Energy oriented Centre of Excellence for computer applications
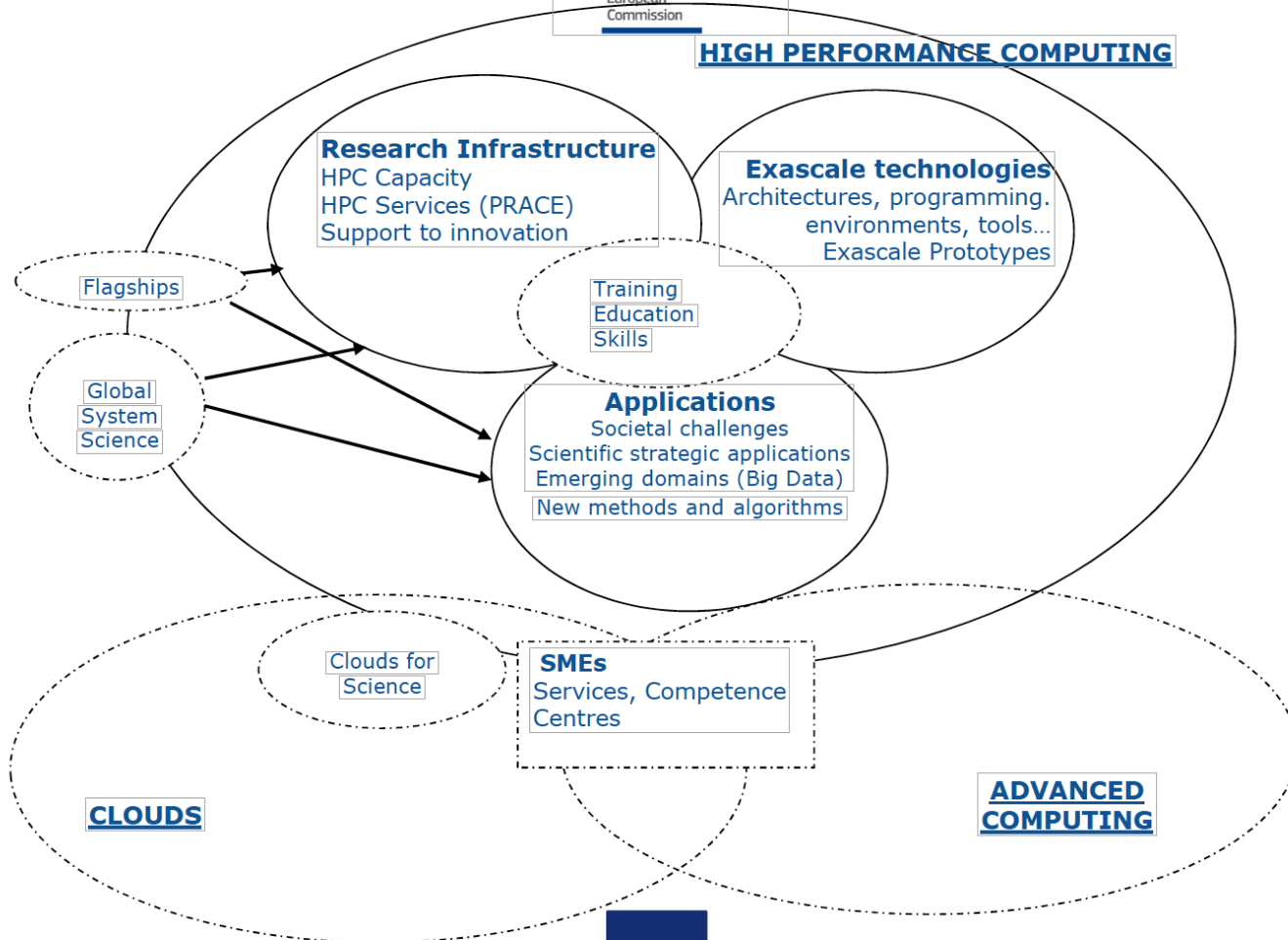
