

EESSI CI/CD Hackathon successfully organized in Copenhagen following the EuroHPC User Days 2025



This exciting event was organized by EuroHPC CoE MultiXscale in collaboration with CASTIEL2, and EuroCC Denmark bringing together experts and innovators from across Europe to advance the European Environment for Scientific Software Installations (EESSI).

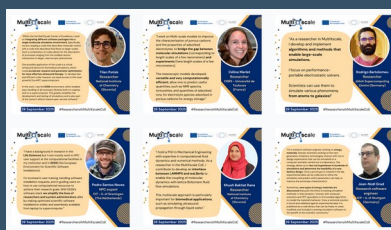
The EESSI CI/CD Hackathon dived deep into the world of Continuous Integration and Continuous Deployment (CI/CD) for scientific software in HPC environments. Participants worked hands-on to improve automation pipelines, streamline software deployment, and contribute to the EESSI ecosystem — a shared infrastructure that simplifies scientific software installation across HPC centers.

[Read More](#)

More news in this issue:



Book of Abstracts of the 2025 ESPResSo Summer School “Systematic coarse-graining and machine learning in soft matter physics with ESPResSo”.



The researchers behind MultiXscale, at the European Researchers' Night, on 26 September 2025.



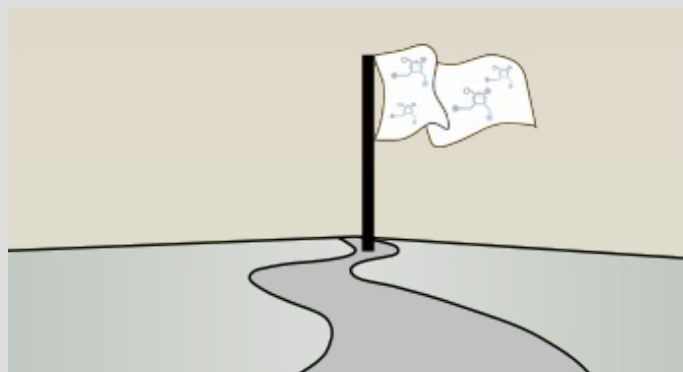
The lectures recorded during the CECAM Flagship Workshop are already available online!



Rethinking scientific applications for exascale and emerging architectures: the Centre of Excellence challenge

2025-12-26

This workshop will be organized in the framework of HiPEAC Krakow, on 27 January 2026. CoE organisers: ChEESE-2P, EoCoE-III, ESIWACE3, ExCELLERAT P2, MaX, MultiXscale, POP3, and SPACE. More details available [here](#).



Milestone Achievement

2025-12-23

We have reached a new milestone by implementing tests for key MultiXscale applications in the EESSI test suite. The current milestone reflects that EESSI test suite, as of [version 0.9.0](#), covers all the key applications developed in WPs 2, 3 and 4 of MultiXscale with a test case. Further info [here](#).

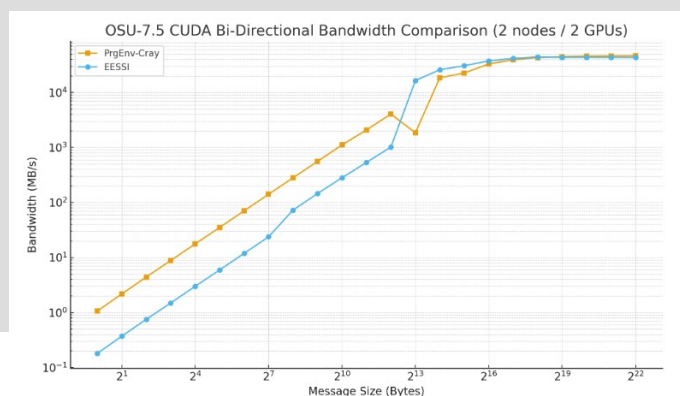


Research Software Engineering Day - RSE Day 2025

2025-12-05

Talk given and poster presented at the event organized by KU Leuven at Campus Arenberg in Heverlee (Belgium).

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MPI at Warp Speed: EESSI Meets Slingshot-11

2025-11-17

In this blog post, we present the requirements for building OpenMPI 5.x with Slingshot-11 support on HPE/Cray systems and its integration with EESSI using the host_injections mechanism of EESSI to inject custom-built OpenMPI libraries. Discover more through this link [here](#).



