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

Philippe Ricoux on behalf of

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Key Objectives

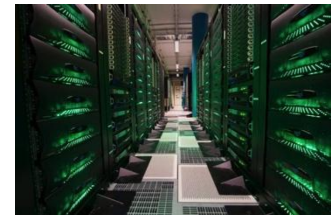
- Investigate on key application breakthroughs and quantify their societal, environmental and economical impacts
- Perform a gap analysis between current situation and Exascale targets
- Evaluate the R&D activity performed by scientific and industrial communities, especially in applications redesign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

General outcome of I&E Applications

- **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**

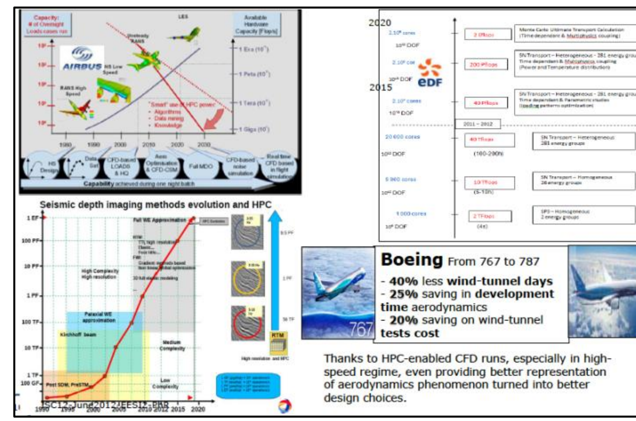
WG3.1- Industrial applications

- 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 furnance and coupled electro-mechanical problem in a heart.

WG3.1- Industrial applications

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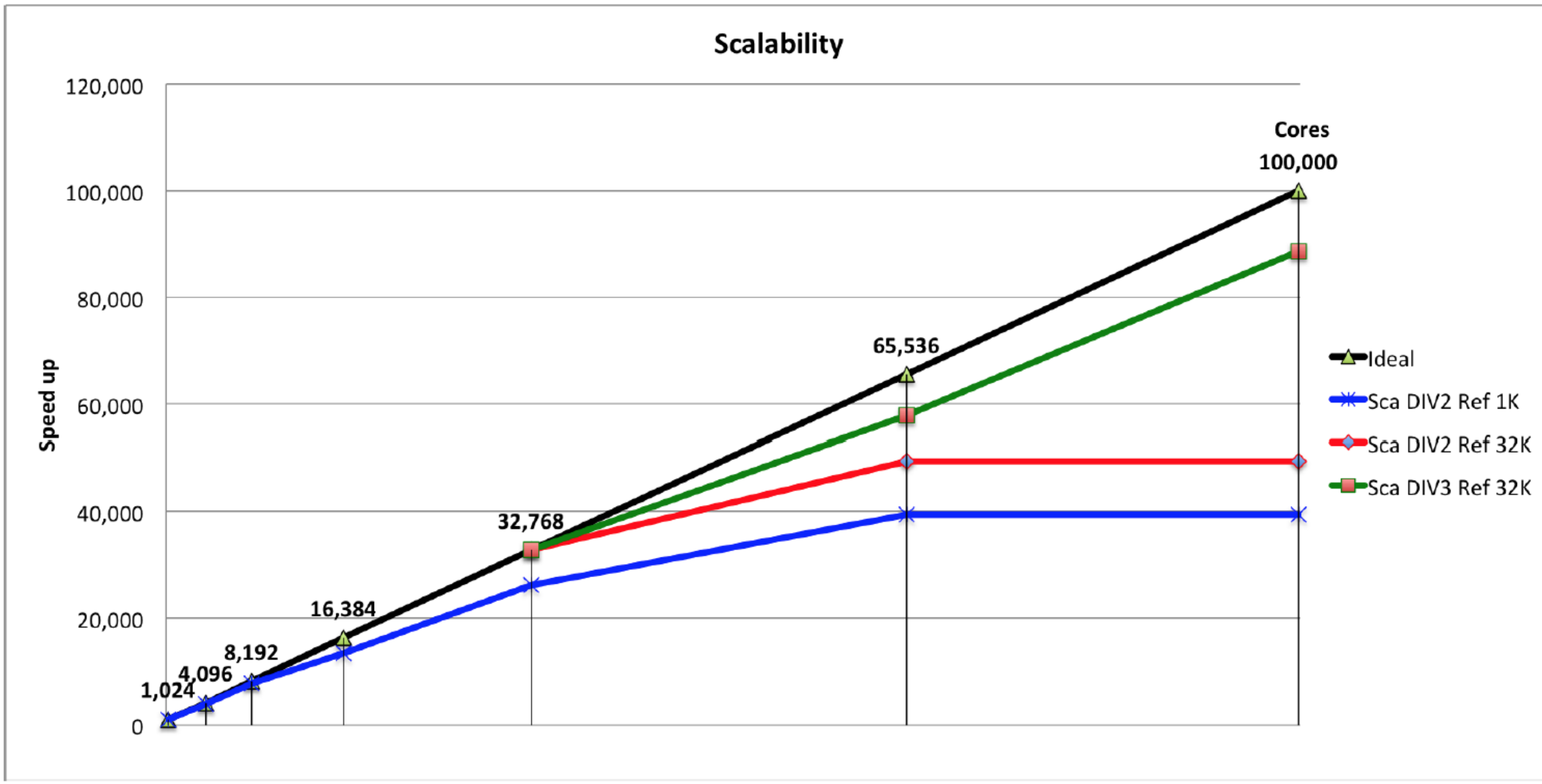


