

EESSI meeting

May 6th 2021

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

Agenda



- Quick introduction by new people
- 2. EESSI-related meetings in last month [Bob, Kenneth, Thomas]
- 3. Update on CZI grant "Essential Open Source Software for Science" [Alan]
- 4. Progress update per EESSI layer [Bob, Peter, Kenneth]
- 2021.03 version of pilot repository: status [Kenneth]
- 6. Build nodes experience report [Thomas, Axel]
- Testing with ReFrame [Caspar]
- 8. AWS/Azure update + infrastructure in AWS [Kenneth, Terje]
- 9. Focus points in coming weeks/months
- 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



- April 13th: Monthly CernVM-FS coordination meeting (attended by Bob)
 - Very short meeting, main (relevant) news: version 2.8.1 was released, solves a few bugs
- April 23rd: Brainstorm about setting up software stacks on new clusters
 see https://github.com/EESSI/meetings/wiki/Brainstorm-software-stacks-new-clusters-Apr-23-2021
- April 30th: NESSI EESSI coordination meeting
 (Thomas, Bob, Kenneth, Alan, Terje, Peter, Caspar, Axel, Andreas, Dan)
 - NESSI development phase started May 2021 (1y, ~24 PMs of effort)
 - Agenda: status & plans for NESSI & EESSI, how to coordinate effort, EESSI "road map", focus points for NESSI (ReFrame, automation, monitoring)
 - https://docs.google.com/document/d/1awxIYTIXYj-6LuopRjR1ifj7d2ciNJL9Oj7TdXdqdmM

Application for CZI grant



- "Essential Open Source Software for Science" (Cycle 4)
 - See https://chanzuckerberg.com/eoss
 - Software projects that are essential to biomedical research
- Proposal with University Medical Centre Groningen
 - Focus on rare diseases and supporting biomedical workflows via EESSI
 - "Community Champion" to act as a gateway to community: outreach, usage, tutorials, docs, requirement gathering,...
 - Couple to (funded) developer within EESSI to translate their needs into something actionable, then implement these
- "Not selected to move forward to the full application stage"

Progress update: filesystem layer



- New patch release (0.3.1) to trigger the creation of a moving "latest" release
 - https://github.com/EESSI/filesystem-layer/releases/tag/latest
- PR #83 to make use of new config packages in container definitions and scripts
 - Also adds a workflow to automatically build and publish containers
 - Now using GitHub Container Registry instead of Docker Hub
 - One multi-arch image for x86_64, aarch64, ppc641e, built using QEMU and Docker Buildx
 - Multi-stage Dockerfile to prevent build packages from ending up in client image
- Idea to use S3 storage for (private) Stratum 1 in AWS
 - Allows us to easily use AWS CloudFront as a cache for clients without a local Squid cache
 - Edge locations around the globe
 - Ansible role does not support this
- Still have to fetch and set up the yubikeys (Bob)...
- Bob is working on documentation, see: https://github.com/EESSI/docs/pull/69

CernVM-FS bug found by ComputeCanada



- "Large scale corruption of a frequently used file in CVMFS"
- In-place update of glibc (\$EPREFIX/lib64/libc-2.30.so) caused trouble
- Significant amount of clients got corrupt version of this file!
- CernVM-FS developers working on (non-trivial) fix
- Workaround possible via symlink to avoid actual in-place update
- All details in https://sft.its.cern.ch/jira/browse/CVM-2001

Progress update: compatibility layer



- Test suite rewritten to make use of ReFrame instead of pytest
 - https://github.com/EESSI/compatibility-layer/pull/94
- Automatically build and publish containers for bootstrapping Gentoo Prefix
 - https://github.com/EESSI/compatibility-layer/pull/98
- CI currently broken, due to (once again...) issues with Lua libraries
 - https://github.com/EESSI/compatibility-layer/issues/99
- TODO: Gentoo security updates in 2021.03 for OpenSSL, SQLite, Python...

