# The HPC Centres of Excellence

*2023-2026*

*A summary of their consortia, objectives, areas of activity, use cases and HPC codes*

Authored by CASTIEL2-WP2

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| ESiWACE-3 | | POP3 | |
| EXCELLERAT-P2 | | SPACE | |

01.01.2023 - 31.12.2026
Life Sciences
https://bioexcel.eu/
3rd Phase - Type 2 (Apps)

| Coordinator: KTH Royal Institute of Technology - SE (PI: Rossen Apostolov) | University of Utrecht NL |
|---|---|
| Barcelona Supercomputing Centre ES | IRB Barcelona ES |
| EMBL-EBI DE | MPG DE |
| Nostrum Biodiscovery ES | Norman Consulting NO |

BioExcel's mission is to provide applications, tools, support, and networking opportunities to Life Science researchers, enabling them to address grand scientific challenges by fully exploiting the power of data and computing e-infrastructure. Powerful and sophisticated software packages are critically important for fundamental and applied research, including industrial development, in particular in the areas of drug design, biotechnology, food and chemical industries.

- Service Portal: https://bioexcel.eu/services/
- Trainings: https://bioexcel.eu/services/training/
- Potential Collaboration with Industry (not partners): Yes

## USE CASES

- Antibody Design through Biomolecular Interactions Engineering
- High-Throughput Modelling of Interactomes
- Electronic Interaction Phenomena: Proton Dynamics and Fluorescent Proteins
- Rational Drug Design

## CODES

- **GROMACS:** one of the most used molecular dynamics codes. Highly tuned assembly kernels with hybrid CPU/GPU execution.
- **HADDOCK:** used for integrative modelling. Python wrapper to execute a series of CNS (Crystallography and NMR system) scripts that also run pre and post-processing analysis.
- **PMX:** used to automate the free energy calculations and assess binding between drug and protein. It uses GROMACS as a backend engine.
- **BioBB:** Python library consisting of a collection of wrappers on top of biomolecular tools (e.g. GROMACS, HADDOCK, PMX), adding interoperability between them, and allowing an easy creation of biomolecular simulation workflows. The library combined with BSC PyCOMPSs workflow manager can be used to launch the workflows in HPC systems using thousands of cores.

# CEEC
## Centre of Excellence in Exascale CFD

01.01.2023 - 31.12.2026
Exascale CFD
https://ceec-coe.eu/
1st Phase - Type1 (Exascale)

| Coordinator: KTH Royal Institute of Technology - SE (PI: Niclas Jansson) | AUTh EL |
|---|---|
| Barcelona Supercomputing Centre ES | FAU - University Erlangen DE |
| University of Stuttgart (HLRS) DE | Umea University SE |
| Denmark Technical University DK | BAM DE |

CEEC's ambition is to enable the use of exascale computers for key computational fluid dynamics (CFD) applications and demonstrate their capabilities through key light-house cases. Understanding the turbulent behavior of gases and liquids has direct societal impact. In fact, it will be key for enabling the transition to a carbon-free economy through optimizations like more fuel efficient airplanes and cargo ships or wind turbines that can be more easily and sustainably installed on the ocean floor. CEEC aims at: implement exascale-ready workflows to solve grand scientific challenges, develop new or improves algorithms that can efficiently exploit exascale systems, improve energy efficiency of simulations, and demonstrate workflows on lighthouse cases that are relevant for academia and industry.

- Service Portal: -
- Trainings: https://ceec-coe.eu/training/
- Potential Collaboration with Industry (not partners): Yes, but not primary target

## USE CASES

- Shock – Boundary layer interaction and buffet on wings at the edge of the flight envelope. - FLEXI
- High fidelity aeroelastic simulation of the SFB 401 wing in flight conditions - ALYA
- Topology optimization of static mixers - Neko
- Localized erosion of an offshore wind-turbine foundation - waLBerla
- Simulation of Atmospheric Boundary Layer (ABL) flows - NekRS/Nek500
- Merchant ship hull - Neko

## CODES

- **ALYA**: Multi-physics / multi-scale simulation framework
- **FLEXI**: DG-Spectral element based CFD code
- **Nek5000 & NekRS**: Spectral element based CFD Codes
- **Neko**: Spectral element based CFD code
- **waLBerla**: Lattice Boltzmann based multiphysics framework