Numerical Simulation & HPC for Safety

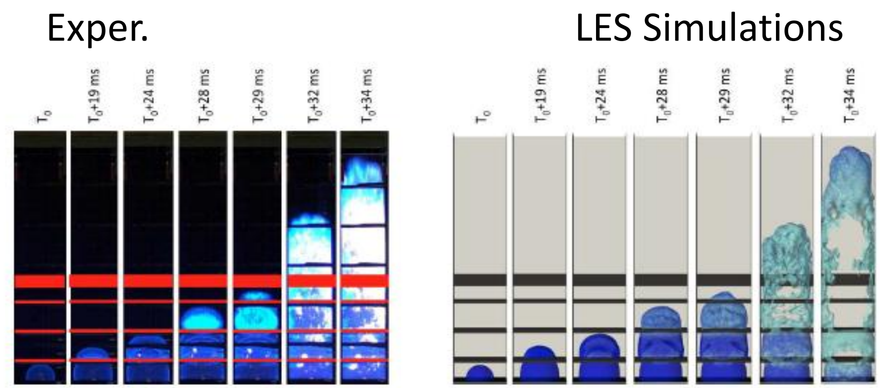
Explosions

CERFACS and TOTAL using INCITE calls

LES simulations for studying accidental gas explosions in buildings

Comparaions with experimental databases and real testings

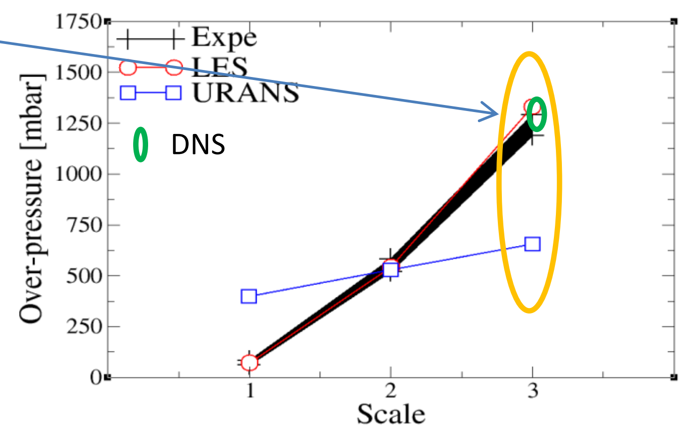
DNS **86 millions core hours on Mira (Argone Labs) using AVBP scalable up to 150000 cores.**



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; Poinsot T; Ricoux Ph
Industrial & Engineering Chemistry Research , Feb.2013
Pierre Quillatre, PhD Thesis, May 2014



LES validated by DNS and Exper.

Simulation/HPC: A tool for Understanding, Conception and Innovation

Intensive Computing for Numerical Simulation : Necessary, Unavoidable

Simulation and HPC for a better Understanding of major complex scientific problems:

- **Earth System**: *Goelogy,Geomecanic*, ***global changes (climate, ocean,…), natural risks, …***
- **Physics**: ***Particles, chemical activity, Astrophysics, Thermodynamics,***
- **Life Sciences**: ***Pharmacy, Genome, Biomechanics …***
- **Industrial challenges**: ***Geosciences, Aeronautics, turbulent combustion, multi-fluid flows, new materials,, …***

Simulation for Conception, Optimization, Innovation

A tool for R&D and Engineering … is in the service of processes

- **Material Structure:** ***Rheology, Fluid/Structure coupling, compounds, …***
- **New Material Design:** ***with more and more Molecular Simulation, nanomaterials, nanosystems***
- **Process Engineering**: ***oil&gas, Automotive, Crash Test, Aeronautics, …***

Benefits of Numerical Simulation :

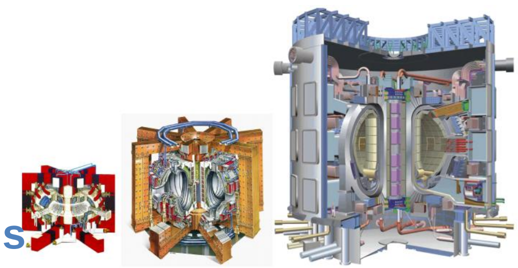
- **Better Understanding with a** ***huge reduction of errors and risks***
- **Increase range of parameters variation** **(closer limits)** ***with reduction of dangerous or expansive experiments***
- **Large «time saving» of development phases, before pilot**

Necessary way to go further: Work together

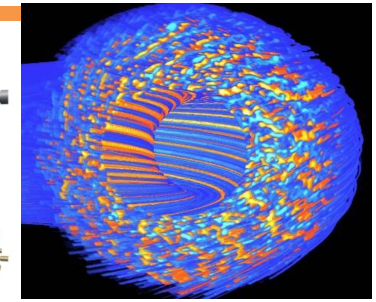
- **Collaboration, Multi disciplinary teams**: ***Share tools and algorithms, merge skill, …***
- **Multi domains** ***Team Building , workgroup : Maths, Computer Science, Applicative experts, Engineers, …***

What about simulations for industrial applications?

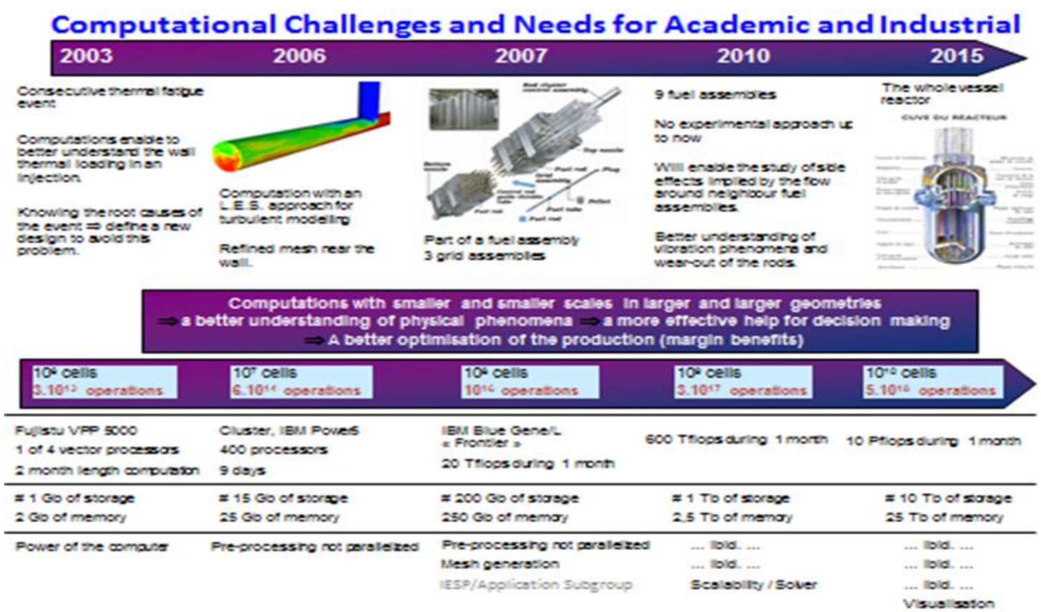
- Nuclear reaction / energy
  - **Nuclear Weapons**
    - **Stop of real experimental tests thanks to numerical simulations**
  - **Nuclear plants**
    - **Safety / Control**

