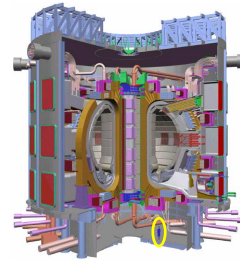


Sustainable Energy and High Performance Computing

Enjeux du Calcul Intensif pour l'Énergie *Recherche et développement dans le domaine de l'énergie*



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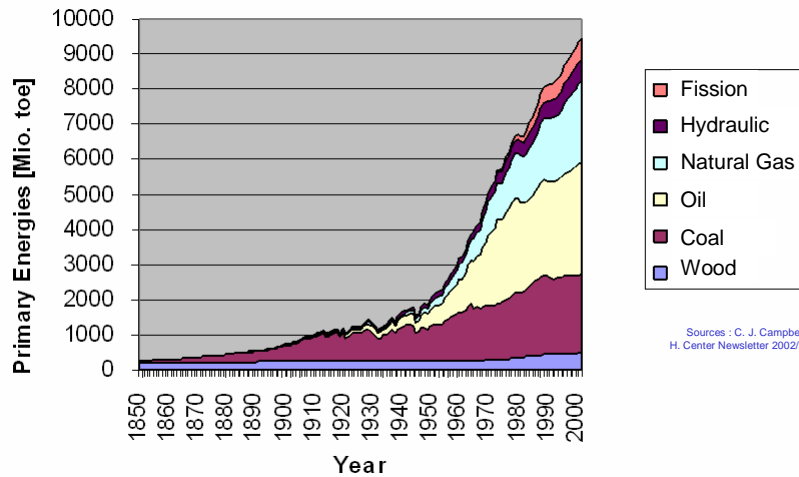


Bernard Bigot,
Haut commissaire à l'énergie atomique

Energy

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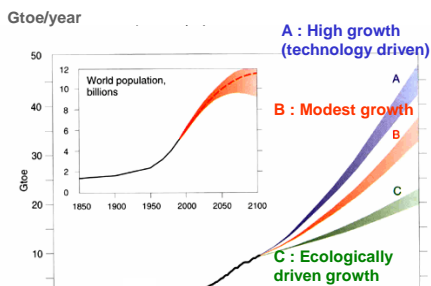
The consumption of worldwide primary energy increased by a factor of 16 during the 20th century !



During the first seven years of the 21th century, the average annual growth is still over +2,7% (a new doubling in 26 years !)

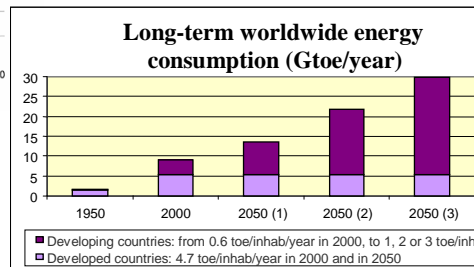
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Whatever energy savings the world will do in the future, the projected world energy demand will increase !



Reference : IIASA/WEC study « Global Energy Perspectives », 2003

For example, the IPCC as well as IEA latest and most conservative forecast is +57% by 2030



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The present world energy landscape

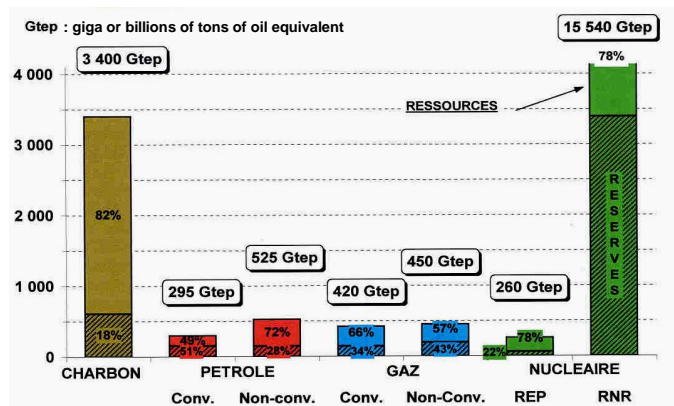
Consumption of primary energy in 2005 : 11.43 Gtoe

	World	EU 25	France
Oil	34.3%	37.3%	33.5%
Gas	20.9%	23.8%	14.8%
Coal	25.1%	17.7%	3.4%
Total of fossil fuels	80.3%	78.8%	51.7%
Nuclear	6.4%	14.6%	42.0%
Hydraulic	2.2%	1.5%	1.9%
Wind, solar, ...	0.5%	0.7%	0.1%
Biomass	10.6%	4.4%	4.3%
Total of renewables	13.3%	6.6%	6.3%

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Estimated world resources and reserves of energy

(renewable energies not included)



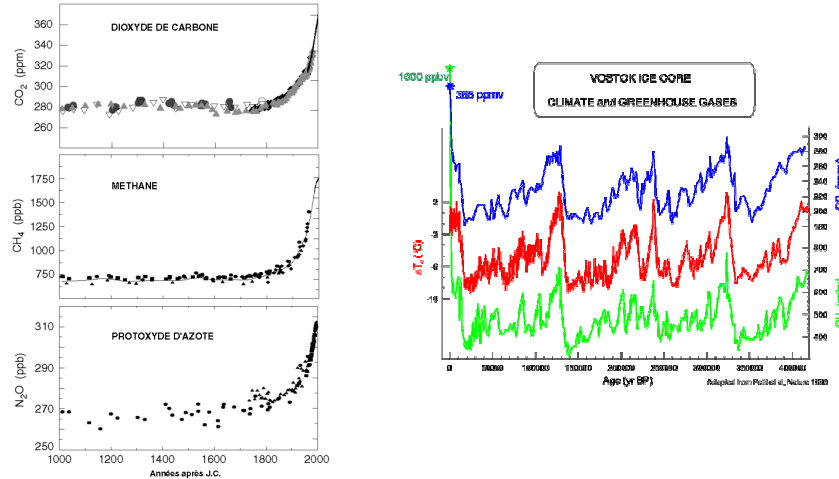
Source : World Council of Energy 2003

Reserves R1 : proved resources which are recoverable at a given fixed mean cost.
 Resources R2 : estimated resources which are recoverable without any consideration of cost.
 In 2003, IEA appraised R1/P to be 223, 40, 63 et 67 years respectively and R2/P to be 850, 124, 102 et 118 years.