01.01.2023 - 31.12.2026
Solid Earth
https://cheese2.eu/
2nd phase - Type 2 (Apps)

| Coordinator: CSIC ES (PI: Arnau Folch) | |
|---|---|
| INGV  IT | Ludwig Maximilian Univerity of Munich DE |
| Barcelona Supercomputing Centre ES | University of Mainz DE |
| CINECA IT | University of Malaga ES |
| Icelandic Metereological Office IS | Norwegian Geotechnical Institute NO |
| ETH Zurich CH | IPGP F |
| EVIDEN F | CNRS F |
| University of Stuttgart (HLRS) DE | Ruder Boscovic Institute HR |
| Technical University of Munich DE | CSC FI |
| Sorbonne University F | E4 Analytics  IT |

ChEESE-2P aims to prepare 11 community flagship codes to address 12 domain-specific Exascale Computational Challenges (ECCs) on, eg., computational seismology, magnetohydrodynamics, physical volcanology. Codes will be optimized in terms of performance on different types of accelerators, scalability, deployment, containerization, and portability. Codes and workflows will combine to form a new generation of 9 Pilot Demonstrators underpinned by concepts like multi-scale, multi-source, and multi-physics, that will materialise in 15 Simulation Cases representing capability and capacity use cases of particular relevance in terms of science, social relevance, or urgency.

- Service Portal: -
- Trainings: https://cheese-coe.eu/events/training
- Potential Collaboration with Industry (not partners): Yes - also public administration targeted

### ECCs

- Full-waveform inversion and high resolution tomography (capability computing)
- Near real-time seismic scenations  (capacity computing)
- Physics-based Probabilistic Seismic Hazard Assessment  (capacity & urgent computing)
- Near real-time tsunami source inversion and characterization (capability computing)
- Faster Than Real Time tsunami scenarios (capacity & urgent computing)
- Probabilistic Tsunami Hazard Assessment (capacity computing)
- Volcanic Explosions and Interactions  (capability computing)
- Probabilistic Volcanic Hazard Assessment (capacity computing)
- The dynamo model and the Earth's magnetic field evolution  (capability computing)
- Landslide triggering  (capability computing)
- Lithospheric stress states and induces seismicity  (capability computing)

### CODES

- **SeisSOL:**  complex earthquake simulation
- **SPECFEM3D:**  linear seismic wave propagation
- **ExaHyPE:** special emphasis on **ExaSeis** collection of seismic models
- **Tandem**: linear elasticity + sequences of earthquakes and seismic slips
- **xSHELLS**: flows, magnetic fields including Geodynamo simulations
- **HySEA**: earthquake –induced Tsunamis
- **FALL3D:** atmospheric transport & ground deposition
- **OpenPDAC:** simulation of volcanic fluids
- **LaMEM:** thermo-mechanical geodynamic modelling
- **pTatin3D**: simulation of long time-scale geodynamics processes
- **ELMER/ICE:** Multi-physics package

# dealii X

01.10.2024 - 31.12.2026
Personalised Medicine
https://www.dealii-x.eu/
1st phase

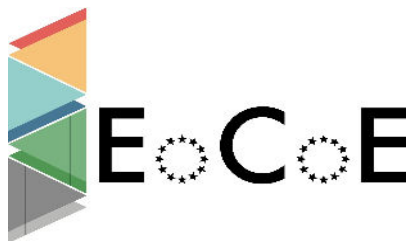| Coordinator: Ruhr-Univ. Bochum DE (PI: Martin Kronbichler) | |
| --- | --- |
| Bayrische Akademie der Wissenschaften  DE | Politecnico di Milano  IT |
| Centre National de la Recherche Scientific CNRS)  FR | Scuala Internazionale Superiore di study avanzati di Trieste  IT |
| Consigio Nationale delle Ricerche (CNR)  IT | Technische Universität München  DE |
| Dualistic SaRL  IT | Università degli studi di Brescia  IT |
| Exact Lab SRL  IT | Università degli studi di Roma Tor Vergata - IT |
| Forschungsverbund Berlin e.V.  DE | Università di Pisa  IT |
| Friedrich-Alexander-Universität Erlangen  DE | Virtual Physiologial Human Institute For Integrative Biomedical Research VZW   BE |
| Institut National Polytechnique de Toulouse  FR | |

**dealii-X** - an Exascale Framework for Digital Twins of the Human Body - aims at developing a scalable, high-performance computational platform to create accurate digital twins of human organs using the deal.II finite element library. The framework will combine sophisticated numerical methods with exascale computing capabilities to create cutting-edge multiphysics and multidisciplinary simulation models. Lighthouse applications representing crucial processes in the human brain, the cardiovascular and respiratory systems as well as the liver will be tackled to gain new insights into biological processes of the human body and aiding in personalized medicine. A primary focus is on a new generation of solvers, including novel methods for large linear, nonlinear and coupled systems, matrix-free finite element algorithms for GPUs and discretization schemes.

