Centres of Excellence view on:

“What are the important research goals for the next 5 years”

Peter Bauer & Erwin Laure 4CoE

1st Generation of CoE

EoCoE - Energy oriented Centre of Excellence for computer

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

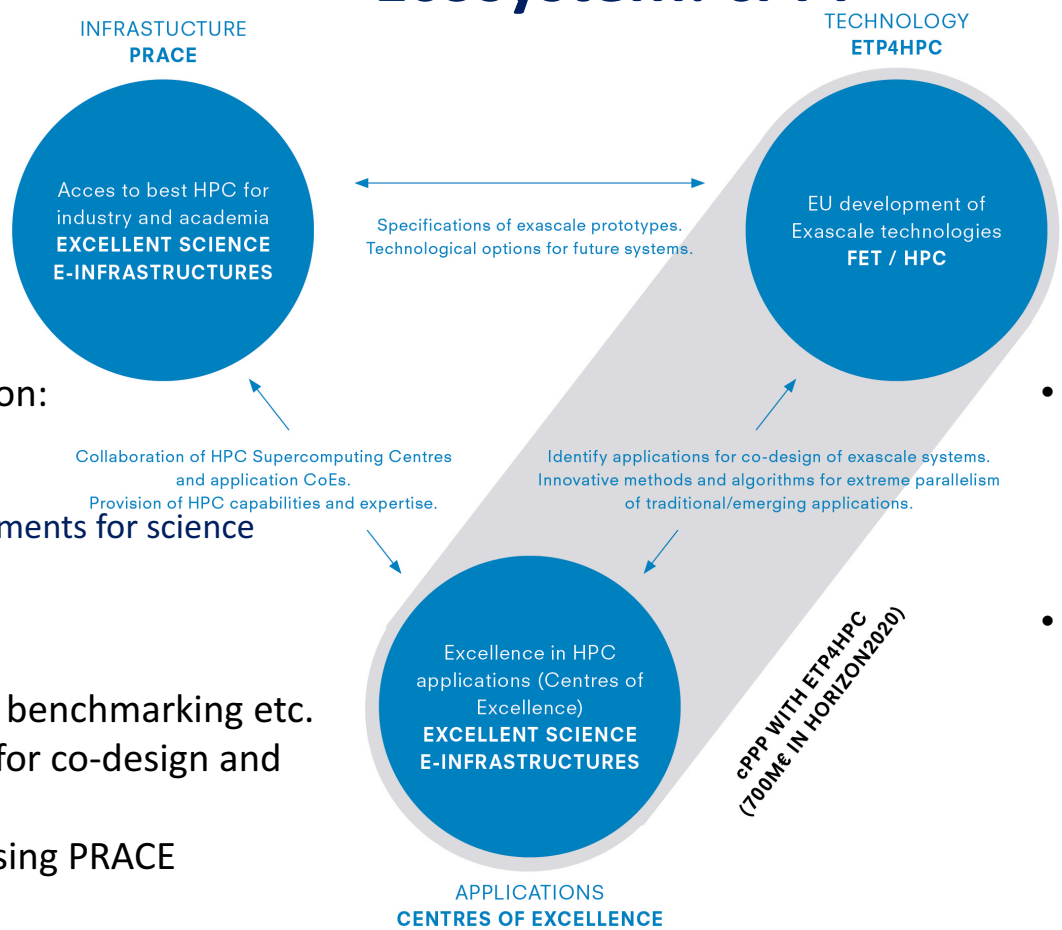
E-CAM - An e-infrastructure for software, training and consultancy in simulation and modelling

POP - Performance Optimisation and Productivity

COEGSS - Center of Excellence for Global Systems Science

CompBioMed - A Centre of Excellence in Computational Biomedicine

Ecosystem: cPPP



- Collaborate with **PRACE** on:
  - best practices
  - software environment
  - organizational requirements for science domains
  - training
- PRACE HLST
- Use PRACE resources for benchmarking etc.
- Use center competence for co-design and exascaling (all tiers)
- Help communities accessing PRACE resources

- Collaborate with **FET research** projects to:
  - harden and integrate results to production quality
  - provide real-world test cases
- Provide for ESDs:
  - provide requirements
  - optimize software for targeted ESDs – will also be important for smaller scales
  - co-design

Goals of CoE

Ensure European competitiveness in the application of HPC to address scientific, industrial or societal challenges:

