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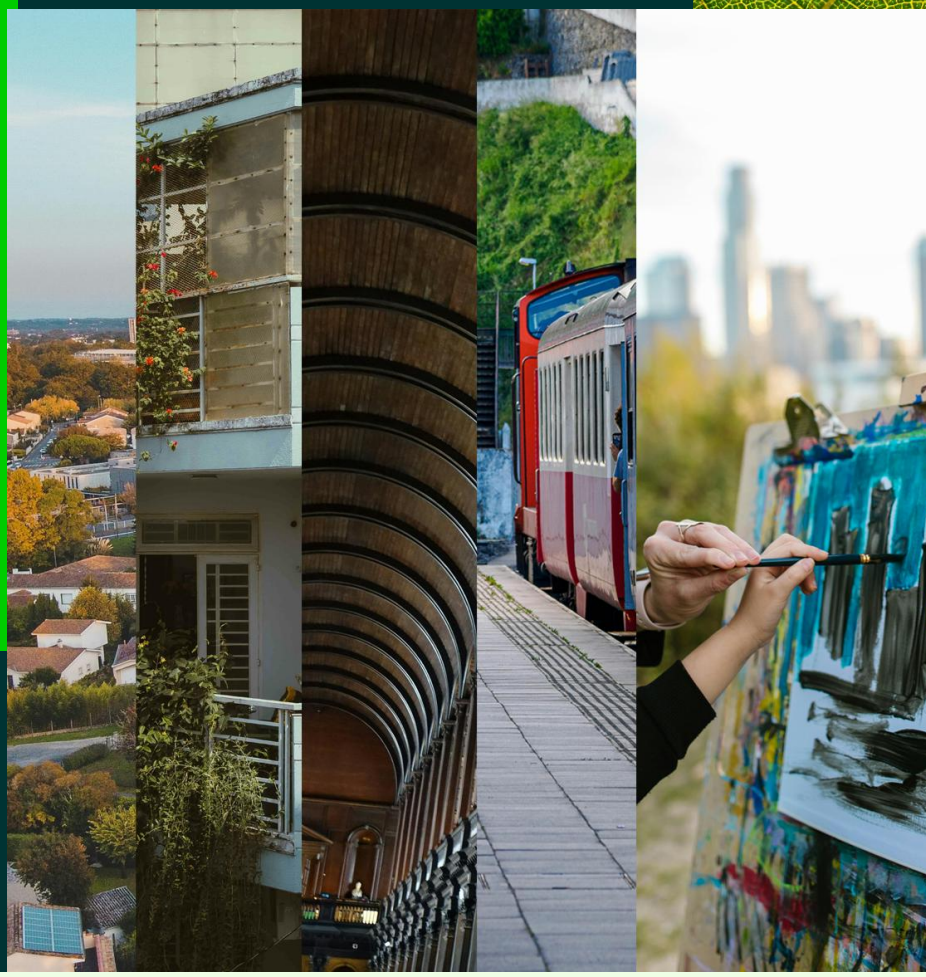

Spoke 6

The workshop **"High Performance Computing to Enhance Efficiency of Scientific Simulations"** is organized within the framework of **ECOSISTER – Ecosystem for Sustainable Transition in Emilia-Romagna**, a project aimed at promoting the ecological transition of the economic and social systems of the region, through the integration of sustainability and digital innovation. In line with the goals of the Climate and Labour Pact, ECOSISTER fosters cutting-edge research and technological transfer to support sustainable development by advancing quality employment, improving quality of life, and protecting the environment. As part of this mission, the workshop provides researchers with advanced training in high-performance computing (HPC) and scientific simulation acceleration, key tools to address complex challenges in materials science and biochemistry while promoting a sustainable and efficient use of HPC resources

Ecosystem for Sustainable Transition in Emilia-Romagna

Codice: ECS_00000033 CUP: B83D21014180006 Missione 04 Istruzione e ricerca – Componente 2 Dalla ricerca all'impresa Investimento 1.5, – NextGenerationEU

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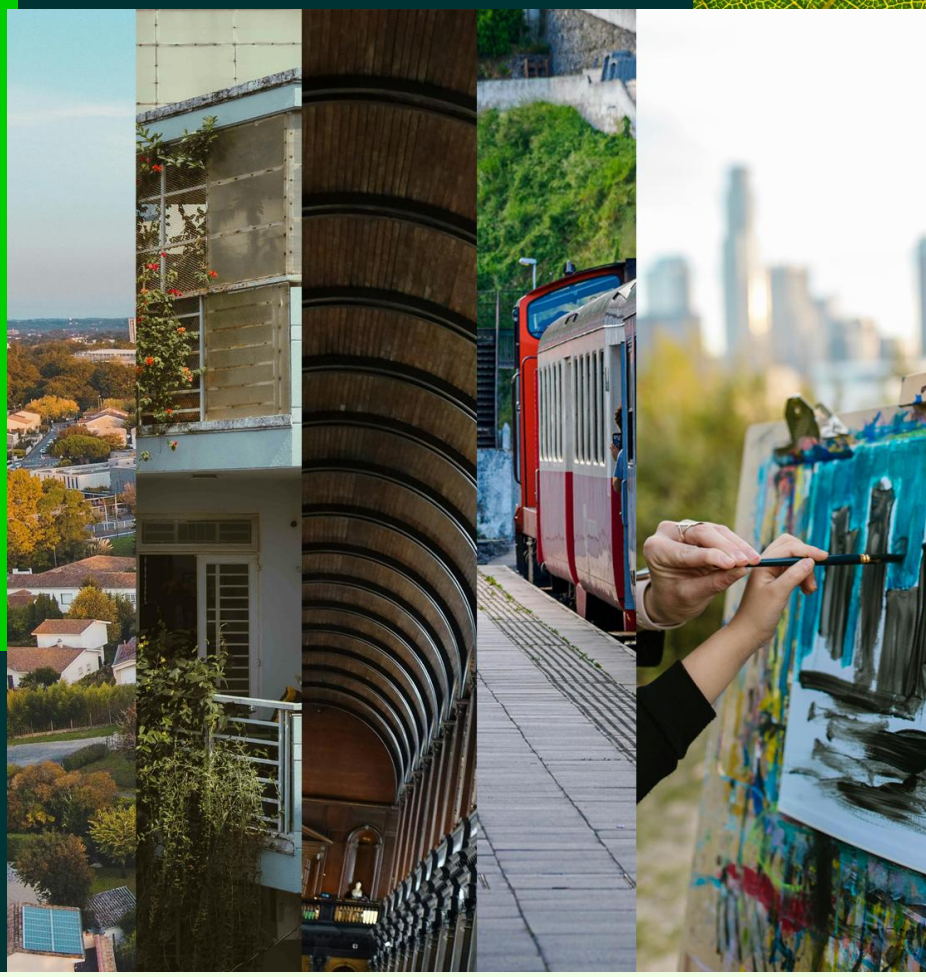

