EESSI

EUROPEAN ENVIRONMENT FOR
SCIENTIFIC SOFTWARE INSTALLATIONS

EESSI meeting

5 Jan 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. bot for software layer)
4. Report on EESSI hackathon Dec'22
5. EESSI pilot repository
6. AWS/Azure sponsorship update + OCRE funding opportunity
7. Update on MultiXscale EU project
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

- Monthly Azure/EESSI sync meeting (9 Dec’22)
    - Primary topics:
        - EOSC Future Grant for requesting OCRE funding - EESSI as “use case”
        - Report on use of EESSI at azhop workshop at SC’22 (see also LinkedIn post)
        - Setting up Slurm cluster in Azure (using CycleCloud)
    - Notes available at https://github.com/EESSI/meetings/wiki/Azure-meeting-Dec-9-2022
- Various sync meetings on development of EESSI build-and-deploy bot
    - Consultant hired by HPC-UGent to work on bot completed their 3-month contract (Oct-Dec’22)
    - Development effort continued by Thomas/Kenneth/Bob/… (in scope of MultiXscale project)
    - Bi-weekly sync meetings planned to coordinate effort

[Kenneth]

EESSI hackathon Dec’22

- Wed 14 Dec - Wed 21 Dec 2022
- ~8 participants, fully remote (kickoff/sync/show&tell meetings via Zoom)
- Progress on:
    - Adding software to EESSI pilot repository
    - Development of build-and-deploy bot
    - GPU support
    - Exporting EESSI filesystem layer to container image for archiving
- Notes at https://github.com/EESSI/meetings/wiki/EESSI-hackathon-Dec'22

[Kenneth]

Security hardening of CI in EESSI repos

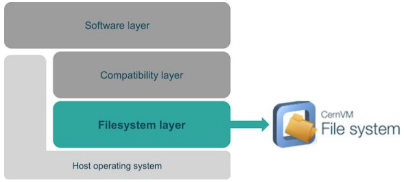
- CI workflows are open to abuse

- Rather than try to figure this out, add a security action
  - Provided by Open Source Security Foundation (OpenSSF)
  - https://github.com/ossf/scorecard

- Solve the issues raised by the security action
  - Minimising the permissions of `GITHUB_TOKEN` (read-only where that's sufficient)
  - Using a specific hash for all actions used
  - Manually listing actions that are permitted to be run by the organisation
  - Integration with Slack was disabled (requires too much permissions)

[Alan]

Progress update: filesystem layer

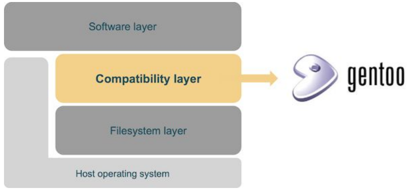


- Pull requests for updates to tarball ingestion script:
  - #138: Functionality for ingesting dataset tarballs (to `data.eessi-hpc.org`)
  - #139: Functionality for ingesting `scripts` directory tarballs

- **2021.06 version of EESSI pilot will be removed** (unless someone objects)
  - No more changes have been made for months
  - Has been replaced by 2021.12 version, which provides same software (and more)
  - init script will be replaced to print a message that 2021.12 should be used instead
  - Everything else in `/cvmfs/pilot.eessi-hpc.org(/versions)/2021.06` will be removed

[Bob, Kenneth]

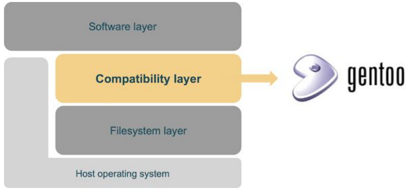
Progress update: compatibility layer (1/2)



- Several security updates (still) required for 2021.12 version of EESSI pilot repository (these were reported by Gentoo's `glsa-check` tool)
  - expat, glibc, gzip, libgcrypt, libxml2, openssl, sqlite, zlib, libksba, …
- Short term:
  - Actually perform the updates via updated update-pkgs-2021.12.sh script
  - Deploy updated compat layer in `/cvmfs/pilot.eessi-hpc.org/versions/2021.12`
- Long term: come up with better approach to follow up on necessary security updates (via Ansible playbook?)

