EESSI

EUROPEAN ENVIRONMENT FOR
SCIENTIFIC SOFTWARE INSTALLATIONS

8 Feb 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

4. Update on EESSI production repository `software.eessi.io`

5. Update on EESSI test suite + build-and-deploy bot

6. EESSI support portal

7. AWS/Azure sponsorship update

8. Update on MultiXscale EuroHPC project

9. Upcoming/recent events: EuroHPC Summit + EasyBuild User Meeting 2024 + ISC'24

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

- *(12 Jan'24)* Bot sync meeting ([notes](#))

- *(15 Jan'24)* EESSI/Azure sync meeting ([notes](#))

- *(18 Jan + 1 Feb'24)* Sync meeting on EESSI test suite ([notes](#), [notes](#))

- *(22 Jan'24)* CernVM-FS Coordination Meeting - CernVM workshop moved to 16-18 Sept (@ CERN)

- *(2 Feb'24)* Meeting with CASTIEL2 and EuroHPC Hosting Entities on CernVM-FS + EESSI

- *(Jan'24)* Meetings to prepare MultiXscale project review (scheduled for 19 Feb'24)

- *(Jan'24)* Weekly support team sync meetings *(notes are in private wiki on EESSI support portal)*

[Bob, Kenneth]

Progress update: filesystem layer
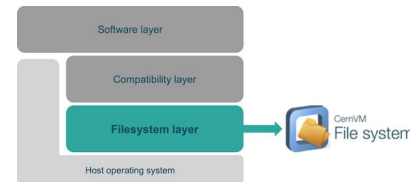
- Issue with building (multi-platform) EESSI Docker images has been resolved (PR [#173](#))

- When ingesting an updated compatibility layer, the old one will now be moved (PR [#176](#))
  - This will allow us to fall back to the old version, if necessary
  - Ideally, this can be controlled by a variant symlink, but this requires changes in the build environment as well to prevent the symlink from being resolved

- Script for updating the Lmod caches of all supported CPU targets (PR [#175](#))
  - Can be run on the Stratum 0
  - Prevents the cache from being overwritten by an older version

    when an older software PR gets merged

- Working on getting the CernVM-FS sync server configured and documented properly

[Bob, Kenneth]

Progress update: compatibility layer
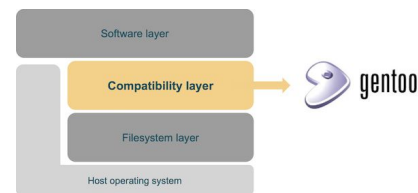
- 2023.06 version for `software.eessi.io` (see [PR#191](#))
  - Again ~30 recent Gentoo Linux Security Advisories, see https://security.gentoo.org/glsa
    - Two of them affect the compatibility layer
    - Updates have been prepared, ready to be ingested (PR [#197](#))
    - Procedure to check security advisories that affect EESSI should be documented/automated…
  - ReFrame tests should be run against the production repo (PR [#196](#))

- 2023.06 version in EESSI pilot repository (`pilot.eessi-hpc.org`)
  - No recent changes here, except for testing some additional host symlinks (PR [#194](#))
  - **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
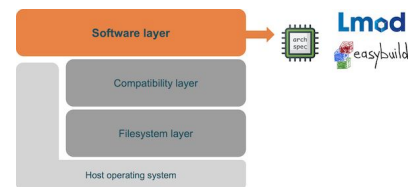
- Recently merged PRs:

  - More software: at-spi2-core 2.49.91 (PR #454), CDO (PR #427),

    ESPResSo v4.2.1 (PR #455), matplotlib v3.8.2 (PR #459), netCDF v4.9.2 (PR #453),

    OpenFOAM v11 (PR #446), ReFrame v4.3.3 (PR #450),

    PyTorch v2.1.2 (CPU-only) (PR #444), QuantumESPRESSO v7.2 (PR #436),

    Rivet 3.1.7 (PR #418), scikit-learn (PR #464), SciPy-bundle with foss/2022b (PR #448)

  - Only pick a software subdir provided by archdetect that is present in the CVMFS repository (PR #460)

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

Progress update: software layer
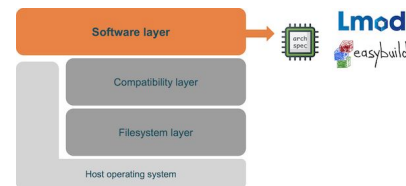
- Recent open PRs:

  - More software: GROMACS (PR #401 + PR #463), OpenFOAM v10 (PR #404),
    GDAL (PR #419), waLBerla (PR #424), CDO (PR #427),
    R-bundle-CRAN (PR #428), BWA (PR #429), ImageMagick (PR #445),
    R v4.2.2 (PR #452), Qt5 (PR #462)

  - Add support for zen4 / AMD Genoa to archdetect (PR #447)

