

5 Sept 2024

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

# Agenda

J'L

- 1. Quick introduction by new people
- 2. EESSI-related meetings and events in last month(s)
- 3. Progress update per EESSI layer
- 4. Update on EESSI production repository software.eessi.io
- 5. Modulefile for initializing the EESSI stack
- 6. Update on EESSI documentation + test suite + build-and-deploy bot
- 7. EESSI as backend in Ramble
- 8. Status page and monitoring
- 9. AWS/Azure sponsorship update
- 10. Upcoming/recent events
- 11. Frequency of EESSI update meeting
- 12. Q&A

# Quick introduction by new people



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

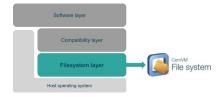
- Who are you, where do you work, on what?
- Why are you interested in the EESSI project?
- Are you planning to actively contribute,
   and if so, to which aspect(s) of the project?

## EESSI-related meetings & events



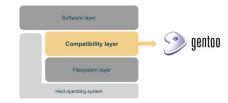
- (8 July + 12 Aug'24) CernVM-FS coordination meeting
   (CVMFS 2.11.4 release, CernVM Workshop, discussions about specific issues)
- (25 July + 8 Aug'24) EESSI test suite sync meeting (notes, notes)
- (30 Aug'24) Sync meeting on CVMFS monitoring dashboard (notes)
- (July+Aug'24) Weekly support team sync meetings (notes are in private wiki on EESSI support portal)
- (30 July + 20 Aug '24) Mini-hackathons: team-up with a colleague to move forward some topic
  - Next dates: 10 Sept and 1 Oct → ask if you want to join

# Progress update: filesystem layer



- Servers have been updated to the latest CernVM-FS release (2.11.5)
- Automatically generate an Lmod admin file for displaying known issues when loading modules (<u>WIP PR #197</u>)
- Working on CVMFS monitoring dashboard: see dedicated slide
- Create a top-level modules directory that will be populated with EESSI initialization module files (see dedicated slide and <u>PR #198</u>)
- PR #198 shows that some CI is now failing due to CentOS 7 being end-of-life
  - We should bump the OS of the affected containers (e.g. the client container)

## Progress update: compatibility layer



• 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 <a href="https://github.com/EESSI/software-layer/pull/685">https://github.com/EESSI/software-layer/pull/685</a>)
- Probably makes sense to wait until EasyBuild 5.0 is released?

# Progress update: software layer (1/3)



#### Recently merged PRs:

- Additional software: CP2K 2023.1 (<u>PR #630</u>), bioinformatics packages (<u>PR #634</u>), Extrae 4.2.0 (<u>PR #640</u>), pystencils 1.3.4 (<u>PR #641</u>), MetalWalls 21.06.1 (<u>PR #642</u>), Blast+ 2.14.0 (<u>PR #649</u>), amdahl 0.3.1 (<u>PR #650</u>), pyMBE 0.8.0 (<u>PR #651</u>), SciTools-iris + xarray (<u>PR #656</u>), BioPerl 1.7.8 (<u>PR #658</u>), grpcio 1.57.0 (<u>PR #660</u>), gnuplot 5.4.6 (<u>PR #661</u>), h5py 3.8.0 (<u>PR #663</u>), MDAnalysis 2.4.2 (<u>PR #664</u>), orjson 3.9.15 (<u>PR #665</u>), STAR 2.7.11b (<u>PR #671</u>), wradlib 2.0.3 (<u>PR #684</u>), MBX 1.1.0 (<u>PR #687</u>), Transrate 1.0.3 (<u>PR #689</u>), Critic2 1.2 (<u>PR #691</u>), HPL 2.3 (<u>PR #692</u>)
- Additional software zen4: ParaView 5.11.2 (<u>PR #632</u>), OpenFOAM 10 + 11 (<u>PR #639</u>), Modflow 6.4.4 (<u>PR #659</u>), BioPerl 1.7.8 (<u>PR #662</u>)
- Additional software A64FX: OpenFOAM 10 + 11 + v2312 (<u>PR #666</u>), R 4.3.2 (<u>PR #681</u>)
- EESSI bash initialization to module file (<u>PR #667</u>, see dedicated slide)

