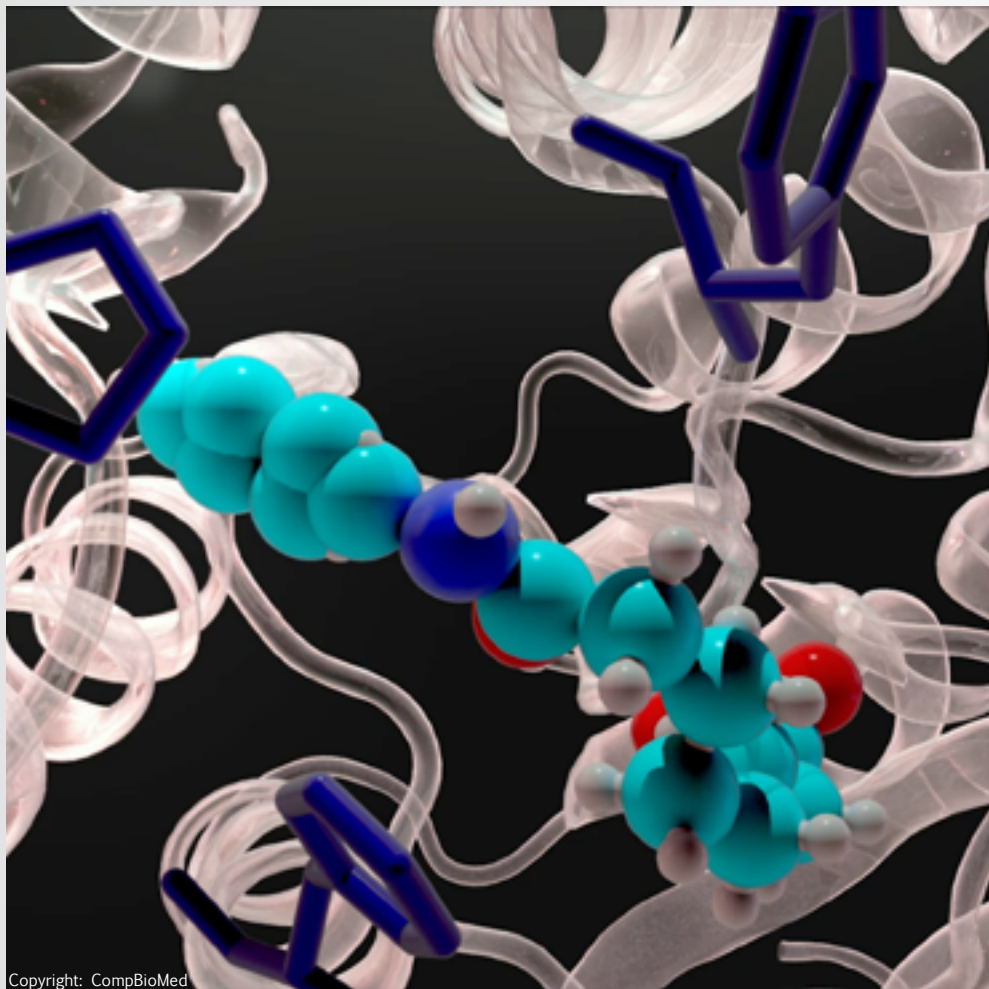




CoE European
Excellence in
HPC Applications

TABLE OF CONTENT

SERVICES CATEGORIES	4 & 5
BIOEXCEL 2	8 & 9
CHEESE	10 & 11
COMPBIOMED	12 & 13
E-CAM	14 & 15
EOCOE-II	16 & 17
ESIWACE2	18 & 19
EXCELLERAT	20 & 21
HIDALGO	22 & 23
MAX	24 & 25
POP 2	26 & 27



Copyright: CompBioMed

SERVICE CATEGORIES

- 1. Codes & Software Packages:** The specific codes, software packages concerning computing and storage aspects, and simulation tools developed and/or supported by the CoE.
- 2. Repository:** Various tools including workflows (user-friendly and efficient systems for workflow executions and data processing) provided by the CoEs.
- 3. Data Catalogue:** Store, share, and access CoE files and their metadata on a global scale.
- 4. Support to Code Optimization:** The CoE experts offer their expertise to develop and optimize customers' codes and tailored solutions adapted to end-users needs.
- 5. Consulting:** Personalized support from the CoEs, for example consultancy services on cutting-edge numerical tools or in modelling and simulation.
- 6. Training:** CoE training programmes, which include face-to-face training events, webinars, and a range of online tutorials and courses.

