energie atomique • energies alternatives

High Performance Computing at CEA

Thierry Massard CEA-DAM

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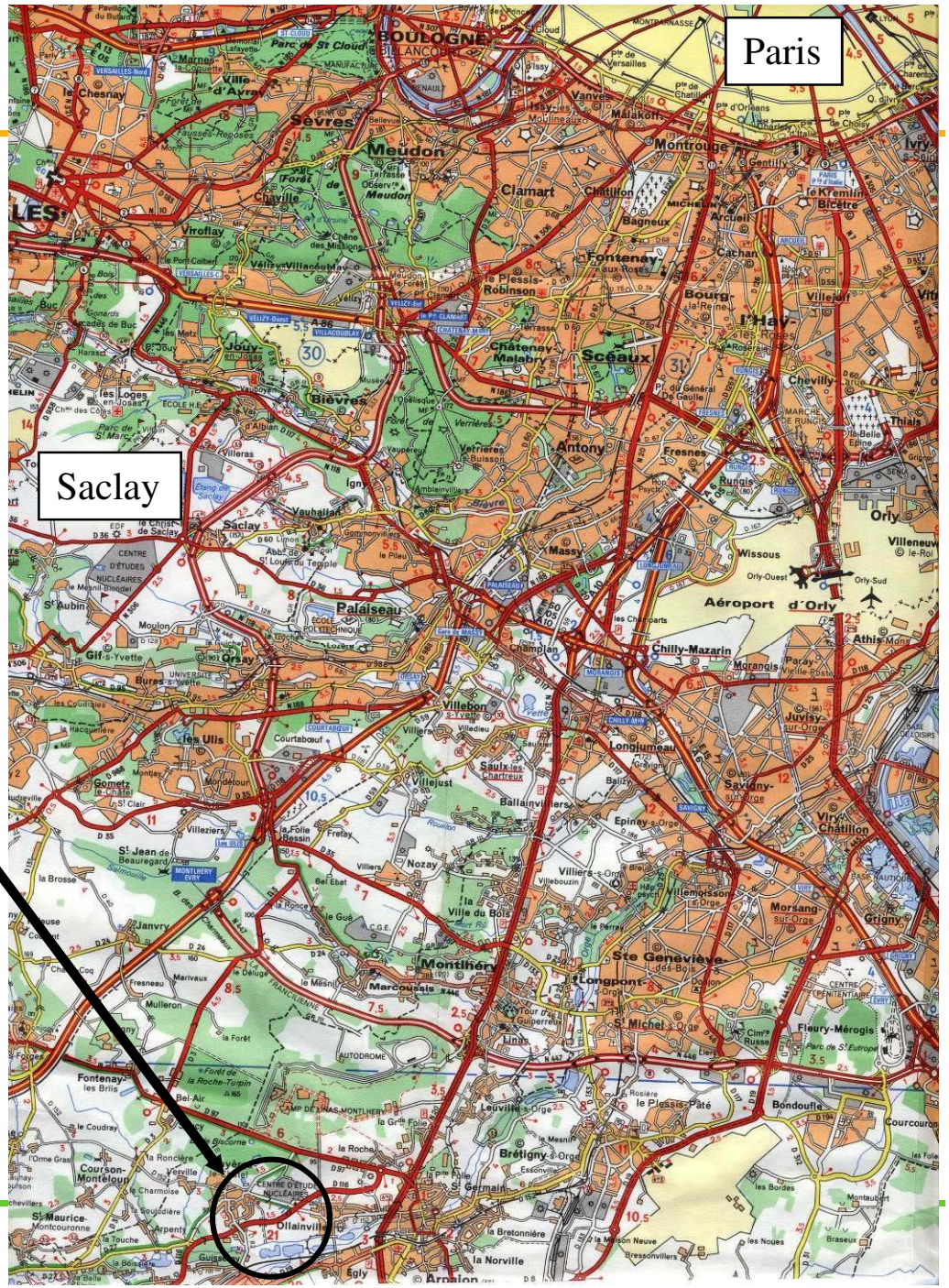
CEA/DIF (Bruyères-Le-Châtel)

CEA Supercomputing Complex



Brief Presentation of CEA

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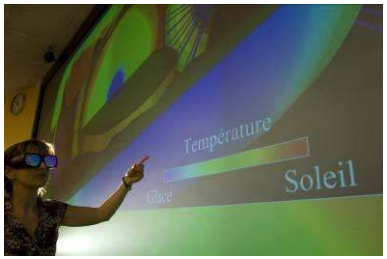

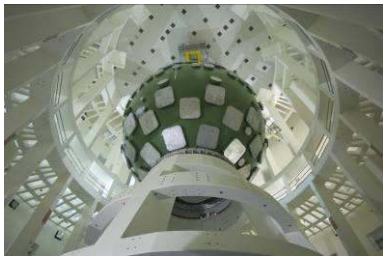

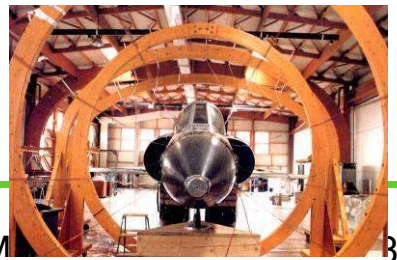

- CEA, namely “Atomic and Alternative Energies Commission”, is a French governmental research organization
  - 15 000+ employees
  - 1 000+ doctoral students
  - 3.9 B€/year budget
  - 4 000+ scientific publications/year
  - 300+ European projects with CEA participation
- Main focuses of CEA are:
  - Defense and global security
  - Energy
  - Information & Health technologies
  - Related and necessary fundamental research
- Other outcomes
  - Teaching and knowledge dissemination
  - Technology transfer (patents, start-up/spin-off companies…)

HPC a huge need for CEA

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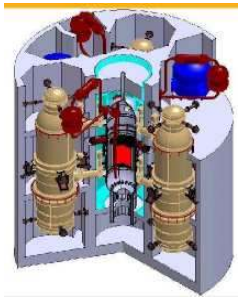
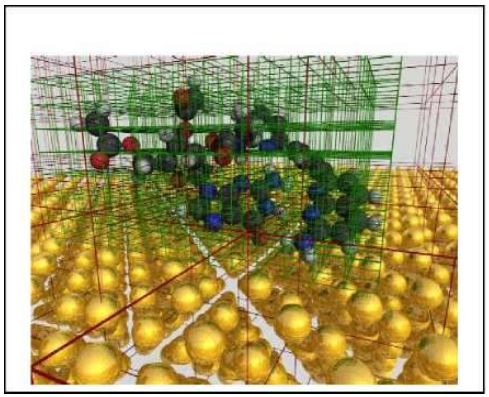
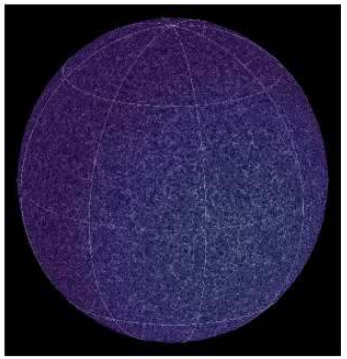
Basic science and applied research for the Simulation program