# Progress update: software layer (2/3)



#### Recent active open PRs + issues:

- Additional software:
  - Single-cell-python-bundle 2024.02 (<u>PR #637</u>)
  - R-bundle-CRAN 2024.06 (<u>PR #686</u>)
- Map tests to software builds (<u>PR #673</u>)
- Add new init scripts for new initialization module (<u>PR #668</u>)
- List modules for which eb --module-only does not work [WIP] (PR #690)
- Use ReFrame's CPU autodetect in test step (PR #682)

# Progress update: software layer (3/3)



#### Additional CPU targets

- AMD Genoa (zen4)
  - ~64% done (467 modules in place vs 731 for fully supported CPU targets)
- Intel Sapphire Rapids
  - New build cluster in AWS is set up incl. Sapphire Rapids partition, need to configure bot
- Arm A64FX (mainly for EuroHPC system Deucalion)
  - 170 modules in place (~23% done), incl. ESPResSo, OpenFOAM, R
  - Requires work in archdetect, see (PR #608)

## EESSI production repository

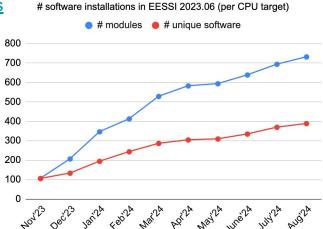
#### eessi.io/docs



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

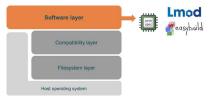
- 8 supported CPU targets: see <u>eessi.io/docs/software\_layer/cpu\_targets</u>
- 3 more CPU targets being added: zen4, a64fx, (sapphirerapids)
- Initial support for NVIDIA GPUs is in place, see <u>eessi.io/docs/gpu</u>
- Currently: 731 software installations per CPU target (+93 in July+Aug'24)
  - 388 different software projects (+54),
     6,505 software installations (across 8+2 CPU targets, +983)



#### Current focus:

- Providing optimized software installations for AMD Genoa (Zen4) + A64FX (+ Intel Sapphire Rapids)
- Adding more software, processing incoming contributions, fixing broken builds/test suites

## Modulefile for initializing the EESSI stack



- New method for initializing the EESSI stack: Lua modulefile (see <u>PR #667</u> of software layer)
- They will be made 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
- Some known issues: trouble when sticky modules are used, only supports bash shell, ...

## Bot for building + deploying software layer



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

- July-August'24
  - Cleanup of shared disk storage when PR has been merged <u>PR#271</u> or closed <u>PR#27</u>
  - Add setting to give all jobs a unique name <u>PR#273</u>
  - Add argument accelerator: X/Y to bot: build command PR#276 (not used yet)
- Ongoing work
  - Test + merge PR that allows customizing Slurm submit options PR#277 (community contrib)
  - Continue work on supporting GPU builds (bot code + target repo changes/additions)
  - Improve deployment (ingestion efficiency, single approval PR, flexible tasks)
- Side note: over 17,000 Slurm jobs have been submitted on AWS Slurm cluster (bot + test suite)

### **EESSI** documentation



<u>eessi.io/docs</u> - GitHub repo <u>github.com/EESSI/docs</u>

Improvements to the EESSI documentation: ~15 merged PRs (+ 23 updates to software overview)

- Add zen4 to software overview (PR #185)
- Blog post about adding Extrae to EESSI (PR #231)
- Updates for EESSI test suite (<u>PR #232</u>): changed scale tags + more info on ESPResSo tests
- Add note about CernVM-FS cache directory (<u>PR #234</u>)
- Clean up the available software script and the tests (PR #239)
- Use a time template in module documentation generation (PR #256 + PR #258)
- Add section on <u>writing portable tests</u> for the EESSI test suite (<u>PR #262</u>)
- Update pip install instructions in README (PR #263)
- Run workflow to update overview of available software only twice a day (<u>PR #267</u>)