CoE	Codes & Software Packages	Repository	Data
	X	X	
 ChEESA	X	X	
	X		
	X	X	
	X		
 esiwace CENTRE OF EXCELLENCE IN SIMULATION OF WEATHER AND CLIMATE IN EUROPE	X		
 HiDALGO	X		
 MAX DRIVING THE EARTHSCALE TRANSITION	X	X	
	X		
	X	X	

Catalogue	Support to Code Optimization	Consulting	Training
	X	X	X
			X
	X	X	X
	X	X	X
	X	X	X
X	X		X
X		X	X
			X
X	X	X	X
	X	X	X



PROJECT COORDINATION:


KTH Royal Institute of Technology,
Sweden

CONTACT:

Rossen Apostolov | rossen@kth.se

WEB INFORMATION:

www.bioexcel.eu

 [@BioExcelCoE](https://twitter.com/BioExcelCoE)

 [www.linkedin.com/company/
bioexcel/](https://www.linkedin.com/company/bioexcel/)

 goo.gl/5dBzmw

CENTRE OF EXCELLENCE FOR COMPUTATIONAL BIOMOLECULAR RESEARCH

BioExcel focuses on the advancement and support of the HPC software ecosystem in the life science domain. Research and expertise covers structural and functional studies of the main building blocks of living organisms (proteins, DNA, membranes etc.) and techniques for modelling their interactions ranging from quantum to coarse-grained models up to the level of a single cell.

SERVICES

Codes:

- Provision and support for molecular dynamics, free energy and docking software packages and workflows
- GROMACS, PMX, HADDOCK, CP2K and CPMD
- Integrated workflows for portable and flexible solutions

Repository:

- Upstream sources of releases are provided on GitHub (<https://github.com/bioexcel>)
- A full stack of components, BioExcel Building Blocks (BioBB), is developed and provided for custom workflow solutions: https://bioexcel.eu/research/projects/biobb_standardization/

Support to Code Optimization:

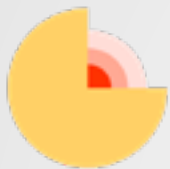
- Code optimisation for efficient and scalable high performance computing

Consulting services:

- Application of biomolecular modelling to industry challenges such as drug discovery
- Tailored solutions adapted to meet end-user needs

Training:

- Support Forums: supporting the community for computational biomolecular research (ask.bioexcel.eu)
- Webinars: covering topics related to the latest development of the supported software packages (bioexcel.eu/category/webinar/)
- Knowledge Resource Centre: repository for computational biomolecular training resources aggregated from BioExcel partners and third party providers (krc.bioexcel.eu)
- BioExcel Training Programme: including face-to-face training events, webinars and a range of online tutorials and courses (bioexcel.eu/services/training/)



ChEESE

PROJECT COORDINATION:


Barcelona Supercomputing Centre (BSC), Spain

CONTACT:

Arnau Folch | cheese-coe@bsc.es

WEB INFORMATION:

www.cheese-coe.eu

 [@Cheese_CoE](https://twitter.com/Cheese_CoE)

 www.linkedin.com/company/cheese-coe/

CENTER OF EXCELLENCE FOR EXASCALE IN SOLID EARTH

ChEESE aims to become a hub for HPC software within the solid earth community. In CheEESE, leading European HPC centers, academia, hardware developers, as well as SMEs, industry and public governance bodies such as civil protection are working together to prepare European flagship codes for upcoming pre-Exascale and Exascale supercomputing systems to tackle global challenges in the domain of solid earth. Potential services include urgent computing, hazard assessment and early warning. ChEESE will promote and facilitate the integration of HPC services to widen the access to codes to the Solid Earth user's community. Finally, ChEESE aims at acting as a hub to foster HPC across the Solid Earth Community and related stakeholders and to provide specialized training on services and capacity building measures.

SERVICES

Code & Software

Packages:

ExaHype, Salvus, Seis-Sol, SPECFEM3D, PARODY_PDAF, XSHELLS, ASHEE, FALL3D, T-HySEA, L-HySEA

Repository:

- Various tools provided, including user-friendly and efficient systems for workflow executions and data processing

Training:

- Workshops:
cheese-coe.eu/events/workshops
- Meetings:
cheese-coe.eu/events/meetings
- Training courses:
cheese-coe.eu/events/training
- Webinars:
cheese-coe.eu/events



PROJECT COORDINATION:


University College London, UK

CONTACT:


Emily Lumley | e.lumley@ucl.ac.uk

WEB INFORMATION:

www.compbiomed.eu

 [@bio_comp](https://twitter.com/bio_comp)

 www.linkedin.com/company/cheese-coe/

 <https://bit.ly/2CyAa31>

CENTRE OF EXCELLENCE IN COMPUTATIONAL BIOMEDICINE

CompBioMed is a user-driven Centre of Excellence in Computational Biomedicine to nurture and promote the uptake and exploitation of high performance computing within the biomedical modelling community, supporting users in academia, industry and clinical practice.

