

## Roadmap for the next 10 minutes



The problem: fragmented, adhoc HPC support



The model: what EPICURE is



The flow: how support works end-to-end



Evidence: who it helps + early impact



What's next + ways to engage



Q&A

#### Consortium









VSB TECHNICAL | IT4INNOVATIONS | NATIONAL SUPERCOMPUTING | CENTER















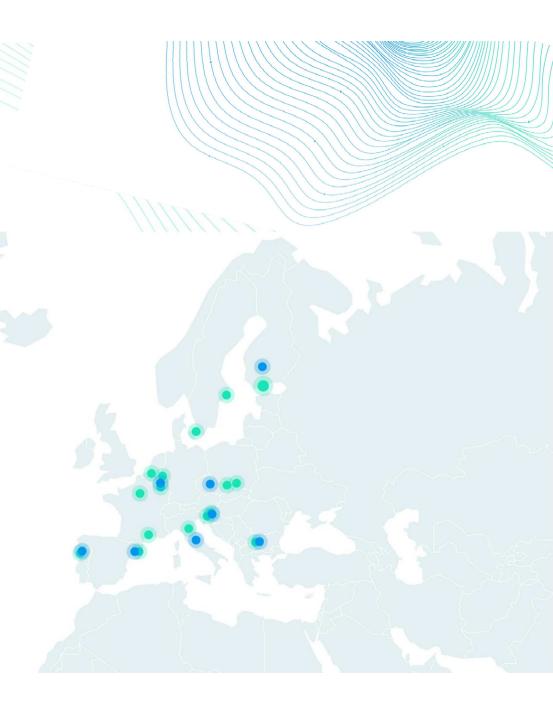












### **EPICURE:** the three pillars

01

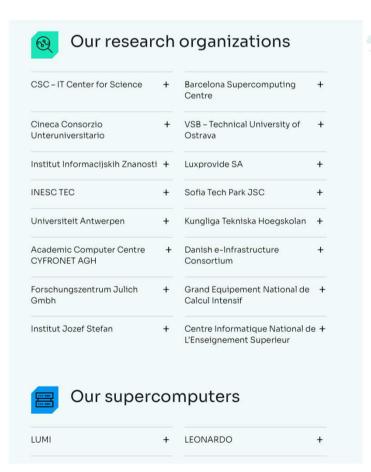
Access — one simple entry point that routes requests to the right experts.

02

Delivery — crosssite teams led by a named lead; timebounded, outcomefocused. 03

Reuse — we package results (containers, playbooks, lessons) so others benefit.

#### **EPICURE:** consortium





#### Who we serve



Academia: researchers, Pls, students, research software engineers.



Industry: startups, SMEs, large R&D teams.



Public labs and national centers collaborating across sites.



Cross-disciplinary communities needing scalable HPC expertise.

## **Operating principles**



User-first scoping and time-bounded engagements.



Reuse by default: document once, apply widely.



Cross-site collaboration with clear roles (lead, contributors, artefact owner).



Transparent metrics and continuous feedback.

## How EPICURE support flows



# **Application Enablement**

Al applications and LLM models support and optimization

Enabling,
Compilation,
porting and
Optimization
Projects

24

Profile, Performance Analysis and Benchmarking

18

HPC Workflow and Job Management, Containerizatio n, Data and I/O

# Example: From methane and iron nanoparticles - catalytic process inside a reactor

- Bottlenecks in the workflow's pre- and post-processing functions
- Update of the Python environment to later version
- Implementation/extension of the unit tests

Simply the update of the python implementation and the replacement of libraries with more efficient ones produced a huge (20x) improvement of the performance.

| Interface       | Old Rbf/old<br>environment | old Rbf/new environment | new Rbf/new environment |
|-----------------|----------------------------|-------------------------|-------------------------|
| Ag(111)/Cu(111) | 54s                        | 12s                     | 11s                     |
| Al(111)/Cu(111) | 1h18m                      | 3m38s                   | 2m12s                   |
| Ti(001)/Mg(001) | > 17h                      | 43m49s                  | 28m27s                  |

| Interface       | serial | parallel |  |
|-----------------|--------|----------|--|
| Ti(001)/V(110)  | 2m12s  | 23s      |  |
| Ti(001)/Fe(110) | 38m45s | 5m33s    |  |
| Ti(001)/Cr(110) | 1h0m1s | 9m4s     |  |
|                 |        |          |  |

