

## EESSI + HPC.NRW collaboration Kickstart meeting

Tue Jan 5th 2021 - 13:00-14:30 CET

## Agenda



- 1. Quick introduction of participants [ALL]
- Very short intro for HPC.NRW competence network [Robert]
- 3. Goals with respect to harmonized software environment in HPC.NRW [Robert]
- 4. Current areas of activity and possible contribution areas in EESSI [Kenneth]
- 5. Discussion of what HPC.NRW could do [ALL]
- 6. Next steps

## Quick introduction of participants



Please introduce yourself (in 1 min or less!)

- Where do you work
- Experience in HPC context
- Primary interests in context of EESSI project

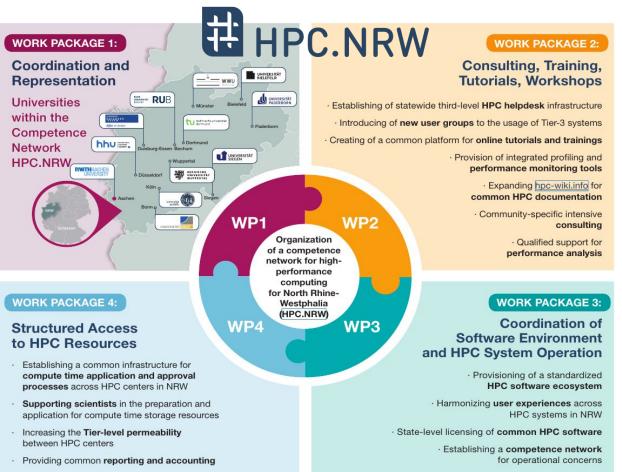
## HPC.NRW competence network



- 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
- .....

[Robert]

## 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)

# Current areas of activity and possible contributions to EESSI



- Fixing problems encountered with iterative revisions of pilot repository,
   see project for 2020.12 revision (<a href="https://github.com/orgs/EESSI/projects/3">https://github.com/orgs/EESSI/projects/3</a>)
- Improvements & bug fixes to EasyBuild (RPATH issues, building in Prefix env)
- Automation: Ansible, scripts
- Continuous Integration (GitHub Actions)
- Testing for (compat &) software layer with ReFrame
- Exploring other platforms (macOS, POWER)

### Discussion of what HPC.NRW could do



#### Automation

- Continue Terje's work with Terraform to leverage cloud resources
- Work towards goal of adding software to repo via pull requests

#### Testing & CI

- Verify aspects of compat & software layer in GitHub Actions workflow
- Software application testing with ReFrame (MPI, GROMACS, OpenFOAM, TensorFlow)

#### Documentation

- Native CernVM-FS access (next to via Singularity)
- Running MPI jobs (+ using CernVM-FS alien cache?)
- Build nodes (<u>https://github.com/EESSI/docs/issues/50</u>)
- 0 ...

## Next steps



- Getting organised
  - Create issues + project (Kanban) board
  - Make sure active contributors are using EESSI Slack (easy communication)
  - Weekly (short) meetings to discuss current/next tasks & progress?
    - Fixed day/time?
    - Maybe only by small focused working groups?
- Prioritize & assign tasks
  - Which tasks should be tackled first?
  - Which aspects does HPC.NRW want to focus on?
  - O Who does what?