### **EESSI** documentation



<u>eessi.io/docs</u> - GitHub repo <u>github.com/EESSI/docs</u>

Overview of available software in EESSI (software.eessi.io, version 2023.06)

- High-level overview available at <u>eessi.io/docs/available software/overview</u>
- Separate page per supported software project with more details,
   see for example <u>eessi.io/docs/available\_software/detail/OpenFOAM</u>
- Does not include CPU targets yet for which installations are very incomplete (a64fx, ...)
- Semi-automatically updated as more software gets added
  - PR is opened automatically by GitHub Actions workflow if update is needed
  - Overview in documentation is updated when PR is merged

### **EESSI** documentation



<u>eessi.io/docs</u> - GitHub repo <u>github.com/EESSI/docs</u>

### Improvements to the EESSI documentation - (recent) open PRs:

- Add a page about sites that are known to support EESSI (<u>PR #145</u>)
- How to build on top of EESSI without EB (PR #175)
- Add information on how to use EESSI in CI: GitHub Actions + GitLab CI/CD (PR #245)

### **EESSI** test suite



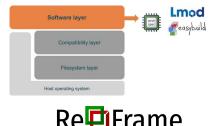
<u>eessi.io/docs/test-suite</u> - <u>github.com/EESSI/test-suite</u>

#### Merged pull requests:



- PyTorch (torchvision-based) (<u>PR #130</u>)
- LAMMPS (<u>PR #131</u>, <u>PR #169</u>)
- CP2K (<u>PR #133</u>)
- mpi4py tutorial, corresponds to tutorial in docs on writing portable tests (<u>PR #149</u>, <u>PR #172</u>)
- Update to various system configs (<u>PR #165</u>, <u>PR #166</u>, <u>PR #168</u>, <u>PR #171</u>, <u>PR #173</u>)
- Report (and fail) on duplicate modules (<u>PR #167</u>).
  - Previously, two tests were generated, but both would use the same module (first on \$MODULEPATH)
- Add hook for measuring memory usage in a job (PR #174)
- Updates to CI config (<u>PR #173</u>, <u>PR #175</u>, <u>PR #176</u>)

### **EESSI** test suite



<u>eessi.io/docs/test-suite</u> - <u>github.com/EESSI/test-suite</u>

#### Open pull requests:

- MetalWalls (<u>PR #164</u>)
- Try using RegressionMixin class to set default hooks (PR #177, draft)
  - When writing docs, a lot of hooks turned out to be 'mandatory'. Inheriting from a RegressionMixin class could run all of those by default for any inheriting test
  - Allows printing informative information for test developers if their test 'misses' information (variables, etc) needed by these mandatory hooks

## EESSI test suite - dashboard (WIP)

Compatibility layer

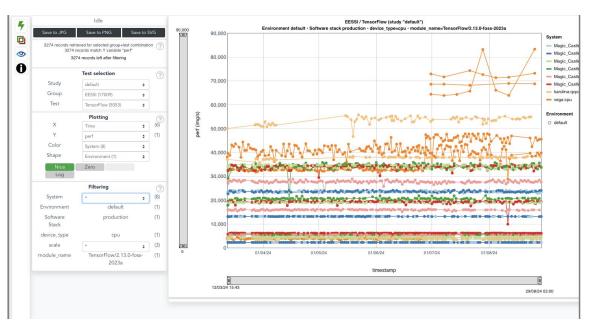
Filesystem layer

Host operating system

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



- Test suite runs daily on Vega & Karolina (EuroHPC systems), and AWS & Azure build clusters
- Test reports pushed to ElasticSearch database daily (since late Aug 2024)



