# The European Centres of Excellence in High Performance Computing (CoE)

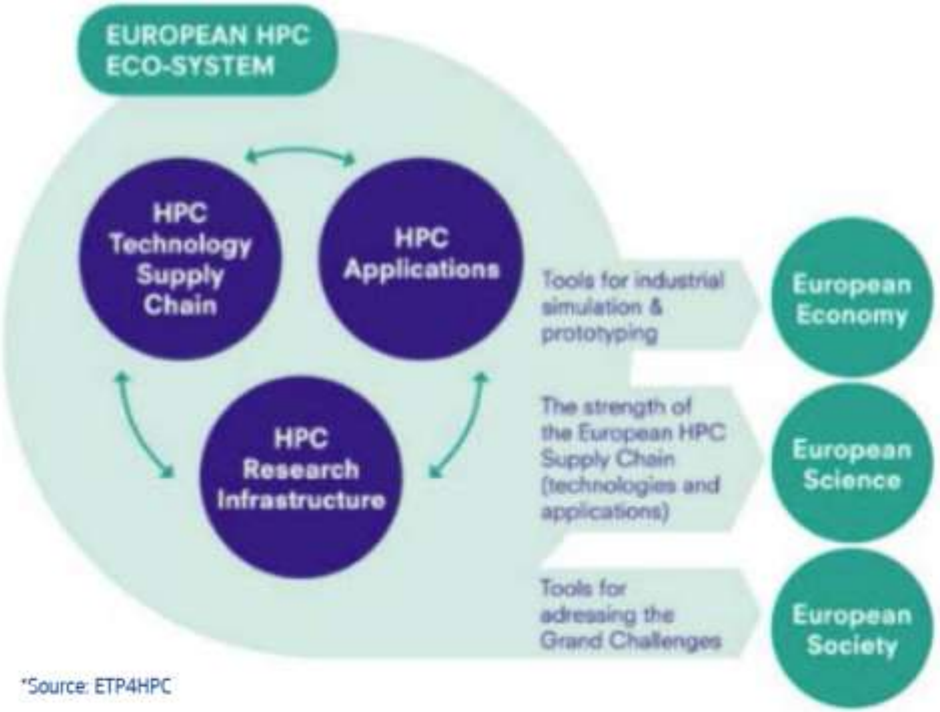
Edouard Audit

CoE European Excellence in HPC Applications

# European Policy – Three pillars

## The European HPC strategy

***The overall strategic goal is to develop a thriving European HPC ecosystem :***




*Source: ETP4HPC

***Infrastructure***: Capacity of acquiring leadership-class computers

***Technology***: Securing our own independent HPC system supply

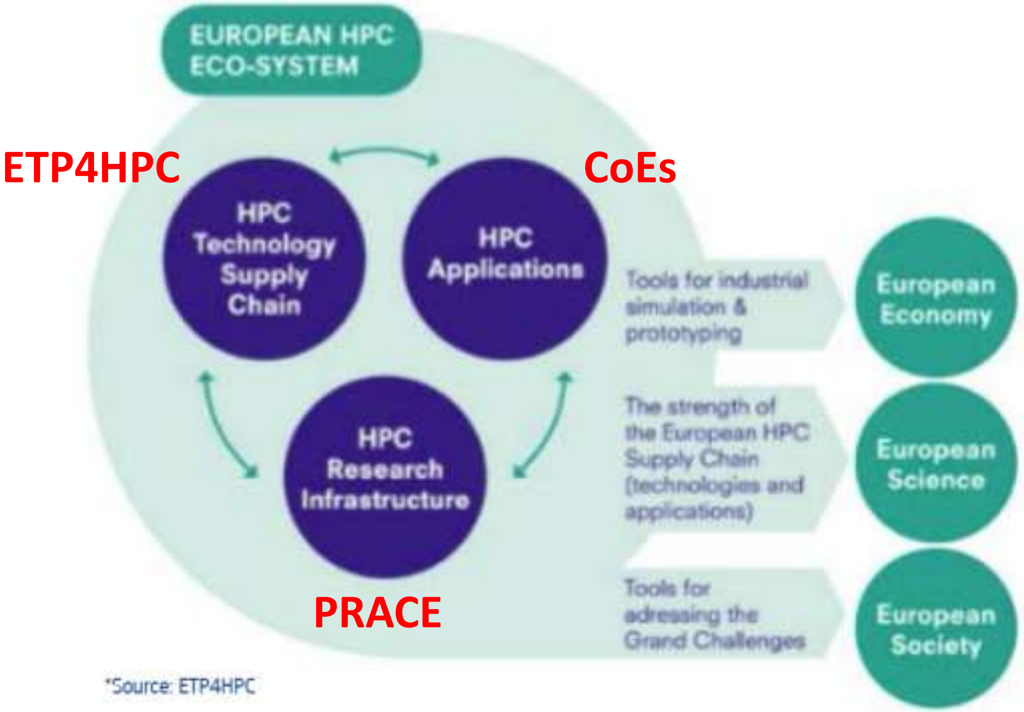
***Applications***: Excellence in HPC applications, and widen HPC use

