

EPICURE and Containers, activities in EuroHPC

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EuroHPC
Joint Undertaking

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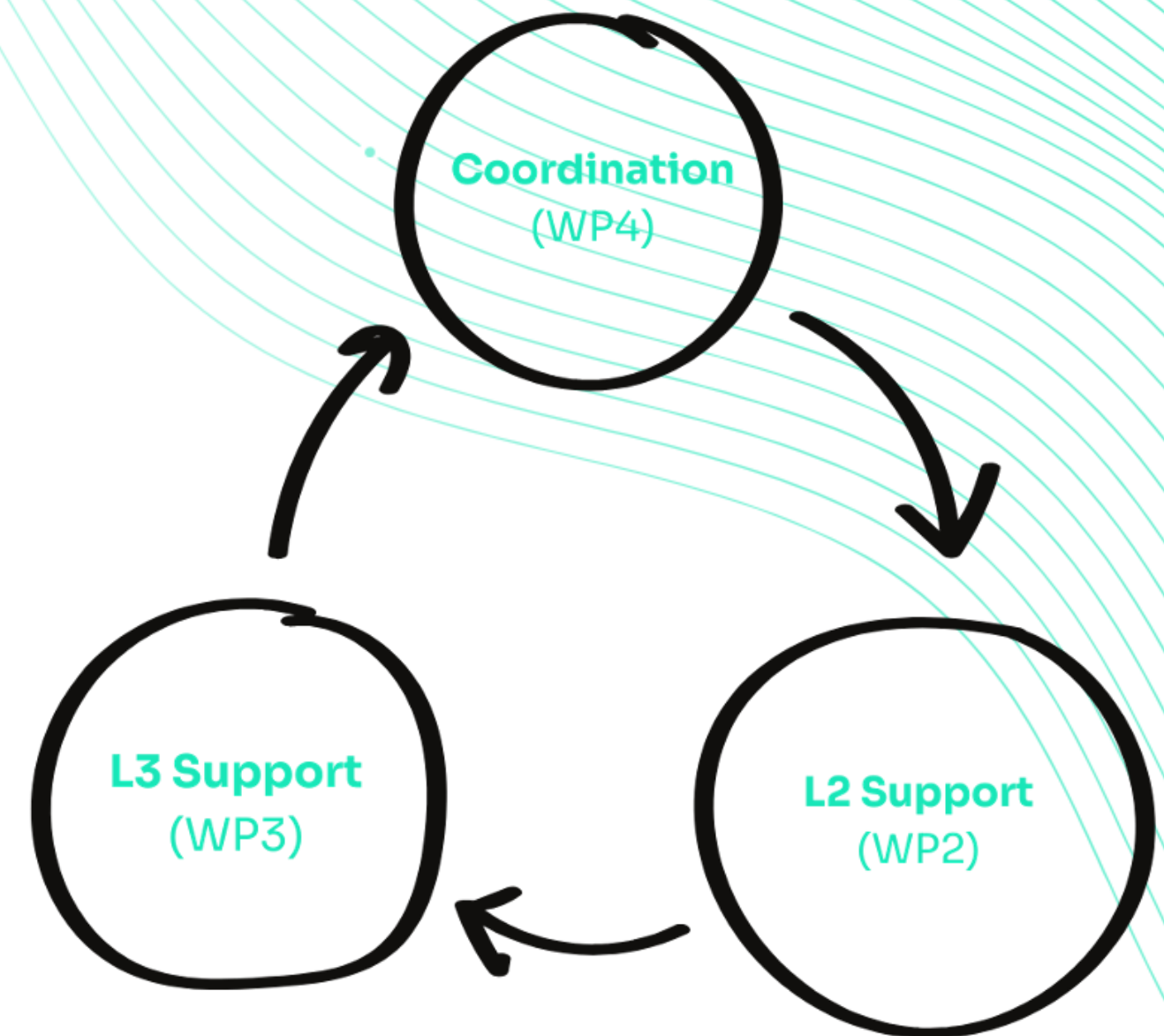
What is EPICURE?

EPICURE draws on the **experience** and **knowledge** of the current and future EuroHPC supercomputer hosting organisations to provide better user support

- Adequate code installation and porting to different architectures (**Level 2**)
- Intra- and inter-node optimisation, focusing on accelerators and scalability (**Level 3**)

Knowledge exchange through the organisation of hardware-specific **training, hackathons, webinars, and workshops** in several EU countries

- Promotes **sharing of expertise** among hosting organisations
- Provides users with a wide knowledge pool



