



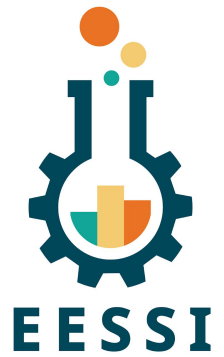
EESSI use cases

EESSI Community Meeting @ Amsterdam

14 Sept 2022

Kenneth Hoste (HPC-UGent) + Alan O'Cais (CECAM)

Overview of use cases enabled by EESSI



- A uniform software stack across HPC clusters, clouds, servers, and laptops
- Can be leveraged in continuous integration (CI) environments
- Significantly facilitates setting up infrastructure for HPC training
- Enhanced collaboration with software developers and application experts
- Enable portable workflows

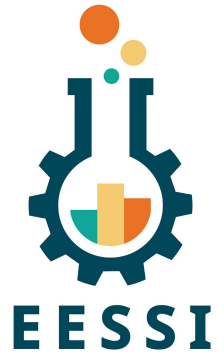
Also discussed in our open-access paper, available via doi.org/10.1002/spe.3075

EESSI provides a uniform software stack



- Main goal: **same software everywhere**: laptop, server, HPC, cloud, ...
- Wide variety of systems supported
 - CPUs: x86_64 (Intel, AMD), aarch64 (Arm), ppc64le (POWER), riscv64 (soon...)
 - OS: any Linux distribution, Windows via WSL, macOS should be possible too
 - High-speed interconnects (Infiniband), GPUs, etc.
- Without compromising on software performance
 - Optimized software installations for specific CPU microarchitectures + auto-detection
 - Large contrast with generic binaries often used in containers
- Facilitates migrating from laptop to HPC, cloud bursting, ...

Leveraging EESSI in CI environments



- EESSI can be used in CI environments like Jenkins, GitHub Actions, ...
- We can provide:
 - Different compilers to test your software with
 - Required dependencies for your software
 - Additional tools like ReFrame, ...
- Other than CernVM-FS, no software installations required
 - Everything that is actually needed is pulled in on-demand by CernVM-FS
- Significantly facilitates also running CI tests in other contexts (laptop, HPC, ...)

Leveraging EESSI in CI environments

Accessing EESSI in a GitHub Actions workflow is very... easy:

```
jobs:
  eessi:
    runs-on: ubuntu-20.04
    steps:
      - name: Check out repository
        uses: actions/checkout@v2
      - name: Mount EESSI CernVM-FS pilot repository
        uses: cvmfs-contrib/github-action-cvmfs@main
        with:
          # name of EESSI pilot repository
          cvmfs_repositories: pilot.eessi-hpc.org
          # EESSI configuration package (long download URL)
          cvmfs_config_package: https://.../latest/cvmfs-config-eessi\_latest\_all.deb
          # direct access to CernVM-FS network, no proxy
          cvmfs_http_proxy: DIRECT
      - name: Set up EESSI environment and run tests
        run: |
          source /cvmfs/pilot.eessi-hpc.org/versions/2021.12/init/bash
          ./run_tests.sh # what the developer really cares about, just load modules for dependencies!
```

See it in action in the `eessi-demo` repository:

github.com/EESSI/eessi-demo/actions/workflows/pilot_repo_native.yml

github.com/EESSI/eessi-demo/blob/main/.github/workflows/pilot_repo_native.yml



Leveraging EESSI in CI environments



Summary

Jobs

- ✓ pilot_repo_native (Bioconduc...
- ✓ pilot_repo_native (Bioconduc...
- ✓ pilot_repo_native (GROMACS...
- ✓ pilot_repo_native (GROMACS...
- ✓ pilot_repo_native (OpenFOA...
- ✓ **pilot_repo_native (OpenFO...**
- ✓ pilot_repo_native (TensorFlo...
- ✓ pilot_repo_native (TensorFlo...

pilot_repo_native (OpenFOAM, 2021.12)
succeeded 2 hours ago in 15m 10s

Search logs

- > ✓ Set up job 2s
- > ✓ Check out software-layer repository 1s
- > ✓ Mount EESSI CernVM-FS pilot repository 47s
- ▼ ✓ **Run demo** 14m 19s

```
1 ▶ Run source /cvmfs/pilot.eessi-hpc.org/versions/2021.12/init/bash
2 Found EESSI pilot repo @ /cvmfs/pilot.eessi-hpc.org/versions/2021.12!
3 Using x86_64/intel/haswell as software subdirectory.
4 Using /cvmfs/pilot.eessi-hpc.org/versions/2021.12/software/linux/x86_64/intel/haswell
5 /modules/all as the directory to be added to MODULEPATH.
6 Found Lmod configuration file at /cvmfs/pilot.eessi-hpc.org/versions/2021.12/software
7 /linux/x86_64/intel/haswell/.lmod/lmodrc.lua
8 Initializing Lmod...
9 Prepending /cvmfs/pilot.eessi-hpc.org/versions/2021.12/software/linux/x86_64/intel/haswell
10 /modules/all to $MODULEPATH...
11 Environment set up to use EESSI pilot software stack, have fun!
12 /home/runner/work/eessi-demo/eessi-demo/OpenFOAM
13 WORKDIR: /tmp/runner/5019
14 /tmp/runner/5019
15 /tmp/runner/5019/motorBike
16 generating mesh...
17 New entry maxGlobalCells 20000000;
```

