

MultiXscale at EuroHPC User Day 22-23 October, in 2024 Amsterdam



MultiXscale CoE will be involved in two sessions at the EuroHPC User Day 2024, carried out from 22 to 23 October 2024 in Amsterdam:

- Tuesday, 22 October 2024, 14:00-15:30 CEST, Kenneth Hoste gave a short presentation on MultiXscale and EESSI during the “HPC ecosystem tools” (parallel) session.

- Wednesday, 23 October 2024, 10:30-12:00 CEST, promotion of MultiXscale and demonstration of EESSI during the “Application Support & Skills” walk-in networking session, including a small prize giveaway with a Raspberry Pi 5 starter kit.

We are already looking forward to engaging with the EuroHPC user community next year in Denmark 2025!



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More news in this issue:



EESSI has been recognized with an HPCwire Award!



Book of Abstracts of the 2024 ESPResSo Summer School “Simulating soft matter across scales” [here](#)



Video of the first Ambassador event organized in collaboration with NCC Austria and Slovenia, on 4 October 2024, is already available on our YouTube channel [here](#)

EESSI has been recognized with an HPCwire Award!

EESSI (European Environment for Scientific Software Installations) has received the HPCwire Readers' Choice Award for the Best HPC Programming Tool or Technology!

This prestigious recognition celebrates the groundbreaking work of EESSI and MultiXscale, showcasing their significant impact on the HPC community.

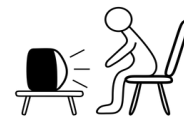
A heartfelt thank you to everyone who contributed their dedication and expertise to push the boundaries of scientific software installations. This award is a true testament to what we can achieve together! Thank you very much to EuroHPC JU for the ongoing support for MultiXscale and EESSI, and thanks to everyone who voted for EESSI!

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Best HPC Programming Tool or Technology

European Environment for Scientific Software Installations (EESSI)



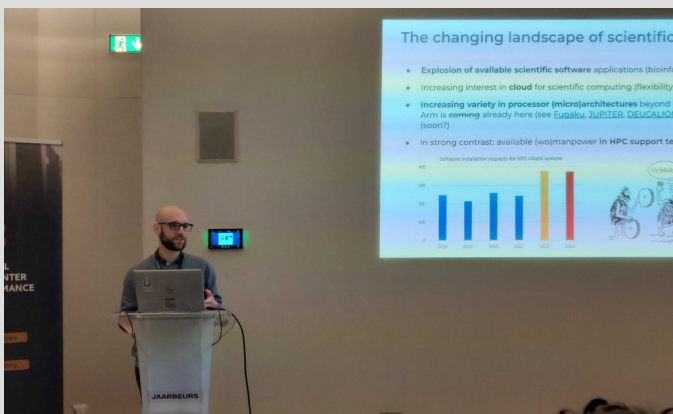
MultiXscale will participate in the following sessions at HiPEAC Barcelona 20-22 January 2025:

- EESSI: European Environment for Scientific Software Installations

This tutorial covers installing and configuring CernVM-FS, the usage of EESSI, installing software into and on top of EESSI, and advanced topics like GPU support and performance tuning. More information [here](#).

- Special CoEs Session

At the upcoming HiPEAC25 conference, the European Centres of Excellence (CoEs) will host two special workshops to delve into the world of HPC while appraising the contributions of women experts in the field. More information [here](#).



SURF Advanced Computing User Day 2024-12-23

“Keeping it Simple, Keeping it #EESSI: Updates from 2023-2024” by Pedro Santos Neves at SURF Advanced Computing User Day, on 12 December 2024, in the Jaarbeurs, Utrecht.

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EESI in the Dutch Federated Computing and Data works

2024-11-19

Bob Dröge presented the European Environment for Scientific Software Installations (#EESI) in the Dutch Federated Computing and Data workshop, organized by EuroCC Netherlands and SURF’s Innovation department.

