EESSI

EUROPEAN ENVIRONMENT FOR
SCIENTIFIC SOFTWARE INSTALLATIONS

7 Nov 2024

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

Agenda

- Quick introduction by new people

- Progress update per EESSI layer

- Update on EESSI production repository `software.eessi.io`

- Modulefile for initializing the EESSI stack

- Update on EESSI documentation + test suite + build-and-deploy bot

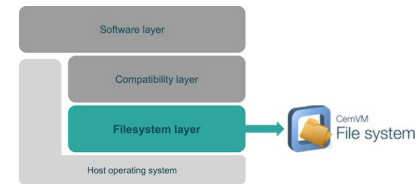- AWS/Azure sponsorship update

- Upcoming/recent events

- Q&A

Quick introduction by new people

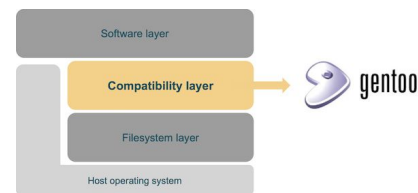**New people on the call: feel free to introduce yourself!**

- ○ 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?

Progress update: filesystem layer

- Client container was updated to RHEL8 (PR #199)

[Bob, Kenneth]

Progress update: compatibility layer

- No significant updates

- Discussion / ideas for compatibility layer of next EESSI version:

  https://gitlab.com/eessi/support/-/issues/56

  - Installation of `foss/2024a` requires this new version,

    as it needs OpenSSL 3 in the compatibility layer

    (see https://github.com/EESSI/software-layer/pull/685)

 - Probably makes sense to wait until EasyBuild 5.0 is released?

[Bob, Kenneth, Thomas, …]

Progress update: software layer (1/3)
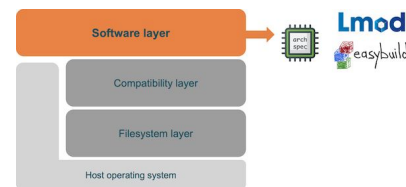
Highlights of recently merged PRs:

- Additional software: EasyBuild 4.9.3 & 4.9.4 (PR #703 & PR #740), bio-packages (PR #706), ReFrame 4.6.2 (PR #708), GROMACS 2024.3 (PR #709), LAMMPS 29Aug2023 (PR #725), waLBerla 6.1 (PR #779)

- Additional software zen4: LAMMPS 2Aug2023 (PR #705), JupyterNotebook 7.0.2 (PR #713), PyOpenGL 3.1.7 (PR #751), SAMtools 1.18 (PR #757), OSU-Micro-Benchmarks 7.1-1 (PR #759)

- Additional software A64FX: LAMMPS 2Aug2023 (PR #707), ESPResSo 4.2.2 + pyMBE 0.8.0 (PR #782), SciPy-bundle 2023.11 (PR #776)

- Many PRs on GPU support (see dedicated slide)

- PRs on support for dev.eessi.io (see dedicated slide)

[Kenneth, Thomas, Richard, Pedro, Bob, Lara, Caspar, Satish, Xin, Alan, …]

Progress update: software layer (2/3, GPU)
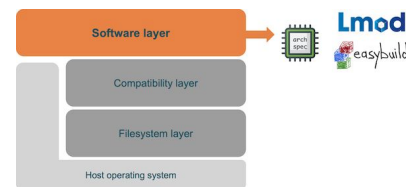
Recent active open PRs + issues for GPU support:

- Redesign of approach

    - `/cvmfs/…/2023.06/software/linux/x86_64/amd/zen3/accel/nvidia/cc80/`

    - Only zen2 (AMD Rome) + cc80 (NVIDIA A100) supported for now

- Accelerator detection added to archdetect ([PR #767](#))

- End-user support added for bash script ([PR #767](#)) and EESSI module ([PR #781](#))

- Initial software added

    - cuDNN ([PR #772](#)), ESPResSo ([PR #748](#)), LAMMPS ([PR #711](#)), *waLBerla ([PR #780](#))*

