

EESSI meeting

December 3rd 2020

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

Agenda



- 1. Quick introduction by new people
- HPC.NRW competence network [Robert]
- 3. Testing of 2020.10 version of pilot repository [Alan, Kenneth]
- 4. Progress update [Bob, Kenneth, Peter, Terje]
- 5. Plans for 2020.12 version of pilot repository [Kenneth, Bob, Terje]
- 6. Fenix project proposals [Alan, Henk-Jan]
- Updates on sponsorship by Azure/AWS [Alan, Bob, Kenneth]
- 8. Starting an EESSI consortium (+ rename without 'European'?) [Jaco, Kenneth]
- 9. Next steps
- 10. Past & upcoming events
- 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?

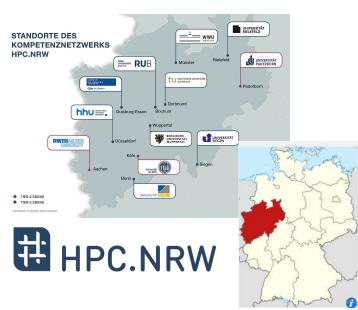
HPC.NRW competence network



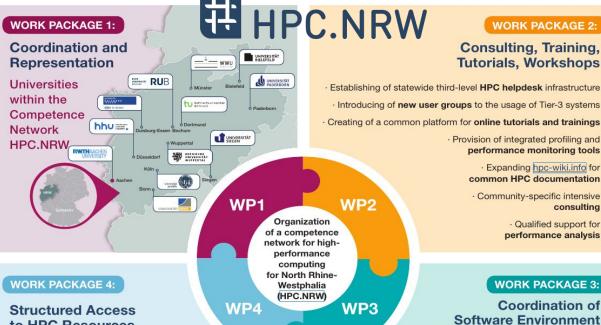
Competence network of all universities with data centers in

North-Rhine-Westphalia (NRW)

- 12 universities
- Established mid 2019
- First funding phase till end of 2022
- Main goals:
 - Support for transitions between HPC-tiers
 - Competent HPC-Support for all researchers in NRW
 - Efficient planning, setup and use of HPC resources
- Funding for personnel (18 FTE) and for state-level software licensing, ...



HPC.NRW competence network





WP3: Coordination of Software **Environment and HPC System** Operation:

- Provisioning of a standardized HPC software ecosystem
- Harmonizing user experiences across HPC systems in NRW

to HPC Resources

- Establishing a common infrastructure for compute time application and approval processes across HPC centers in NRW
- Supporting scientists in the preparation and application for compute time storage resources
- Increasing the Tier-level permeability between HPC centers
- Providing common reporting and accounting

Software Environment and HPC System Operation

> · Provisioning of a standardized **HPC** software ecosystem

· Harmonizing user experiences across HPC systems in NRW

· State-level licensing of common HPC software

· Establishing a competence network for operational concerns

HPC.NRW competence network



WP3: Coordination of Software Environment and HPC System Operation:



Efforts so far for a standardized HPC software ecosystem:

- Investigation and analysis of available software and software usage in NRW
- Internal Easybuild Workshop and Best-Practice guides
- Concept for an "HPC.NRW-module-tree"
 - In addition to the existing module-trees, deployment with Easybuild
 - → instead of setting up a similar initiative

We think we can contribute to EESSI because:

- we have developers and system administrators in the project (6 FTE for WP3)
- we have sites that have experience with/use Easybuild and/or CVMFS
- we have many different clusters (for testing purposes)

Testing of 2020.10 version of pilot repository



- <u>EESSI demos</u> used during imakefoss/SORSE/Nordic RSE talks
 - (Kenneth) on 4-node Raspberry Pi cluster (native CernVM-FS, built from source)
 - (Kenneth) Cloud (single node): Azure (Intel, native CernVM-FS), AWS (Graviton2, Singularity)
 - (Kenneth) On HPC-UGent AMD Rome pilot cluster (via Singularity, only single node)
 - (Thomas) On Saga cluster @ <u>Sigma2</u> + VM on OpenStack platform at (<u>NREC</u>)
- Alan: MPI benchmarks on JUWELS @ JSC (via Singularity):
 - OSU benchmarks comparable to system for latency and bandwidth (need set of ReFrame tests)
 - o GROMACS: 54.16 ns/day for 1 node, 98.46 ns/day for two (compared to 56.5/107 for system)
- Alan @ JSC + Magic Castle
 - Couple of PRs to Magic Castle to get things working
 - Requires some PRs in EESSI too (related to JupyterHub and shell initialisation)
 - Successfully tested on AWS and Azure (including infiniband)
- Jaco: further testing in WSL with ParaView + ImageMagick (GUI)