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Induction of climate change and health issues

In addition to the prospect of an energy shortage during the next century, the massive use of fossil fuels (80% of the world energy consumption) induces serious risks for human health, and climate and environment changes : +2/+4.5°C by 2100 ? (IPCC , 2007)



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GLOBAL ENERGY NEEDS AND SUSTAINABLE DEVELOPEMENT

Summary :

- The growth in the world's population and the legitimate aspiration of emerging countries to raise their standard of living will increase the world energy needs unavoidably during the first part of the 21th century.
- Fossil energy resources will be depleted over the coming decades for oil and gas, and during the next century for coal, while they are assuring 85% of the world energy consumption.
- The growth in energy needs could impact on our environment seriously, the greenhouse gas emissions and other pollutants in the atmosphere having potential large consequences on the climate and the functioning of the biosphere.
- Meeting humanity growing energy needs within a sustainable development policy is a major issue for the 21st century.
- To face the challenge, the most reasonable approach is to save energy, diversify energy sources and intensify R&D on innovative technologies (today, R&D represents 0.3% of the 3.7 G€ world energy market).

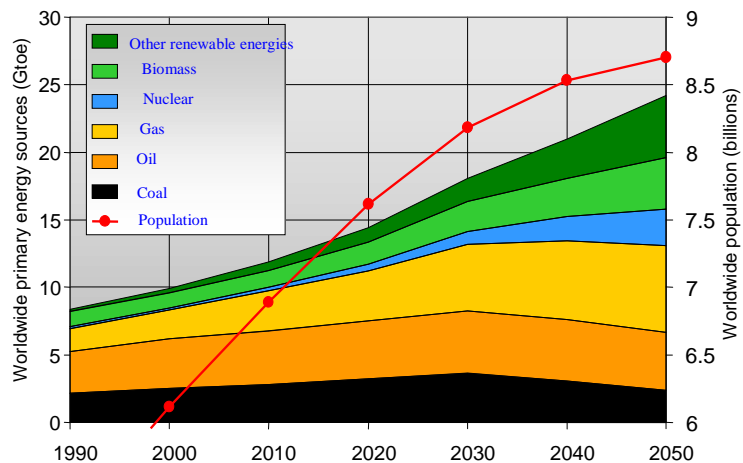
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There is a need for a new world energy policy !

- Saving energy and resources (changing the behaviours and processes, improving energy efficiency, recycling the wastes,...) to lower the energy intensity further
- Developing the use of renewable resources (best use of biomass, solar, wind, hydraulic, geothermic, resources)
- Decreasing further the carbon emissions as long as there are still fossil fuels (developing the CO₂ bio-sequestration and geological sequestration...) : we need to divide the annual CO₂ emission by a factor of 4 before 2050
- Strengthening the nuclear option (safety, operability, economic efficiency)
- ... **Modelling and simulation could largely contribute to the required R&D and to the innovation development!**

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Future Energy Mix? How to speed up the changes ?



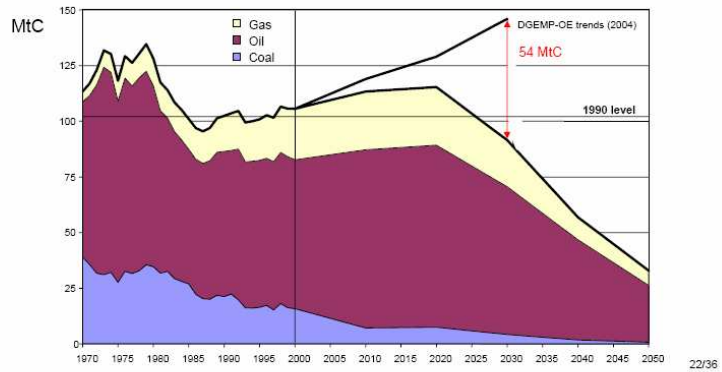
Source IEA: International Energy Agency
Energy to 2050 - Scenarios for a Sustainable Future

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CO2 emissions due to energy by 2050 (DGEMP-OE(2005) – “Factor 4”)

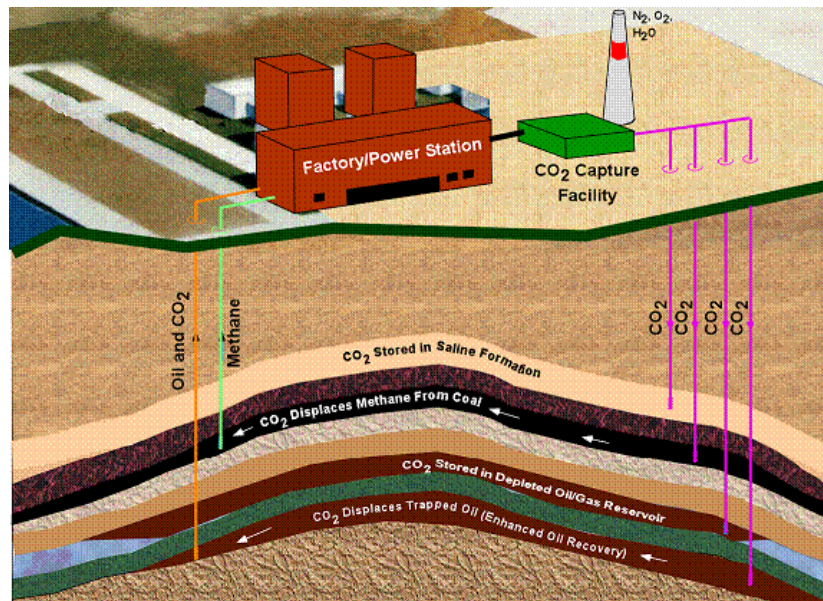


- “CO2 stabilisation at 450 ppm” worldwide and “factor 4” in the industrialised countries => **Developing CO2 capture and sequestration ?**
- CO2 emissions due to fuel combustion in France:



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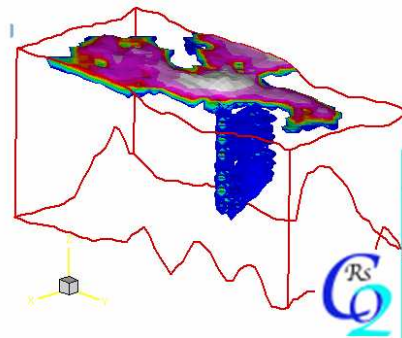
CO2 capture and sequestration



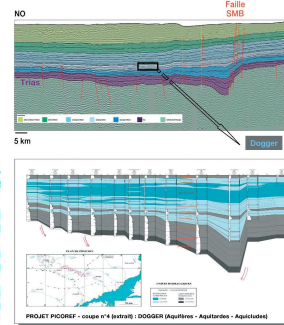
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CO₂ sequestration : the HPC involvment

CO₂ Distribution after 25 years of injection in a layered saline aquifer



COORES Simulator (IFP)



Projet PICO

Le Gallo Y et al " Long-term flow simulations of CO₂ storage in saline aquifer" Proceedings of International Conference on Greenhouse Gas Control Technologies, Trondheim, 19-23, June 2006



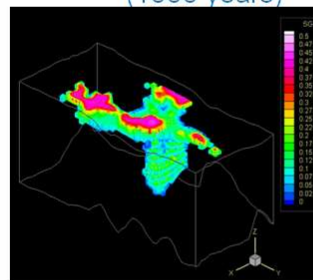
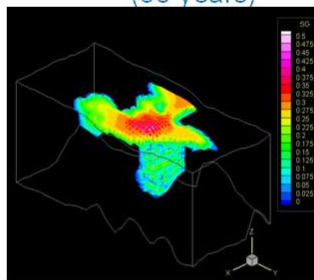
CO₂ distribution

end of CO₂ injection

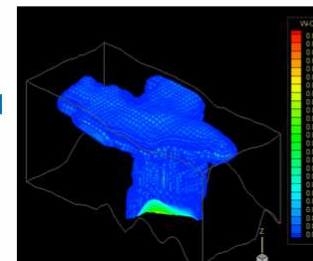
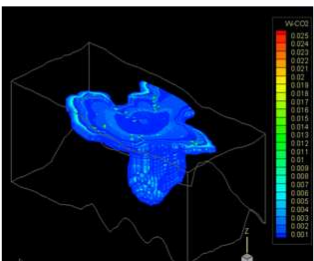
end of CO₂ storage

(30 years)

(1000 years)

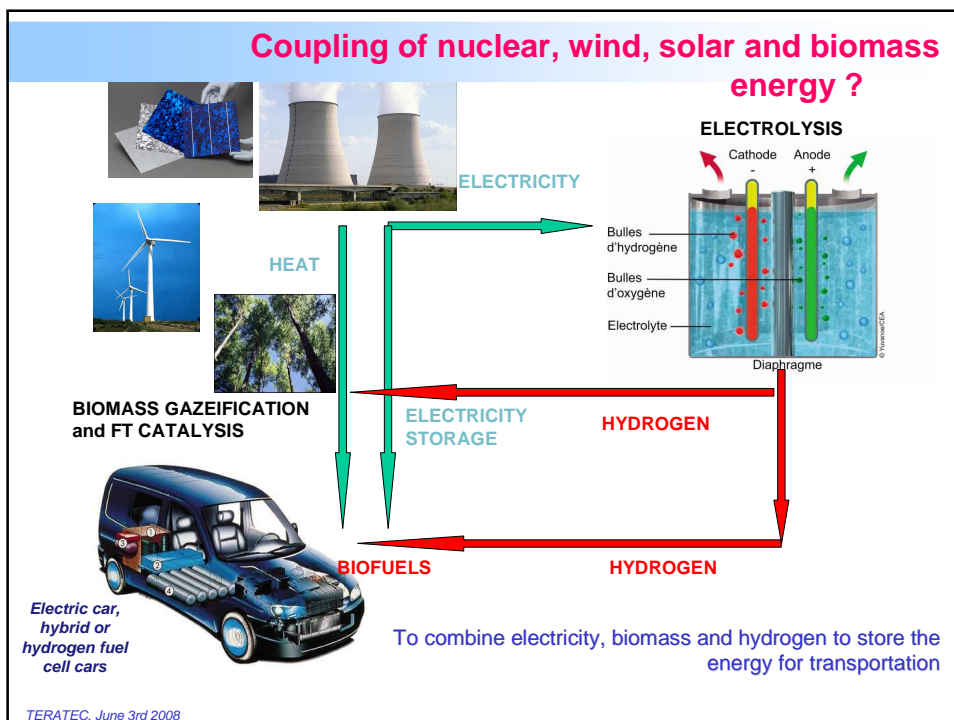
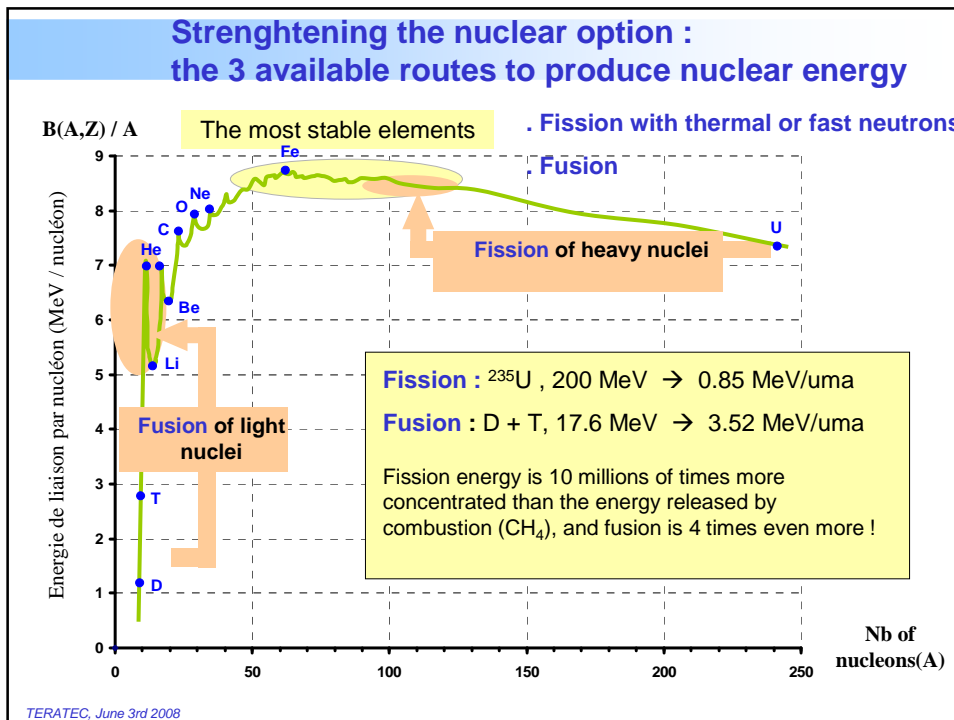