    - Rebuilds of previous packages

- Logistics of testing GPU builds a concern (due to cost and complexity)

- No sanity check to confirm compute capability ([issue #92](#))

[Kenneth, Thomas, Richard, Pedro, Bob, Lara, Caspar, Satish, Xin, Alan, …]

Progress update: software layer (3/3)
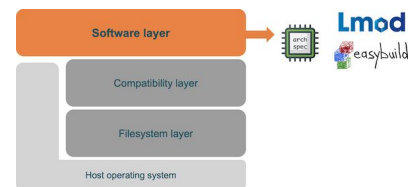
Highlights and PRs on dev.eessi.io:

- Separate CVMFS repository with development builds, already accessible and with deployed software

- Example repository with first installations:

  - ESPResSo dev build (PR #1)

  - LAMMPS small build with OBMD (PR #6)

- Software-layer PRs for dev.eessi.io:

  - Tweak installation scripts to support dev.eessi.io installations (PR #771)

  - [WIP] Ensure installations land in project subdirectories (PR #804)

- Currently only for AMD Rome (zen2)

- See also docs PR #321

[Kenneth, Thomas, Richard, Pedro, Bob, Lara, Caspar, Satish, Xin, Alan, …]

EESSI production repository
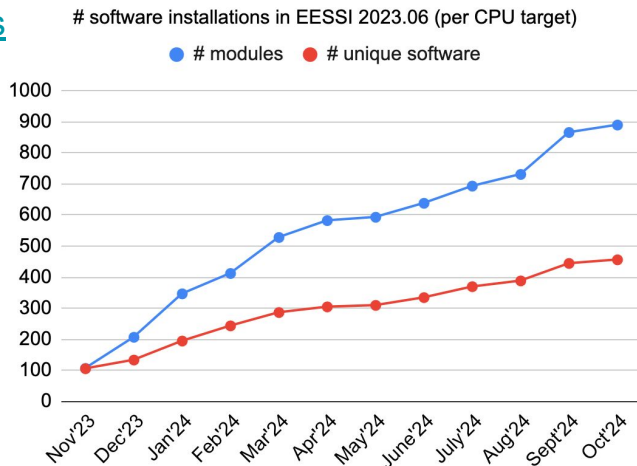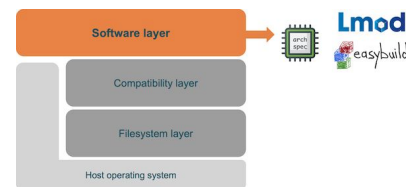
`software.eessi.io` is the **production-ready EESSI repository**

Version 2023.06 is being populated with software via PRs to software-layer repo + build-and-deploy bot

- 8 supported CPU targets: see eessi.io/docs/software_layer/cpu_targets

- 3 more CPU targets being added: `zen4, a64fx, (sapphirerapids)`

- Initial support for NVIDIA GPUs is in place, see eessi.io/docs/gpu

- **Currently: 890 software installations per CPU target**
  (+159 in Sept+Oct'24)

    - 456 different software projects (+68),
      8,066 software installations (across 8+2 CPU targets, +1,561)

- Current focus:

    - Providing optimized software installations for AMD Genoa (Zen4) + A64FX (+ Intel Sapphire Rapids)

    - Adding more (CUDA) software, processing incoming contributions, fixing broken builds/test suites, …

\# software installations in EESSI 2023.06 (per CPU target)
● # modules ● # unique software

[Kenneth, Bob, Alan, Caspar, Lara, Thomas, Richard, Pedro, Xin, …]
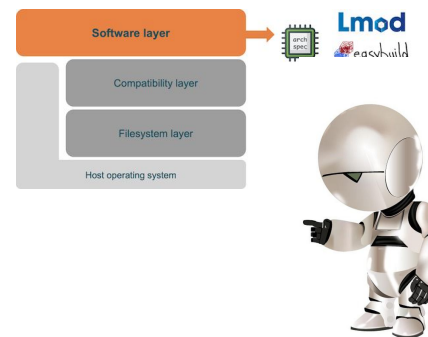
Modulefile for initializing the EESSI stack