Applied research, industrial applications in the field of Energy and Health and Communication technology



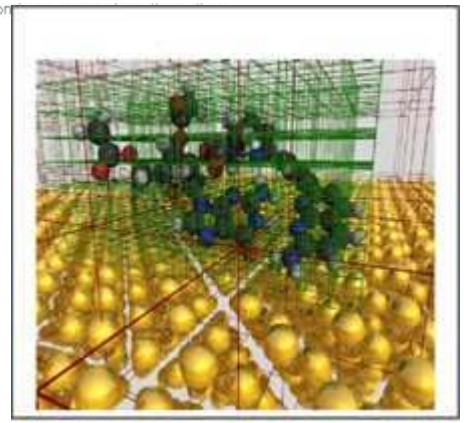
Fundamental research (Matter and Biology)



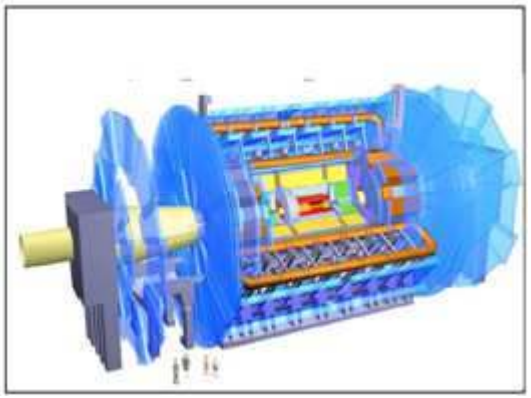


Fundamental Sciences of Matter

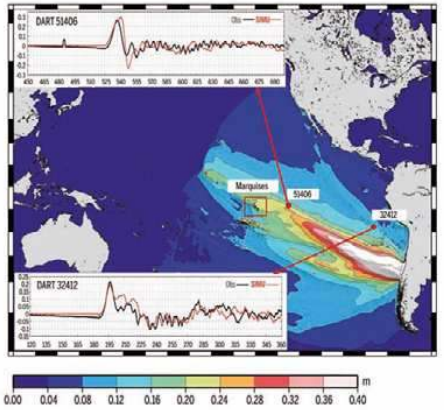
Nanosciences



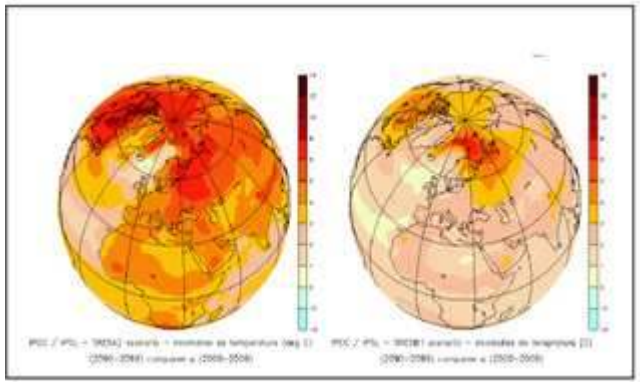
Particles Physics



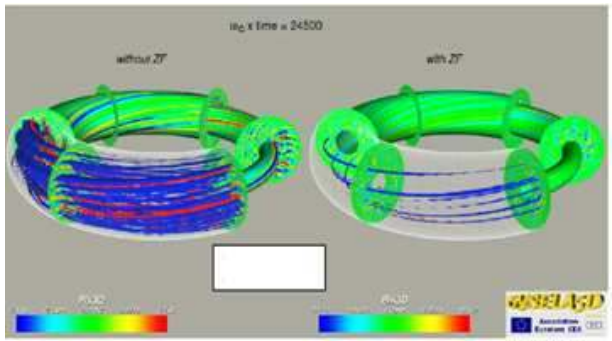
Environmental risks tsunamis



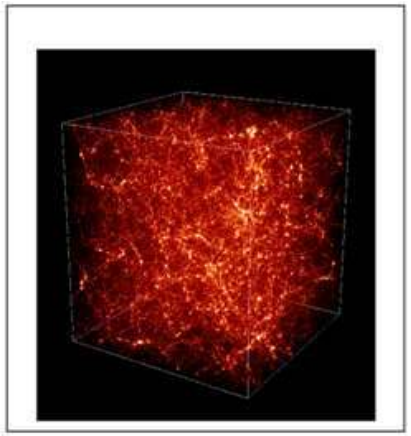
Global warming



Fusion



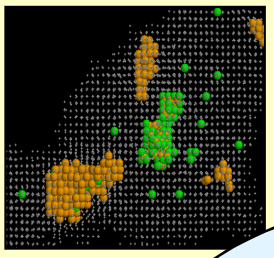
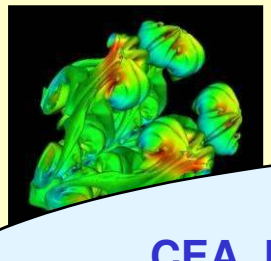
Structure of the Universe



