EESSI

EUROPEAN ENVIRONMENT FOR
SCIENTIFIC SOFTWARE INSTALLATIONS

8 Dec 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. Update on new EESSI production repository `software.eessi.io`
5. Update on EESSI NVIDIA GPU support
6. Update on EESSI test suite
7. Infrastructure and monitoring
8. EESSI support portal
9. AWS/Azure sponsorship update
10. Update on MultiXscale EuroHPC project
11. Upcoming/recent events: “Best Practices for CernVM-FS in HPC” tutorial + talks on EESSI/MultiXscale
12. Q&A

Quick introduction by new people

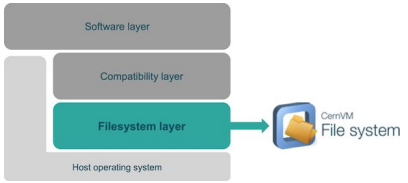
New people on the call: feel free to introduce yourself!

- 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+22 Nov'23 + 6 Dec'23)* Sync meetings on EESSI test suite (notes)
- *(13 Nov'23)* CernVM-FS coordination meeting (notes)
- *(14 Nov'23)* MultiXscale WP1+WP5 sync meeting *(notes are private to MultiXscale project partners)*
- *(20 Nov'23)* Sync meeting with CernVM-FS dev team on tutorial (notes)
- *(21 Nov'23)* Sync meeting on GPU support (notes)
- *(Nov'23)* Sync meetings on MultiXscale deliverables *(notes are private to MultiXscale project partners)*
- *(Nov'23)* Weekly support team sync meetings *(notes are in private wiki on EESSI support portal)*

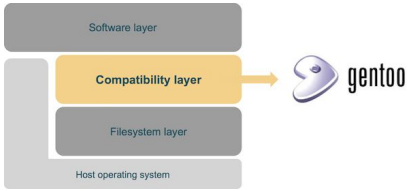
Progress update: filesystem layer



- New Stratum-0 server and Stratum-1 servers for new `software.eessi.io` CernVM-FS repository
  - MFA-secured jumphost in place to access the servers
  - Initial setup of an S3-backed Stratum 1 that can be used as public Stratum 0
    - Can be used for setting up and synchronising a private Stratum 1
    - Still has to be included in the Ansible configuration
- Build + client container images for new CernVM-FS repository have been created (PR #163)
- New release of `cvmfs-config-eessi` packages (`pilot.eessi-hpc.org` + `software.eessi.io`) (v0.5.0)
- A README file has been added to the EESSI CernVM-FS repository (PR #168)
- `software.eessi.io` **is available in default CernVM-FS configuration since Mon 20 Nov'23!**
- We should still improve/rethink the ingestion workflow (separate PRs for each CPU target is a hassle)

[Bob, Kenneth]

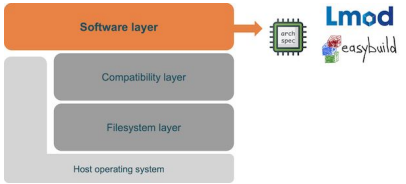
Progress update: compatibility layer



- 2023.06 version for `software.eessi.io` (see PR#191)
  - Built by the bot, manually uploaded to S3 bucket, ingested by automated procedure on Stratum 0
  - Same set of packages as in 2023.06 version of `pilot.eessi-hpc.org`
  - Updated to address recent Gentoo Linux Security Advisories (see PR#193)
  - Updated compat layer has been ingested on Fri 17 Nov'23
  - Software has been built on top already
- 2023.06 version in EESSI pilot repository (`pilot.eessi-hpc.org`)
  - No recent changes here
  - We should apply updates (see PR#193) for the pilot too

[Thomas, Bob, Kenneth]

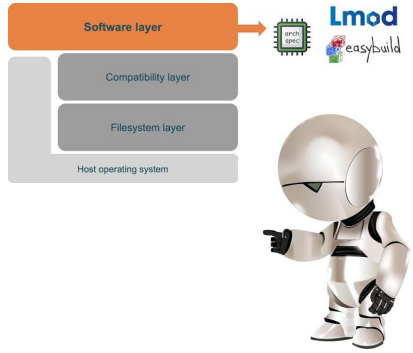
Progress update: software layer



- ~25 merged PRs since previous EESSI update meeting
  - Various updates to scripts to start building for `software.eessi.io`
  - PRs to build & deploy EasyBuild v4.8.2, `foss/2023a`, SciPY-bundle, TensorFlow, Qt5, X11, …
  - Initial steps towards adding GPU support
- Various open PRs to build & deploy for `software.eessi.io`

