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MultiXscale: Centre of Excellence in exascale-oriented application co-design and delivery for multiscale simulations

Description

The MultiXscale Centre of Excellence will increase performance, productivity and portability (the Three P's) across the entire spectrum of scientists active in the domain of multiscale simulation. It couples the scientific expertise of the CECAM network, represented by leading experts in multiscale simulations from different European institutions, with the technical expertise of the EESSI collaboration, and targets the computational laboratories of EuroHPC and beyond.

It will shoulder much of the technical burden of developing and distributing domain-relevant applications for (pre-)exascale through application co-design for exascale technologies, and the provisioning of exascale-oriented libraries and services that nudge the community to adopt battle-tested, future-oriented, scalable workflows and portable technologies. Together, these will allow application developers to pursue domain-relevant scientific innovation without being over-burdened by technical detail, and empower industrial and academic application users to painlessly adopt bleeding-edge technologies from the domain on whatever computational resource they may have access to.

To drive the development of the libraries and services, and to showcase the scientific and industrial potential of truly multiscale approaches, MultiXscale will pursue three pilot 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.

MultiXscale will extend the applications, user-base and domains that are actively engaged in the current CoE and EuroHPC ecosystem by addressing specific and critical needs and advancing the transition towards the use of exascale resources by scientific and industrial users in the multiscale modelling community.

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