CEA Scientific Computing Complex

Defense Computing Center
TERA



R&D
on HPC
Technologies

Très Grand Centre de calcul du CEA
TGCC

PRACE

GENCI
GRAND EQUIPEMENT NATIONAL DE CALCUL INTENSIF

CCRT

cea · AREVA · EDF · SAFRAN · CERFACS · INERIS · ONERA · EADS astrium

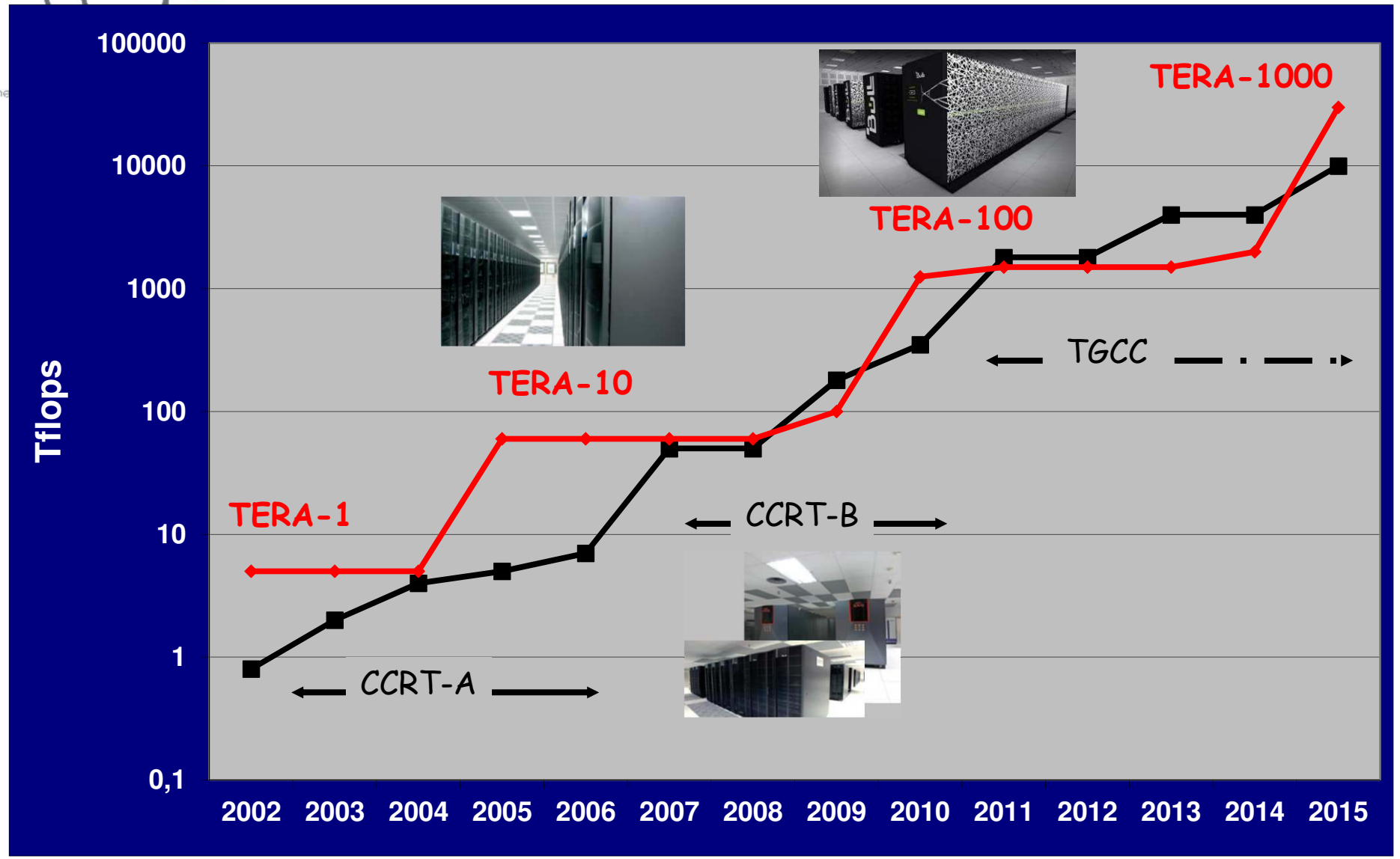
Address the needs of
CEA, French & European Research Communities
and Industry in terms of High Performance Simulations

While developing and assessing news technologies
for more powerful and efficient HPC systems

Joint Laboratories

- Extreme Computing Lab (BULL, CEA)
- Exascale Computing Research (INTEL, GENCI, CEA, UVSQ)

Compute Complex Capacity Roadmap




TERA Computing Centre
Classified computing resources for the CEA/DAM
“Simulation Program”

TERA 100

1st european supercomputer in 2010 above the sustained Petaflops

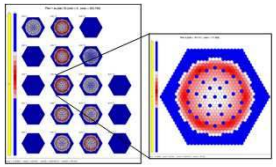
1,25 Petaflop/s peak
4 300 nodes
140 000 coresIntel Xeon® Nehalem EX
QDR Infiniband interconnect
System software Open source

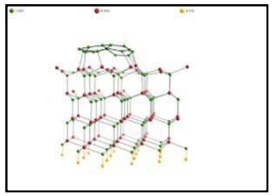
300 TB memory
20 PB storage disk
500 GB/s bandwidth
toward the storage system

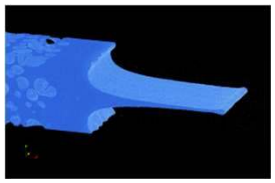
High reliability machine to meet the strategic needs of CEA/DAM

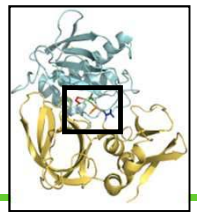
Grand Challenges on TERA 100

- We have taken advantage of the pre-production phase to «invite » a selection of frontier extreme computing cases :
  - Part of the V&V process for the global system
  - Reach the limit of the machine
  - To observe the behavior of other software than those in CEA-DAM's portfolio
- Sampling from the nov 2010 – feb.2011 campaign :





