



FP7 Support Action - European Exascale Software Initiative
DG Information Society and the unit e-Infrastructures



European Exascale Software Initiative

EESI2

Towards exascale roadmap implementation

WP3.1 - Industrial & Engineering Applications

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Key Objectives



- Investigate on key application breakthroughs and quantify their societal, environmental and economical impacts
- Perform a gap analysis between current situation and Exascale targets
- Evaluate the R&D activity performed by scientific and industrial communities, especially in applications redesign and development of multiscale/multiphysics frameworks;
- Foster the structuration of scientific communities at the European level and assess the rise of Co Design Centers



- **ONLY Few heros** apps scalable to Exascale so need :
 - support both Capability and Capacity simulations
 - rethink/rewrite applications and incorporate legacy apps
- Multi disciplinary optimization (UQ, ...) using **farming mode**
- **Multi-scale / Multi-Physics** simulations
 - **Coupling** tools for multi-physics and multi-components simulations on HPC systems: Proposal from CERFACS strongly supported by Safran, Onera, TOTAL, Inria, Eu DEEP Project, ENES, ...
 - Code coupling and **automatic/adaptive mesh generation** tools as mandatory R&D actions to be incorporated into future H2020 WP
- **Data Management and BigData**
 - simplify the end-to-end science workflows, improve massive data management, bridge together data and compute specialists
 - New skills in both extreme-scale and data-intensive computing
- **Train and retain skills**

WG3.1- Industrial applications

10 experts with representatives from 5 companies & ISV



EESI applications roadmaps

- In oil & gas, energy, aeronautics, automotive, ...
- Revisited but still valid with a one year delay

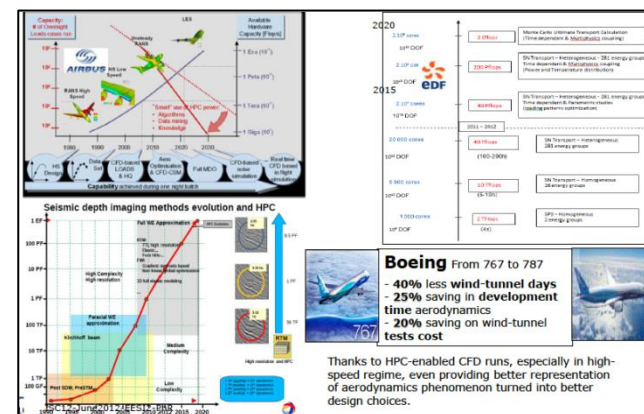
Deployment/use of big HPC facilities by industry

- Internally : TOTAL, BP, ENI, EDF, Airbus, ...
- Remotely: using large-scale research infrastructures like PRACE and Incite

→ Strong R&D needs on meshers, solvers, resilience, reproducibility, comm avoiding, ...

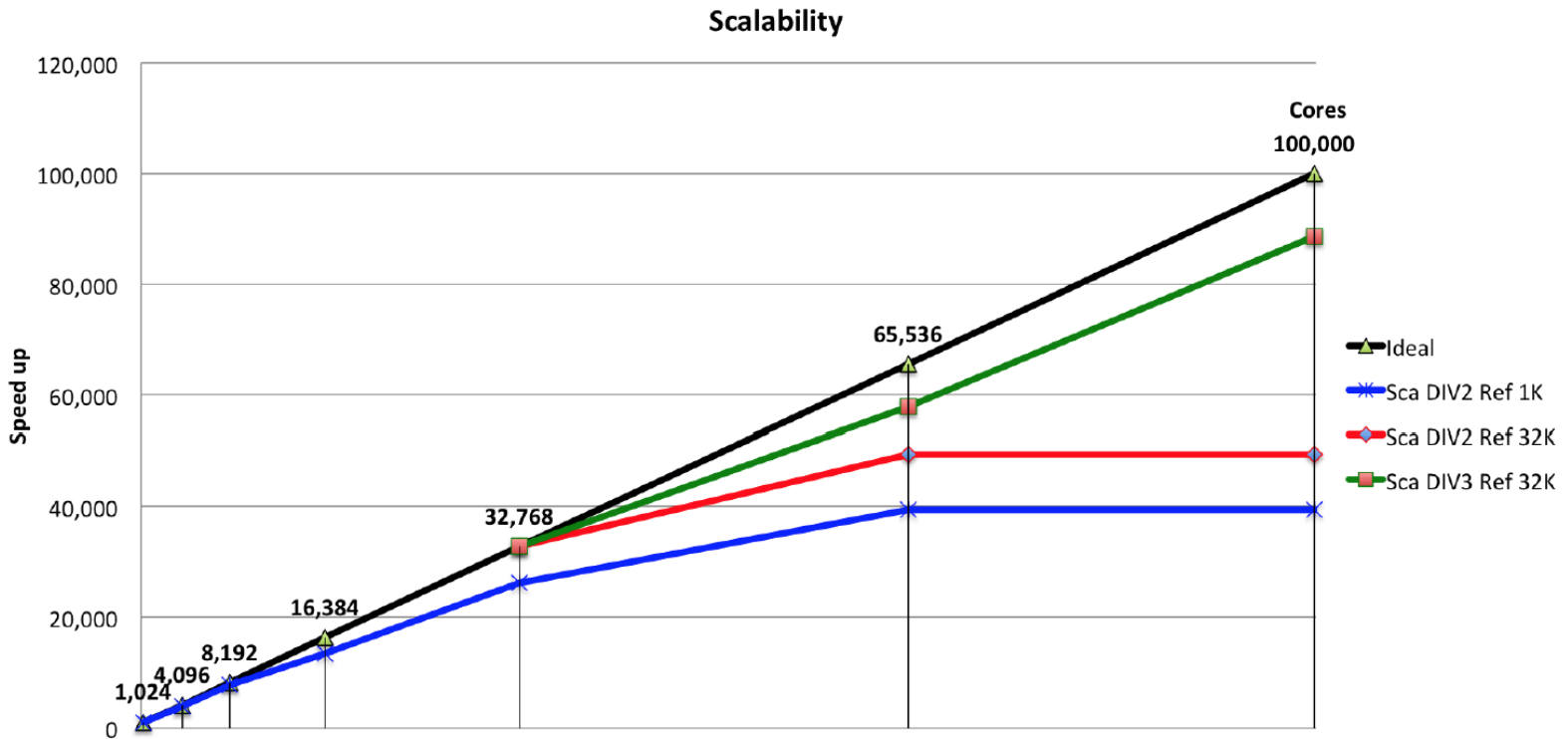
Some new breakthroughs reported

- Scalability ALYA to up to 100 000 cores of BlueWaters (NCSA)
 - Scalability proven on Cray system using test case from incompressible flow in human respiratory system, low mach combustion in kiln furnace and coupled electro-mechanical problem in a heart.



WG3.1- Industrial applications

- 10 experts with representatives from 5 companies & ISV
- EESI applications roadmaps
 - In oil & gas, energy, aeronautics, automotive, ...