Spoke 6

High Performance Computing to enhance efficiency of scientific simulations

A comprehensive overview of current techniques for parallelizing and accelerating material science and biochemistry simulations, with a particular emphasis on performance optimization for HPC architectures

- ***specifically designed for ECOSISTER researchers and scientists who want to improve their technical skills in parallel computing***

15-19 September 2025 **Workshop**

Workshop registration

https://tinyurl.com/ecosister-workshop

Program

15 Sept 2025

[09:00 – 18:00]

Spoke 6

Speakers: Fabio Affinito, Andrew Emerson, Tommaso Gorni, Laura Bellentani, Lara Querciagrossa, Angela Acocella

CINECA – HPC Department

09:00 **Welcome and Introduction**

Fabio Affinito
Welcome and goals of the workshop

Parallel computing

09:30 **. Basic principles and essential role of parallel computing in modern science**
Computers and Computational Science: an overview of key computational challenges and fundamental concepts and metrics of parallel computing

10:30 **. Introduction to High Performance Computing**
Basics of high-performance computing, architectures, and parallel processing and workflow management for scientific applications

12:00 **. CINECA HPC environment**

12:30 **Lunch Break**

14:00 **. Compilation and Optimization with a short hands-on session**
Compilers and common optimization techniques in FORTRAN and C programs

16:00 **. Library Integration with a short hands-on session**
Best practices for incorporating libraries to optimize code performance and compatibility within HPC workflows

18:00

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CINECA – HPC Department

Program

16 Sept 2025

[09:00 – 18:00]

Distributed and Shared Memory Parallelization

09:00 . Exploring MPI: Message Passing for Distributed Computing
Principles of message-passing programming, point-to-point and collective communications, Non-blocking, load balancing

10:45 . Hands-on session on MPI programming

12:30 Lunch Break

14:00 . Parallel Programming with OpenMP: Shared Memory Model and Basic Syntax
Shared memory parallelism for multi-core systems, Key OpenMP constructs: Directives, parallel loops

16:00 . Hands-on session on OpenMP and hybrid MPI/OpenMP programming

18:00

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CINECA – HPC Department

Program

17 Sept 2025

[09:00 – 18:00]

Hybrid Programming and Advanced Optimization

09:00 . Introduction to accelerated computing
An overview of GPUs hardware and execution model. Programming solutions for accelerating scientific codes

10:45 . Accelerating Computations with OpenACC
Overview of OpenACC directives to offload compute-intensive code sections to accelerators

12:30 Lunch Break

14:00 . Hands-on session on OpenACC
Introduction to OpenACC directives to offload compute-intensive code sections to accelerators

16:15 . Advanced Code Optimization Techniques
Measuring systems performance (profiling tools), reducing communication overhead in hybrid calculations

18:00

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CINECA – HPC Department

Program

18 Sept 2025

[09:00 – 18:00]

Parallelization in Complex Simulations

09:00 . Parallelization Strategies in software for Material Science Simulations
An exploration of software parallelization strategies for material simulations, including an analysis of how popular QM codes implement parallelization

10:30 . Real Applications and Case Studies
Evaluating parallelism levels in QuantumESPRESSO

12:30 Lunch Break

14:00 . Parallelization Strategies in software for Biochemistry Simulations
Overview of parallelization approaches for MD algorithms, addressing key challenges such as communication and load balancing

15:30 . Real Applications and Case Studies
Evaluating multi-level parallelism in GROMACS

18:00

Spoke 6

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Speakers: Fabio Affinito, Andrew Emerson, Tommaso Gorni, Laura Bellentani, Lara Querciagrossa, Angela Acocella

CINECA – HPC Department

Program

19 Sept 2025

[09:00 – 15:00]

Introduction to ML models

09:00 . An overview of ML models and their relevance to computational materials science and biochemistry
Exploring machine learning techniques and their growing relevance in computational materials science and biochemistry

10:45 . Real Applications and Case Studies

12:30 Lunch Break

14:00 . Closure and Reflections

15:00

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