C2S@Exa Inria Project Lab
Computer and Computational Sciences at Exascale

Nuclear energy production application
Kickoff meeting - May 17, 2013
Inria Sophia Antipolis - Méditerranée

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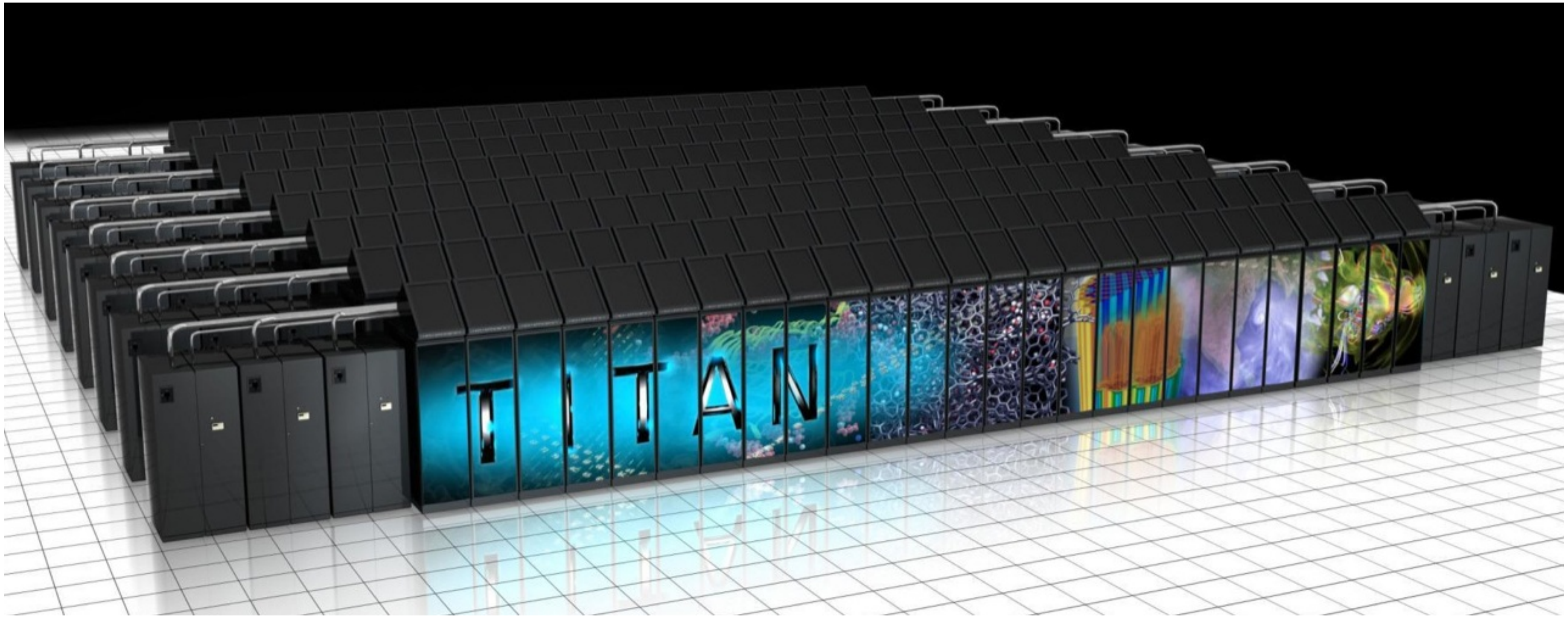

Titan system, Oak Ridge National Laboratory
Cray XK7 , AMD Opteron 6274 16C 2.2 GHz, Cray Gemini interconnect, NVIDIA K20x
560640 cores, 27112.5 TFlop/s peak