## EXASCALE COMPUTATIONAL CHALLENGES / USE CASES

- Simulation of airflow in the human lung coupled to gas exchange processes through fully resolved coupled Navier-Stokes / poromechanics models for capturing pathologies at full scale
- Simulation in cardiac computational medicine by multiscale and multiphysics models with extreme spatial and temporal resolution to gain novel insights
- Simulation of brain tissue mechanics through refined nonlinear routines for inverse parameter identification and related problems in the study of physiological and pathological scenarios
- Development of a digital twin of the human liver through multiscale representations of the vascular structure by effective biomechanical properties to enable data-driven enhanced personalization
- Novel simulators for cellular interactions through space-time FEM applied to sophisticated governing equations for single and collective cellular motility & relocation of receptors on advecting lipid membranes
- Hardware-driven algorithm development from mathematics to application needs
- Efficient infrastructure for surrogate modeling

## CODES & LIBRARIES

- deal.II: Library providing algorithmic and data structure building blocks to create cutting-edge numerical solvers for solving PDEs with the finite element method (FEM) using mixed-dimensional methods, parallel multigrid preconditioners and rich matrix-free/matrix-based features
- PSCToolkit: A parallel sparse linear algebra toolkit implementing massively parallel sparse solvers and preconditioners for a wide range of multi-physics and multi-scale simulations
- MUMPS: Direct solver for sparse linear systems with symmetric, unsymmetric, real-valued and complex matrices, implementing novel block low-rank approximate factorizations
- lifex: Multiphysics and multiscale modelling for a wide range of cardiovascular models and computational medicine based on the deal.II library
- 4C: A comprehensive multi-physics framework for research in solid mechanics, fluid mechanics, scalar transport and chemical reactions, slated to use advanced exascale capabilities of the deal.II library
- ExaDG: High-order CFD and multiphysics application solver using deal.II
- polyDEAL: Polytopal DG solvers based on deal.II for algorithms on agglomerated entities with high flexibility
- LiverX: A deal.II-based multiphysics simulation to analyze multiscale coupling in vascularized tissues
- ExaBrain: A simulator for poro-viscoelastic processes in the human brain

| Coordinator: CEA F (PI: Edouard Audit) | |
|---|---|
| CEA F | FZJ DE |
| Barcelona Supercomputing Centre ES | CNRS F |
| INRIA F | CERFACS F |
| ENEA IT | E4 IT |
| MPG DE | CNR IT |
| FAU Erlangen DE | ULB BE |
| PSNC PL | DDN F |
| U. Roma Tor Vergata IT | IFPEN F |
| UNITN IT | CIEMAT ES |

01.01.2024 - 31.12.2026
Energy - Engineering
https://www.eocoe.eu/
3rd Phase

EoCoE III demonstrates the benefit of HPC for the net-zero energy transition for research institutes and also for key industries in the energy sector, channeling its efforts into 5 exascale lighthouse applications covering the key domains of Energy Materials, Water, Wind and Fusion.

The multidisciplinary effort of the consortium partners harnesses innovations in computer science and mathematical algorithms within a tightly integrated co-design approach to overcome performance bottlenecks, to deploy the lighthouse applications on the coming European exascale infrastructure, and to anticipate future HPC hardware developments.

- Service Portal: https://www.eocoe.eu/services/
- Software as a Service portal: https://eocoe.psnc.pl/
- Training events: https://www.eocoe.eu/
- Potential Collaboration with Industry: Yes

## CODES

- **Gysela-X**: 5-D code enabling simulations of the nonlinear turbulent core-edge plasma region at unprecedented spatial and temporal resolution length scales
- **libNEGF**: Non-equilibrium Green's function library, combined with density functional theory (DFT) models of material properties to enable new advances in photovoltaics
- **Parflow**: Groundwater modelling framework, combined with the hydropower infrastructure management system HYPERstreamHS to provide high-resolution hydrological forecasting at the continental scale
- **ALYA**: High Performance Computational Mechanics code focusing on incompressible flow for Wind over complex terrain, including physics required by wind community
- **waLBerla-wind** : fluid dynamics solver to achieve multiscale offshore and flat terrain onshore wind farms modeling
- **AGMG**, **PSCToolkit**, **GmgPolar**, **Maphys++**, **MUMPS** : Exascale-ready Linear Algebra libraries
- **Deisa**: Library that ensures coupling MPI simulation codes with the Dask Framework