    - On hold until we actually have software installations for `x86_64/amd/zen4`

  - Script to determine license for software being included in EESSI (PR #457)

  - Run EESSI test suite after building software with bot (PR #467)

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

Progress update: software layer
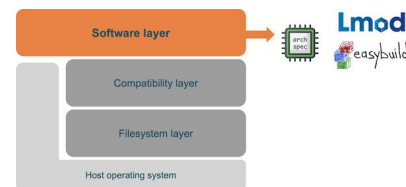
We are starting to see help/input/interest from software developers,
for example for GROMACS (see https://gitlab.com/eessi/support/-/issues/47):

Mark Abraham @mark.j.abraham · 1 day ago

Upstream will be interested to see more detail on these, e.g. from `ctest -V`

Kenneth Hoste @boegel · 16 hours ago   Owner

@mark.j.abraham It would be great to get some insight on this from upstream!

For the failing `GmxapiMpiTests` we see, all we basically see in the detailed test output is this:

```
Program:      gmxapi-mpi-test, version 2023.3-EasyBuild_4.9.0
Source file: src/gromacs/utility/futil.cpp (line 454)
MPI rank:     1 (out of 2)

File input/output error:
/tmp/bot/easybuild/build/GROMACS/2023.3/foss-2023a/easybuild_obj/api/gmxapi/cpp/tests/Testing/Tempo
```

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

Bot for building + deploying software layer

https://github.com/EESSI/eessi-bot-software-layer
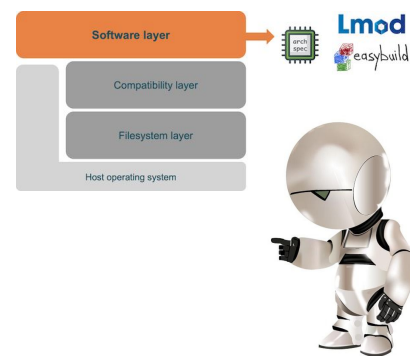
- Discussed future developments (12 Jan'24, notes)

  - Priority: improvements to deployment procedure
    (single staging PR, multiple bot instances, delete action, ...)

- Release of the bot v0.3.0, 30 Jan'24

  - PR#237 New command `bot: status` which shows a
    summary of finished build jobs.

  - PR#238 Renew token to access GitHub earlier
    (already after 30 minutes), attempt to avoid some of the
    crashes of the job manager.

This is the status of all the `bot: build` commands:

arch	result	date	status	url
zen2-ib	😊 SUCCESS	Nov 09 14:23:49 UTC 2023	finished	#4 (comment)
skylake-ib	🤷 UNKNOWN	Nov 09 15:26:56 UTC 2023	finished	#4 (comment)
cascadelake-ib	😊 SUCCESS	Nov 09 15:24:51 UTC 2023	finished	#4 (comment)
cascadelake-ib	😊 SUCCESS	Nov 09 15:34:09 UTC 2023	finished	#4 (comment)
cascadelake-ib	😊 SUCCESS	Nov 09 15:38:19 UTC 2023	finished	#4 (comment)
cascadelake-ib	😊 SUCCESS	Nov 09 15:42:28 UTC 2023	finished	#4 (comment)
cascadelake-ib	😊 SUCCESS	Nov 09 15:46:36 UTC 2023	finished	#4 (comment)
cascadelake-ib	😊 SUCCESS	Nov 09 16:11:09 UTC 2023	finished	#4 (comment)
cascadelake-ib	😊 SUCCESS	Nov 09 16:22:24 UTC 2023	finished	#4 (comment)
cascadelake-ib	😊 SUCCESS	Nov 22 14:10:13 UTC 2023	finished	#4 (comment)
zen3x-ib	😊 SUCCESS	Nov 23 08:57:26 UTC 2023	finished	#4 (comment)
zen3x-ib	😊 SUCCESS	Nov 23 08:58:30 UTC 2023	finished	#4 (comment)
zen3x-ib	😟 FAILURE	Nov 23 08:57:24 UTC 2023	finished	#4 (comment)
zen3x-ib	😊 SUCCESS	Nov 23 08:58:28 UTC 2023	finished	#4 (comment)
zen2-ib	😟 FAILURE	Nov 23 08:56:13 UTC 2023	finished	#4 (comment)
zen2-ib	😟 FAILURE	Nov 23 08:56:11 UTC 2023	finished	#4 (comment)
zen2-ib	😟 FAILURE	Nov 23 08:57:21 UTC 2023	finished	#4 (comment)
zen2-ib	😊 SUCCESS	Nov 23 08:57:22 UTC 2023	finished	#4 (comment)

[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 <u>PRs to software-layer repo</u> + build-and-deploy bot