<https://github.com/EESSI/eessi-demo/actions/runs/3044103853/jobs/4904114694>

Leveraging EESSI in CI environment (short version)



We also have an EESSI GitHub Action as a shorthand for this:

```
name: ubuntu_gromacs
on: [push, pull_request]
jobs:
```

```
  build:
```

```
    runs-on: ubuntu-latest
```

```
    steps:
```

- uses: actions/checkout@v2
- uses: eessi/github-action-eessi@main

```
    with:
```

```
      eessi_stack_version: '2021.06'
```

- name: Test EESSI

```
    run: |
```

```
      module load GROMACS
```

```
      gmx --version
```

```
    shell: bash
```

See it in action in the `github-essi-action` repository:

github.com/EESSI/github-action-eessi

github.com/EESSI/github-action-eessi/blob/main/.github/workflows/gromacs-usage.yml



Leveraging EESSI GitHub Action



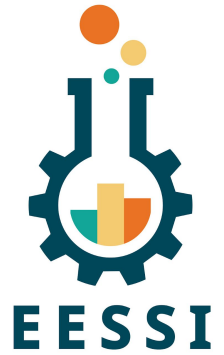
```
build
succeeded 2 minutes ago in 1m 1s
Search logs

> ✓ Set up job 2s
> ✓ Run actions/checkout@v2 0s
> ✓ Run eessi/github-action-eessi@main 52s
▼ ✓ Test EESSI 5s
  1 ▼ Run module load GROMACS
  2   module load GROMACS
  3   gmx --version
  4   shell: /usr/bin/bash --noprofile --norc -e -o pipefail {0}
  5   env:
  6     EESSI_SILENT: 1
  7     BASH_ENV: /cvmfs/pilot.eessi-hpc.org/versions/2021.06/init/bash
  8
  9     -: GROMACS - gmx, 2020.4-MODIFIED (-:
 10
 11     GROMACS is written by:
 12     Emile Apol      Rossen Apostolov   Paul Bauer   Herman J.C. Berendsen
 13     Par Bjelkmar    Christian Blau     Viacheslav Boznykh   Kevin Boyd
 14     Aldert van Buuren  Rudl van Drunen   Anton Feenstra   Alan Gray
 15     Gerrit Groenhof  Anca Hamuraru     Vincent Hindriksen M. Eric Irrgang
 16     Aleksei Iupinov  Christoph Junghans  Joe Jordan     Dimitrios Karkoulis
 17     Peter Kasson     Jiri Kraus        Carsten Kutzner   Per Larsson
 18     Justin A. Lemkul  Viveca Lindahl    Magnus Lundborg   Erik Marklund
 19     Pascal Merz      Pieter Meulenhoff  Teemu Murtola    Szilard Pall
 20     Sander Pronk     Roland Schulz     Michael Shirts   Alexey Shvetsov
 21     Alfons Sijbers   Peter Tieleman    Jon Vincent      Teemu Virolainen
 22     Christian Wennberg  Maarten Wolf     Artem Zhmurov
 23     and the project leaders:
```

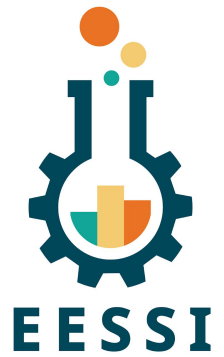
<https://github.com/EESSI/github-action-eessi/actions/runs/3044539257/jobs/4905040409>

Facilitate HPC training

- EESSI can significantly reduce effort required to set up infrastructure for HPC training sessions (introductory, software-specific, ...)
- Setting up a throwaway Slurm cluster in the cloud is easy via CitC or Magic Castle
- EESSI can provide (scientific) software that is required for the training
- Attendees can easily set up the *same* software environment later on their own system(s) by leveraging EESSI



Collaboration with software developers + experts



- A central software stack by/for the community opens new doors...
- We can work with software developers/experts to verify the installation
 - Check how installation is configured and built
 - Help to verify whether software is functional for different use cases
 - Show us how to do extensive testing of their software
 - Evaluate performance of the software, enable performance monitoring
 - **“Approved by developers” stamp for major applications included in EESSI**
- Relieve software developers from burden of getting their software installed
 - Remove need to provide pre-built binary packages?
- Developers can also leverage EESSI themselves: dependencies, CI, ...

EESSI enables portable workflows

- Portable workflows are significantly easier when relying on EESSI
- They often involve running a broad set of tools, which all need to be available
- Workflows definitions (Snakemake, ...) can be included in EESSI along with software
- Community-specific view on software provided by EESSI can be provided





Paper (open access): <https://doi.org/10.1002/spe.3075>

Website: <https://www.eessi-hpc.org>

Join our mailing list & Slack channel

<https://www.eessi-hpc.org/join>

Documentation: <https://eessi.github.io/docs>

GitHub: <https://github.com/eessi>

Twitter: [@eessi_hpc](https://twitter.com/eessi_hpc)

[YouTube channel \(brand new!\)](#)

[Monthly online meetings](#) (first Thursday, 2pm CEST)