm64` Prefix profile has been merged upstream (https://bugs.gentoo.org/892876)
- PR for missing `bc` build dependency for `Lmod` has been merged upstream
- To reduce the number of installed Python versions, we stick to Python 3.11 in compat layer (PR #182)
- Ansible playbook now creates a `reprod` dir at the end (see PR #180)
  - Contains copy of the bootstrap script, list of all the installed packages in the compat layer, metadata file with additional build details
- Cleanup task at the end of the playbook now removes `CMake, Ninja, Go, Rust` (PR #181)
- **Tarballs for new compatibility layer (2023.04, `aarch64` and `x86_64`) have been created and staged**
  - Still needs to be approved, after which they will be ingested
  - Goal of automating build + deploy of compat layer with bot not reached (yet)

[Bob, Thomas, Kenneth]

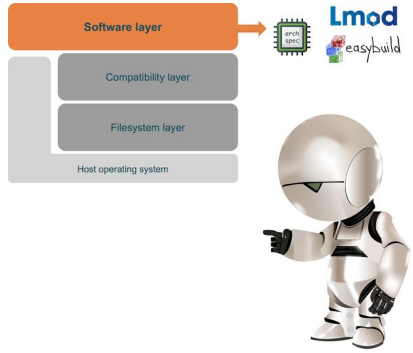
Progress update: software layer



- `bot/check-result.sh` script (PR #241 - draft)
- Dealing with GPU applications that only build for a single GPU target like LAMMPS, CP2K (issue #242)
- Script to check for missing installations reports false positive (issue #243 + PR #244 - open)
- Enable `--read-only-installdir` EasyBuild config option (PR #245 - merged)
- Initial test builds on top of (candidate) build of 2023.04 compat uncovered some problems…
  - GCC problem fixed by updating GCC easyblock to ensure that `--sysroot` is passed to linker
- Easyconfig for ESPResSo, relevant for MultiXscale project (easyconfigs PR #17709 - merged)
- **Sync meeting for building 2023.04 software layer being planned, see #software-layer in Slack**
  - First meeting likely Mon 8 May 2023 at 10:00 CEST

[Kenneth, Thomas]

Bot for building + deploying software layer



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

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

- April'23
  - PRs: 2 merged - 5+1 open (ready + draft) PRs
  - issues: 2 closed, 2 opened - 61 still open (+0 in April'23)

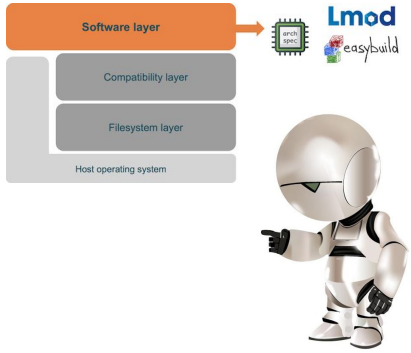
- PR #171: add logging if labeler has no permission
- PR #172: send commands to bot
- WIP PR #174: move job result checking to target repository
- PR #177: fix handling non bot jobs
- PR #178: replay a GitHub event locally
- PR #179: unit tests for two functions in the job manager

date	status	comment

04/28/2023 03:34	finished	▼ 😄 SUCCESS *(click triangle for detailed information)*
		Details
		✔️ job output file `slurm-4682.out`
		✔️ no message matching `ERROR:`
		✔️ no message matching `FAILED:`
		✔️ no message matching `required modules missing:`
		✔️ found message(s) matching `No missing modules!`
		✔️ found message matching `tar.gz created!`
		Artefacts
		▼ `eessi-2023.04-software-linux-x86_64-generic-1682696567.tar.gz`
		size: 234 MiB (245366784 bytes)
		entries: 1234
		modules under *2023.04/software/linux/x86_64/intel/cascadelake/modules/all/*
		`GCC/9.3.0.lua`
		`GCC/10.3.0.lua`
		`OpenSSL/1.1.lua`
		software under *2023.04/software/linux/x86_64/intel/cascadelake/software/*
		`GCC/9.3.0/`
		`CMake/3.20.1-GCCcore-10.3.0/`
		`OpenMPI/4.1.1-GCC-10.3.0/`
		other under *2023.04/software/linux/x86_64/intel/cascadelake/*
		`.lmod/cache/spiderT.lua`
		`.lmod/cache/spiderT.luac_5.1`
		`.lmod/cache/timestamp`