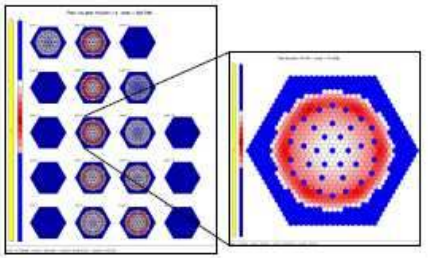


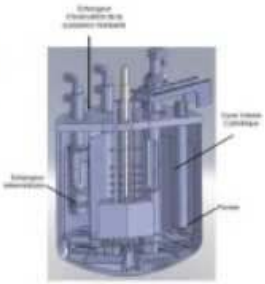


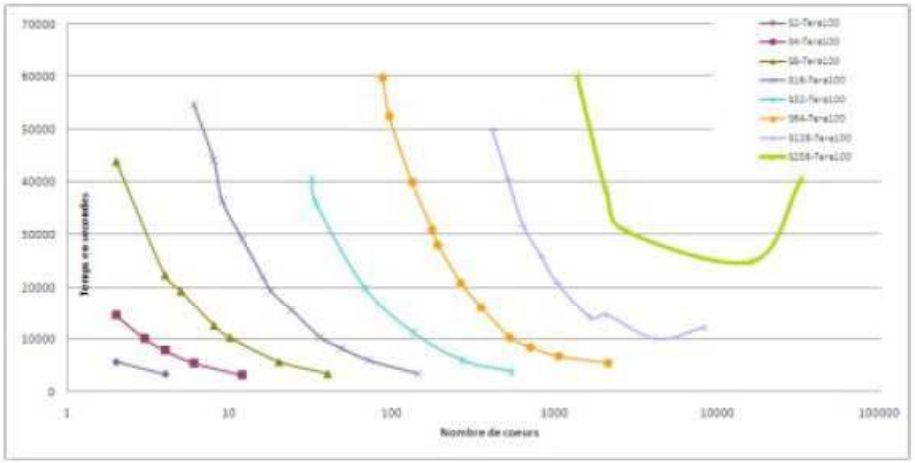
- **Massive parallell Calculation for the 3D transport of a sodium fast reactor using APOLLO3**
  R. Baron, C. Calvin, J. Dubois, J-J. Lautard, S. Salmons
  CEA/DEN/DANS/DM2S/SERMA
  up to 30000+ cores
- **Simulation of graphene growth on Silicon Carbibe (BigDFT)**
  Thierry Deutsch, Luigi Genovese, Pascal Pochet, Eduardo Machado-Charry
  CEA/DSM/INAC – Grenoble
- **Classical Molecular Dynamics Simulations (STAMP)**
  L. Soulard et al. , CEA/DAM/DPTA
  up to 10000 cœurs
- **Design of artiificial enzymes (STAMPS)**
  - G. Debret, M. Masella, P. Cuniasse, G. Collet CEA/DSV/iBiTecS

APOLLO3 au Pétaflop sur TERA-100 pour GENIV

« Calcul massivement parallèle en transport 3D d'un réacteur rapide sodium avec APOLLO3 »

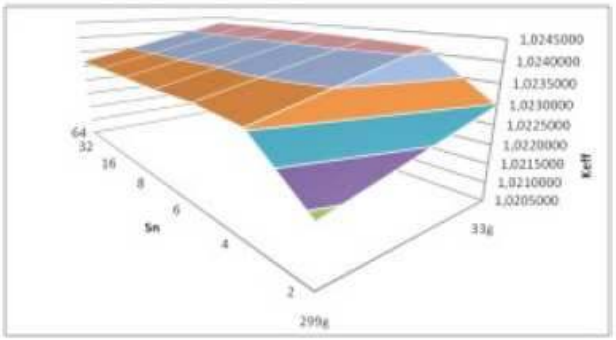




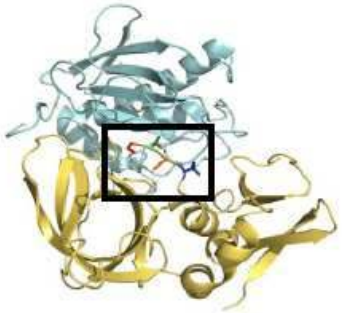


- **Détermination d'une solution de référence – Minimisation des incertitudes**
  - Résolution de l'équation du transport par une méthode Sn (solveur MINARET)
  - Ordre de méthode de S2 à S256 → utilisation jusqu'à **33.000** cœurs de calcul

- **Etude paramétrée – corrélation entre options de calcul et précision**
  - 48 cas de calcul sur **6.000** cœurs de calcul en 12h (6 mois en séquentiel)



Design of artificial enzymes



Natural Protein

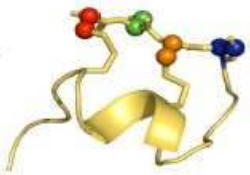
Functional Site
Geometric features

STAMPS

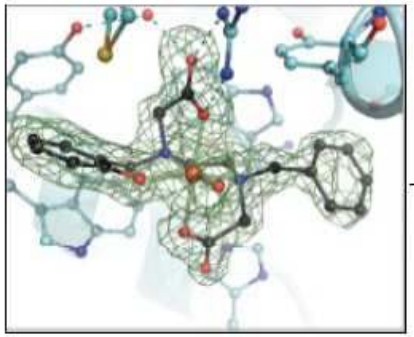
Recursive Search
at Atomic resolution
Including flexibility

RCSB PDB
PROTEIN DATA BANK

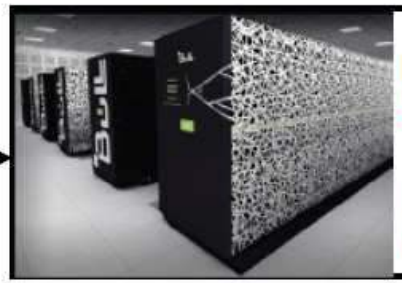
~56000 3D structures



Artificial Enzymes



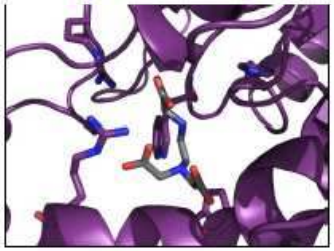
Cavazza et al.
Nature Chem (2010)