SERVICES

Code & Software Packages:

- Cardiovascular: Alya, HemeLB, HemoCell, OpenBF, Palabos, PolNet, InSilicoMRI, Living Heart HumanModel
- Molecular Medicine: BAC, HTMD, Playmolecule, VisualGec, HTBAC, Virtual Assay
- Neuro-musculoskeletal Medicine: CT2S, Insigneo Bone Tissue Suit, Palabos
- Software Hub: www.compbiomed.eu/services/software-hub/

Support to Code Optimization:

- Expertise to develop and optimize customers' codes
- Tailored solutions adapted to end-users needs

Consulting:

- Code auditing
- Consultancy on services such

- as cutting-edge numerical tools or modelling and simulation
- CompBioMed Associate Partner scheme (www.compbiomed.eu/associate-partners/)
- Help with accessing data and e-infrastructure
- Online HPC allocation requests to gain access to several large scale HPC resources (www.compbiomed.eu/high-performance-computer-allocations/)

Training:

- Regular webinars, training events and training repository (www.compbiomed.eu/training-3)
- Visitor Programme: a flexible scheme designed to support knowledge exchange (www.compbiomed.eu/innovation/visitor-programme/)

**PROJECT COORDINATION:**

Ecole Polytechnique Fédérale de
Lausanne, Switzerland

CONTACT:

- Luke Drury (Proj. Chair) | ldcp.dias.ie
- Ana Catarina Mendonça (Proj. Coordinator) | ana.mendonca@epfl.ch
- Ignacio Pagonabarraga (Proj. Tech. Manager) | ignacio.pagonabarraga@epfl.ch

WEB INFORMATION:

www.e-cam2020.eu

 [@ECAM2020](https://twitter.com/ECAM2020)

CENTRE OF EXCELLENCE FOR SOFTWARE, TRAINING AND CONSULTANCY IN SIMULATION AND MODELLING

The overall objective of E-CAM is to create, develop and sustain a European infrastructure for computational science applied to simulation and modelling of materials and of biological processes of industrial and societal interest.

SERVICES

Code & Software Packages:

- Molecular dynamics: LAMMPS, GRO-MACS, OPS, NAMD
- Electronic Structure: ESL, ELSI, Wannier90, QMCPACK, QuantumEspresso, SIESTA, Aiida
- Quantum Dynamics: PaPIM, Quantics, CP2K, Q-Chem, CPMD, EIVibRot
- Meso- and multi-scale modelling: MP2C, ESPResSo++, DL_MESO_DPD, GC-AdResS

Repository:

- Open access to E-CAM software repository (www.e-cam2020.eu/software-library/)

Support to Code Optimization:

- Expertise to develop and optimize customers' codes
- Tailored solutions adapted to end-users needs

Consulting and interaction with industry:

- Pilot projects focused on industrially oriented problems
- Industrial involvement and participation in E-CAM state-of-the-art and scoping workshops
- Broker for industry

- Assist on business decision as to whether computational methods can be effectively applied to a given problem with good cost/benefit ratio
- Define of the most appropriate modeling strategy for a given problem within and across the scientific areas of E-CAM
- Survey existing methods to establish whether a given modelling strategy requires new developments or can be enacted with existing tools
- Evaluate the accuracy of available methods for a given problem
- Develop, document, validate and benchmark of new software, for packages structured by combining modules already present in the E-CAM repositories or of interfaces with community codes belonging to the E-CAM partnership
- Assist in selecting the most appropriate hardware architecture

Training:

- Extended Software Development Workshops (www.e-cam2020.eu/calendar/)
- Webinars / lecture streaming
- On-demand industry training courses on specific methods, software and tools
- Online training material (training.e-cam2020.eu)



PROJECT COORDINATION:

Maison de la Simulation (MdlS) at
CEA, France

CONTACT:

Edouard Audit | contact@eocoe.eu

WEB INFORMATION:

www.eocoe.eu

 [www.linkedin.com/company/
hpc-energy/](https://www.linkedin.com/company/hpc-energy/)

ENERGY ORIENTED CENTRE OF EXCELLENCE

EoCoE will use the prodigious potential offered by the ever-growing computing infrastructure to foster and accelerate the European transition to a reliable and low carbon energy supply via targeted support to five carbon-free energy pillars: Meteorology, Materials, Water, Wind and Fusion, each with a heavy reliance on numerical modelling.

