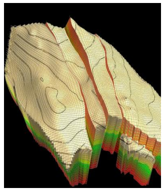
Numerical simulation and HPC in Oil & Gas Industry TOTAL Group

Philippe Ricoux

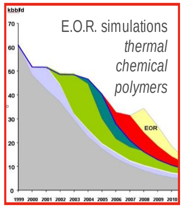
TOTAL/DS

Calculs Parallèles et Applications – ASPROM- 1er Octobre 2014

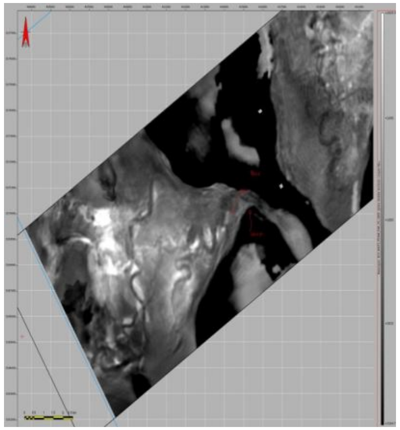
TOTAL: POOL OF ENERGIES

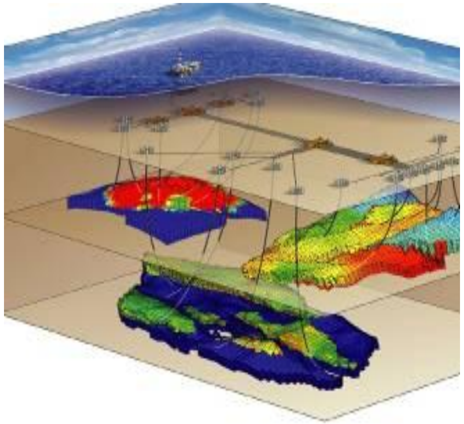


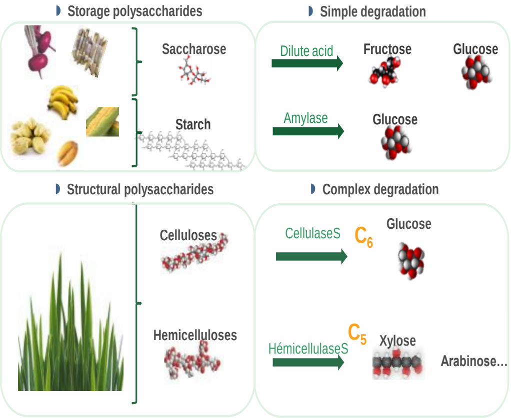
Heavy Oil production



E.O.R. simulations
thermal
chemical
polymers







Storage polysaccharides

Saccharose

Starch

Simple degradation

Dilute acid → Fructose Glucose

Amylase → Glucose

Structural polysaccharides

Celluloses

Hemicelluloses

Complex degradation

CellulaseS C_6 → Glucose

HémicellulaseS C_5 → Xylose Arabinose...

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, …***

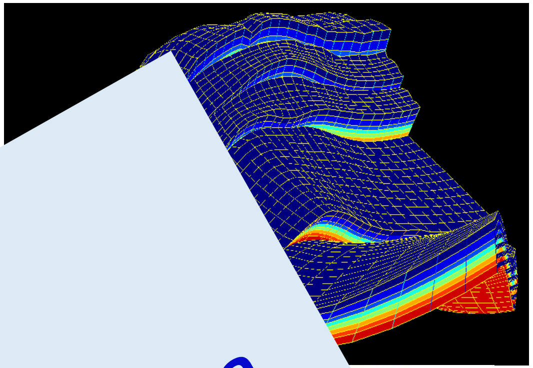
Benefits of Numerical Simulation :

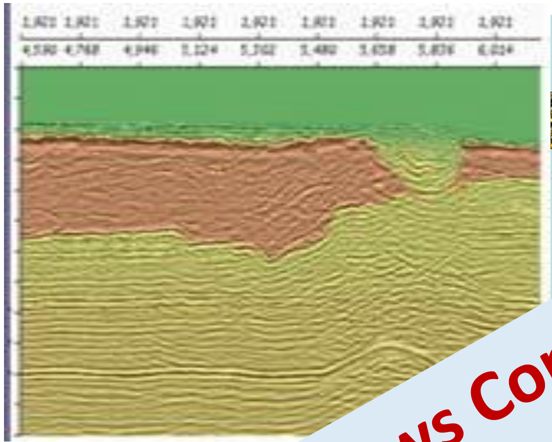
- **Better Understanding with a** ***huge reduction of errors and risks***
- **Increase range of parameters variation** (closer limits) ***with reduction of dangerous or expansive experiments***
- **Large «time saving» of development phases, before pilot**

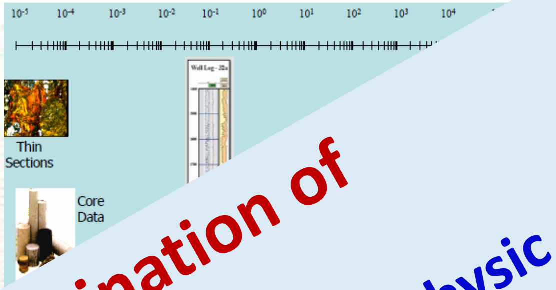
Necessary way to go further: Work together