**TouCAM. 6-7 November 2025 at
Université de Toulouse (France)**
2025-11-11

MultiXscale expert El Hassane Lahrar presented the talk “Towards efficient and accurate simulations of porous carbon based energy storage systems” on Thursday 6th of November 2025, during the TouCAM event, organized in Toulouse (France).

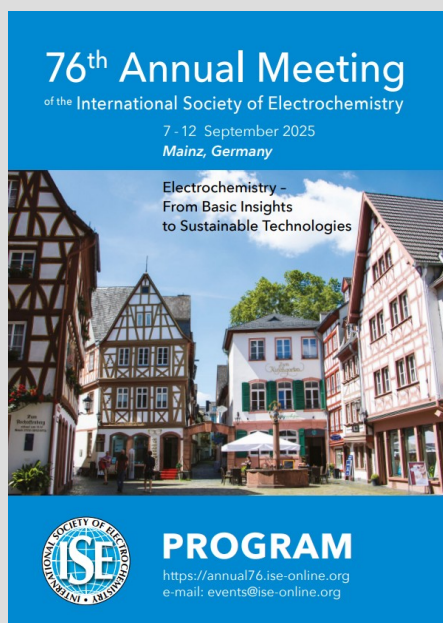
[Read More](#)



**Book of Abstracts of the 2025 ESPResSo
Summer School “Systematic coarse-
graining and machine learning in soft
matter physics with ESPResSo”**
2025-10-20

The ESPResSo summer school is a CECAM flagship school organized every year by the Institute for Computational Physics at the University of Stuttgart to train students and scientists in simulation software for soft matter physics and foster synergies between simulation experts and experimentalists. The 2025 edition focused on coarse-graining and machine learning methods. The event attracted 63 attendees and featured 14 talks and 18 posters.

[Read More](#)



**76th Annual Meeting of the Int. Society of
Electrochemistry. 7-12 September in
Mainz, Germany**
2025-09-15

MultiXscale expert Céline Merlet (CIRIMAT, CNRS – Université de Toulouse, Toulouse, France) gave the keynote talk “Modelling high power devices across scales” on Monday 8th September, during the 76th Annual Meeting of the International Society of Electrochemistry, in Mainz, Germany.

[Read More](#)

The researchers behind MultiXscale, at the European Researchers' Night

2025-09-26

We were excited to shine a light on the incredible work of our MultiXscale CoE team during the European Researchers' Night, on 26 September 2025.

Meet the team of researchers driving innovation behind MultiXscale and discover their key roles in the project:

MultiXscale Co-funded by the European Union EuroHPC

"Within the MultiXscale Center of Excellence, I work on **integrating different software packages into a single multiscale simulation environment**. Specifically, we are coupling a code that describes molecular motion with a code that describes fluid flows on larger scales. Such a combination of codes allows for the description of processes ranging from the smallest atomic interactions to larger, macroscopic phenomena.

One possible application of this code is a virtual ultrasound device for biomedical simulations, which could **accelerate research and parameter optimization for more effective ultrasound therapy**. To develop fast and efficient code, however, we need access to the most powerful EuroHPC supercomputers.

In this work, I use the EESSI environment, which enables easy handling of all necessary libraries both on a laptop and on a supercomputer. This greatly simplifies the development and testing of simulations and is also part of the center's efforts toward open-access software."

Tilen Potisk
Researcher
National Institute of Chemistry (Slovenia)

26 September 2025 #ResearchersAtMultiXscaleCoE

MultiXscale Co-funded by the European Union EuroHPC

"I work on Multi-scale models to improve the characterisation of porous carbons and the properties of adsorbed electrolytes, to **bridge the gap between molecular simulations** (corresponding to length scales of a few nanometers) **and experiments** (here length scales of a few micrometers).

The mesoscopic models developed, **versatile and very computationally efficient**, allow one to predict useful quantities, such as NMR spectra, tortuosities, and quantities of adsorbed ions, for electrolyte species adsorbed in porous carbons for energy storage."

Céline Merlet
Researcher
CNRS - Université de Toulouse (France)

26 September 2025 #ResearchersAtMultiXscaleCoE

MultiXscale Co-funded by the European Union EuroHPC

"As a researcher in MultiXscale, I develop and implement **algorithms and methods that enable large-scale simulations**.

I focus on performance-portable electrostatic solvers.