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

Bot for building + deploying software layer



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

- Patch release v0.1.1 (14 Nov'23)
  - PR#217 tool to clean up disk space
  - PR#220 omit header lines in `squeue` output
  - PR#221 clarify permissions for GitHub App
  - PR#224 ensure compatibility with PyGithub v2.1.1
- Minor release v0.2.0 (26 Nov'23)
  - PR#222 support for running tests
  - PR#229 enable bot build for pilot and `software.eessi.io`
  - PR#233 README for smee client on `aarch64`
  - PR#230 repository-specific buckets via `bucket_name` cfg
- TODO:
  - v0.3.0: Remove code in the deployment function that is specific to EESSI/software-layer
  - Look into separate test phase (to test in different contexts before deployment)

[Thomas, Kenneth, Bob]

EESSI pilot repository

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

NOT FOR PRODUCTION USE!

- 2021.12 version is “frozen”, no more changes planned there, but it's still the default ("`latest`") version
- 2023.06 version is not being actively used any longer
  - Build-and-deploy bot can still build software via branch `2023.06-pilot.eessi-hpc.org`
  - Might still be used for experimenting…
  - We currently have **~480 software installations** per CPU target => **~3,900 installations in total !**

[Kenneth, Bob, Caspar, Lara, Richard, …]

New EESSI production repository

https://www.eessi.io/docs

- `software.eessi.io` is the new **production-ready EESSI repository**, and is now the default
- 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
  - Recently added software installations (for all supported CPU targets) for 2023a toolchain:
    - TensorFlow (PR #386)
    - OSU Micro Benchmarks (PR #412)
    - Nextflow (PR #409)
    - SciPy-bundle v2023.07 (PR #403)
  - **We currently have ~110 software installations per CPU target => ~900 installations in total !**
  - Next goal is to add software that was already included in `pilot.eessi-hpc.org`
  - Already seen two new contributions after EESSI tutorial (5 Dec 2023):

    LHAPDF (PR#417) and Rivet (PR#418)

[Kenneth, Bob, Caspar, Lara, Richard, …]

Contribution policy - v0.1.0 released Nov 9th

https://eessi.io/docs/adding_software/contribution_policy

- Has been reiterated a couple of times in an open process starting in early July '23
- Additions to software stack shall comply with this policy
- Future changes are anticipated
- 8 requirements:
  1. Software must be **freely redistributable software**, and preferably open source;
  2. Software being added must be *built and deployed by the* **bot**;
  3. Software must be *built and installed with* **EasyBuild**;
  4. The **compiler toolchain** used must be *supported by EasyBuild*;
  5. A **recent toolchain** should be used;
  6. **Recent software versions** are preferred;
  7. The software should work on **all CPU targets** *supported by EESSI* version being targeted;
  8. It should be possible to **test** *the built software packages* being added using the EESSI test suite.

[Kenneth, Thomas]

EESSI Documentation

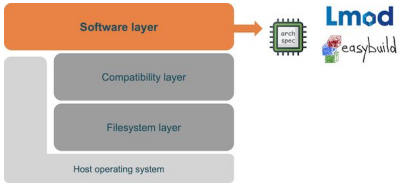
https://www.eessi.io/docs/ - GitHub repo https://github.com/EESSI/docs

Improvements to the EESSI documentation

- Better landing page: https://eessi.io/docs
- Contribution policy: https://eessi.io/docs/adding_software/contribution_policy
- Improved overview on adding software to EESSI: https://eessi.io/docs/adding_software/overview
- Update page on opening PR changed branch: https://eessi.io/docs/adding_software/opening_pr
- Debugging failed builds: https://www.eessi.io/docs/adding_software/debugging_failed_builds/
- How to build on top of EESSI: https://www.eessi.io/docs/using_eessi/building_on_eessi

[Kenneth, Thomas, Xin, Caspar]

EESSI NVIDIA GPU support



Four challenges:

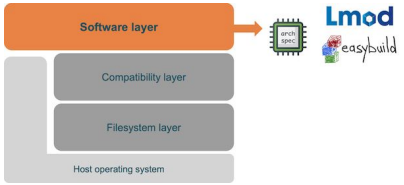
1. CUDA SDK only allows partial redistribution (e.g. runtime, not compilers)
2. GPU drivers on host need to be found by software in software layer
3. CUDA software in software layer needs sufficiently new GPU drivers or CUDA Compatibility Libraries
4. CUDA needs to work in build container

See also [software-layer issue #375]

Goal is to have initial support for GPU software in software.eessi.io by end of 2023