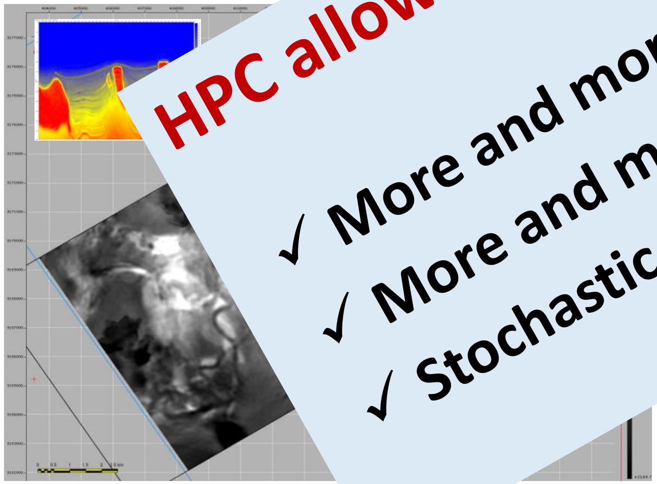
- **Collaboration, Multi disciplinary teams**: ***Share tools and algorithms, merge skill, …***
- **Multi domains** ***Team Building , workgroup : Maths, Computer Science, Applicative experts, Engineers, …***

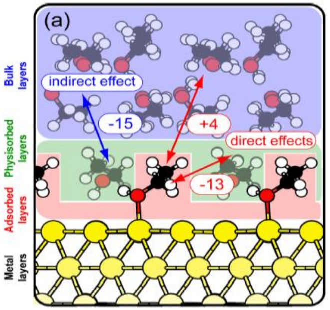
TOTAL
NUMERICAL SIMULATION AND HPC

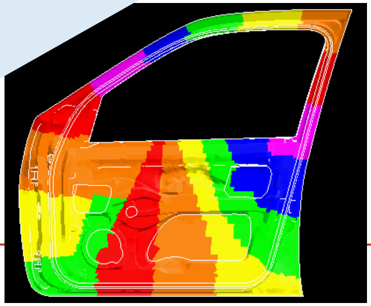


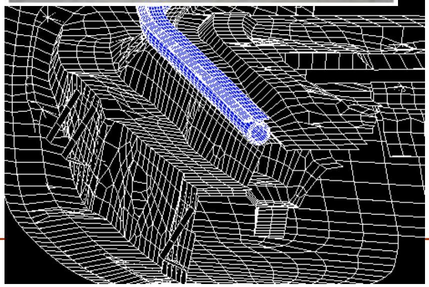


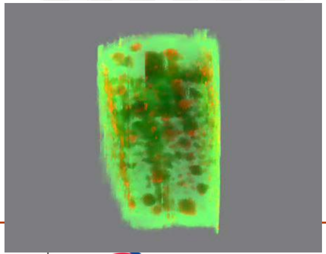










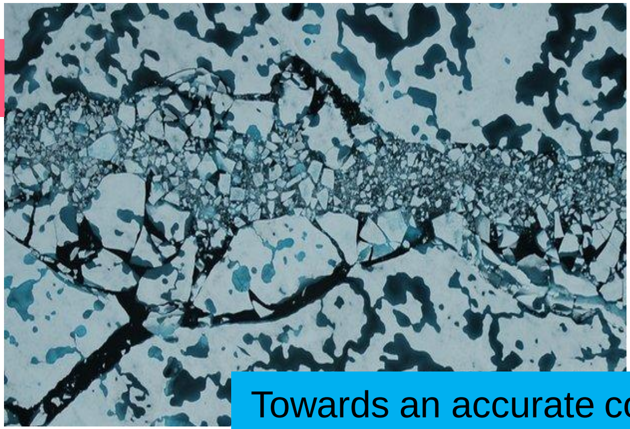


HPC allows Combination of

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

SEA ICE MODELLING

Sea Ice Floes



Towards an accurate continuum dynamical model for sea ice

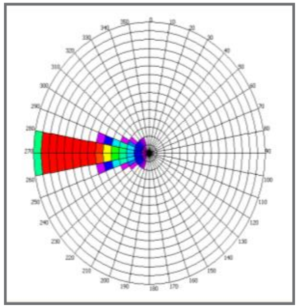
Dynamics of an Assembly of Rigid Ice Floes

