

1st Year of MultiXscale project



MultiXscale is a EuroHPC JU Centre of Excellence in multiscale modelling. It is a collaborative 4-year project between the CECAM network and EESSI that will allow domain scientists to take advantage of the computational resources that will be offered by EuroHPC.

You can download our poster [here](#)

Partner Networks:



EuroHPC Centre of Excellence
Presented by Alan O'Caís (University of Barcelona), Thomas Rößlitz* (University of Bergen)

OBJECTIVES	OUTCOMES
<ul style="list-style-type: none"> Scientific <ul style="list-style-type: none"> Increase performance, productivity and portability ("the Three P's") across the entire spectrum of scientific activity in the domain of multiscale simulation Pilot multiscale use cases of societal and industrial significance: <ul style="list-style-type: none"> Hydrogen design and certification for safe transport Battery applications to support the sustainable energy transition, optimized for non-invasive diagnostics and biomedical applications. Technical <ul style="list-style-type: none"> Focus on performance, automation, testing, collaboration Application and system co-design for multiscale technologies Reduce technical barriers in domain scientists Provisioning of multiscale-oriented libraries and services (such as CUDAS) Scalable workflows and portable technologies. 	<ul style="list-style-type: none"> Project workflows running at scale on EuroHPC systems Dramatic growth in the number of applications supported by the shared software stack (EESSI – European Environment for Scientific Software Installations) Accelerated adoption of EuroHPC compute services among the community Increasing HPC sites explicitly supporting the shared software stack EESSI Cloud providers promoting the EESSI stack in cloud environments Large number of developers using our CI tools Training Panels with our training courses and additional training content Adoption of MultiXscale software and workflows in the industrial community

ACHIEVEMENTS

- EESSI: A streamlined, production-quality, multi-platform, optimized scientific software stack
- Working proof of concept (see <https://eessi.github.io/eessi02023/>)
- Another physics-based, energy issue (<https://github.com/eessi>)
- CentAI-PS, Station 0 @ Univ. of Groningen + four Station 1 servers
- Software (CPU-only): Bioconductor, GROMACS, OpenFOAM, R, TensorFlow, ...
- Hardware targets:
 - jeanrak4.gwdg.de, ABE, K4I (premier)
 - arni1@newell, skylake_jev512, arn16 (arn12,arn13), arn164 (graftron2,graftron3), ppc64le/power9c
- Supported by EuroHPC and HPC4U sponsored credits to develop necessary infrastructure.

EESSI: Design

User software contribution workflow to EESSI

MILESTONES

Partners:



MultiXscale at EuroHPC User Day 11/12/2023 – Brussels, Belgium

The MultiXscale EuroHPC Centre-of-Excellence was explicitly called out at the [EuroHPC User Day](#) as an example that fits quite well in the strategy of the EuroHPC Joint Undertaking, in particular the European Environment for Scientific Software Installations (EESSI) project, which provides the technical backbone for MultiXscale.

NEW VIDEO! - ONLINE TUTORIAL - 05/12/2023



Introduction to EESSI
EUROPEAN ENVIRONMENT FOR SCIENTIFIC SOFTWARE INSTALLATIONS



Alan O'Cais
University of Barcelona/CECAM
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Streaming Optimised Scientific Software: an Introduction to EESSI

Have you ever wished that all the scientific software you use was available on all the resources you had access to, without having to go through the pain of getting them installed the way you want/need?

In [this tutorial](#), we'll explain what EESSI is, how it is being designed, how to get access to it, and how to use it.

We'll give a number of demonstrations and also give access to a resource where you can try EESSI out for yourself.

NEW VIDEO! - ONLINE TUTORIAL - 04/12/2023



Best Practices for CernVM-FS in HPC

online tutorial
Mon 4 Dec 2023

Best Practices for CernVM FS in HPC

[Introductory tutorial](#) to CernVM-FS, the CernVM File System, with a focus on employing it in the context of High-Performance Computing (HPC).

In this tutorial you will learn what CernVM-FS is, how to get access to existing CernVM-FS repositories, how to configure CernVM-FS, and how to use CernVM-FS repositories on HPC infrastructure. Tutorial website: click [here](#)



EESSI
EUROPEAN ENVIRONMENT FOR SCIENTIFIC SOFTWARE INSTALLATIONS

Did you know that the production repository of [EESSI](#) is available *by default* in CernVM-FS since 20 November 2023?

If you have access to a Linux system that has CernVM-FS installed, try it yourself by running the following shell command:

```
source /cvmfs/software.eessi.io/versions/2023.06/init/bash
```

More information: [here](#)

NEW VIDEO!

Making scientific software EESSI - and fast

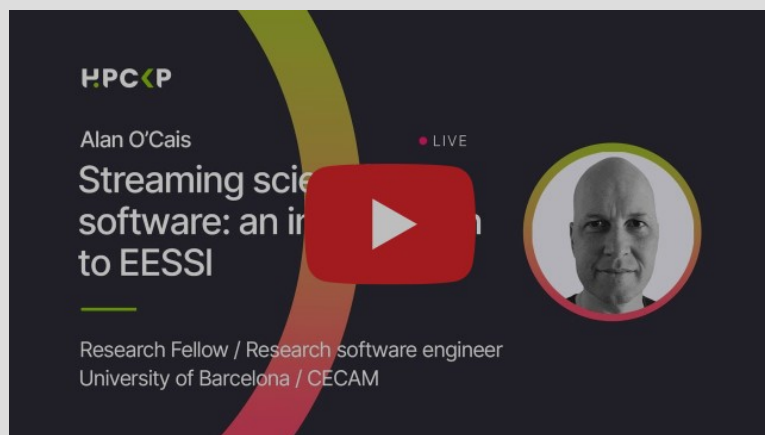


Scientific software is almost defined by its complexity. But just because it was hard to write doesn't mean it should be hard to build and even harder to run well. EESSI is a project that aims to change that by making architecture-specific binaries available to be streamed to your machine or your cluster, just by reaching out and asking it for them. Kenneth and Alan - two leaders from the EasyBuild and EESSI projects - came to show us what this idea is, and how it works. Genius.

