



EESSI meeting

1 Dec 2022

<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. bot for software layer)
4. 2021.12 version of pilot repository + outlook to next pilot version
5. AWS/Azure sponsorship update + OCRE funding opportunity
6. Update on MultiXscale EU project
7. Upcoming events: EESSI hackathon Dec'22
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



- *(no CernVM-FS coordination meeting in Nov'22)*
- Meeting on use of EESSI at azhop workshop at SC'22 (7 Nov'22)
 - Attended by Kenneth, Hugo, Davide
 - *(see next slide)*
- BioHackathon Europe sync calls (7-11 Nov'22)
 - Attended by Anthony, Elisabeth, Jurij, Kenneth, Sebastián
 - *(see separate slide)*
- Meetings on applying for OCRE funding (cloud credits) (4 Nov'22 + 17 Nov'22)
 - Attended by Alan, Caspar, Ivar, Kenneth
- Various calls on development of build-and-deploy bot (~twice a week in Nov'22)
 - Attended by Hafsa, Kenneth, Thomas

EESSI at azhop workshop at SC'22



- <https://azure.github.io/az-hop>
 - Adding of OpenFOAM v9 + OSU Micro-Benchmarks to EESSI (see [PR #195](#) + [#201](#))
 - Tutorial at SC'22
- [az-hop tutorial - exercise 6: Run OpenFOAM DrivAer-Fastback simulation using EESSI stack](#)
- "Everybody was very surprised by how quick and easy it was to run OpenFOAM from EESSI.
We had a good amount of questions on how EESSI works.
The compatibility layer was one of the most appreciated features."

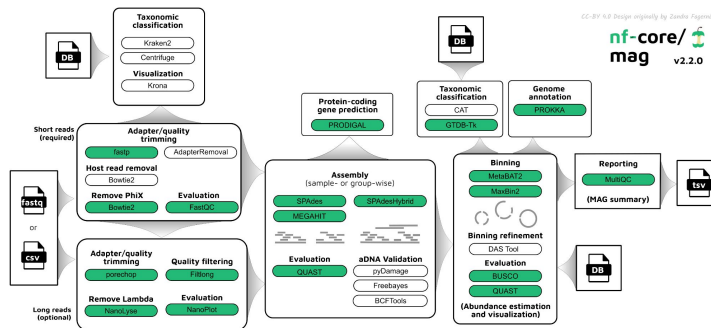


[Hugo, Davide]

BioHackathon Europe 2022

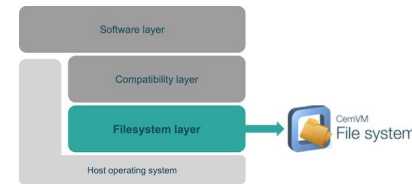


- <https://biohackathon-europe.org> – 7-11 Nov'22 – near Paris
- Project #16:
“***Make your own or favourite software available on your cluster with EasyBuild/EESSI***”
- Only Sébastien was on-site, others (Anthony, Elisabeth, Jurij, Kenneth) joined remotely
- Main goal: support running Nextflow workflow <https://nf-co.re/mag> via EESSI
- **27 merged PRs** in central easyconfigs GitHub repository (see [BioHack2022 label](#))
- Effort not completed yet, open PRs to add software to EESSI (PRs [#197](#) + [#202](#) + [#203](#))



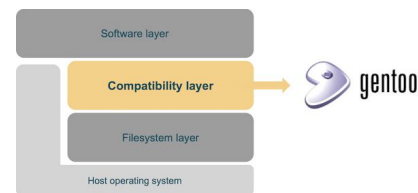
[Sébastien, Kenneth]

Progress update: filesystem layer



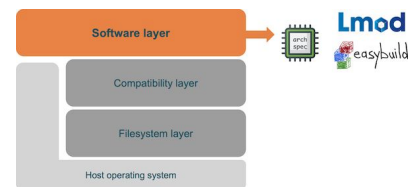
- New repository for datasets available: `data.eessi-hpc.org` ([PR #119](#))
 - Added to all 4 EESSI Stratum 1 servers
 - Still empty, working on updated ingestion script and procedures for adding/defining data
- Build container updated to Debian 11.5, CVMFS 2.10.0, fuse-overlayfs 1.9, awscli 1.27.8
 - See [PR #113](#)
 - Needs more testing to find out if the issue with `fuse-overlayfs` is really solved
- Workflow for building `cvmfs-config-eessi` package for macOS disabled (it's broken)
 - See PRs [#134](#) + [#136](#) + [issue #135](#)

