

EESSI meeting

6 Oct 2022

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

Agenda



- 1. Quick introduction by new people
- 2. EESSI-related meetings in last month (incl. EESSI Community Meeting)
- 3. Progress update per EESSI layer (incl. bot for software layer)
- 4. archdetect alternative to archspec
- 5. 2021.12 version of pilot repository + outlook to next pilot version
- 6. AWS/Azure sponsorship update + OCRE funding opportunity
- 7. Update on MultiXscale EU project
- 8. Past & upcoming events
- 9. 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



- Mon-Tue 12-13 Sept: CernVM-FS workshop in Amsterdam
 - See https://indico.cern.ch/event/1079490
 - Attended by Kenneth Hoste & Hugo Meiland
 - Presentation on EESSI by Kenneth Hoste => lots of interesting questions
 - Slides + recording available via https://indico.cern.ch/event/1079490/timetable
 - News about funding (via MultiXscale project) was well received
 - Bug for corruption issue (<u>CVM-2001</u>) should be fixed
 - Fix is fully client-side (no relevant changes to CernVM-FS server)
 - In theory problems may still occur when doing in-place updates of files
 - We should try and verify that the problem is indeed fixed (via glibc in-place update)

EESSI Community Meeting in Amsterdam









- First physical EESSI community meeting since March 2022
- Physical attendees: ~16 (6 outside of NL), remote attendees: ~10
- More info via https://eessi.github.io/docs/meetings/2022-09-amsterdam

EESSI Community Meeting in Amsterdam



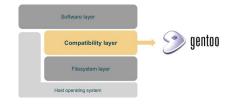
- Introductory sessions on various aspects, incl. hands-on sessions
- More in-depth sessions on different layers, infrastructure, bot, GPU support, testing, ...
- Presentation on the MultiXscale project and the relation to EESSI
- Site reports from NESSI, NLPL, HPCNow, Microsoft Azure
- Discussions on various topics, incl. governance, what could make or break EESSI, etc.
- Hacking sessions on using EESSI, installing EESSI, archdetect, ...
- Slides & recorded talks available: https://eessi.github.io/docs/meetings/2022-09-amsterdam
- Ideas for (location of) next edition are welcome! Maybe in conjunction with EasyBuild User Meeting?

Progress update: filesystem layer



- Fix for CernVM-FS bug (CVM-2001) merged in devel branch in CernVM-FS GitHub repo
 - See <u>PR #3043</u>, changes will be part of next CernVM-FS release
 - Fix is fully client-side, no changes in CernVM-FS server
 - We should try and validate this fix!
- EESSI build/client containers updated to hide extended attributes used by CernVM-FS (PR #125)
 - + update to CernVM-FS v2.9.4
 - Needed to avoid trouble when files are being copied from EESSI (see <u>issue #110</u>)
- Ingest script was updated to support deploying compat layer updates (<u>PR #127</u> + <u>PR #130</u>)
- archspec was added to build container to facilitate CPU detection (PR #129)
- CI workflows for testing Ansible playbooks updated to Ubuntu 22.04 (PR #128)
- Attempt at updating client/build containers to also support RISC-V 64-bit (open PR #132)

Progress update: compatibility layer



- Several security updates required for 2021.06 and 2021.12 compat layers (these were reported by Gentoo's glsa-check tool)
 - Updated for 2021.12 (aarch64/ppc64le/x86_64): libarchive, lxml, vim (+ indirect Python update)
 - Updates performed using script added in <u>PR #155</u>, should be done via Ansible playbook instead?
 - o TODO:
 - 2021.06: expat, glibc, gzip, libarchive, lxml, vim
 - 2021.12: update expat, glibc (?), gzip
- Initial scan with <u>trivy</u> vulnerability scanner showed that it only reports some outdated packages
 - Only reports lxml package being vulnerable in 2021.06 version (doesn't flag glibc, ...)
 - Needs more work...

