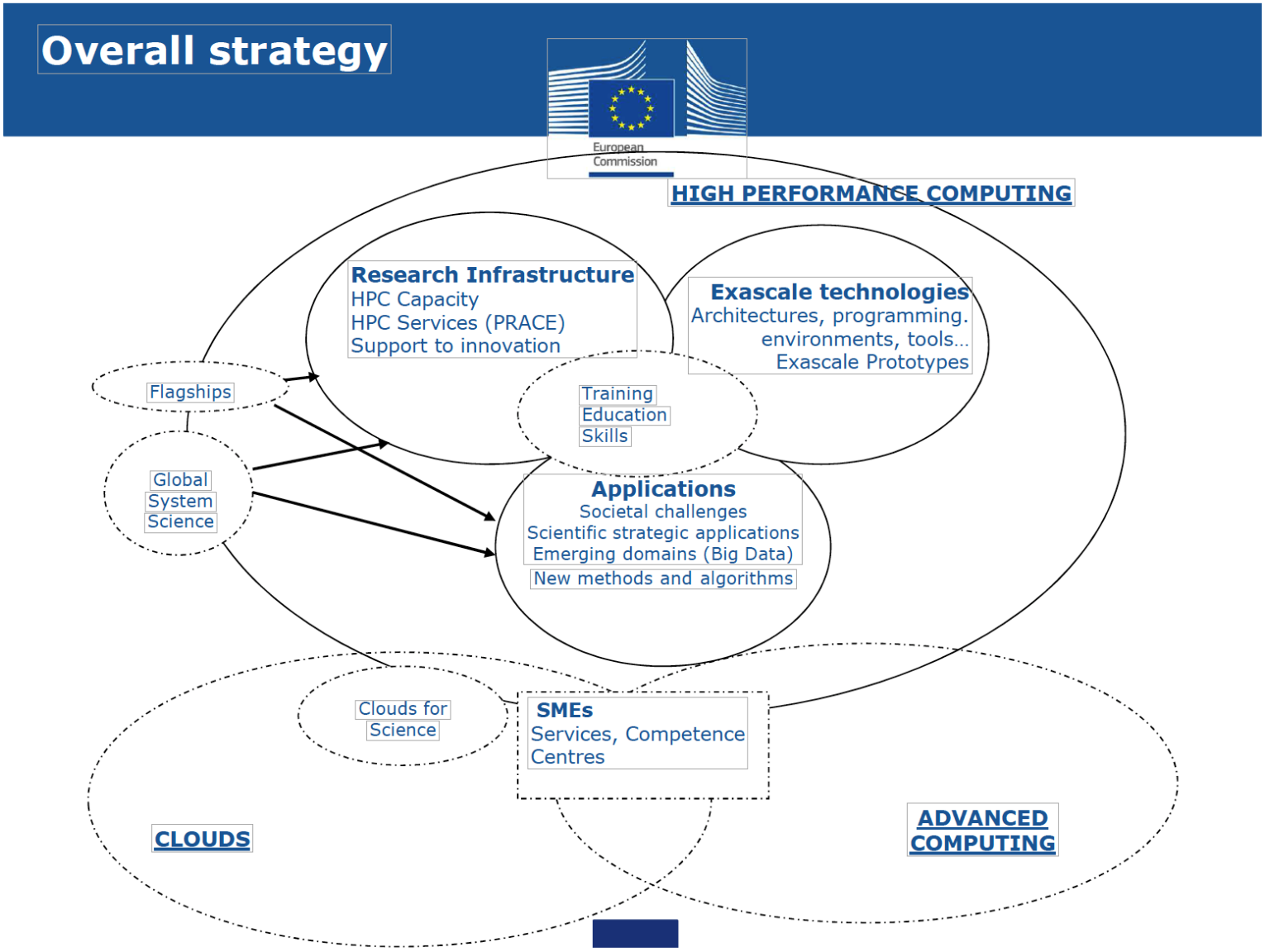
Energy oriented Centre of Excellence for computer applications