[Thomas, Kenneth]

Bot for building + deploying software layer



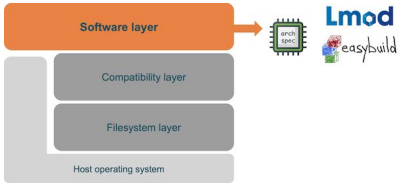
Progress on *use* of build-and-deploy bot in NESSI project

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

- April'23:
  - Building for 5 `x86_64` + 1 `aarch64` CPU architectures across 3/4 clusters (AWS CitC + 2/3 in Norway)
  - 17 PRs ongoing, 27 PRs finished and ingested
    - 8 PRs for NESSI/2023.04
      - So far only GCC/10.3.0 plus a few basic packages (CMake, Perl, OpenMPI)
      - Rust/1.52.1 (dependency for Python/3.9.5) does not build -> replacing it with v1.60.0
  - Having a test (suite) available before ingesting would be very welcome!
  - Continuing work on wiki page for troubleshooting
- Goals for May/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



ReFrame

See https://github.com/EESSI/test-suite (recent meeting notes here)

Merged PRs in past month for GROMACS test:

- Add support for custom executable options (PR #23)
- Moved as much ‘generic’ logic out of GROMACS test, into (reusable) hooks (PR #26)

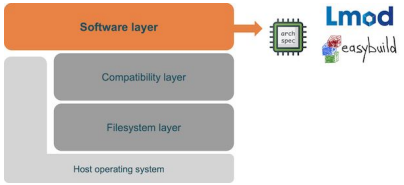
EESSI test suite (with only a GROMACS test) is now ready to experiment with!

Work in progress:

- TensorFlow
  - Written Python code for test using `tf.distribute`
  - TODO: create ReFrame test based on it
- OSU Microbenchmarks

[Caspar, Sam, Satish, Kenneth]

EESSI test suite



ReFrame

Future work

- Restructure namespace of Python package for EESSI test suite (#25)
  - Now: `eessi_utils.hooks`, probably want something like `eessi.testsuite.hooks`
  - Test implementations should go in `eessi.testsuite.tests.apps.*`
- Replace text strings (e.g. partition features such as ‘gpu’) by constants (#30)
- Run EESSI test suite in GitHub Actions workflow (mainly to test the test suite) (#6)
  - Using ReFrame’s dry-run feature
  - Also actually run (selected) small-scale tests, using EESSI
- Add example configuration files for different systems (#24)
- 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 authentication

How do we grant people access to resources? Specifically, computing resources…

- “Everyone”, especially those who contribute to the project, has a GitHub account
- GitHub accounts rely on SSH keys
- GitHub supports teams (groups) within organizations
- What if… We could give everyone in a GitHub team access to a computer?

Enter github-authorized-keys! Originally developed by Cloudposse. GitHub as IAM!

- Runs as a service (or in docker/podman)
- Validates memberships of users, and fetches public keys directly from GitHub
- Uses `AuthorizedKeysCommand` in `sshd` under the hood
- Tested on RHEL8+, Fedora 35+, Ubuntu… ***Very*** easy to install.

[Terje]

EESSI pilot repository

NOT FOR PRODUCTION USE!