EPICURE and containers

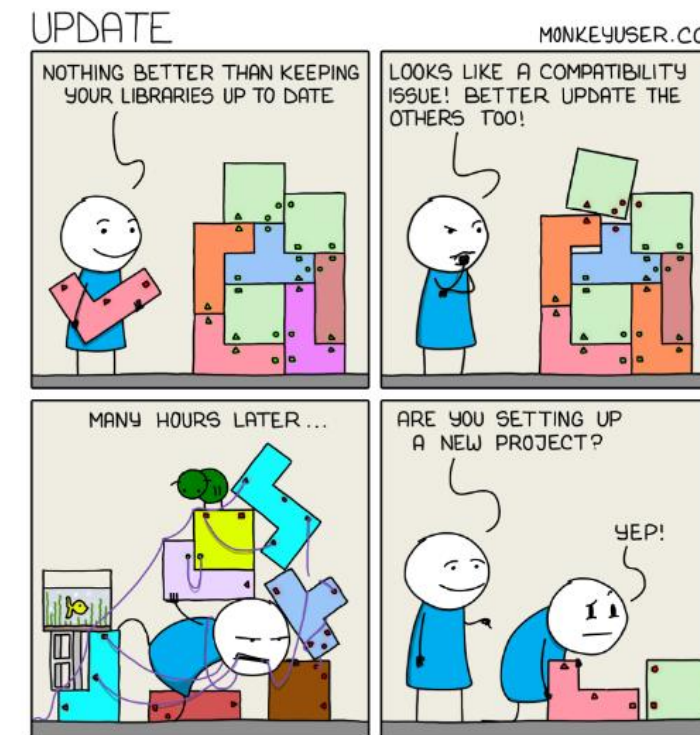
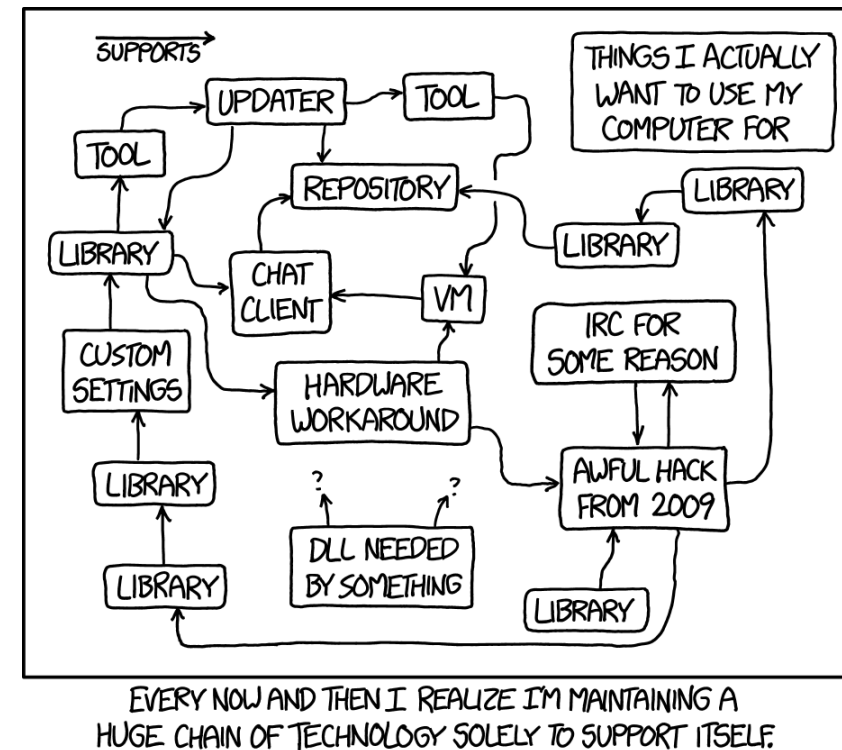
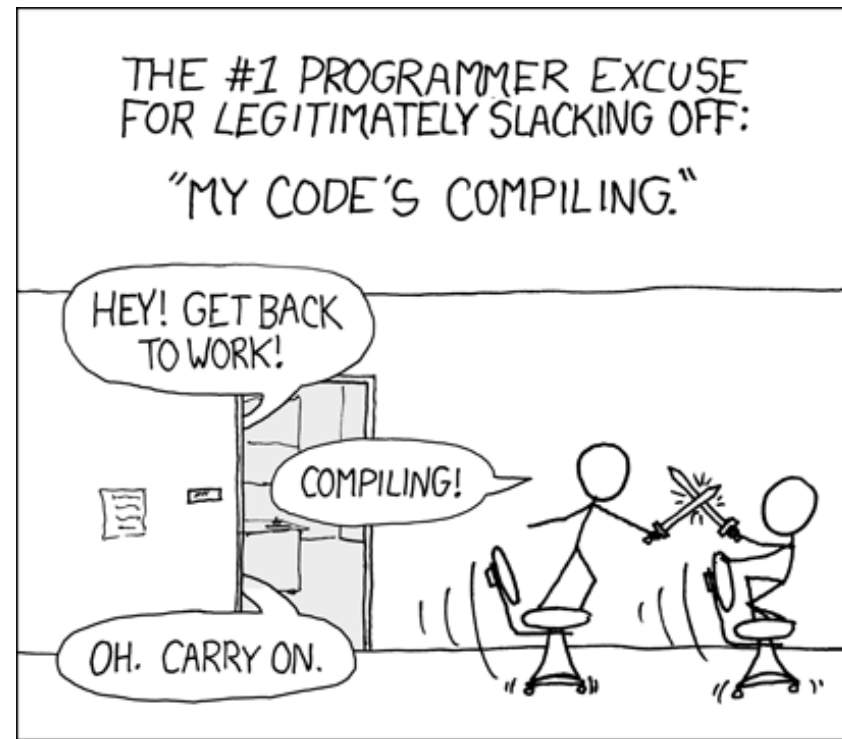
From project proposal:

When possible, **provide containerized applications** or the receipts used to compile the software to be **distributed among sites**, in order to provide a similar software stack between machines sharing the same architecture.