- **Excellence** in research, development and service;
- **User-driven**, with the application users and owners playing a decisive role in governance;
- **Integrated**: encompassing not only HPC software but also relevant aspects of hardware, algorithms, data, workflows, connectivity, security, etc., covering the full scientific/industrial workflow and addressing full-scale, widely used applications with proven impact, not just application kernels or mini-apps;
- **Multidisciplinary**: with teams that combine application domain and user expertise together with HPC system, software and algorithm expertise;
- **Distributed** with a possible central hub, federating capabilities around Europe, exploiting available competences, and ensuring synergies with national/local programmes;
- Showing a clear path towards **Exascale** covering both **computing** and extreme **data**
- Committed to a culture of **collaboration** and sharing of best practice among CoEs on cross-cutting topics, such as co-design and Exascale technologies, software sustainability, and potential business models;
- Committed to collaborate with the upcoming **Extreme Scale Demonstrators**, providing them with a high performance and scalable **application base**;
- Actively contributing to **economic and societal benefit**, by facilitating high-impact research and collaborating with industry and SMEs.

Present CoE

Vertical (domain) CoEs, which provide services to well defined communities:

- Software development, support & consultancy, training
- Frontier developments towards exascale

→ requirements in Material Sciences, Weather&Climate or Bio may be very different

Horizontal (transversal) CoEs, which cover topics of importance to several vertical CoEs:

- Software development, support & consultancy, training
- Performance analysis

→ potentially complex interaction matrix

Future CoE

Vertical (domain) CoEs, which provide services to well defined communities:

- Current themes

+ Engineering?
+ Fundamental physics?
+ Environmental sciences (adaptation to environmental change)?

→ Cover entire value chain (from science to industry)

→ Compute and data (from exaflop to exabyte)

Horizontal (transversal) CoEs, which cover topics of importance to several vertical CoEs:

- Current themes

+ High-performance data analytics?
+ Software sustainability?
+ Mathematics and algorithms?

→ Enhance culture of collaboration (CoE matrix)

Future CoE: Considerations

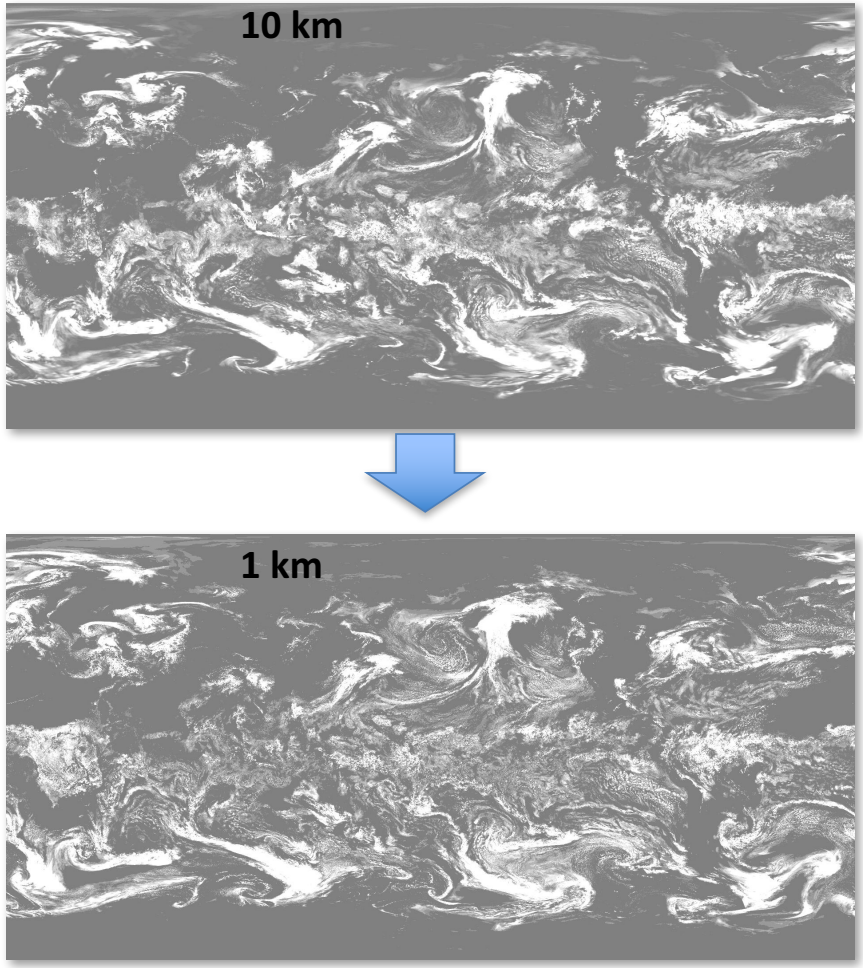
- Potentially merging of existing CoE (cf. Flagships):
  - smaller number of domains that have shown a clear path to exascale/co-design <u>or</u> larger variety?
  - may provide more efficient x-benefit for several communities towards exascale <u>but</u> effectiveness may suffer (weak links affect wider area)
  - providing support for merged communities will be challenging
- Importance of Exascale:
  - addressing key science challenges is most important (≠ Exaflop)
  - technological developments (e.g. co-design → EsD → top 3 in 2022) run away from applications
  - only few CoE have really big data tasks (e.g. ESiWACE)
- Stimulation of SME:
  - smaller dedicated efforts may be more effective (e.g. SHAPE, Fortissimo)
  - unified software development vs specialized SME niches
- Sustainability:
  - assimilating cutting-edge FET developments
  - business model needs simple/realistic approach (and public funding for some time to come)

