EESSI meeting

3 Feb 2022

https://github.com/EESSI/meetings/wiki

Agenda

1. Quick introduction by new people

2. EESSI-related meetings in last month

3. WRF on Azure via EESSI

4. EESSI hackathon (Jan'22) report

5. Progress update per EESSI layer

6. 2021.12 version of pilot repository

7. AWS/Azure sponsorship update

8. Update on EESSI paper

9. Past/upcoming events

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 (1/2)

- Jan 11th: EESSI/Azure sync meeting

  - Follow-up on activities with EESSI on Azure resources

  - Request to include WRF into EESSI (see https://github.com/EESSI/software-layer/pull/162)

  - Work-in-progress by Hugo (+ Matt): supporting Azure in Cluster-in-the-Cloud

  - Sponsored Azure credits have been "donated" to SURF, so **no end date** to consume them

  - Meeting notes at https://github.com/EESSI/meetings/wiki/Azure-meeting-11-Jan-2022

[Kenneth]

EESSI-related meetings (2/2)

- Jan 11th: monthly CernVM-FS coordination meeting

  - Version 2.9.1 will probably be released in (the beginning of) February

    - Fix for the GEO API issue on EL8 systems

  - CernVM workshop (12-14 Sept 2022, Amsterdam):

    - See https://indico.cern.ch/event/1079490/

    - online, offline, hybrid?

  - Some site saw issues with replicating files due to virus scanning tools: best to disable these

[Bob]

WRF on Azure with EESSI and more….

- CitC integration started (going through subscription hoops)

- Integration with Azure HPC OnDemand Platform, [PR submitted](#)

- Tested WRF3 on Az-HOP with 64-80 nodes

  - WRF module not longer included in Lmod cache since today? (thanks ReFrame!) => [issue #165](#)

- Setting up ReFrame testing

  - STREAM benchmark

  - OSU: bandwidth and alltoall

  - WRF

    - Need to add performance….

    - Can we start hosting benchmark data?

- [Archspec not detecting Zen3 on Azure](#)

- Glibc-devel question => in Gentoo or host OS?

```
[EESSI pilot 2021.12] $ reframe -C config/settings.py -c checks --recursive -n Wrf* -r
[ReFrame Setup]
  version:            3.10.0
  command:           '/cvmfs/pilot.eessi-hpc.org/versions/2021.12/compat/linux/x86_64/usr/lib/python-exec/python3.9/r
  launched by:        clusteruser@ondemand.internal.cloudapp.net
  working directory: '/anfhome/clusteruser/azhop-reframe'
  settings file:     'config/settings.py'
  check search path: (R) '/anfhome/clusteruser/azhop-reframe/checks'
  stage directory:   '/anfhome/clusteruser/azhop-reframe/stage'
  output directory:  '/anfhome/clusteruser/azhop-reframe/output'

[==========] Running 2 check(s)
[==========] Started on Thu Feb  3 08:18:51 2022

[----------] start processing checks
[ RUN      ] WrfConusDownload @azhop:execute+builtin
[      OK  ] (1/4) WrfConusDownload @azhop:execute+builtin [compile: 0.018s run: 1469.999s total: 1470.046s]
[ RUN      ] WrfCheck @azhop:hc44rs+eessi-foss-2020a
[ RUN      ] WrfCheck @azhop:hb120v2+eessi-foss-2020a
[ RUN      ] WrfCheck @azhop:hb120v3+eessi-foss-2020a
[     FAIL ] (2/4) WrfCheck @azhop:hc44rs+eessi-foss-2020a [compile: 0.019s run: 702.221s total: 702.367s]
=> test failed during 'sanity': test staged in '/anfhome/clusteruser/azhop-reframe/stage/azhop/hc44rs/eessi-foss-202
[      OK  ] (3/4) WrfCheck @azhop:hb120v3+eessi-foss-2020a [compile: 0.020s run: 662.020s total: 753.389s]
[      OK  ] (4/4) WrfCheck @azhop:hb120v2+eessi-foss-2020a [compile: 0.020s run: 722.794s total: 783.695s]
[----------] all spawned checks have finished

[   FAILED ] Ran 4/4 test case(s) from 2 check(s) (1 failure(s), 0 skipped)
[==========] Finished on Thu Feb  3 08:56:25 2022
```

[Hugo]

EESSI hackathon report (1/3)

https://github.com/EESSI/meetings/wiki/EESSI-hackathon-Jan'22

- 2nd EESSI hackathon: Jan 17-21, 2022

- **Main goal: focused effort on various tasks in EESSI**

- About 11 participants, working in small teams on 6 topics (out of ~16 proposed)