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

- 2021.06: considered “end of life”: **will soon be removed** (no changes in April’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]

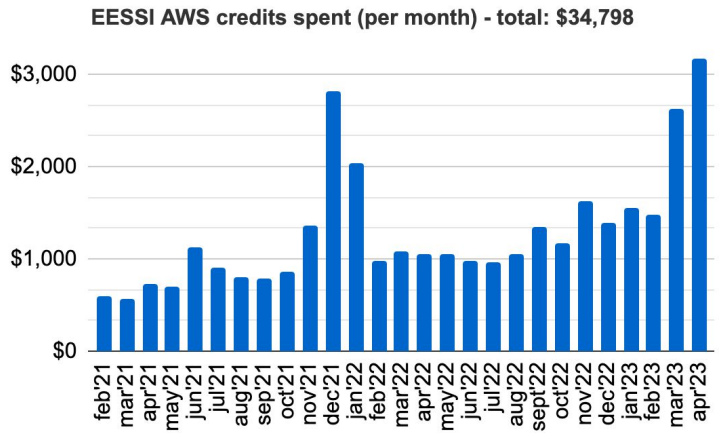
Outlook to next pilot version (2023.04)

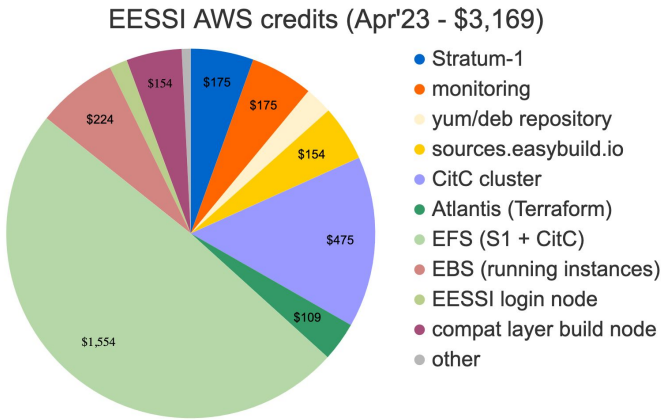
- Small changes to compatibility layer: updated Lmod, **less packages installed**, …
- Include enhancements/changes that are necessary for CUDA GPU support
- Work towards getting rid of ugly install script, aim for easystack-only (if possible)
- **Ideally build/deploy compat + software layer via bot, 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) - when available
- **Effort is ongoing** (Bob, Thomas, …)**, compat layer built, looking into software layer**
- Hopefully using EasyBuild v4.7.2 (to be released soon - mid April'23) for software layer…

[Bob, Thomas, Kenneth]

Sponsored AWS credits

- **Ask in #aws-resources Slack channel to get access!**
- **Currently ~$3,962 worth of sponsored credits left (valid until Sept'23) - OK for May'23**
- **~$3,169** "spent" in Apr'23 on Stratum-1, monitoring, sources.easybuild.io, **Slurm cluster (build bot)**
- ~$34,798 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