Numerical simulation of ice performance of ships

Forecast of gas dispatch schedule from Artic area

SEISMIC DATA

Conventional NAZ

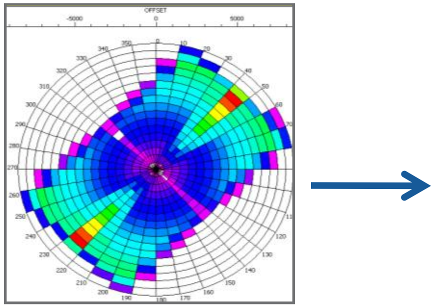


7-9 M$

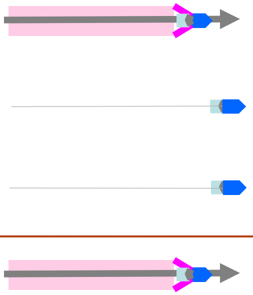
Cost for ~200 km²

WAZ Explo 2

Larger Xline offset

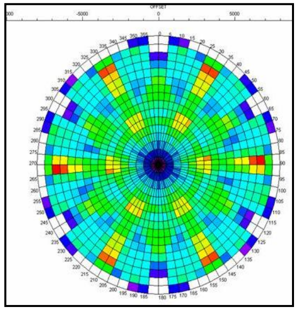


30-70M$

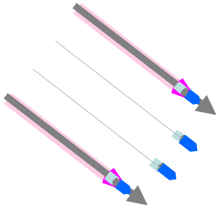


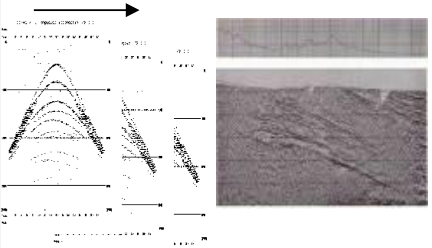
RAZ/Full WAZ

Development



50-110M$



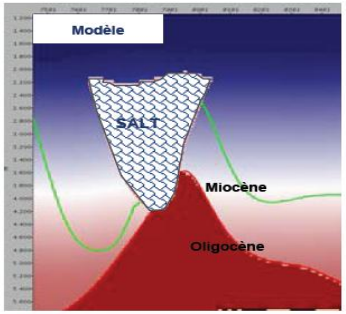


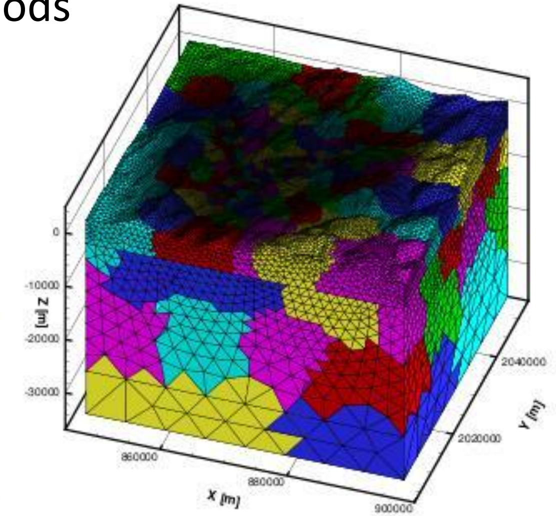
Seismic and geological Data

unconventional

HPC for Depth Imaging : 3 fundamental steps

Numerical analyst
Numerical Methods

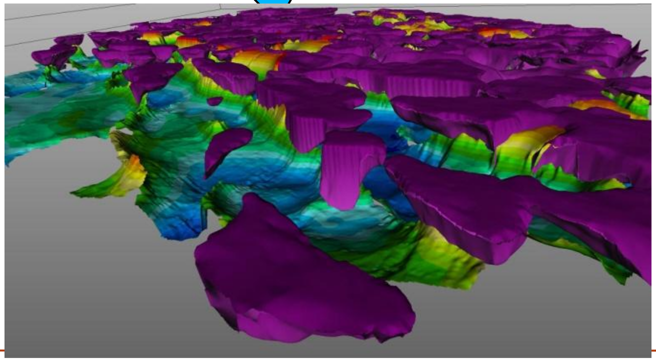