- Using prepared infrastructure with EESSI pilot on Azure, AWS & FENIX

  - Temporary Magic Castle clusters (https://github.com/EESSI/hackathons/tree/main/2022-01/magic_castle)

    - `eessi-aws` on AWS with fast interconnect (EFA) + GPU (G4 instances - NVIDIA T4)

    - one on Azure with Intel Skylake nodes + Infiniband

    - one with GPUs on FENIX resources at JUSUF @ JSC (AMD EPYC + NVIDIA V100)

  - CitC cluster on AWS: Intel Haswell + Skylake + Cascade Lake, AMD Rome, Graviton2 (https://github.com/EESSI/hackathons/tree/main/2022-01/citc) - **still available!**

- Dedicated GitHub repository: https://github.com/EESSI/hackathons

- Live notes via HackMD documents (one per hackathon task)

[Thomas]

EESSI hackathon report (2/3) - key results

https://github.com/EESSI/meetings/wiki/EESSI-hackathon-Jan'22

- **Task 02: Building on top of EESSI** (Kenneth, Frank, Martin, Jacob)

  - see 2022-01/02_software_on_top subdir in EESSI/hackathons

  - work on adding RPATH wrappers to GCC + building LAMMPS manually on top of EESSI

- **Task 03: Workflow for additions to EESSI** (Bob, Jörg, Kenneth)

  - Scripts to enable fully autonomous building of software for EESSI (see PR #163)

  - Limited progress, but good understanding of next steps (see hackathon notes)

- **Task 05: GPU support** (Alan, Bartek, Michael)
  - GPU support is working, initial script for new pilot version 2021.12:
    https://github.com/EESSI/hackathons/tree/05_gpu/2021-12/05_gpu
  - GROMACS with GPU support has been installed in test setup and seems to work \o/

[Thomas]

EESSI hackathon report (3/3) - key results

https://github.com/EESSI/meetings/wiki/EESSI-hackathon-Jan'22

- **Task 06: EESSI test suite (with ReFrame)** (Thomas)
  - very little progress during Jan'22 hackathon :(

- **Task 07: Monitoring** (Terje)
  - little progress during Jan'22 hackathon

- **Task 16: Exporting EESSI to a tarball/container** (Jure)
  - Worthwhile to note:
    - Using EESSI init scripts is problematic in noninteractive container startup
    - We now have ability to pick up generic modules instead of optimized ones
    - Overall pretty happy with "minimum viable product" resulting from hackathons
 - Script available in hackathon repo

[Thomas]

# Progress update: filesystem layer
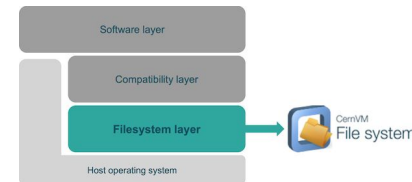
- It *seemed* that the "`Operation not permitted`" errors were solved in latest `fuse-overlayfs` version

  - We built new EESSI build/client containers ([PR #113](#))

  - However, while testing them more thoroughly, we did run into the same issue again :(

  - So, the change has been reverted, and we're sticking to the ancient version again ([PR #114](#))

  - See also https://github.com/containers/fuse-overlayfs/issues/232

- Good progress by Jure on exporting software installations in EESSI to a container image

  - Mainly for archiving purposes

  - (see [Jan'22 hackathon](#))

[Bob]

Progress update: compatibility layer
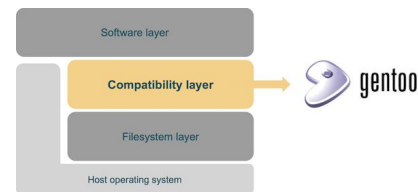
- No security updates required for 2021.06 or 2021.12 compat layers

  (as reported by Gentoo's `glsa-check` tool)

  - New GLSAs reported by Gentoo for Polkit, Chromium/Chrome, WebkitGTK+

  - These are not installed in our compat layers

Progress update: software layer (1/2)
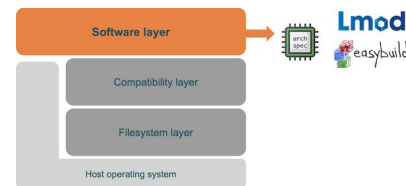
- Scripts were added to enable fully autonomous building of software for EESSI

```
mkdir -p /tmp/$USER; cd /tmp/$USER

git clone https://github.com/EESSI/software-layer; cd software-layer

./build_container.sh run /tmp/$USER/EESSI $PWD/install_software_layer.sh
```