## GRAND CHALLENGES / USE CASES

- Large-scale calculations of non-equilibrium charge carrier transport across the heterostructure of two-dimensional layers
- High Fidelity Microscale wind simulations and wind resource assessment, optimal complex terrain scale resolving simulations on GPUs
- Weak and strong scalings on the 4D Gysela axisymmetric version up to 100 GPUs, and up to 5000 GPUs with Gysela-X, i.e. the 5D non-axisymmetric version
- Integrated hydrologic and hydropower infrastructure information at the resolution of a reservoir, stream reach and neighborhood from the continental to the global scale
- Promotion of solutions and codes in the largest European Alliance on Energy research (EERA)

01.01.2023 - 31.12.2026
Weather - Climate
https://www.esiwace.eu/
3rd Phase - Type 2 (Apps)

| Coordinator: Barcelona Supercomputing Centre **ES** (PI: Mario Acosta) | NLeSC NL |
|---|---|
| ECMWF UK | SMHI SE |
| ATOS F | CSC FI |
| DKRZ DE | University of Helsinki FI |
| CMCC IT | Juelich Forschungzentrum DE |
| Max Planck Institute for Metereology DE | Latest Thinking DE |

ESiWACE3 focuses on the community's support to reach a higher readiness level regarding exascale supercomputing and knowledge transfer between the different Earth System modelling centres and teams across Europe. The project focuses on three main pillars: (i) the transfer and establishment of knowledge and technology for efficient and scalable simulations of weather and climate across the Earth system modelling community, (ii) closing common technology knowledge gaps and providing toolboxes for high-resolution Earth system modelling via joint developments and (iii) serve as a sustainable community hub for training, communication and dissemination for high-performance computing for weather and climate modelling in Europe. ESiWACE3 will bring the various approaches to address these challenges from the different modelling groups together to transfer knowledge across the weather and climate domain, generate synergies between the local efforts, provide targeted support to modelling groups via customised high-performance computing services, and provide training to educate the next generation of researchers.

- Service Portal: https://www.esiwace.eu/services
- Training events: https://www.esiwace.eu/training
- Potential Collaboration with Industry (not partners): Yes, but it is not the primary target.

## CODES

- **EC-Earth:** coupled Earth System Model for climate simulations
- **NEMO**: ocean model for climate simulations
- **ICON:** coupled Earth System Model for climate simulations
- **IFS:** Atmospheric model for weather simulations
- **HPCW:** Set of weather & climate benchmarks

## GRAND CHALLENGES

- Increase the efficiency of weather and climate simulations on state-of-the-art supercomputers.
- Design tools to close technology gaps for high-performance computing.
- Develop tools to tackle the data challenge of high-resolution weather and climate modelling.
- Support the wider weather and climate modelling community using state-of-the-art supercomputers via targeted services, training and capacity building.
- Build a well-connected and inclusive community for high-resolution Earth System modelling across Earth system science and HPC.

# EXCELLERAT P2

| Coordinator: Univ. of Stuttgart (HLRS) - DE (PI: Bastian Koller) | |
|---|---|
| Barcelona Supercomputing Centre ES | DLR DE |
| CINECA IT | University of Roma "La Sapienza" IT |
| SIPEARL F | RWTH AACHEN DE |
| University of Ljubljana SI | SICOS DE |
| KTH Royal Institute of Technology SE | SSC DE |
| ARCTUR SI | Teratec F |
| CERFACS F | Fraunhofer SCAI DE |

01.01.2023 - 31.12.2026
Engineering - Manufacturing
https://www.excellerat.eu/
2nd phase - Type 2 (Apps)

EXCELLERAT P2 spans the whole domain of engineering – ensuring that innovations produced are applicable to other engineering challenges, that co-design is handled properly, that success stories are created and distributed. EXCELLERAT P2 strives to show the contribution of HPC, HPDA and AI in engineering to a low-carbon, more environmentally friendly and socially responsible product development and manufacturing as well as the mobility and energy sector. The holistic view of EXCELLERAT P2 to the usage of HPC (and HPDA and AI) is needed, if engineering applications shall be supported to increase the European competitiveness.

- Service Portal: https://services.excellerat.eu/
- Trainings: https://services.excellerat.eu/searchevents/training
- Potential Collaboration with Industry (not partners): Yes

## USE CASES

1. External aircraft aerodynamics - Aircraft and Aerospace - DLR - CODA
2. Hydrogen combustion for propulsion - Automotive, Aircraft & Aerospace - CERFACS - AVBP
3. Migration of aeroacoustic noise - Automotive, Aircraft & Aerospace, Energy - RWTH Aachen - m-AIA
4. Fully integrated aircraft simulations with emission models - Aircraft & Aerospace - BSC - Alya
5. High-fidelity simulations of rotating parts -Aircraft & Aerospace, Energy KTH - Neko
6. Active control for drag reduction of transonic airfoils - Aircraft & Aerospace- CINECA - FLEW
7. Engineering design of digital twin of the first wall of tokamak fusion reactor - Energy - University of Ljubljana - OpenFOAM/Raysect