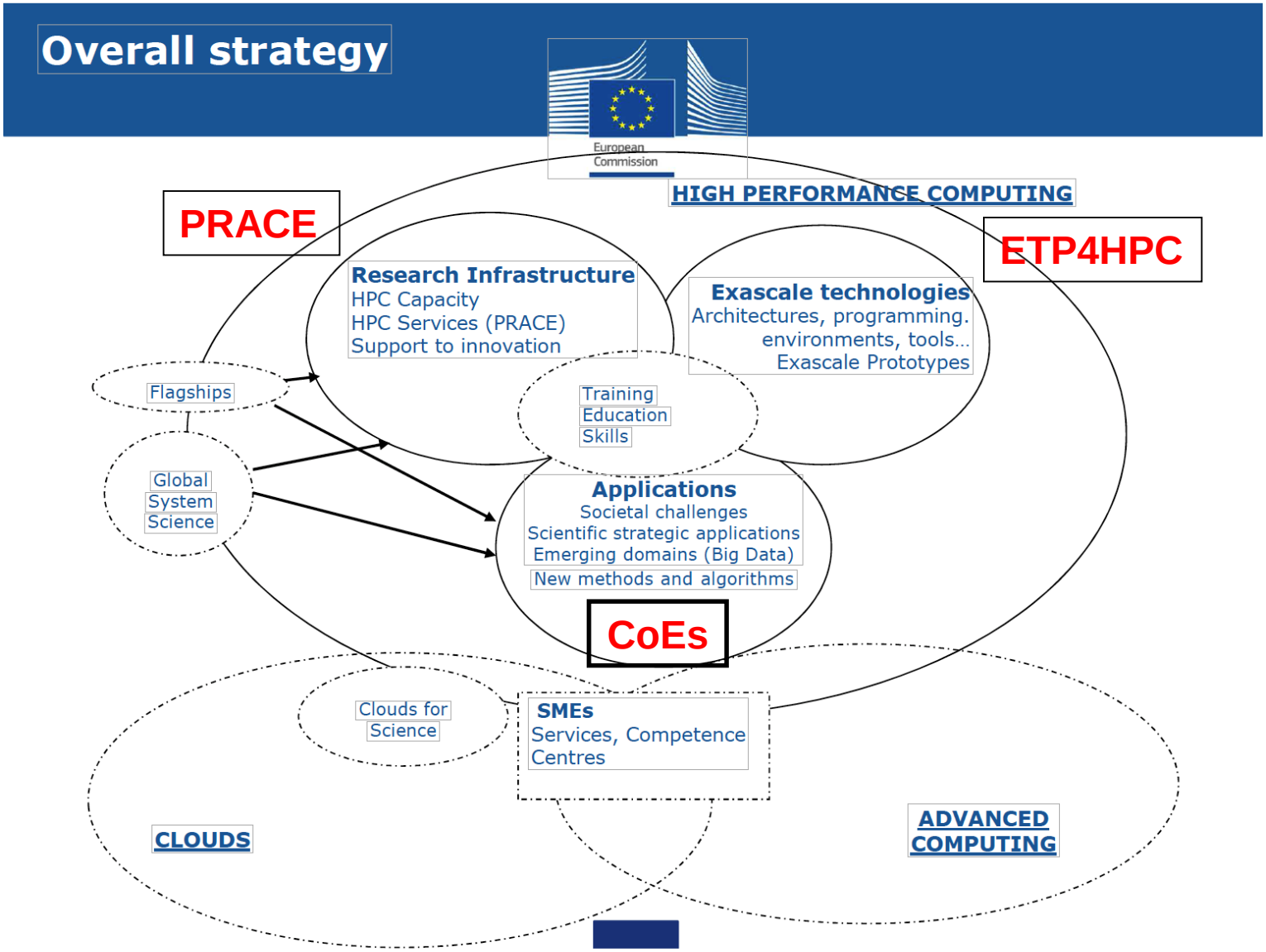
Edouard Audit

Horizon 2020
European Union funding
for Research & Innovation

European HPC strategy



European HPC strategy



8 CoEs

EoCoE - Energy oriented Centre of Excellence

BioExcel - Centre of Excellence for Biomolecular Research