100 000
Cores
+
Options
GPU

HPC Computing
HPC implementation

Studies

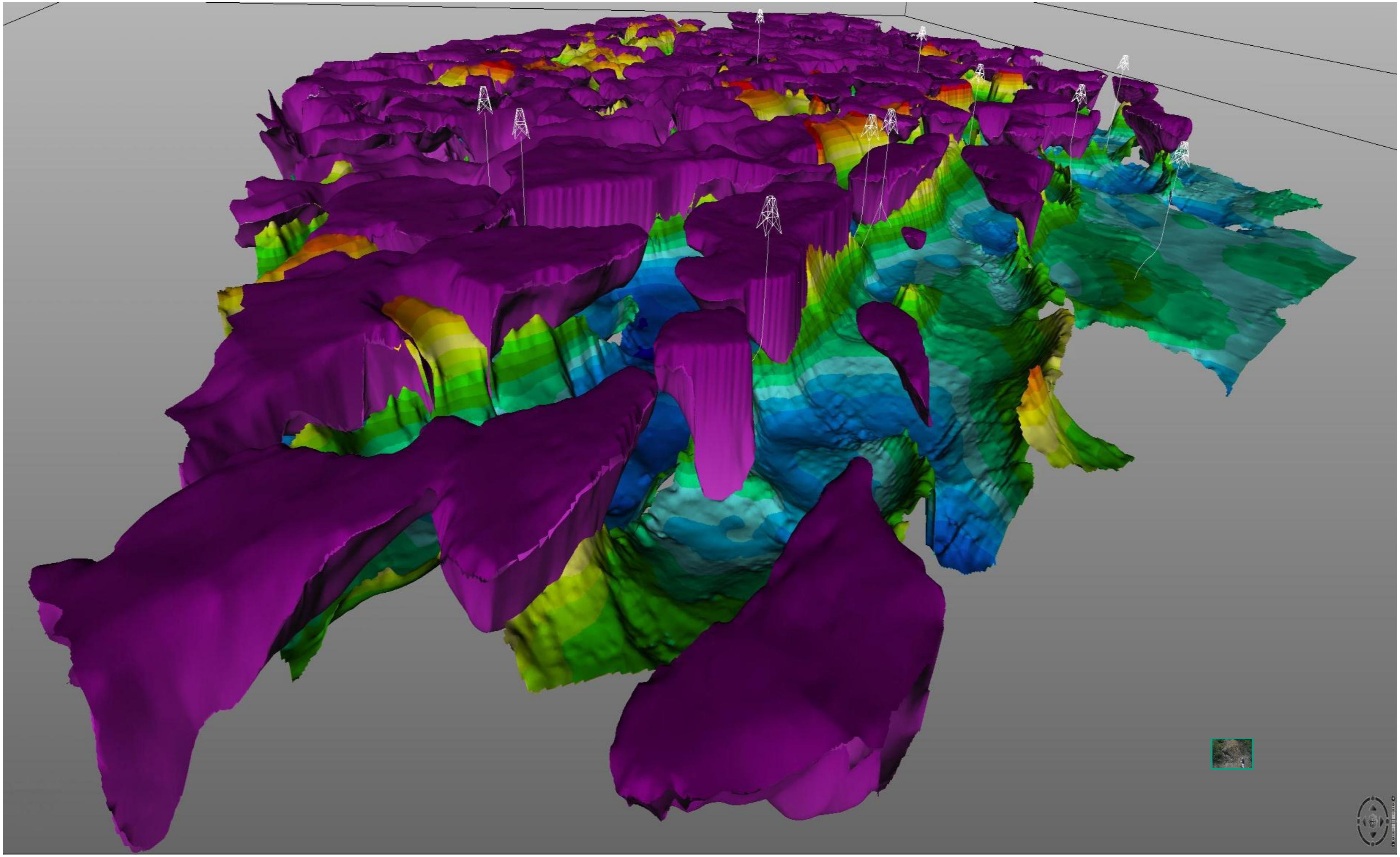


Geo-physics
Maths for Physic Modeling

$$\frac{\partial \mathbf{q}_p}{\partial t} + \mathbf{A}_{pq}\frac{\partial \mathbf{q}_q}{\partial x} + \mathbf{B}_{pq}\frac{\partial \mathbf{q}_q}{\partial y} + \mathbf{C}_{pq}\frac{\partial \mathbf{q}_q}{\partial z} = \mathbf{E}_{pq}\mathbf{q}_q + \mathbf{s}_p,$$

Embarrassingly Parallel approximation

WEST AFRICA



DEPTH IMAGING: AN ALGORITHM

$$\left(\nabla^2 - \frac{1}{c^2}\frac{\partial^2}{\partial t^2}\right) u(\mathbf{r},t) = 0.$$

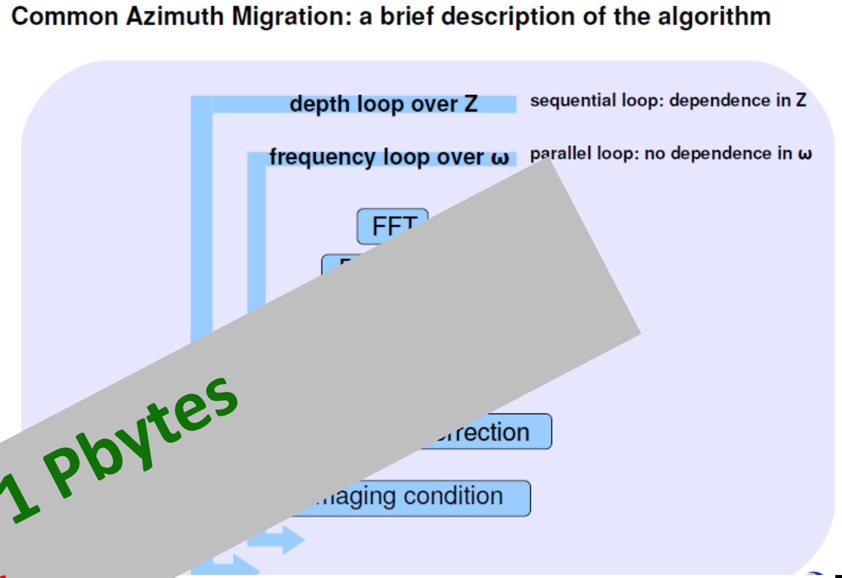
Wave Equation (hyperbolic)