- New method for initializing the EESSI stack via a Lua module file

- Now available in `/cvmfs/software.eessi.io/init/modules`

- In some sense better than init/bash script, since it's reversible (via `module unload`)

- If you already have Lmod, you can simply do:

  ```
  module use /cvmfs/software.eessi.io/init/modules
  module load EESSI/2023.06
  ```

- **Please give it a try, and report any issues**

- eessi.io/docs/using_eessi/setting_up_environment/#loading-an-eessi-environment-module

[Kenneth, Thomas, Richard, Pedro, Bob, Lara, Caspar, Satish, Xin, Alan, …]

Bot for building + deploying software layer

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

- September-October'24

  - allow customizing Slurm submit options PR#277 (community contrib)

  - use github API for downloading the diff PR#278

  - add docs on private repos PR#279

  - add accelerator value to job cfg and extend PR comment PR#280 & PR#282

  - release v0.6.0

- Ongoing work

  - Installing bot on clusters with support for GPUs

  - Improve deployment (ingestion efficiency, single approval PR, flexible tasks)

- Side note: over 27,000 Slurm jobs have been submitted on AWS Slurm cluster (bot + test suite)

[Thomas, Bob, Kenneth, Lara, Pedro]

EESSI documentation

eessi.io/docs - GitHub repo github.com/EESSI/docs

Improvements to the EESSI documentation: ~24 merged PRs (+ 30 updates to software overview)

- Blog post about EuroHPC User Day 2024 (PR #332)

- Blog post on using EESSI in CI (PR #323)

- Blog post on EESSI being nominated for HPCwire Readers' Choice Awards 2024 (PR #293)

- Updates on documentation on how to use EESSI (PR #317)

- Updates on how to build on top of EESSI to use EESSI-extend (PR #316)

- Slides for EESSI CASTIEL2 NCC Ambassador workshop (PR #307)

- Use a time template in module documentation generation (PR #256 + PR #258)

- Page with overview on systems on which EESSI is available natively (PR #303 + PR #308+ PR #309 + PR #311 + PR #312 + PR #315)

[Lara, Pedro, Helena, Bob, Xin, Kenneth, Caspar…]
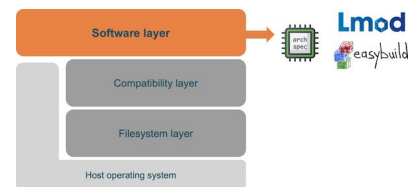
EESSI documentation

eessi.io/docs - GitHub repo github.com/EESSI/docs

- Auto-updates to overview of available software: eessi.io/docs/available_software/overview

- New section with overview of systems where EESSI is known to be available already:

  eessi.io/docs/systems

- Additional blog posts: eessi.io/docs/blog

[Lara, Pedro, Helena, Bob, Xin, Kenneth, Caspar…]