Progress update: filesystem layer



- Some updates on issue with fuse-overlayfs + Singularity, but still not solved...
- Symlink /cvmfs/pilot.eessi-hpc.org/latest that points to the latest version
- Manually built client package for macOS
 - Needs some effort to build it automatically with the existing Github Action (see <u>PR #54</u>)
- cvmfs_server enter now available in nightly CernVM-FS builds
 - Could be useful for quickly getting a writable overlay for testing purposes
- Monthly CernVM-FS coordination meeting (Nov 10th)
 - aarch64 / Debian builds of CernVM-FS packages
 - Adding CernVM-FS as component to OpenHPC (ongoing effort with Jakob (CERN) + Karl (OpenHPC))
 - Github Action for mounting CernVM-FS (see <u>cvmfs-contrib/github-action-cvmfs</u>)

[Bob, Kenneth]

Progress update: compatibility layer



- End-to-end Ansible playbook (see <u>EESSI/compatibility-layer/ansible/playbooks</u>)
 - Now includes a step to first bootstrap Gentoo Prefix, then install packages (Lmod, archspec, ...)
 - Building compat layer is fully automated: ansible-playbook -i hosts -b install.yml
- Playing with macOS/x86_64 and Linux/POWER
 - Gentoo Prefix devs fixed the bootstrap script for macOS (see <u>bug #730476</u>)
 - Very good support from Gentoo for adding a ppc641e profile to Prefix
- Libraries go in different places on x86_64 vs aarch64: /usr/lib vs /usr/lib64?
- Architecture-specific package sets on top of one base set (see <u>gentoo-overlay/etc/portage/sets</u>)
 - Some packages only work / are only needed on a specific architecture / OS (rdma-core, opa-psm, ...)

Progress update: software layer



- Containers for build nodes
 - Debian 10 OS + CernVM-FS + fuse-overlay, images for both x86_64 and aarch64
 - Available through Docker Hub (<u>eessi/fuse-overlay</u>), can be run via Singularity
 - Easy to create writable overlay on top of read-only /cvmfs mount
 - TODO: documentation on usage + use GitHub container registry?
- Quick demos (run in minutes) for applications in pilot repo
 - https://github.com/EESSI/eessi-demo
 - Good starting point for proper application tests to run in CI!
- Some CMake problems popped up when building for aarch64/generic ...
 - CMake fails to find libraries in compat layer; only looks in lib, not lib64 (or vice versa)?!
 - Best workaround seems to be to patch CMake; WIP in EasyBuild, see PR https://github.com/easybuilders/easybuild-easyblocks/pull/2248
 - Not entirely clear why this didn't pop up before...

[Kenneth]

Progress update: testing with ReFrame



ReFrame: single file defines a test

- What to compile
- What to run
- Sanity check
- Performance check
- Valid systems & prog environments
- #tasks
- #tasks-per-node

System specific

Progress update: testing with ReFrame



How to make ReFrame test generic?

- ReFrame 'abstract tests': https://github.com/eth-cscs/reframe/issues/1555
 - Define all non-system specific things. Reusable.
 - Each site needs to create derived classes to set num_tasks etc.
- #tasks: --flex-alloc-nodes: at runtime selection of #nodes
 (SLURM backend only)
- #tasks per node: get from a 'config', instead of hardcoding, e.g.
 - o self.num_tasks_per_node = system_properties.ncorespernode
- #tasks_per_node: define tests for all core counts (parametric test),
 and select with tag
 - reframe -r ... --tag ncpn16
- https://github.com/casparvl/software-layer/tree/mpihello/tests/reframe

Progress update: other stuff



- GPLv2 licenses are now in place in all repositories @ github.com/EESSI
- Initial support for "easystack" files has been merged in EasyBuild
 - See https://github.com/easybuilders/easybuild-framework/pull/3479
 - Will eventually replace dirty shell script we use for installing stuff in software layer
 - Initial support will be included in upcoming EasyBuild v4.3.2, but insufficient for our purposes...
- Access to OSU OSL infrastructure (Linux/POWER)
 - Temporarily used Easybuild's access for testing on POWER8
 - Requested Openstack access to POWER9 machines on behalf of EESSI
 - Approved, but waiting for IP addresses to become available
- Script for mounting the EESSI repository under Windows (WSL) [Jaco]
 - Will soon be added to the Github repository

EESSI pilot repository

NOT FOR PRODUCTION USE!