# European Policy – Three pillars

## The European HPC strategy

EuroHPC Joint Undertaking

*The overall strategic goal is to develop a thriving European HPC ecosystem :*




*Source: ETP4HPC

EuroHPC Joint Undertaking

CoE European Excellence in HPC Applications

# 14 Centres of Excellence

14 Centres of excellence are active at the moment. They were created during three calls (2015, 2018 and 2019)

bioexcel
Centre of Excellence for Computational Biomolecular Research

CoE for Computational Biomolecular Research

ChEESE

CoE for Exascale in Solid Earth

CompBioMed

Computational methods for biomedical applications

coec
Center of Excellence in Combustion

ecam

CoE of the CECAM community

EoCoE

Energy oriented CoE : toward exascale for energy

CoE European Excellence in HPC Applications

# 14 Centres of Excellence

esiwace
CENTRE OF EXCELLENCE IN SIMULATION OF WEATHER AND CLIMATE IN EUROPE

HiDALGO
HPC and Big Data Technologies for Global Challenges

EXCELLERAT
CoE for Engineering Applications

MAX
Materials design at the exascale

NOMAD
NOVEL MATERIALS DISCOVERY

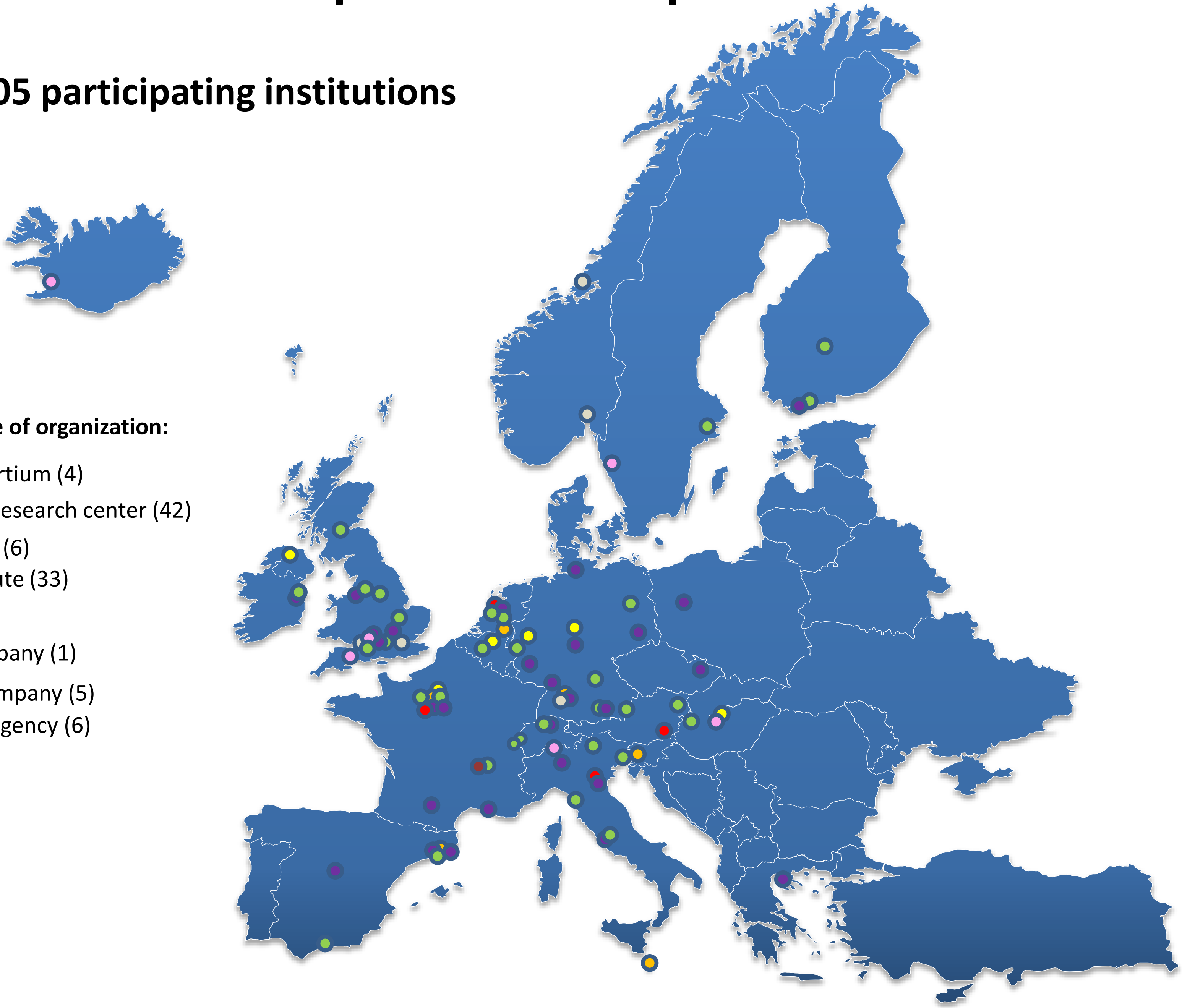
PerMed CoE

POP
Performance Optimisation and Productivity

TREX
Targeting Real chemical accuracy at the EXascale

# A pan-European network

**105 participating institutions**



**CoE actors by type of organization:**

- Research consortium (4)
- University and research center (42)
- Large company (6)
- Research institute (33)
- SME (8)
- Non-profit company (1)
- Consultancy company (5)
- Governement agency (6)

**CoE actors by country:**

| | |
|---|---|
| Austria | 3 |
| Belgium | 2 |
| Czech Republic | 1 |
| Finland | 3 |
| France | 12 |
| Germany | 17 |
| Greece | 1 |
| Hungary | 3 |
| Iceland | 1 |
| Ireland | 2 |
| Italy | 9 |
| Malta | 1 |
| Netherlands | 5 |
| Norway | 2 |
| Poland | 1 |
| Slovenia | 1 |
| Spain | 8 |
| Sweden | 2 |
| Switzerland | 5 |
| UK | 19 |

## A CSA (Coordination and Support Action ) to "*coordinate*" CoEs

FocusCoE contributes to the success of the EU HPC Ecosystem and the EuroHPC Initiative by supporting the EU HPC CoEs to more effectively fulfil their role within the ecosystem and initiative: ensuring that extreme scale applications result in tangible benefits for addressing scientific, industrial or societal challenges.