## CODES

- **m-AIA**: CFD-related, multi-physics code in C++ with hybrid MPI/OpenMP parallelization and some solvers ported to NVIDIA GPUs
- **AVBP**: 3D parallel Navier-Stockes solver for reactive multi-phase multi-physics problems using Large Eddy Simulation on unstructured grids (runs on any CPU and NVIDIA GPUs).
- **Neko**: SME code running on CPU and GPUs using native accelerator kernels (HIP, Cuda, OpenCL).
- **Alya**: Navier-Stokes solver exploiting a Spectral Element discretization. Runs fully on GPUs (mostly tested on Nvidia V100 and A100 GPUs. Poor performance on AMD GPUs).
- **CODA**: CFD software, Python frontend, C++ backend, supports hybrid MPI/GASPI + OpenMP + NVIDIA GPUs
- **OpenFOAM:** free, open source CFD software
- **Mitsuba2**: Monte Carlo Ray tracing for optical and radiative heat transfer simulations (runs on GPUs)
- **FLEW:** FVM solver for DNS of compressible flow, written in Fortran and OpenACC.

| Coordinator: PSNC - PL (PI: Marcin Lawenda) | | Univeristy of Strasbourg F |
|---|---|---|
| ATOS ES | | ICCS EL |
| University of Stuttgart (HLRS) DE | | Meteogrid SL ES |
| SZE HU | | Future Needs CY |

01.01.2023 - 31.12.2026
Simulations for global challenges
http://www.hidalgo2.eu/
2nd phase - Type 2 (Apps)

HiDALGO2 explores synergies between modelling, data acquisition, simulation, data analysis and visualisation. It will also efficiently utilise current and future HPC and AI infrastructures to develop highly scalable solutions to global climate and social challenges (e.g. violent weather, floods, pollution). HIDALGO2 aims at bringing together advanced solutions (HPC-AI-HPDA) to provide decision makers and stakeholders tools that would mitigate tragic consequences of climate and civilization phenomena, by delivering necessary knowledge.

- Service Portal:
- Trainings: -
- Potential Collaboration with Industry (not partners): Yes (also targets public services)

## USE CASES & CODES

- Urban Air Project: evolution of air in urban areas considering pollution, wind, comfort and planning. The core is the Urban Air Flow (UAP.AF) computational model, based on two main software: OpenFOAM and Fluid-Solver. For both solvers, modelling of more physical properties will be developed including thermal convection, solar heat radiation, transport and reaction between several species.
- Urban Building: advanced building models for better integration with architecture and for pollutants and heat models.
- Renewable Energy Sources: Solutions for production of renewable energy accustomed to urban and rural areas. Multiscale weather prediction based on Fortran and MPI coupled energy production estimation (based on AI/HPDA)
- Wildfires: Simulations of wildfires and atmosphere interaction and smoke dispersion in forest and urban areas. Forecast of weather conditions from WRF and LES at very detailed scales, generating ensembles of weather scenarios over the landscape and coupling of CFD solutions for the detailed modeling of air flow at the settlement scale.

All HiDALGO2 Pilots will be integrated into a newly developed dashboard, a key entry point for internal and external stakeholders of these global challenges.

Additional transversal activities:
- Setup an efficient benchmarking and profiling process
- Optimize pilot towards efficient execution
- Combine simulations and AI models
- Evaluate impact of emerging architectures and technologies

# MaX
## DRIVING THE EXASCALE TRANSITION

01.01.2023 - 31.12.2026
Material Design
http://www.max-centre.eu/
3rd phase - Type 1 (Exascale)

| Coordinator: CNR IT (PI: Elisa Molinari) | ICN2 ES |
|---|---|
| Barcelona Supercomputing Centre ES | SISSA IT |
| CINECA IT | E4 IT |
| SIPEARL F | Jozef Stefan Institute SI |
| CEA F | IT4I CZ |
| ATOS BULL F | Leonardo IT |
| Julich Forschungzentrum DE | University of Modena&Reggio IT |
| CSIC ES | University of Bremen DE |

MaX-3 targets lighthouse codes for material simulations aimed at understanding, predicting, and discovering the properties and performance of materials. The aim is: to upscale the MaX codes and their performance to multiple heterogeneous exascale architectures; to endow these codes with innovative capabilities enabled by such architectures; to co-design the hardware and software in collaboration with the relevant European stakeholders; to enable turn-key simulation capabilities that meet the power of exascale resources and deliver the resilience needed; to disseminate the entire ecosystem of codes, workflows, and data; and to train and engage developers and users in fully leveraging such powerful instruments for discovery and innovation.

