

EESSI meeting

3 Nov 2022

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

Agenda



- 1. Quick introduction by new people
- 2. EESSI-related meetings 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. Past & upcoming events
- 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



- CernVM-FS coordination meeting (10 Oct)
 - CernVM-FS 2.10.0 is tagged, call for testing (especially client side)
 - Includes fix for corruption bug (<u>CVM-2001</u>)
- EESSI/Azure/SURF sync meeting (28 Oct)
 - Recent developments discussed, incl. MultiXscale EuroHPC project & OCRE
 - Is anyone planning to attend SC'22 in Dallas (13-18 Nov'22)?
- EESSI/AWS sync meeting (31 Oct)
 - No action taken yet by AWS on additional batch of sponsored credits
 - Will to keep sponsoring EESSI still very much there, will be followed up
 - Additional expertise will be pulled into next meeting w.r.t. EFA support in EESSI
- Various calls to coordinate effort on MultiXscale project

Next EESSI hackathon + community meeting?



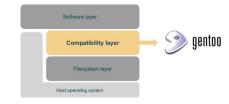
- EESSI hackathon before end of the year?
 - Week of 19-23 Dec'22?
 - Focused effort on build-and-deploy bot, GPU support, next EESSI pilot version, ...
- Next EESSI community meeting?
 - Coincide with EasyBuild User Meeting (likely to take place in spring 2023)?
 - Coincide with a MultiXscale meeting/event?
 - Jörg has been polling for interest for an EESSI meeting @ London

Progress update: filesystem layer



- Fix for corruption issue for files that are changed in-place is included with CernVM-FS 2.10.0
 - Clients that have a library open (glibc, ...) see mix of old/new chunks if library was updated
 - See <u>CVM-2001</u> for more details
 - CernVM-FS 2.10.0 release is there, but not announced yet?
 - We should verify that a glibc update doesn't cause trouble anymore for active clients...
- Old and outdated container images in eessi organisation on Docker Hub were removed (see compat layer issue #129)

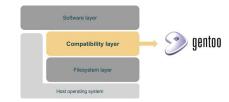
Progress update: compatibility layer (1/2)



- Several security updates (still) required for 2021.06 and 2021.12 versions (these were reported by Gentoo's glsa-check tool)
 - o 2021.06: expat, glibc, gzip, libarchive, lxml, vim, libgcrypt, libxml2, openssl, sqlite, zlib, libksba
 - o 2021.12: update expat, glibc, gzip, libgcrypt, libxml2, openssl, sqlite, zlib, libksba

- Script (<u>see PR #155</u>) to install security updates should be replaced by tasks in Ansible playbook
 - We should explore this while installing the additional security updates?

Progress update: compatibility layer (2/2)



Ongoing effort to build new version of compat layer (2022.11?)

- Done:
 - Update Gentoo Prefix bootstrap script, fix problems that occur during build of compat layer (EESSI/compatibility-layer PR #160)
 - Updated package sets for 2022.11 in <u>EESSI/gentoo-overlayPR #84</u>
 - Incl. update version-fixed packages to latest version (Lmod, ReFrame, archspec, opa-psm2)
 - Fix failing tests for Lmod (see also <u>Lmod issue #611</u>)

TODO:

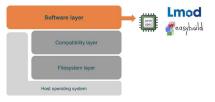
- Also test on ppc641e, to see if we can keep ppc64le support with minimal effort for now
- Install additional packages: htop, rpm, libnss, direnv
- Remove ReFrame from compat layer, only install as module in software layer?