Gas



Dissolved
















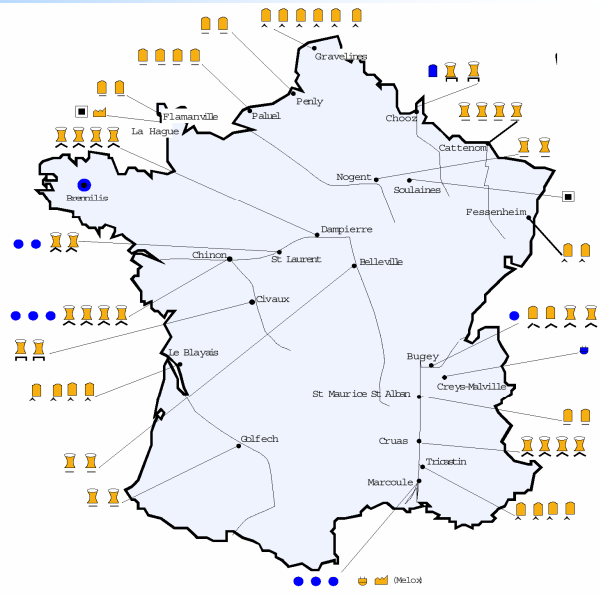
Nuclear Fission

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The fission route in France

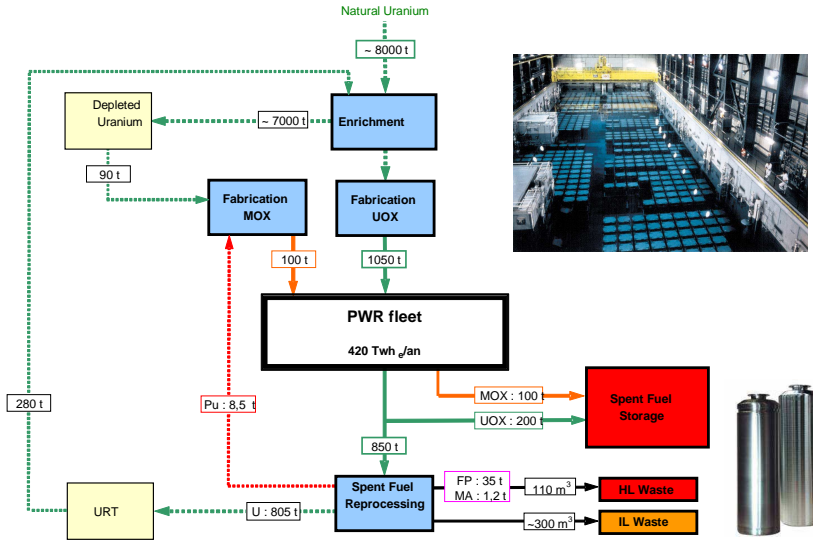
58 thermal neutrons PWR reactors produce over 80% of the French electricity

-  In service
-  Decommissioned
-  900 MWe
-  1300 MWe
-  1450 MWe
-  UNGG
-  PWR cooling tower
-  PWR direct cooling
-  FBR
-  Fuel facility
-  LLW sites



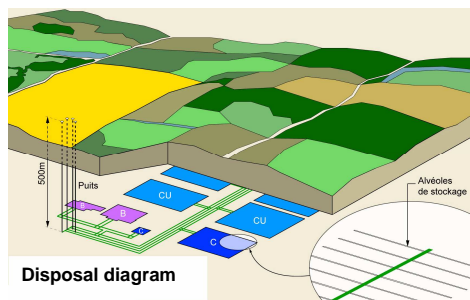
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French nuclear fleet : annual flow of materials and wastes

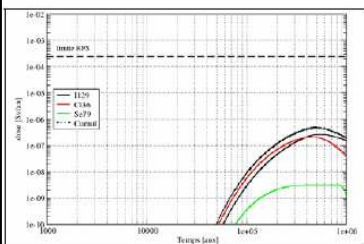


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The reference option : geologic disposal

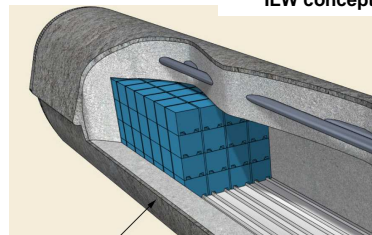


C1 + C2 vitrified waste

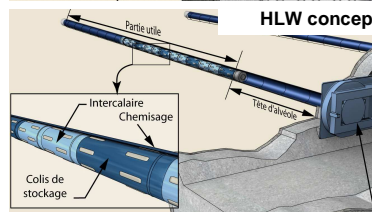


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ILW concept



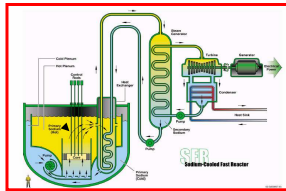
HLW concept



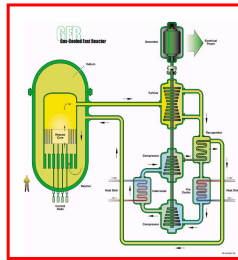
The law decides to prepare a plan for construction of a reversible depository of vitrified LLW and compacted MLW in order to be able to take a formal decision by 2015 and to make it to be operative by 2025.