→ **Manage expectations of CoE what will be able to achieve & sustain – given the available funding**

CoE in SRA-2

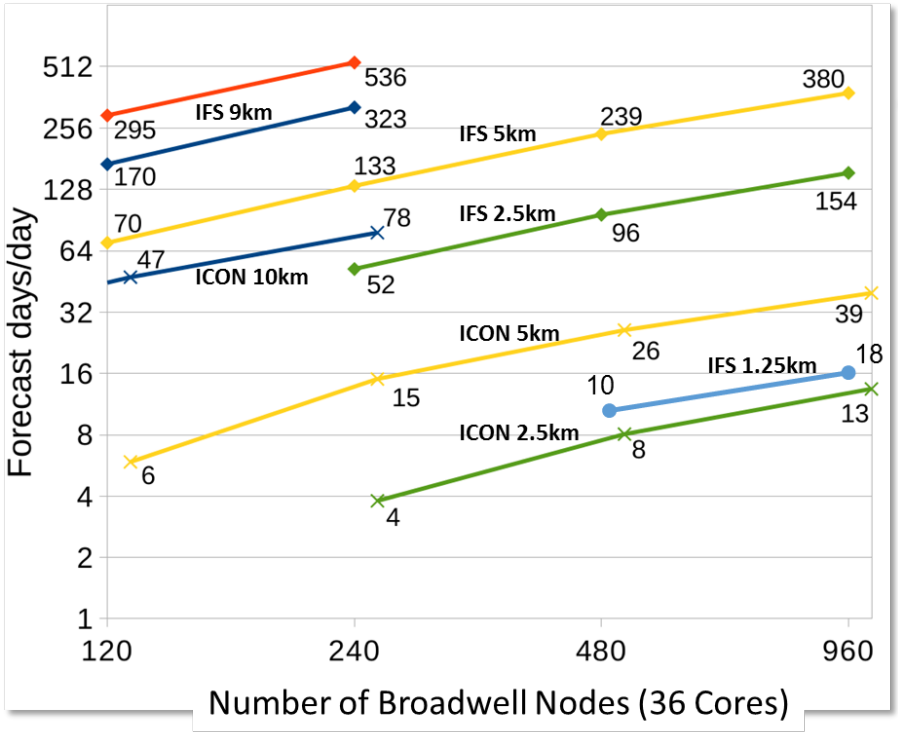
- Section 8 **EsD introduction**, page 67: “These EsDs should provide platforms deployed by HPC centres and used by CoEs for their production of new and relevant applications.”
- Section 8.2, **Proposal of ETP4HPC for EsD Calls**: “This and other hardware characteristics (energy efficiency, I/O bandwidth, resiliency, etc.) will be detailed in the 2017 release of the SRA, also taking into account results from the FETHPC projects and requirements from the CoEs.”
- Section 9.3, **Centres of Excellence for Computing Applications**: “The Centres of Excellence in Computing Applications (CoEs) form one of the three pillars of the European HPC Ecosystem and represent the European Application expertise […]. ETP4HPC will be working to include the CoEs in the processes of the contractual Public-Private Partnership for HPC and synchronise their efforts with those of the other two pillars of the European HPC Ecosystem (i.e. ETP4HPC and the FETHPC projects, PRACE).

Example: ESiWACE Science Challenge



Target for addressing key science challenges in weather & climate prediction:

Global 1-km Earth system simulations @ ~1 year / day rate



CoE and SRA-3

Domain CoE: What are the key scientific challenges and what does it take to achieve them?

