

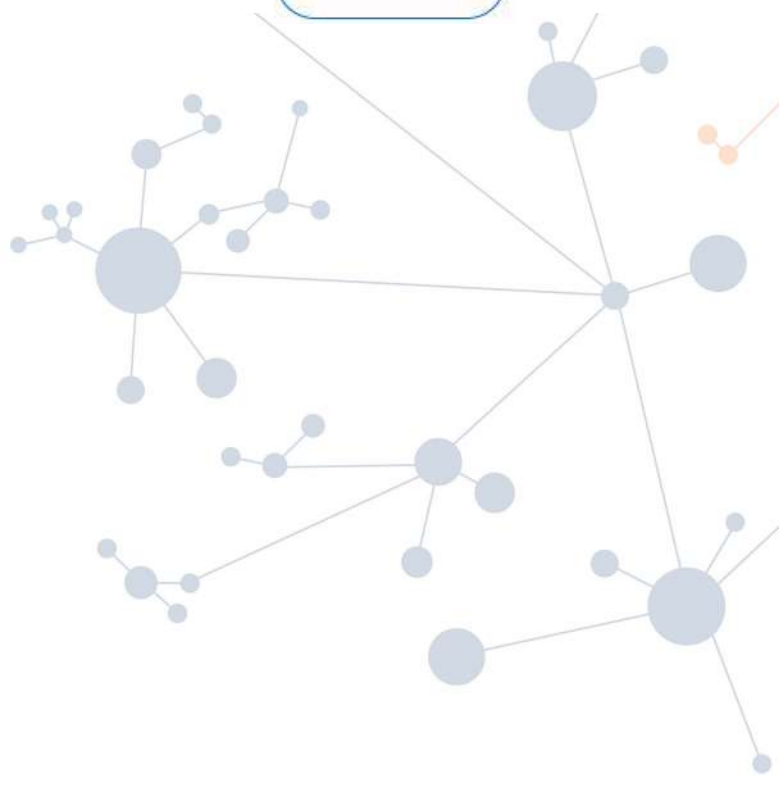
MultiXscale project celebrated its General Assembly 2024 after EuroHPC Summit in Antwerp, Belgium

MultiXscale project gathered a European group of experts on High-Performance Computing (HPC) in its General Assembly (GA), in Antwerp, Belgium from 21 to 22 March 2024.

The main activities to be developed during the second year of this EuroHPC Joint Undertaking funded project were discussed in this two-days meeting, celebrated after the EuroHPC Summit event, organized from 18 to 21 March.

The EuroHPC Summit brought together top experts working in the field of European supercomputing, enabling a perfect place to share the latest technological developments, define synergies, express their current and future needs, and participate in shaping the future of European supercomputing.

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MultiXscale at InPEX Workshop 2024

2024-06-28

The technical manager of MultiXscale (Alan O’Cais) was invited to participate in the 2024 InPEX Workshop, and in particular contributed to the “Software production and management” topic of the workshop. Lively discussions were held as part of that topic with a general agreement that creating a software installation description format could be very useful to encourage collaboration between the various software installation tools being used “in the wild” (at this particular workshop EasyBuild/EESSI, Spack and Guix were represented).

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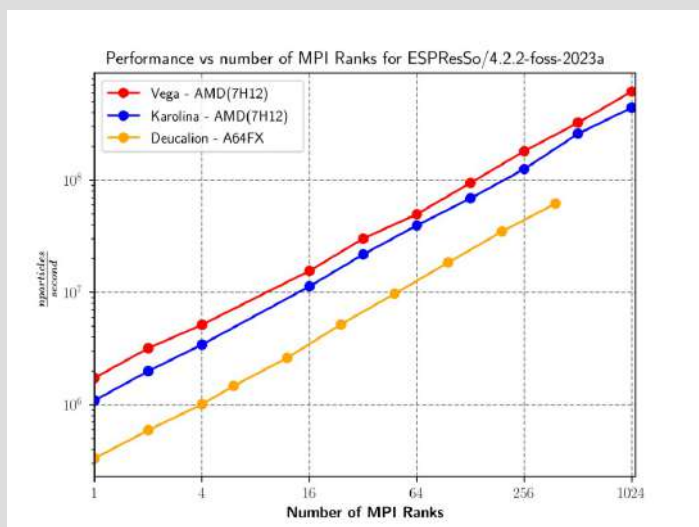