[Kenneth, Bob, Thomas]

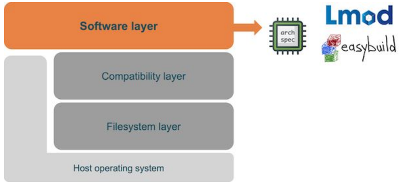
Progress update: compatibility layer (2/2)



- 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, …
- Recent attempt to build compatibility layer failed
  - using a recent Gentoo commit failed because of https://bugs.gentoo.org/886123
  - rebuilding with a previously working commit (early Nov) failed too, for other reasons though
- IDEA: use the bot to build compat layers more regularly to detect regressions early
  - probably requires to port current Ansible scripts to a shell script

[Kenneth, Bob, Thomas]

Progress update: software layer (1/2)

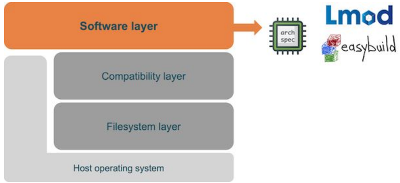


- Merged PRs + deployed to EESSI pilot 2021.12
  - also install SciPy-bundle-2021.05-foss-2021a.eb into 2021.12 pilot (PR #160)
  - enhance EasyBuild hooks to fix installation of MetaBAT in EESSI (PR #203)
  - use correct easyblock to install OpenBLAS/0.3.15-GCC-10.3.0 for `*/generic` (PR #211)
  - ignore failing FlexiBLAS tests for `ppc64le/generic`(PR #211)

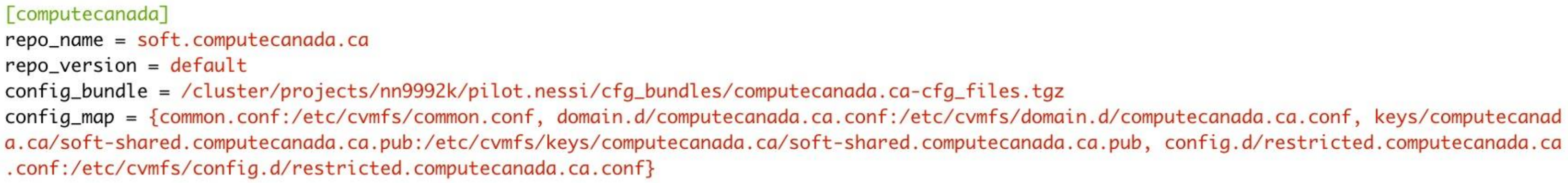
- WIP PRs:
  - add R 4.1.0 with foss/2021a to EESSI pilot 2021.12 (PR #210)
  - add software required for 'mag' Nextflow pipeline to EESSI 2021.12 (PR #202) (requires R 4.1.0 with foss/2021a)
  - use single source file for pilot version and repository (PR #215)
  - addd OSU-Micro-Benchmarks/5.7.1-gompi-2021a to EESSI pilot 2021.12 (PR #201)
  - add OpenFOAM v9 to EESSI pilot 2021.12 (PR #195)

[Kenneth, Thomas]

Progress update: software layer (2/2)



- Unified script to access EESSI (read-only and read & write) via container (WIP PR #216)
  - `./eessi_container.sh`--> ready to go
  - `./eessi_container.sh --access rw`--> make changes to /cvmfs/... (build pkgs)
  - `./eessi_container.sh --repository computecanada`--> access a different repository

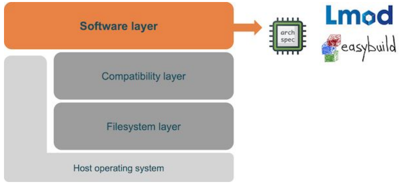


```
[computecanada]
repo_name = soft.computecanada.ca
repo_version = default
config_bundle = /cluster/projects/nn9992k/pilot.nessi/cfg_bundles/computecanada.ca-cfg_files.tgz
config_map = {common.conf:/etc/cvmfs/common.conf, domain.d/computecanada.ca.conf:/etc/cvmfs/domain.d/computecanada.ca.conf, keys/computecanad
a.ca/soft-shared.computecanada.ca.pub:/etc/cvmfs/keys/computecanada.ca/soft-shared.computecanada.ca.pub, config.d/restricted.computecanada.ca
.conf:/etc/cvmfs/config.d/restricted.computecanada.ca.conf}
```

  - TODO: reuse tmp storage to speed-up container launch & to facilitate debugging (bot)