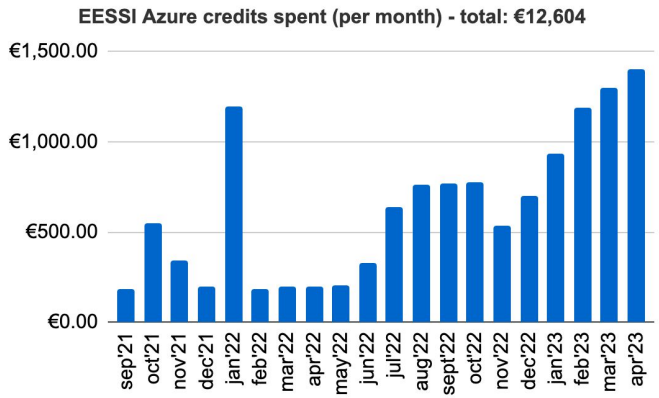


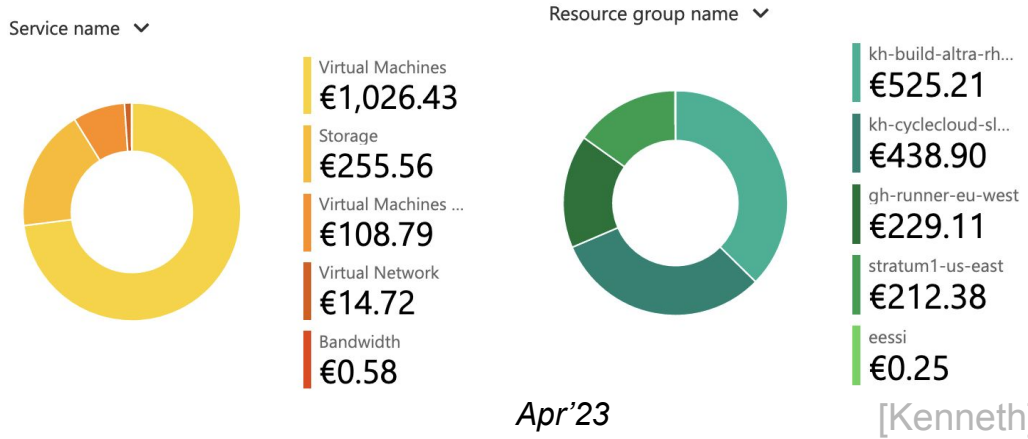


[Kenneth]

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: ~€1,406 worth of credits spent
- ~€12,604 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…)





[Kenneth]

www.multixscale.eu github.com/multixscale

- CI/CD collaboration with Deucalion (Portugal) via CASTIEL2
  - We're also applying for development access to other EuroHPC sites
- Two training events planned this year
  - Hybrid EESSI introductory user training event at HPCKP'23 meeting
  - "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
- Support portal for EESSI is a deliverable in MultiXscale due by end of 2023
  - MultiXscale task 5.1
  - Currently evaluating/comparing alternatives like GitHub, GitLab, JIRA, etc.

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

8th EasyBuild User Meeting 2023

https://easybuild.io/eum23 - ~30 on-site attendees + ~30 remote attendees

All talks were recorded, and are available via YouTube

"EESSI: status update" presentation by Caspar

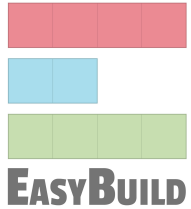
- Introduction to EESSI
- Relation between EESSI ⇔ MultiXscale
- Current & future activities
- Recording available on YouTube here, slides (PDF) available here

Interest/potential to collaborate on ReFrame tests with Digital Research Alliance of Canada

- Challenge: The Alliance uses a hierarchical module naming scheme

[Kenneth, Alan, Caspar]

8th EasyBuild User Meeting 2023



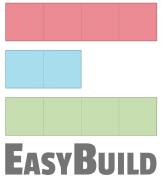
Questions/thoughts raised by Kurt Lust during his talk on use of EasyBuild at LUMI:

- Who to turn to for support on EESSI?
  - Site user support probably has limited knowledge on EESSI
  - EESSI community has limited knowledge on site-specific setup
- Being able to build on top of EESSI is an essential feature
- Extra daemons not always an desirable (OS jitter)
  - We should also support other ways of distributing next to CVMFS?

See slide 28+29 (PDF available here)

[Kenneth, Alan, Caspar]

EasyBuild + EESSI UK workshop



https://easybuild.io/eb-eessi-uk-workshop-2023-04

- Introduction to EasyBuild + EESSI
  - 50% basic EasyBuild (incl. hands-on)
  - 25% advanced EasyBuild (incl. demos)
  - 25% introduction to EESSI (incl. demos/hands-on)
- Tutorial materials available at https://tutorial.easybuild.io/2023-eb-eessi-uk-workshop
- Sessions were also recorded, see YouTube playlist
- Lots of interest in EESSI part, attendees were impressed

[Kenneth, Alan]

Upcoming events: HPCKP

- Website: hpckp.org/annual-meeting
- 17-18 May 2023 - Barcelona, Spain
- Hybrid (in-person and remote)
- Agenda https://hpckp.org/annual-meeting/agenda/
- Registration is free! (our lovely sponsors cover the expenses)
- 12 May: Registration deadline
- **2-hour EESSI tutorial will be part of HPCKP'23 program**
    - Thu 18 May (afternoon)

[Danilo]

Upcoming events:

- ISC'23 website: https://www.isc-hpc.com
- When: 21-25 May 2023
- Where: Hamburg, Germany
- MultiXscale poster + EESSI Talk/demo at EuroHPC booth by Elisabeth (HPCNow!)
- 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! (booth #D404)

[Elisabeth]