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

Plans for 2020.12 version of EESSI pilot repository

- Tweak compat layer: 2020.12/compat/{linux/macos}/{x86_64,aarch64}
- Same software? (GROMACS, OpenFOAM, Bioconductor, TensorFlow, foss/2020a)
- Same targets:
 - x86_64/generic, x86_64/amd/zen2, x86_64/intel/{haswell,skylake_avx512}
 - aarch64/generic, aarch64/graviton2 (maybe aarch64/{thunderx2,a64fx})
- Look into GPU installations with fosscuda/2020a (GROMACS, TensorFlow)
 - Fat installations, optimized for all CUDA compute capabilities
 - Evaluate pros/cons of fat vs GPU-specific installations
- Experiment with software built for Linux/POWER and macOS clients?

Fenix project proposals



- Both project proposals accepted! \o/
- Project 1 (submitted by Henk-Jan)
 - 36,000 node hours on scalable resources (EPYC)
 - 2vCPU + object store at CINECA, 4vCPU+vGPU at JSC (EPYC)
 - Additional info required by Dec 7th
- Project 2 (submitted by Alan)
 - Related to EESSI + Magic Castle and HPC training
 - 40vCPU and 2vGPU at JSC (EPYC), 40vCPU at CINECA
- PRACE-ICEI resources at both JSC (soon) and CINECA (~ April'21)

Update on sponsorship by Azure/AWS

- EESSI SCHOOL SCH
- Credits for several people available in both Azure/AWS to play with
- **Azure**

Kenneth, Alan, Terje



- Looking into more structured sponsorship
 - EESSI "project" in both Azure/AWS
 - Univ. of Groningen as receiving party
 - People involved in EESSI can get access to develop/test EESSI
- Currently working on the red tape + agreements with Azure/AWS on specifics

Starting an EESSI consortium



- Current collaboration is voluntary, no official agreement or consortium
- Time to change that, make it "official"?
- Task for Dell Technologies (Jaco) + SURF?
- Look into what setting up a consortium actually involves...
- Maybe also rename first 'E' in EESSI from "European" to "Easy"
 - The "European" part has been raising questions, feels restrictive
 - "EESSI is the Easy Environment for Scientific Software Installations"

Next steps



- Improve support for "easystacks" in EasyBuild
- GPGPU software installations (GROMACS, TensorFlow)

Testing & continuous integration

- More & better CI checks for EESSI layers (leverage software demos?)
- Tests for software layer via ReFrame (smoke tests, apps, benchmarks, ...)
- Documentation: build nodes, "native" CernVM-FS access, HPC clusters, ...

Automatic deployment of software to EESSI repository

- Triggered by pull requests in GitHub
- Bots negotiating with each other?
- Leveraging both cloud resources in Azure/AWS + resources at HPC sites
- EESSI pilot stack for Linux/POWER + macOS clients?

Past events

https://github.com/EESSI/docs/tree/master/talks



- Terje's talk on EasyBuild on ARM (+ EESSI pitch at the end)
 - ARM HPC Users Group @ Supercomputing'20
 - Recording (YouTube)
- Kenneth's interview during IMakeFoss live stream (Nov 24th)
 - Slides recording (YouTube)
- Kenneth's "software demo" talk at SORSE (Nov 25th)
 - Slides recording (YouTube) (Q&A chat transcript available)
- Thomas's talk at Nordic RSE meeting (Dec 2nd)
 - <u>Slides</u> <u>Q&A</u> (good starting point for Q&A section in docs?)

Upcoming events



- Kenneth's talk at HPC Champions workshop (UK HPC sites)
 - Dec 15th 2020, 1.15pm UTC, free to attend
 - https://www.archer2.ac.uk/training/courses/201215-champions
 - Maybe including demo on Isambard system (Arm64 ThunderX2 + A64FX)...
- EasyBuild User Meeting (virtual): week of 25-29 Jan 2021
 - https://github.com/easybuilders/easybuild/wiki/6th-EasyBuild-User-Meeting
 - Talks on CernVM-FS, Gentoo Prefix, EasyBuild, Lmod, ReFrame, ...
 - CernVM-FS tutorial, co-org. by Kenneth/Bob, CernVM-FS developers, Compute Canada
 - ReFrame tutorial, organised by ReFrame developers
- CernVM-FS Workshop: 1-3 Feb 2021: https://indico.cern.ch/event/885212
 - o Incl. talk by Bob on EESSI (by invitation)
- HPC devroom at FOSDEM'21 (virtual): Sun Feb 7th 2021: https://hpc-bigdata-fosdem21.github.io
 - Submissions for HPC devroom are open NOW (deadline is Tue Dec 15th!)