### EESSI as backend in Ramble



https://googlecloudplatform.github.io/ramble

- Ramble is a tool developed by Google to easily run experiments for software applications
- EESSI is now documented as a supported "package manager" backend for Ramble,
   see <a href="mailto:readthedocs.io/en/latest/package\_managers.html#eessi-package-manager">readthedocs.io/en/latest/package\_managers.html#eessi-package-manager</a>
- Software installations available in EESSI can be used to run tests with Ramble
- See also tutorial: <u>ramble.readthedocs.io/en/latest/tutorials/EESSI\_package\_manager.html</u>

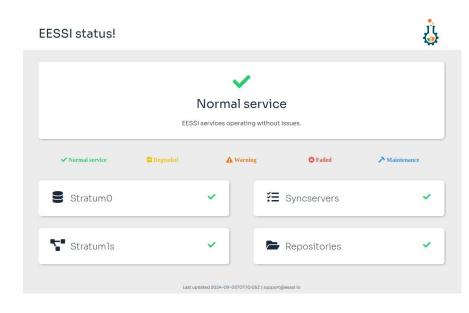
# EESSI status page: <a href="https://status.eessi.io">https://status.eessi.io</a>



Rewritten in Rust:

https://github.com/terjekv/cvmfs-status-page-rust

- Shows an overall status of the CernVM-FS infrastructure, and also more detailed ones
- Scrapes CVMFS information from all servers
  - New version also shows the sync server
- Exports all statuses as Prometheus metrics



# Monitoring EESSI (WIP)



- Working on a setup of Grafana + Prometheus + Prometheus Alertmanager + several exporters
- Using Ansible for configuring all servers
- Except for installing some CVMFS-specific Prometheus exporters, most of the main work has been done; now it's mostly a matter of customizing things (dashboards, notifications)

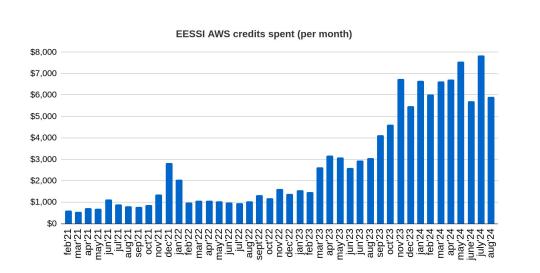


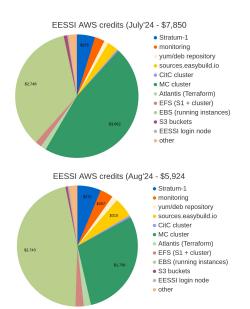


## Sponsored AWS credits

aws

- Ask in #aws-resources Slack channel to get access!
- ~\$7,850 + \$5,924 "spent" in July + Aug'24 on Stratum-1 servers, monitoring, sources.easybuild.io, EESSI debugging (build) issues, demos, Slurm clusters (build bot), testing on Sapphire Rapids, ...
- Bulk of consumed credits due to EESSI build-and-deploy bot
- ~Bi-monthly sync meetings with AWS





## Sponsored Azure credits





- Ask in #azure-resources Slack channel to get access!
- In June: ~€2,288 worth of credits spent
- Used for: Slurm cluster for bot (Zen4), Stratum-1 mirror servers, GitHub Runners
- Slurm cluster with Magic Castle in place for EESSI build-deploy bot



## Upcoming events

- CernVM Workshop 2024: 16-18 Sept 2024 @ CERN (Geneva)
   <a href="https://indico.cern.ch/event/1347727/overview">https://indico.cern.ch/event/1347727/overview</a>
  - Talk on EESSI will be presented by Thomas
- - We plan to have a strong presence at this event...
  - Kenneth & Lara & Richard & Thomas will be attending, anyone else?
- Proposal for EESSI Birds-of-a-Feather session at SC'24 accepted

# Frequency of EESSI update meeting

- Monthly or every two months?
- Proposal: bi-monthly meeting from now on.

Next meetings:

- Thu 7 Nov 2024 14:00 CET
- Thu 9 Jan 2025 14:00 CET
- Thu 9 Mar 2025 14:00 CET
- Thu 1 May 2025 14:00 CEST