- Service Portal: http://www.max-centre.eu/services
- Trainings: http://www.max-centre.eu/training-and-education
- Potential Collaboration with Industry (not partners): Yes (but not primary target)

## CODES

- **Quantum ESPRESSO** is an integrated suite of open-source computer codes for electronic-structure calculations and materials modeling at the nanoscale. It is based on density-functional theory (DFT), plane waves, and pseudopotentials.
- **SIESTA** is a code that performs efficient electronic structure calculations and ab initio molecular dynamics simulations of molecules and solids. SIESTA's efficiency stems from the use of a basis set of strictly-localized atomic orbitals.
- **YAMBO** is an open-source code implementing first-principles methods based on Green's function theory to describe excited-state properties of realistic materials.
- **FLEUR** is a code family for calculating ground-state as well as excited-state properties of solids within the context of DFT. A key difference lies in the treatment of all electrons on the same footing.
- **BigDFT** is an electronic structure pseudopotential code that employs Daubechies wavelets as a computational basis, designed for usage on massively parallel architectures.

## ADDITIONAL RESOURCES

- Max Libraries: http://www.max-centre.eu/software/libraries
- Features and algorithms: http://www.max-centre.eu/software/features-and-algorithms
- Workflows (AiiDA): http://www.max-centre.eu/software/workflows
- Data: http://www.max-centre.eu/data

# MICROCARD

**01.11.2024 - 30.04.2027**
**Personalised Medicine**
https://www.microcard.eu
1st phase

| Coordinator: Univ. de Bordeaux FR (PI: Mark Potse) | |
|---|---|
| INRIA  FR | Università degli studi di Pavia  IT |
| Karlsruhe Institure for Technology (KIT)  DE | Università degli studi di  Trento  IT |
| Megware GmbH  DE | Université de Strasbourg  FR |
| Simula  NO | Zuse-Institut Berlin (ZIB)  DE |
| Technische Universität München  DE | |

Cardiac function is coordinated by an electric system whose disorders are among the most frequent causes of death and disease. Numerical models of this complex system are mature and widely used, but to match observations in aging and diseased hearts they need to move from a continuum approach to a representation of individual cells and their interconnections. This makes the problem more complex, harder to solve, and four orders of magnitude larger, necessitating exascale computers.

**MICROCARD-2** builds software that can meet this challenge of simulating cardiac electrophysiology using whole-heart models with sub-cellular resolution, on exascale supercomputers, building on and scaling up the results of the forerunner project MICROCARD.

On a technical level, the project will further develop  numerical schemes, moving to second-order spatial discretisation. Based on MICROCARD results, the team will develop mixed-precision preconditioners and data compression to reduce communication bandwidth. The highly successful efforts towards automated compilation of high-level model descriptions into optimised, energy-efficient system code for different CPUs and GPUs will be extended to upcoming architectures. The project will continue efforts to robustify parallel remeshing software and add necessary functionality for parallel mesh partitioning and production of realistic synthetic tissue meshes needed for simulations.

The platform will be benchmarked with realistic test cases and be made accessible for a wide range of users with tailored workflows. The platform will be adaptable to similar biological systems such as nerves, and several of the products such as improved solvers, preconditioners, remeshers, and partitioners will be reusable in a wide range of applications.

## EXASCALE COMPUTATIONAL CHALLENGES / USE CASES

- Whole-heart model of cardiac electrophysiology at sub-cellular resolution

## CODES & LIBRARIES

- **openCARP**  A widely-used simulation code and toolset for cardiac electrophysiology simulation.
- **Ginkgo**   A high-performance numerical linear algebra library for many-core systems, with a focus on solution of sparse linear systems. Notably, it allows linear algebra problems to be solved efficiently on NVIDIA, AMD and Intel GPUs.
- **mmg3d**  A remeshing code for (large) tetrahedral meshes, with functionality to discretize complex level sets and the ability to preserve internal boundaries.
- **ParMmg**   A process-parallel version of mmg3d able to run on distributed-memory systems.