NoMaD - The Novel Materials Discovery Laboratory

MaX - Materials design at the eXascale

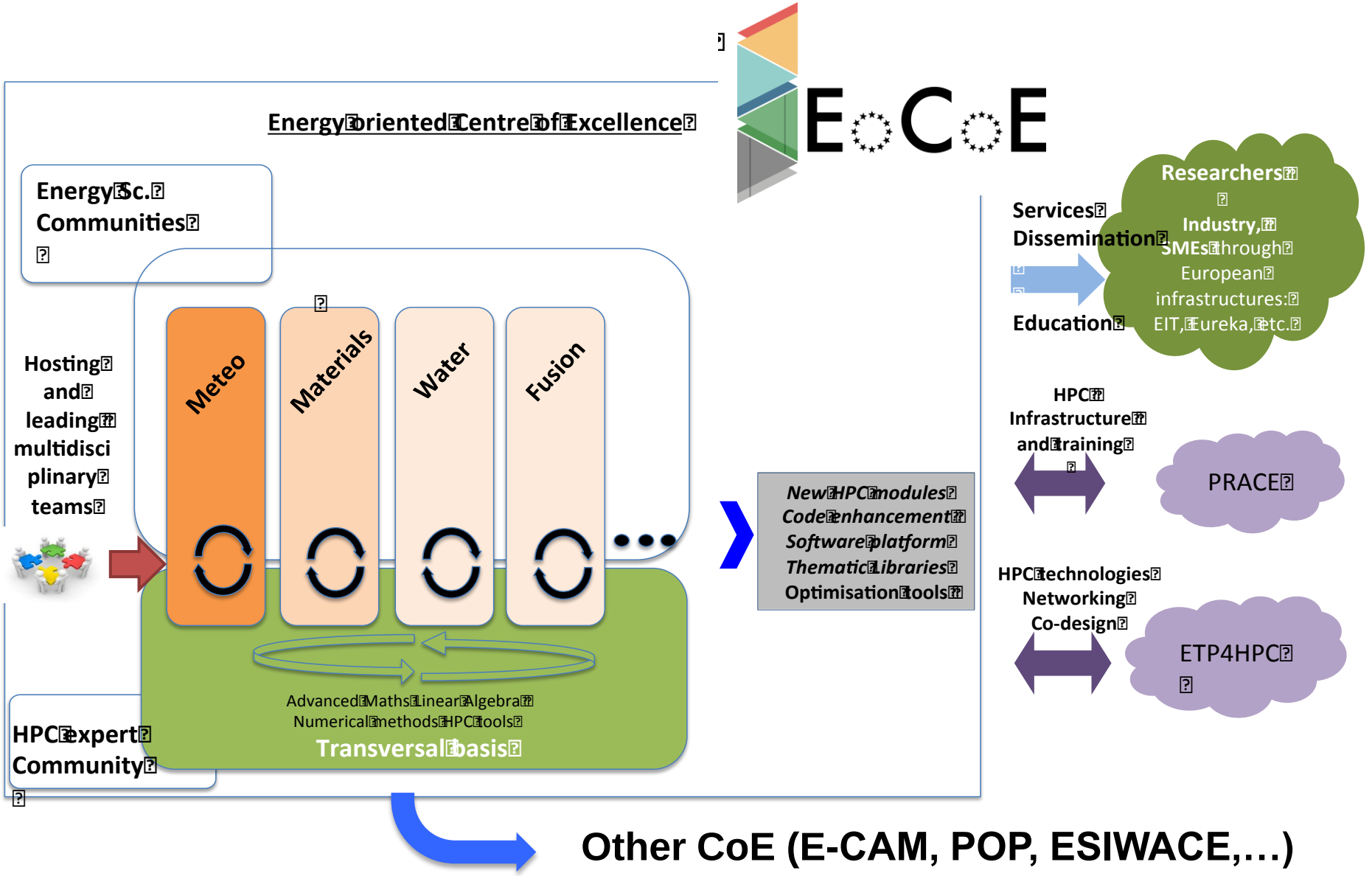
ESiWACE - Excellence in SImulation of Weather and Climate in Europe

E-CAM - An e-infrastructure for software, training and consultancy in simulation and modelling