- ❑ To create a platform, the EU HPC CoE General Assembly, that allows all HPC CoEs to collectively define an overriding strategy and collaborative implementation for interactions with and contributions to the EU HPC Ecosystem.
- ❑ To support the HPC CoEs to achieve enhanced interaction with industry, and SMEs in particular, through concerted out-reach and business development actions.
- ❑ To instigate concerted action on training by and for the complete set of HPC CoEs: providing consolidating vehicle for user training offered by the CoEs and by PRACE (PATCs) and providing cross-area training to the CoEs (e.g. on sustainable business development)
- ❑ To promote and concert the capabilities of and services offered by the HPC CoEs and development of the EU HPC CoE brand raising awareness with stakeholders and both academic and industrial users.

European Excellence in HPC Applications

**$HPC^3$ HPC CoE Council**

# HPC$^3$ : HPC CoE Council

Created by all the active CoEs to promote and ensure the strong support for application development within the HPC landscape shaped by EuroHPC. Applications are essential in order to yield any science or innovation from a computer and they require important and long-term support.

- The EuroHPC policy needs to be clearly articulated around three pillars: Infrastructure – Technology – Applications. In particular, **application development** is a central ingredient in order to produce science and innovation using the Exascale infrastructure. It should therefore be supported in the long term and at a proper level, as is done in other exascale projects outside Europe.
- The **co-design** approach is often mentioned and is an important aspect of the global HPC policy. However, the way to implement this co-design is not always clear.
- **Large legacy** codes are key tools for many scientific and industrial communities. These codes often need to be heavily refactored for new architectures. Long term and sufficient support towards “performance portability” of these essential codes is therefore needed.
- More specific plans are needed for the **sustainability of, & long-term vision** for, middleware (MW) software stacks.
- There is a need to have a strong link with other initiative concerning AI and data analytics.

