



Co-funded by
the European Union



EuroHPC
Joint Undertaking

MultiXscale

arnes
povezujemo znanje

EuroHPC JU Centre of Excellence

Matej Praprotnik

National Institute of Chemistry, Ljubljana, Slovenia

MultiXscale Hackathon, SLING days, Ljubljana

3.12.2024

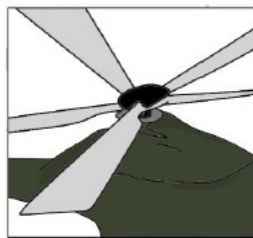


What is MultiXscale?

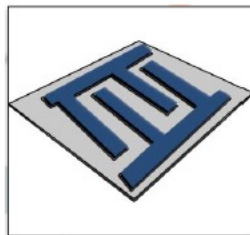
- Collaboration between scientific partners (CECAM nodes) who deliver **3 pilot use cases**, and technical partners (EESSI members) who provide the tools to allow application software to be seamlessly used on any available hardware
- MultiXscale targets improving the
 - **Productivity** of scientists who develop and/or use open source codes
 - **Performance** of those codes on EuroHPC hardware (and beyond)
 - **Portability** of the codes and workflows from laptop to server to cloud to HPC
- The focus of MultiXscale is multiscale modelling and leveraging the opportunities that EuroHPC offers
- Advances the transition towards use of exascale resources for the community

Solving societal challenges by HPC

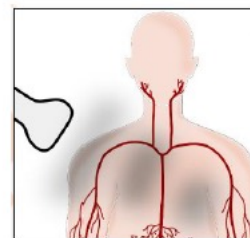
SCIENTIFIC SHOWCASES



Advanced parallel aerodynamic code for rotor aeroelastic analyses



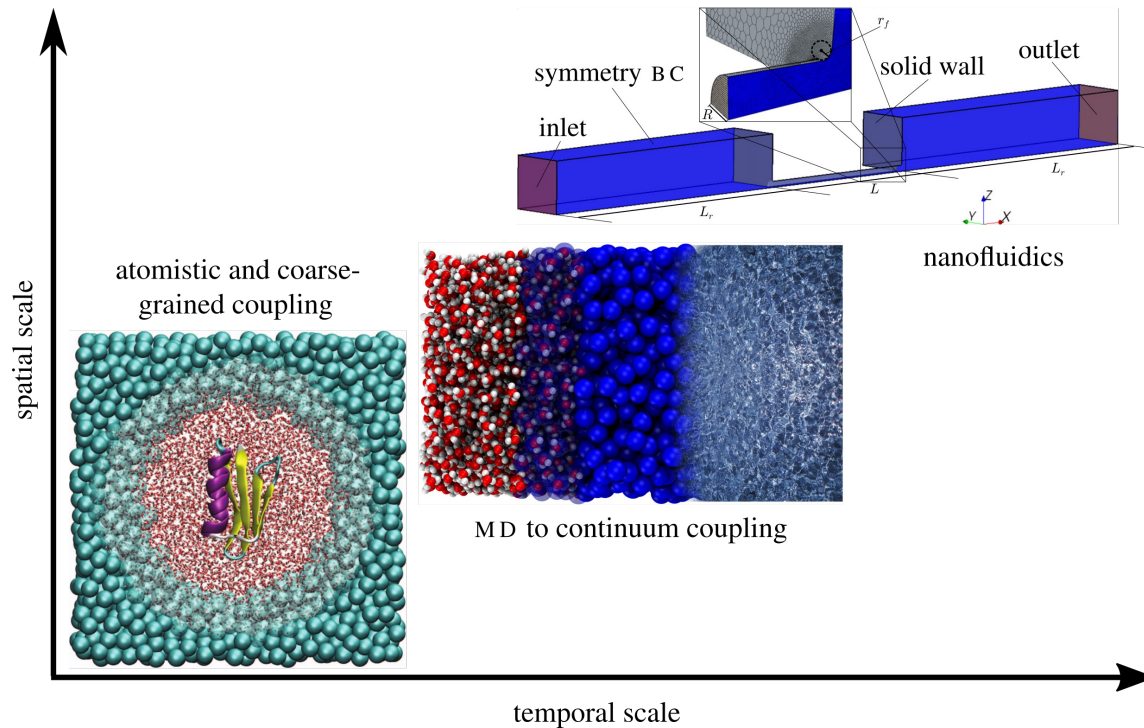
*High-power battery
Applications:
Towards enhanced supercapacitor systems*