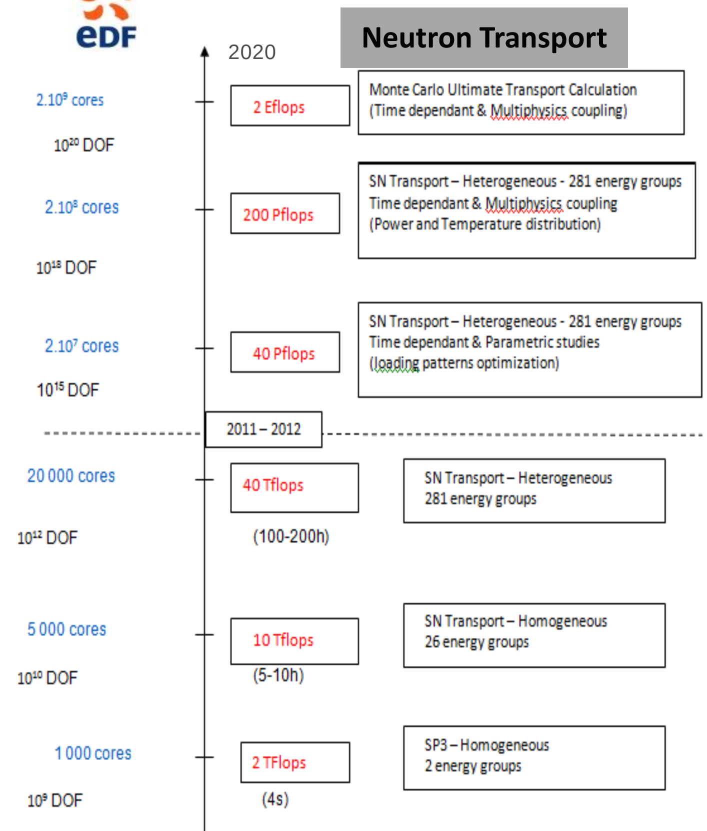


Tore Supra G~0 | JET G~1 | ITER G~10



EDF Nuclear Plant vision: Thermal





Industrial Numerical Simulations: Aeronautics

 # Wing prototypes: 77

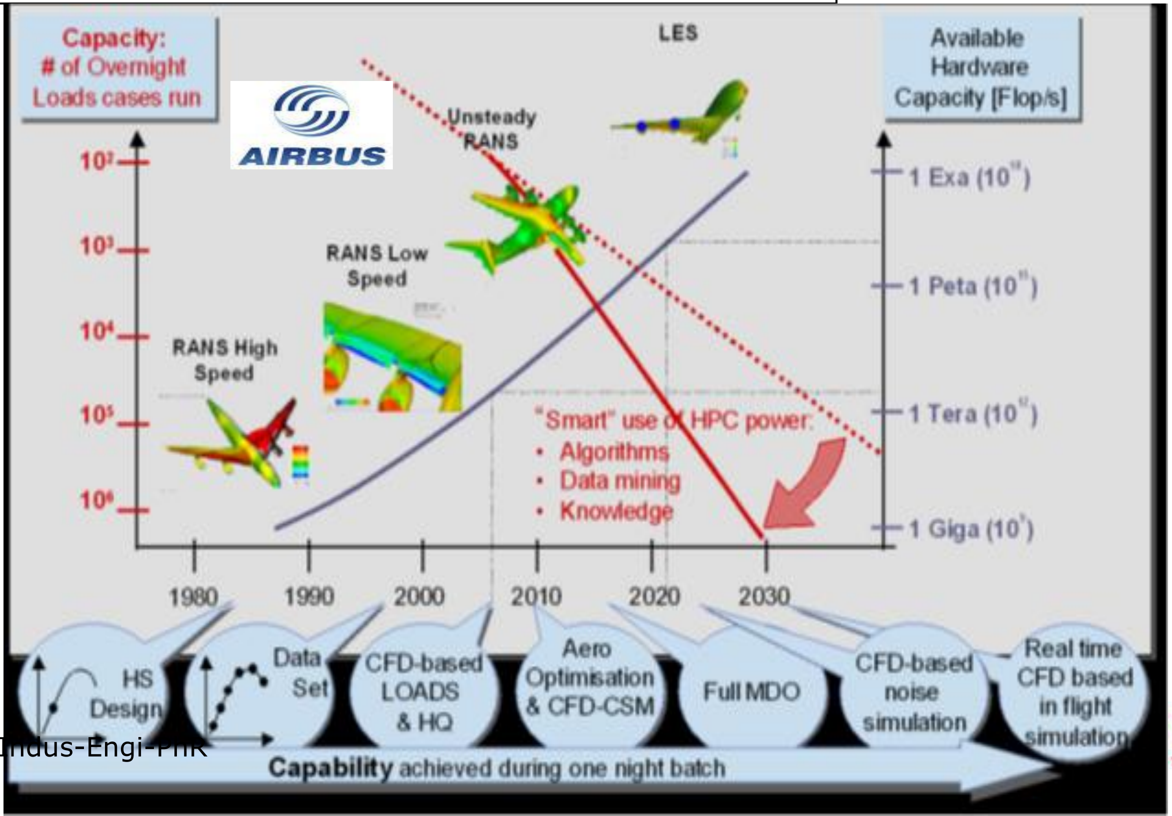
Boeing From 767 to 787

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

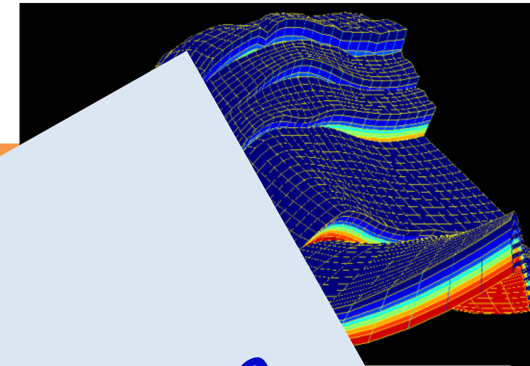
Thanks to HPC-enabled CFD runs, especially in high-speed regime, even providing better representation of aerodynamics phenomenon turned into better design choices.