Progress update: compatibility layer



- Attempt to let software bot build for a new architecture failed (when installing EasyBuild)
 - Lots of testing revealed that update to compatibility layer (5 Sep) likely causes this
- Started trying to build new compatibility layer (working "title" 2022.10)
 - Updated bootstrap-prefix.sh script to latest Gentoo Prefix version (+ EESSI changes)
 - Several issues: can't build gcc-config-2.6 (recent version bump), see <u>bugzilla#875377</u>
 - Needs GCC >= 10 (which we have masked currently)
- We may want to add new tools like direnv (see issue #159)
- Observations/Ideas:
 - Would be nice if building compatibility layer runs completely in container
 - If we had a bot also for the compatibility layer, we could build it "daily" to detect regressions

Progress update: software layer



- Alternative to archspec by Hugo (see <u>PR #187</u>)
 - See separate slides coming up
- Some tweaks may be necessary to script to facilitate implementation of build/deploy bot
 - See overview of changes made by Thomas in PR #184
- <u>Software build script</u> doesn't correctly control EasyBuild version being installed (?)
- GCC provided by EESSI does not (by default) use compat linker (see <u>issue #185</u>)
- Kenneth & Caspar have been trying to find time to make progress on easystack support in EasyBuild... (see PRs #4021 + #4057)

Bot for building + deploying software layer

Compatibility layer

Filesystem layer

Host operating system

- Goal: get procedure good enough to build next pilot release; expecting lots of needed improvements
- Status:
 - o PR #24: monitor build jobs and report result back to PR in software-layer repo
 - More testing and debugging for pilot.eessi-hpc.org(both completed)
 - Starting a new software subdirectory (cascadelake) failed already at building EasyBuild
 - Developed script to resubmit job locally with optional changes; updates PR comment
 - Problem with EESSI pilot is likely due to an update of the compat layer on 5 Sept.
- Next steps:
 - o 1) Get PR#24 merged!
 - o 2) Add collected issues for future improvements
 - o 3) Implement eessi-bot-deploy.sh script that ingests built software into repo: ETA: ~ end of Oct'22
 - o In parallel: use bot to build more packages; analyse failures -> collect needed improvements

archdetect script (alternative to archspec)



- archspec (<u>github.com/archspec</u>) is not sufficient for our purpose
 - Too focused on strict CPU architecture definition instead of 'enough' for binary compatibility
 - Mis-identifying Ampere Altra (in Azure) as AWS Graviton2
 (graviton2 instead of neoverse-n1)
 - Relies on Python in compatibility layer
 - O No capabilities in e.g. GPU identification (for e.g. PR #172) or interconnect identification
- Proposing alternative "archdetect" with pure shell script (PR #187)

```
# determine subdirectory in software layer

if [ -z $EESSI_USE_ARCHDETECT ]; then

# if archdetect is enabled, use internal code

export EESSI_SOFTWARE_SUBDIR=$(${EESSI_INIT_DIR_PATH}/eessi_archdetect.sh cpupath)

echo "archdetect says ${EESSI_SOFTWARE_SUBDIR}" >> $output

else
```

archdetect script (alternative to archspec)



build (x86 64/intel/haswell/archspec-linux-E.

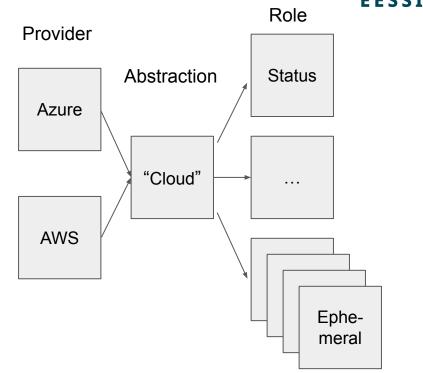
build (x86_64/intel/skylake_avx512/archspec

build (ppc64le/power9le/unknown-power9le)

- Proposing alternative "archdetect" with pure shell script (PR #187)
 - Identify CPU architecture based on minimal required features and align with EESSI tuned binaries
 - Currently tested against 8 cpuinfo examples:
 - -action- Please provide more cpuinfo examples!
 - Extensible to supported CPU architectures (RISC-V?)
 - Extensible to understand more CPU/memory capabilities,
 like L3 cache in Milan and Milan-X, NUMA domains, hierarchical system memory, ...
 - Extensible to identify e.g. GPU architecture / GPU driver / interconnect
 - Next steps discussed in #archdetect channel
 - Activating step 1 (merge PR): add as optional to init scripts
 - Activating step 2: become default script used by init

Infrastructure update: Terraforming EESSI

- Azure and AWS have different approaches
- Can we abstract away such differences?
- Kinda. Maybe. Sort of.
- Terraform isn't very agreeable
- Conditional creation is fine
- Conditional module output is harder
- The end problem is consuming the roles