[Read More](#)



European Environment for Scientific Software Installations (EESSI) Community BoF at Supercomputing Atlanta 2024

2024-11-19

Birds of a Feather (BoF) session organized on Tuesday, 19 November 2024, from 12h15 to 13h15 by MultiXscale members at Supercomputing Atlanta 2024, the International Conference for High Performance Computing, Networking, Storage, and Analysis.



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NRIS Talks : How to build on top EESSI using EasyBuild

2024-11-18

This webinar, organized by the Norwegian Research Infrastructure Services, as part of it's outreach program NRIS Talks, showed how to use EasyBuild to build (scientific) software on top of EESSI for all users, for a specific project account or individual users.



[Read More](#)

EPICURE Webinar: Streaming Optimised Scientific Software: an Introduction to EESSI

2024-11-14

This webinar covered the design and usage EESSI, different ways to accessing EESSI, how to add software to EESSI, and highlight some more advanced features including support for NVIDIA GPUs and facilitating the deployment of pre-release builds of scientific software.



[Read More](#)



Video of the first MultiXscale Ambassador event online!

2024-11-12

The video of the first Ambassador event organized in collaboration with NCC Austria and Slovenia, on 4 October 2024, is already available on our YouTube channel [here](#).



MultiXscale CECAM Webinar Video Now Available!

2024-11-12

We're excited to announce that the recording of our recent MultiXscale CECAM webinar: Supporting the Development of Multiscale Methods via the European Environment for Scientific Software Installations (EESSI) is now available to view [here](#)!

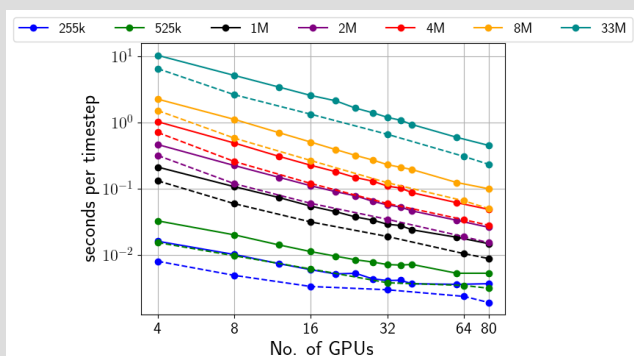


Exascale Day: Inspiring Future Scientists

2024-10-22

To celebrate Exascale Day, the MultiXscale CoE in partnership with NCC Slovenia and SLING, opened the doors of the National Institute of Chemistry (NIC) to students from local primary and high schools.

[Read More](#)



Pre-exascale Workloads of DPD Fluid Simulations Using OBMD on EuroHPC Vega System – Achieving Another Milestone in MultiXscale

2024-10-18

We are excited to announce the successful completion of Milestone 5 in the MultiXscale project: “WP4 Pre-exascale workload executed on EuroHPC architecture”.

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Book of Abstracts of the 2024 ESPResSo Summer School “Simulating soft matter across scales”

2024-10-17

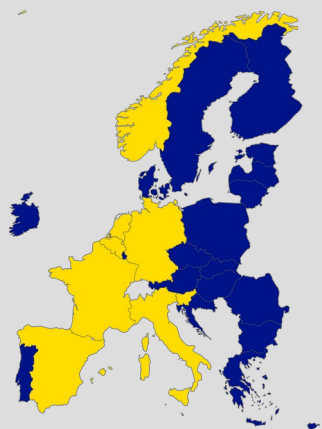
The conference contributions have been collected into [this book of abstracts](#). The talk slides can be obtained from [the event website](#), and recorded lectures are available on the [YouTube channel](#).



Code for Thought podcast: “HPC software installations made EESSI”

2024-10-15

In the latest episode, MultiXscale project members Kenneth Hoste and Alan O’Cais discussed about EESSI and how it can help make scientists more productive...and reduce the technical burden of working with HPC resources. [Click here to access the episode](#).



CI workflow leveraging EESSI

2024-10-11

EESSI’s CI workflows are available on GitHub Actions and as a GitLab CI/CD component. Enabling this is as simple as adding EESSI’s CI to your workflow of choice, giving you access to the entire EESSI software stack optimized for the relevant CPU architecture(s) in your runner’s environment.