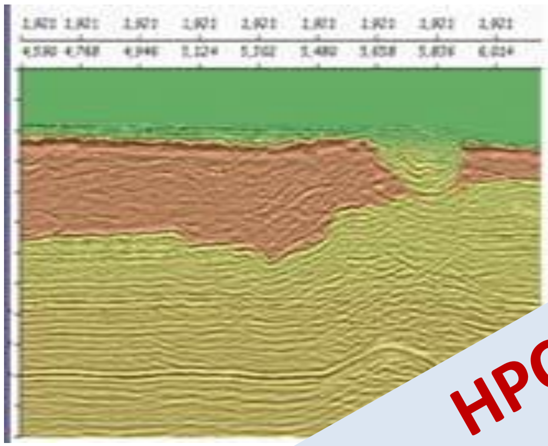
But ... Digital Aircraft will require at least 1 ZetaFlop !

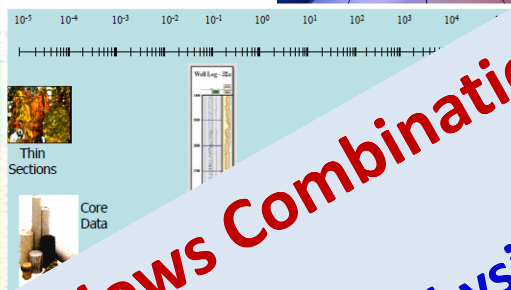
 # Wing prototypes: 11 (2008) → 7 by new methods and HPC (2015)