01.01.2023 - 31.12.2026
Multiscale Modelling
https://www.multixscale.eu/
1st Phase - Type 2 (Apps)

| Coordinator: Kemijski Institut SI (PI: Matej Praprotnik) | | IIT IT |
|---|---|---|
| Barcelona Supercomputing Centre ES | | University of Ghent BE |
| University of Barcelona ES | | SURF NL |
| Max Planck Society DE | | HPC Now! ES |
| University of Stuttgart (HLRS) DE | | Forschungzentrum Julich DE |
| University of Bergen NO | | Leonardo IT |
| Sorbonne University F | | Univerity of Groningen NL |
| CNR IT | | Univerity of Tolouse F |

MultiXscale aims at increasing performance, productivity and portability in the domain of multiscale simulation. It couples the scientific expertise of the CECAM network, represented by leading experts in multiscale simulations from different European institutions, with the technical expertise of the EESSI collaboration, and targets the computational laboratories of EuroHPC and beyond. It will shoulder much of the technical burden of developing and distributing domain-relevant applications for (pre-)exascale through application co-design for exascale technologies, and the provisioning of exascale-oriented libraries and services that nudge the community to adopt battle-tested, future-oriented, scalable workflows and portable technologies. These will allow application developers to pursue domain-relevant scientific innovation without being over-burdened by technical detail, and empower industrial and academic application users to painlessly adopt bleeding-edge technologies from the domain on whatever computational resource they may have access to.

- Service Portal: -
- Trainings: -
- Potential Collaboration with Industry (not partners): Yes (no PoC budget)

## USE CASES

- Helicopter design and certification for civil transport
- Battery applications to support the sustainable energy transition
- Ultrasound for non-invasive diagnostics and biomedical applications

## CODES

- **EESSI** (European Environment for Scientific Software Installation): complete build and deployment environment for all MultiXscale applications and beyond. Provides a streaming service for scientific software, automatically distributing hardware-optimised applications and updates to all hardware types: supercomputers, servers, laptops…even a Raspberry Pi!

Applications used and contributed to that enter into the multiscale workflows:

- **ESPResSo**: highly versatile software package for performing and analyzing scientific Molecular Dynamics many-particle simulations of "coarse-grained" bead-spring models as they are used in soft-matter research in physics, chemistry and molecular biology.
- **LAMMPS**: classical molecular dynamics code with a focus on materials modeling.
- **waLBerla**

01.01.2023 - 31.12.2026
Plasma Simulations
https://plasma-pepsc.eu/
1st Phase - Type 1 (Exascale)

| Coordinator: KTH Royal Institute of Technology - SE (PI: Stefano Markidis) | FORTH EL |
|---|---|
| Barcelona Supercomputing Centre ES | HZDR DE |
| Max Planck Society DE | IPP CZ |
| SIPEARL F | University of Helsinki FI |
| Technical University of Munich DE | University of Ljubljana SI |

Plasma-PEPSC aims at reaching scientific breakthroughs in plasma science Grand Challenges through exascale computing and extreme-scale data analytics, by enabling unprecedented simulations on current pre-exascale and future exascale platforms to control plasma-material interfaces, optimize magnetically confined fusion plasmas, design next-generation plasma accelerators and predict space plasma dynamics in the Earth's magnetosphere. Plasma-PEPSC aims at achieving these goals by maximizing the parallel performance and efficiency of four European flagship plasma codes with a large user base: BIT, GENE, PIConGPU, and Vlasiator, by building on algorithmic advances as well as on programming model and library developments (MPI, accelerator and data movement APIs and runtimes, in-situ data analysis). Plasma-PEPSC ensures an integrated HPC software engineering approach for deploying, verifying, and validating extreme-scale kinetic plasma simulations that can serve as a community standard.

- Service Portal: -
- Trainings: -
- Potential Collaboration with Industry (not partners): Yes, but more likely at later stage


**GRAND CHALLENGES**

- Controlling Plasma-Material Interfaces - BIT1
- Optimizing Magnetically Confined Plasmas - GENE
- Enabling Next-Generation of Plasma Accelerators for Real World Applications - PIConGPU
- Predicting Near-Earth Space Dynamics - Vlasiator

**CODES**

- **GENE**: Plasma microturbulence based on Eulerian calculation and MPI domain decomposition.
- **BIT1:** full-size kinetic modelling of plasma edge
- **Vlasiator**: Semi-Lagrangian simulation of the Vlasov Equation and MPI domain decomposition. OpenMP/MPI hybrid parallelizations, sparse grids.
- **PIConGPU** plasma accelerators at full resolution and scale

01.01.2024 - 31.12.2026
Performance - Productivity
https://pop-coe.eu/
3rd Phase - Type 1 (Exascale)

| Coordinator: Barcelona Supercomputing Center (BSC) - ES - PI: Jesus Labarta | |
|---|---|
| Barcelona Supercomputing Center ES | INESC ID PT |
| Forschungszentrum Jülich DE | Teratec FR |
| RWTH Aachen University DE | U. Versailles FR |
| VŠB - TU Ostrava (IT4I) CZ | University of Stuttgart (HLRS) DE |

Since its first phase in 2015, the Centre of Excellence on Performance Optimisation and Productivity (POP CoE) assists a broad community of HPC application developers and users in both science and industry domains helping them to understand the performance-related issues of their applications and thus improve their efficiency and productivity. This fundamental purpose is reached by externally and objectively auditing the performance of the codes of all interested users, by providing not only qualitative but also quantitative analysis through the use of POP tools and methodology.