Number of nodes
4096

Runtime
18h30

Tera-100



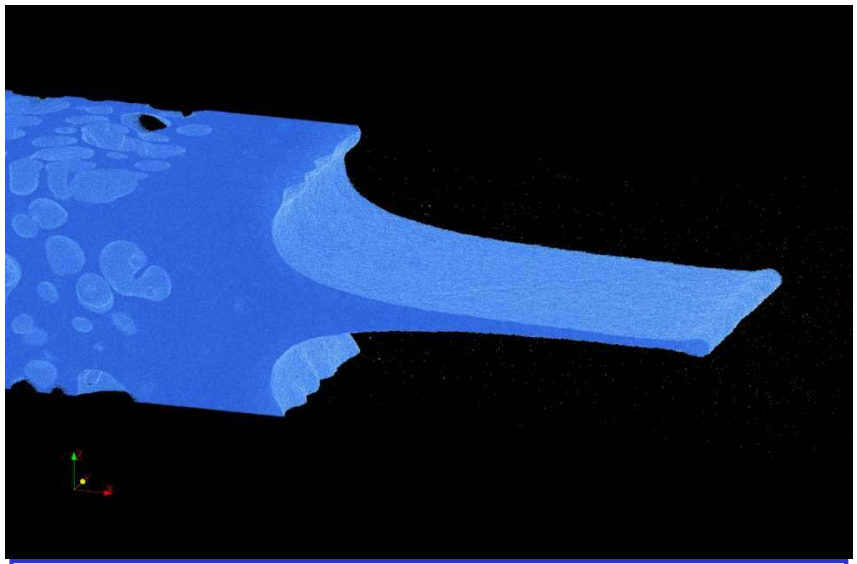
1222 Solutions identified

Currently analyzed by biochemists

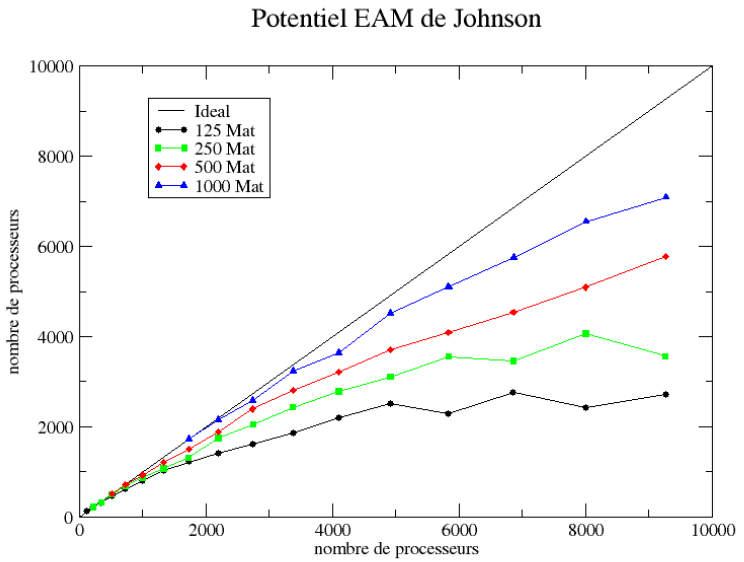
Applications : Biofuel, Green Chemistry…

Simulations de dynamique moléculaire TERA-100

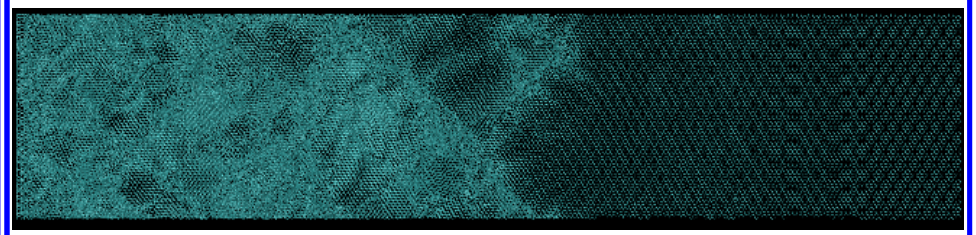
La dynamique moléculaire résout l'équation fondamentale de la dynamique pour un ensemble de *N* particules en interaction mutuelle.
Pourvu que *N* soit suffisamment grand, elle peut permettre de faire le lien entre le calcul quantique et la mécanique des milieux continus.



Ejection de matière lors de la réflexion d'un choc sur une surface libre. 125 millions d'atomes, 4000 cœurs, potentiel interatomique assez simple mais temps physique de simulation très long (pour la dynamique moléculaire) : de l'ordre de la nanoseconde.



Performances du code Stamp sur TERA-100 entre 250 millions et un milliard d'atomes, et jusqu'à 10 000 processeurs.



Plastification du diamant au passage d'une onde de choc. Relativement peu d'atomes (1,3 millions, 6400 cœurs) mais potentiel interatomique extrêmement complexe.

TERA-100: Co-designed by BULL and CEA/DAM

TERA-100 has been the first European computer to reach the Petaflops.

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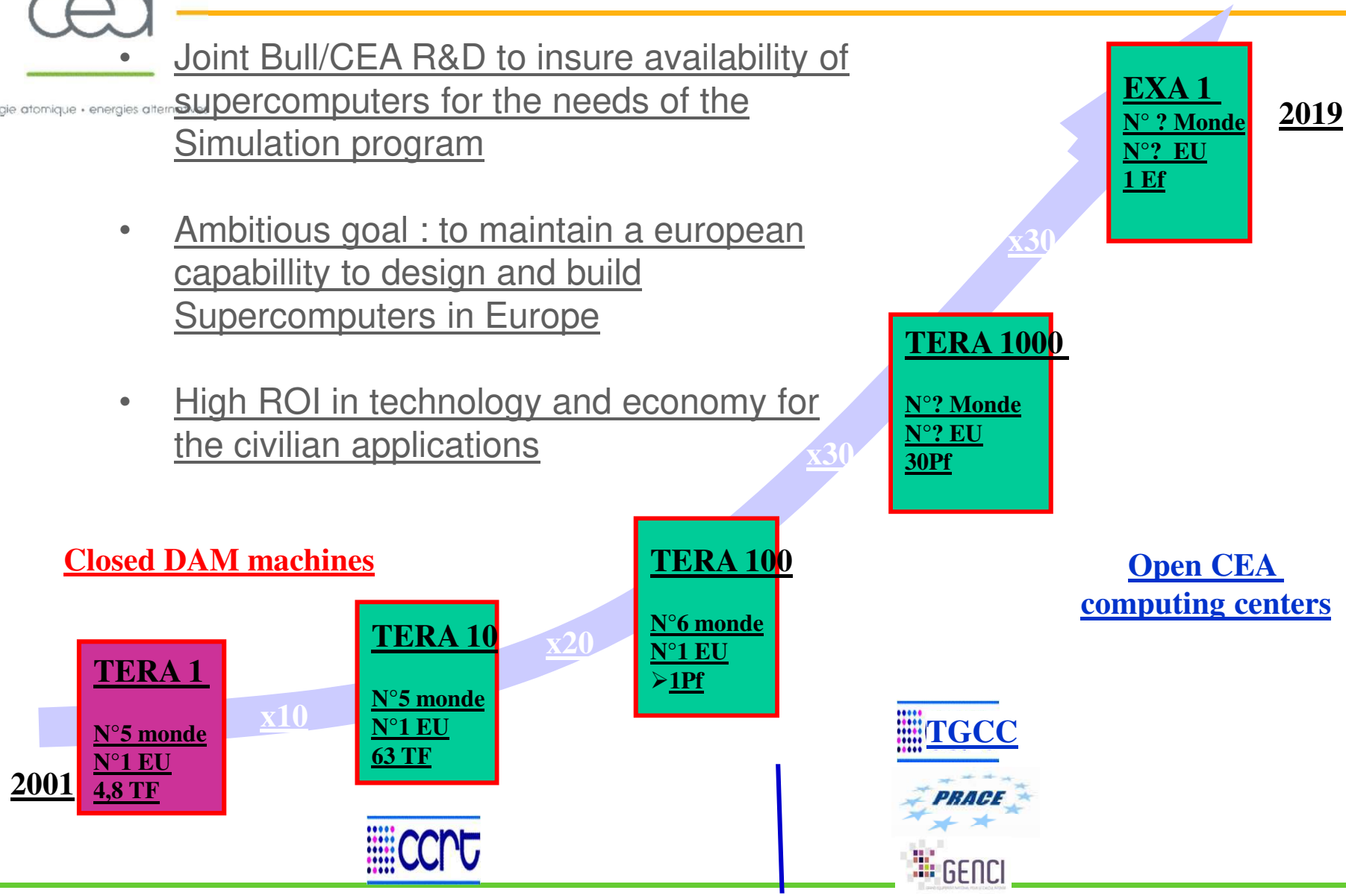
General Purpose production system with a tremendous effectiveness and reliability (1.05 Pflops, 83,7% of the peak performance in a 22 hours run)