Numerical Simulation & HPC for Safety

Explosions



CERFACS and TOTAL using INCITE calls

LES simulations for studying accidental gas explosions in buildings

Comparaions with experimental databases and real testings

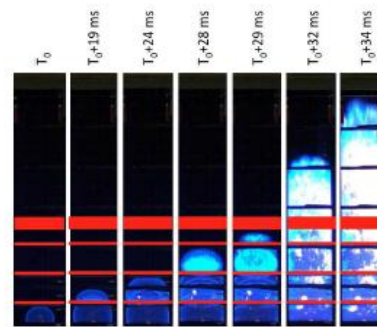
DNS **86 millions core hours on Mira (Argone Labs) using AVBP**
scalable up to 150000 cores.

Understanding for safety

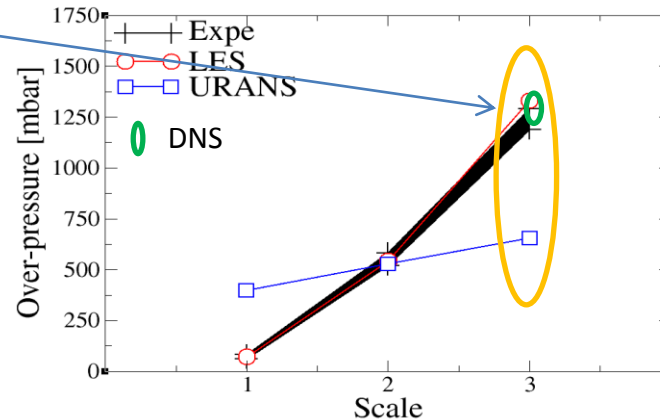
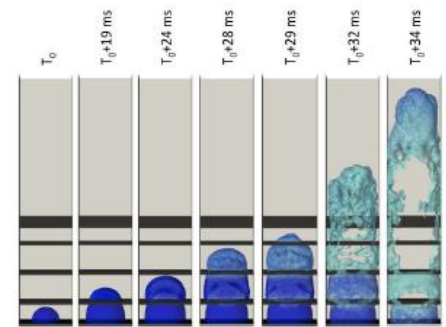
Integration in “on using” codes of danger studies (large economical issue)

Ref: *Large Eddy Simulation of Vented Deflagration*
Quillatre P; Vermorel O; Poinso T; Ricoux Ph
Industrial & Engineering Chemistry Research ,
Feb.2013
Pierre Quillatre, PhD Thesis, May 2014

Exper.



LES Simulations



**LES
validated
by DNS
and Exper.**

What about simulations for industrial applications?



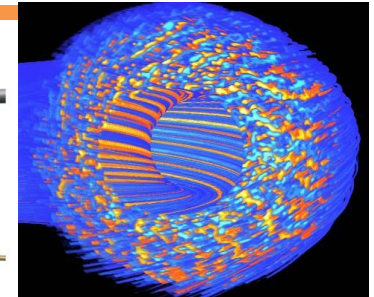
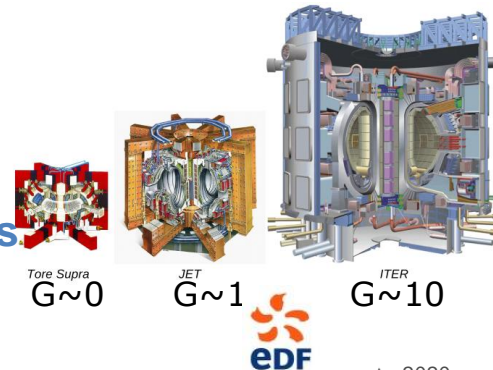
□ Nuclear reaction / energy

■ Nuclear Weapons

- Stop of real experimental tests thanks to numerical simulations

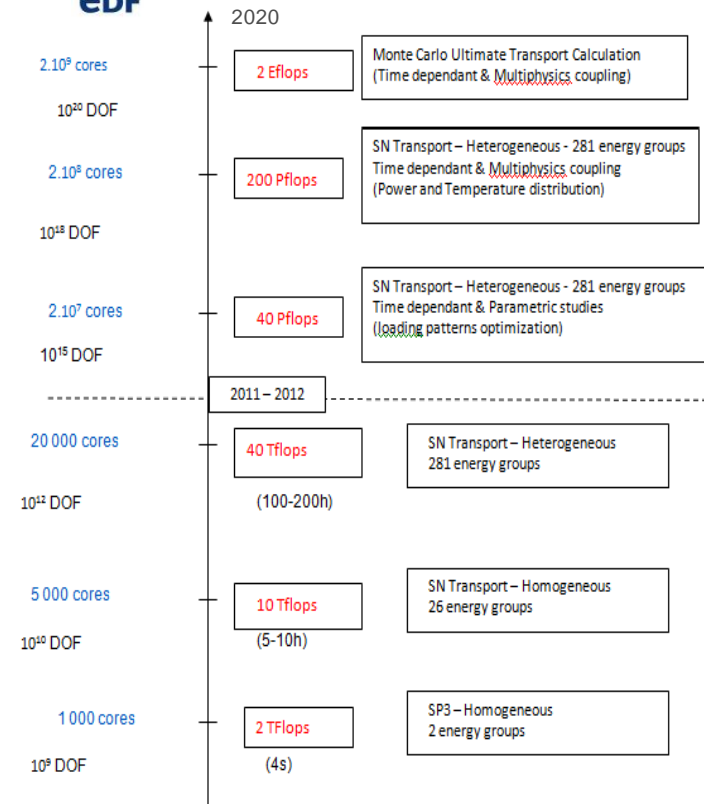
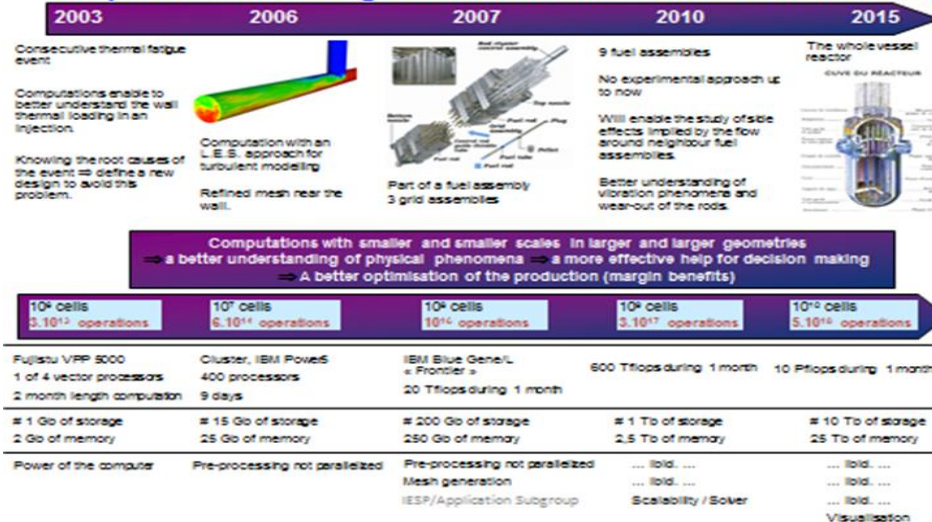
■ Nuclear plants

- Safety / Control



American Nuclear Plant vision

Computational Challenges and Needs for Academic and Industrial



TOTAL



767

Wing prototypes:
77

Boeing From 767 to 787

- **40% less** wind-tunnel days
- **25% saving** in aerodynamics development time
- **20% saving on wind-tunnel tests cost**