[Kenneth, Thomas]

Progress update: GPU support

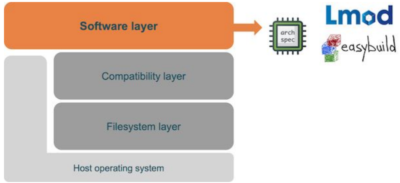


- Plan: split up PR#172 into smaller and more manageable chunks
  - Has become quite large and difficult to review
  - Leave the PR open as reference point
- Merged PRs
  - Adding CUDA-Samples to EasyBuild: PR#16914
    - Allows us to build and ship binaries that we can use to test if the CUDA runtime works
    - Central managing of CUDA-Samples instead of having to build them manually (within scripts)
    - Unified approach for multiple CUDA versions

      (samples are not a part of the CUDA toolkit anymore starting from version 11.6)

[Michael, Alan]

Progress update: GPU support



Software layer

Compatibility layer

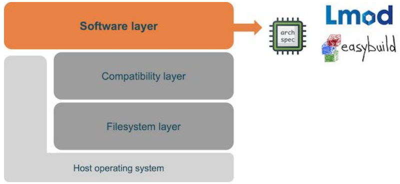
Filesystem layer

Host operating system

- Opened PRs
  - Add CUDA to software layer: PR#212
    - Install CUDA using EESSI-pilot-install-software.sh together with p7zip and CUDA-Samples
      - p7zip is needed to unpack the CUDA compatibility libraries
    - Use EasyBuild hook to only ship CUDA runtime (and everything else we're allowed to ship according to the EULA), replace everything else with symlinks pointing to `host_injections`
    - Add script to install CUDA in `host_injections`, unbreaking the shipped symlinks; to be used by admins/users locally (should be moved to new scripts subdir, see below)
    - Add EasyBuild hook to tag software depending on CUDA with a `gpu` tag
  - Create new scripts subdirectory in software-layer: PR#213
  - Add new scripts subdirectory to ingestion scripts: PR#139

[Michael, Alan]

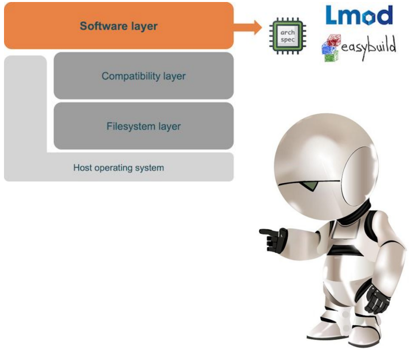
Progress update: GPU support



- PRs in preparation
  - CUDA compatibility libraries
    - Still needs some clean up but functionality is already there in PR#172, depends on PR#212
  - CUDA tests
    - Needed some rework/simplification now that we ship CUDA-Samples (don't need to build manually anymore)
    - Depends on PR#212, tests will be finalized once the other PR is merged
  - Lmod hooks
    - Hide and refuse to load modules depending on CUDA if CUDA is not installed in `host_injections`
  - Documentation
    - Will come last, depends on exact layout of all other PRs

[Michael, Alan]

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



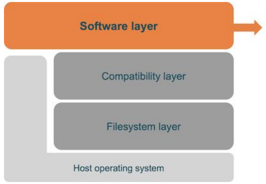
Progress on implementation of build-and-deploy bot

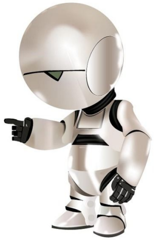
https://github.com/EESSI/eessi-bot-software-layer

- Working minimal bot
    - Who wants to test this for the current or next EESSI pilot?
- Dec'22 (PRs: 13 merged/3 open/2 drafted, issues: 7 closed/51 open)
    - PR #77/#129 improved error handling (Jacob, UiO)
    - PR #78 using run_cmd everywhere (Hafsa, INUITS)
    - PR #79 non-bot jobs leaking into known jobs (Thomas, UiB)
    - PR #80 split up argument parsers (Hafsa, INUITS)
    - PR #83 identify PR comment (Hafsa, INUITS)
    - PR #84 determine username (Hafsa, INUITS)
    - PR #116 show running state of jobs (Hafsa, INUITS)
    - PR #117 security CI action (Alan, CECAM)
    - PR #119 LICENSE added (Thomas, UiB)
    - PR #120 keep testing with Python 3.6 (Kenneth, UGent)
    - PR #123 improve start of bot (Hafsa, INUITS)
    - PR #124 check build permission (Hafsa, INUITS)
    - PR #130 generic read_config (Hafsa, INUITS)