$$u(\mathbf{r},t) = A(\mathbf{r})T(t).$$

$$(\nabla^2 + k^2)A = 0$$

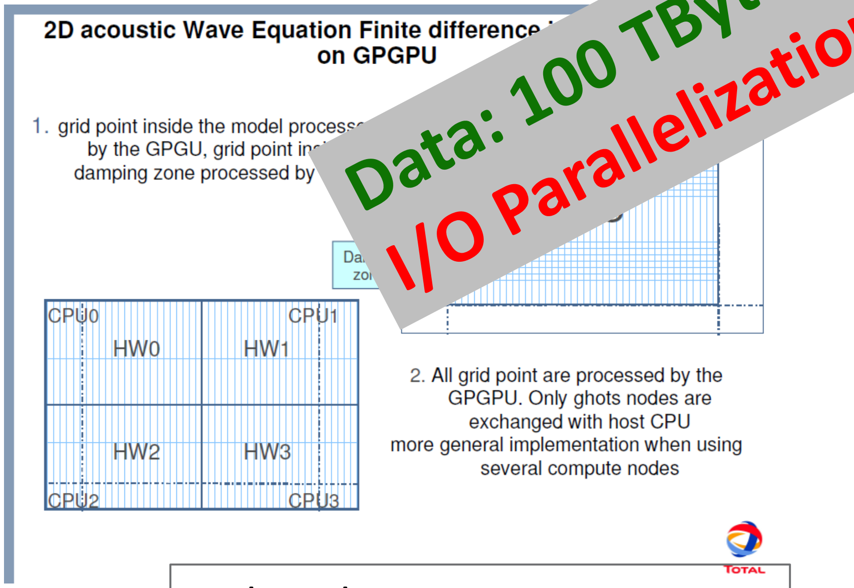
Approximation :
Helmholtz Equation (elliptic)

Billions unknown variables ,
Large solvers


Common Azimuth Migration: a brief description of the algorithm

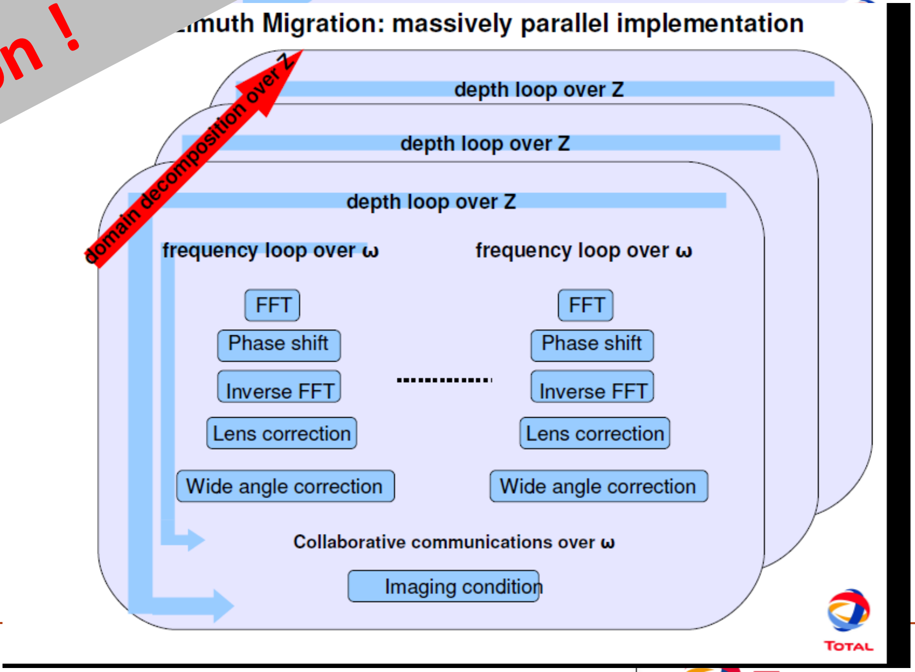
Data: 100 TBytes to 1 Pbytes

I/O Parallelization !


2D acoustic Wave Equation Finite difference ... on GPGPU

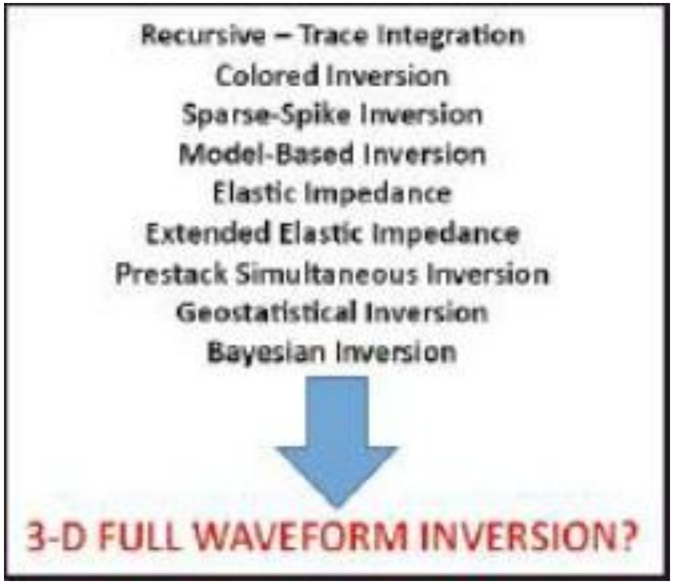
1. grid point inside the model process... by the GPGU, grid point in... damping zone processed by

2. All grid point are processed by the GPGPU. Only ghots nodes are exchanged with host CPU more general implementation when using several compute nodes