POP - Performance Optimisation and Productivity

COEGSS - Center of Excellence for Global Systems Science

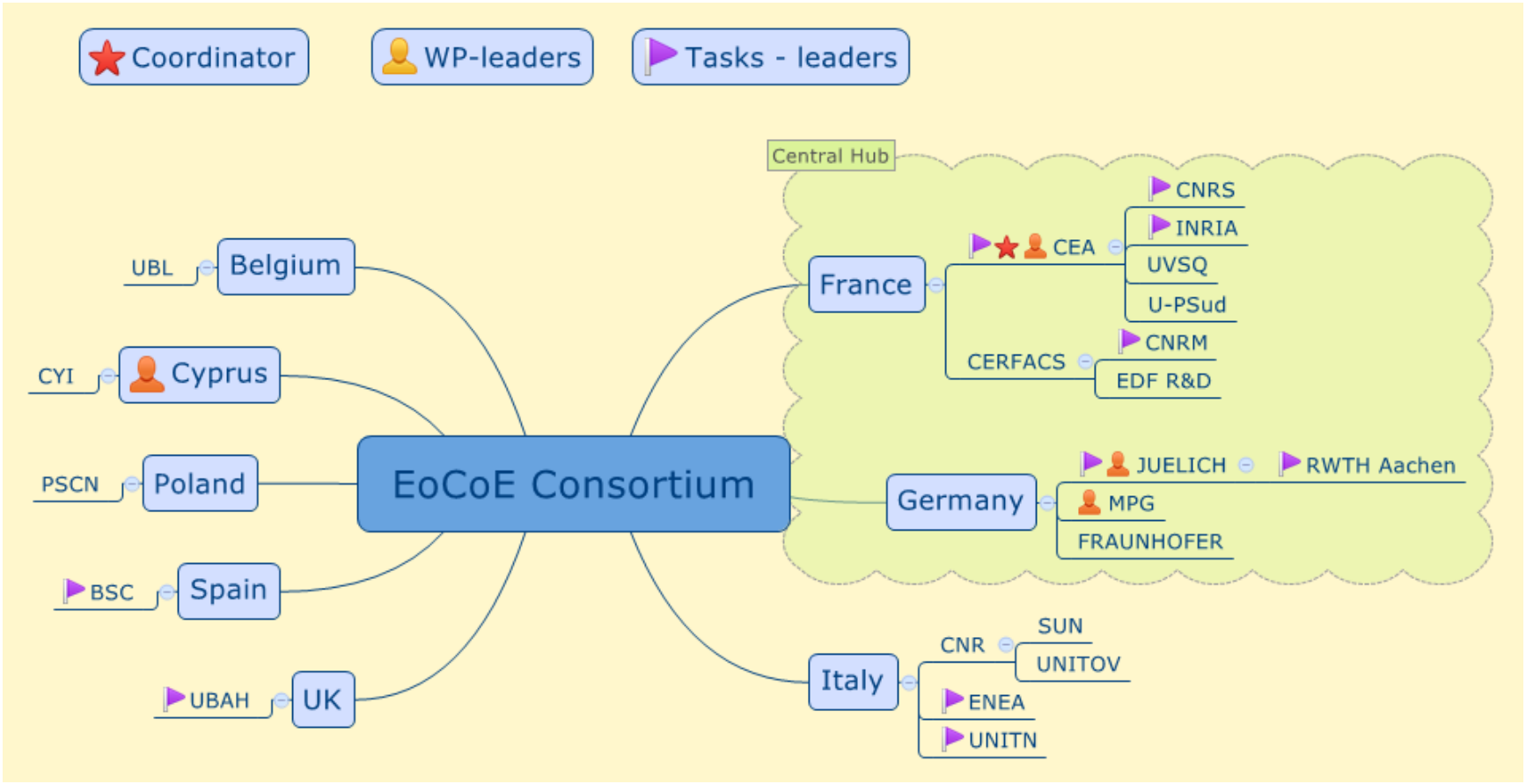
EoCoE


Energy oriented Centre of Excellence
Energy Sc. Communities
Hosting and leading multidisciplinary teams
Meteo
Materials
Water
Fusion
Advanced Maths Linear Algebra
Numerical methods HPC tools
Transversal basis
HPC expert Community
New HPC modules
Code enhancement
Software platform
Thematic Libraries
Optimisation tools
Services
Dissemination
Education
Researchers
Industry, SMEs through European infrastructures: EIT, Eureka, etc.
HPC Infrastructure and training
PRACE
HPC technologies
Networking
Co-design
ETP4HPC
Other CoE (E-CAM, POP, ESIWACE,…)