- WRF 3.9.1.1 built with `foss/2020a` was added to EESSI pilot 2021.12 (to test on Azure)

  - Not correctly reflected in Lmod cache, see https://github.com/EESSI/software-layer/issues/165

- Install SciPy-bundle with `foss/2021a` into EESSI pilot 2021.12

  - See https://github.com/EESSI/software-layer/pull/160

  - Built + ingested for all `x86_64` + `aarch64` CPU targets

  - Not yet for `ppc64le`, due to problems with FlexiBLAS (included in `foss/2021a`)
    cfr. https://github.com/easybuilders/easybuild-easyconfigs/issues/12968

[Kenneth]

Progress update: software layer (2/2)
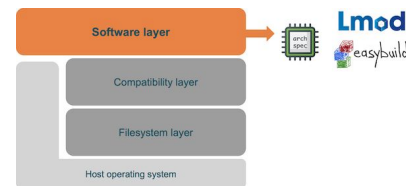
- First experiments with EasyBuild in RISC-V emulated environment

    - One top of pre-built Gentoo for RISC-V (not yet a proper compat layer built for EESSI!)

    - Using QEMU to emulate RISC-V, on an AWS `c6i.8xlarge` instance (Intel Icelake)

    - Worked: installing vim, git, Lmod (from source using Gentoo's `emerge`)

    - Handful of small installations with EasyBuild (so Python 3.9 + Lmod working fine)

    - Ran into a wall with `binutils` because `ld.gold` is not supported for RISC-V (see also https://github.com/easybuilders/easybuild-easyblocks/issues/2657)

    - Detailed notes at https://gist.github.com/boegel/6530823d57629b69aa3b0384870fdd8d

[Kenneth]

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:
  - New path: `/cvmfs/pilot.eessi-hpc.org/`**`versions`**`/2021.12`
  - Compatibility layer: in place for `aarch64` / `ppc64le` / `x86_64`
    - List of installed packages is pretty much identical \o/
  - 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
  - TODO:
    - Move "latest" symlink from 2021.06 to 2021.12
    - Update documentation at https://eessi.github.io/docs/pilot

[Kenneth]

Progress update: infrastructure (1/3)

- Preliminary monitoring of stratum1s is operational

  - Cvmfs-servermon -> Blackbox-exporter -> Prometheus -> Grafana

  - All remote, nothing required installed on stratum1s

- Current checks via cvmfs-servermon (https://github.com/cvmfs-contrib/cvmfs-servermon):

  - Repos are (recently) updated

  - Repos have (recently) run a garbage collection

  - Repos have a working GEO api

- A more complete option in the pipeline

  - Track repo versions

  - node_exporter

- Lots of manual work right now, lots and lots of moving parts and configuration files

[Terje]

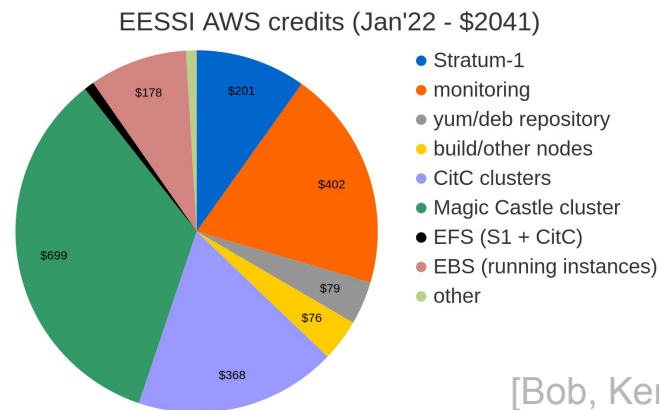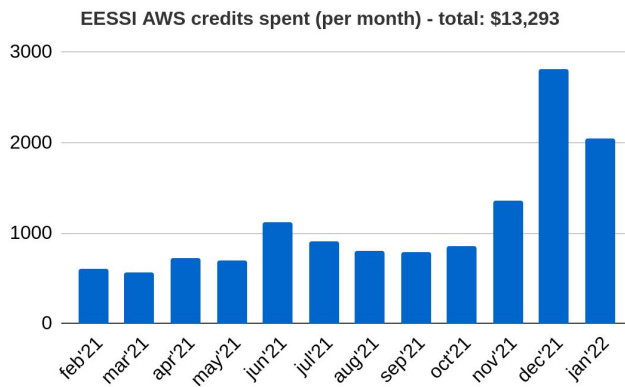# Progress update: infrastructure (2/3)