Scientists can use them to simulate various phenomena, **from atoms to galaxies!**"

Rodrigo Bartolomeu
Researcher
Jülich Supercomputing Centre (Germany)

26 September 2025 #ResearchersAtMultiXscaleCoE

MultiXscale Co-funded by the European Union EuroHPC

"I have a background in research in the **Life Sciences** but I now mostly work in HPC user support at the computational facilities in my institution and in EESSI (the European Environment for Scientific Software Installations).

I'm involved in user training, handling software installation requests, and in guiding users on how to use computational resources to achieve their research goals. With EESSI's software stack **we simplify the lives of researchers and system administrators** alike by making optimized scientific software installations widely and seamlessly available from laptop to supercomputer."

Pedro Santos Neves
HPC expert
CIT - U. of Groningen (The Netherlands)

26 September 2025 #ResearchersAtMultiXscaleCoE

MultiXscale Co-funded by the European Union EuroHPC

"I hold a PhD in Mechanical Engineering with expertise in computational fluid dynamics and numerical methods. As a researcher in the MultiXscale CoE, I contribute to develop an **interface between LAMMPS and waBerla** to enable the coupling of molecular dynamics with lattice Boltzmann fluid flow simulations.

This multiscale approach is particularly important for **biomedical applications**, such as simulating ultrasound propagation through liquid water."

Khush Bakhat Rana
Researcher
National Institute of Chemistry (Slovenia)

26 September 2025 #ResearchersAtMultiXscaleCoE

MultiXscale Co-funded by the European Union EuroHPC

"I'm a research software engineer working on **energy materials**. Domain scientists working on the next generation of battery technologies interact with me to design experiments that can be simulated on a computer and later carried out in a laboratory. This strategy allows us to **test out hypotheses in hundreds of simulations and determine the feasibility of a new battery design**. Once a prototype is created in the lab, experimental data can be collected to refine the simulation and predict which parameters can help us improve the prototype characteristics.

Sometimes, **new types of energy materials are discovered** that push the limits of existing simulation methods; in that situation, I interact with computer scientists and HPC specialists to find suitable algorithms to model the material's behavior. Once a technical solution is found and validated against experimental data, it is published as a code library that can be freely re-used, modified, and included in existing simulation software to the benefit of the scientific community."

Jean-Noël Grad
Research software engineer
ICP - U. of Stuttgart (Germany)

26 September 2025 #ResearchersAtMultiXscaleCoE

MultiXscale Co-funded by the European Union EuroHPC

"The design of helicopter rotors is a complex task as it requires a coupled analysis of the aerodynamic and mechanical behaviour of the elastic rotor blades. This type of analysis is even more delicate whenever the rotor interacts with external obstacles as it occurs during landing in rescue operations.

Leonardo's activity within the MultiXscale project is to develop computational workflows capable of describing the aerodynamic and structural properties of helicopter rotors in this demanding flight configurations, reaching a higher physical accuracy w.r.t. currently used mid-fidelity approaches while keeping an high computational efficiency.

These **simulations** are currently developed exploiting the open-source Lattice Boltzmann solver **waBerla** whose remarkable scalability properties on GPU-based hardware are expected to dramatically reduce the time needed for these aero-structural simulations while offering the necessary high level of physical accuracy required in the rotor design process."

Matteo Zanfagnini
Researcher
Leonardo (Italy)

26 September 2025 #ResearchersAtMultiXscaleCoE

MultiXscale Co-funded by the European Union EuroHPC

"I assist scientists and researchers across **all disciplines, including Humanities**, who use supercomputers in their work.

Together with my colleagues, I strive to **improve access to scientific software** and simplify its use. Our efforts are currently focused on the European Environment for Scientific Software Installations (EESSI), a shared scientific software stack designed to streamline access for researchers."

Lara Peeters
Scientific Software Support
Ghent University (Belgium)

26 September 2025 #ResearchersAtMultiXscaleCoE

MultiXscale Co-funded by the European Union EuroHPC

"I hold a Ph.D. in Mechanical Engineering from the Indian Institute of Technology Bombay and specialize in the **mathematical modelling and numerical simulation** of complex multiscale, multiphysics systems. At the MultiXscale Center of Excellence, I am responsible for the development of cutting-edge Lattice Boltzmann algorithms for **simulating the fluid dynamics associated with helicopters**.