First portable test run on two systems with different architectures

2024-06-28

One of the milestones that we have in MultiXscale is to be able to run the EESSI test suite on at least two different architectures. In the context of EuroHPC that means running on different partitions of the available EuroHPC Supercomputers. Our initial effort focused on getting the test suite portable between two different supercomputers: Karolina and Vega.

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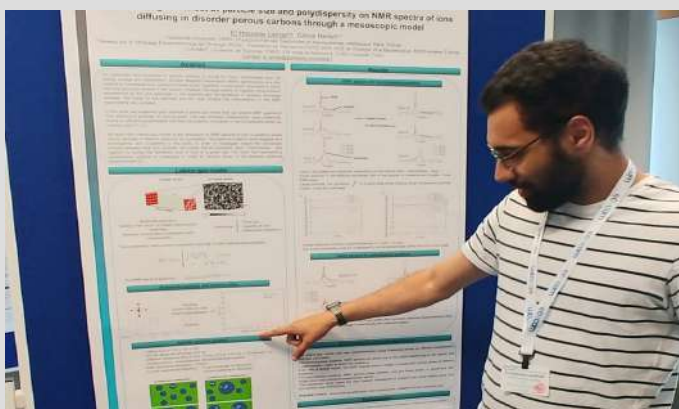


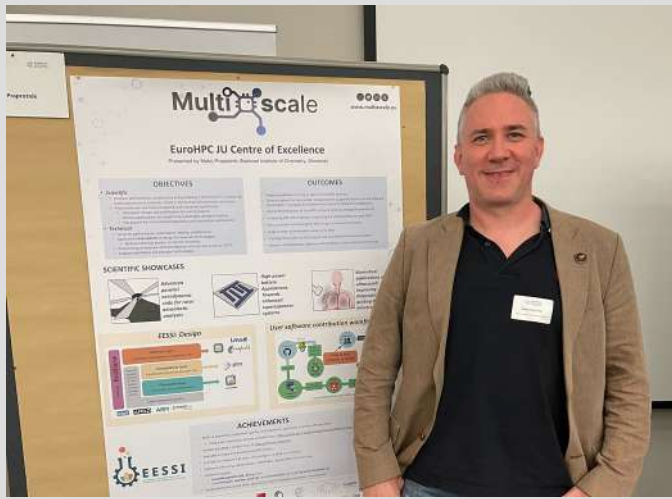
New Paper available at Faraday Discussions Journal

2024-06-19

“Investigating the effect of particle size distribution and complex exchange dynamics on NMR spectra of ions diffusing in disordered porous carbons through a mesoscopic model”. The document is accessible for download [here](#).

The poster was presented at CECAM workshop in Lausanne (Switzerland).





Austrian-Slovenian HPC Meeting 2024 – ASHPC24

2024-06-17

Our coordinator, Matej Praprotnik, gave a talk and presented MultiXscale poster at the Austrian-Slovenian HPC Meeting 2024 – ASHPC24. He also chairs the Program committee.

The event was carried out at Seeblickhotel Grundlsee (Austria) from 11-13 June 2024.