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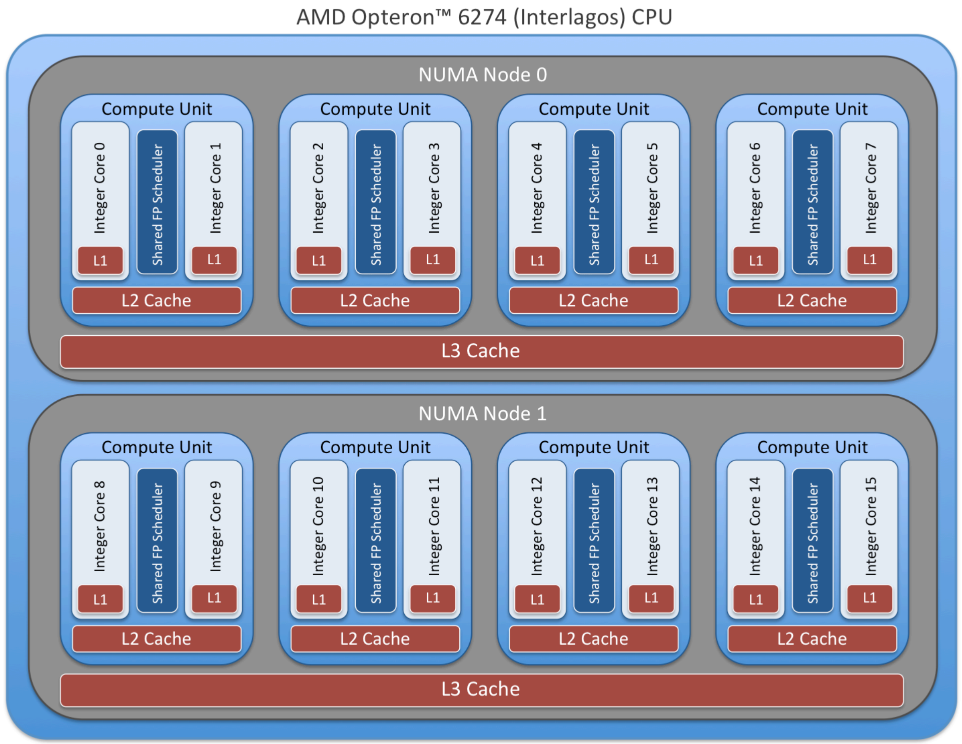

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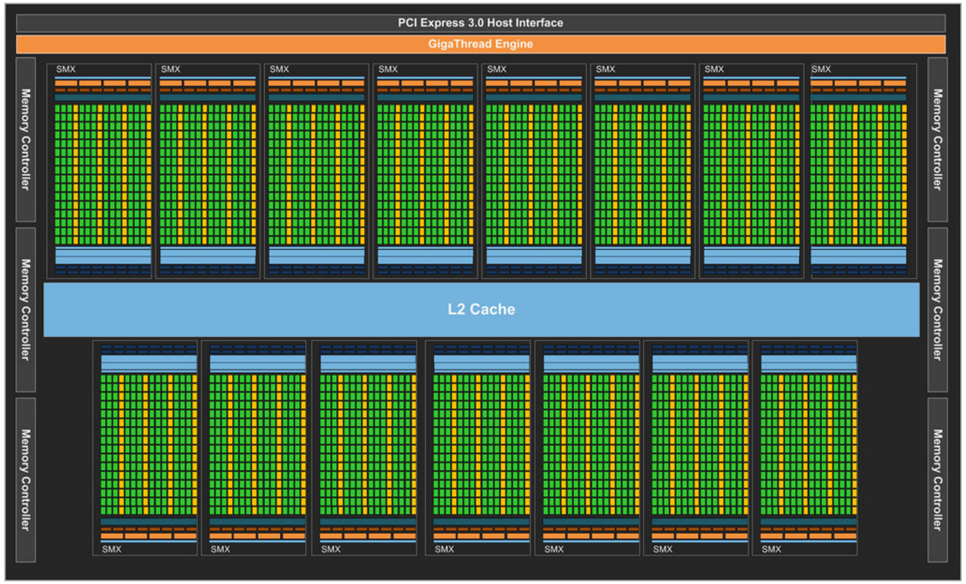

	TESLA K10[a]	TESLA K20	TESLA K20X
Peak double precision floating point performance (board)	0.19 teraflops	1.17 teraflops	1.31 teraflops
Peak single precision floating point performance (board)	4.58 teraflops	3.52 teraflops	3.95 teraflops
Number of GPUs	2 x GK104s	1 x GK110	
Number of CUDA cores	2 x 1536	2496	2688
Memory size per board (GDDR5)	8 GB	5 GB	6 GB
Memory bandwidth for board (ECC off)[b]	320 GBytes/sec	208 GBytes/sec	250 GBytes/sec
GPU computing applications	Seismic, image, signal processing, video analytics	CFD, CAE, financial computing, computational chemistry and physics, data analytics, satellite imaging, weather modeling	
Architecture features	SMX	SMX, Dynamic Parallelism, Hyper-Q	
System	Servers only	Servers and Workstations	Servers only