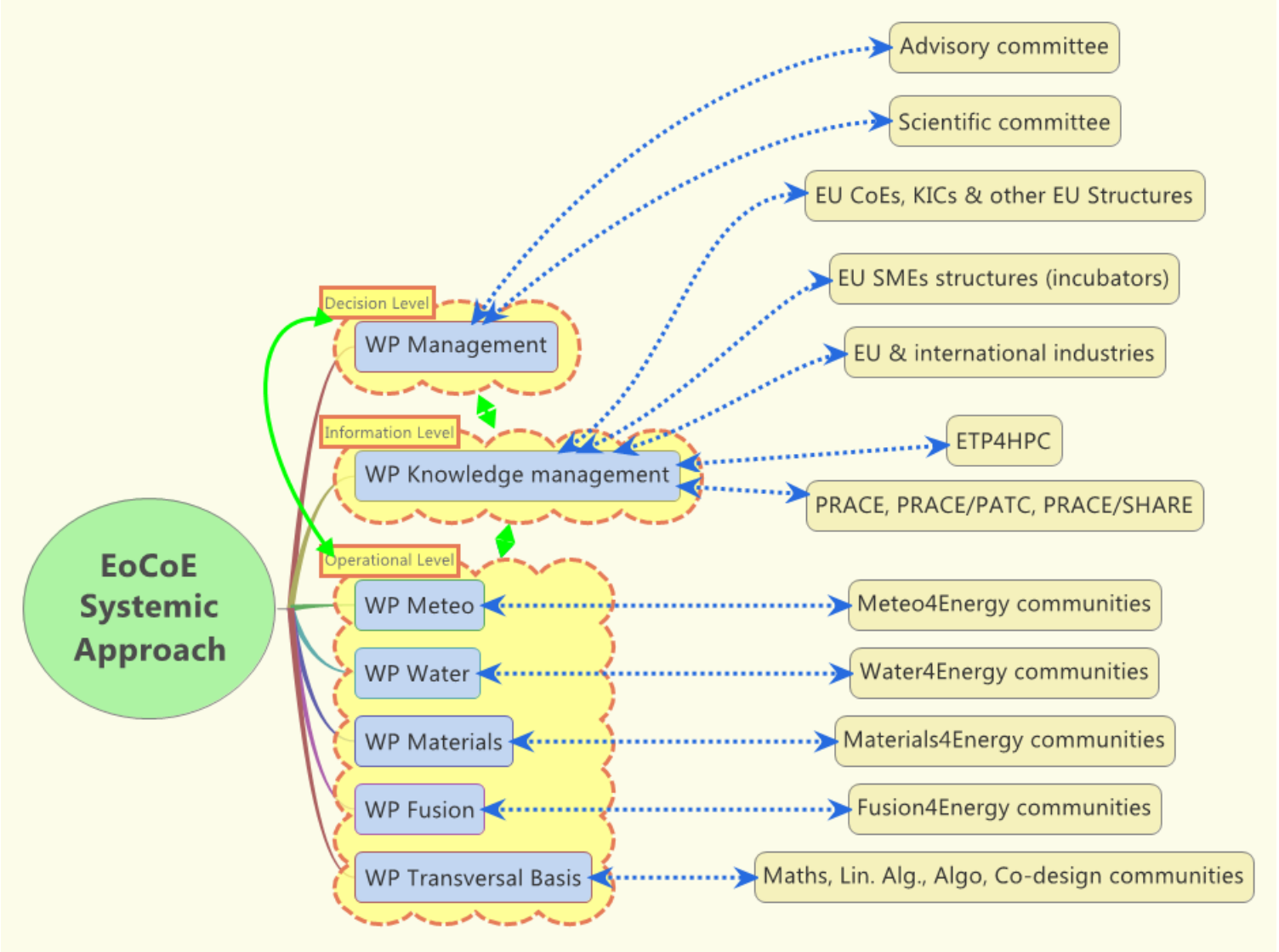
EoCoE consortium

Foster the European transition to a reliable low carbon energy supply using HPC

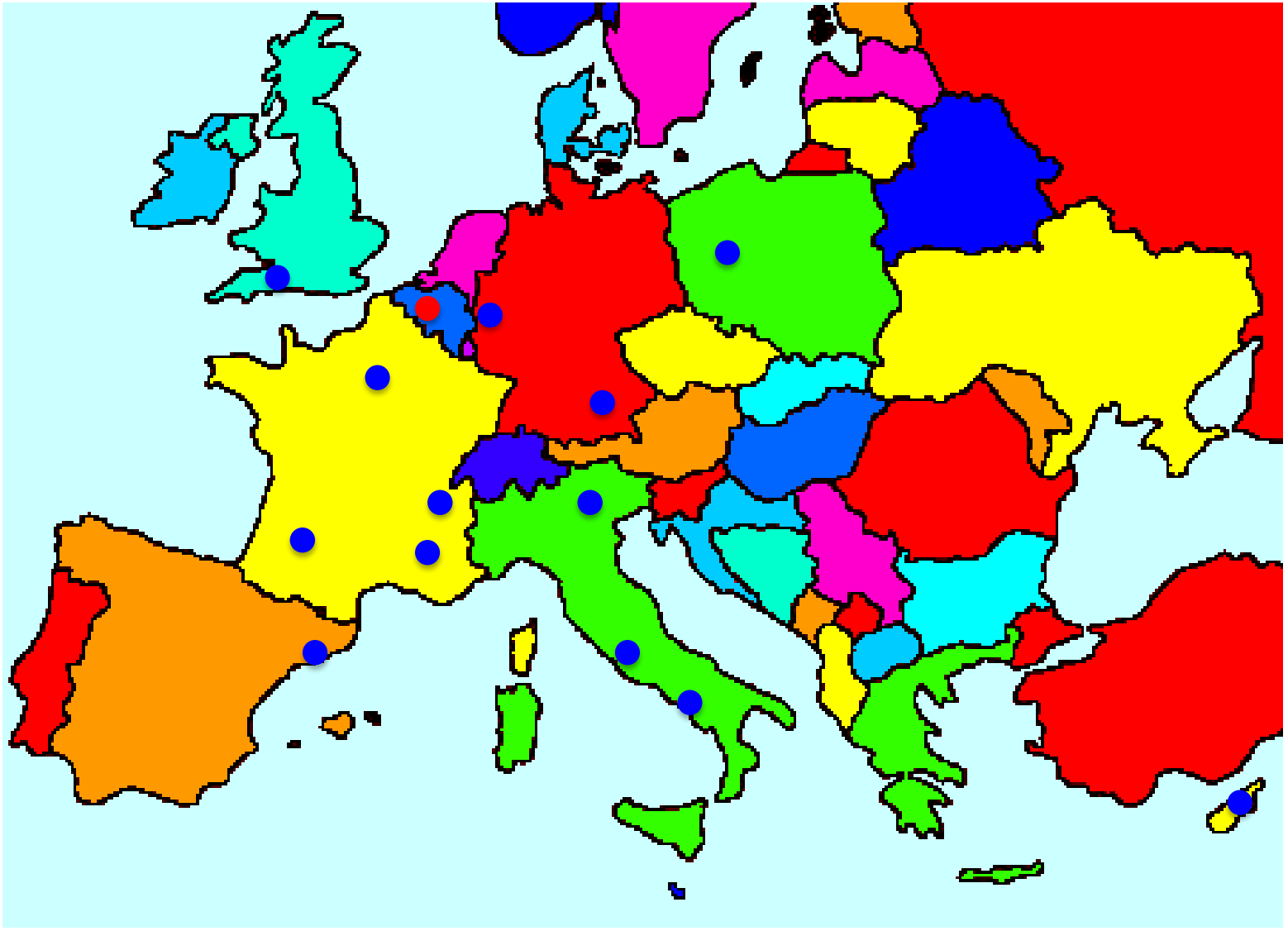
8 countries, 22 partners, 5.5 M€, lead by MdS