Progress update: compatibility layer



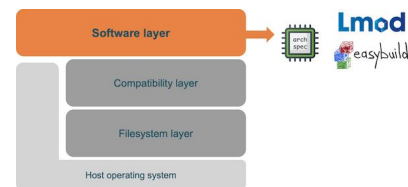
- Several security updates (still) required for 2021.06 and 2021.12 versions (these were reported by Gentoo's `glsa-check` tool)
 - 2021.06: expat, glibc, gzip, libarchive, lxml, vim, libgcrypt, libxml2, openssl, sqlite, zlib, libksba
 - 2021.12: update expat, glibc, gzip, libgcrypt, libxml2, openssl, sqlite, zlib, libksba
- Script ([see PR #155](#)) to install security updates should be replaced by tasks in Ansible playbook
 - We should explore this while installing the additional security updates?
 - Need a good way to evaluate impact on software layer (like broken EasyBuild install due to setuptools update)
 - Bob & Kenneth have been trying to find time for this...
- PRs to build compat layer for new EESSI pilot (2022.11) by Thomas
 - [gentoo-overlay PR #84](#): package sets (incl. updated archspec, ReFrame, Lmod)
 - [compatibility-layer PR #160](#): updated bootstrap script, pinning to GCC 10.4, ...

Progress update: software layer (1/2)



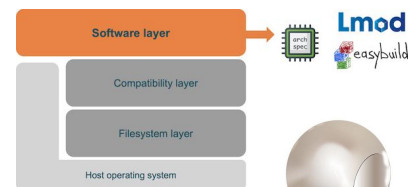
- `archdetect` alternative to `archspec` deployed in EESSI pilot 2021.12 ([PR #187](#) + [PR #200](#))
 - Pure bash alternative, more lightweight and quicker than `archspec`, fully under our control
 - Opt-in by setting `$EESSI_USE_ARCHDETECT` to 1 before sourcing init script
 - TODO: add symlinks for `aarch64/arm/neoverse-*` to `aarch64/graviton*`
- PRs to add software to EESSI pilot 2021.12
 - SciPy-bundle for foss/2021a ([PR #160](#)), still problematic on `ppc64le`
 - OpenFOAM ([PR #195](#)) + OSU Micro-Benchmarks ([PR #201](#)) for azhop workshop (partially deployed)
 - Bioinformatics + workflow tools (in context of BioHackathon Europe 2022)
 - Nextflow 22.10.1 ([PR #194](#))
 - snakemake ([PR #197](#))
 - software for 'mag' Nextflow pipeline ([#202](#))
 - PR to enhance EasyBuild hooks to fix installation of MetaBAT ([PR #203](#))

Progress update: software layer (2/2)



- Meson does not like the `ld` wrapper used by EasyBuild ([issue #196](#))
- Support for easystack files in EasyBuild was enhanced
 - See [PR #4021](#) + [PR #4057](#)
 - Only in `develop` branch for now, to be included with upcoming EasyBuild v4.7.0 release
 - See updated (develop) documentation at docs.easybuild.io/en/develop/Easystack-files.html
 - Easystack files can now specify custom configuration options for specific installations
 - Can be used to pull in fixes from PRs with `--from-pr` or `--include-easyblocks-from-pr` (?)
 - First step towards getting rid of ugly [EESSI-pilot-install-software.sh](#) script
 - EESSI software layer can be specified through a set of easystack files
 - Necessary to allow community contributions to propose software to add into EESSI via PRs

Bot for building + deploying software layer (1/3)

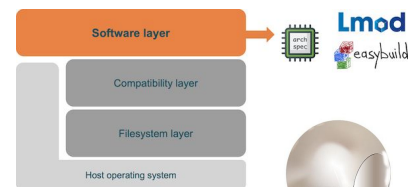


Progress on implementation of build-and-deploy bot

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

- Working minimal bot ([PR#62](#) merged) - bot in action [example software-layer PR](#)
 - Used for building larger stack (nessi.no/2022.11)
 - Who wants to test this for the current or next EESSI pilot?
- Focus for Dec'22
 - Redo PR for `resubmit.py` script that helps with debugging failing build jobs
 - Create issues for ideas collected during bot development and use
 - Plan what should be included in a first release
 - Improve code quality
 - Improve efficiency when building across multiple clusters for multiple CPU architectures