[Alan, Caspar, Kenneth]

EESSI NVIDIA GPU support



PR #368 (merged):

- host sysadmin installs CUDA in `host_injections` dir using `install_cuda_host_injections.sh`
- host sysadmin Links CUDA driver libs to `host_injections` dir using `link_nvidia_host_libraries.sh`
- modifies build container (`eessi_container.sh`) to use GPUs in container

PR #381 (open):

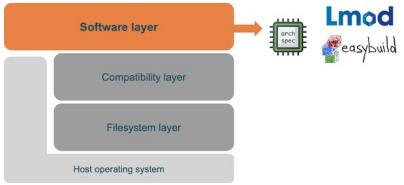
- Hook for adding GPU Lmod property to CUDA-dependent modules
- Hook for *only* installing redistributable part of CUDA in software-layer
- Adds CUDA and CUDA-Samples to software-layer

TODO:

- ship `install_cuda_host_injections.sh` and `link_nvidia_host_libraries.sh` as part of EESSI
- have bot run these on build clusters (when needed)

[Alan, Caspar, Kenneth]

EESSI test suite



ReFrame

Merged pull requests:

- Add option to specify memory requests to ReFrame configs (PR #96)
- Update CI driving scripts, document how to periodic runs on new systems (PR #93)
  - Periodic runs on Vega, Karolina and AWS cluster
- Refactoring of hooks (PR #95)

Open pull requests:

- OSU tests (PR #54)

Next steps

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

[Caspar, Sam, Satish, Kenneth, Lara]

Support portal for EESSI (MultiXscale task 5.1)

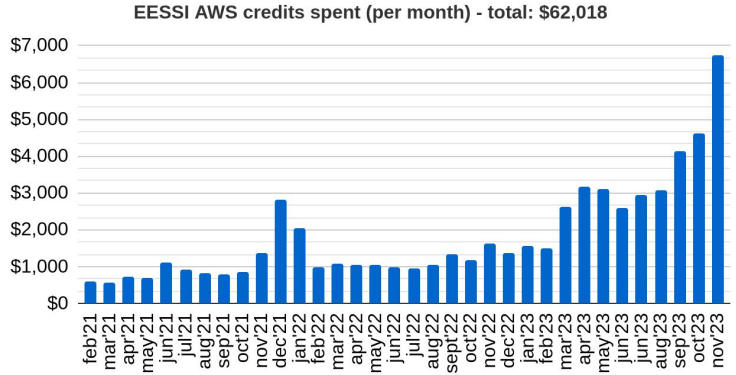
- EESSI support portal set up at https://gitlab.com/eessi/support
  - Tickets can be created by:
    - Opening an **issue in GitLab**
    - Sending an **email** to `support@eessi.io`
  - **Information on support portal and initial support policy => https://eessi.io/docs/support**
  - Support is “reasonable effort” + only for problems with how software was installed in EESSI
  - Proposal for the support rotation in the wiki (https://gitlab.com/eessi/support/-/wikis/Proposal-for-rotation)

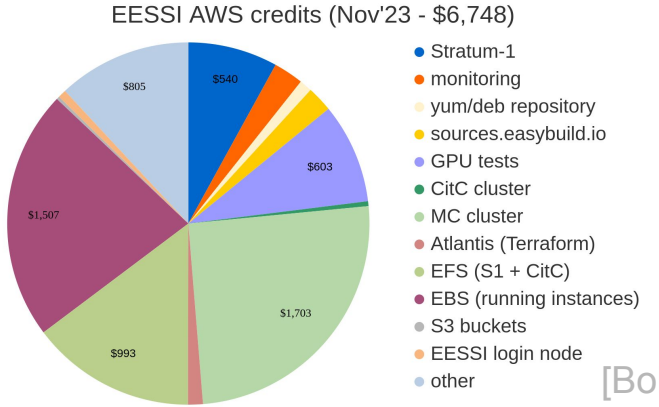
- 1 Oct’23 - end of 2023: (experimental) support rotation between the MultiXscale partners
  - A MultiXscale partner is “first-line” for incoming support requests for 2 weeks
  - Weekly regular support sync or hand-over meetings
  - Tickets are starting to be opened and are followed up

[Lara, Kenneth, …]

Sponsored AWS credits

- Ask in #aws-resources Slack channel to get access!
- Currently ~$16.7k worth of sponsored credits left (valid until 29 Feb'24)
- ~$6,748 "spent" in Nov'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
- ~$62k 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**
- Monthly sync meetings with Brendan/Angel/Matt/Francesco (AWS) every 2nd Thursday of the month