[Thomas, Kenneth]

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



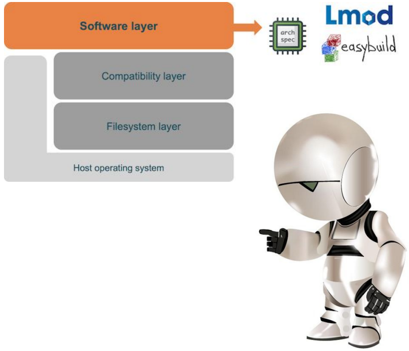


- Dec’22 (PRs: 13 merged/3 open/2 drafted, issues: 7 closed/51 open)
  - Draft PR #85 for `resubmit.py` script that helps with debugging failing build jobs
  - Draft PR #127 for improved overview of status of a pull request (hackathon)
  - Created issues for ideas collected during bot development and use (currently 51 open issues)

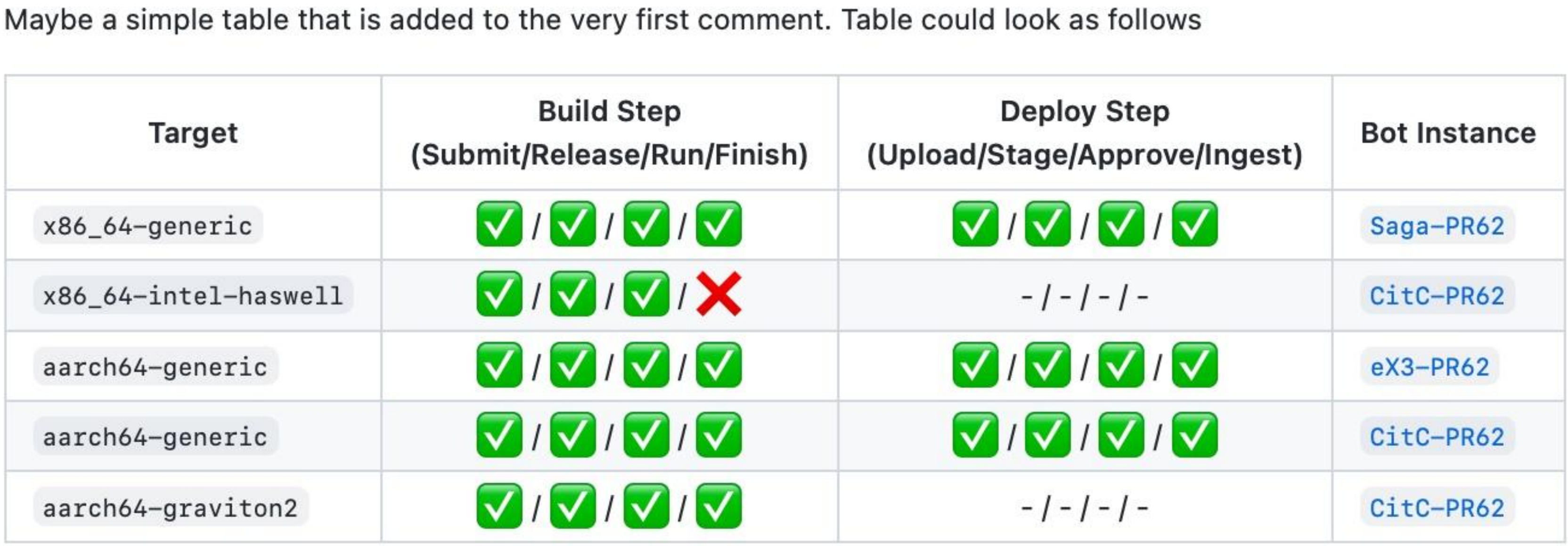
- Focus in Jan'23
  - Get work for MXS started - Task 5.3 "Facilitating community contributions to the central software stack"
    - 1st coordination meeting, 5 Jan’23 (Bob, Kenneth, Thomas)
    - Related PRs to software-layer:
      - PR #214 `init/eessi_defaults`
      - WIP PR #216 `eessi_container.sh`
  - Merge open PRs, finish PR drafts, code/doc cleanup
  - Plan a first release of bot (v0.1.0) to be used in a production environment

[Thomas, Kenneth]

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



Example for status overview of a pull request to the software-layer.

