

EuroHPC Centre of Excellence

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OBJECTIVES

• Scientific

- Increase performance, productivity and portability ("the Three P's") across the entire spectrum of scientists active in the domain of multiscale simulation
- Pilot multiscale use cases of societal and industrial significance:
 - Helicopter design and certification for civil transport,
 - Battery applications to support the sustainable energy transition,
 - Ultrasound for non-invasive diagnostics and biomedical applications.

• Technical

- Focus on performance, automation, testing, collaboration
- Application and system co-design for exascale technologies
 - Reduce technical burden on domain scientists
- Provisioning of exascale-oriented libraries and services (such as CI/CD)
- Scalable workflows and portable technologies

OUTCOMES

- Project workflows running at scale on EuroHPC systems
- Dramatic growth in the number of applications supported by the shared software stack (EESSI – European Environment for Scientific Software Installations)
- Accelerated adoption of EuroHPC compute services among the community
- Increasing HPC sites explicitly supporting the shared software stack EESSI
- Cloud providers promoting the EESSI stack in cloud environments
- Large number of developers using our CI tools
- Training Portal with our training courses and additional training content
- Adoption of MultiXscale software and workflows in the industrial community

ACHIEVEMENTS



- EESSI: A streamed, production-quality, multi-platform, optimised scientific software stack
 - Working proof of concept (see <u>https://eessi.github.io/docs/pilot</u>)
- Ansible playbooks, scripts, docs at https://github.com/eessi
- CernVM-FS: Stratum 0 @ Univ. of Groningen + four Stratum 1 servers
- Software (CPU-only): Bioconductor, GROMACS, OpenFOAM, R, TensorFlow, ...
- Hardware targets:
 - {aarch64,ppc64le,x86_64}/generic
 - intel/{haswell, skylake_avx512}, amd/{zen2,zen3}, aarch64/{graviton2,graviton3}, ppc64le/power9le
- Supported by Azure and AWS: sponsored credits to develop necessary infrastructure



EESSI: Design

User software contribution workflow to EESSI