...muth Migration: massively parallel implementation

Link with computer science

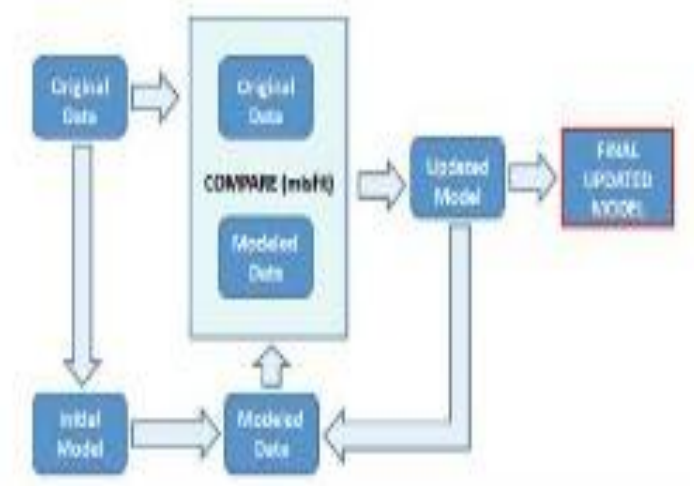
FWI ALGORITHM



Recursive – Trace Integration
Colored Inversion
Sparse-Spike Inversion
Model-Based Inversion
Elastic Impedance
Extended Elastic Impedance
Prestack Simultaneous Inversion
Geostatistical Inversion
Bayesian Inversion

3-D FULL WAVEFORM INVERSION?

FWI is the best Approach today to determine reservoir properties.

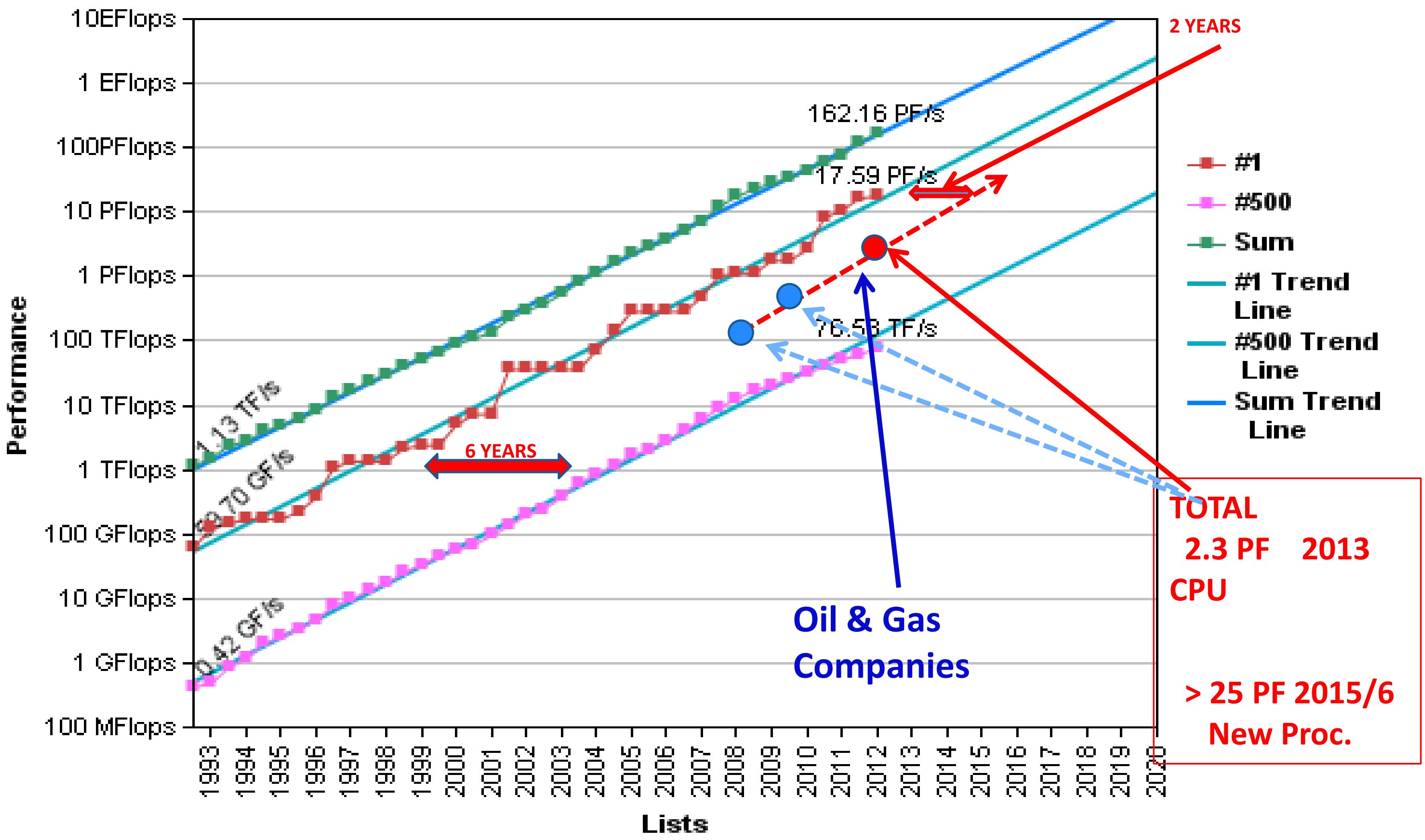


General workflow for FWI, initial model:
legacy velocities, well logs, and non-seismic measurements for velocity analysis.