Next Generation of nuclear power plants : fast neutrons reactors

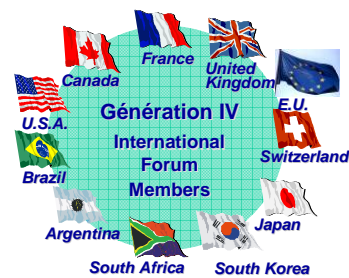
With this technology and the stocks of depleted uranium and plutonium expected to be available in 2040, France could fulfill all the national energy needs for 8-10 000 years



Sodium cooled reactor



Gas cooled reactor



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An example of HPC utility policy : EDF Strategy*

- EDF has strategically decided to use HPC for helping to solve global energy issues in the company
- EDF computation investments are shared with other organizations (CCRT) or in-house (to-day 150 Teraflops are in operation)
- Industrial CFD computations have run on more than 10 000 processors.
- A large range of business applications benefit from EDF investments on high performance simulation (nuclear energy production, safety demonstration, education training, electricity distribution,...).
- EDF is convinced that research-industry partnerships are needed: the size and the scientific complexity of industrial problems to be solved need the cooperation of both types of organizations..

* Data provided by Jean-François Hamelin

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EDF Strategy. A challenging computation example

- Computation of time-dependent asymmetric flow in the internal structures of a nuclear reactor vessel, for determining the thermal-hydraulic strain on the fuel assemblies.
- Massively parallel HPC (Code-Saturne) is intended to evaluate “mixing grids” effects (a few millimeters compared to multi meters flows in the core).
- 10 000 processors computations allow to represent a simplified fuel assembly (a few fuel pins); the treatment of actual assemblies and the detailed flow inside the internal structures clearly need multi-petaflops computers

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Vessel Thermal-hydraulics

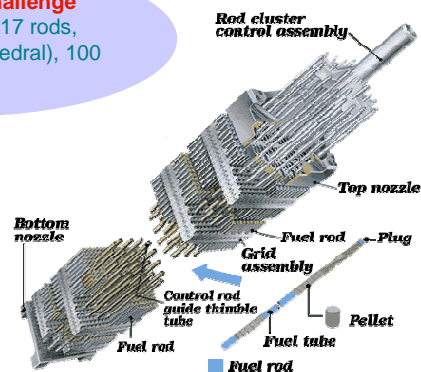
What is at stakes

- mechanical behaviour of assemblies, taking into account complex realistic geometries (fretting)
- Thermal hydraulics critical Design of the **EPR vessel**

2007 HPC Challenge
3D RANS, 5x5 rods,
100 millions cells
(tetrahedral), 2
Mheure.cpu

2008-2009 HPC Challenge
3D RANS/LES, 17x17 rods,
220 millions (hexahedral), 100
Mheure.cpu

2010 –2015 HPC Challenge
Full vessel, 10^{10}
cells, 10 Pflops

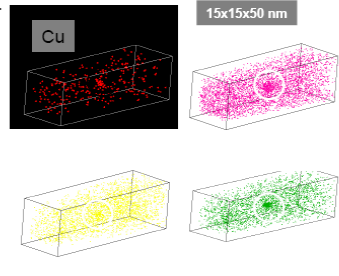


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Material Science: ab initio Calculation - HPC applications for Nuclear Plant

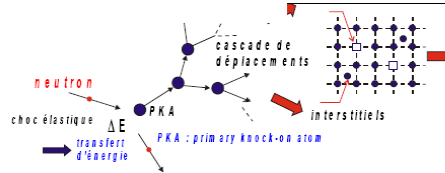
➤ Irradiation damages (materials structure) :

- Vessels
- Internal structure
- rod (or casing)



➤ HPC Applications :

- Material Corrosion
- Corrosion in primary circuit



IBM involvement: VASP, CPMD assessment

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The need of scientific european cooperation : NURESIM



NUclear REactor SIMulation
European Integrated Project (2005-2008)
13 Countries, 18 Partners

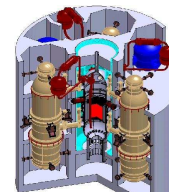
Present NPP



GEN-III



GEN-IV



Optimisation of the present
 NPP technology
 (safety/operability/efficiency)

Technological rupture

Integration of Reference Coupled Codes
 → **SNETP: Sustainable Nuclear Energy Technology Platform**

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State of the art R&D programs : Light Water Reactors

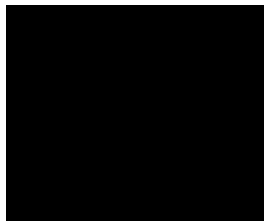


Future challenges:

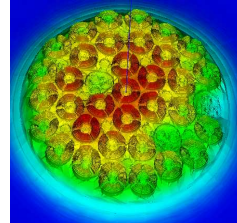
3D core with coupling between neutronics, thermal-hydraulics and fuel
 Detailed description of boiling

→ > 500 Tflops
 → > 500 Tflops

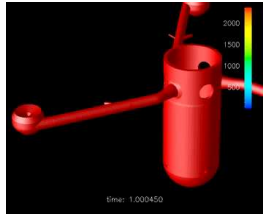
Bubbles in a duct



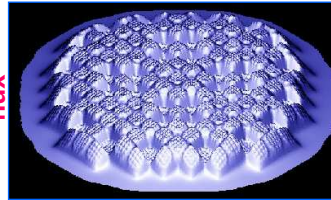
JHR neutron flux



Flow mixing



PWR neutron flux

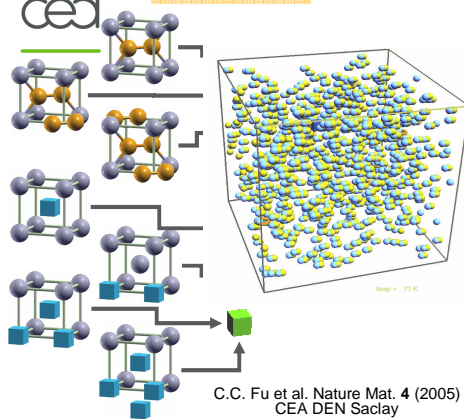


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Ab initio modeling of defects in nuclear materials