Bot for building + deploying software layer (2/3)



Progress on implementation of build-and-deploy bot

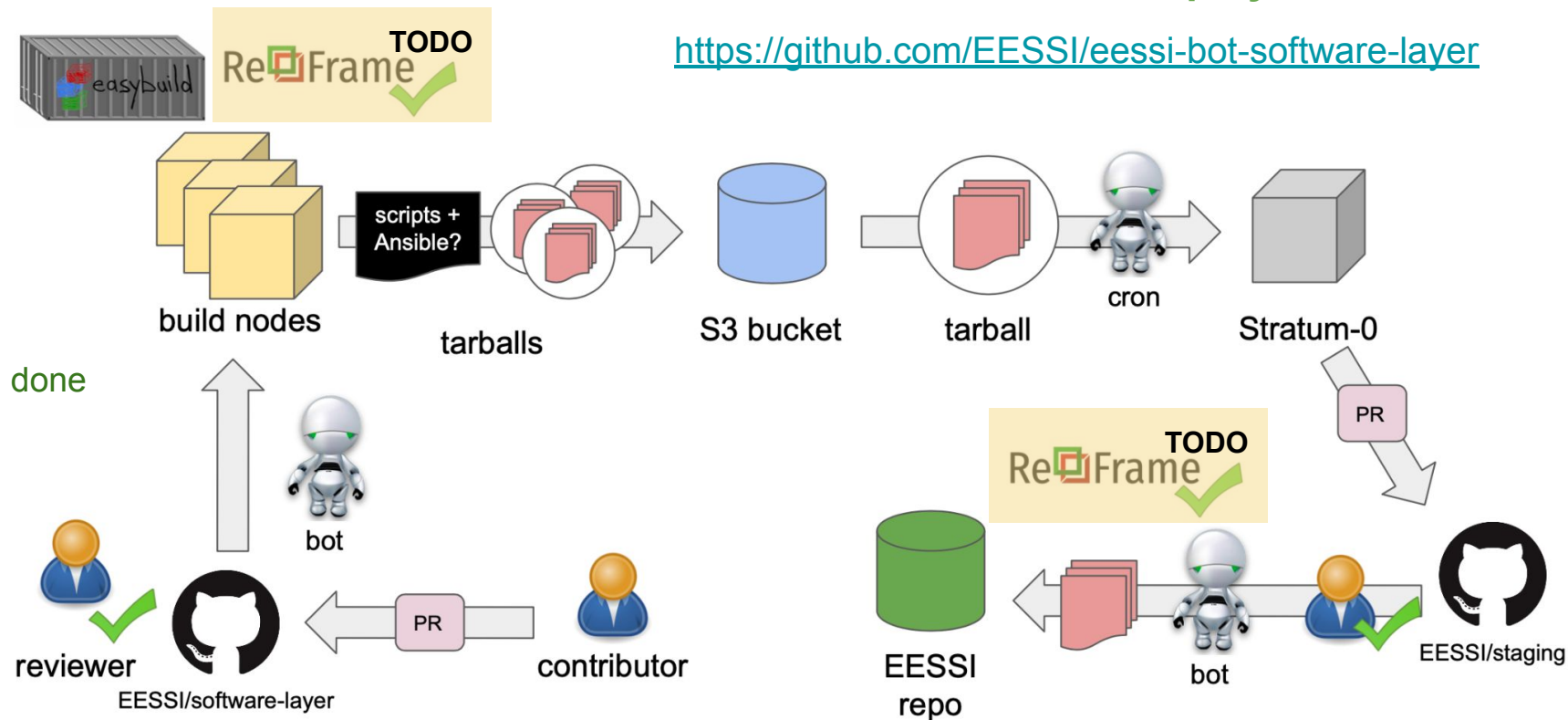
<https://github.com/EESSI/eessi-bot-software-layer>

- Merged [PRs](#):
 - [PR#56](#): Use `run_cmd` everywhere (instead of using `subprocess.run`) and add unit testing
 - [PR#53](#): More refactoring/renaming in `tasks/build.py`
 - [PR #63](#): Ignoring non bot jobs in `process_new_job` + `process_finished_job` to fix job manager crashes when it encounters a non-bot job
 - [PR #80](#): Separate handling of command line arguments for event handler/job manager
 - [PR #84](#): Change method for determining name of user that runs the job manager
- Work in progress: [PR #83](#): Function for identifying PR comment to be updated (to fix [issue #32](#))
- Next Steps:
 - Get [PR #83](#) merged
 - [Issue #27](#): Update PR comments when job starts running
 - [Issue #9](#): Improve start of app (in PyGHee)