Progress update: software layer (1/2)



- Security updates in 2021.12 compat layer caused trouble in software layer
 - Update of setuptools broke installation of EasyBuild with EasyBuild
 - Underlying cause: we were still using setup.py installrather than pip install...
 - Fixed in updated EasyBuildMetaeasyblock included with EasyBuild v4.6.2 (see issue #191)
- Not setting \$LD_LIBRARY_PATH breaks some corner cases (see <u>issue #192</u>)
 - Example: dynamic loading of libraries in Python via cdll.LoadLibrary
 - See <u>upstream issue #65241</u>
 - Fixed by ComputeCanada by patching Python's built-in ctypes library (see here)
- archdetect pure bash alternative to archspec (PR #187)
 - Requires that symlinks are added for aarch64/arm/neoverse-v1in 2021.12
 - Should be included in init/ dir of 2021.12 version of EESSI pilot

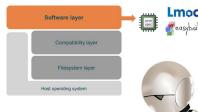
Progress update: software layer (2/2)



- Progress on enhancing (experimental) support for easystack files in EasyBuild
 - Easystack files can now specify custom configuration options for specific easyconfigs
 - Custom options are parsed but ignored in EasyBuild v4.6.2
 - EasyBuild framework <u>PR #4057</u> to actually apply these options is ready to merge
 - Also drops support for "software" key in easystack file
 - Preference goes to specifying installations via easyconfig filename
 - PR will be merged when companion PR #832 for docs is ready to merge...
 - Example (YAML format):

```
easyconfigs:
 - binutils-2.25-GCCcore-4.9.3:
       options: {
           'debug': True,
           'from-pr': 12345,
       }
```

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



Progress on implementation of build-and-deploy bot

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

- PR #24 was finally merged (7 Oct): complete implementation of build phase of bot
 - Two parts: event handler (GitHub App) + job manager (for loop)
 - o In use across 6 clusters, building for 11 targets (1+7 x86_64, 1+2 aarch64)
- Proof-of-concept implementation of deploy phase of bot (<u>PR #49</u>)
 - Upload script works with AWS S3 and Minio S3 buckets (config setting)
 - o O(100) ingests done
 - Added some metadata to enable auto ingest script (running on S0) to update PR comments
 - WIP because code refactoring work by Hafsa should be reused (see next two slides)

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



Progress on implementation of build-and-deploy bot

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

- Created new <u>issues</u> for code cleanup such as <u>#51</u> to separate bot code from runtime environment
- Merged <u>PRs</u>:
 - PR #36: Refactor build_easystack_from_printo smaller functions
 - PR #37: Rename eessi_bot_software_layerto eessi_bot_event_handler
 - PR #35: Hardcode holding of jobs bug
 - PR #55: Set up CI workflow for running test suite + add trivial test for mkdir function
- Work in progress: PR #56: add run_cmd method and unit testing (to fix issue #44)
- Next Steps:
 - Get <u>PR #56</u> merged
 - <u>Issue #33</u>: Job manager crashes when it encounters a non-bot job bug
 - <u>Issue #53</u>: More refactoring/renaming in tasks/build.py

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



Example of the bot doing the build phase for a PR (see here):

Oct 26 14:21:29 UTC

Oct 26 14:29:40 UTC

2022

2022

released

finished

add CaDiCaL v1.3.0 with GCC/9.3.0 #16 <> Code -Hafsa-Naeem wants to merge 1 commit into Hafsa-Naeem:main from EESSI:add-CaDiCaL-9.3.0 [다 Conversation 2 +11 -0 -o- Commits 1 F. Checks 0 + Files changed 2 Hafsa-Naeem commented 8 days ago Owner 🕤 ··· Reviewers 193 No reviews No description provided. Assignees 193 add CaDiCaL v1.3.0 with GCC/9.3.0 Verified dc60643 No one-assign yourself Pafsa-Naeem added the bottbuild label 8 days ago Labels (6) bot:build eessi-bot-app bot commented 8 days ago • edited -⊕ … 193 **Projects** Job 2661 on My-eessi-bot-app for x86_64-generic injob dir /mnt/shared/home/hafsa/jobs/2022.10/pr_16/2661 None yet job (6) Milestone date comment status No milestone Oct 26 14:17:42 UTC iob waits for release by iob manager submitted 2022