	BioExcel	CompBioMed	MaX	ESiWACE	E-CAM	POP	CoEGSS
HPC System Architecture and Components	Large width vector units, low-latency networks, high-bandwidth and large memory; fast CPU<->accelerator transfer rates, Heterogeneous acceleration, floating-point	Hybrid systems, GPUs, high-bandwidth memory	Scientific challanges: accurate computations requiring more powerful HPC systems, heterogeneous systems designed to optimize end-to-end workflows	High-bandwidth memory, networks, NVRAM	High memory bandwidth, large RAM	Throughput oriented devices (vectors), memory architectures and how to use them, architectural support for runtimes, mechanisms to monitor progress and notify runtimes in cases of resource preemptions	Convergence between HPC & HPDA, NVRAM, Fast networks
System Software and Management	Dynamic (task) scheduling, Support for workflows	Dynamic scheduling, urgent computing	Virtual Machine model supported	Dynamic scheduling, compilers	Cross compiling, archiving tools	Dynamic, interactive use of available resources, tight and bidirectional communication/cooperation between job schedulers and runtimes	Dynamically scaling jobs, Integration of HPC & HPDA, Visualization (in situ), Data analytics (in situ) Programming Environment
Programming Environment	Standardization, portability, task parallelism, fast code driven by Python interfaces	Portability, ease of scale out, MPI extensions	support new MPI and OpenMP standards + new development tools like python	Fast standardization, DSL	Interactive testing, OpenCL support, sustainable support of standards	Programming model and runtime support for malleability, asynchrony/out of order task execution, hide heterogeneity and tolerate latency and variability, powerful performance analytics in tools, tools for task dependencies and memory access patterns, programmers mindset from bottom-up latency dominated to throughput oriented mentality	Well-defined standards /and tools that implement the standards) for agent-based modeling, Compilers, Debuggers
Energy and Resiliency	Distributed computing techniques to handle resiliency/fault tolerance	Reduced cost, improved fault tolerance	Energy optimized workflows: HPC systems including energy monitoring and profiling.	Fault handling, less precision	Energy aware algorithms	Better integration between algorithmic based fault detection techniques and mechanism in the infrastructure from detected errors	Not important for CoeGSS

CoE and SRA-3 (cont'd)

Domain CoE: What are the key scientific challenges and what does it take to achieve them?

	BioExcel	CompBioMed	MaX	ESiWACE	E-CAM	POP	CoEGSS
Balance Compute, I/O and Storage Performance	Post-processing on the fly, Data-focused workflows, handling lots of small files in bioinformatics	Post-processing on the fly, easy transfer between storage tiers	HT material science workload becomes quickly memory and I/O bound: systems with high IOPS and post posix data objects are required.	Post-processing on the fly, multi-tier software	Fast access of archive data, multi-platform workflows, multi-threaded applications for hybrid production/analysis applications	Integration of asynchronous I/O interface in programming model, better integration of programming models/languages and persistent storage	Converged systems, Live data analytics, Strong data movement capabilities
Big Data and HPC usage Models	Proximity of data generation and analysis/visualization resources, workflows, machine learning for analyzing simulation data, high-throughput sampling	Analytics of simulation outputs, visualisation	Workflows, intelligent data analytics	Recomputing, data analytics	Fast access to data bases, data mining	Better integration between programming model and storage interface, more dynamic, interactive supercomputing practices, make users/programmers aware of cost/benefit of each individual data and computation for better resource/storage scheduling	HPDA Platform support, Algorithms / Models for efficient HPDA
Mathematics and algorithms for extreme scale HPC systems	Multi-scale algorithms, task-parallel algorithms, Electrostatics solvers, ensemble sampling & clustering theory, ensemble simulations	Novel time stepping algorithms, automated implementation of multiscale computing patterns	New algorithms avoiding synchronous (unnecessary) data dependency and exploiting unreducible data dependency tree (nesting), to improve concurrency and locality	Disruptive numerical methods (discretization), data placement	Memory/cache aware algorithms, asynchronous algorithms, efficient handling of long range/collective correlations	Algorithm complexity (computation/communication). asynchrony and variability tolerance, algorithm based fault detection	Algorithms for efficient data analytics

CoE and SRA-3/EsD

Assumption: EsD will be precursors of European exascale HPC facilities hosting novel technologies and software stack

→ EsD are FLOP focused, CoE application areas may not be!

If the key role of CoE is to provide wider (domain) user community with expertise, software etc.:

1. How is transition from 'novel' to 'applicable' be managed? What is the role of FET projects in this context? (there is also no certainty for sustainability of FET projects per domain)
2. How are key applications, to be run on EsD in operational mode, adapted to novel architecture, stack, programming models etc.? By whom? With what funding?
3. If future CoE become wider (less domain specific):
   a. how can the above be realized?
   b. will the horizontal CoE do the job?