CoE European Excellence in HPC Applications

# CoE area of expertise

CoE develop strong expertise in their specific application fields as well as more transversal HPC skills needed to achieve science at exascale.

**Disciplinary Expertise**

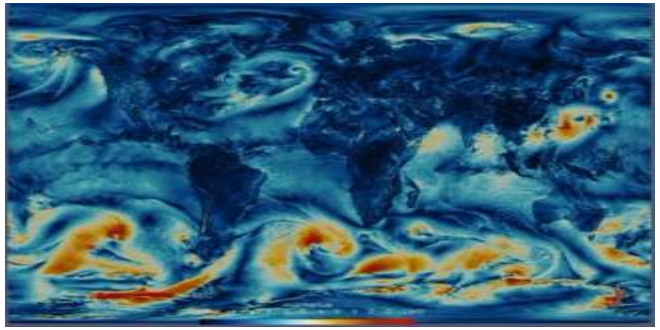
- Energy production (wind, hydro, fusion,…)
- Material science
- Material for energy (batteries, PV cells,…)
- Climate sciences and weather forecasts
- Molecular biology
- Biomedical applications (Cardiovascular Medicine, Neuro Musculoskeletal Medicine,…)
- Global challenges (health-relevant social habits, green growth, dynamics of global urbanisation.)
- Engineering (automotive, aerospace,…)
- Solid earth physics
- Combustion
- Personnalized medicine
- Chemistry

**HPC expertise**

- Programming models for exascale
- Performance monitoring, optimization and scalability
- Tools for HPDA in complex workflows
- Workflows
- Scalable solvers, linear algebra
- Data flow, in-situ data analysis and I/O
- Ensemble runs
- Implementing co-design and technology integration

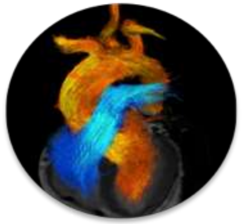
CoE European Excellence in HPC Applications

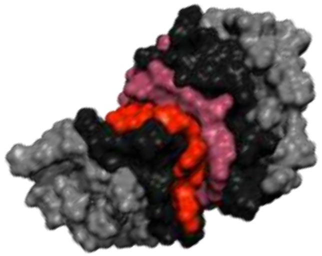
# CoE goals and main objectives



- ❑ CoEs are user driven, scientific communities are at the centre
- ❑ Enable transformational science breakthroughs in their fields
- ❑ CoEs are working toward a sustainable "*business*" model

- Code optimization, performance portability,…
- Co-design, link with technology projects (EPI,…)
- Re-write or re-design community flagship European codes from their user communities for the upcoming pre-Exascale (2020) and Exascale (2022) supercomputer
- Design and develop cutting-edge computational methods, production-ready HPC softwares and software modules to bring the scientific numerical tools to exascale computing levels and manage the data generated
- Develop processing tools, benefit from the synergies between HPC, HPDA and IA
- Promote all these tools and software in academia and industry
- Train scientists from industry and academia on the development of methods and software scaling towards the high end of HPC systems
- Provide expertise and advanced training to end-users and promoting best practices in the field.





CoE European Excellence in HPC Applications

# CoE services

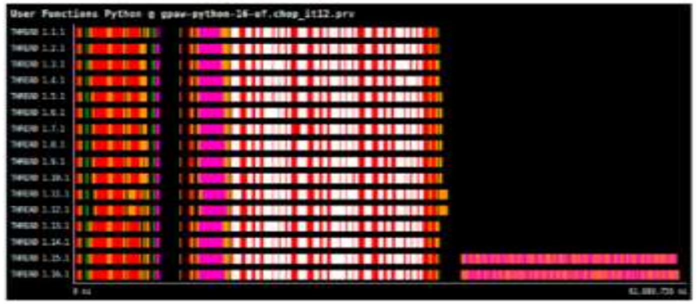
**CoEs provide a wide range of services for academic and industrial users**