SUCCESS tarball eessi-2021.12-software-linux-x86 64-generic-

job awaits launch by Slurm scheduler

1666794527.tar.gz (0.001 GiB) in job dir

Notifications

open/close state

2 participants

💬 🦱

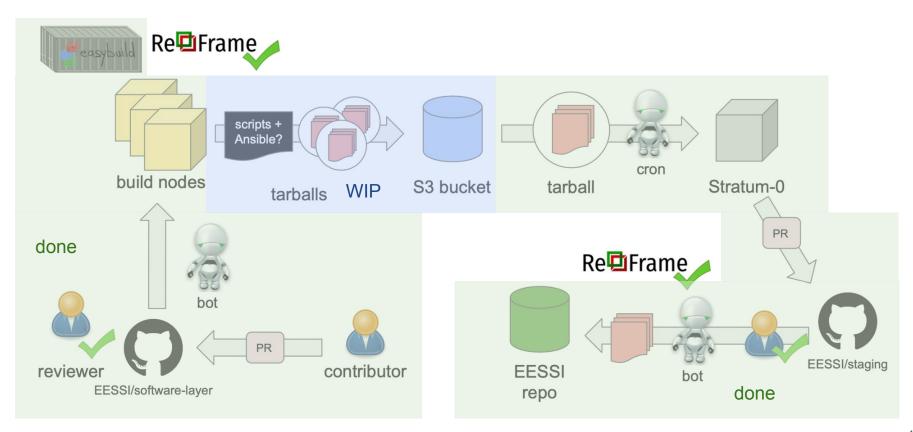
Unsubscribe

You're receiving notifications because you modified the

[Hafsa, Thomas, Kenneth]

Customize

Bot for building + deploying software layer: goal



Progress update: Infrastructure



Terraform woes:

- No native way to abstract away providers in modules
- No native way to abstract away regions/locations in modules
- So, one will have to specify each provider and each region/location explicitly for each resource
- Looking to make something work for ephemeral nodes, where you have to pick provider (Azure/AWS), and regions are locked.



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 / ppc64le / x86_64
 - Security updates for a handful of packages were installed (ingested on 8 Sept'22) more are 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. 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?

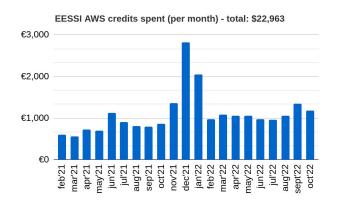


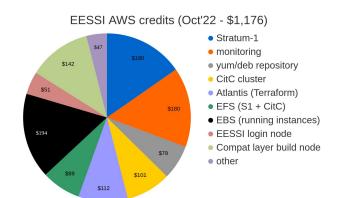
- Small changes to compatibility layer: updated Lmod, more tools, ...
- Include enhancements/changes that are necessary for CUDA GPU support
- Work towards getting rid of ugly install script, aim for easystack-only
- Only add software installations via bot, no more manual deployments!
- Initially include 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



- 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
- ~\$5,319 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 Oct '22: ~\$1,176 worth of credits spent on Stratum-1, monitoring, CitC cluster, test VMs, ...
- ~\$22,963 worth of credits spent in total so far (since Feb'21), all covered by sponsored credits



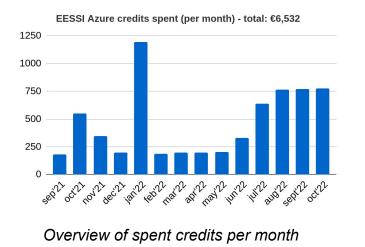


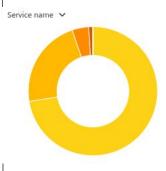
Azure sponsorship





- Sponsored credits (€40,000) are being put to good use!
- Ask in #azure-resources Slack channel to get access!
- In Oct'22: ~€777 worth of credits spent: Stratum-1 + VM for GSoC RISC-V project + GH Runners
- ~€6,532 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)









Oct'22

EU project: MultiXscale







- 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 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

Near Paris (7-11 Nov'22)

- {**B**其**H**}
- 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
- Project #16:
 - "Make your own or favourite software available on your cluster with EasyBuild/EESSI"
- Only a small number of people selected our project, but this is still subject to change...
- Sébastien Moretti will prepare a quick demo on EESSI to showcase during the event
- Accounts at CitC AWS cluster can be provided