A systemic approach



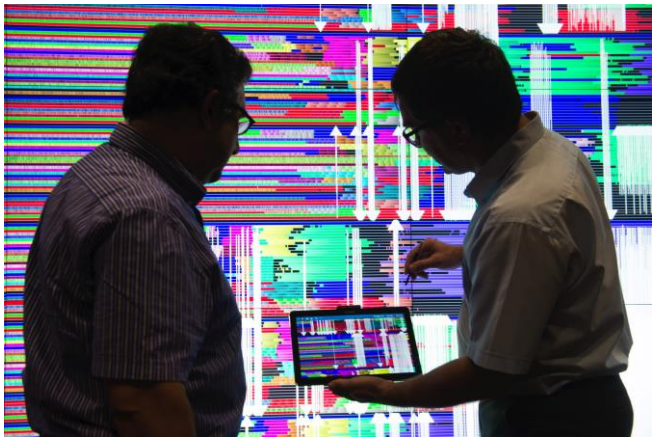
EoCoE : A European project

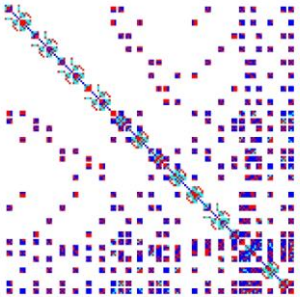


Objectives - I

Develop or optimise high end tools and software for all the communities. Get ready for exascale computer

- Applied math and numerical methods
- Linear algebra
- System tools for HPC
- New programing model



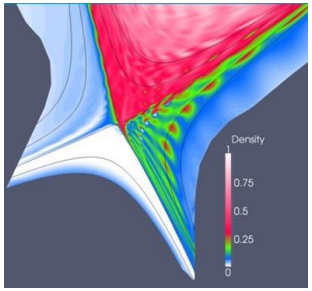


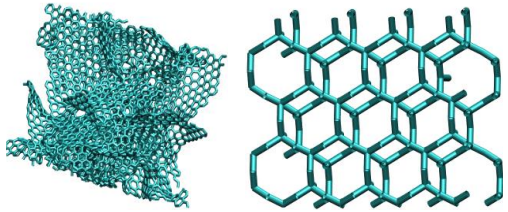
Objectives - II

Improve means of **production**, **storage** and **distribution** of electricity with **short**, **middle** and **long** term goals

Meteorology for energy : Very short term forecast to predict the production of solar and winf farm – Efficient coupling to the grid, energy trading.

Fusion for energy : Coupling kinetic and fluid codes, mesh aligned with equilibrium configurations.





Material for energy : Photovoltaic cells, battery and super-capacitors

Water for energy : Geothermy et hydro-electricity – Managment of ressource, strategy of usage - influence of climate change.

First Phase objectives for users

Community partners objectives are organised in short, mid and long terms impacts and in production, storage and delivery of energy.

(Table below shows the EoCoE first phase applications and in *italic red text* expected later subjects).

Energy features	Short-term*	Mid-term**	Long-term***
Production	Water WP (Geothermal energy) *Water WP (ocean energy)*	Materials WP (enhanced Photovoltaic cells)	Fusion WP (ITER)
Storage		Materials WP (Batteries and super capacitors) Water WP (Reservoirs strategy according to climate change) *Water WP (heat geological storage)*	
Delivery	Meteorology WP (solar and wind energy prediction)		

WP (work package).
*short-term: mature technology; simulation will help efficient and cost effective implementation
**Mid-term: enhancing researches; simulation will reduce time to market
***Long-term: fundamental research; simulation will accelerate research

First Phase objectives for users

Meteorology for Energy community:

1. Power grid control and power trading by ultra large meteorological ensemble runs (IEK 8-IWES)

2. Statistical calibration of ensemble forecasts (CNRM)

3. Optimal operation of Concentrated Solar Power (CSP) under Weather Uncertainty (RWTH Aachen, CyI)

4. Solar power nowcasting from image assimilation (INRIA)

First Phase objectives for users

Materials for Energy community:

1. Ab initio method (BigDFT) for large system with a given accuracy (FZJ)
2. Screening/PES (ENEA)
3. Ab-initio methods for large system (CEA)
4. Boosting the calculation of the electronic properties (CNRS)
5. Embedded method (CNRS)
6. Aging and diffusion properties (CEA)
7. Virtual materials for devices (inoPV, OLED, batteries, supercapacitors) (UBAH)

First Phase objectives for users

Water for Energy community:

1. Geothermal energy HPC issues / link to transversal activity (RWTH)
2. Geothermal energy application (RWTH)
3. Setup of TerrSysMP at 1km resolution over continental Europe (FZJ)
4. Hydropower energy application (UNITN)

First Phase objectives for users

Fusion for Energy community:

1. Constructing flux-surface aligned mesh-grids in the poloidal plane (MPG)

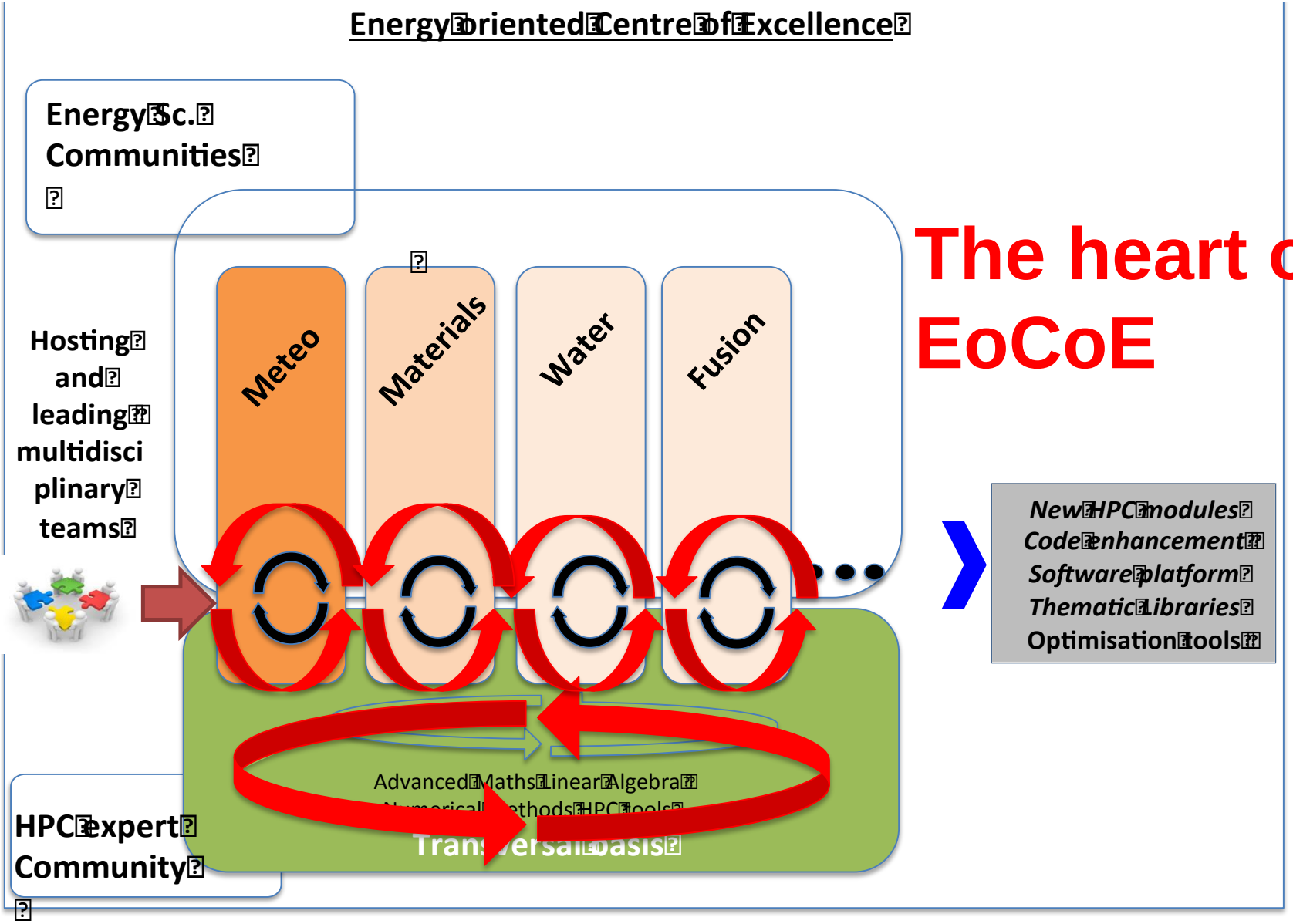
2. Coupling of MHD or fluid descriptions with the gyrokinetic and Monte-Carlo approaches (FZJ)

Transversal Basis

The EoCoE is intended to foster cross-cutting skills in massively parallel algorithms for many-cores architectures in a co-design (algorithms/software/hardware) approach, such as

1. Numerical methods – applied mathematics (INRIA)
2. Linear algebra (INRIA)
3. System tools for high performance (CEA)
4. Advanced programming methods and tools (FZJ)
5. Tools and services for HPC (FZJ)

The heart of EoCoE



Example : IO

Usage of XIOS by other communities :

The climate communities has a very strong experience in IO :

- Large volume of data to manage
- Complexe post-treatment and workflow

Larger simulation generate larger and larger dataset.

→ Other communities are/will face the same challenge….

Adapt XIOS for a wider usage :

- Relax geometrical constraints (ie 5D array for kinetic codes)
- Different management of calendar
- More general back-end NetCDF, HDF5, sionlib,….