*Biomedical applications of ultrasound:
Improving diagnostics and guiding drug delivery*

The common feature of these complex systems is that they are inherently **multiscale**, i.e., their physical properties are determined by the interplay of disparate length and time scales!

Multiscale modeling & simulation

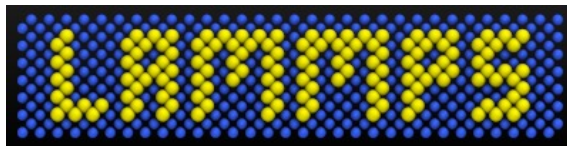


Multiscale simulation techniques that couple multiple models at different resolutions provide the most efficient way to span many orders of magnitude in the spatiotemporal scales involved in these systems.

Towards exascale-ready multiscale software

To fully exploit the methodological potential of multiscale methods they need to be integrated into community software packages with the following properties:

- scalable couplings between particle-based simulation codes (e.g., ESPResSo, LAMMPS) and CFD codes (e.g., waLBerla)
- open and user-friendly so they can be easily adopted by scientific and engineering communities for solving relevant groundbreaking scientific and industrial problems
- easy to install on various HPC systems with different architectures with sustainable user support



MultiXscale – Performance, Portability, Productivity

Accelerate development for exascale



Application co-design for exascale



Deploy scientific workflows across exascale systems



Community knowledge and skills development

Attract user community with groundbreaking science and ease of use

Efficient Access to Developed Software



EESSI in a nutshell

- *European Environment for Scientific Software Installations (EESSI)*
- **Shared repository of (optimized!) scientific software installations**
- Avoid duplicate work across (HPC) sites by collaborating on shared software stack
- Uniform way of providing software to users, regardless of the system they use!
- Should work on any Linux OS (+ WSL, and macOS) and system architecture
 - From laptops and personal workstations to HPC clusters and cloud
 - Support for different CPUs, interconnects, GPUs, etc.
- **Focus on performance, automation, testing, collaboration**



E E S S I

EUROPEAN ENVIRONMENT FOR
SCIENTIFIC SOFTWARE INSTALLATIONS

<https://www.eessi.io>

<https://www.eessi.io/docs/>

This project has received funding from the European High Performance Computing Joint Undertaking under grant agreement No. 101093169



EuroHPC
Joint Undertaking

HPCwire 2024 Readers' Choice Award as the Best HPC Programming Tool or Technology



MultiXscale objectives

Scientific

- Co-design multiscale modeling applications for exascale through the provision, support and maintenance of key community software packages
- Pilot multiscale use cases of societal and industrial significance:
 - **Helicopter design and certification for civil transport**
 - **High-power battery applications to support the sustainable energy transition**
 - **Ultrasound for non-invasive diagnostics and biomedical applications**

Technical

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

MultiXscale

Web page: www.multixscale.eu

Facebook: MultiXscale

X: @MultiXscale

LinkedIn: multixscale

YouTube: @MultiXscale



Co-funded by
the European Union



EuroHPC
Joint Undertaking



UNIVERSITAT DE
BARCELONA



Universität
Stuttgart



SORBONNE
UNIVERSITÉ



Université
de Toulouse



Consiglio Nazionale
delle Ricerche



MAX-PLANCK-GESSELLSCHAFT



Funded by the European Union. This work has received funding from the European High Performance Computing Joint Undertaking (JU) and countries participating in the project under grant agreement No 101093169.