Tera100 key figures :

- 220 racks in 650 m²
- 4370 servers interconnected with IB-QDR
- 17480 Intel X7560 processors
- 140 000 compute cores
- 300 TB of memory
- 500 GB/s I/O bandwidth
- System software mostly based on Open source developments (Linux, LUSTRE, SLURM..)

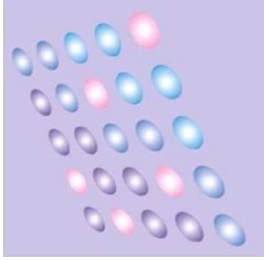
Supercomputers... A roadmap to Exaflops

- Joint Bull/CEA R&D to insure availability of supercomputers for the needs of the Simulation program
- Ambitious goal : to maintain a european capabillity to design and build Supercomputers in Europe
- High ROI in technology and economy for the civilian applications



CCRT
“Computing Centre for Research and Technology”

A partnership approach to gather academic research and industrials high end simulation in the same computing centre



Computing Center for Research and Technology

- A successful business model since 2003
- CCRT major goals
  - Meet CEA & partners simulation needs for research
  - Synergy between research organizations, universities and industry
    - Promoting exchanges and scientific collaborations between partners
    - Usages of HPC, code scaling and optimization
    - Centralized application support, workshops…
- Industrial partners
  - Multi-year agreements for a “share” based on total cost of ownership (sharing risk and opportunities)

CCRT Partnership Overview (2011)

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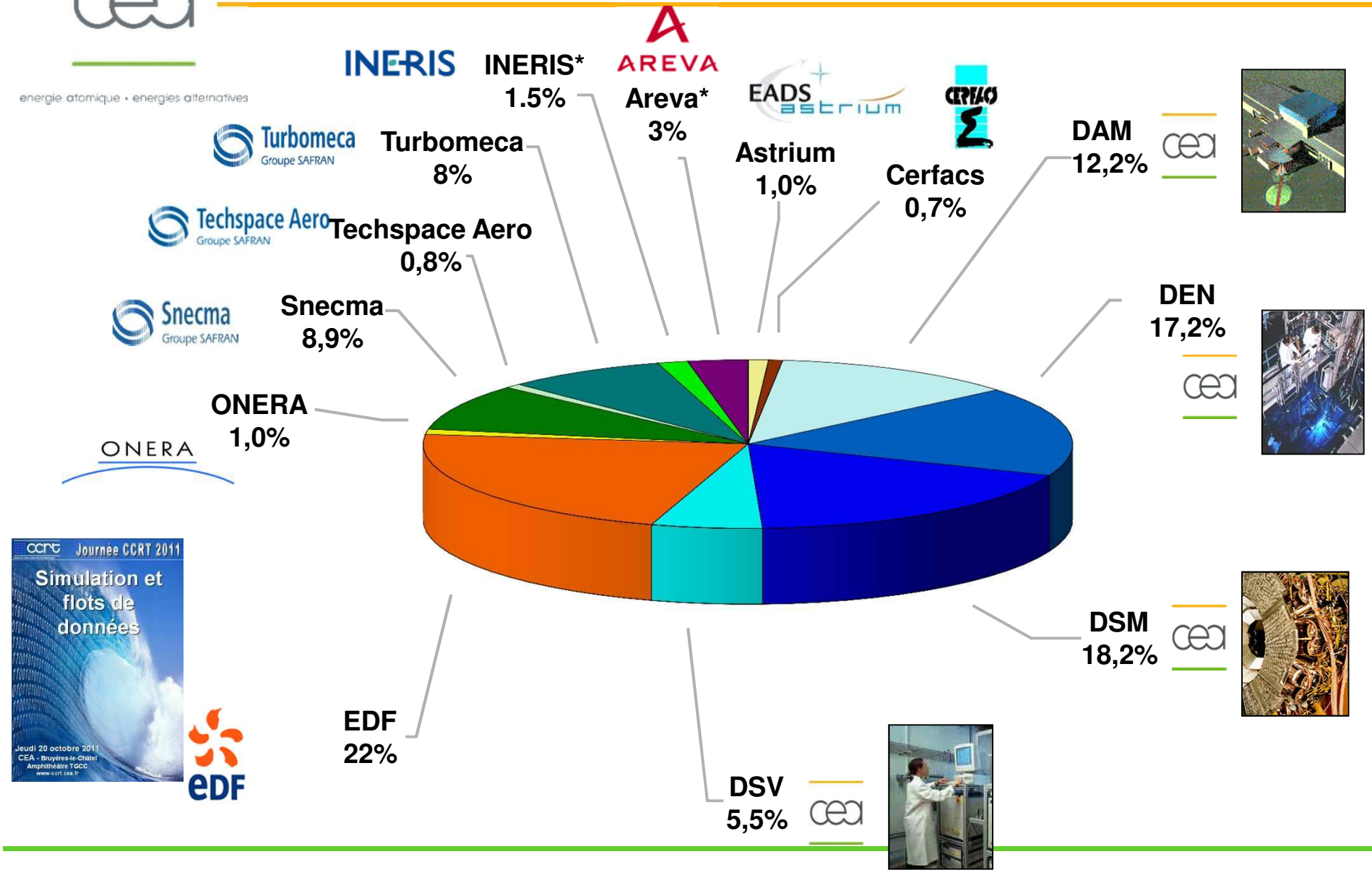