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Sequoia system, Lawrence Livermore National Laboratory
IBM BlueGene/Q, Power BQC 16C 1.6 GHz, custom interconnect
1572864, 20132 TFlop/s peak

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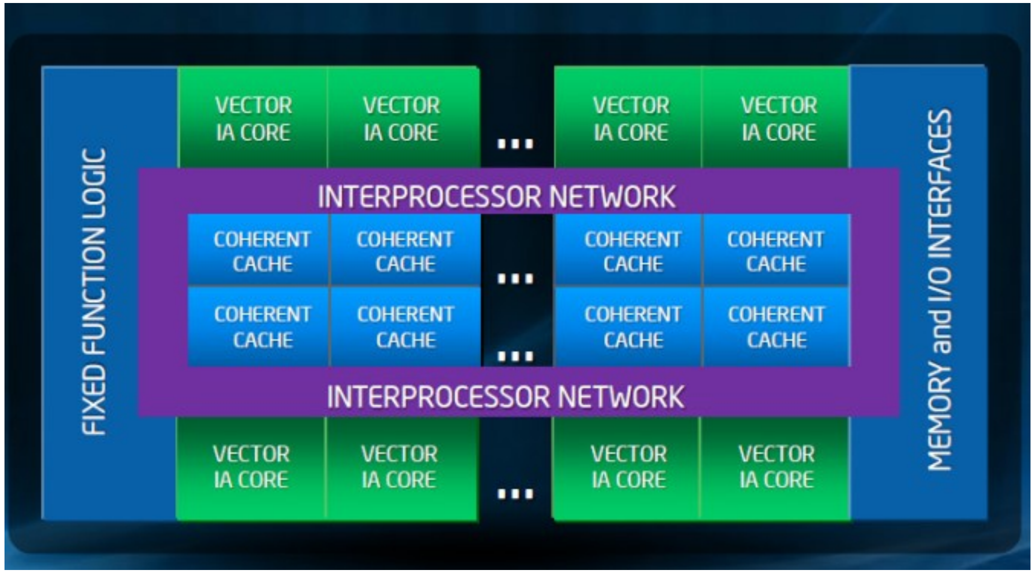

Intel Many Integrated Core (MIC) architecture
32 cores, 1.2 GHz, 128 threads (4 threads/core), > 1TFlop/s peak

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In recent computer systems, parallelism spreads over many architecture levels including nodes, processors, cores, threads, registers, SIMD-like and vector units

Several different levels of parallelism (from coarse to fine or very fine grain parallelism) need to be harnessed in order to maximize computational efficiency and scalability

Moreover, heterogeneity of the memory is growing at the node as well as at the chip level

The NUMA penalty in data accesses is one of the main critical issues for parallel performances and one must take care of locality access and memory affinity when distributing data on cores

All these heterogeneous characteristics of hardware resources keep effective performance far from theoretical peak

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Most applications and algorithms are not yet ready to utilize these available architecture capabilities

Developing large-scale scientific computing tools that efficiently exploit this processing power, of the order of petaflops with current generation systems, is a very complicated task and will be an even more challenging one with future exascale systems

Heterogeneity characteristic and hierarchical organization of modern massively parallel computing systems are recognized as central features that impact at all the layers from the hardware to the software with issues related to computer science and numerical mathematics as well

At the current state of the art in technologies and methodologies, a **multi-disciplinary approach** is required to tackle the obstacles in manycore computing, with contributions from **computer science**, **applied mathematics**, **high performance computing**, and engineering disciplines

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General objective and contributions

Establishment of a continuum of skills in the applied mathematics and computer science fields for a multidisciplinary approach to the development of numerical simulation tools that will take full benefits of the processing capabilities of emerging high performance massively parallel architectures

Activities and contributions are organized along a three-level structure from **generic building-blocks** to **large-scale applications**

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Project structure and activities (1/3)
Level 1 – Towards generic and scalable algorithms

- ✓ **Computer science topics**
  Upstream from the core topics which are centered on *the development of high performance numerical schemes and algorithms*

- ✓ **Algorithmic aspects**
  *E*mphasis on the development of generic numerical libraries and solvers in order to benefit from all the parallelism levels with the main goal of optimal scaling on very large numbers of computing entities

- ✓ **Robustness, accuracy and scalability issues of numerical schemes**
  Generic design issues of high performance numerical schemes for systems of partial differential equations

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Project structure and activities (2/3)
Level 2 – Towards robust, accurate and highly scalable numerical schemes for complex physical problems