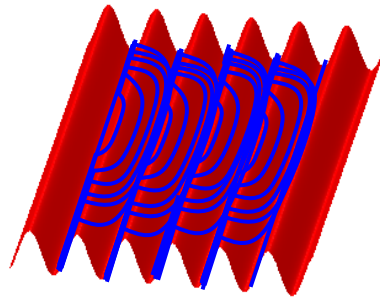
Present



C.C. Fu et al. Nature Mat. 4 (2005)
 CEA DEN Saclay

Defect clusters (0D)
 200-400 atoms
 Input for kinetic codes
 (recovery of defects in iron after electron irradiation)

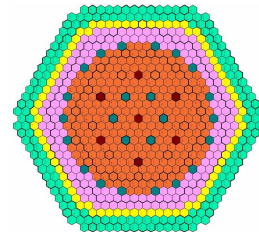
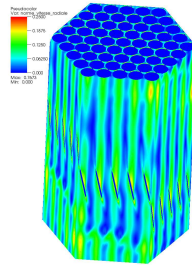
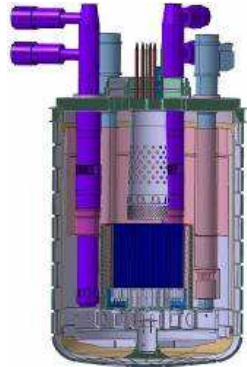
Future Challenge



Dislocation lines (1D)
 (interaction with solutes and radiation defects)
 3000 atoms (~20 000 proc. for 10 days)
 Input for plasticity codes
 Application: degradation of the mechanical properties of nuclear materials under irradiation

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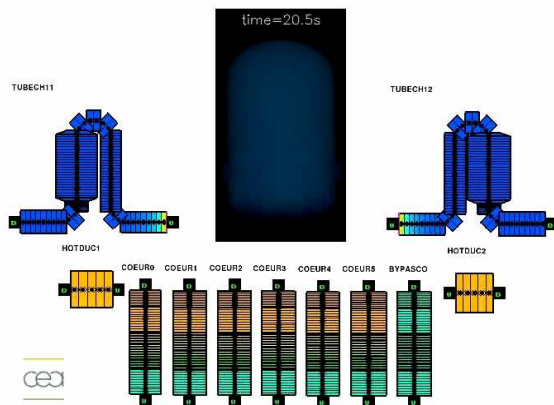
Sodium Fast Reactor



Future challenge:
 Core calculation with Monte-Carlo methods
 including fuel depletion
 → > 500 Tflops

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Gas Cooled Fast Reactor



Heat removal during a transient

Future challenge: same as for Sodium Fast Reactor

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Energy conversion and turbines

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There is a real need for larger and more efficient steam turbines : Alstom « Arabelle » design is expected to require much less time and experimental testing than previous turbines for large nuclear power plant .

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Challenge

LP Steam Turbines exhaust flow simulation requirement

Steam Turbines LP Exhaust flow simulation

Aerodynamics team within R&D steam turbines would like to perform 3D simulations with the following configuration :

Full **stage-diffuser-hood-condenser** flow 3D simulation including:

- a- Unstructured-structured mesh including general interfaces.
- b- Flow phase change (condensing steam) with heat transfer.
- c- Full detailed complex geometry.
- d- Supersonic flows and water injection system simulation.

To perform this kind of simulation, the hardware resources was always the most crying weak point which has put this action into dusty drawer.

Current estimation for Hardware needs: 74-75 Million nodes requires **296-300 GB** live memory for direct calculation. This would be easily done on parallel **80 processors**.

Alstom Power Steam Turbines R&D. M. Lakehel - 03/03/2007 - P 9

POWER SYSTEMS | **ALSTOM**

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Alstom goals and challenges *

- In close partnership with EDF, Alstom will carry out the engineering, procurement, construction and commissioning of the whole 1750 MW turbine island and directly supply all the major turbine island components, including Arabelle steam turbine, generator, condenser and moisture separator reheaters.
- « Arabelle » turbine technology is installed in four 1550 MW units in the EDF nuclear power plants located in Chooz and Civaux, and is currently being installed in the extension of Ling Ao power plant in China. The « Arabelle » steam turbine at Flamanville will be the biggest ever built in the world.

* Data provided by Frédéric Lamarque

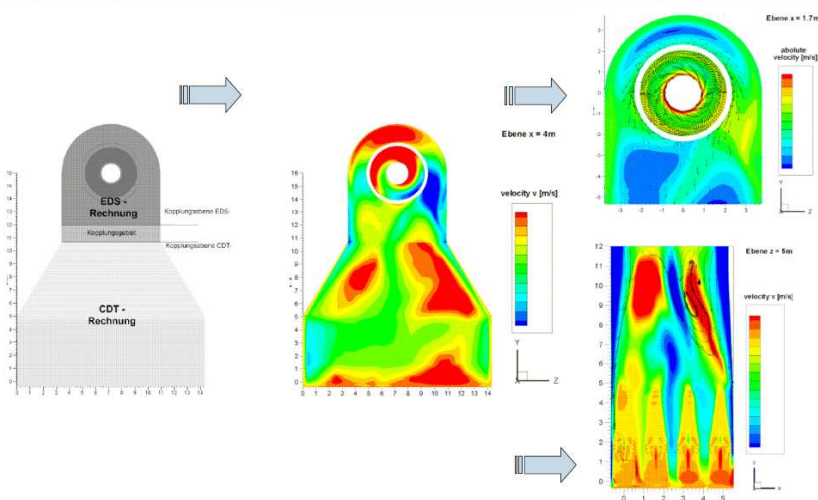
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The challenge of HP computation for HP turbine development

- There is expectation of the computation of a full low pressure exhaust for a high power steam turbine : the geometry includes the last turbine stage, the diffuser, the outer hood and the condenser.
- Optimizing the design of this assembly intends to reduce pressure loss significantly and improve the global efficiency of the turbine.
- For solving this problem, there is no other way than more research and development and more computing resources.