Current CCRT Architecture (~200 Tflops)

energie atomique

BULL Itanium Cluster

47.7 Tflops
Mémoire 23.2 To
Disques 420 To

6 * 10 Gb/s

NEC Vector system

SX8	SX9 GENCI
8 nodes	3 nodes
2 Tflops	4.8 Tflops
0.9 To	3 To
40 TB of Disk	

8 * 1Gb/s

Extension CCRT-2010 40 Tflops

Hybride (CPU/GPU) Bull Cluster

1 092 nœuds Bull **8736** Intel/Nehalem cores **3 GB/core** **103 TFlops** GENCI	**48serveurs Tesla S1070** **46 080** NVIDIA cores **4 GB/GPU** **192 Tflops-SP**

500 TB of disk

8 * 10 Gb/s

8 * 10 Gb/s

HP Post-processing Cluster

38 graphic nodes
3.2 TB of memory, 100 TB of disk

Backbone Ethernet 10Gb/s

2 Gb/s

Users

NFS Server

SGI Altix 450
DMF

Level 1:
1 Po of DDN Sata disk

Level 2:
SUN-SL8500 (9940 & T10000 tapes)

Storage System

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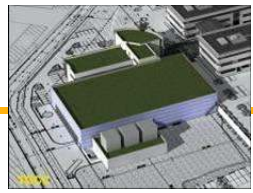

TGCC

"Très Grand Centre de calcul du CEA"

A completely new computing centre
built by CEA to host the French contribution
to the PRACE Research Infrastructure
and other high end HPC resources

PRACE

GENCI
GRAND EQUIPEMENT NATIONAL DE CALCUL INTENSIF

TGCC Overview


Designed to host :

- 2nd system of the PRACE Research Infrastructure (European –Tier0)
- 3rd generation of the CCRT (French - Tier1)
- High speed network node (10+ GIGE links)

Main characteristics of the infrastructure

- New power line 225 kV / 60 MW
- Initially configured for ~12 MW (7.5 MW of IT equipments)
- 2600 m² machine rooms floor space
- Conference room for 200 people
- Operated by CEA/DAM-Ile-de-France site teams

Très Grand Centre de Calcul du CEA « in one glance »

The European strategy for HPC

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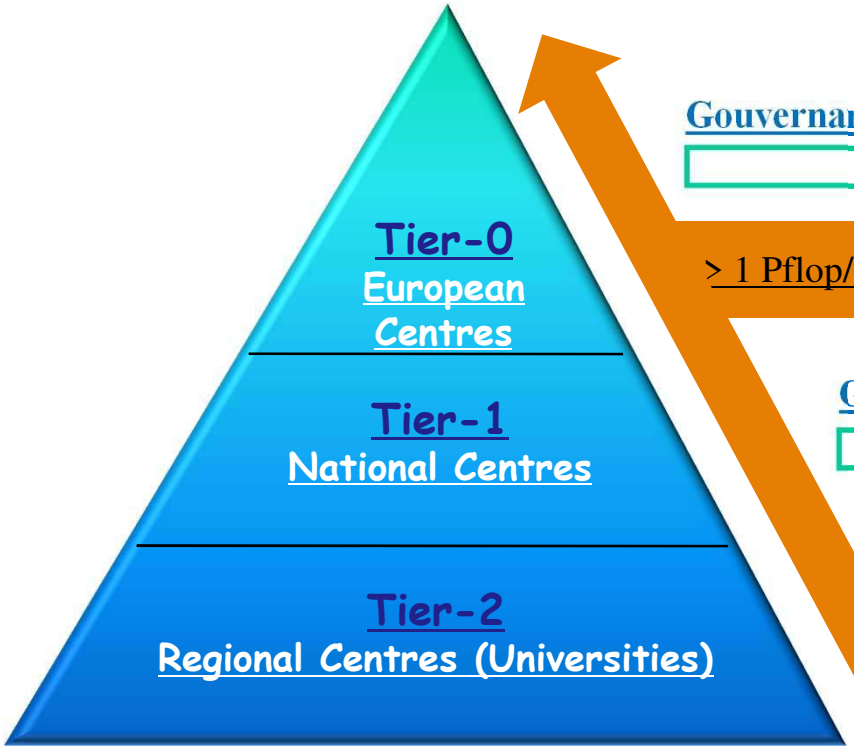


PRACE

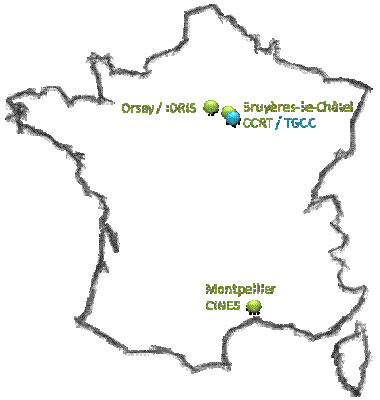
21 pays membres dont la France représentée par GENCI

Gouvernance européenne

> 1 Pflop/s

GENCI

Gouvernance nationale



< 50 Tflop/s

Gouvernances régionales

Equip@meso

GENCI

PRACE supercomputers

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➔ 2012: approx. 14,6 PF Peak Performance

