

# **EESSI** meeting

June 3rd 2021

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

# Agenda

EESSI

STORY OF STANKE NOTALATORS

- Quick introduction by new people
- 2. EESSI-related meetings in last month [Bob, Kenneth]
- 3. Progress update per EESSI layer [Bob, Peter, Kenneth]
- 4. 2021.03 version of pilot repository: status [Kenneth]
- Outlook to next pilot version [Kenneth]
- 6. Testing with ReFrame [Caspar]
- AWS/Azure update + infrastructure in AWS [Kenneth, Terje]
- 8. EESSI paper [Thomas, Kenneth]
- 9. NESSI update [Thomas]
- 10. Upcoming events [Kenneth]
- 11. Q&A

# Quick introduction by new people



#### New people on the call: feel free to introduce yourself!

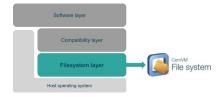
- Who are you, where do you work, on what?
- Why are you interested in the EESSI project?
- Are you planning to actively contribute,
   and if so, to which aspect(s) of the project?

#### **EESSI-related meetings**



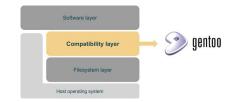
- May 11th: Monthly CernVM-FS coordination meeting (Bob, Kenneth)
  - Mostly about adding user code to repositories (using containers)
  - Discussion about the in-place updates corruption issue
    - Tricky to change this part of the code, will not be fixed anytime soon...
    - In-place updates are discouraged: will also be highlighted in the docs
    - Workaround: use symlinks to avoid in-place updates of files...
- May 19th: Chat with Stefano Angioni Univ. of Bath, UK (Kenneth, via MS Azure)
- May 19th, May 26th, May 28th: EESSI paper meetings (Alan & co)
- June 1st: Chat with Wageningen University & Research (Jaco, Bob, Kenneth)
- June 2nd: Discuss application of ReFrame library tests (Caspar)
  - See "Testing with ReFrame" slide

### Progress update: filesystem layer



- Stratum 1 @ RUG is currently down due to maintenance in OpenStack platform
  - But doesn't affect availability of EESSI pilot repository thanks to Stratum 1 at UiO
  - Highlights the need for monitoring of our CernVM-FS network...
- Small updates to the PR for automatically building the client container images
  - See <a href="https://github.com/EESSI/filesystem-layer/pull/83">https://github.com/EESSI/filesystem-layer/pull/83</a>
  - Also includes fuse-overlayfs
- 2020.12 pilot version was removed from the repository

### Progress update: compatibility layer



- Various security updates were installed for EESSI pilot 2021.03
  - Only relevant ones were for misc/curl and x11-libs/libX11
  - Updates are currently applied best effort by Bob
  - Process is currently very slow (emerge --sync takes hours)
- Initial version of a GitHub Action that automatically reports about Gentoo security
  - vulnerabilities (by using Gentoo's glsa-check tool)
    - Reports to private subchannel in EESSI Slack
    - Can be run as a daily cron job
    - Also reports how to fix the issue
    - Issues in the screenshot still need to be fixed :-)



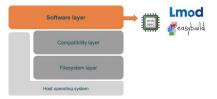


#### Progress update: software layer



- New software added to EESSI pilot 2021.03:
  - Horovod 0.21.3
  - GROMACS 2020.4
  - QuantumESPRESSO 6.6
- PR for a script that facilitates creating the tarball containing software to be ingested
  - See <a href="https://github.com/EESSI/software-layer/pull/111">https://github.com/EESSI/software-layer/pull/111</a>
  - First step in automating process of getting software installs from build node to Stratum 0
- Meeting with NVIDIA w.r.t. including CUDA happening soon (hopefully) ...
- EasyBuild 4.4.0 release \o/

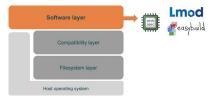
#### EasyBuild 4.4.0: what's relevant for EESSI