Bot for building + deploying software layer

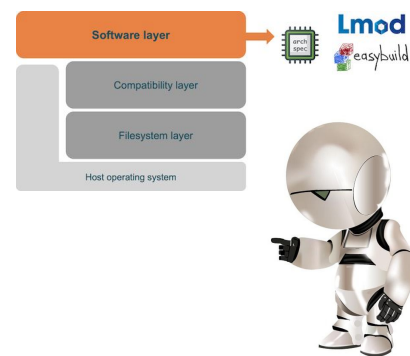
Minimal version of build-and-deploy bot now works!

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



Bot for building + deploying software layer

Example 1 of the bot doing the build + deploy phase for a PR (see [here](#)):



add CaDiCaL v1.3.0 with GCC/9.3.0 #18

Open boegel wants to merge 1 commit into boegel:main from EESSI:add-CaDiCaL-9.3.0

Conversation 3 Commits 1 Checks 110 Files changed 2 +11 -0

boegel commented 14 days ago

No description provided.

add CaDiCaL v1.3.0 with GCC/9.3.0 Verified ✓ dc60643

boegel added the bot:build label 14 days ago

test-eessi-bot-... bot commented 14 days ago · edited

New job on instance test-eessi-bot-software-layer for architecture x86_64-generic in job dir /mnt/shared/home/boegel/eessi-bot-software-layer/jobs/2022.11/pr_18/3156

date	job status	comment
Nov 16 14:41:05 UTC 2022	submitted	job id 3156 awaits release by job manager
Nov 16 14:42:04 UTC 2022	released	job awaits launch by Slurm scheduler
Nov 16 14:49:07 UTC 2022	finished	🎉 SUCCESS tarball eessi-2021.12-software-linux-x86_64-generic-1668610123.tar.gz (0.001 GiB) in job dir
Nov 16 14:56:58 UTC 2022	not uploaded	transfer of eessi-2021.12-software-linux-x86_64-generic-1668610123.tar.gz to S3 bucket failed
Nov 16 15:13:22 UTC 2022	uploaded	transfer of eessi-2021.12-software-linux-x86_64-generic-1668610123.tar.gz to S3 bucket succeeded

Reviews

No reviews

Still in progress? Convert to draft

Assignees

No one—assign yourself

Labels

bot:build bot:deploy

Project

None yet

Milestone

No milestone

Notifications

Customize

Unsubscribe

You're receiving notifications because you authored the thread.

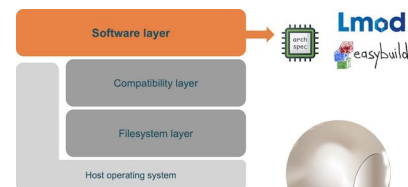
1 participant

Build phase is triggered by
`bot:build` label being added.

Deploy phase is triggered via
`bot:deploy` label
(restricted to specific people)

Bot provides feedback on
status by updating table in
comment (one per target CPU)

Bot for building + deploying software layer



Example 2 of the bot doing the build + deploy phase for a PR (see [here](#)):

Merged nessi.no/2022.11 - adding CMake, OpenBLAS, OpenMPI, Python, Perl with GCC/9.3.0 #47
trz42 merged 1 commit into [trz42:nessi.no-2022.11](#) from [poksumdo:nessi.no-2022.11-CMak](#) 8 days ago