Study of the systems of PDEs that model the scientific and engineering use cases considered in the project

Topics of interest include discretization in space of underlying systems of PDEs (high order approximation, adaptivity, etc.), solution algorithms base on continuous models (domain decomposition algorithms, physics base preconditioners, etc.) and numerical methods adapted to multi-scale and multi-physics problems

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Project structure and activities (3/3)
Level 3 – Towards exascale computing for the simulation of frontier problems

Large-scale simulations using high performance numerical computing methodologies resulting from the activities undertaken in the bottom and intermediate levels

With the involvement of external partners from research laboratories or industrial groups that will help in defining and dimensioning a number of frontier problems

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Core project-teams: numerical mathematicians

BACCHUS [INRIA Bordeaux – Sud-Ouest]
Parallel tools for numerical algorithms and resolution of essentially hyperbolic problems

HIEPACS [INRIA Bordeaux – Sud-Ouest]
High-end parallel algorithms for challenging numerical simulations

NACHOS [INRIA Sophia Antipolis – Méditerranée
Numerical modeling and high performance computing for evolution problems in complex domains and heterogeneous media

SAGE [INRIA Rennes – Bretagne Atlantique]
Simulations and algorithms on Grids for environment

TONUS [INRIA Nancy – Grand-Est]
Tokamak numerical simulations

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Core project-teams: computer scientists

ALPINES [INRIA Paris - Rocquencourt]
Algorithms and parallel tools for integrated numerical simulations

AVALON [INRIA Grenoble – Rhône-Alpes]
Large algorithms and software architectures for service oriented platforms

MOAIS [INRIA Grenoble – Rhône-Alpes]
Programming and scheduling design for applications in interactive simulation

ROMA [INRIA Grenoble – Rhône-Alpes]
Resource optimization: models, algorithms, and scheduling

RUNTIME [INRIA Bordeaux – Sud-Ouest]
Efficient runtime systems for parallel architectures

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Scientific and technical challenges: ANDRA use case

In the field of phenomenological description and performance/safety assessment, ANDRA has to perform many numerical simulations, in particular to quantify flow, from the waste package to the human being, and through the repository and geological environment

Simulations have to take into account many physical processes, applied to different components (from the waste packages to the geological media) and material (clay, concrete, iron, glass, etc.) on very large time (up to one million years) and scale (from centimeter to tens of kilometers

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Scientific and technical challenges: ANDRA use case

ANDRA is developing TRACES is a computer program for the simulation of flow and reactive transport in saturated porous media

Two levels of simulations are considered

- ✓ Complex physicochemical processes, involving strong couplings (such as chemical-transport, 2 phase-flow with radionuclide transfer, thermo-hydro-mechanics problems) but solved on small systems with grids up to many thousands of elements
- ✓ Simplified physicochemical processes (leak coupling) consisting of modifying in space and time hydraulic and solute transfer parameters, but solved on big systems with grids of many millions of elements. Global system is split into embedded compartments whose scales are bigger and bigger

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Scientific and technical challenges: ANDRA use case

Ex : deep geological repository

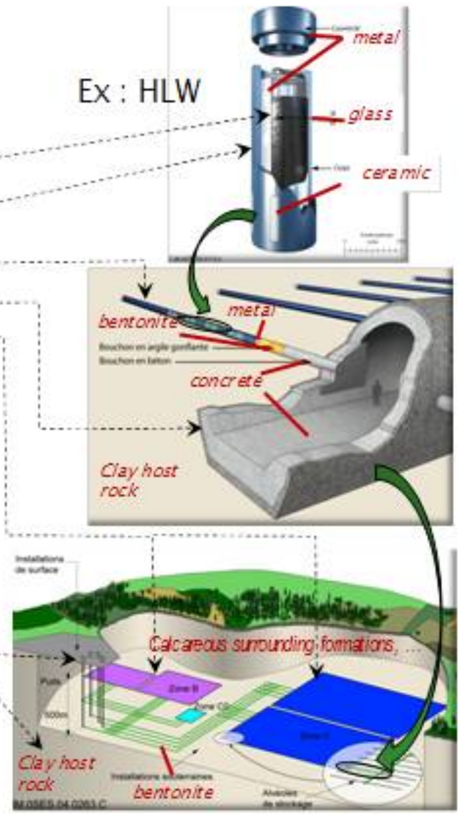
Multi components

Waste — Waste package
Galleries — Disposal cell
Access (shaft…) — Modules and zones
Geological medium