catalytic

reactor

# Example: DEAREL: Large-scale Deep rEinforcement leARning for activE fLow control in wings

- Performed in-depth tracing analysis (Nsight) to identify bottlenecks and synchronization issues
- Optimization targeted several kernels (OpenACC Fortran)
  - Memory access patterns (stride, indirect access)
  - Cache utilization
  - · Reduction of atomic operations
  - Improved register utilization
  - Loop optimization
- Significant improvement for parallel construct in save\_hdf5\_restartfile resulting in 1400x speedup

| Kernel Name                | Time Before | Time After | Speedup |
|----------------------------|-------------|------------|---------|
| visc_dissipationRate       | 140.08 ms   | 72.75 ms   | × 1.93  |
| save_hdf5_restartfile      | 542.27 ms   | 370.53µs   | × 1463  |
| eval_laplacian_diag        | 30.51 ms    | 3.41 ms    | × 8.95  |
| full_diffuision_ijk_incomp | 1.21 ms     | 1.18 ms    | × 1.03  |
| smart_visc_spectral_incomp | 2.63 ms     | 785.41 μs  | × 3.35  |
| eval_gradient              | 701.12 µs   | 486.08 μs  | × 1.44  |
| full_convec_ijk_incomp     | 2.53 ms     | 1.40 ms    | × 1.81  |

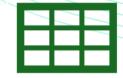
# **Early impact**



Time-to-engagement reduced from X weeks to Y days for intake sprints.



Performance gains of A--B% on key applications after optimisation.

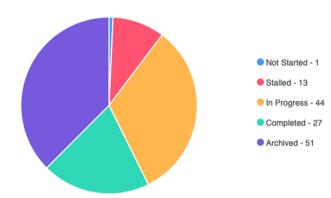


Reusable artefacts (containers, scripts, playbooks) adopted across sites.

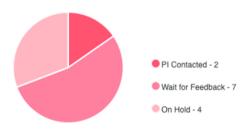
# Portfolio Snapshot (End of M18)



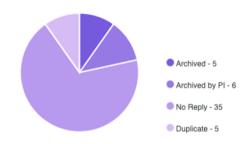




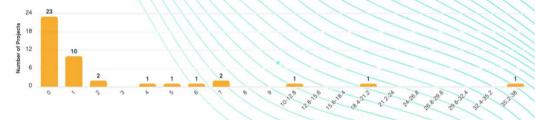
Stalled reasons (n=13)



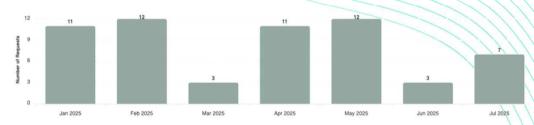
Archived reasons (n=51)



ESM - Assign to Lead Partner or Rejected Avg. time (Days) [N=48]



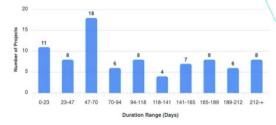
**ESM - User Support Received** 



**ESM - Person-months per project** 



ESM - Project duration (days)



#### **User Feedback Metrics**







## What's next & how to engage



GROW THE EXPERT POOL; LIGHTWEIGHT ONBOARDING AND MATCHMAKING.



PUBLISH A PUBLIC CATALOGUE OF REUSABLE ARTEFACTS AND PLAYBOOKS.



DEEPER INTEGRATION WITH EUROHPC CALLS AND SITE SUPPORT CHANNELS.



CLOSE THE LOOP: SIMPLE USER FEEDBACK, SHARED METRICS DASHBOARD.

### We're Hiring — High Level Support Team

#### **IT4Innovations National Supercomputing Center**

#### What you'll do

- Tackle complex HPC user cases: profiling, scaling, and code optimization.
- Co-design and tune workflows on national/EuroHPC systems.
- Mentor researchers and deliver hands-on trainings & best practices.
- Collaborate technical publications with domain scientists

#### What we're looking for

- Solid C/C++/Fortran and parallel programming (MPI, OpenMP; GPU: CUDA/SYCL/OpenACC a plus).
- Performance analysis & tuning tools (e.g., VTune, Arm MAP, TAU, Nsight).

#### Why IT4Innovations

- Work directly on cutting-edge Tier-1/Tier-0 HPC systems.
- Impact national and EU research across disciplines.
- Collaborative, international team with real user impact.z



João Barbosa joao.barbosa@vsb.cz

IT4Innovations National Supercomputing Center VSB – Technical University of Ostrava Studentská 6231/1B 708 00 Ostrava-Poruba, Czech Republic www.it4i.cz



IT4INNOVATIONS
NATIONAL SUPERCOMPUTING
CENTER