- Code optimization, profiling, refactoring
- Training course in HPC for industrial and academic users (HPC, HPDA, I/O, DLS, …)
- Train scientists from industry and academia on the development or usage of methods and software scaling towards the high end of HPC systems
- Training courses for industrials, on specific families of methods, software and HPC tools
- Webinars
- Bridging the skill gap, especially between academic research and industrial practice
- Disseminate software and libraries, especially high-end tools. Software repositories
- Organize workshop with industries to identify areas of mutual interest as well as the possibility to engage in direct discussions.
- Tailored training, consultancy and expertise
- Provide/develop tailored numerical tools
- Set-up pilot projects targeted at solving specific problems posed by industrial partners
- Sass portal
- Support discussion forums, act as a hub in their fields


CoE European Excellence in HPC Applications

# Main bottle-neck for exascale

- Load balancing
- Programming models for exascale
- Performance Portability of codes, standardization of programming models
- dynamic (task) scheduling
- Scalable solvers
- Data flow, in-situ data analysis and I/O
- Ensemble runs
- Implementing co-design and technology integration
- post-processing on the fly, data-focused workflows
- Using large width vector units
- Using heterogeneous architectures, strong memory hierarchy
- Visualisation and data processing/analysis
- Workflows combining HPC simulations with associated data management and analytics capabilities

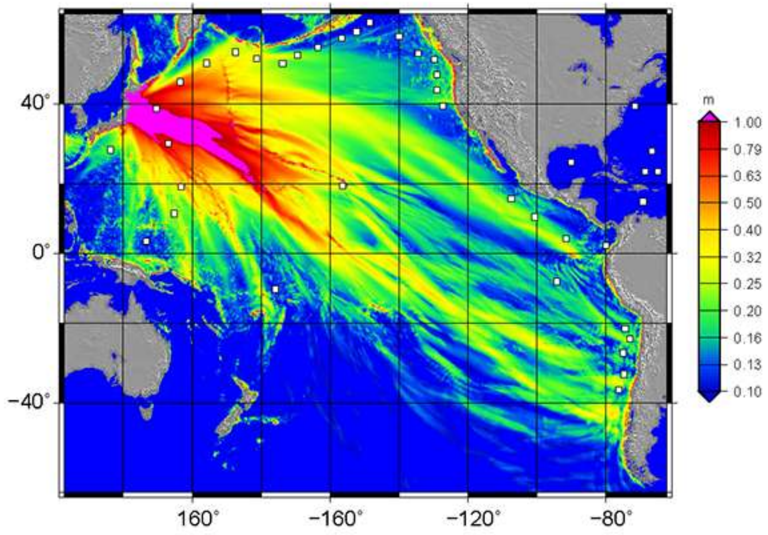


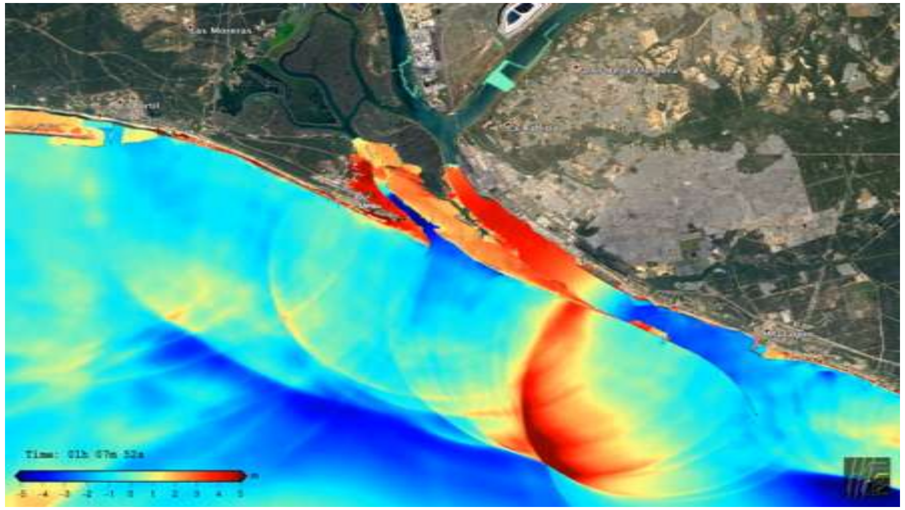
CoE European Excellence in HPC Applications

# Scientific perspectives

**Earth Science :**

- Physics-based Probabilistic seismic/volcanic/tsunami hazard
- High resolution Forecast of volcanic ash clouds, volcanic ash fallout and volcanic ash resuspension
- Faster-than-real-time simulations for Tsunami Early Warning Systems