SERVICES

Support to Code Optimization:

- Improvement of third-party applications
- Code performance assessment and optimization
- Porting codes on new architectures
- Software integration, special purpose algorithms
- Usage of developed/provided codes and numerical tools

Code & Software Packages:

- Wind: Alya
- Meteorology: ESIAS-Chem, ESIAS-Meteo, EURAD-IM
- Materials: QMPACK, libNEGF, KMC/DMC
- Water: ParFlow, SHEMAT-Suite
- Fusion: Gysela

Consulting:

- Consultancy for running simulation with industrial focus
- Consultancy services in modeling energy-oriented processes
- Code auditing
- Consultancy on cutting-edge numerical tools
- General topics related to high-performance computing

Training:

- Workshops and hackathons (www.eocoe.eu/workshops)
- Interactive webinars
- Online training and tutorials (www.eocoe.eu/video_resource/)



PROJECT COORDINATION:

Deutsches Klimarechenzentrum
(DKRZ), Germany

CONTACT:

Joachim Biercamp
esiwace@lists.dkrz.de

WEB INFORMATION:

www.esiwace.eu
🐦 @ESIWACE

CENTRE OF EXCELLENCE IN SIMULATION OF WEATHER AND CLIMATE IN EUROPE

ESiWACE2 aims to link, organise and enhance Europe's excellence in weather and climate modelling to enable leading European weather and climate models to leverage the performance of pre-exascale systems as soon as possible and prepare the weather and climate community to be able to make use of exascale systems when they become available.

SERVICES

Code & Software Packages:

- Leading European Weather & Climate Models: ICON, IFS, NEMO, Dynamico
- Support to other models, e.g. UM from the UK Met Office

Data Catalogue:

- Via links to the sister project IS-ENES3, the centre provides services to store, share, and access weather and climate model result data and metadata on a global scale

Support to Code Optimization:

- Expertise to develop and optimize customers' codes
- Tailored solutions adapted to end-users needs

Training:

- IO and HPC awareness
- DSL
- C++ for HPC
- OASIS3-MCT
- High-Performance Data Analytics
- Docker
- Summer school in HPC for weather and climate



PROJECT COORDINATION:

Universität Stuttgart (HLRS), Germany


CONTACT:

Bastian Koller | koller@hlrs.de

WEB INFORMATION:

www.excellerat.eu

 [@EXCELLERAT_CoE](https://twitter.com/EXCELLERAT_CoE)

 www.linkedin.com/company/excellerat/

CENTRE OF EXCELLENCE FOR ENGINEERING APPLICATIONS

EXCELLERAT's goal is to facilitate the development of important codes for high-tech engineering, including maximizing their scalability to pre-exascale and exascale architectures and supporting the technology transfer that will enable their uptake within the industrial environment.

SERVICES

Code & Software

Packages:

- Nek5000: a fast and scalable high-order solver for computational fluid dynamics
- Alya: large scale computational mechanics
- AVBP: software tool for Computational Fluid Dynamics
- FEniCS: FEniCS is a popular open-source computing platform for solving PDEs
- Flucs: FLEXible Unstructured CFD Software
- TPLS: open-source program for simulation of two-phase flows

Repository:

- Development of dedicated general purpose tools and plug-ins that are of interest to the community

Support to Code Optimization:

- Porting
- Optimizing code

Consulting:

- Expertise on the ecosystem
- Network consulting

Training:

- Training programmes (<https://www.excellerat.eu/wp/training/training-event/>)



HiDALGO

PROJECT COORDINATION:

Atos Spain, Spain

CONTACT:

Francisco Javier Nieto
francisco.nieto@atos.net

WEB INFORMATION:

www.hidalgo-project.eu
🐦 @EU_HiDALGO

HPC AND BIG DATA TECHNOLOGIES FOR GLOBAL SYSTEMS

HiDALGO enables the assessment of Global Challenges problem statements by enabling highly accurate simulations, data analytics, artificial intelligence and data visualisation, but also by providing knowledge on how to integrate the various workflows and the corresponding data.