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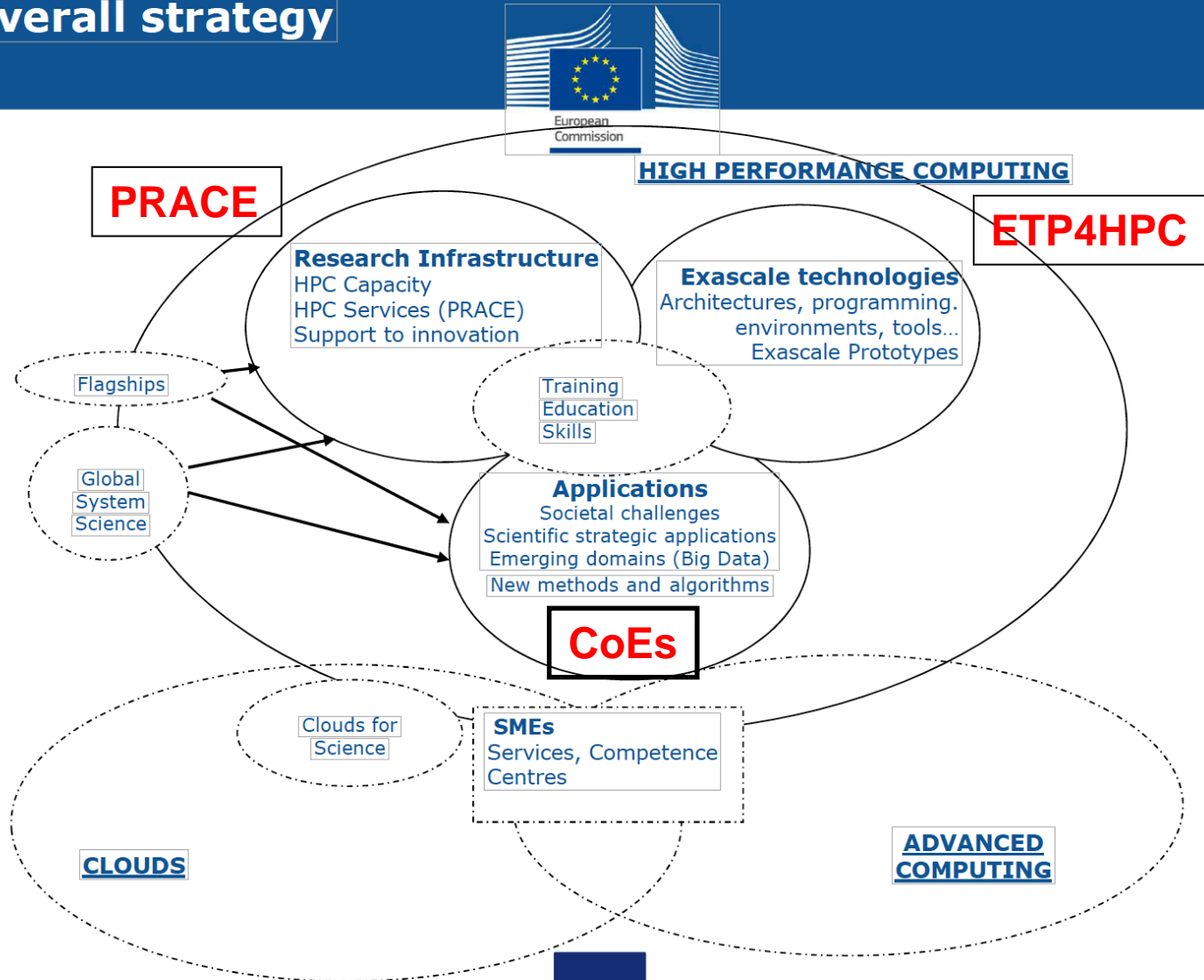
Overall strategy