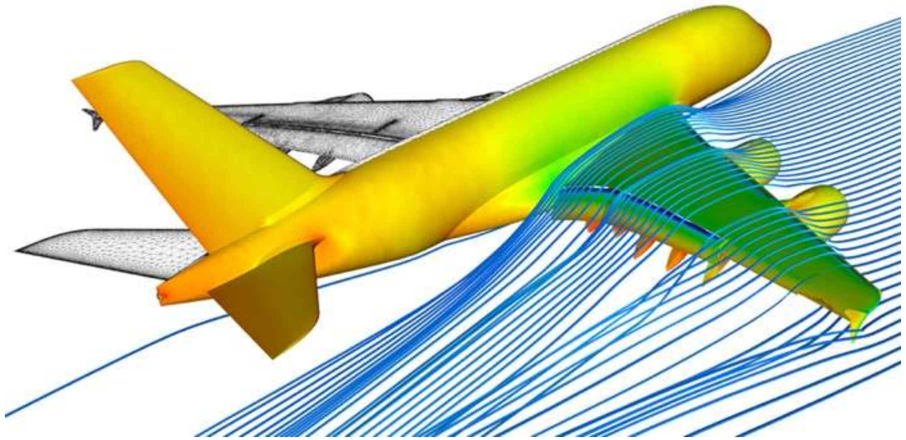



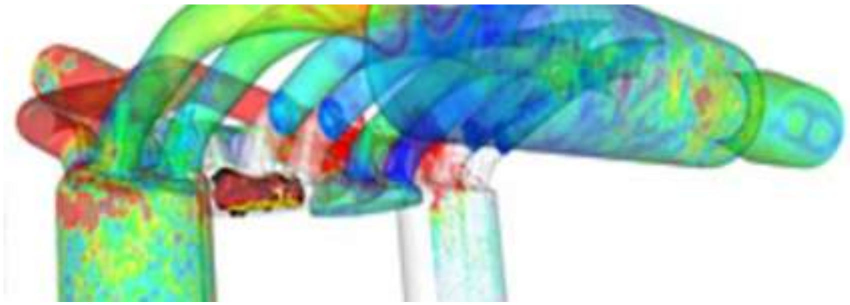
CoE European Excellence in HPC Applications

# Scientific perspectives

**Engineering :**

- Emission prediction of internal combustion  and gas turbine engines
- Tidal Energy Generation Modelling of drag and sedimentation effects of tidal turbines
- Active flow control of aircraft aerodynamics