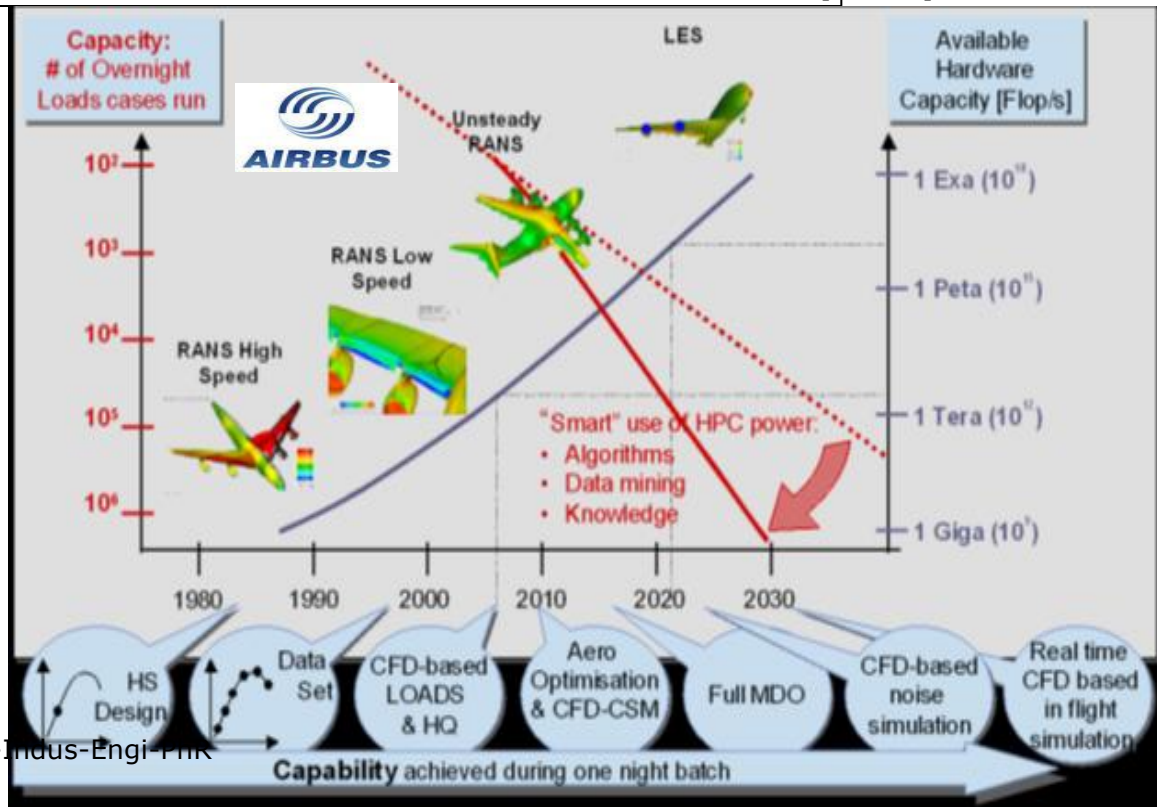
Thanks to HPC-enabled CFD runs, especially in high-speed regime, even providing better representation of aerodynamics phenomenon turned into better design choices.

But ... Digital Aircraft will require at least 1 ZetaFlop !



787

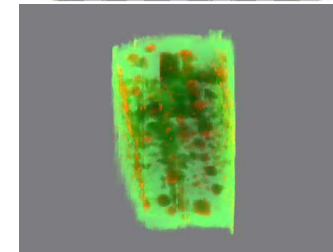
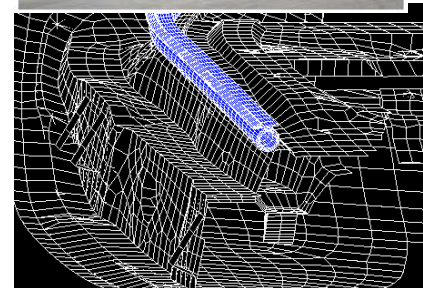
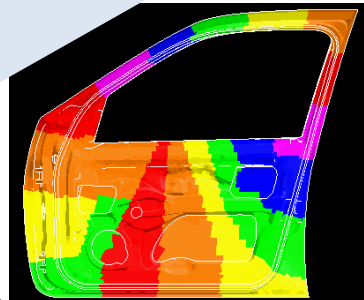
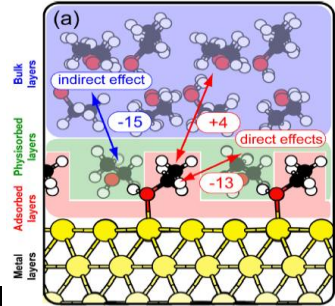
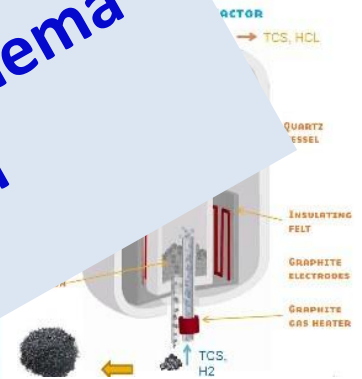
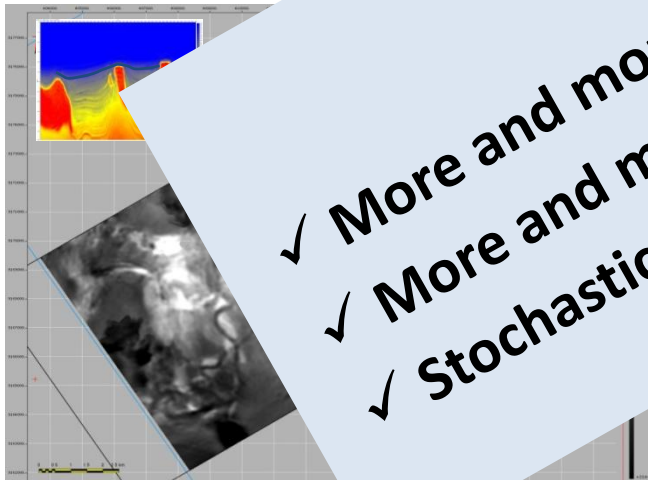
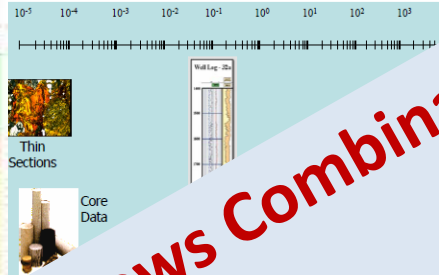
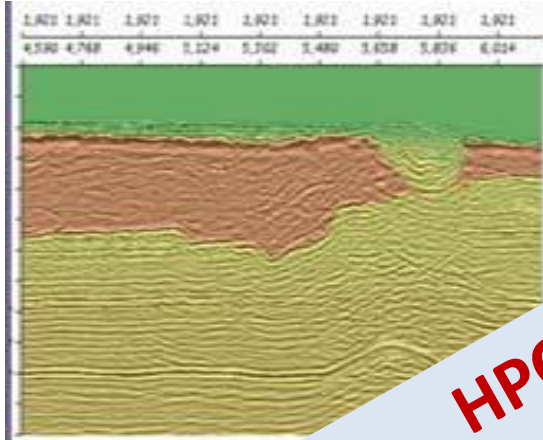
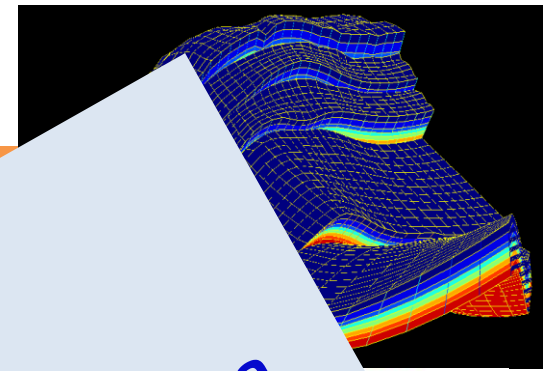
Wing prototypes: **11** (2008)
→ **7** by new methods and HPC (2015)