SERVICES

Code & Software

Packages:

- Agent-based Modelling: AMOS, RepastHPC, MASON, SUMO, FLEE, MUSCLE2
- Data Analytics: Apache Spark, Apache Flink, Apache Storm
- Machine Learning: TensorFlow, Torch
- Visualization: COVISE, VISTLE
- Computational Fluid Dynamics (CFD): FEniCS

Data Catalogue:

- Store, share, and access CoE files and their metadata on a global scale

Consulting:

- Code auditing
- Consultancy on services such as cutting-edge numerical tools or modelling and simulation

Training:

- HPC, HPDA, AI and Global Challenges simulation trainings with different community foci



PROJECT COORDINATION:

CNR Nano, Modena, Italy


CONTACT:

Mariella Ippolito


mariella.ippolito@max-centre.eu

WEB INFORMATION:

www.max-centre.eu

 [@max_center2](https://twitter.com/max_center2)

 www.linkedin.com/company/max-centre/

 bit.ly/2YvSwue

MATERIAL DESIGN AT EXASCALE

MAX (MAterials design at the eXascale) is a European Centre of Excellence which enables materials modelling, simulations, discovery and design at the frontiers of the current and future High Performance Computing (HPC), High Throughput Computing (HTC), and High Performance Data Analytics (HPDA) technologies.

MAX gives great importance to engaging academic and industrial communities: on the one hand, by providing workflows and turn-key solutions, and on the other by organizing training events for different pools of users and developers.

SERVICES

Code & Software Packages:

- Codes: Quantum Espresso, Yambo, Fleur, Siesta, BigDFT, CP2K
- Workflows platform: AiiDA
- Domain Specific Libraries: Sirius, FFTXLib & LAXLib, CheSS
- Software developed by MAX is open-source

Repository:

- AiiDA implements, runs and shares workflows and turnkey solutions, and it ensures reproducibility and reuse of computational research, as well as data analytics

Data Catalogue:

- Materials Cloud: open-access, moderated repository for research data in computational materials science, in which data can be uploaded, visualized, analyzed and shared

Consulting:

- High Level Consultancy service supports the end-users in using the MAX flagship codes. The service helps, generally, in finding ad-hoc solutions for the users (best parameters for the optimal run on a given architecture, performance optimization, ...), and possibly it comprises code development (new features/algorithms)

Training:

- Integrated training and education in the field of HPC developments and in the computational materials science domain, with workshops, schools and hackathons
- Contributions to university courses
- Training through research in the CoE labs

**PROJECT COORDINATION:**

Barcelona Supercomputing Centre (BSC), Spain

CONTACT:

Jesus Labarta | pop@bsc.es

WEB INFORMATION:

www.pop-coe.eu

 [@POP_HPC](https://twitter.com/POP_HPC)

 youtube.com/POPHPC

PERFORMANCE OPTIMISATION AND PRODUCTIVITY

The POP Centre of Excellence gathers leading experts in performance methods and tools and programming models to offer services to all academic and industrial communities to help them better understand the behaviour of their parallel applications, suggest the most productive directions for optimizing the performance of the codes, and help implementing those transformations in the most productive way.

SERVICES

Code & Software Packages:

- Open-source parallel performance tools: Extrae, Paraver, Dimemas, Scalasca, Cube, Extra-P, Score-P, MAQAO
- Open-source correctness tools: MUST, ARCHER

Support to Code Optimization

(<https://pop-coe.eu/services>):

- Parallel Application Performance Assessment (Primary Service): Initial analysis measuring a range of performance metrics to assess quality of performance and identify the issues affecting performance. If needed, also identifies the root causes of the issues found and recommend approaches to address them
- Proof-of-Concept (Follow-up service): Experiments and mock-up tests for customer codes, Kernel extraction, parallelisation, and mini-apps experiments to demonstrate the actual benefits of proposed optimisations

Data Catalogue:

- Co-design data repository, which includes statistics about common performance issues of HPC applications as well as micro-kernels, extracted from real applications each characterising fundamental performance behaviour. Hardware architects or system software designers from other EU projects will be able to get quantitative information of how to estimate the potential impact of an architectural or system software approach they may be developing.

Consulting:

- Consulting services related to parallel performance analysis and optimization tools and methods

Training:

- Performance tool tutorials and Application tuning workshops (pop-coe.eu/news/events)
- Offline training material including webinars (pop-coe.eu/further-information/learning-material)

 Funded under the Horizon 2020 research & innovation programme from European Union



www.focus-coe.eu



Twitter: @FocusCoE

Höchstleistungsrechenzentrum Stuttgart (HLRS) | Nobelstraße 19, 70569 Stuttgart | Tel.: 0711 68587269