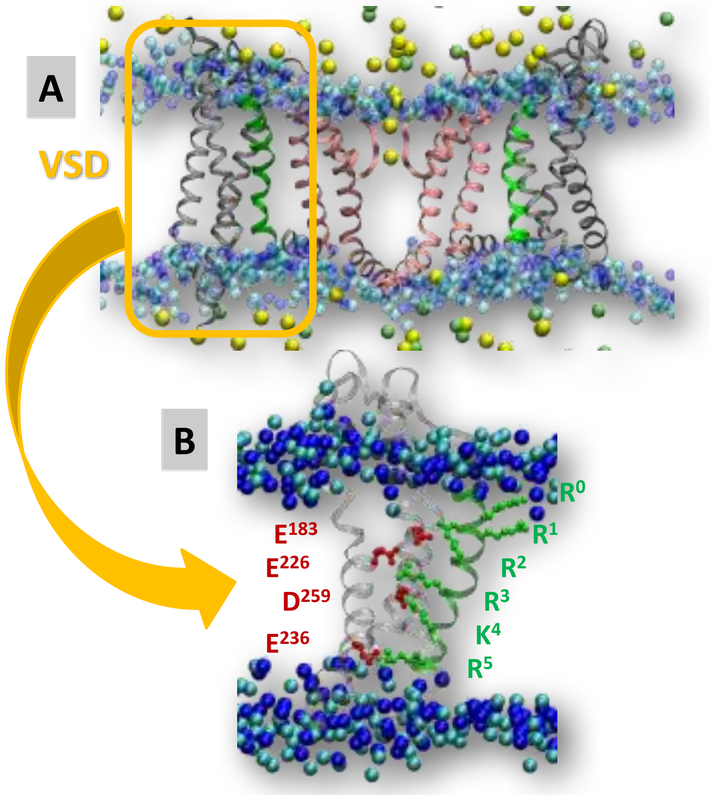




CoE European Excellence in HPC Applications

# Scientific perspectives

## Molecular Dynamics on the exascale for drug design

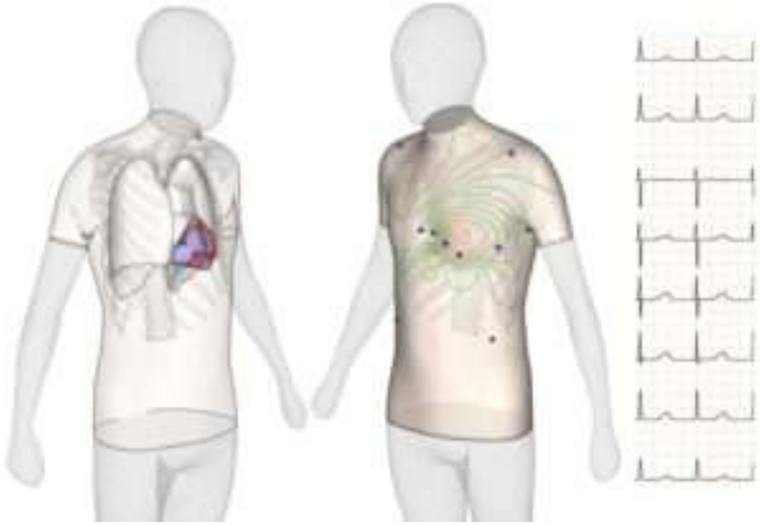


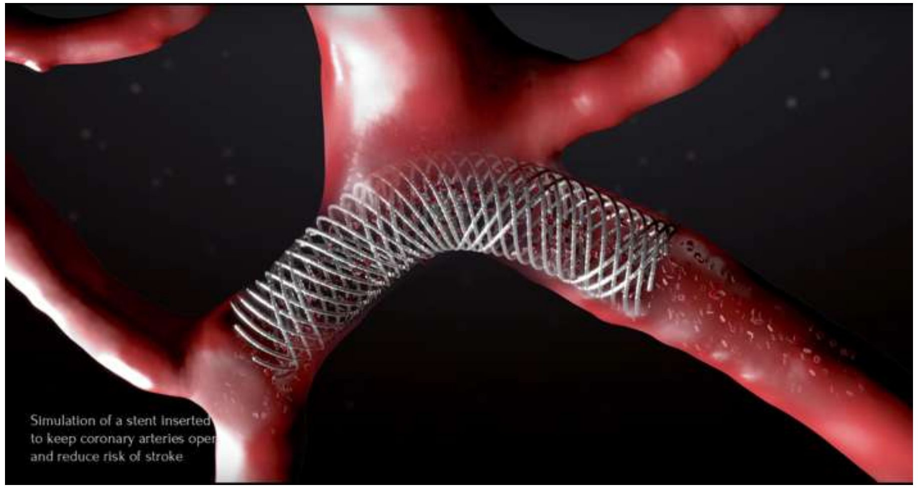

- Understanding proteins and drugs
- A 1 µs simulation: 10 exaflop
- Many structural transition: many simulations needed
- Study effect of several bound drugs
- Study effect of mutations
- All this multiplies to >> zettaflop
- Question: how far can we parallelize?

# Scientific perspectives

**Health :**

- In silico heart assays on High Performance Computing
- Simulate the blood flow through a stent (or other flow diverting device) inserted in a patient’s brain.
- in silico drug trials in populations of human cardiac cell models for predictions of drug safety and efficacy