TOTAL: Numerical Simulation and HPC

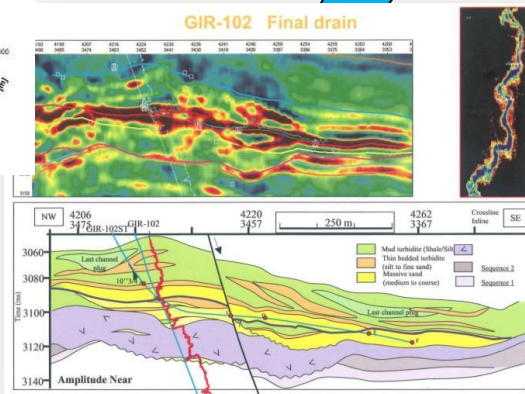
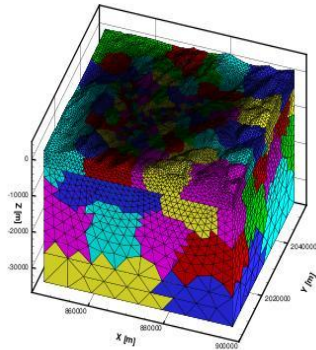
HPC allows Combination of

- ✓ More and more accurate physic modeling
- ✓ More and more performing numerical schema
- ✓ Stochastic methods, Robust optimization



DEPTH IMAGING: 3 Fundamental Steps

**Numerical analyst
Numerical Methods**



**Pangea
2,3 PF
>100
000
Cores**

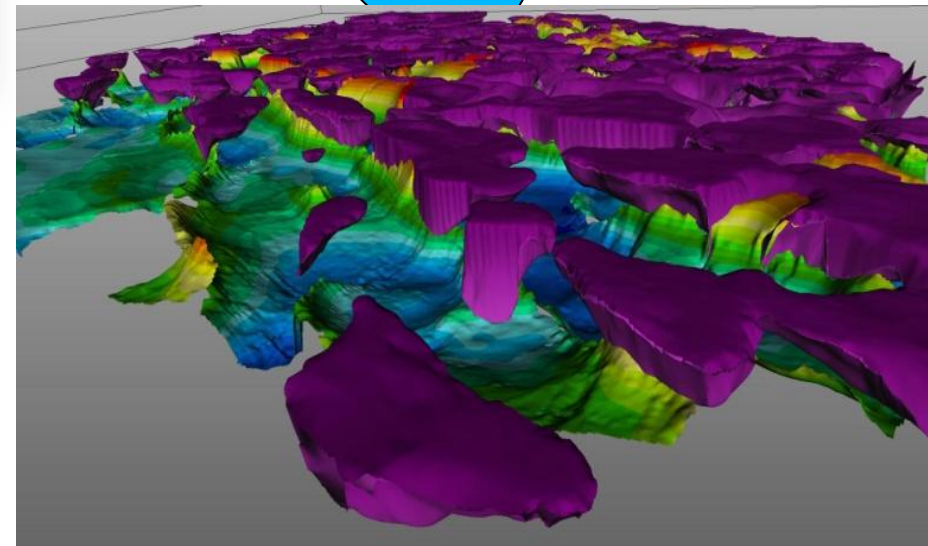
**HPC Computing
HPC implementation**



**Geo-physics
Maths for Physic Modeling**

$$\frac{\partial q_p}{\partial t} + A_{pq} \frac{\partial q_q}{\partial x} + B_{pq} \frac{\partial q_q}{\partial y} + C_{pq} \frac{\partial q_q}{\partial z} = E_{pq} q_q + s_p,$$

**Embarrassingly Parallel
approximation**

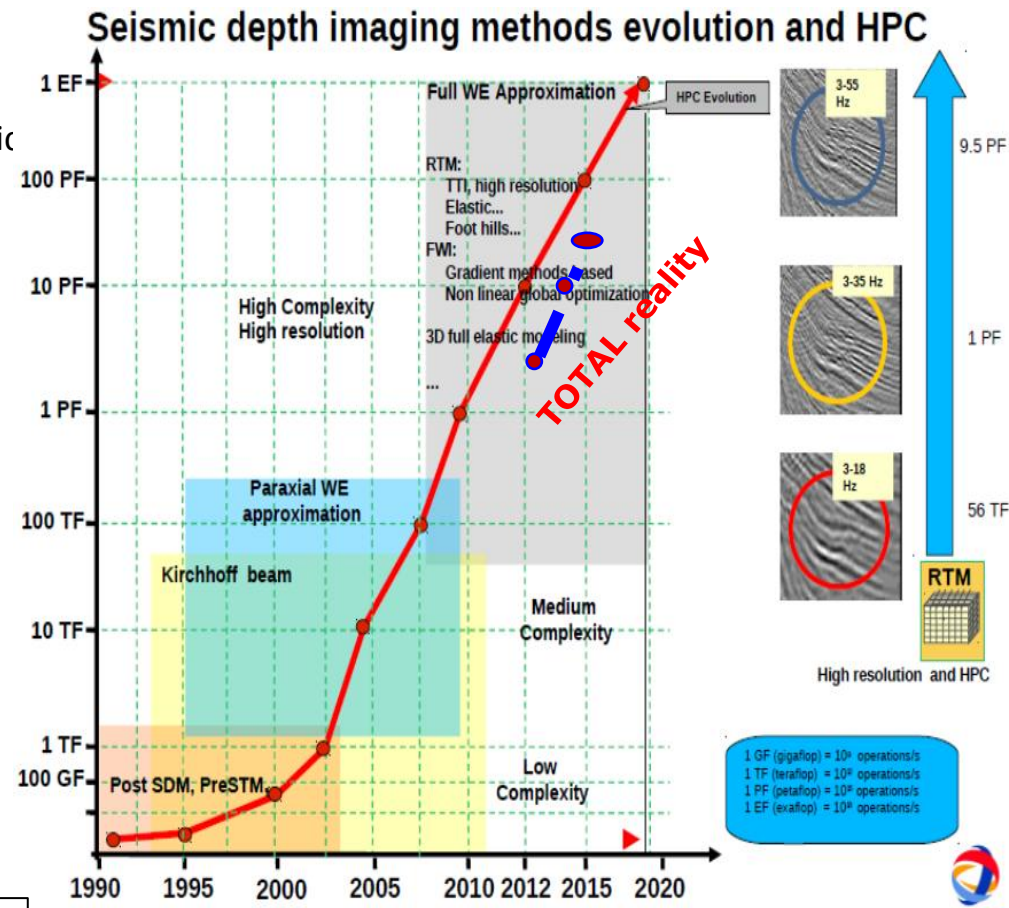


HPC Opportunities in TOTAL: Next steps in Depth Imaging



Combinaison of Physics, Numerics, Uncertainties (UQ)