  - Supported CPU targets: see <u>eessi.io/docs/software_layer/cpu_targets</u>

  - Initial support for NVIDIA GPUs is in place, see <u>eessi.io/docs/gpu</u>

  - **We currently have ~360 software installations per CPU target** (+90 compared to last month)
    - 199 different software projects (+60), ~2,510 software installations (across 8 CPU targets, +360)

  - Current focus:
    - Adding software relevant for MultiXscale project + EESSI demos
    - 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 status page: status.eessi.io

- Shows status of production EESSI CernVM-FS repository (software.eessi.io) & related servers

- Dedicated server in AWS (ap-southeast-2, Melbourne) with https from Let's Encrypt + Certbot (auto-updated)

- Uses https://github.com/EESSI/cvmfs-server-scraper + https://github.com/EESSI/status-page

- The backend software has been cleaned up and modernized:

  - Python typing hints and pydantic models attempt to make things better

  - Saner error checking, but things like CernVM-FS using locale for date fields is… interesting:
    "do 9 mrt 2023 13:39:26 UTC" as a timestamp from a server? Sure. Great. Thanks.

- Currently no automated reporting (there has been talk of Slack integration)

- Maintenance messages are effectively not supported :(

[Terje]

EESSI Documentation

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

Improvements to the EESSI documentation

- Add page about production repository `software.eessi.io` (PR #141)

  and replace pilot repository by production repository (PR #144 and PR #146)

- Add and update documentation about test suite (PR #143, PR #149, PR #150)

- Add link to join EESSI Slack (PR #151)

Planned: auto-updated overview of available software in EESSI

[Kenneth, Thomas, Xin, Caspar, Lara, Pedro]
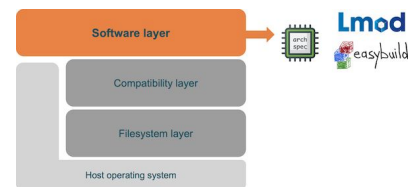
EESSI test suite

Merged pull requests:

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

- Unify test names (PR #108)

- Config file for automatically running test suite after software layer build jobs by the bot (PR #112)

- CI fixes (various PRs)

Open pull requests:

- Minor fixes for OSU-MicroBenchmark test (PR #110)

- New hook to filter invalid scales based on features set in the config file (PR #111)

Next steps

- Add more tests (ESPResSo, CUDA samples, EasyBuild sanity check, …)

- Make GROMACS skip test if too many cores for given test case

[Caspar, Sam, Satish, Kenneth, Lara]

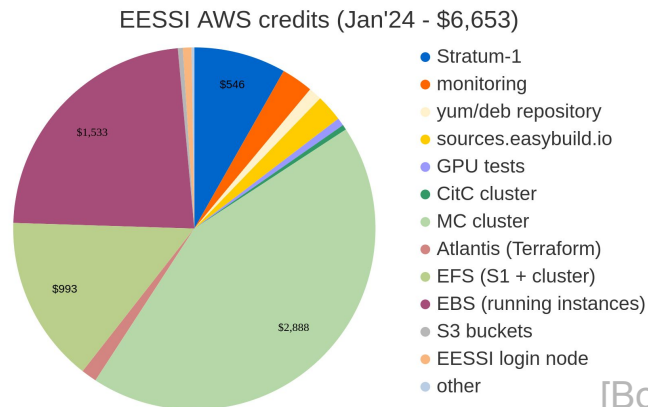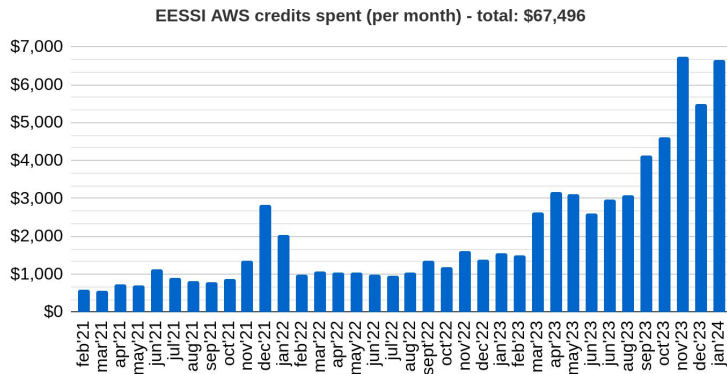# Support for EESSI (MultiXscale task 5.4)

- 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!