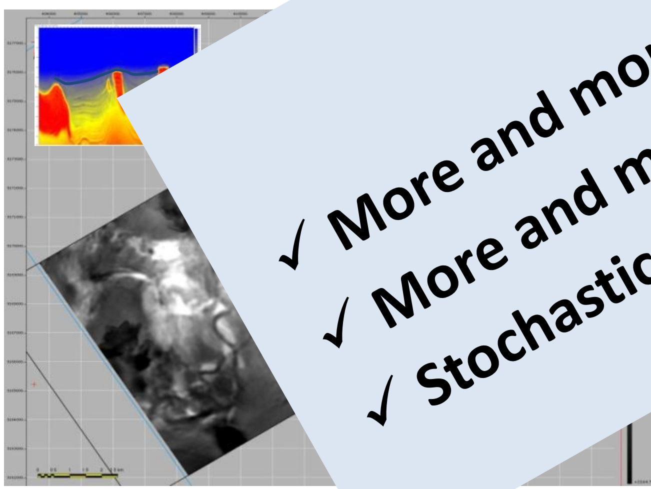


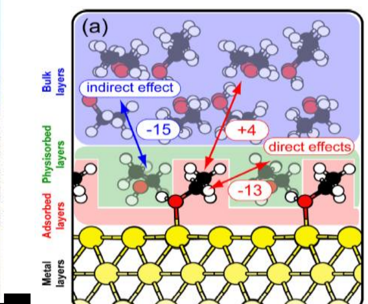
TOTAL: Numerical Simulation and HPC

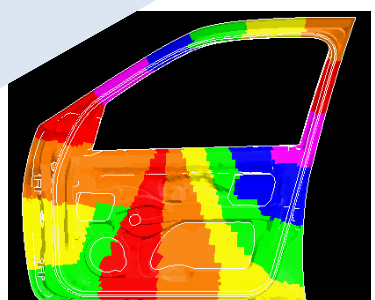


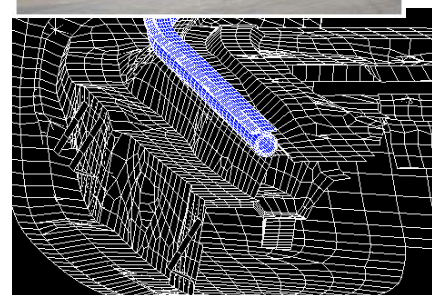


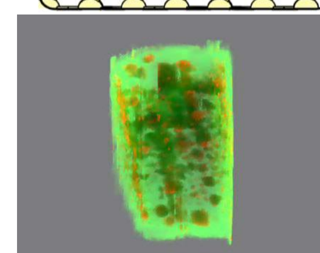










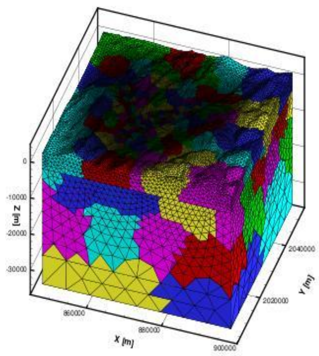


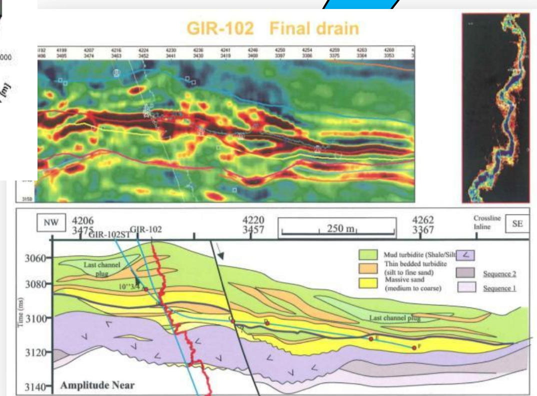
HPC allows Combination of

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

DEPTH IMAGING: 3 Fundamental Steps

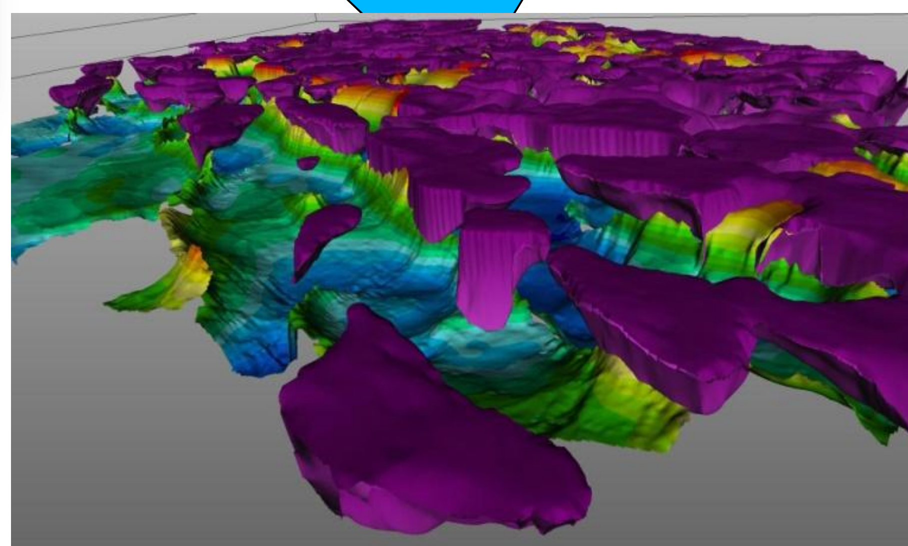
Numerical analyst
Numerical Methods





HPC Computing
HPC implementation

Pangea
2,3 PF
>100 000 Cores



Geo-physics
Maths for Physic Modeling

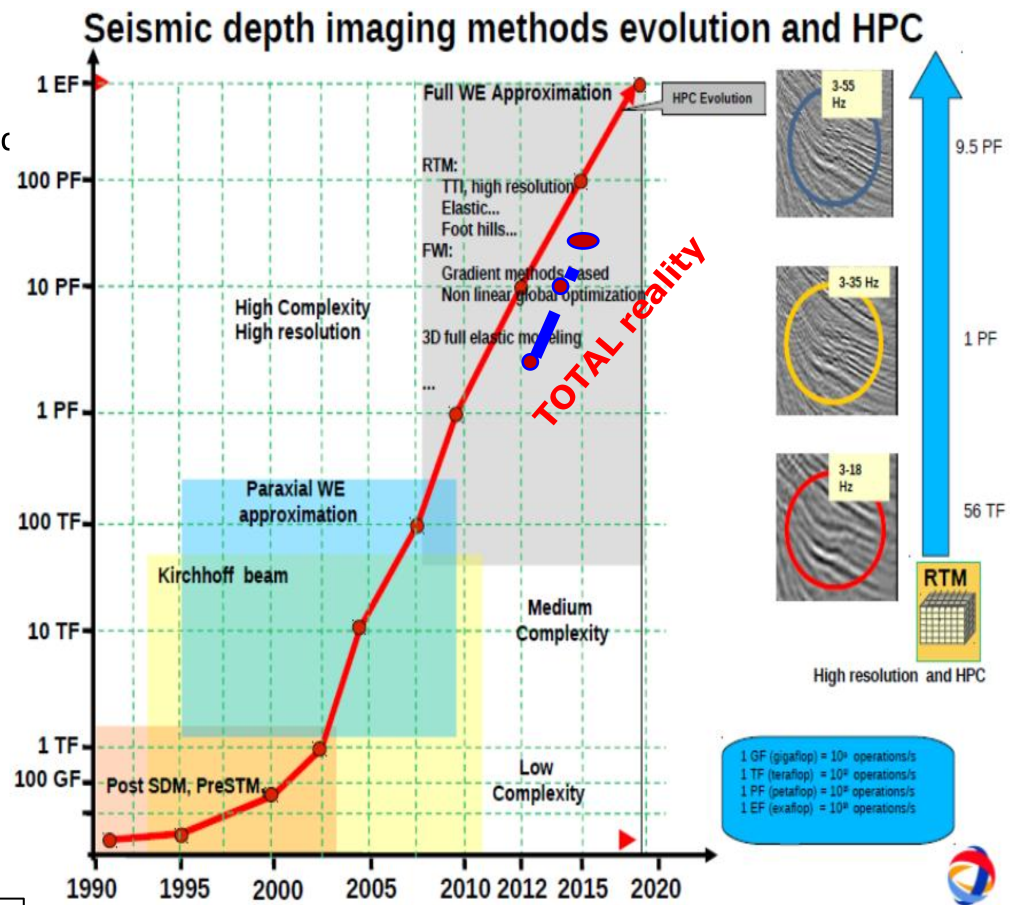
$$\frac{\partial q_p}{\partial t} + A_{pq}\frac{\partial q_q}{\partial x} + B_{pq}\frac{\partial q_q}{\partial y} + C_{pq}\frac{\partial q_q}{\partial z} = E_{pq} q_q + s_p,$$

Embarrassingly Parallel approximation

HPC Opportunities in TOTAL: Next steps in Depth Imaging

Combinaison of Physics, Numerics, Uncertainties (UQ)

- Involving maths modling 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, …