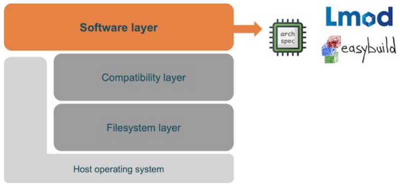


Maybe a simple table that is added to the very first comment. Table could look as follows

Target	Build Step (Submit/Release/Run/Finish)	Deploy Step (Upload/Stage/Approve/Ingest)	Bot Instance
`x86_64-generic`	✅ / ✅ / ✅ / ✅	✅ / ✅ / ✅ / ✅	`Saga-PR62`
`x86_64-intel-haswell`	✅ / ✅ / ✅ / ❌	- / - / - / -	`CitC-PR62`
`aarch64-generic`	✅ / ✅ / ✅ / ✅	✅ / ✅ / ✅ / ✅	`eX3-PR62`
`aarch64-generic`	✅ / ✅ / ✅ / ✅	✅ / ✅ / ✅ / ✅	`CitC-PR62`
`aarch64-graviton2`	✅ / ✅ / ✅ / ✅	- / - / - / -	`CitC-PR62`

[Thomas, Kenneth]

Progress update: software testing



- Separate GitHub repository created: [EESSI/test-suite]
- Goal is to develop portable software tests, using ReFrame
- Initial test for GROMACS already merged, based on work done by Caspar (SURF)
  - Feedback welcome! See README for basic info on getting started
- Result of meeting between SURF & VSC on collaborating on a common test suite using ReFrame
- Idea is to leverage this for EESSI, but also in other contexts (system-specific software stacks maintained with EasyBuild, …)
- Aligns well with one of the goals in MultiXscale

[Kenneth, Thomas]

EESSI pilot repository

NOT FOR PRODUCTION USE!

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

- 2021.06: considered “end of life”: **will soon be removed**
- 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 (**also for `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
    - 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)

[Kenneth]

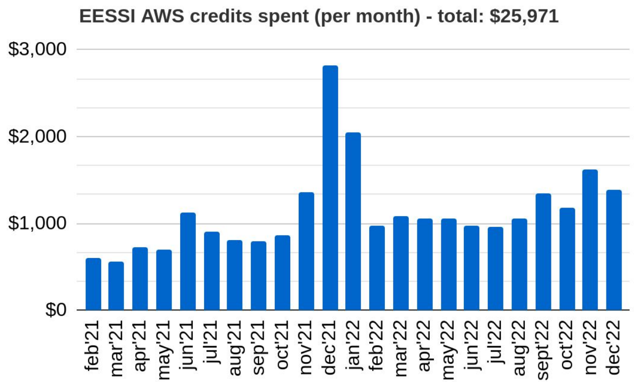
Outlook to next pilot version (2023.x)

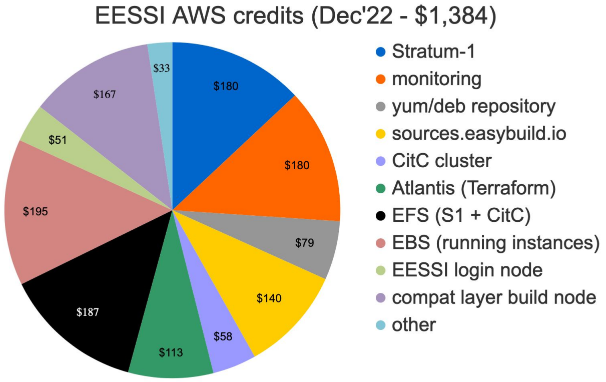
- Small changes to compatibility layer: updated Lmod, more tools, …
- Include enhancements/changes that are necessary for CUDA GPU support
- Work towards getting rid of ugly install script, aim for easystack-only (if possible)
- **Only add software installations via bot, no more manual deployments!**
- 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`) - start considering RISC-V
- Alpha/beta for production EESSI repository
- Switch to `eessi.io` domain + new Stratum 0 (dedicated hardware, yubikey) - if available
- **Effort already started by Thomas: see compat layer PR #160 + gentoo-overlay PR #84**
  (more work needed to get a new working pilot version - 2023.x)