HIGH PERFORMANCE COMPUTING

Research Infrastructure
HPC Capacity
HPC Services (PRACE)
Support to innovation

Exascale technologies
Architectures, programming.
environments, tools...
Exascale Prototypes

Flagships

Training
Education
Skills

Global
System
Science

Applications
Societal challenges
Scientific strategic applications
Emerging domains (Big Data)
New methods and algorithms

Clouds for
Science

SMEs
Services, Competence
Centres

CLOUDS

**ADVANCED
COMPUTING**

Overall strategy

PRACE

ETP4HPC

HIGH PERFORMANCE COMPUTING

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CoEs

Clouds for
Science

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CLOUDS

ADVANCED COMPUTING

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 CIimate in Europe**

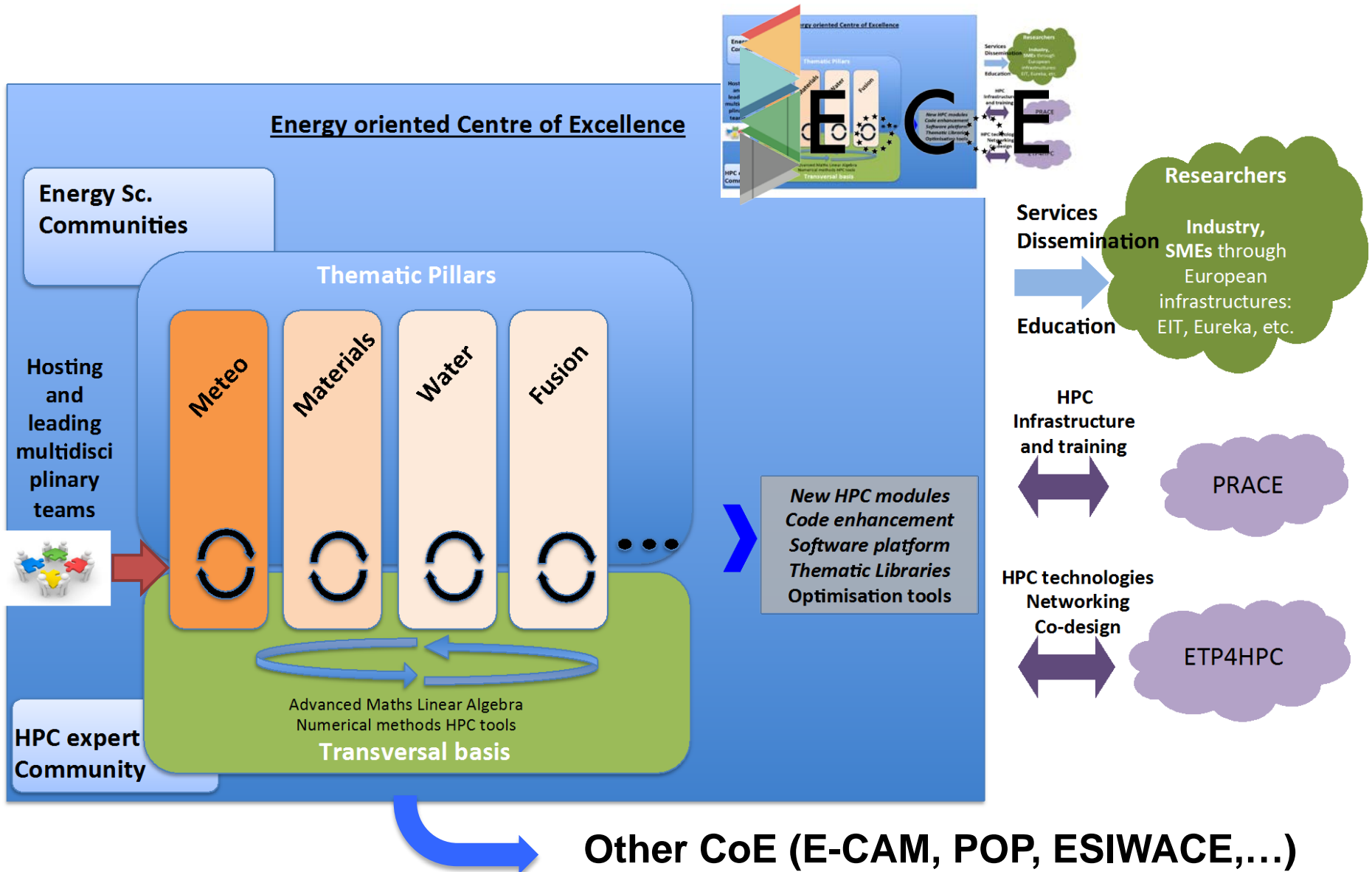**E-CAM - An e-infrastructure for software, training and consultancy in simulation and modelling**
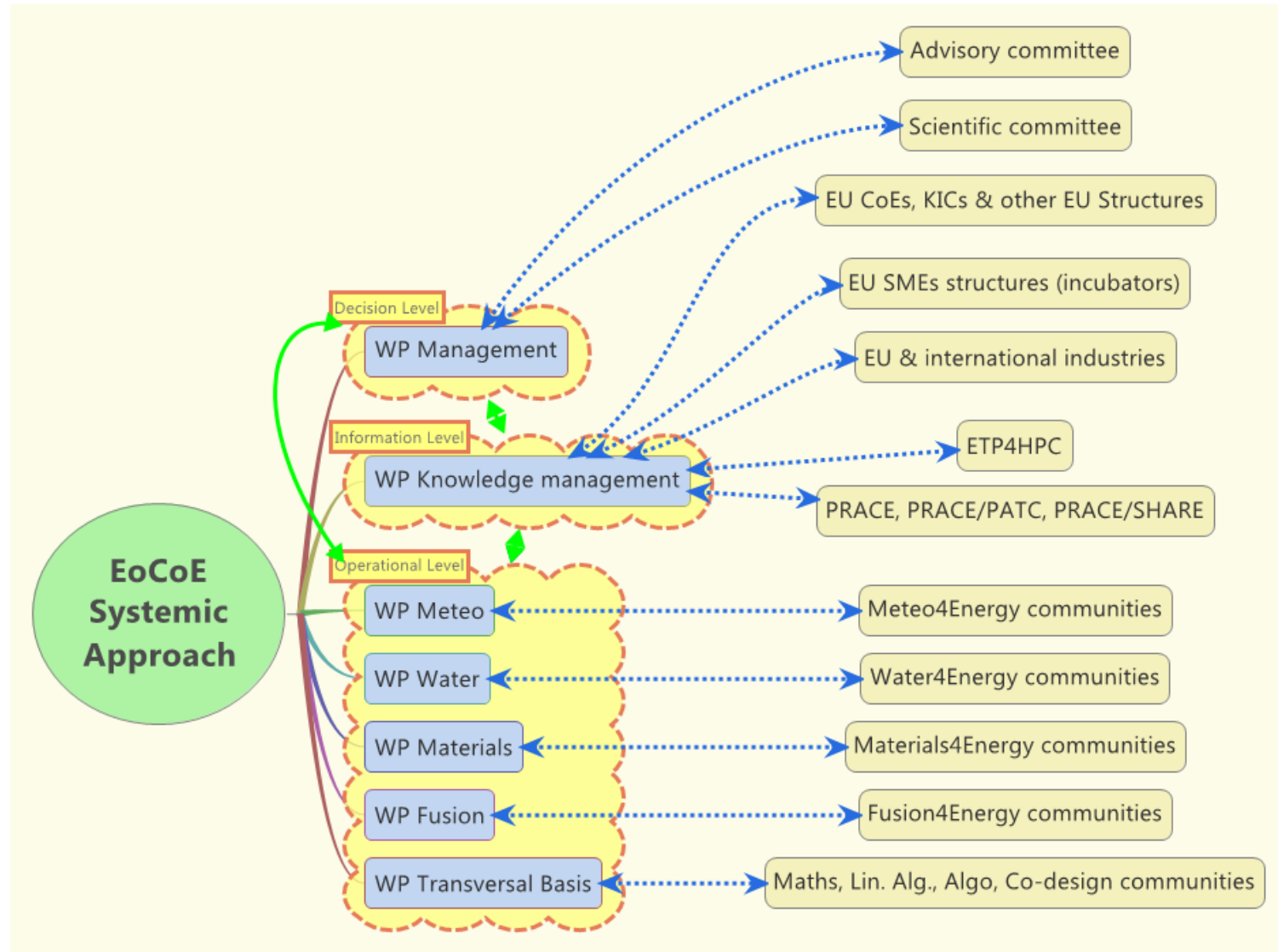
POP - Performance Optimisation and Productivity
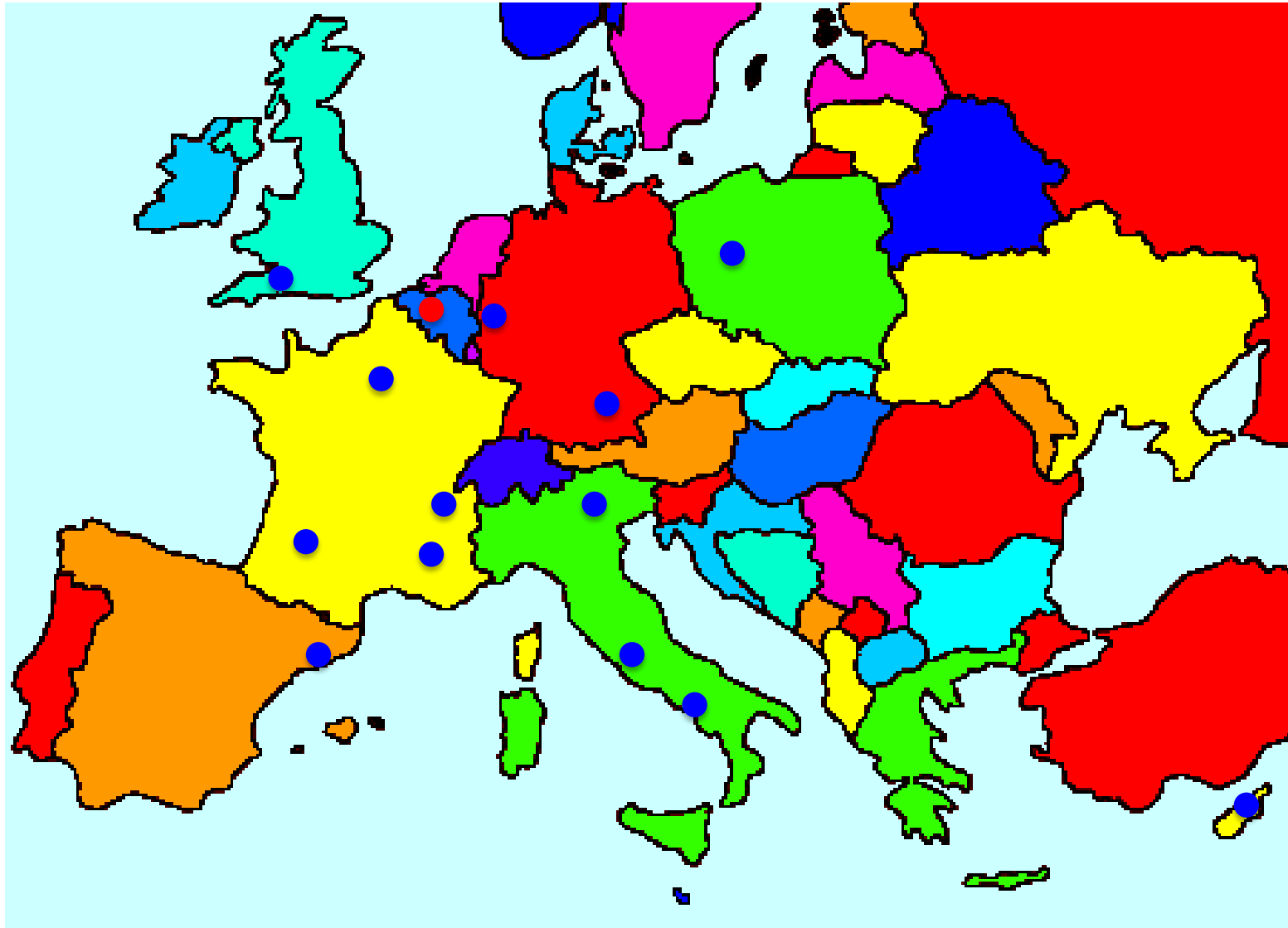
COEGSS - Center of Excellence for Global Systems Science