You can get more information about the project at <https://eessi.github.io/docs/> or by joining their slack at <https://www.eessi-hpc.org/join> and getting involved.

NEW VIDEO!

Streaming scientific software: an introduction to EESSI



Have you ever wished that all the scientific software you use was available on all the resources you had access to without having to go through the pain of getting them installed the way you want/need? The European Environment for Scientific Software Installations (EESSI – pronounced “easy”) is a common stack of scientific software installations for HPC systems and beyond, including laptops, personal workstations and cloud infrastructure. In many ways it works like a streaming service for scientific software, instantly giving you the software you need, when you need it, and compiled to work efficiently for the architecture you have access to.

During this tutorial, we explain what EESSI is, how it is being designed, how to get access to it, and how to use it. We also give a number of demonstrations that you can try out for yourself.



- In the media:

15/06/2023 – HPC Tech Shorts – Making scientific software EESSI – and fast

30/03/2023 – HPCNow! website – MultiXscale EuroHPC funded project launched to increase the productivity of software and workflows for scientists working in the field of multiscale simulation

23/03/2023 – RTV 365 – Znanost in tehnologija

23/03/2023 – STA – Chemistry Institute spearheading EUR 6m multiscale simulation project

23/03/2023 – STA – Nov Center odličnosti MultiXscale na kemijskem inštitutu za pospešitev prehoda na superračunalniške vire

22/03/2023 – Sio1NET – Slovenski superračunalniški prispevek k reševanju svetovno pomembnih vprašanj

27/01/2023 – HPCNow! website – HPCNow! takes part in the New Centre of Excellence MultiXscale

26/01/2023 – NIC website – New Centre of Excellence MultiXscale

26/01/2023 – EuroHPC JU website – Kick-off of 10 Centres of Excellence in HPC to support the transition towards exascale

26/01/2023 – HPCwire – EuroHPC Announces Launch of 10 Centers of Excellence

- Newsletters:

MultiXscale Newsletter Issue 1 2023

- Press Releases:

MultiXscale EuroHPC funded project launched to increase the productivity of software and workflows for scientists working in the field of multiscale simulation.

- Posters

“Genomics made EESSI: from HPC to cloud, the benefits of a shared appstack”, by Erica Bianco at the XI Symposium of Bioinformatics and Genomics, 15-16 December 2023, in Barcelona (Spain)

MultiXscale Poster at the European Corner of the European Researchers' Night, September 2023 (Nit Europea de la Recerca)

MultiXscale NEWSLETTER
ISSUE #1 2023

MultiXscale EuroHPC funded project launched to increase the productivity of software and workflows for scientists working in the field of multiscale simulation

The National Institute of Chemistry in Ljubljana, Slovenia, hosted from 23rd to 24th March the kick-off meeting of MultiXscale project, one of the new 10 Centres of Excellence funded by the European High Performance Computing Joint Undertaking (EuroHPC JU) to support research and innovation actions that will develop and adapt HPC applications for the exascale and post-exascale era. Funded for a period of four years, MultiXscale gathers 13 partners joining from the academic and industrial sectors across Europe.

Read the press release [here](#)

- Deliverables

- D8.2 – Project data management plan
- D8.3 – Project collaboration plan
- D2.1 – Report on the current scalability of ESPResSo and the planned work to extend it
- D7.1 – Dissemination and Communication Plan



- Training

“One scientific software stack for all systems, that’s EESSI”, by Bob Dröge, at The Power of “High-Performance Computing session” SURF Advanced Computing User Day, 7 December 2023, in Amsterdam (The Netherlands)

“Streaming Optimised Scientific Software: an Introduction to EESSI”, 5 December 2023, Online

“Best Practices for CernVM-FS in HPC”, 4 December 2023, Online

Presentation on MultiXscale and EESSI, by Alan O’Cais, at CATIEL2’s fifth Code of the month, 28 November, Online

“Magic Castle: Terraforming the Cloud to Teach HPC”, at SC23, 12 November 2023, in Denver (USA)

ESPResSo Summer Schools, 9-13 October 2023, Stuttgart University, in Germany

“About EESSI – European Environment for Scientific Software Installations”, by Helena Vela, at WHPC 1st MAR chapter Workshop, 9 October 2023, in Barcelona (Spain)

“Distributing software the #EESSI way”, by Caspar Martijn van Leeuwen, at CompBioMed2023 Conference, 12 September 2023, in Garching (Germany)

NCC Training Coffee Break, by Alan O’Cais, 7 September 2023, Online

“When Portability and Reproducibility also meets Performance”, by Jordi Blasco, at ALCS2023, 15 June 2023, in Canberra (Australia)

EasyBuild/EESSI UK workshop, 27-28 April 2023, in London (UK)

“EESSI: status update”, by Caspar van Leeuwen, at 8th EasyBuild User Meeting, 25 April 2023, in London (UK)





ISC

High Performance

MAY 21 – MAY 25, 2023 | HAMBURG, GERMANY



Elisabeth Ortega presented EESSI and MultiXscale at EuroHPC Joint Undertaking booth B20 at ISC Hamburg, on May 23rd, 2023



Contact Us:

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