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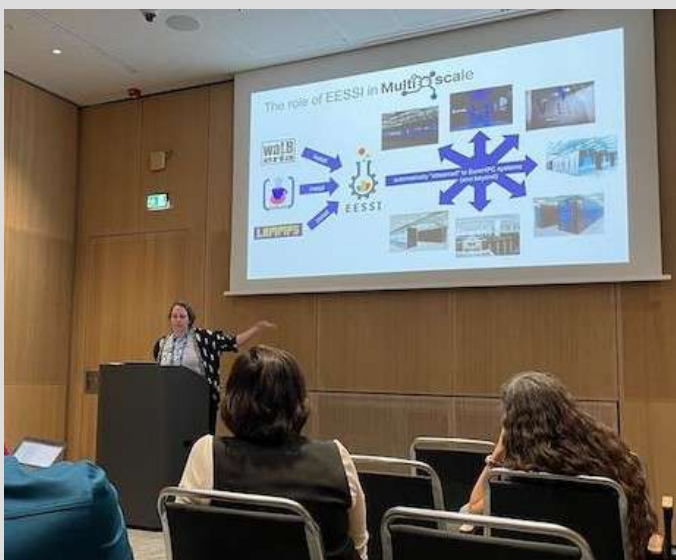
Europa Village space at Teratec Paris

2024-05-30

MultiXscale participated together with other CoEs at the Europa Village space at Teratec Forum, carried out from 29 to 30 May 2024 in Paris (France).

Teratec Forum is the meeting place for high-powered digital experts. Numerical Simulation - HPC/HPDA - Artificial Intelligence - Quantum Computing

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MultiXscale at ISC Hamburg, May 2024

2024-05-23

Several members of MultiXscale CoE participated from 12 to 16 May at the ISC High Performance 2024, in Hamburg (Germany). This event connects public, industry users and technology developers in the fields of High Performance Computing, Machine Learning, Data Analytics & Quantum Computing.

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University of Stuttgart
Institute for Computational Physics

Simulating soft matter across scales
CECAM Flagship School
October 7-11, 2024, Stuttgart, Germany

This school teaches coarse-grained and lattice-based simulations methods to model soft matter systems at different length- and time-scales using the software ESPResSo and waLBerla.

After an introduction to particle-based simulations and the software interface, we will explore the lattice-Boltzmann method for hydrodynamic interactions, machine-learned effective potentials, coarse-grained ionic liquids, polymers, and electrokinetics and catalysis with diffusion-advection-reaction solvers.

Lectures are followed by hands-on sessions tutored by developers of the software. Hence, users can get advice on their specific simulation projects.

Research talks will illustrate practical applications of the simulation software and provide further background in the field of multiscale simulations.

Attendance is free of charge. To apply and submit a poster abstract, follow the registration link below and write a short motivation + CV.

Invited speakers:
Timm Krüger, University of Edinburgh (United Kingdom)
Tristan Berau, University Heidelberg (Germany)
Christine Peter, University of Konstanz (Germany)
Frederik Hennig, University of Erlangen-Nuremberg (Germany)
Matej Praprotnik, National Institute of Chemistry (Slovenia)
Pablo M. Blanco, Norwegian University of Science and Technology (Norway)

Registration link: <https://www.cecami.org/workshop-details/1324>

Logos: MultiXscale, CECAM, DFG, ESPResSo, Institute for Computational Physics

ESPResSo Summer School, “Simulating soft matter across scales”, October 7-11, 2024, Stuttgart, Germany

2024-05-13

We invite all interested to attend the ESPResSo summer school “Simulating soft matter across scales” on October 7-11, 2024, University of Stuttgart, Germany. The school will focus on coarse-grained and lattice-based simulations methods to model soft matter systems at mesoscopic length and time scales. Attendance to the summer school is free of charge. You can submit a poster abstract until September 1, 2024.

[Read More](#)



HPC Knowledge Portal annual meeting – HPCKP24 Barcelona

2024-05-09

Alan O’Cais, technical manager of MultiXscale, presented “Streaming scientific software has never been so EESSI” at HPCKP24 event, carried out from 8 to 9 May in Barcelona (Spain). HPC Knowledge Portal motivates new initiatives and collaborations in the HPC, AI and Quantum Science fields, enabling fluent communication and interaction with key active members of the HPC community.

More information about the event: [here](#)



9th EasyBuild User Meeting from 23-25 April 2024, at Umeå, Sweden

2024-04-25

Lara Peeters kicked off the 3rd day of the 9th EasyBuild User Meeting with an introduction to EESSI.

The recording is available on YouTube through [this link](#).