EESSI test suite

eessi.io/docs/test-suite - github.com/EESSI/test-suite

Test suite v0.4.0 release

- Lammps, PyTorch, CP2K

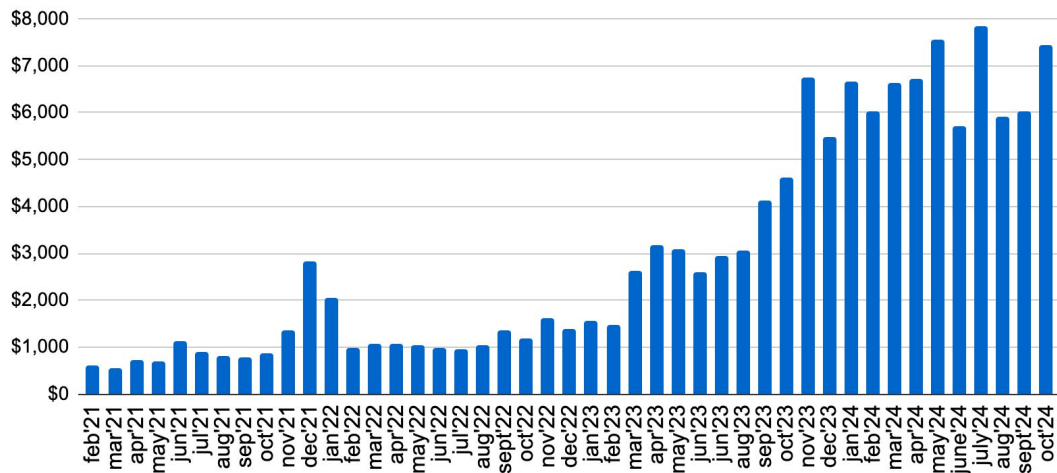- Various bug fixes & other updates, full release notes here

Post-release merges

- eessi_mixin class: facilitate easier creation of portable test (PR #177)
  - Nearly every test in EESSI test suite should inherit from this (except special cases)
  - Provides feedback if child classes are missing information
- MetallWalls (PR #164)

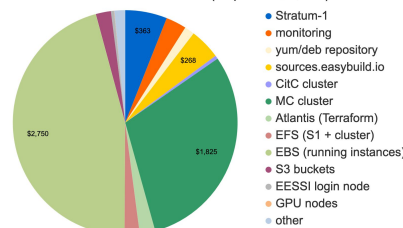[Caspar, Sam, Satish, Kenneth, Lara]

Sponsored AWS credits

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

- ~$6,016 + $7,441 "spent" in Sept'24 + Oct'24 on Stratum-1 servers, monitoring, demos, sources.easybuild.io, debugging (build) issues, Slurm clusters (build bot), testing on GPU nodes, …

- **Bulk of consumed credits due to EESSI build-and-deploy bot**

- Regular sync meetings with AWS - **more sponsored credits have been provided for coming months**

EESSI AWS credits spent (per month)

EESSI AWS credits (Sept'24 - $6,016)

Legend: Stratum-1, monitoring, yum/deb repository, sources.easybuild.io, CitC cluster, MC cluster, Atlantis (Terraform), EFS (S1 + cluster), EBS (running instances), S3 buckets, EESSI login node, GPU nodes, other

$363, $268, $1,825, $2,750

EESSI AWS credits (Oct'24 - $7,441)

Legend: Stratum-1, monitoring, yum/deb repository, sources.easybuild.io, CitC cluster, MC cluster, Atlantis (Terraform), EFS (S1 + cluster), EBS (running instances), S3 buckets, EESSI login node, GPU nodes, other

$375, $3,294, $2,776

[Kenneth, Bob]
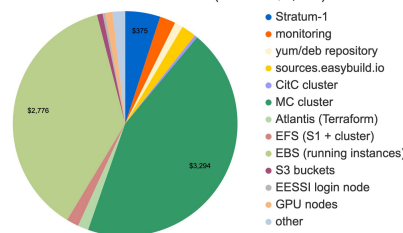
Sponsored Azure credits

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

- In Sept+Oct'24: €5,230+€3,811 worth of credits spent

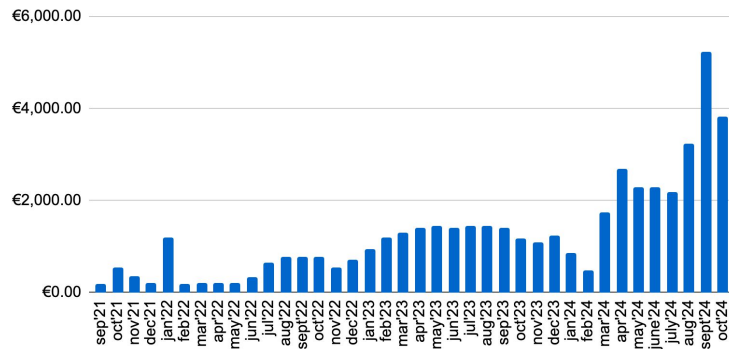- Used for: **Slurm cluster for bot (Zen4)**, Stratum-1 mirror servers, GitHub Runners, GPU nodes, …