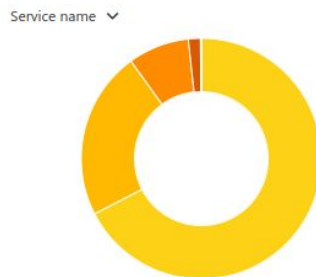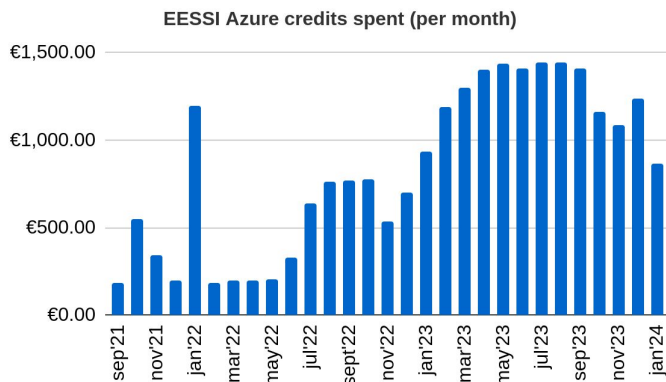[Lara, Kenneth, Caspar, Bob, Danillo, Alan, Thomas, …]

Sponsored AWS credits

- Ask in #aws-resources Slack channel to get access!

- ~$6,653 "spent" in Jan'24 on Stratum-1 servers, monitoring, sources.easybuild.io, **Slurm clusters (build bot)**

- **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

EESSI AWS credits spent (per month) - total: $67,496

EESSI AWS credits (Jan'24 - $6,653)

- Stratum-1
- monitoring
- yum/deb repository
- sources.easybuild.io
- GPU tests
- CitC cluster
- MC cluster
- Atlantis (Terraform)
- EFS (S1 + cluster)
- EBS (running instances)
- S3 buckets
- EESSI login node
- other

[Bob, Kenneth]

Sponsored Azure credits

- Ask in #azure-resources Slack channel to get access!

- In Jan'24: ~€862 worth of credits spent

- Used for: Stratum-1 mirror servers, GitHub Runners

- Slurm cluster using Azure Cyclecloud has been removed

- Looking into to set up a Slurm cluster with Magic Castle, same tool as used in AWS

EESSI Azure credits spent (per month)

Service name	
Virtual Machines	€581.12
Storage	€194.99
Virtual Machines Lic...	€70.98
Virtual Network	€14.00
Bandwidth	€0.89

| Resource group name	
stratum1-us-east	€216.76
qh-runner-eu-west	€209.37
eessi.io-stratum1-us...	€206.22
kh-cyclecloud-slurm...	€156.38
test_group	€40.12

Jan'24

[Bob, Kenneth]

Multi scale

- MultiXscale deliverables covering activity in 2023 are now available via multixscale.eu/deliverables

- **MultiXscale project partners are currently preparing project review meeting (19 Feb'24)**

- Via CASTIEL2 CoE, we are in touch with EuroHPC Hosting Entities to make EESSI available

  - First meeting on Fri 2 Feb'24, next sync meeting on Fri 9 Feb'24

  - EESSI is already available on Vega (Slovenia) and Karolina (Czech Republic)

  - Kenneth is meeting with MeluXina team in Luxembourg on Tue 20 Feb

  - Some reluctance from BSC (MareNostrum 5) & CSC (LUMI) w.r.t. security, networking, OS jitter, etc.

  - **Some pressure from EuroHPC JU to have a common software stack adopted everywhere (and EESSI is gaining momentum as the viable option)** [Alan, Kenneth, Lara, Bob, Thomas, Caspar, Satish, Elisabeth, …]

EuroHPC Summit 2024
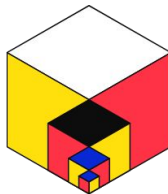
- 18-21 March 2024 in Antwerp (Belgium) - https://www.eurohpcsummit.eu

- Busy week for MultiXscale project partners…

- Various interesting sessions relevant to EESSI

- **Great event to promote EESSI!**

- There will be a MultiXscale poster (incl. EESSI), hopefully also live demos with EESSI

- We will also try to make EESSI part of "EuroHPC Demo Lab",

  https://www.eurohpcsummit.eu/demo-lab

[Kenneth, Lara, Alan, Thomas, Elisabeth, …]

EasyBuild User Meeting 2024
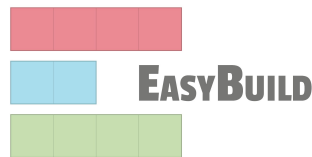
- Tue-Thu 23-25 April 2024 @ Umeå University (Sweden) - https://easybuild.io/eum24

- Yearly meeting, focus on EasyBuild & related projects

- **Registration for on-site attendance + virtual attendance is open!**

- EasyBuild 5.0 will definitely be a hot topic…

- Thursday 25 April will be focused on EESSI, session ideas (to be confirmed):

  - Intro to EESSI + Status Update

  - Contributing to EESSI

  - Hands-on sessions (sysadmin, user, contributor)

  - EESSI test suite, GPU support in EESSI, …

[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**

- Acceptance notifications expected by 9 Feb'24 (tutorials) and 14 Feb'24 (BoF)
  (**still waiting, no info yet…**)

[Kenneth, Alan, Lara, Elisabeth, …]