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

8 countries, 22 partners, 5.5 M€, lead by MdS
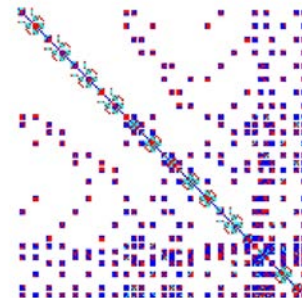
EoCoE
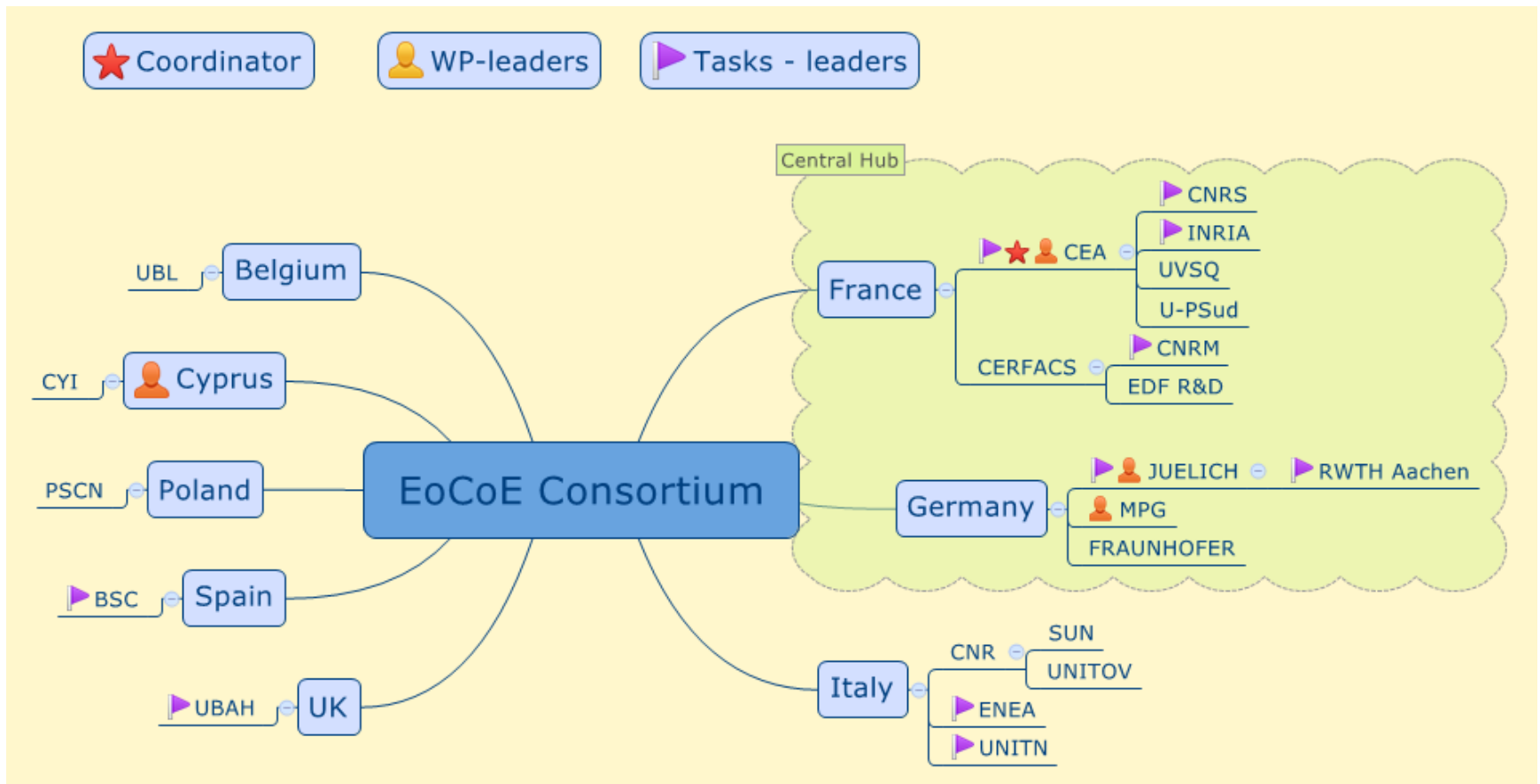
Develop or optimise high end tools and software for all the communities. Get ready for exascale computer

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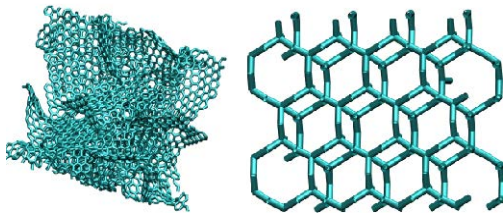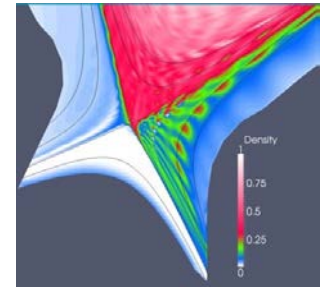
Material for energy : Photovoltaic cells, battery and super-capacitors

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

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)

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)

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)

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 EoCoE is opened to the HPC-users European Ecosystem using a dedicated "Multi-services Access Point" (MAP):

- Education through close partnerships
  with PRACE/PATC and other organisations and partners
  training facilities to disseminate the skills, best practices and
  know-how of the CoE
- Industry and SMEs through close partnerships to help SMEs
  reach competitiveness using high performance simulation
  - related EIT/KICs - Climate, ICT Labs, InnoEnergy,…
  - European Structures – EUROGIA[2020], European Mathematical
    Society,…
  - Incubators networks

- Research Institutes with the links established
  by the 4 Scientific Pillars and the Transversal Basis with their
  respective communities to answer their specific needs

Knowledge Management

- Organise capitalisation, dissemination and communication of results

- Realise provision of services and exploitation of results

- Promote HPC education and build training session modules

- Build a Strategic HPC Energy oriented Ecosystem network and international relations