- ▶ Involving maths modeling for a more accurate approximation of the physics of propagation:
 - More realistic: elastic, visco-elastic, poro-visco elastic
 - Hybrid representations of waves equation
 - Others physics: EM, micro gravimetric, ...
- ▶ More and more adapted numerics:
 - Sub domains, automatic mesh generation
 - Finite Elements, ... explicit or implicit ... Massively parallel solvers, embedded solvers, .
 - Performing approximations
- ▶ **Uncertainties, Optimization**
 - Stochastic Methods thank to HPC.
 - Robust optimization basis of inverse problem
- **Computer Science**
 - Load Balancing
 - Programming,
 - Resilience, ...



Integrated Approach of Oil System :
 interaction geology – geophysic :
 foot hills, non conventional reservoirs, ...

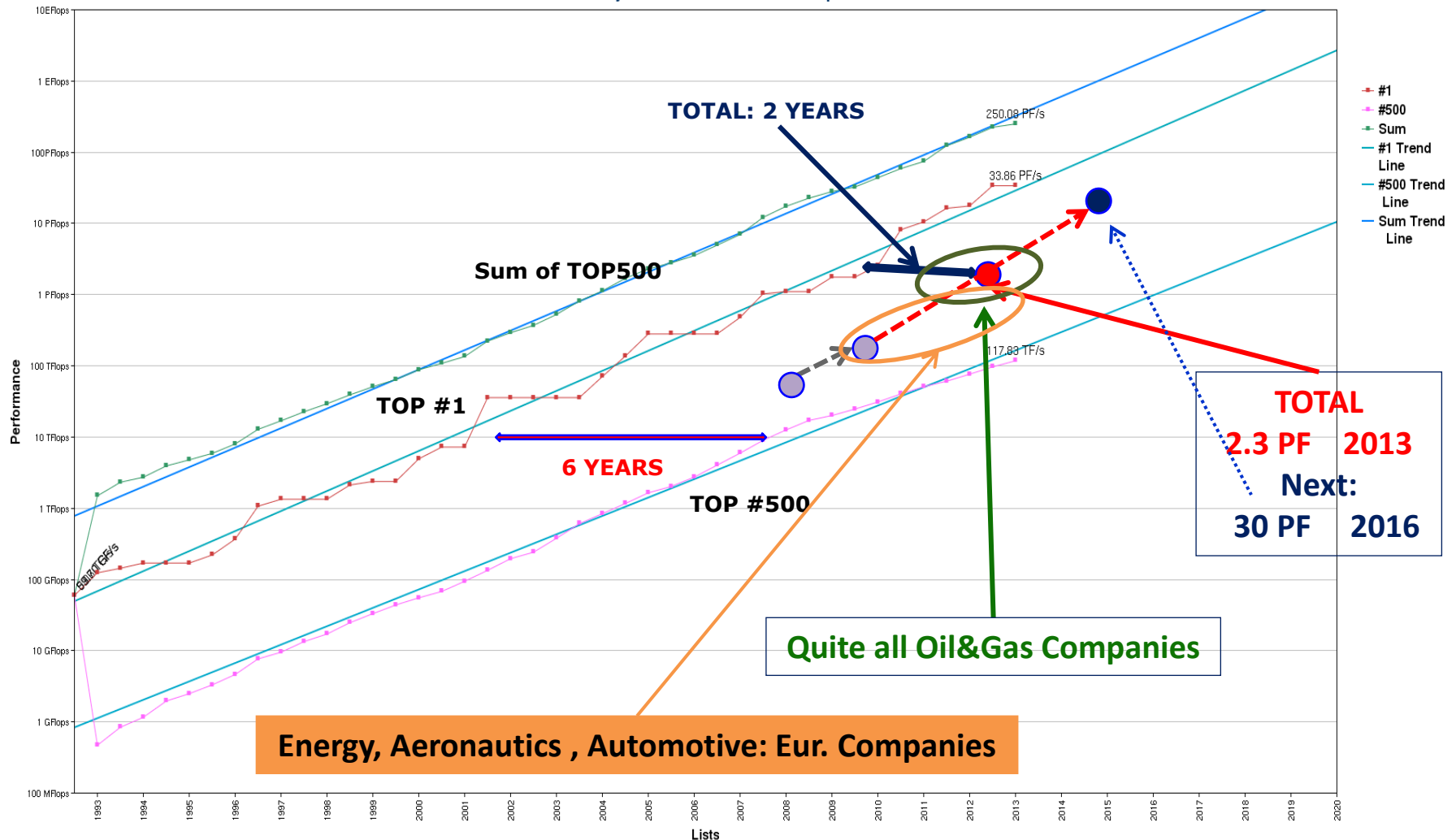
**Same Roadmap in BP ,
 Chevron**

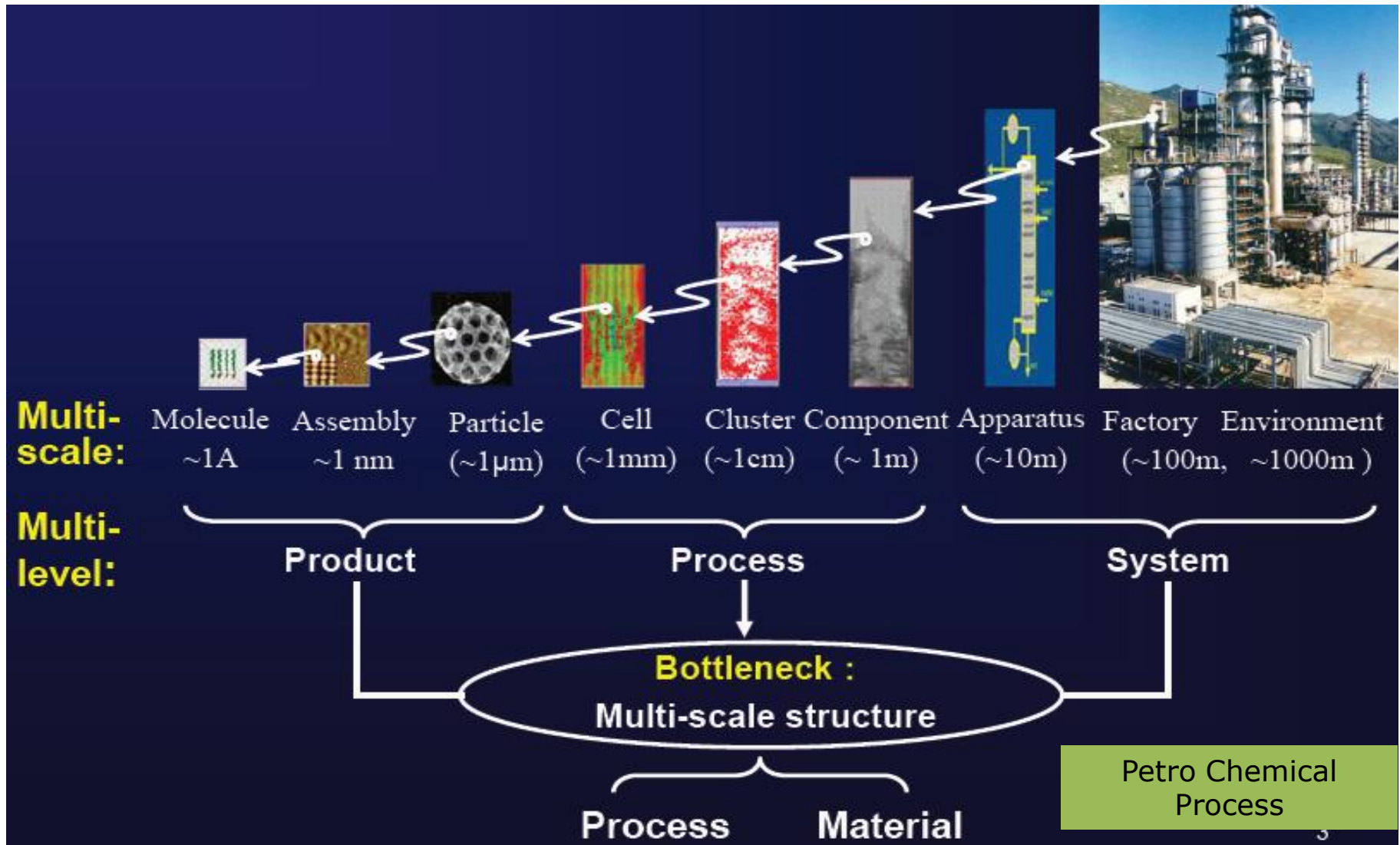
Absolute Need of multi skills

Industries in Top500: Insight into HPC Performance



Projected Performance Development **November 2014**





What about simulations for industrial applications?

Automotive

Crash Test

- 100 parameters on optimal numerical “experimental” design
- 2 Mhcores on HPC simulations and UQ (Uncertainties)
- 2 years of experimental crash tests saving