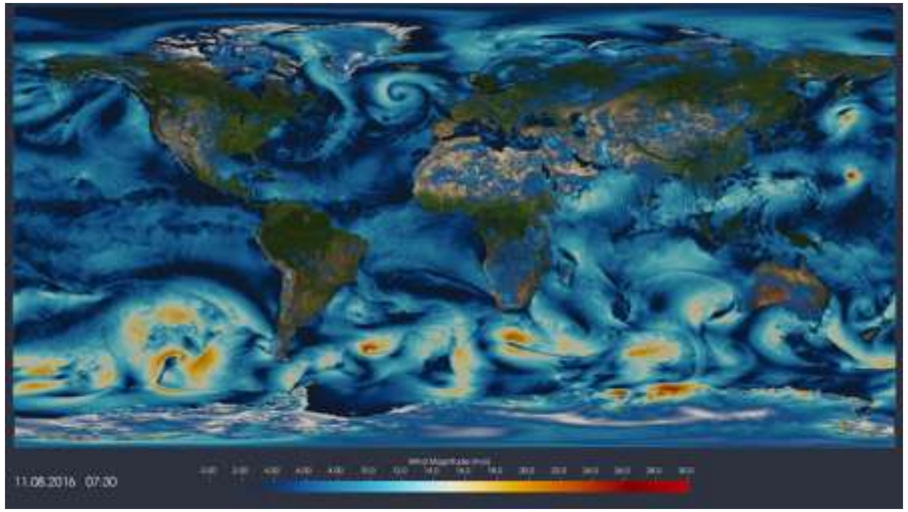


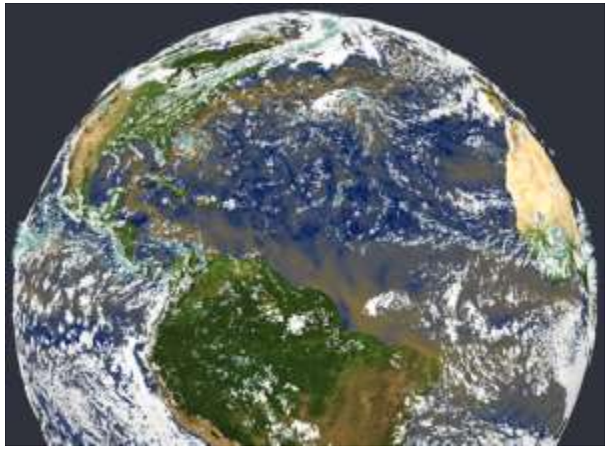


# Scientific perspectives

## Climate and weather forecast :

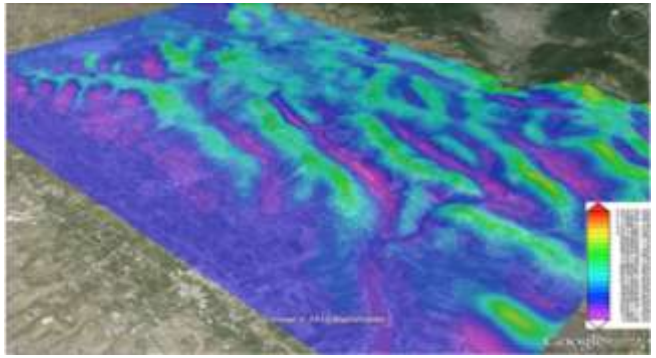
- Run simulations at a kilometre-scale horizontal resolution to explicitly resolve features such as deep convection, gravity waves and meso-scale to small-scale ocean eddies
- Enable a new quality of simulations and forecasts, allowing for a step change in the level of detail of predictions, such as patterns of extreme events in a changing climate
- Pave the way towards extreme resolution ensemble methods in operational climate and weather forecasting
- Storm-resolving simulations with resolutions from 5km to up to 150m



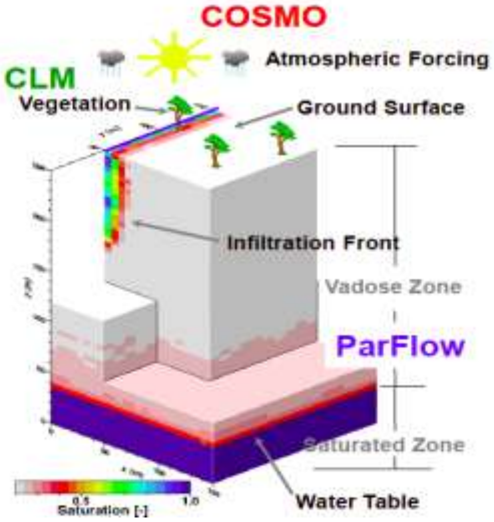


CoE European Excellence in HPC Applications

# Scientific perspectives



**Wind for energy:**
*Turbulent flows in turbine wakes* are an important factor in *wind farm modelling*. Requires huge number of grid points and time steps; complex geometries requiring unstructured grids; wall-layer and subfilter-scale modelling.




**Water for energy:**

Challenge is to apply very high-spatial resolution physically-based models to produce useful predictions: leads to a very large number of forward model runs. Exascale simulation challenge is a *fusion of physically-based terrestrial models with observations* providing the current state of the hydrologic states and fluxes.

# Conclusions

- CoEs are now well established produce great science and prepare for upcoming super-computers
- A long term vision and sustained efforts are necessary to develop high-end applications
- HPC3 will work on this long term vision and promote it, especially toward EuroHPC