Progress update: software layer

Software layer

Compatibility layer

Filesystem layer

Host coerating system

- Build script updated for EasyBuild v4.3.4 (see PR #85)
- Arrow, Spark, IPython added (see <u>PR #91</u> + <u>PR #94</u>)
- Qt5 broken for clients with Linux kernel older than 3.17 (see <u>issue #99</u>)
- amd/zen2 in 2021.03 pilot version installed with EasyBuild v4.3.3 (not v4.3.4) (issue #102)
- Work by Alan on creating different "view" via separate module tree
 - Via "eb --module-only", several fixes needed in EasyBuild...
 - See also <u>PR #100</u> + <u>issue #101</u>
- Proposal by Caspar to add Horovod (for testing TensorFlow multi-node)
 - See https://github.com/EESSI/software-layer/pull/104
- Some progress on speeding up installation of R by installing extensions in parallel...
 - See https://github.com/easybuilders/easybuild-easyblocks/pull/2408



EESSI pilot repository

NOT FOR PRODUCTION USE!



TODO: remove 2020.12 pilot version?

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

2021.03 version of pilot software stack

Current status:

Compatibility layer in place for x86_64 + aarch64
 (ppc641e on hold due to Gentoo Prefix bootstrap issue)

- Target CPUs:
 - 0 {aarch64,x86_64}/generic
 - o intel/{haswell,skylake_avx512}, amd/zen2, aarch64/graviton2
- Software: Bioconductor (R), GROMACS, OpenFOAM, TensorFlow, Spark, IPython, ...
- Init script updated
- Docs updated: https://eessi.github.io/docs/pilot
- GPU installations: on hold (cfr. discussion with NVIDIA on CUDA)



Build nodes experience report



2021.03 Haswell stack on NREC (by Axel)

- Followed the build instructions found here:
 - https://eessi.github.io/docs/software_layer/build_nodes
- Need: 50GB disk space
- Local cloud VM only has 20GB on /
- Need extra volume of 50GB attached to VM
- Then environment variables need to be set to bind /tmp in the build container to the attached volume.
 - Opened PR to add these instructions: https://github.com/EESSI/docs/pull/77

Build nodes experience report



2021.03 Skylake stack on Saga (by Thomas)

- very slow (1/5 or so even using a full node with 40 cores)
 - would be great to understand why it was so slow
- attempt to use /dev/shm did not speed up build
- sometimes only few cores were used, sometimes more than 40
- sources for one package DB... weren't available temporarily
- building on compute nodes within batch jobs might benefit from a more incremental procedure or more inbuilt fault tolerance
- would be nice to have some reference values for build times
 - alternatively some progress info (10%, 20%, ... done) could be useful

Testing with ReFrame



- Current status:
 - PR for GROMACS: https://github.com/EESSI/software-layer/pull/65
 - PR for TensorFlow: https://github.com/EESSI/software-layer/pull/106
 - Docs: https://eessi.github.io/docs/software_testing
- Planning brainstorm + hackathon to expand, also with NESSI
 - Agree on test selection (tags, programming environments, modules)
 - Agree on fixed test sizes, max runtimes (#nodes etc)
 - Agree on native vs EESSI-container based tests
 - Shortlist of new tests to be created + hackathon
- Who's in?

Update on sponsorship by Azure/AWS

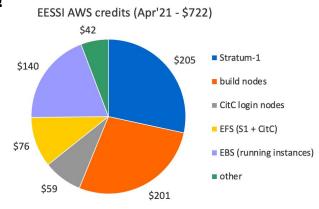




- Sponsored credits (\$25,000) are being put to good use!
- In Mar'21: ~\$722 worth of credits spent on Stratum-1, build nodes, EB testing, ...
- Ask in #aws-resources Slack channel to get access!



- No follow-up meetings planned for now...
- Blog post on CernVM-FS tutorial:



https://techcommunity.microsoft.com/t5/azure-compute/azure-hpc-powers-cernvm-fs-tutorial/ba-p/2261437

AWS infrastructure: status





- Bob has used the script a bit, works well given >1GB of RAM...
- Slack bot interface being worked on, albeit very slowly...
- Route53 up and running, both for infra.eessi-hpc.org and eessi-infra.org
- monitoring.eessi-hpc.org is on its way.
 Zabbix + Grafana for Stratum servers and the wider EESSI infrastructure
- Ask in #aws-resources Slack channel to get access

Focus points in coming weeks/months



- Target architectures: x86 64 and aarch64 (cfr. 2021.03 pilot)
 - o x86 64:intel/{haswell,skylake avx512} + amd/zen2 is sufficient?
 - o aarch64: only generic and graviton2 for now?
 - Can all be tackled via AWS EC2 instances!
 - ppc641e on hold due to Gentoo bootstrap issue + limited interest?
- Software: additional packages can be added if there are interesting use cases
- Primary focus should be on automation, testing, monitoring, documentation, ...