- Safety / Competitiveness



Courtesy of Renault

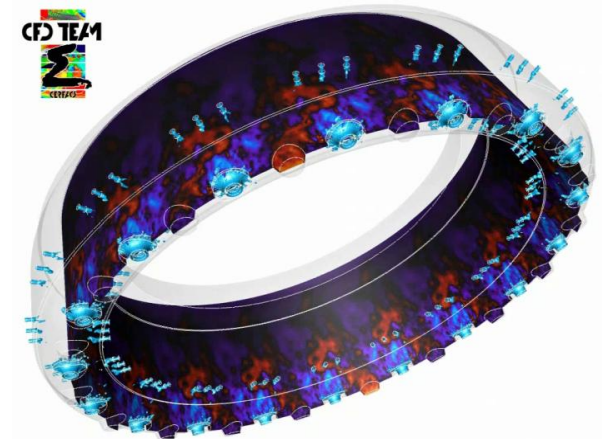
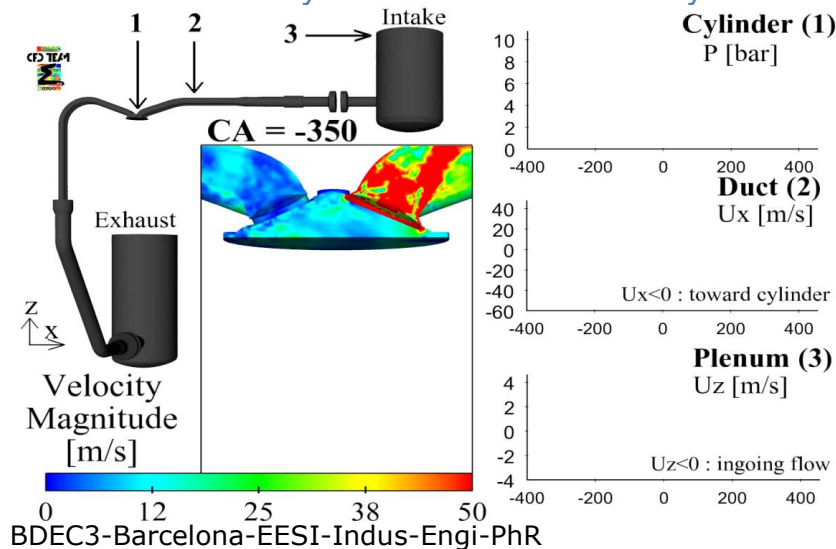
Engine combustion, Turbulent Combustion

Aerospace, Gas Turbine, Helicopter, Oil equipment

- Efficiency / **Safety** / Competitiveness

Automotive

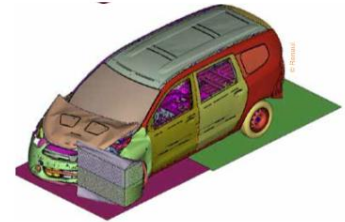
- Efficiency / Environment / Life Cycle



Validation by experiments thanks to High Speed Imaging, Particle Image Velocimetry (HS PIV)

PRACE Project : FMOC awarded by 42M core hours on CURIE@GENCI

- World premiere for the size / number of core for a PAM CRASH model :
 - this kind of model is usable on HPC ?
 - lower scattering of the result ?
- Optimization study with a very big model :
 - More than 200 different parameters on 20M+ elements meshes on 2048 cores (size of an element = 5mm)
 - it's work : HPC allows to reduce duration of this phase.
 - Ratio between accuracy of 1 run and number of run available id better with big model
- Industrial impact for Renault :
 - To assess new large scale optimisation methodologies
 - To anticipate future EuroNCAP 6 safety regulations
 - To reduce CO₂ emissions by introducing new materials into a design process



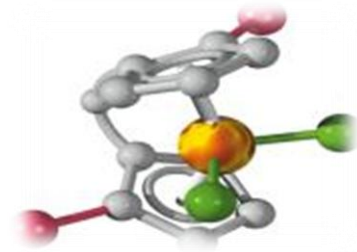
Crash Model Reduction : useful for optimization ?