- Support for checking for unwanted linking to libraries by registering "banned" libraries
  - Allows for checking for accidental linking to OS libraries from build host
  - o Can also check for linking with required libraries via same mechanism (libc.so in compat layer?)
- Support for --sanity-check-only (easy smoke testing of existing software installations)
  - Should be doable to leverage this via ReFrame by using EasyBuild as a library...
- foss/2021a toolchain with FlexiBLAS to allow runtime switching to different BLAS/LAPACK libraries
- Support updating of specific build options after initializing the EasyBuild configuration
- Fixes for eb --module-only relevant to create other/custom "views" on the provided software
- Support for prepending custom library paths in RPATH section via --rpath-override-dirs
- Support for using EasyBuild on a system with more than 1,024 cores:)

[Kenneth]

#### EasyBuild 4.4.0: TODOs related to EESSI



- Patching of CMake to make it aware of compatibility layer
   <a href="https://github.com/easybuilders/easybuild-easyblocks/pull/2248">https://github.com/easybuilders/easybuild-easyblocks/pull/2248</a>
- Make CMakeMake generic easyblock aware of --sysroot configuration option <a href="https://github.com/easybuilders/easybuild-easyblocks/pull/2247">https://github.com/easybuilders/easybuild-easyblocks/pull/2247</a>
- correctly determine path to active binutils in TensorFlow easyblock
   <a href="https://github.com/easybuilders/easybuild-easyblocks/pull/2218">https://github.com/easybuilders/easybuild-easyblocks/pull/2218</a>
- Failing numpy tests on aarch64 (bug in OpenBLAS?)
   <a href="https://github.com/easybuilders/easybuild-easyconfigs/issues/11959">https://github.com/easybuilders/easybuild-easyconfigs/issues/11959</a>
- Broken installation of TensorFlow 2.4.1 with foss/2020b on aarch64 <a href="https://github.com/easybuilders/easybuild-easyconfigs/pull/12667">https://github.com/easybuilders/easybuild-easyconfigs/pull/12667</a>
- Better support for easystack files...

## **EESSI** pilot repository

# NOT FOR PRODUCTION USE!



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

#### 2021.03 version of pilot software stack

#### Current status:

2020.12 pilot version was removed!

- 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,
   Horovod, QuantumESPRESSO, ...
- Demo scripts (incl. Script to do native installation of CernVM-FS): <a href="https://github.com/EESSI/eessi-demo">https://github.com/EESSI/eessi-demo</a>
- GPU installations: on hold (cfr. discussion with NVIDIA on CUDA)



### **EESSI** pilot repository

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

Next pilot version: 2021.06?

#### Goals:

- Linux only, same CPU targets, same software applications
- Use new container image for build nodes
- Software installations with more recent compiler toolchain?
- Look into automating ingestion of software installations from build node to Stratum 0 via S3 bucket
- Also run smoke tests on node different from build node? (eb --sanity-check-only)
- Look into GPU builds of GROMACS, TensorFlow
   (once discussion with NVIDIA w.r.t. CUDA has been settled)
- We need helping hands to tackle small parts of this!

#### Testing with ReFrame



#### Discussed ReFrame 'library tests'

- Separate tests into test-specific (in library test) and system specific (derives from library test) parts. E.g.
  - Sanity pattern = test specific
  - Number of tasks per node = system specific
- Library test != turn-key test suite, but EESSI requires turn-key test suite...
   We will need to implement the 'system-specific' part too, but 'generically'.
  - EESSI goal: limit all system-specific things to ReFrame config
  - E.g. set number of tasks per node based on num\_cpus in ReFrame config

## Testing with ReFrame



Discussed ReFrame 'library tests'

We plan to adopt this structure.

Benefits for EESSI:

- Provides structure in designing tests
- Library test (also) maintained by ReFrame community
- Practical: will initially develop in EESSI software-layer GitHub (or in separate repo?)
   Keep library tests and derived tests.
  - Library tests: in e.g. tests/ReFrame/libtests/...
  - Derived tests: in e.g. tests/ReFrame/eessi/...
  - Future: libtest will be moved/PR-ed to ReFrame (or separate) repo.