eessi-bot-devel... bot commented 10 days ago • edited by trz42		
New job on instance <code>CitC-PR62</code> for architecture <code>aarch64-graviton2</code> in job dir <code>/mnt/shared/home/trz42/pilot.nessi/PR62/jobs/2022.11/pr_47/3183</code>		
date	job status	comment
Nov 21 05:30:25 AM UTC 2022	submitted	job id <code>3183</code> awaits release by job manager
Nov 21 05:30:47 AM UTC 2022	released	job awaits launch by Slurm scheduler
Nov 21 07:41:11 AM UTC 2022	finished	👍 SUCCESS tarball <code>eessi-2022.11-software-linux-aarch64-graviton2-1669016371.tar.gz</code> (0.346 GiB) in job dir
Nov 22 11:31:33 AM UTC 2022	uploaded	transfer of <code>eessi-2022.11-software-linux-aarch64-graviton2-1669016371.tar.gz</code> to S3 bucket succeeded
Nov 22 01:01:09 PM UTC 2022	staged	tarball <code>eessi-2022.11-software-linux-aarch64-graviton2-1669016371.tar.gz</code> downloaded to S0, merge PR trz42/staging#175 for approval
Nov 22 01:28:24 PM UTC 2022	approved	👍 tarball <code>eessi-2022.11-software-linux-aarch64-graviton2-1669016371.tar.gz</code> approved, see PR trz42/staging#175
Nov 22 01:31:04 PM UTC 2022	ingested	👍 tarball <code>eessi-2022.11-software-linux-aarch64-graviton2-1669016371.tar.gz</code> successfully ingested at <code>2022.11/software/linux/aarch64/graviton2/</code>

Build phase is triggered by
`bot:build` label being added.

Deploy phase is triggered via
`bot:deploy` label
(restricted to specific people)

Bot provides feedback on status by
updating table in comment (one per
target CPU),
here using enhanced ingest script

EESSI pilot repository

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

**NOT FOR
PRODUCTION USE!**



- 2021.06: considered “final”: no further changes, except security updates in compat layer if needed
- Current status for 2021.12 (default version)
 - Compatibility layer: in place for `aarch64` / `ppc64le` / `x86_64` (security updates needed!)
 - 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 (excl. `ppc64le`), WRF, **Nextflow, OpenFOAM v9 (partial!), OSU Micro-Benchmarks (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:
 - Ensure that Lmod cache update is done correctly, includes *all* available modules (first step: [PR #168](#))
 - Bot to automate workflow of adding software to EESSI (to avoid losing time doing it manually)
 - Build the stack for Azure's Ampere Altra (Arm) CPUs ([generally available since 1 Sept'22](#))

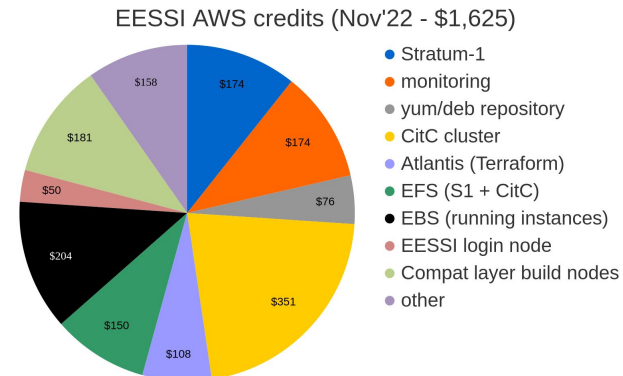
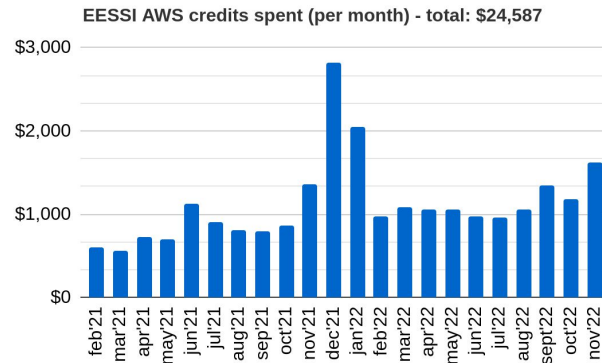
Time for the next pilot version?

- 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
- **Only add software installations via bot, no more manual deployments!**
- Initially include same software installations in software layer, then **gradually expand**
- Also install software with more recent toolchains + more applications
- Stop wasting time with supporting POWER (ppc64le), not used broadly enough
- Alpha/beta for production EESSI repository
- Switch to `eessi.io` domain + new Stratum 0 (dedicated hardware, yubikey)
- **Effort already started by Thomas: see [compat layer PR #160](#) + [gentoo-overlay PR #84](#)**