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3- Coupled Exhaust hood and Condenser (EDS & CDT)



Alstom Power Steam Turbines R&D, M. Lakehel - 01/01/2007 - P. 9.

POWER SYSTEMS | **ALSTOM**

Courtesy of Christian Heneka

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Tokamak

In russian
Tok: current
Mak: machine

Poloidal field created by I_p

Toroïdal field created by magnetic coils

Total field

- The lines of the magnetic field create some magnetic closed surfaces,
- Ions et electrons of the plasma wind around the lines of the magnetic field,
- The plasma is confined within the magnetic surfaces leading to its spatial and thermal isolation,

➔ The magnetic field must be larger than 200 000 times the earthly fields !

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International Thermonuclear Experimental Reactor (ITER)

– Main features

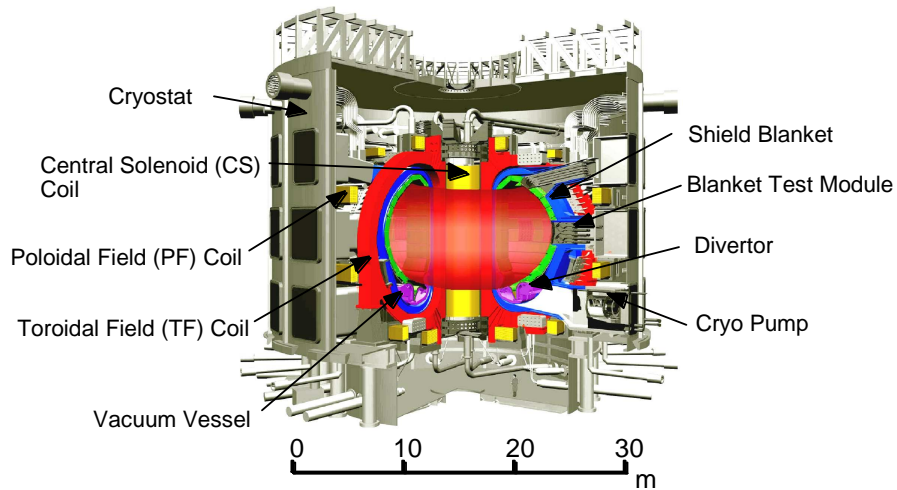
- Grand radius (vessel) : 6,2 m
- Small radius (vessel) : 2 m
- Internal volume : 840 m³
- Magnetic field : 5,3 T
- Electrical intensity : 15 MA
- Height (cryostat) : 24 m
- Radius (cryostat) : 14 m

– Main goals

- 500 MW of fusion energy during 400 s
- Amplification of energy of 10
- Continuous operation at 250 MW
- Key ITER technologies fabricated and tested by industry
- Aim is to demonstrate integrated physics and engineering on the scale of a power station

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Sectional view of Tokamak ITER

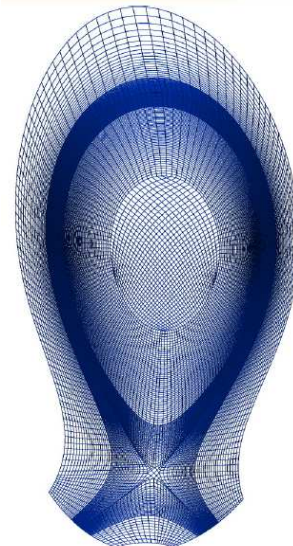


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Tokamak Plasmas - Simulation

Most advanced numerical methods are needed

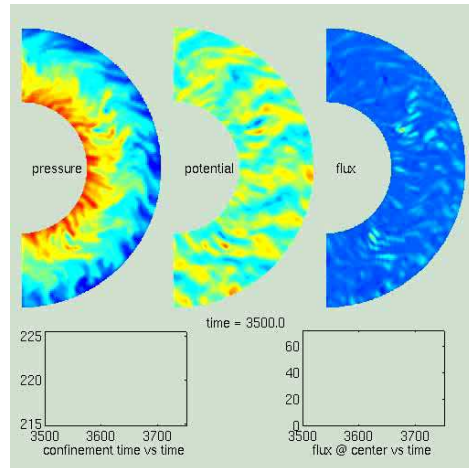
Example: adaptive meshgrid for the simulation of MHD instabilities of ITER



G. Huysmans CEA Cadarache

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- The origin of heat losses is turbulence phenomena
- These losses are to be minimized and turbulence controlled

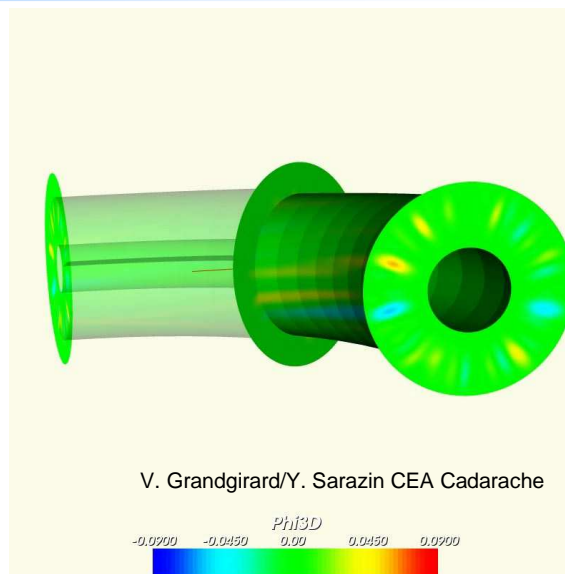


P. Beyer U. Provence

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These simulation are highly computing time consuming