Infrastructure update: The problem, part 1

Jį W

- Defining the modules
- Calling the right one
- Ignoring the other(s?)

```
modules > cloud > ¥ main.tf > ⟨ module "aws_version" > □ type
      module "aws_version" {
          source = "../aws/"
          count = var.cloud provider == "aws" ? var.node count : 0
          size = var.size
          type = var type
          hostname = var.hostname
          placement = var.placement
           security_group = local.security_group
      module "azure_version" {
          source = "../azure/"
          count = var.cloud_provider == "azure" ? var.node_count : 0
          size = var.size
          type = var.type
          hostname = var hostname
          placement = var.placement
           security_group = local.security_group
```

Infrastructure update: The problem, part 2



- We need output so we can tell callers (users) what the IPs and ssh keys created are...
- How do we get the address from the created module?
- Non-created modules are empty, so we can't "dot" into them...

EESSI pilot repository

NOT FOR PRODUCTION USE!



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

- 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 / ppc641e / x86_64
 - Security updates for a handful of packages were installed (ingested on 8 Sept'22)
 - 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. ppc641e), WRF
 - Targets: aarch64/generic, aarch64/graviton2, aarch64/graviton3, ppc64le/generic (partial!), ppc64le/power9le (partial!), x86_64/generic, x86_64/amd/zen2, x86_64/amd/zen3 (Milan), x86_64/intel/haswell, x86_64/intel/skylake_avx512
 - o 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?

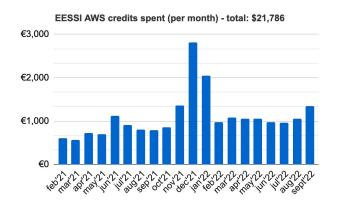


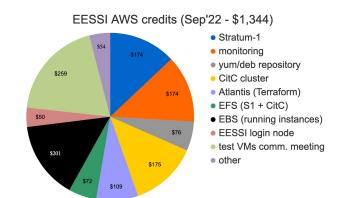
- Small changes to compatibility layer: updated Lmod, more tools, ...
- Include enhancements/changes that are necessary for CUDA GPU support
- Work towards getting rid of ugly install script, aim for easystack-only
- Only add software installations via bot, no more manual deployments!
- Initially include same software installations in software layer, then gradually expand
- Also install software with more recent toolchains + more applications
- Stop wasting time with supporting POWER (ppc641e), not used broadly enough
- Alpha/beta for production EESSI repository
- Switch to eessi.io domain + new Stratum 0 (dedicated hardware, yubikey)

Usage of sponsored AWS credits

aws

- 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
- ~\$6,495 worth of sponsored credits left (should be sufficient until Mar'23 at current spending rate)
- Shared document with outline of how sponsored credits can be leveraged was shared with AWS
- In Sept '22: ~\$1,344 worth of credits spent on Stratum-1, monitoring, CitC cluster, test VMs, ...
- ~\$21,786 worth of credits spent in total so far (since Feb'21), all covered by sponsored credits



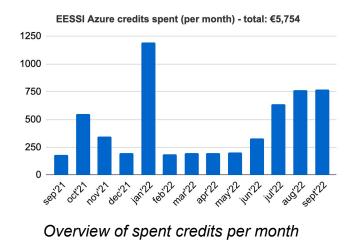


Azure sponsorship





- Sponsored credits (€40,000) are being put to good use!
- Ask in #azure-resources Slack channel to get access!
- In Sept'22: ~€768 worth of credits spent: Stratum-1 + VM for GSoC RISC-V project + GH Runners
- ~€5,754 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)





[Kenneth]

EU project: MultiXscale







- MultiXscale 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 working through red tape towards grant agreement
- Expected 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: BioHackathon Europe 2022

EESSI

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- Near Paris (7-11 Nov'22)
- Our project proposal is accepted:
 "Make your own or favourite software available on your cluster with EasyBuild/EESSI"
- Registration is open
 - All on-site seats taken for now (but there's a waiting list)
 - Remote participation also possible
- Biology-oriented hackathon but potentially a good place to:
 - Reach new users and developers
 - Meet Galaxy users and community
- More information via https://easybuild.io/biohackathon-eu-2022.html