To facilitate deployment on multiple systems we will consider improving or developing recipes for deployment systems such as EasyBuild and Spack, and the **development of containerized installations** that are good solutions to move between systems with a very similar architecture. The different hosting sites participating in this task will **share** the recipes to build the software and **the container images** with the other sites and with the EuroHPC user community.

Guidelines for using containers: Which conditions should containers satisfy to run efficiently on a system, or what should be taken into account when building a container that also has to run efficiently on that architecture or system.

Building scientific software



- code **lacking comments**
- no examples
- lack of detailed documentation
- often written by **scientists-turned-coders**
- not supported/developed anymore
- **non-standard** installation (usually time consuming)
- **dependency hell**

Why containers?

- portability/adaptability/reproducibility of SW
- legacy SW = hard/not possible to build
- definition file acts as SBOM/documentation (dependency management)
- users can make their own (--fakeroot)
- comparable to bare-metal
- run on different EuroHPC clusters

industry = **BYOC**(ontainer)

- different requirements, quality assurance
- workflow isolation, reproducibility, transferability



Problems

- container is not comparable to bare-metal
- lack of skills, technical knowledge
- MPI integration
- HEs sometimes hesitant to support containers (potential security issues)

... and solutions

- EPICURE! technical cooperation/collaboration
- offer (national) image registry
- optimized container images for architecture
- building on top of optimized images
- + EuroHPC container forum, CoEs, NCCs



Current status

- **per-project basis**
- Project #6: provided container image with Python software stack for use on LUMI (**VASP, LAMMPS**)
- Project #13: optimized **PyTorch** distributed communication package for use on Leonardo (resolving NCCL issues)
- Project #53: provided guidance for deploying **AlphaFold** using container on MareNostrum5
- Project #55: working on providing optimized container for **Nemo** for use on Leonardo
- Project #66: deployed **VLLM** in a Singularity container for use on MareNostrum5
- Project #67: created an image that encapsulates the entire build environment, including all dependencies, libraries, and compilers
- Project #95: scalability tests with **CALICO** container, up to 64 nodes on LUMI
- Project #99: prepare **PyTorch** container including HDF5 to use on LUMI

Consortium



Current status



- prepared a webinar on containers as part of WP5 (Training)



WEBINAR: Containerization in HPC Environments



March 31, 2025
11 a.m. (CET)
Online

Teo Prica | IZUM (HPC Vega)

The webinar on basic containerisation for HPC environments provided an overview of key tools and techniques. It covered how to use Singularity/Apptainer containers from various aspects, such as parallelisation with MPI and CUDA for GPU-accelerated workloads and including management and environment systems such as Conda for managing smaller, lightweight environments. The session emphasised practical strategies to optimise HPC workflows with containerised solutions.

Current status



WEBINAR: Scientific Visualisation at the Argonne Leadership Computing Facility



Silvio Rizzi
Joseph Insley
Victor Mateevitsi

July 10, 2024
4 pm (CET)
Online



WEBINAR: Heterogeneous computing with SYCL and oneAPI on CINECA's Leonardo nne Leadership Computing Facility



Biagio Cosenza
University of Salerno

October 10, 2024
9:30am (WEST)
Online



WEBINAR: Streaming Optimised Scientific Software: an Introduction to EESSI



Kenneth Hoste
Alan O'Cais
Pedro Santos Neves

November 15, 2024
2 pm (CET)
Online



WEBINAR: Building Software With Ease: an Introduction to EasyBuild



Kenneth Hoste
Pedro Santos Neves
Caspar van Leeuwen

December 13, 2024
4 pm (CET)
Online



WEBINAR
Unlocking exascale: a first look at JUPITER



Jolanta Zjupa
Junxian Chew

January 17, 2025
2 p.m. (CET)
Online



WEBINAR: Computational Challenges in Advancing Earth Sciences



Oriol Tintó
Barcelona Supercomputing Center

January 17, 2025
2 p.m. (CET)
Online

Subscribe to
the newsletter!



EPICURE HPC in ARM Architecture Hackathon
4-7 February 2025
Braga, Portugal



EPICURE GPU Hackathon
28-31 October 2024
CINECA, Bologna, Italy



Hackathons

Webinars

Getting EPICURE help

Having a EuroHPC project allocation is required (no national project support can be offered)!

Don't have one yet – we can help you apply!



Check **EuroHPC Access Calls**.



Then apply for **EPICURE support**.



<https://pm.epicure-hpc.eu/support/request/>



EPICURE meets Slovenia

May 29, 2025

Online





EPICURE
Unlocking European-level HPC Support

**T
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M**



Dejan Lesjak
Alja Prah
Sebastien Strban



Samo Miklavc
Teo Prica
Žiga Zebec

Thank you!

Follow us



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