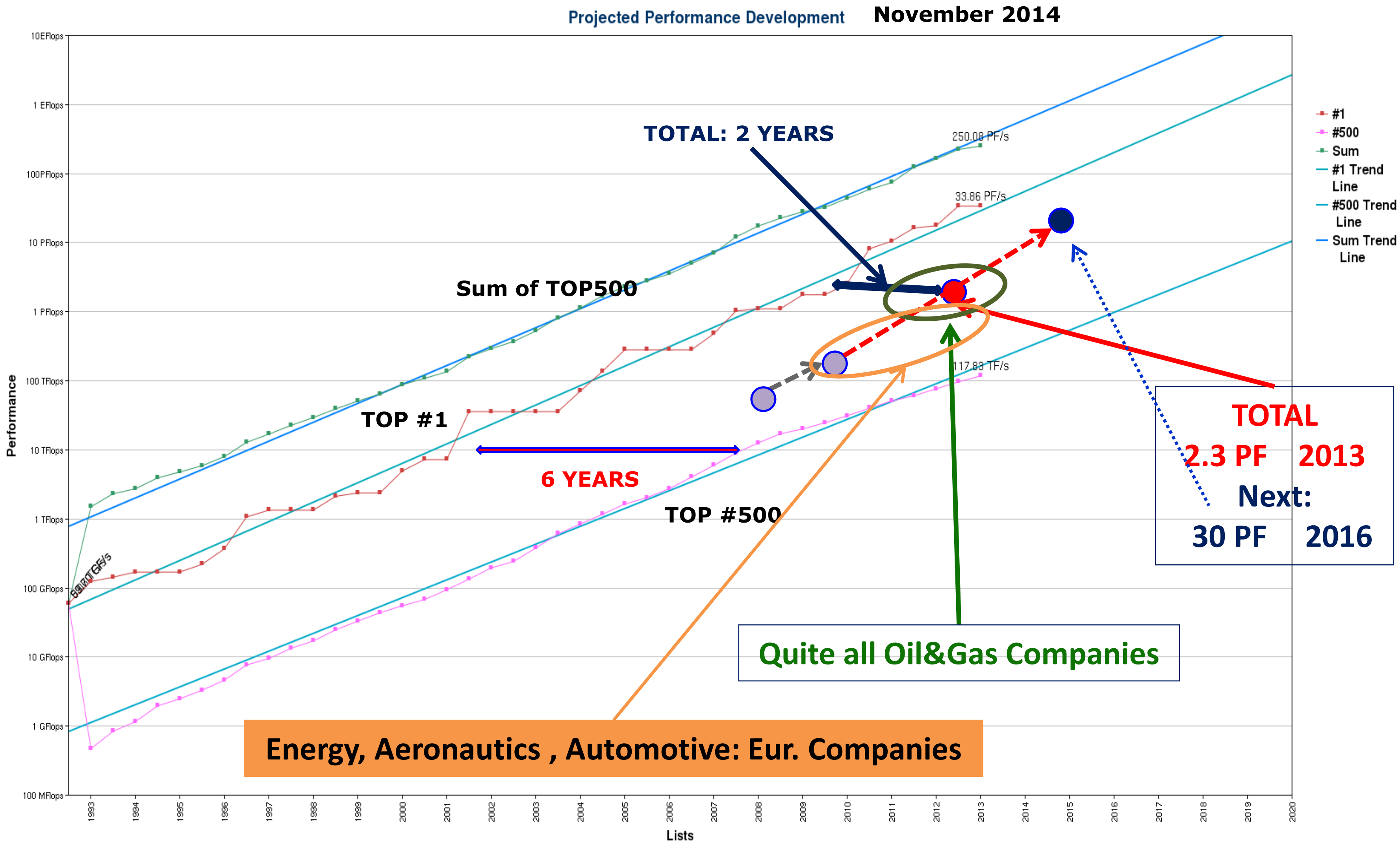


Integrated Approach of Oil System :
interaction geology – geophysic :
foot hills, non conventional reservoirs, …