#### Update on sponsorship by Azure/AWS

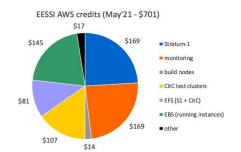




- Sponsored credits (\$25,000) are being put to good use!
- Ask in #aws-resources Slack channel to get access!
- In May'21: ~\$701 worth of credits spent on Stratum-1, monitoring node, EB testing, ...
- ~\$2600 spent in total







- Ball is rolling!
- Azure is actively looking into if/how they can sponsor EESSI (via SURF RUG)
- Probably more news about this soon...

#### AWS infrastructure: status





- Monitoring server up and running
  - Idea is to use Prometheus to monitor services/machines
  - First step: monitor the Stratum 0/1 servers using custom Prometheus metrics
- S3 bucket for software and compatibility layer up and running
  - Publicly readable, writable for EESSI AWS accounts and from infra nodes
  - eessi-upload-to-staging eessi-2021.03-software-linux-zen2-1622000000.tar.gz

#### EESSI paper



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

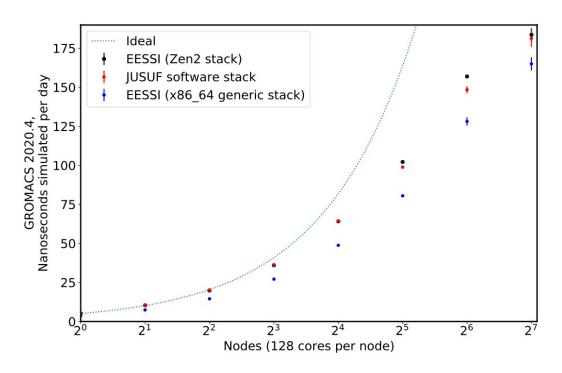
**Submitted** to special issue *New Trends in High Performance Computing: Software Systems and Applications* in Software: Practice and Experience<sup>1</sup>

- Aim to have a publication which we can cite: presentations, project proposals, ...
- Covering what works in the pilot (layers), discussing use cases, performance evaluation, ideas on testing and future work
- Authors: Bob, Victor, Kenneth, Alan, Caspar, Thomas
  - Thanks to Adam for proofreading!
- If you're interested in reading the paper, contact Thomas (thomas.roblitz@uib.no)

https://onlinelibrary.wiley.com/pb-assets/assets/page/journal/1097024x/SPE-SI-HPC-1607014410373.pdf

#### EESSI paper - GROMACS performance





Large-scale (up to 16k cores) performance test with GROMACS on JUSUF @ JSC **EESSI** is competitive with system installation of GROMACS!

#### **NESSI** update from Norway



- EESSI pilot available via native CernVM-FS on HPC cluster Saga in Norway
  - CentOS 7.9, Intel Skylake, ~ 16k cores, Infiniband
  - Next cluster: Fram (Broadwell, ~ 32k cores)
- Work in progress: module to make EESSI accessible
- Work in progress: monitoring instance
- Work in progress: automation of build & ingest procedure
- Starting work on risk analysis & mitigation measures
- Starting work on building packages on top of EESSI

#### Upcoming events



- Half-day EasyBuild tutorial at ISC'21
  - Kenneth (HPC-UGent), Alan (JSC), Maxime (Compute Canada)
  - Fri June 25th 2021, 2pm 6pm CEST
  - https://www.isc-hpc.com/tutorials-2021.html
  - If you're attending ISC'21, please join us!
  - Session will be recorded and available publicly shortly afterwards...
- AWS Arm-HPC hackathon (not directly related to EESSI, yet...)
  - Virtual, week of July 12-16 2021
  - An Apple M1 Macbook per team member for the winning team!
  - Using Spack + ReFrame
  - https://aws.amazon.com/blogs/hpc/aws-arm-hpc-hackathon-2021