- Take part to co-design activities for Exascale Hardware and Software with ETP4HPC structure and related industrial companies
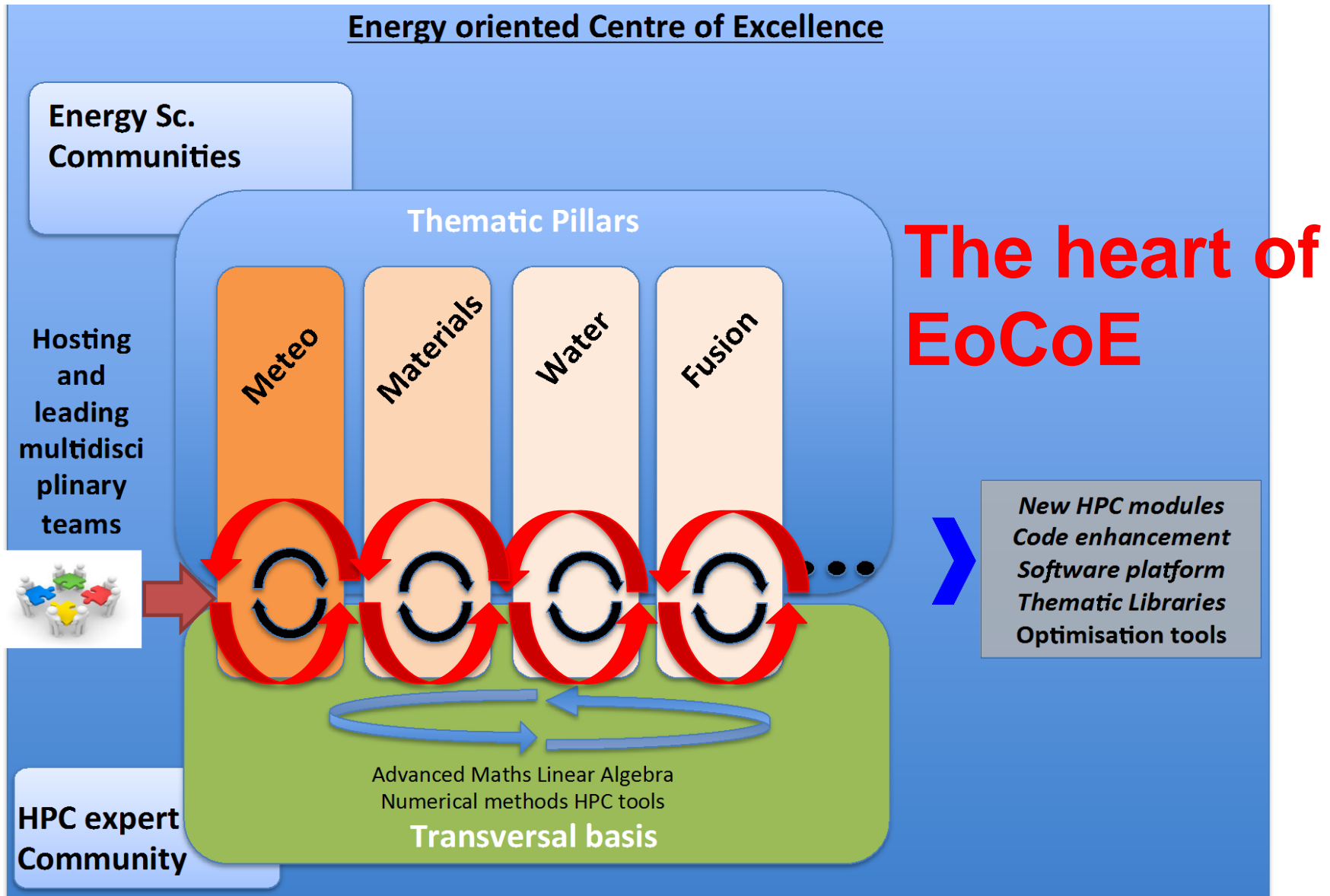
Usage of XIOS by other communities :

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,….