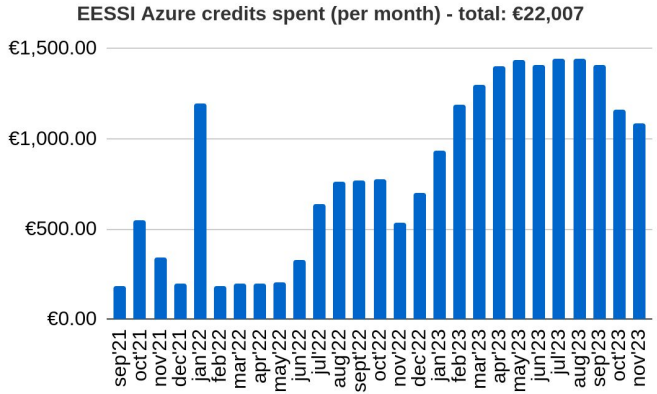


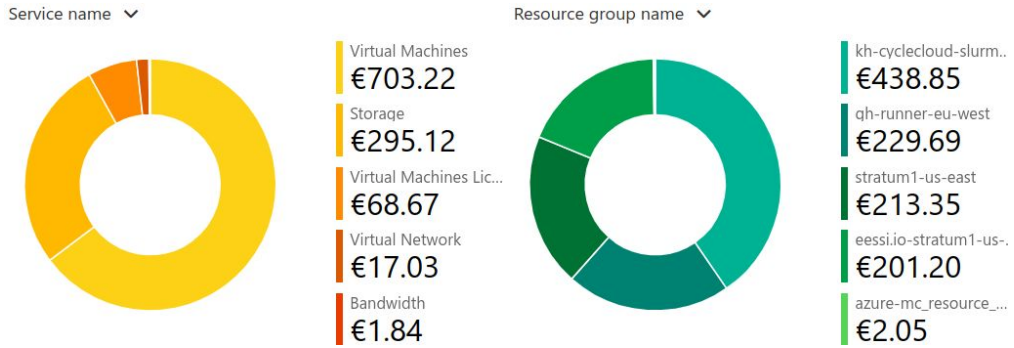


[Bob, Kenneth]

Sponsored Azure credits

- Sponsored credits (€40,000) are being put to good use!
- **Ask in #azure-resources Slack channel to get access!**
- In Nov'23: ~€1,086 worth of credits spent
- ~€22k worth of (sponsored) credits spent in total (since Sept'21)
- Used for: Stratum-1 mirror servers, GitHub Runners, heterogeneous Slurm cluster (with Cyclecloud)
- Current Slurm cluster using Azure Cyclecloud is not used
- Will start over with Magic Castle, same tool as used in AWS (WIP)





Nov'23

[Bob, Kenneth]

Multiscale

EuroHPC Joint Undertaking

EESSI

www.multixscale.eu github.com/multixscale

- “Best Practices for CernVM-FS on HPC systems” tutorial (4 Dec 2023, 13:30-17:00 CET)
- Introduction to EESSI tutorial (5 Dec 2023, 14:30-16:30 CET)
- CI/CD collaboration via CASTIEL2
  - Still not clear what demands will come from this
  - **Funding call expected from EuroHPC in this space**
- Relevant deliverables due end of 2023
  - D1.1: Report on shared software stack prototype *(90% done)*
  - D1.2: Plan for design of a portable test suite *(90% done)*
  - D5.1: Community contribution policy and GitHub App *(95% done)*
  - D5.2: Support portal for EESSI *(75% done)*
- Also some involvement in CASTIEL2 deliverable D5.8 to include CernVM-FS as CD option