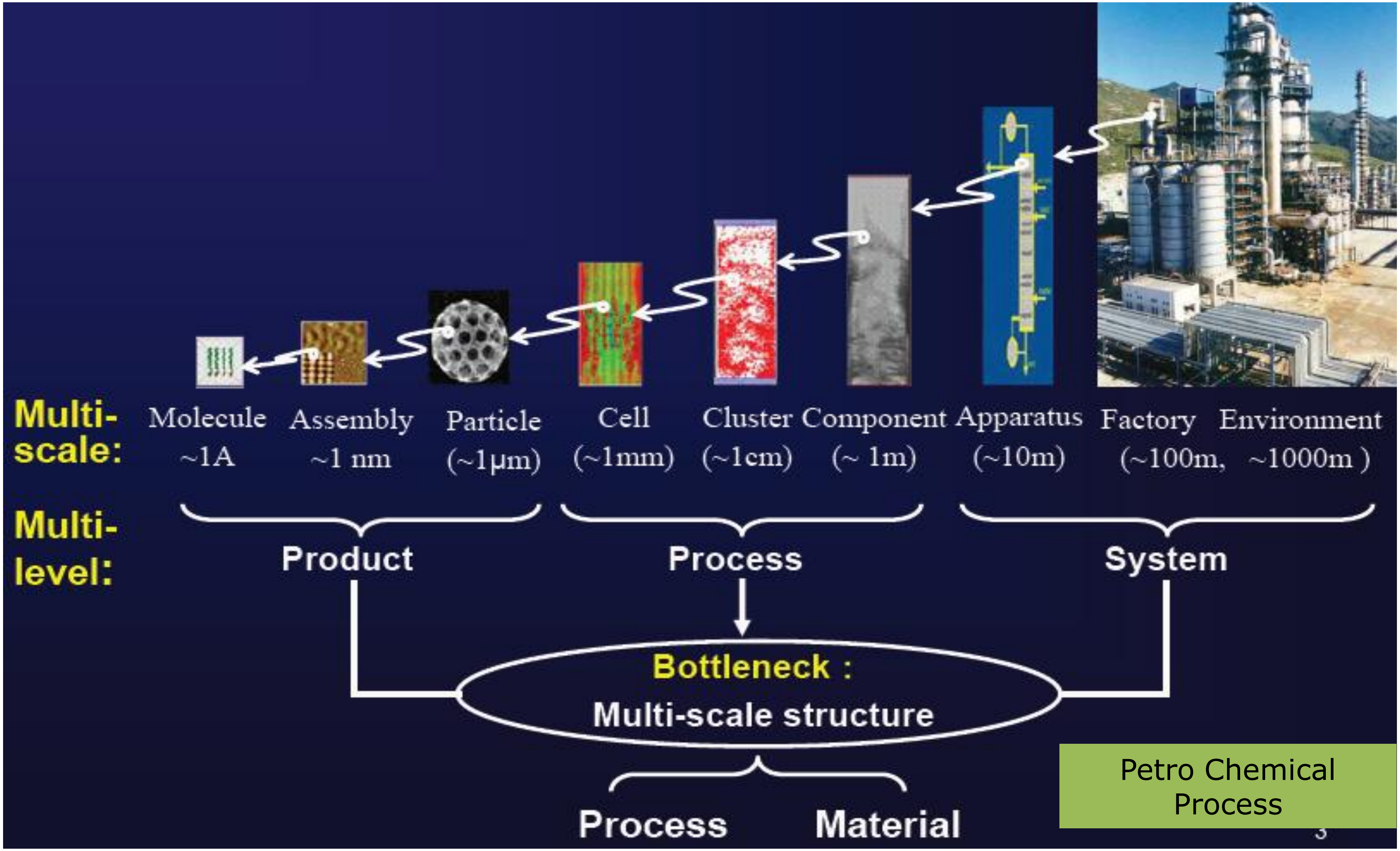
Same Roadmap in BP , Chevron

Absolute Need of multi skills

Industries in Top500: Insight into HPC Performance



HPC for Industrial Engineering Multi Scale Problems



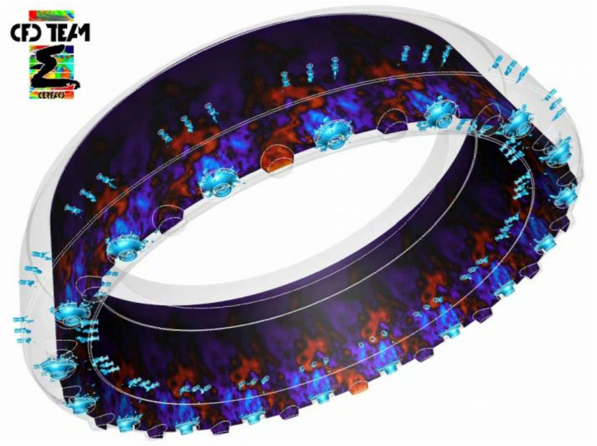
Petro Chemical Process

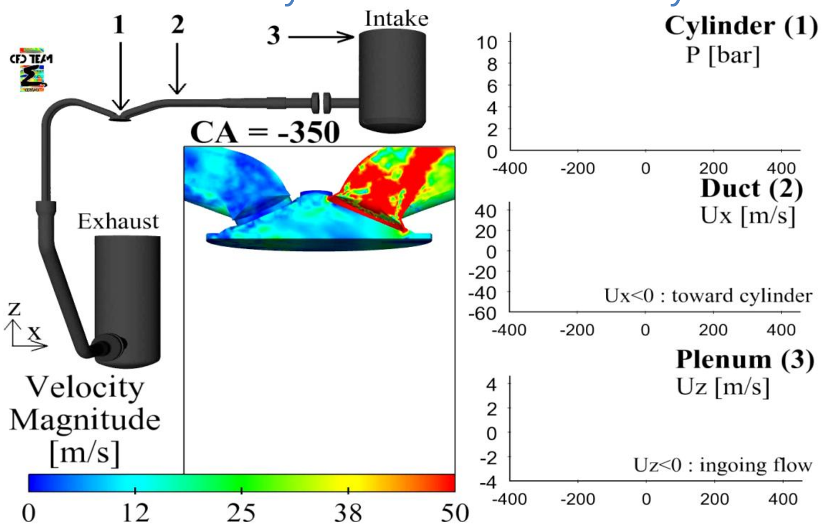
What about simulations for industrial applications?

- **Automotive**
  - **Crash Test**
    - **100 parameters on optimal numerical “experimental” de**
    - **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 equipement**
    - Efficiency / **Safety** / Competitiveness
  - **Automotive**
    - Efficiency / Environment / Life Cycle



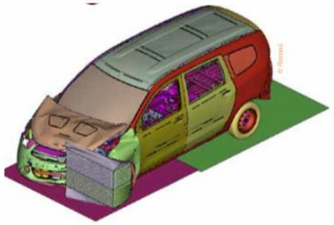


Validation by experiments thanks to High Speed Imaging, Particle Image Velocimetry (HS PIV)

Feedback on PRACE PROJECT / FMOC

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 CO_2 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

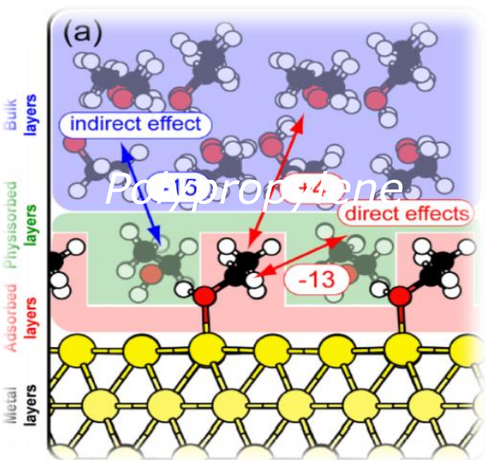
➔ Model reduction and HPC are not competing but complementary

➔ Model reduction combined with HPC will allow to exploit new immersive 3D visualization tools for interactive calculations and optimization

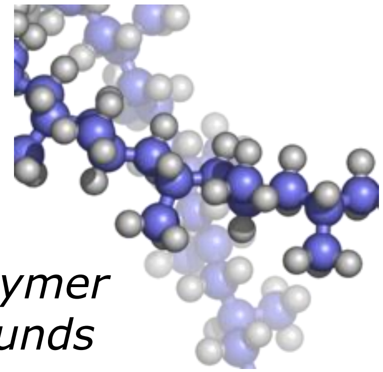
➔ Example : 20 hours elapsed time reduced to few seconds with 10% loss on accuracy (enough to optimize).

TOTAL Formulas(Lubricants, adhesives, Recovery…), Materials, Catalyst, …

Molecular Simulation is now a key technology

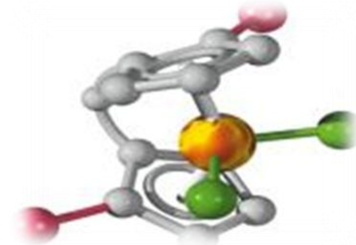


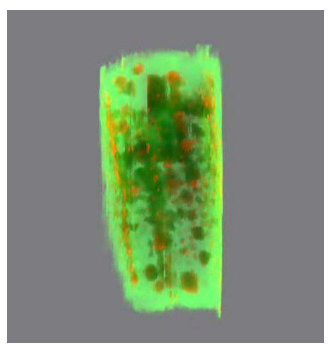
Adhesion



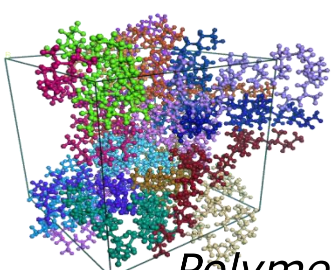
EOR polymer Compounds

Metallocene catalysts



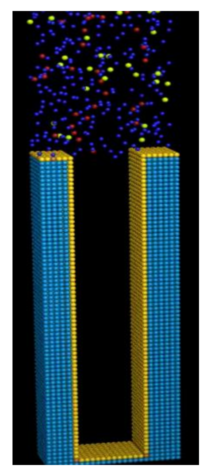


Heterogeneous catalysts (4 nm Cube)



Polymer solubility

KMC simulations for flat copper surface



EESI2 recommandation on UUVQ

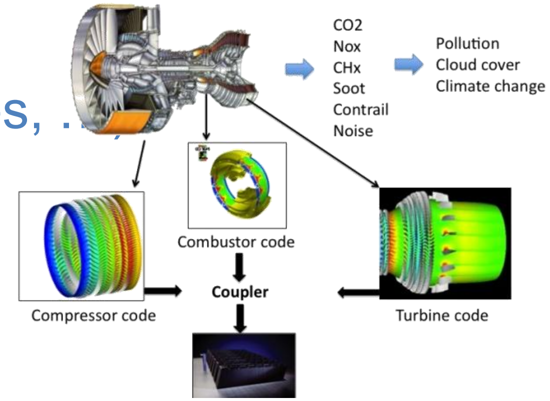
- Multiscale/multiphysics + big data ➔ UUVQ
  - Multiple sources of uncertainties due to
    - lack of knowledge on a physical parameter (epistemic uncertainty)
    - parameter with a random nature (aleatory uncertainty)
    - uncertainty related to the model (model error, too simplified model)
    - 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 ultrascalable UUVQ tools (scheduling, optimisation, …)
- Embeeding UQ loops at the lowest levels of the simulation code
- Use of surrogate models and reduced basis models