The current phase, POP3, is articulated in three main pillars: services, users, and co-design. POP services mainly focus on performance assessments with the goal to evaluate code performance and scaling, identifying the main sources of inefficiency and providing some insight and recommendation about how to improve it. POP3 also provides extended second level services that include proof of concepts, energy efficiency and advisory studies.

While POP3 will continue targeting all scales and types of users (incl. SMEs), POP3 focuses on much larger scales, assessing the execution on the EuroHPC hosting sites of some of the European flagship HPC applications for other CoEs.

- Service Portal: https://pop-coe.eu/services
- Training events: https://hpc-portal.eu/node/2015
- Potential Collaboration with Industry (not partners): Yes

## SERVICES

- Performance assessments
- Proof of concept prototype implementations
- Energy efficiency assessments
- Advisory studies

## TOOLS

**Open source tools:**

- **BSC:** Extrae, Paraver, Dimemas
- **JSC:** Scalasca, Cube, Score-P, Extra-P
- **Other:** MAQAO **(UVSQ),** MERIC **(IT4I),** MUST **(RWTH),** TAU (U.Oregon), Darshan (ANL)

**Commercial tools (when available on system):**

- Vampir
- Intel Trace Analyzer and Collector, VTune Amplifier
- HPE Cray Performance Measurement and Analysis Tools
- Linaro MAP, Performance Reports
- Nvidia developer tools

**01.01.2023 - 31.12.2026**
**Astrophysics / Cosmology**
https://www.space-coe.eu
1st phase - Type 1 (Exascale)

| Coordinator: University of Turin (PI: Andrea Mignone) ||
|---|---|
| INAF IT | University of Oslo NO |
| CINECA IT | E4 IT |
| KU Leuven BE | FORTH EL |
| IT4I CZ | EnginSoft IT |
| LMU DE | Eviden (Bull) F |
| CNRS F | HITS DE |
| Johann Wolfgang Goethe University DE | BSC ES |

SPACE CoE aims to extensively re-engineer astronomy and cosmology (A&C) codes for Exascale, adopting new computational solutions and innovative programming paradigms, software solutions, and libraries, to be able to extract information from the extremely complex and voluminous data that will be produced by the forthcoming missions/telescopes (e.g. SKA, Euclid). SPACE will address the high-performance data analysis of the data torrent produced by exascale A&C simulation applications, also with machine-learning and visualization tools.

- Service Portal: -
- Trainings: -
- Potential Collaboration with Industry (not partners): NO

## CODES

- **PLUTO**: an Eulerian, finite-volume, shock-capturing code based on high-order Godunov methods providing several integration algorithms. It supports both classical and relativistic flows and it is equipped also with a particle module for hybrid MHD-PIC simulations.
- **OpenGADGET**: one of the most used codes It is a N-body code that solves the gravitational and hydrodynamical equations in their Lagrangian form for a large ensemble of particles.
- **CHANGA/GASOLINE:** Tree and Smoothed Particle Magnetohydrodynamics codes that are widely used for cosmological galaxy formation simulations. The two codes have the same implementation, but CHANGA features parallelisation design with Charm++ which enables scaling up to 128K cores for highly-clustered datasets.
- **iPic3D**: fully electromagnetic massively parallel particle in cell based on the semi-implicit approach to address multiple scale problems in plasma physics.
- **RAMSES**: code to to model astrophysical systems, featuring self-gravitating, magnetised, compressible, radiative fluid flow. Based on the Adaptive Mesh Refinement (AMR) technique.
- **WhiskyTHC**: code aimed at solving the general-relativistic hydrodynamics equations on AMR grids by means of high-resolution shock capturing methods. It leverages a high-level C++ programming paradigm to achieve a high degree of efficiency.
- **FIL**: it employs a fourth-order accurate finite differencing scheme to solve the equations of general-relativistic magnetohydrodynamics. It includes a framework for realistic microphysics through the use of temperature and composition dependent Equation of State tables.
- **BHAC**: multidimensional general relativistic magnetohydrodynamics code based on the MPI-AMRVAC framework. BHAC solves the equations of ideal general relativistic magnetohydrodynamics in one, two or three dimensions on arbitrary stationary spacetimes.