[Terje]
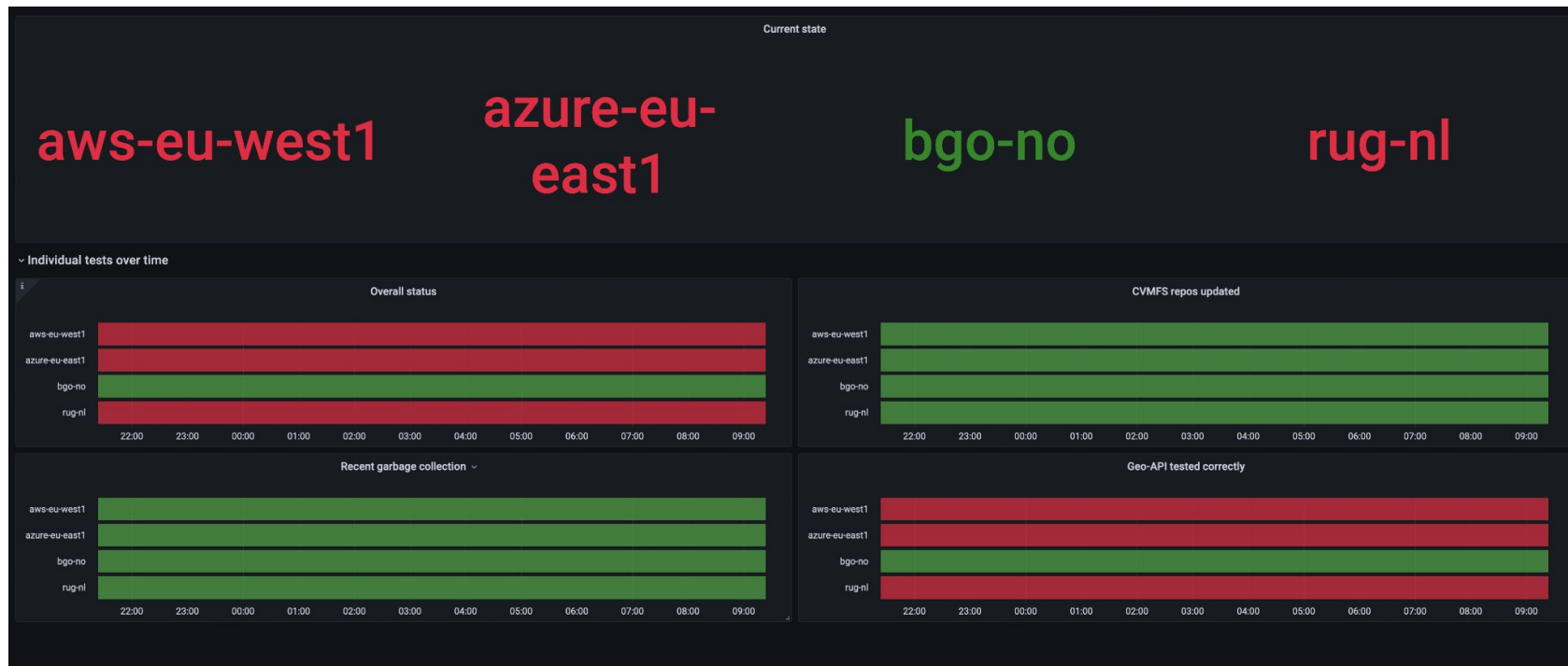
Progress update: infrastructure (3/3)

- Ansible roles for both internal and external use: https://github.com/terjekv/ansible-eessi-roles

  - Supports Clients, Proxies, Stratum1, and Stratum0

  - Feature parity with today's ansible scripts

  - Supports RedHat and Debian based distributions

  - Adds some local monitoring, CVMFS parts not really functional

- Looking at lifecycle management for AWS nodes

  - https://docs.aws.amazon.com/AWSEC2/latest/UserGuide/snapshot-lifecycle.html

  - Managed via terraform, snapshotting tagged instances

  - Good for rapid undos if stuff breaks

  - What about Azure?