15th Annual HPC-AI Swiss Conference

2024-04-17

Danilo González gave the talk "Science Made EESSI: From Desktop to HPC/Cloud, The Benefits of an Agnostic Appstack" at the 15th Annual HPC-AI Swiss Conference, celebrated at Palacinema, in Locarno, Switzerland, from 15 to 17 April 2024.

More information about the event is available [here](#).



4th Baltic HPC and Cloud Computing Conference

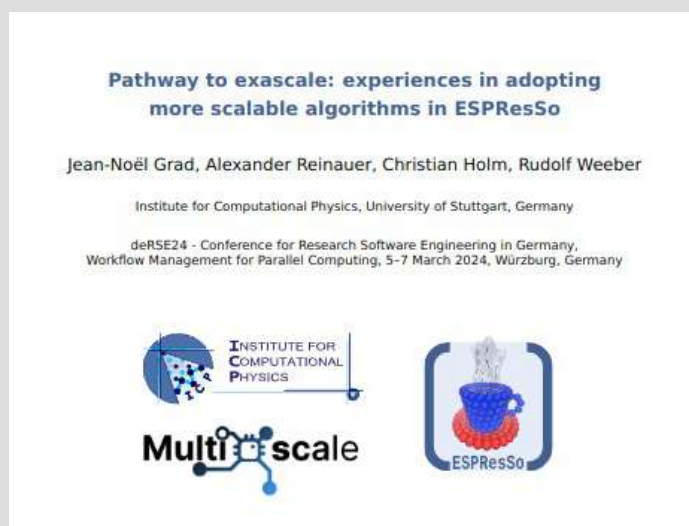
2024-04-15

MultiXscale CoE contributed with a poster at the 4th Baltic HPC and Cloud Computing Conference, carried out in Riga (Latvia), from 11 to 12 April 2024.

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deRSE24 – Conference for Research Software Engineering in Germany, Würzburg

2024-04-11



Jean-Noël Grad shared his experience improving the scalability of the software ESPResSo with applications in energy storage for MultiXscale[2] and using the EESSI GitHub Action to automatically test software and executable papers in the cloud. Dörte Carla Stenel presented the NHR Alliance, a German HPC organisation that assists domain scientists in applying for compute time, organises HPC conferences and summer schools, and provides HPC training via courses, workshops and fully-funded three-year PhD scholarships.

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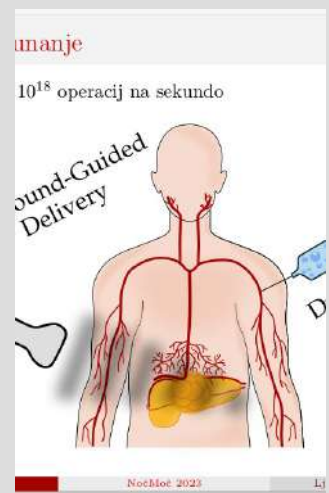
MultiXscale at EuroHPC Summit in Antwerp, Belgium 2024-03-13

During the week of 18-21 March 2024, the EuroHPC community was gathered in Antwerp (Belgium) for the EuroHPC Summit. Partners of the MultiXscale EuroHPC Centre-of-Excellence were actively involved with various aspects of the program.

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New section on MultiXscale website:

In this section, you can download the [MultiXscale dissemination material](#):



Subscribe to our newsletter

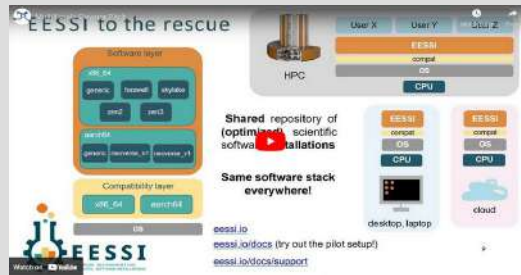
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Elevator Pitch



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MultiXscale | Center of Excellence

Funded by the European Union, the European High Performance Computing Joint Undertaking (JU) and countries participating in the project under grant agreement No 101093169.