A data misfit results after several iterations, producing local and global minima depending on the starting models.

One of the challenges with FWI using gradient or gradient-descent methods is the convergence to the local minima.
Technique very sensitive to the starting velocity model, especially when 3-D is considered

THE TOP500 LIST: TWENTY YEARS OF INSIGHT INTO HPC PERFORMANCE



Projected Performance Development Nov. 2013

Oil & Gas Companies

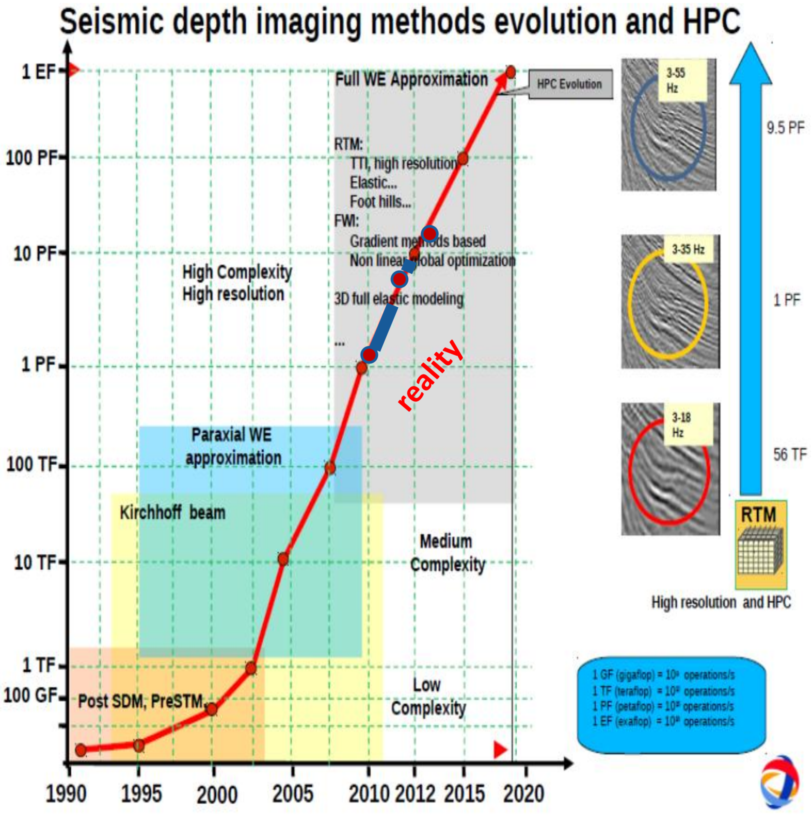
TOTAL
2.3 PF 2013
CPU

> 25 PF 2015/6
New Proc.

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, …



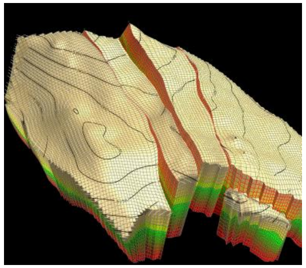
Same Roadmap in BP , Chevron

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

Absolute Need of multi skills
Multidisciplinary teams

HPC & Reservoir Modeling From Pore to Darcy

Needs of new and efficient reservoir simulations



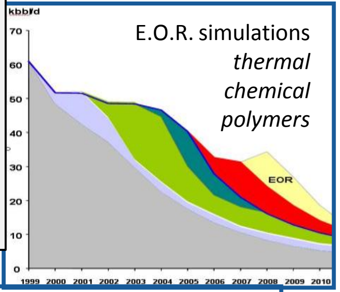
- **Heavy oil** :
  SAGD (evo
- **E.O.R.** mec
  chemical r
- **CO2 proje**
  integrity, predicting long term behavior

Multi Fluids including polymers, MultiPhase Flows,

Multi Physics, including geomechanic, Chemistry, …

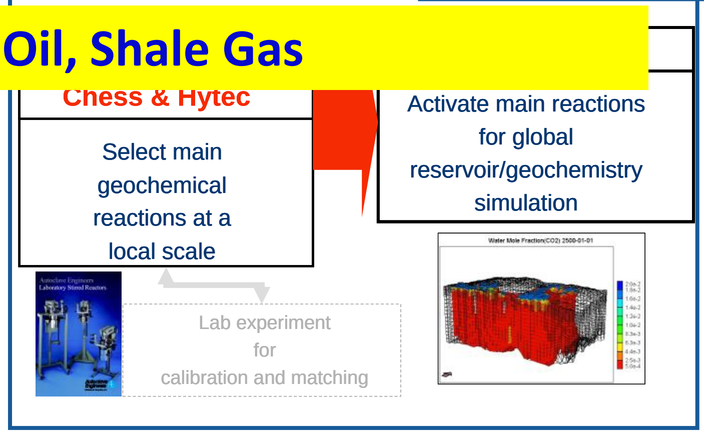
Multi Scale, Different Physics at different scales