EESI2 recommandation on couplers

- 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

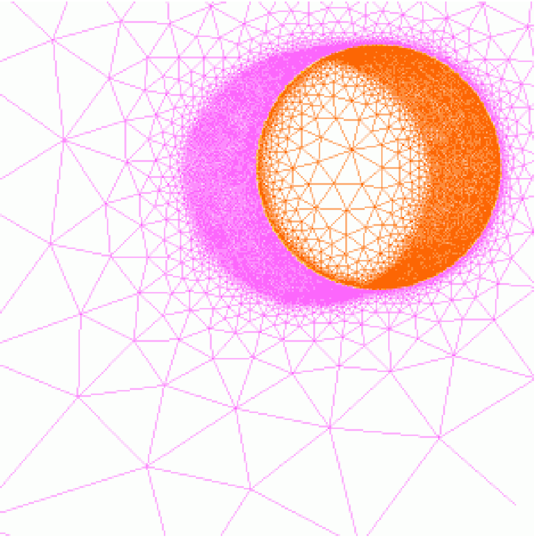


- Europe owns multiple coupler tools
  - OpenPALM, OASIS, MpCCI, …
- 2 approaches
  - Direct coupling (multiple binaries) vs coupling via top-level interfaces (one unified binary)
- But strong challenges to face for Exascale
  - Standard coupling API
  - memory footprint, use of asynchronous (reduced) communications, …
  - Interpolation methods, smart search algorithms, ….

EESI2 recommandation on Mesh

Mesh Generation

- Automatic, Adaptive, Intelligent
- From billions « regular »meshs … to millions !



With numerical methods for solving differential equations such as

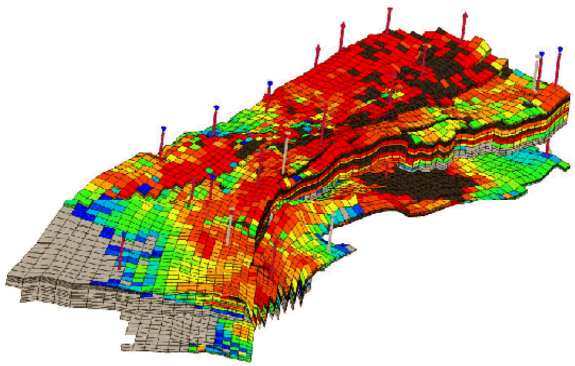
Disontinuous Galerkin: combining features of the finite element and the finite volume framework

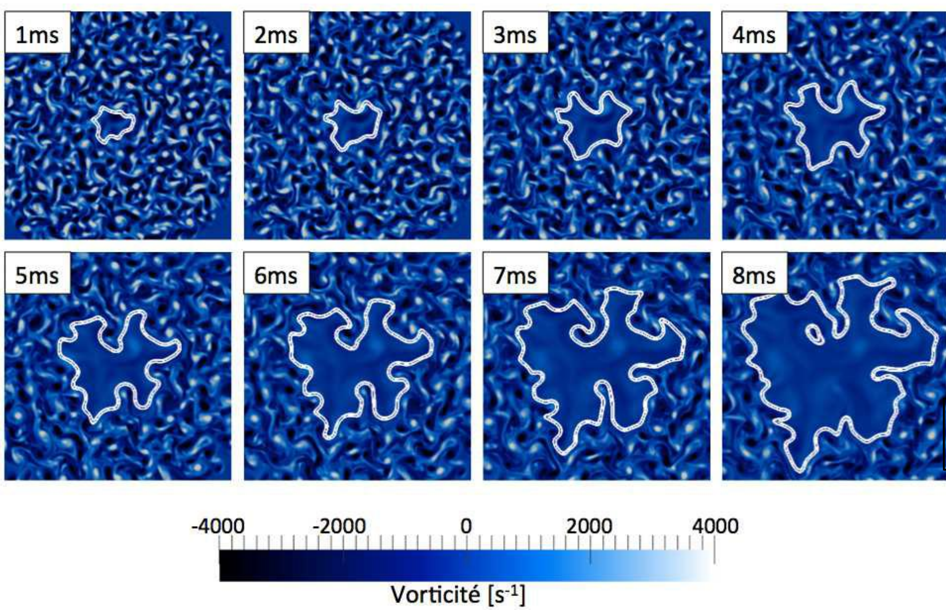
DG methods have a huge interest for electrodynamics, fluid mechanics and plasma physics equations.

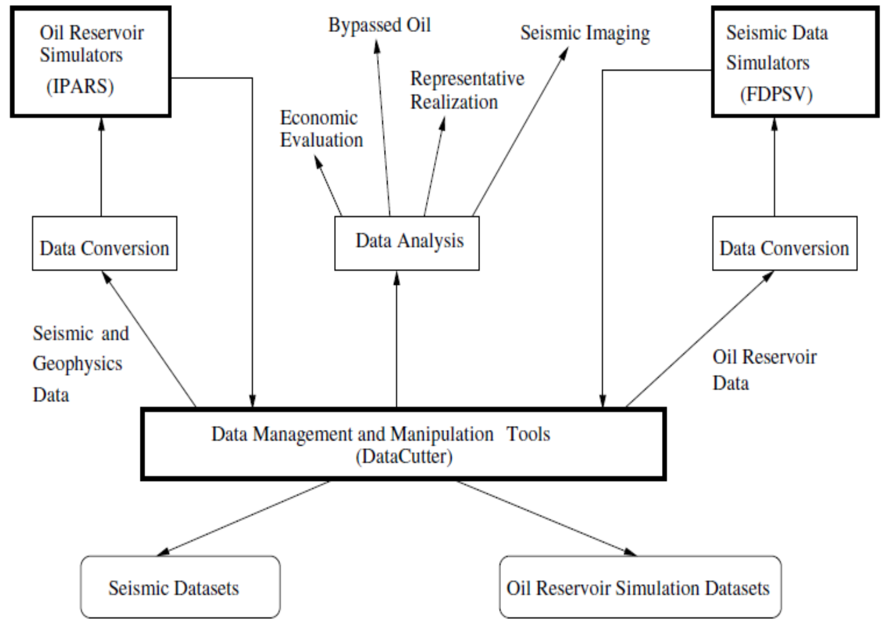
Industrial support for Data Management

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

Even VISUALIZATION !







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