[Terje]

Usage of sponsored AWS credits

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

- In January '22: ~$2,041 worth of credits spent on Stratum-1 server, monitoring node, repository node, EESSI hackathon cluster (CitC, Magic Castle)

- **Original batch of $25,000 worth of sponsored credits expired on Jan 31, 2022!**

- ~$13,293 worth of credits spent in total so far (since Feb'21), all covered by sponsored credits

- Request for new credits is WIP, extra $10k worth of credits already received to bridge the gap

- Christian is leaving AWS, working on finding new contact

EESSI AWS credits spent (per month) - total: $13,293

EESSI AWS credits (Jan'22 - $2041)

Legend:
- Stratum-1
- monitoring
- yum/deb repository
- build/other nodes
- CitC clusters
- Magic Castle cluster
- EFS (S1 + CitC)
- EBS (running instances)
- other
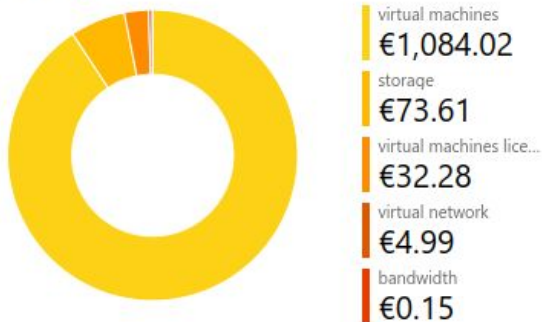
Pie values: $201, $402, $79, $76, $368, $699, $178

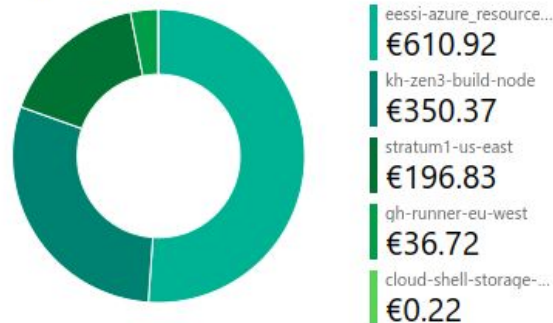[Bob, Kenneth]

Azure sponsorship

- Sponsored credits (€40,000) are being put to good use!

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

- In Jan'22: ~€ 1,195 worth of credits spent

- On Stratum 1, clusters for Jan'22 hackathon, AMD Rome build node, (stopped) GitHub Runners

- ~€2,470 worth of credits spent in total (since Sept'21)

Service name ⌄

virtual machines
€1,084.02

storage
€73.61

virtual machines lice…
€32.28

virtual network
€4.99

bandwidth
€0.15

Resource group name ⌄

eessi-azure_resource…
€610.92

kh-zen3-build-node
€350.37

stratum1-us-east
€196.83

gh-runner-eu-west
€36.72

cloud-shell-storage-…
€0.22

[Bob, Kenneth]

Update on EESSI paper

- *EESSI: A cross-platform ready-to-use optimised scientific software stack*

- **Paper got accepted! \o/**

- Original submission on 31 May 2021, revised on 19 Nov 2021, accepted on 24 Jan 2022

- Now: proofreading, license agreement, open access - all the fun stuff :-)

- Could become available anytime (today+3 days or tomorrow+3 days ...).
    - Journal of Software: Practice and Experience (https://onlinelibrary.wiley.com/journal/1097024x)
    - Special issue *New Trends in High-Performance Computing: Software Systems and Applications*

- We have a DOI: 10.1002/spe.3075

- Will give more visibility to EESSI.

- Thanks to everyone who contributed!

- **Pre-print available for those interested**
  (contact any of Thomas, Bob, Alan, Kenneth, …)

[Thomas]

Past/upcoming events

- 7th EasyBuid User Meeting (EUM'22)

  - 24-28 Jan 2022 (virtual), **all talks recorded** and available on YouTube

  - Talks related to EESSI:

    - *Getting started with EESSI* (presented by Thomas)

    - *Leveraging EESSI for WRF simulations at scale on Azure HPC* (Hugo + Davide, MS Azure)

    - *Semi-automated workflow for adding software to EESSI* (presented by Jörg)

    - *ReFrame update, Lmod update, Singularity to Apptainer, RISC-V, etc.*

  - YouTube links + slides available at https://easybuild.io/eum22/#program

- FOSDEM'22: HPC, Big Data, and Data Science devroom (5-6 Feb 2022, virtual)

  - https://fosdem.org/2022/schedule/track/hpc_big_data_and_data_science

  - Talks on containers in HPC (by Christian), AMD GPUs, Exascale PMI (MPI startup), etc.

[Kenneth]