[Read More](#)



OpenModel Exploitation Workshop in Hamburg (Germany)

2024-10-03

Our coordinator, Matej Praprotnik from Kemijski inštitut – National Institute of Chemistry, was invited to present MultiXscale CoE at the OpenModel Exploitation Workshop, on 18 September, in Hamburg (Germany).

[Read More](#)



MultiXscale at the Nordic Industry Days 2024-09-25

Alan O 'Cais presented MultiXScale and EESSI as part of the Nordic Industry Days 2024 – Supercomputing the gateway to AI, which took place 2-3 September 2024 in Copenhagen.

Watch the video [here](#).



Leveraging EESSI for SKA Radio Astronomy Data on Global SRCnet Infrastructure 2024-08-21

In collaboration with the SKA project, we demonstrated the successful use of European Environment for Scientific Software Installations (EESSI) to run radio astronomy analyses on the globally distributed SRCnet infrastructure. More information [here](#).



Extrae available in EESSI 2024-07-26

Thanks to the work developed under MultiXscale CoE we are proud to announce that as of 22 July 2024, Extrae v4.2.0 is available in the EESSI production repository software.eessi.io, optimized for the 8 CPU targets that are fully supported by version 2023.06 of EESSI. This allows using Extrae effortlessly on the EuroHPC systems where EESSI is already available, like Vega and Karolina. More information [here](#).

Using EESSI in GitHub Action workflows 2024-07-23

GitHub workflows are routinely used to execute test suites, generate and deploy software documentation, and run executable papers. As a real-world example, we will explore pyMBE3, a molecular builder that simplifies and automates the creation of complex molecular models in the molecular dynamics engine ESPResSo.



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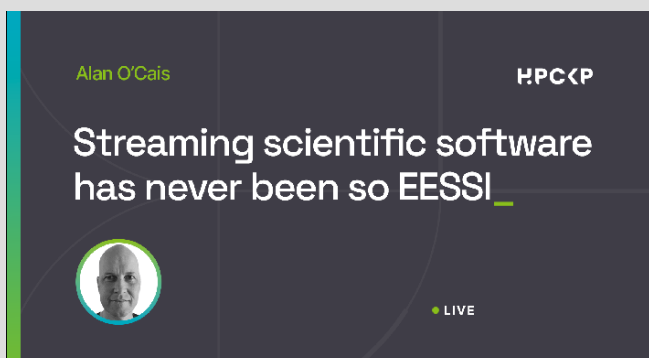


pyMBE: The Python-based molecule builder for ESPResSo

2024-07-18

We are happy to announce the first release of pyMBE, an open-source Python package designed to facilitate the design of custom coarse-grained models of polyelectrolytes, peptides and proteins in ESPResSo (<https://doi.org/10.5281/zenodo.12102635>).

[Read More](#)



HPC Knowledge Meeting – HPCCKP Barcelona, May 2024

2024-07-17

The recording and presentation of the talk “Streaming scientific software has never been so EESSI”, by Alan O’Cais, at HPCCKP’24 Barcelona are already available online [here](#).

New MultiXscale social media corporate profile on Bluesky !!

Follow us [here](#)





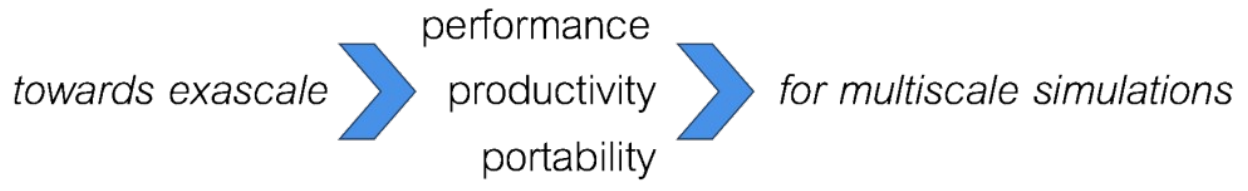
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MultiXscale | Center of Excellence
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