- Accounting for time and space lead to refined mesh grids
- A full turbulence ITER calculation would consume 10 000 years on a standard PC

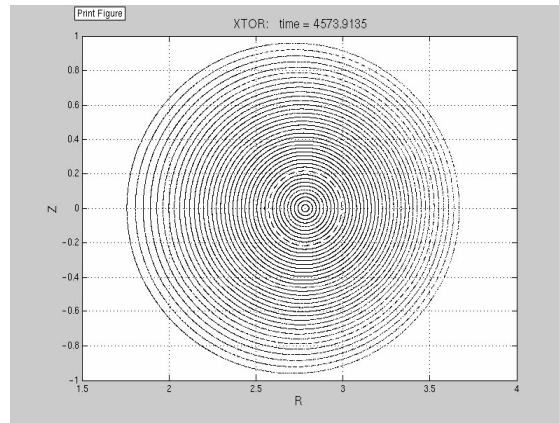


V. Grandgirard/Y. Sarazin CEA Cadarache

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Control of large scale instabilities

- Differences of pressure and flow in the plasma lead to instabilities
- They define the operational domain of the Tokamak



H. Lütjens, CPhT Ecole Polytechnique

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Peta-Scaling Simulation

Two routes :

- Integrated modelling : simulations to provide interpretation of experiments
- « ab-initio » modelling: simulation for prediction ; needs very high computational power

Ideally, one of these simulations in the ITER case

- Either for design (whole) case study
- Or experiments Interpretation
 - 100 Teraflops \approx 10.000 cores
 - 1 year
 - Petaflops
 - \approx 1 month

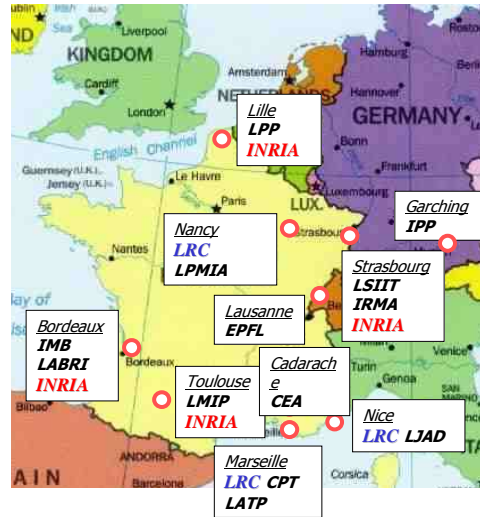
HPC-in-Europe Task Force : typical applications are expected to require:

- 70 to 100 Teraflop/s (sustained) over a few months to one year per application in 2007 – 2009
- > 500 to 1000 Teraflop/s (sustained) in the years past 2009

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GYSELA

- National networking of mathematicians, physicists et computer scientists
- Sponsored by Universities, CNRS, INRIA, CEA and ANR Research Agency



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Petaflops perspectives

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BLUE WATERS

PETASCALE COMPUTING SYSTEM

Work begins now on the first petascale computing system for open scientific research

The Blue Waters petascale computing system will revolutionize science and engineering research and education.

Some announcements !

Blue Waters will deliver sustained performance of one to two petaflops for many real-world scientific and engineering applications. These are codes scientists and engineers use every day, not simple benchmarks commonly used to rank high-performance computers

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The Keisoku Keisan-ki Project

Kei (10¹⁶) Soku (Speed, fast) Keisan-ki (Computer)

Development & Application of Next-Generation Supercomputer

RIKEN
Next-Generation Supercomputer R&D Center

Tadashi Watanabe
Project Leader
Next-Generation Supercomputer R&D Center, RIKEN
May, 2007

- This project is a key milestone for Japan to keep capability of developing supercomputer.
- The Supercomputer will be designed as a series of supercomputers with different performance
- The supercomputer will be completed in March, 2012 with effective more than 1 PFLOPS and serve as a national infrastructure
- Focused application area: Nano and Life sciences. So far, 21 applications have been chosen to make a benchmark suite.
- Budget 110 billions of Yens (800 Millions d'€), funded by MEXT

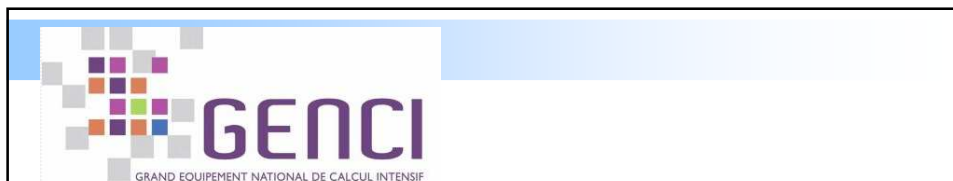
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- The Partnership for Advanced Computing in Europe prepares the creation of a persistent pan-European HPC service, consisting several tier-0 centres providing European researchers with access to capability computers and forming the top level of the European HPC ecosystem.
- PRACE is a project funded in part by the EU's 7th Framework Programme.



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- GENCI, Grand Equipement National de Calcul Intensif, is a «société civile» under French law, owned for 50 % by the the Ministry for Higher Education and Research, for 20 % by the CEA, 20 % by the CNRS et 10 % by the Universities.
- Created in january 2007, GENCI has the following mission:
 - promote the use of modelling, simulation and high performance computing in fundamental and industrial research;
 - promote the organisation of European high performance computing and participate to its actions;
 - set in place and coordinating the major computer equipment for the French computer centers for civilian research, by providing for their financing and assuming their ownership;
 - perform all research required for developping and optimising the utilisation of computing equipment
 - open the equipment it owns to all interested scientific communities, academic or industrial, national, European or international.

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High level cursus for simulation

For using the new HPC capabilities efficiently and developing the next generations of HPC technologies, we must sustain HPC expertise through high quality training programs.

The availability of high quality, abundant human resources in algorithmic sciences, applied mathematics, computing sciences, ,... will be a key issue in the future.

We must build an attractive education offer involving a sustainable and large cooperation among academic institutions, research organisation and industrial and service companies.