GSC@Juelich
JUGENE : IBM BG/P 1 PF

GENCI@TGCC
CURIE : BULL Bullx, 2 PF

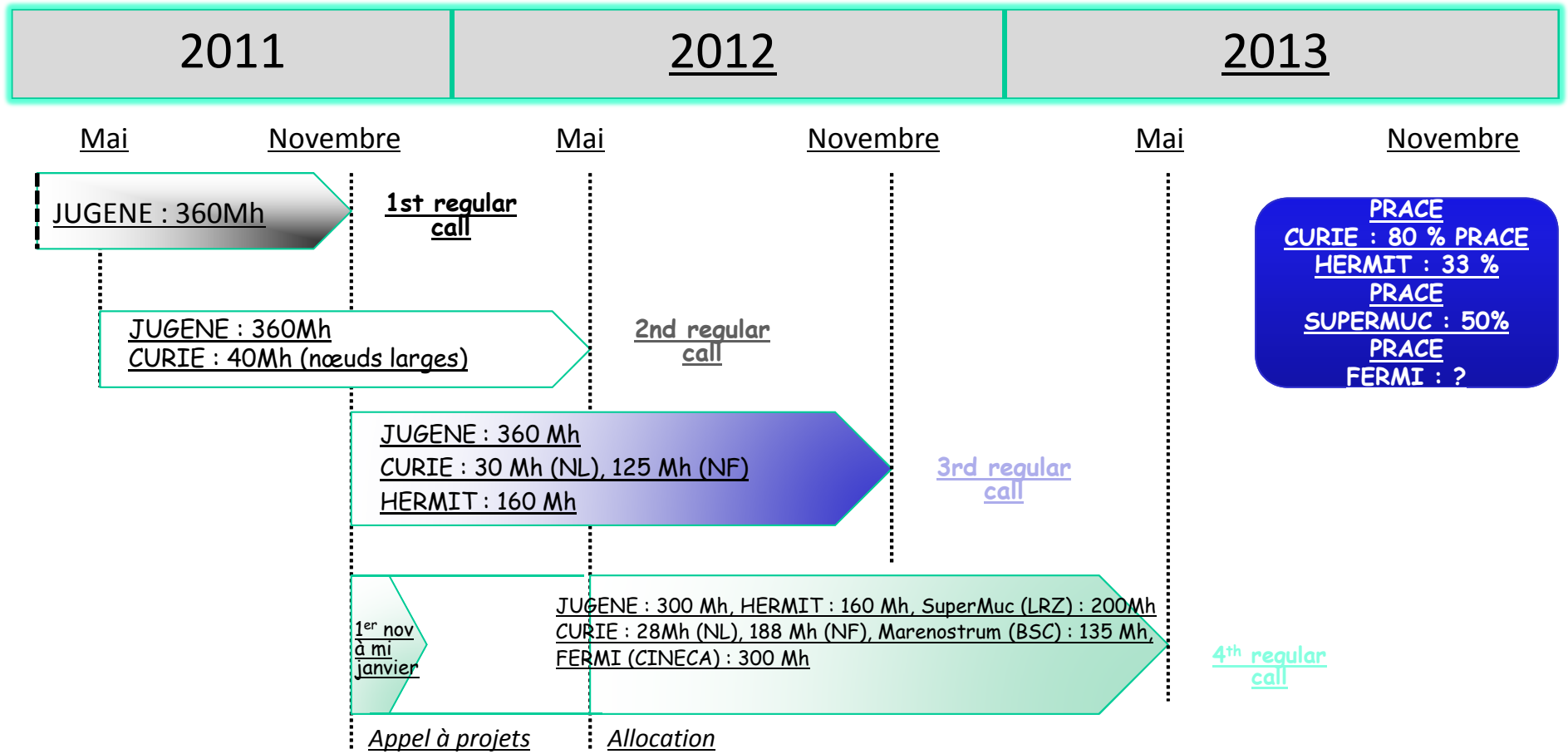
GSC@Juelich & CINECA
IBM BG/Q systems (Fermi)

GSC@HLRS
Hermit : Cray XE6, 1 PF

GSC@LRZ
SuperMUC : IBM iDataplex, 3 PF

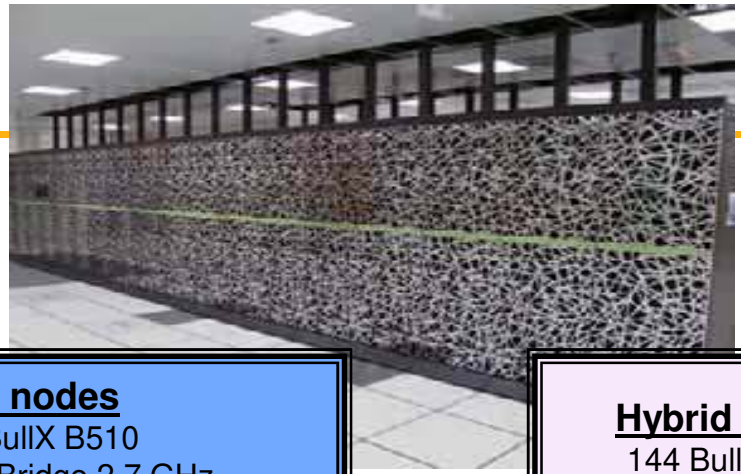
BSC
IBM

PRACE : calls in progress



Curie: The BULL Tier0 System

Curie configuration



Fat nodes
360 BullX S6010
Intel NH EX 2,26 GHz
11520 cœurs
32 =>128 core/node
128 GB => 512 GB/node
4 GB/core
105 TFlops

Thin nodes
5040 BullX B510
Intel Sandy Bridge 2,7 GHz
80 640 cœurs
16 core/node
4 GB/core
1 740 TFlops

Hybrid nodes
144 Bullx B505
288 Nvidia M2090

192 + 12 TFlops

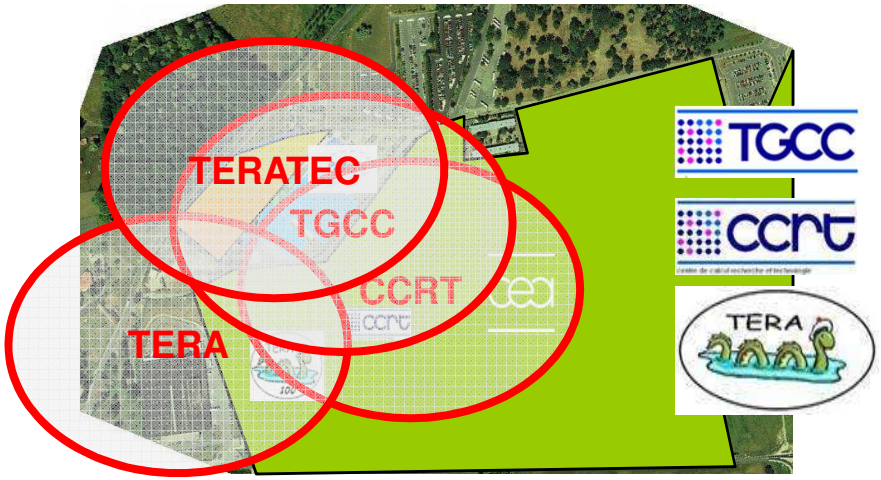
Interconnect Infiniband QDR

5 Po - 150 GB/s

Lustre file system

CEA Supercomputing Complex Summary

A single operator mutualizing expertise developed at CEA/DAM
A rich ecosystem connected from regional to worldwide scale
Collaborations with academics and industry ranging
- from design of HPC system and their environment (I/O, storage..)
- to applications and usages
- through system and management software, algorithms and middleware



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