MultiXscale

EESSI Community Meeting @ Amsterdam
16 Sept 2022
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MultiXscale: Key Points

- EuroHPC Centre of Excellence

  - 4 year project, likely start Q1 2023

- Budget of ~6M EUR (50% EU funding, 50% national funding)

  - Roughly 50% of funding for EESSI-related activities

- Collaboration between EESSI and CECAM (total of 16 partners)

  - EESSI primarily addresses technical aspects

  - CECAM network provides scientific expertise

- Scientific target are multiscale simulations with 3 key use cases

  - Helicopter design and certification for civil transport

  - Battery applications to support the sustainable energy transition

  - Ultrasound for non-invasive diagnostics and biomedical applications

MultiXscale: Objectives

MultiXscale – Performance, Portability, Productivity
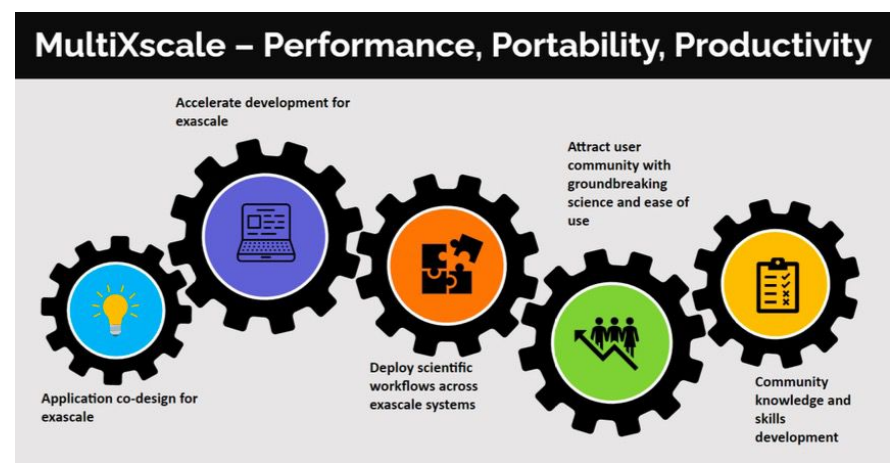
- Co-design multiscale modelling applications for exascale through the provision, support and maintenance of key software packages

- Accelerate domain application development for the exascale era

- Porting, verification, and distribution of community-developed applications to support the full scientific/industrial workflow on all supported architectures

- Attract domain scientists by addressing a set of relevant groundbreaking scientific and industrial problems using MultiXscale co-design approach

- Knowledge and skills development for both domain application developers and users

Scientific Work Packages

- Preparation and optimization of community software codes towards Exascale-readiness
    - Creation of performance-portable electrostatics solver, and load-balancing libraries
    - Implementation of exascale-oriented tools (Kokkos, HPX, OpenACC) in community codes

- Development + efficient implementation of interfaces for coupling different length scales
    - Tight and loose coupling between community codes and libraries (LAMMPS, MDFT, ESPResSo, waLBerla, URANS)
    - Coupling of concurrent tasks on modular architectures

- Multiscale/physics workflows for sustainable industrial design
    - Environmental-friendly rotorcraft design, multiscale design of new families of energy-saving materials and ultrasound propagation in liquid water for biomedical applications
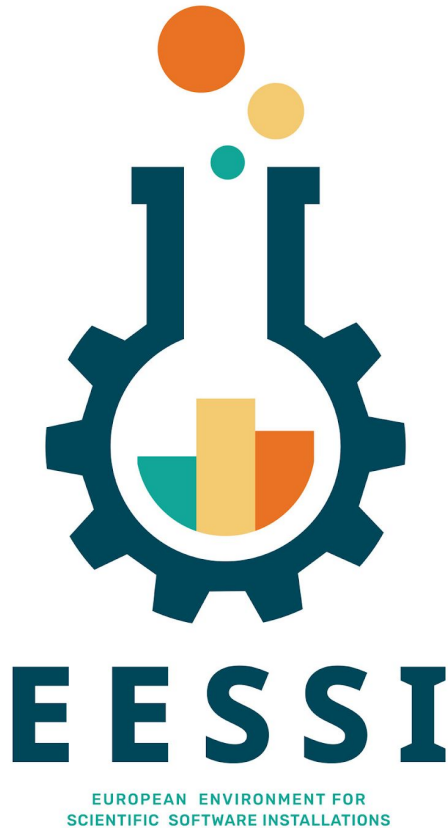
Technical Work Package:
Developing a Central Platform for Scientific Software on Emerging Exascale Technologies

- Create a stable, shared software stack
    - Based on the concept developed in the EESSI initiative: performance-tuned for and accessible from a wide range of computer platforms

- Expand the scope of the shared software stack by supporting current and emerging system architectures
    - Accelerators, interconnects, CPU architectures, operating systems and computer platforms

- Support software developers to adopt emerging hardware architectures
    - Providing developer-oriented services, e.g., continuous integration across a broad range of platforms

- Improve quality assurance of the shared software stack
    - Development of extensive software testing and benchmarking suite, and software testing workflows

- Provide services that facilitate development of the RISC-V software ecosystem
    - Provisioning of early RISC-V toolchains within the shared software stack

Technical Work Package:
Building, Supporting and Maintaining a Central Shared Stack of Optimized Scientific Software Installations

- Provide a production-quality central stack of optimized scientific software installations for a broad range of systems and platforms
  - including personal workstations, cloud environments, and HPC infrastructure (up to and including EuroHPC exascale platforms)

- Offer support to the community for using the central shared software stack and related services

- Ensure that the central shared software stack and related service are robust, reliable, and perform well
  - Actively monitor, test, and maintain all components

- Facilitate and process community contributions to the central software stack in an efficient way

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

youtube.com/channel/UCKLS5X7_oMWhUrAZuzSwBxQ

Monthly online meetings (first Thursday, 2pm CEST)

EESSI

EUROPEAN ENVIRONMENT FOR
SCIENTIFIC SOFTWARE INSTALLATIONS