Multi materials

Glass Ceramic Metal
Concrete
Clay based (bentonite)
Clay host formation
calcareous, …

Ex : HLW



Multi processes

Thermal (T), Hydraulical-Gas (H) ,
Mechanical (M), Chemical (C), Radiological (R)
Solute Transfer in porous media (Tr).

with or without couplings (strong to low)

Multi spatial scale

- *centimetric to metric:* waste
- *metric to decametric:* disposal cell
- *hectometric to kilometric:* disposal
- *pluri-kilometric:* geological medium

→ Management > 7 orders of magnitude

Multi temporal scale

Up to 1 million years

Inria

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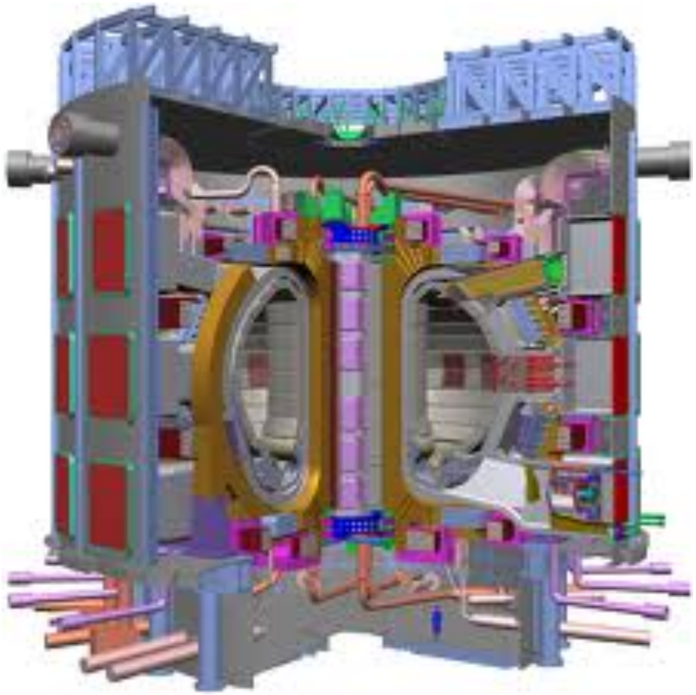
Scientific and technical challenges: CEA/IRFM use case

The IRFM (Research Institute on Magnetic Fusion) institute at CEA (French Alternative Energies and Atomic Energy Commission - Cadarache center) is conducting research activities on nuclear fusion in the context of the ITER project with studies that are concerned with Magneto HydroDynamic (MHD) stability, turbulent transport, plasma-wall interaction, and RF heating



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Scientific and technical challenges: CEA/IRFM use case

Significant recent progress in simulations of fine-scale turbulence and in large-scale dynamics of magnetically confined plasmas has been enabled by access to terascale supercomputers. These progress would have been unreachable without innovative analytic and computational methods for developing reduced descriptions of physics phenomena

Accelerated progress on this critical issue is especially important for ITER, because the size and cost of a fusion reactor are determined by the balance between 1) loss processes and 2) self-heating rates of the actual fusion reactions. Realistic models, simulations and highly parallel algorithms are essential in dealing with such challenges because of the huge range of temporal and spatial scales involved