- Ongoing discussions to extend sponsored credits into 2025

EESSI Azure credits spent (per month)

Resource group name ∨

azure-almalinux93-2...	€3,263.38
azure-almalinux93-2...	€1,375.90
stratum1-us-east	€210.28
eessi.io-stratum1-us-...	€201.70
gh-runner-eu-west	€178.27

Sept'24 (€5,230)

Resource group name ∨

azure-almalinux93-2...	€1,869.63
azure-almalinux93-2...	€1,397.02
stratum1-us-east	€215.18
eessi.io-stratum1-us-...	€206.69
gh-runner-eu-west	€122.87

Oct'24 (€3,811)

[Kenneth, Bob]

CernVM workshop

- 16-18 Sept 2024 at CERN (Geneva, Switzerland)

- https://indico.cern.ch/event/1347727

- Presentation by Thomas: *CernVM-FS makes software EESSI to use*

  - Slides available here

- General interest in EESSI:

  - EESSI being added to EGI

  - Some LHC experiments building software for aarch64 and riscv64 (experimental)

  - Interest in building their software on top of compat layer

CernVM-FS
CernVM File System

EuroHPC User Day 22-23 Oct 2024 (Amsterdam)

- Presentation on MultiXscale and EESSI by Kenneth in *HPC ecosystem tools* session

- Live demo of EESSI at walk-in networking session
  - Raspberry Pi cluster running ESPResSo demo provided by EESSI
  - Contest to win a Raspberry Pi 5 starter kit

- [Link to blog post](#) with more details & pictures + links to slides

[Kenneth, Lara, Caspar, Satish, Thomas, Richard, Bob, Pedro]

Supercomputing'24

- 17-22 Nov 2024 in Atlanta, Georgia (US)
  https://sc24.supercomputing.org

- **Birds-of-a-Feather session** on EESSI: Tue 19 Nov 12:15-13:15 EST
  https://sc24.conference-program.com/presentation/?id=bof126&sess=sess657

  Organised by Elisabeth/Helena/Jordi (HPCNow!) + Kenneth/Lara (HPC-UGent)

- **Presentation at Microsoft Azure booth** at SC'24 exhibit by Kenneth/Lara
  on Wed 20 Nov 14:40-15:00 EST

- *+ some nice news which we can't disclose yet…*

- Maybe also some informal meetup of EESSI (+ EasyBuild) community?

Past/upcoming webinars on EESSI

- MultiXscale Ambassador Event: Introduction to EESSI (4 Oct 2024)
  Recording available at https://www.youtube.com/watch?v=Xf6KqSCIAqw

- EPICURE webinar (Fri 15 Nov'24 14:00-15:30 CET)
  Streaming Optimised Scientific Software: an Introduction to EESSI
  https://epicure-hpc.eu/2024/10/17/webinar-streaming-optimised-scientific-software-an-introduction-to-eessi

- NRIS talks on EESSI

  - 3 Oct 2024: Introduction to EESSI

    https://documentation.sigma2.no/training/nris_talks/2024-10-03-nris-talks.html

  - 28 Nov 2024: How to build on top EESSI using EasyBuild

    https://documentation.sigma2.no/training/nris_talks/2024-11-28-nris-talks.html

Frequency of EESSI update meeting

- From now on EESSI update meetings will be **bi-monthly**, only in odd months

- Next meetings:

  - Thu **9** January 2025 14:00 CET

  - Thu 6 March 2025 14:00 CET

  - Thu 1 May 2025 14:00 CEST

  - Thu 3 July 2025 14:00 CEST