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

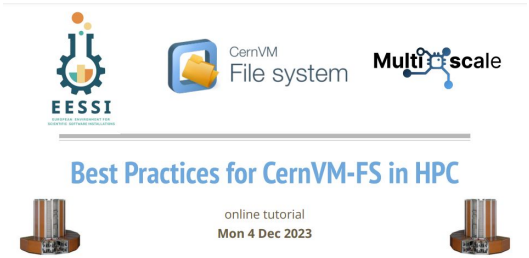
EESSI @ Supercomputing'23

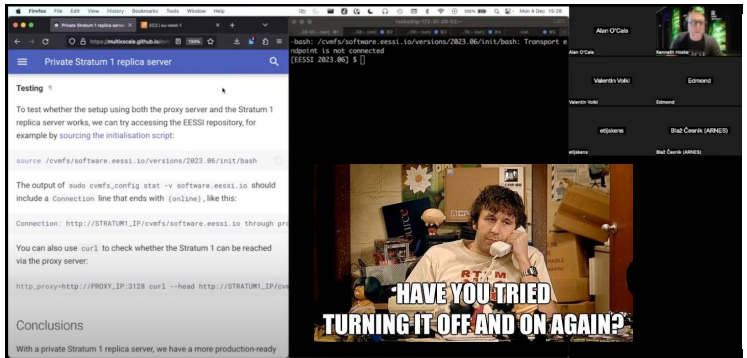
- 12-17 Nov'23 in Denver (US) - https://sc23.supercomputing.org
- Attended by Alan, Henk-Jan, HPCNow!
- Magic Castle tutorial by Alan with Félix-Antoine (Magic Castle lead dev)
- MultiXscale presence in EuroHPC booth (video only)
- 3-min lightning talk on EESSI by Alan at Better Scientific Software BoF session
- **Great networking opportunities!**

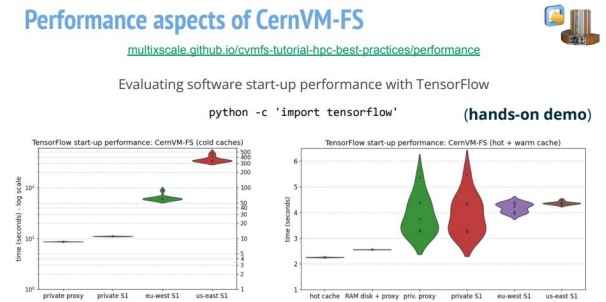
[Alan, Kenneth]

Best Practices for CernVM-FS in HPC tutorial

- 4 Dec'23 via Zoom, by Kenneth Hoste & co, **in collaboration CernVM-FS developers**
  https://multixscale.github.io/cvmfs-tutorial-hpc-best-practices (tutorial website + minimal slide deck)
- Incl. **hands-on demos** of setting up CernVM-FS client/proxy/Stratum 1, troubleshooting, etc.
- Using **EESSI as example** CernVM-FS repository, incl. initial study of TensorFlow start-up performance
- **205 registrations** (!!!), about 130 people actually attending the Zoom session
- Recording available on MultiXscale YouTube channel

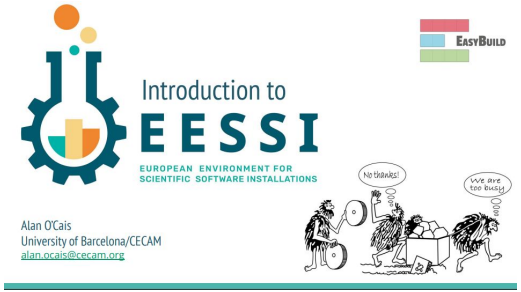


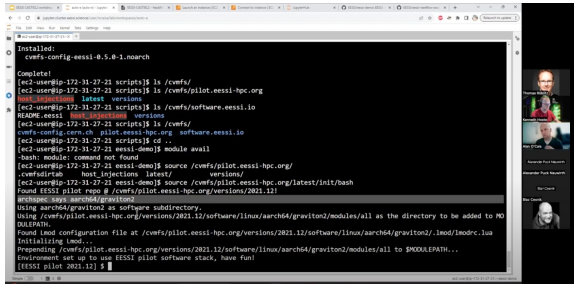


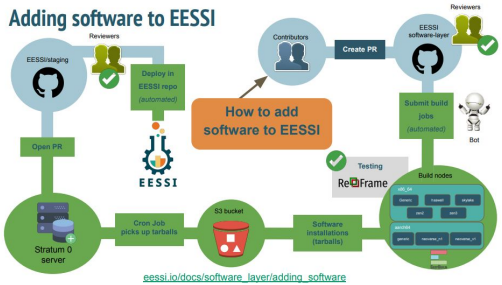


Streaming Optimised Scientific Software: Introduction to EESSI

- 5 Dec'23 via Zoom, by Alan O'Cais, in context of EuroHPC (via CASTIEL2 project)
  https://event.ugent.be/registration/eurohpcncceessi202312
- Incl. hands-on demos of using EESSI in terminal, in CI environment, diff. use cases, etc.
- **134 registrations** (!!!), about 60 people actually attending the Zoom session
- Slides (PDF) available here
- Recording available on MultiXscale YouTube channel







[Alan]

EESSI @ SURF Advanced Computing User Day

- 7 Dec'23 in Amsterdam - https://www.surf.nl/en/agenda/advanced-computing-user-day
- *One scientific software stack for all systems, that's EESSI*

[Bob]