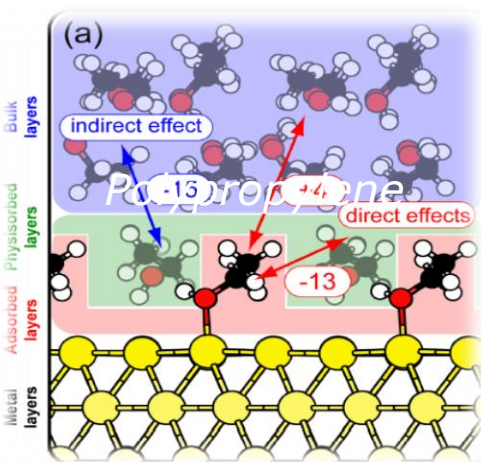
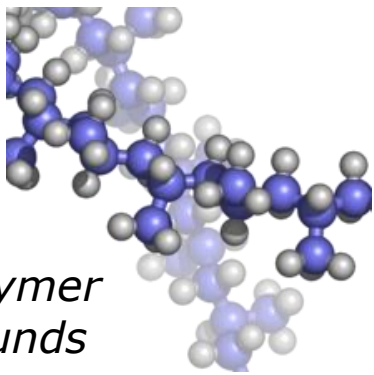
- Crash simulations are more and more costly
 - Model size rise quicker than HPC
 - Near-interactive crash simulation is just a dream
 - ➔ elapsed time do not decrease
 - Future multi physics optimization studies will be bigger and combinatorial ones, complexity increase quicker than HPC
 - Crash simulation needs commercial software
 - ➔ license price can be a barrier to the use of optimization
-
- ➔ Model reduction and HPC are not competing but complementary
 - ➔ Model reduction combined with HPC will allow to exploit new immersive 3D visualization tools for interactive calculations and optimization
 - ➔ Example : 20 hours elapsed time reduced to few seconds with 10% loss on accuracy (enough to optimize).

Molecular Simulation is now a key technology

Metallocene catalysts

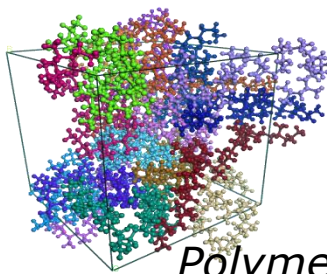
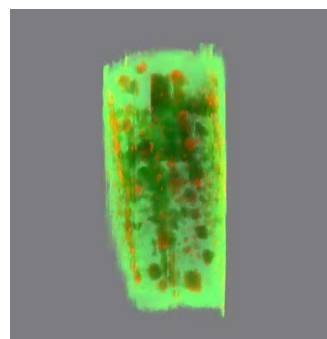


EOR polymer Compounds



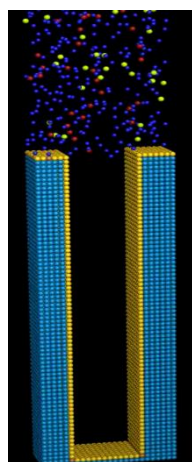
Adhesion

KMC simulations for flat copper surface



Polymer solubility

Heterogeneous catalysts (4 nm Cube)



Uteat

- Multiscale/multiphysics + big data → UUVQ
 - Multiple sources of uncertainties due to
 - lack of knowledge on a physical parameter (epistemic uncertainty)
 - parameter with a random nature (aleatory uncertainty)
 - uncertainty related to the model (model error, too simplified model)
 - uncertainty related to the numerical errors (numerical errors of the model, to the input and output data, ...).
 - Understanding uncertainties essential for acceptance of numerical simulation for decision making
 - Strong impact in industry (automotive, oil & gas, aeronautics, nuclear,...) and academia (climate)
 - EU well positionned in UUVQ : Uranie and OpenTurns
- Toward an unified UUVQ env. for Exascale
- Dev of ultrascaleable UUVQ tools (scheduling, optimisation, ...)
 - Embeeding UQ loops at the lowest levels of the simulation code
 - Use of surrogate models and reduced basis models

□ Coupler : a major software component

- Multiphysics simulations / legacy and new codes
- Crucial for industry (aeronautics, automotive, ...) and academia (climate, astrophysics, life sciences, ...)
- Coupling of 100k cores applications is a good driver for Exascale

□ Europe owns multiple coupler tools

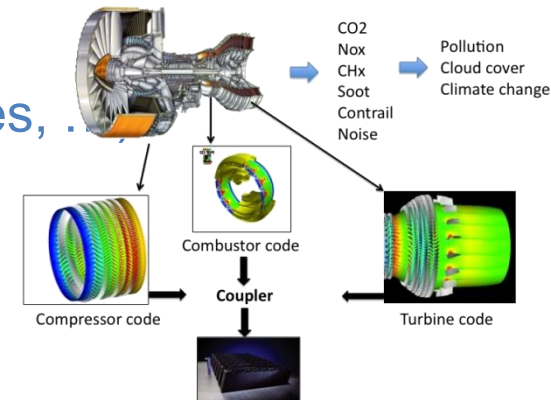
- OpenPALM, OASIS, MpCCI, ...

□ 2 approaches

- Direct coupling (multiple binaries) vs coupling via top-level interfaces (one unified binary)

□ But strong challenges to face for Exascale

- Standard coupling API
- memory footprint, use of asynchronous (reduced) communications, ...
- Interpolation methods, smart search algorithms,