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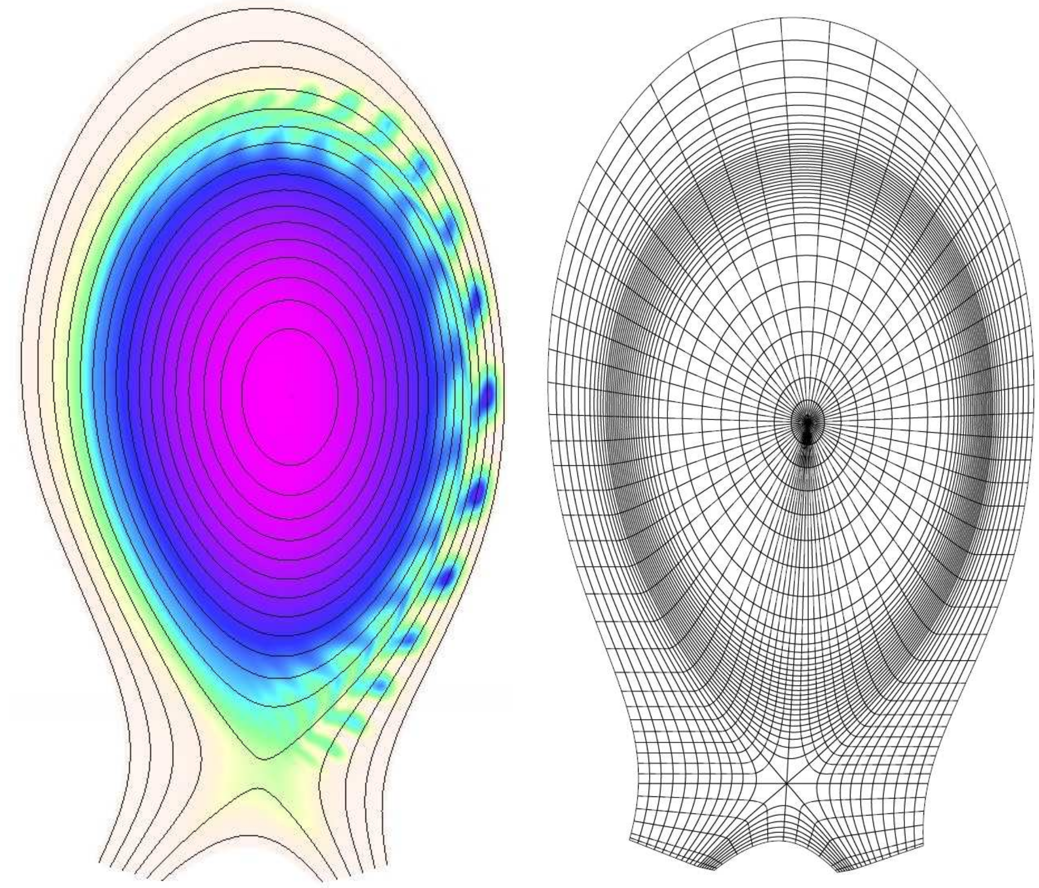
Scientific and technical challenges: CEA/IRFM use case

Two simulations software are considered in C2S@Exa:

- JOREK is dedicated to the numerical study of Edge Localized Modes (ELMs) and disruptions
- GYSELA is a global non-linear electrostatic code which solves the gyrokinetic equations (Vlasov) in a five dimensional phase space with a semi-Lagrangian method



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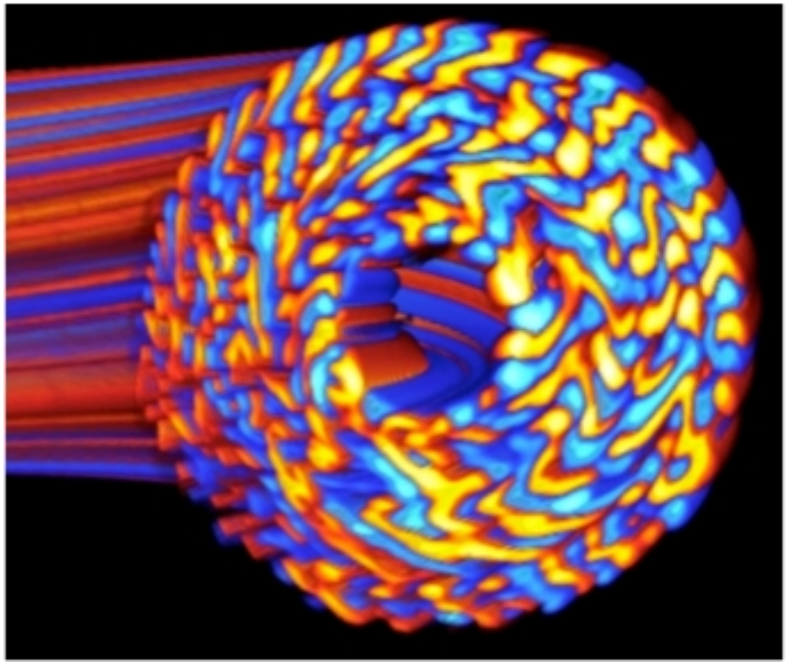

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Meshes in C2S@Exa

- ✓ Physical problems
  - ✓ Complex flows in porous media
  - ✓ Plasma dynamics (Vlasov-Poisson)
  - ✓ Magnetohydrodynamics
- ✓ Discretization schemes
  - ✓ Finite element and finite volume type methods
  - ✓ Tetrahedral and hexahedral meshes
  - ✓ Parallelization strategies based on mesh partitioning