Usage of sponsored AWS credits



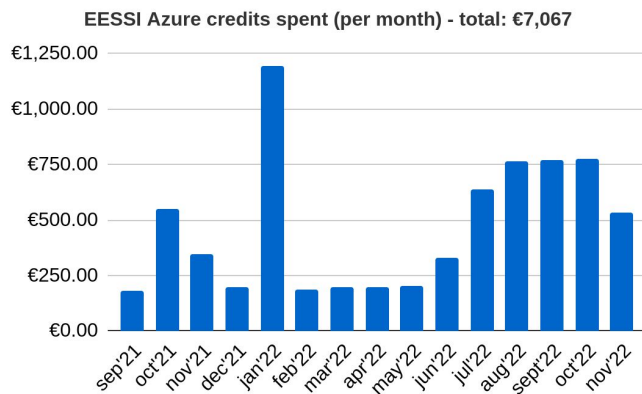
- **Ask in #aws-resources Slack channel to get access!**
- Original batch of \$25,000 worth of sponsored credits expired on Jan 31, 2022
- Request for new credits is WIP, extra \$15,000 worth of credits received to bridge the gap
- **~\$3,694 worth of sponsored credits left** (should be sufficient until Feb'23 at current spending rate)
- **Shared document with outline of how sponsored credits can be leveraged was shared with AWS**
- In Nov '22: ~\$1,625 worth of credits spent on Stratum-1, monitoring, CitC cluster, build nodes, test VMs, ...
- ~\$24,587 worth of credits spent in total so far (since Feb'21), all covered by sponsored credits



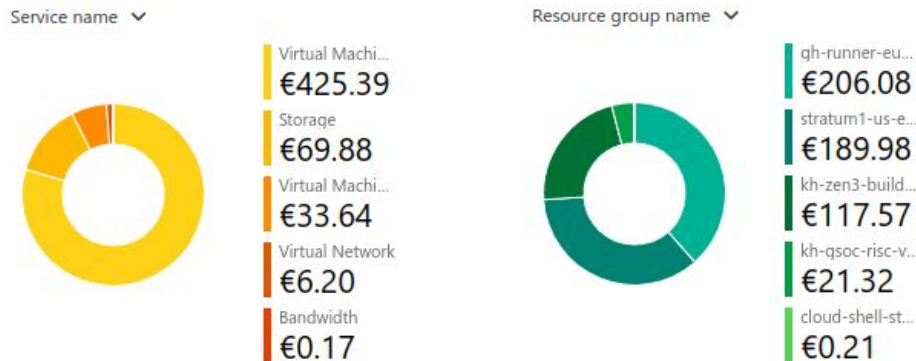
Azure sponsorship



- Sponsored credits (€40,000) are being put to good use!
- **Ask in #azure-resources Slack channel to get access!**
- In Nov'22: ~€535 worth of credits spent: Stratum-1 + GH Runners
- ~€7,067 worth of credits spent in total (since Sept'21)
- We should look into setting up a CitC cluster in Azure as well... (using Hugo's PRs [#118](#) + [#68](#))



Overview of spent credits per month



Nov'22

EU project: MultiXscale



EuroHPC
Joint Undertaking



- MultiXscale is a EuroHPC project: *Increasing performance, productivity and portability in the domain of multiscale simulations*
- 16 partners in 8 countries
- Total budget: ~6M EUR (of which ~50% for WPs related to EESSI)
- 4 year project (~2023-2027), ~5 FTE for WPs related to EESSI
- **Currently (still) working through red tape towards grant agreement**
- **Project start: 1st January 2023**
- Presentation on MultiXscale project & relation to EESSI at EESSI Community Meeting see <https://eessi.github.io/docs/meetings/2022-09-amsterdam/#fri-16-sept-2022>

Upcoming events: EESSI hackathon Dec'22



- **Wed 14 Dec - Wed 21 Dec'22** (Mon-Fri 19-23 Dec would be too close to Christmas)
- **Focused effort** to make progress on various tasks related to EESSI
 - Self-organising small groups working on a (single) specific task
 - You determine how much time you spend on the hackathon (aim for 1h/day, or more)
 - With support from “experienced” EESSI contributors
 - 3 Zoom sessions: kickoff on Wed 14 Dec, sync on Mon 19 Dec, show & tell on Wed 2 Dec
 - More information: <https://github.com/EESSI/meetings/wiki/EESSI-hackathon-Dec'22>
- Dedicated channel in EESSI Slack: [#hackathon](#) + GitHub repo [EESSI/hackathons](#)
- **If you plan to participate, please register and select tasks you are interested in!**
<https://terminplaner4.dfn.de/jNOHCCL2nNTEzrWn>