[Kenneth]

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
- **~$2,301 worth of sponsored credits left, should be sufficient until end of Jan’23 at current spending rate**
- **Meeting scheduled with Brandon Bouffler (AWS) on Wed 11 Jan’23 to get additional sponsored credits**
- In Dec ‘22: ~$1,384 worth of credits spent on Stratum-1, monitoring, sources.easybuild.io, build node, CitC cluster
- ~$25,971 worth of credits spent in total so far (since Feb’21), all covered by sponsored credits



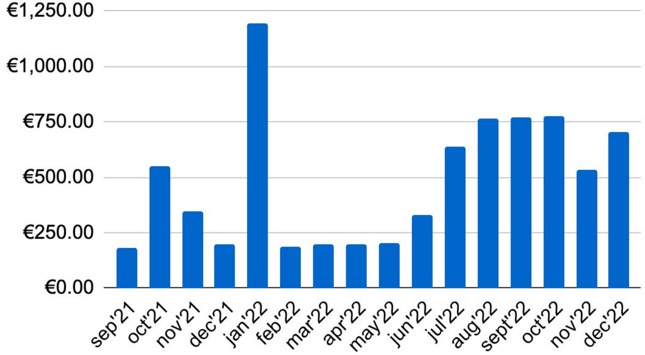


[Kenneth]

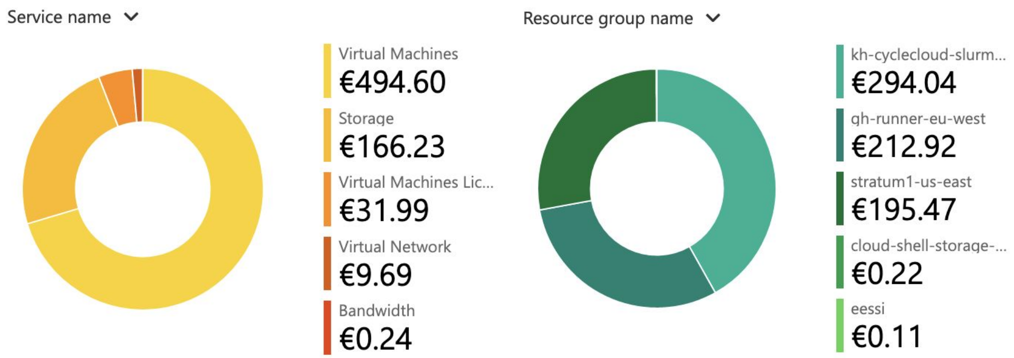
Azure sponsorship

- Sponsored credits (€40,000) are being put to good use!
- **Ask in #azure-resources Slack channel to get access!**
- In Dec: ~€702 worth of credits spent: Stratum-1 + GitHub Runners + virtual Slurm cluster
- ~€7,770 worth of (sponsored) credits spent in total (since Sept'21)
- **New: virtual Slurm cluster in Azure (set up using Azure Cyclecloud) - more info here**
  - TODO: properly set up partitions for different CPU types (to the extent that's possible…)

EESSI Azure credits spent (per month) - total: €7,770



Overview of spent credits per month



Service name ⌄

Virtual Machines
€494.60

Storage
€166.23

Virtual Machines Lic...
€31.99

Virtual Network
€9.69

Bandwidth
€0.24

Resource group name ⌄

kh-cyclecloud-slurm...
€294.04

gh-runner-eu-west
€212.92

stratum1-us-east
€195.47

cloud-shell-storage-...
€0.22

eessi
€0.11

Dec'22

[Kenneth]

EU project: MultiXscale

- **MultiXscale** is a EuroHPC project: *Centre of Excellence in Exascale-Oriented Application Co-Design and Delivery for Multiscale Simulations*
- 16 partners in 8 countries (incl. UGent, RUG, UBergen, UBarcelona, …)
- 8 work packages (WPs) - 2 directly related to EESSI (+ training, dissemination, …)
- Total budget: ~6M EUR (of which ~50% for WPs related to EESSI)
- 4 year project (~2023-2027), ~5 FTE for WPs related to EESSI
- **Grant agreement and collaboration agreements have been signed**
- **Project was started on 1 Jan 2023** - proper (physical) kickoff meeting is being planned
- 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

[Alan, Bob, Kenneth]