All solid Li-ion batteries

High throughput computing allow to test a large variety of material
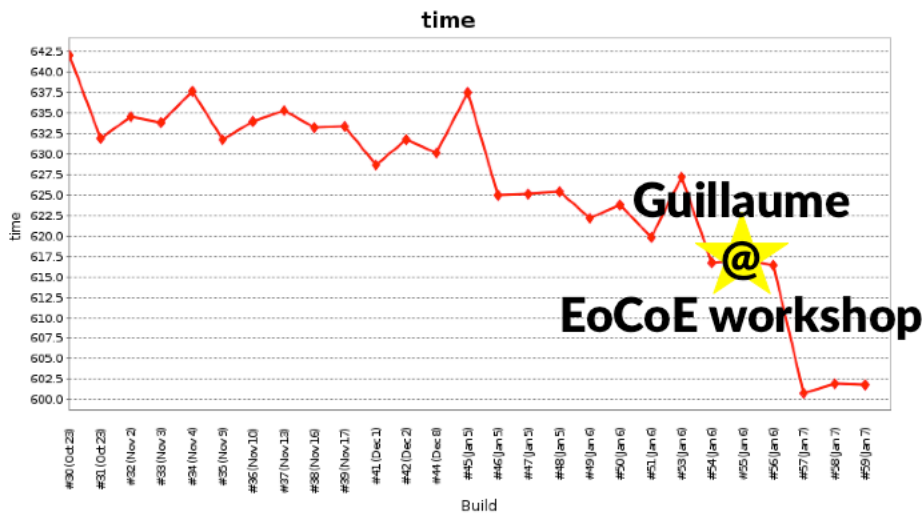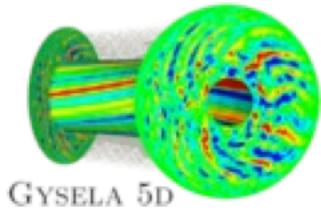
Solid electrolyte solide : $Li_7La_3Zr_2O_{12}$ (LLZO)

Low temperature : tetragonal structure, bad conductor
High temperature : cubic structure, very good conductor
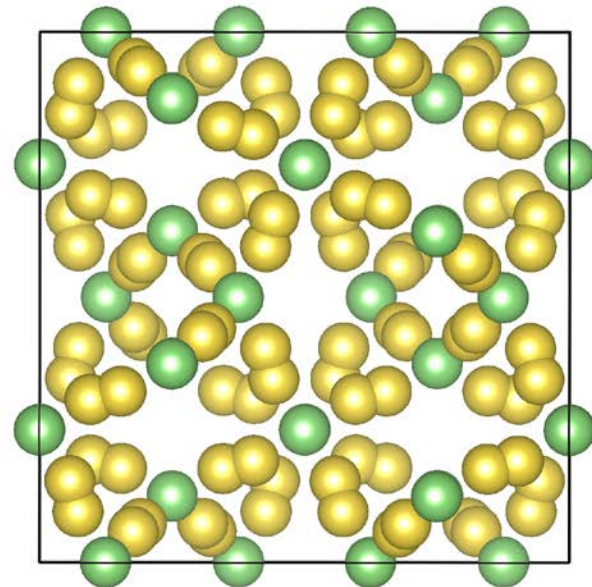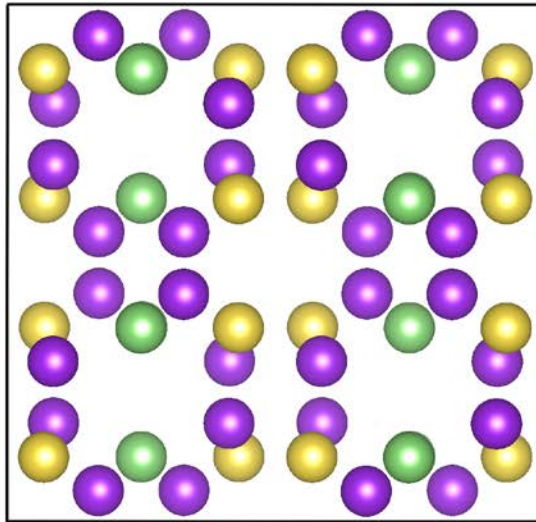
- **Similar structures but very different diffusive mecanisms**
- **Tetragonal phase : Li^+ ions have concerted and difficult movement**

Burbano et al., PRL

- Development of a complet metric sheet and associated tools to evaluate codes in a systematic way.

- Joint workshop with POP gathering HPC expert, and code/tools developers

- Test of a plateform for continous integration

- ❑ Joint workshop and continous work with POP

- ❑ Expertise on software architecture for E-CAM

- ❑ Link with EsiWace for IO

- ❑ ……

CoEs should help to build a strong HPC community in Europe