Additionally, I am also involved in the development of performance portable Lattice Boltzmann implementations within the **waBerla** high performance software framework and large-scale numerical simulations on European supercomputing facilities."

Anirudh Jonnalagadda
Researcher
Istituto Italiano di Tecnologia (Italy)

26 September 2025 #ResearchersAtMultiXscaleCoE

MultiXscale Co-funded by the European Union EuroHPC

"Working as a Project Manager at the MultiXscale Centre of Excellence, I am responsible for administrative and financial management, which for example includes monitoring project resources and their utilization, identifying deviations, participating in the preparation of periodic reports, and ensuring that deliverables are delivered on time. In this way, I **make sure that the project is implemented in accordance with the work plan and within the budget**.

As a researcher, I work on the implementation and exploitation of the open-boundary molecular dynamics method as a virtual ultrasound machine. With the latter, ultrasound parameters such as frequency and amplitude can be easily varied and studied in silico, without the need for a patient. This method ultimately provides us with a **powerful tool** that allows us to study the key parameters that determine the **outcome and safety of real biomedical applications in a non-invasive manner**. In addition, I also maintain the MultiXscale website."

Petra Papež
Researcher
National Institute of Chemistry (Slovenia)

26 September 2025 #ResearchersAtMultiXscaleCoE

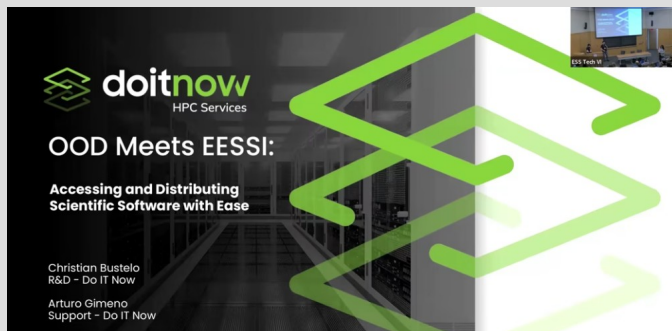
MultiXscale Co-funded by the European Union EuroHPC

"As a Project Coordinator at the MultiXscale Centre of Excellence, I **oversee project implementation**, analyze potential risks and deviations, and, when required, assist in developing strategies for their mitigation. By reviewing project deliverables, I ensure that the work performed is following the project's plan.

Being closely involved in dissemination, communication, and training activities, I **help raise the visibility of MultiXscale within and beyond the EuroHPC ecosystem** and facilitate contacts with stakeholders."

Matej Praprotnik
Project Coordinator
National Institute of Chemistry (Slovenia)

26 September 2025 #ResearchersAtMultiXscaleCoE



The recording of the talk “OOD Meets EESSI” is now accessible on Vimeo platform

2025-09-11

A 2025 Global Open OnDemand Conference presentation entitled ‘OOD Meets EESSI: Accessing and Distributing Scientific Software with Ease.’ The presentation was given by Christian Bustelo and Arturo Gimeno on Wednesday, March 19, 2025, at Harvard University, Cambridge (USA). Access the video [here](#).



The lectures recorded during the CECAM Flagship Workshop are already available online!

2025-09-10

At the CECAM Flagship Workshop “Modeling & Simulation of Fluid-Structure Interactions Across Scales” held at the National Institute of Chemistry in Ljubljana (Slovenia) on 8-11 April 2025, over four inspiring days, we welcomed 55 participants from 10 countries, to explore cutting-edge topics in multiscale modeling for biomedical applications, the transition to sustainable energy and civil transport, AI-enhanced simulation techniques, and HPC workflows. Access the videos [here](#).

EESSI Happy Hour sessions (Mondays, 14:00–15:00 CEST)

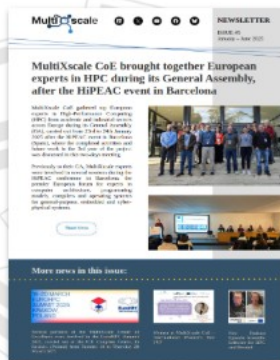
2025-08-13

Join us for EESSI Happy Hour, an informal, weekly online session to explore and discuss key EESSI topics and updates with the community.

Each series will focus on a specific main topic over several sessions, giving participants the opportunity to ask questions, get hands-on guidance, and share experiences.



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Issue 3
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