The EoCoE Matrix

Task in WP 1	Expertise in WP 1	WP 2: METEOROLGY	WP 3: MATERIALS	WP 4: WATER	WP5: FUSION
5 - Tools and services for HPC	Performance evaluation, services and tools	**ALYA wind farm CFD code** Evaluation of the hybrid OpenMP/MPI implementation			
	Post-processing and visualization	**Ensemble calibration** Visualization of large ensembles of simulations, and derived products, including uncertainty quantification **Concentrated Solar Power** Tools needed to visualize the effectiveness of parallelization **Solar nowcasting** Post-processing and visualization of nowcasting results	**Electronic properties** Visualisation of the electronic and solvent 3D densities and their associated local properties for large molecular systems. **Atomic structure** Visualisation of large set of data containing atomic configurations	**SHEMAT geothermal energy** rapid 3D visualization and recording of animated movies, e.g.: from time series of subsurface geothermal reservoir behaviour	High order finite element reader in HDF5-Pixie format in Visit and Paraview.
	Big Data	**WRF super ensemble** Integration of a data mining tool to implement suitable metric for evaluating a phase space distance between ensemble members and the observation stream **Ensemble calibration** Development of novel approaches regarding diagnostics for extreme events related to high impact weather, utilizing reforecast data sets (including graphical applications)	**Storage of big data** for post processing analysis	**SHEMAT** devise solutions to handle the BigData output for high resolution, time dependent 3D geothermal reservoir behaviour **TerrSysMP** Data formats and metadata standards will be communicated for development of the big data analyses and visualization tools **Hydropower** Management of historical data and quality control **Hydraulics** Simulation outputs from 1D and 2D modelling will be provided for development of big data analyses and visualization tools. Movie generation will be needed for inundation scenario simulation. Visual solution for comparing model and observations will be needed.	
	Continuous integration platform (Jenkins) JUBE Benchmarking Environment	**WRF super ensemble** JUBE performance analysis to candidate implementation strategies, including consequences from particle selection		**TerrSysMP** Support for coupled multiphysics geoscience codes and benchmarking	Development of automatic integration and benchmarking tools for fusion codes including non-regression tests

Example : IO

- Interaction matrix establishes contact points between application fields and transversal HPC activity (math algorithms, solvers, I/O, performance, tools). This revealed over 20 unique community codes in need of performance improvements which will contribute to the project goals.

- Formal procedure and template for developer teams to request HPC support via Project Executive Committee established

- Implementation of pre-triggered application requests identified at proposal time: 2 such actions already under way

- Framework for comprehensive application performance audit defined in cooperation with POP CoE, including: code ID cards, performance metrics and diaries to monitor progress. Implementation via joint workshop series plus follow-up actions.

EoCoE optimization workshop

First EoCoE optimization workshop in Julich in December.

- Gathering HPC experts from WP1 and code developpers.
- Organized in collaboration with POP
- 7 EoCoE core applications where participating

Allowed important progress → Next workshop in may

Code Optimisation

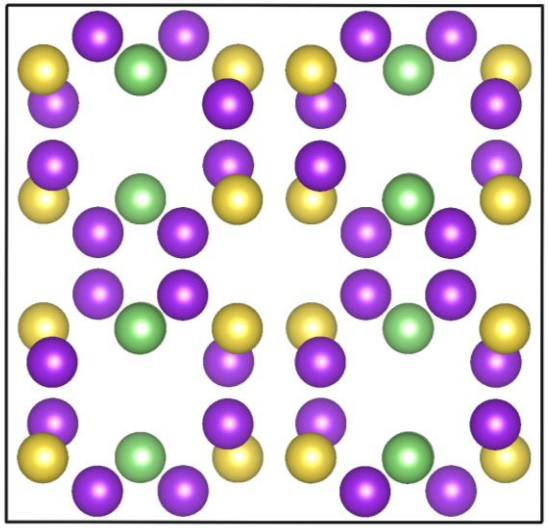
- Development of a complet metric sheet and associated tools to evaluate codes in a systematic way.
- **The evaluation procedure workflow will be fully automated**
- Test of a plateform for continous integration

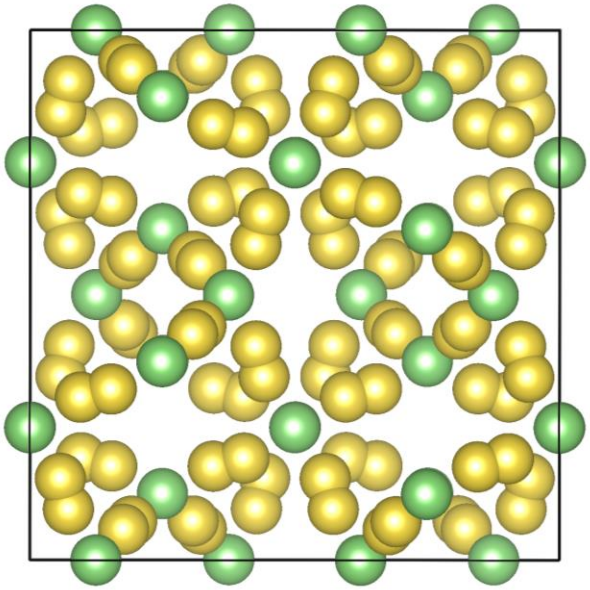
All solid Li-ion batteries

High throughput computing allow to test a large variety of material

Solid electrolyte solide : $Li_7La_3Zr_2O_{12}$ (LLZO)

Low temperature : tetragonal structure, bad conductor
High temperature : cubic structure, very good conductor





- **Similar structures but very different diffusive mecanisms**
- **Tetragonal phase : Li^+ ions have concerted and difficult movement**

Burbano et al., PRL

Conclusions

- Joint workshop and continous work with POP
- Expertise on software architecture for E-CAM
- Link with EsiWace for IO
- ……

CoEs should contribute to build a strong HPC community in Europe