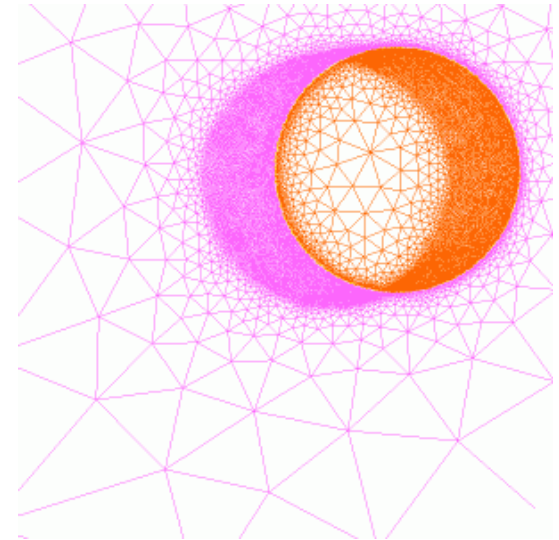


EESI2 recommendation on Mesh



Mesh Generation

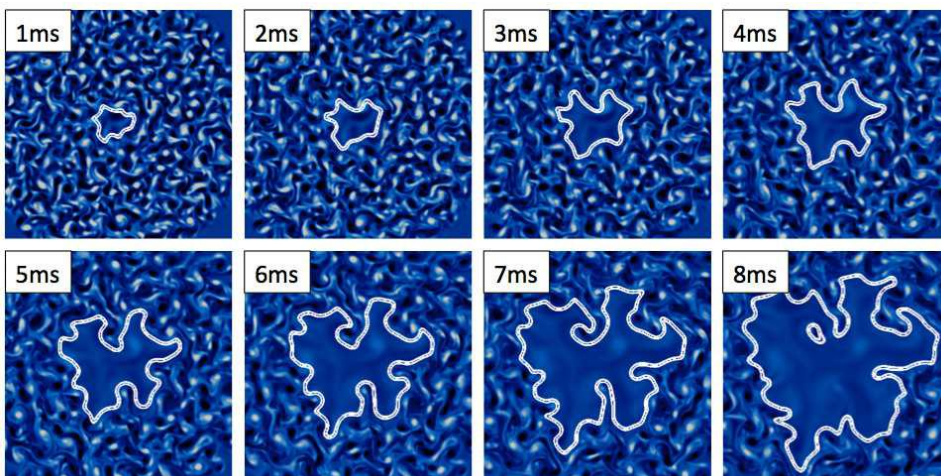
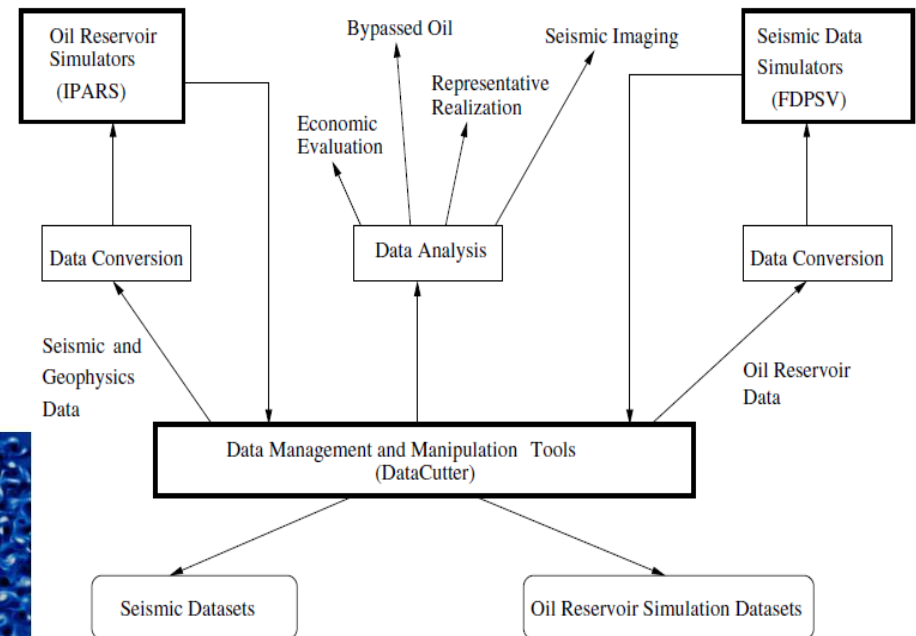
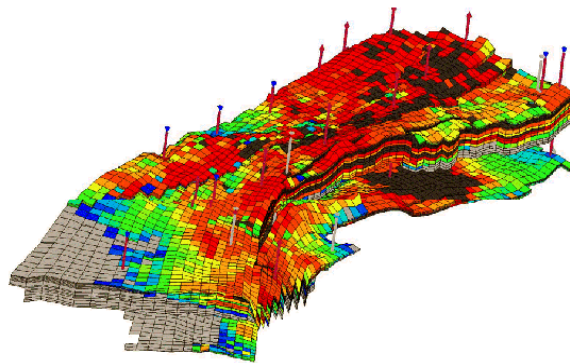
- Automatic, Adaptive, Intelligent
- From billions « regular » meshes ... to millions !



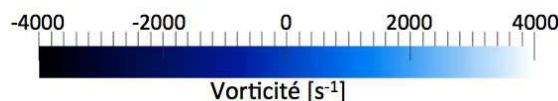
With numerical methods for solving differential equations such as
Discontinuous Galerkin: combining features of the finite element and the finite
volume framework

DG methods have a huge interest for electrodynamics, fluid mechanics and
plasma physics equations.

In Situ Extreme Data Processing in massively parallel numerical simulations: A necessary approach for Exascale (Cf Paper from EESI)



Turbulent combustion



Conclusions



IDC 2014 Study for EESI: **HPC must produce ROI**

There is the only way for Exascale!

Industrial applications are the key factors of potential Exascale viability

**-> Exascale applications must be efficient for ROI !
largely than they are today!**

So, need of R&D programs, need of innovation, disruptive methods on all scientific domains ...

Please Submit EU Calls on concrete R&D for Exascale

**Thank you for your attention and
... your future active contribution**

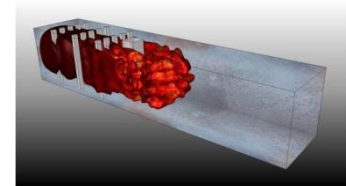
WG3.1- Industrial applications (2/5)

Some new breakthroughs reported (cont.)



■ CERFACS and TOTAL using INCITE calls

- LES simulations for studying accidental gas explosions in buildings
- Comparisons with experimental databases and real testings
- 86 millions core hours on Mira (Argonne Labs) using AVBP



■ Large scale Seismic risk management

- Politecnico di Milano and MunichRe on PRACE systems
- Based on improvement of DGSE (Discontinuous Galerkin Spectral Element)
- Multi-scale seismic wave propagation analyses using open-source spectral element computer code (SPEED), 40 M hours on Fermi (CINECA)

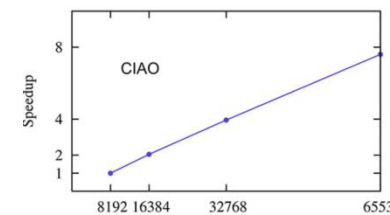
■ QUAntum Simulation of ultimate NanO-devices

- STMicroelectronics and CEA with 6.5 Mh on PRACE (CURIE)
- Studying scattering of electrons by impurities, lattice vibrations, etc into next gen transistors of 16 nm



■ Influence of injector geometry in the primary atomisation process

- Improve the combustion by optimising spray models using the CIAO code (Nav. Stokes second order, semi-implicit finite difference code)
- RWTH Aachen University with 30Mh on PRACE (Marenostrum)



WG3.1- Industrial applications (3/5)

Some new initiatives reported



- Success of PRACE Open R&D access to industry
 - Close to 25 companies supported in less than 2 years
 - More than 300 millions core hours allocated to large companies and SMEs
- Development of the PRACE' SHAPE initiative towards HPC enabling of SMEs
- Launch of the VERIFI program @ ArgonneLabs (US) (Working with industry for addressing combustion challenges)
 - Virtual Engine Research Institute and Fuels Initiative
 - Experimental facilities + access to Mira (10 PF BG/Q) HPC and combustion experts
 - First scale out of CONVERGE CFD to >2000 cores
 - Cooperative Research and Development Agreement between Argonne and interested companies



WG3.1- Industrial applications (4/5)

WG3.1 plans for EESI second year activity (1/2)



- Launch a survey among ISV (and beyond) using the **NAFEMS network** (International Association of the Engineering Modelling, Analysis and Simulation Community)
 - Will provide alternative view of needs and challenges from the commercial software side
 - launched in June, results compiled in EESI2 2nd report
- Provide feedback on disruptive apps to WGx.5
 - Topic of the day : already some discussed ideas around meshless methods, rise of composite materials into automotive and aerospace (will change everything in crash modeling with multi-scale/physics simulations and big data)
- Enlarge apps assessment with Insurance/Finance ?
- Assess and support rise of industrial CoE
 - Call EINFRA-5-2015 – Centres of Excellence for computing applications - open until 14/01/2015 → 8 to 10 CoEs supported
 - combustion, turbulence as potential CoE ?



- Refine 1st EESI2 recommendations especially in
 - Assessment and proposal of mini applications
 - Work done on oil & gas (RTM) and combustion (YALES2)
→ Need to be improved with new mini apps this year
 - R&D on Big Data : smart data extraction / viz of pertinent structures on massive datasets from turbulent simulations
 - Large scale features extraction using selective high-order filters
 - Multi grid techniques for data visualization and processing
 - Interactive run time capabilities and on-the-fly visualization
→ Could fit to any turbulent problems : combustion, climate, cosmology, ...
- Make new recommendations
 - R&D on automatic mesh generation/adaptation on billions of cells meshes and parallel load balancing