Upscaling laws from nanometer to meter



E.O.R. simulations
thermal
chemical
polymers

Essential for new fractured reservoirs, Shale Oil, Shale Gas



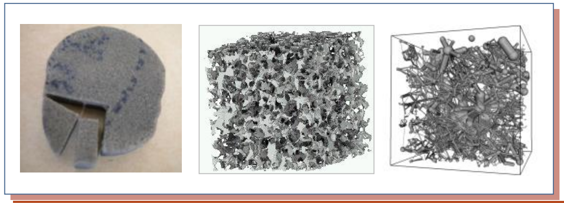
Chess & Hytec

Select main geochemical reactions at a local scale

Activate main reactions for global reservoir/geochemistry simulation

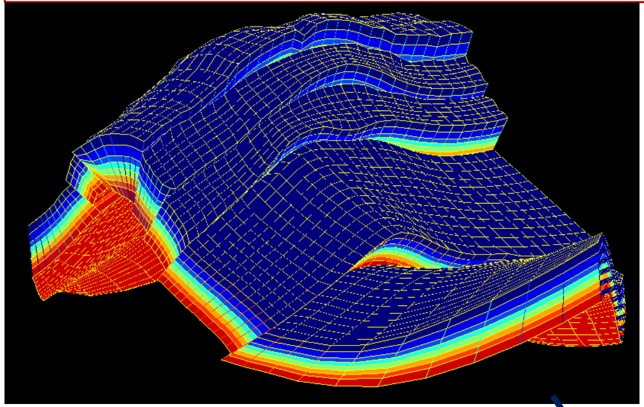
Lab experiment for calibration and matching

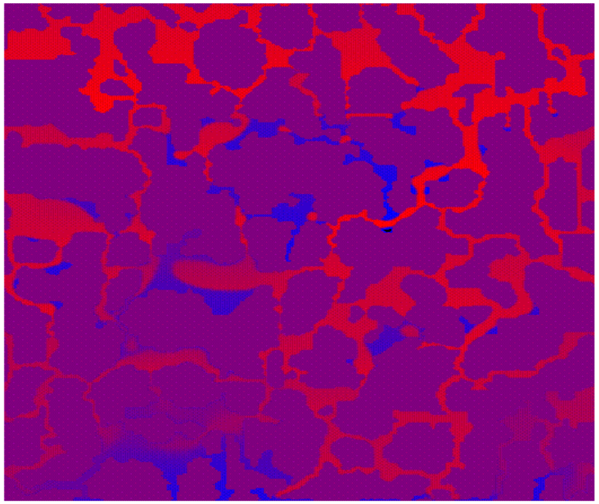
- **Pore Network Modeling**:
  - Modeling mechanisms at pore scale
  - Processing requirements could result in resources comparable to seismic imaging.



Matching performance needs by applying parallelism techniques at all levels

RESERVOIR SIMU. MULTI PHYSICS, MULTI SCALE





Maximization of Oil reservoir production , Oil recovery (EOR)

Multi-phase flow, Darcy's law modified with stochastic relative permeability:
(stochastic PDE, macro law)

$$\mathbf{u}_\beta = -k\frac{k_{r\beta}}{\mu_\beta}(\nabla p_\beta - \rho_\beta \mathbf{g})$$

for each phase of each component

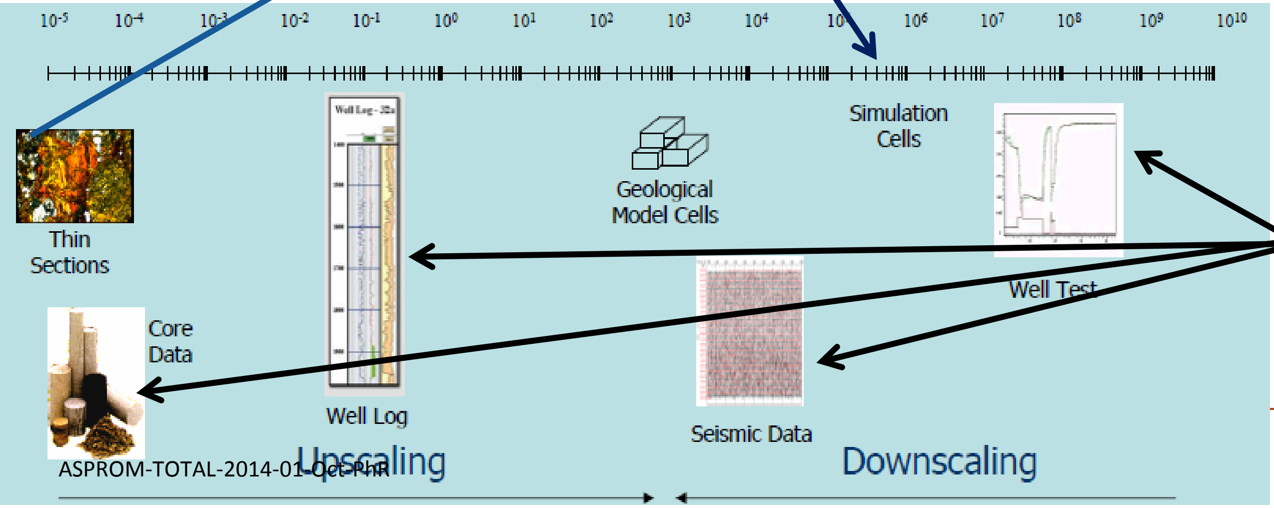
Where β indicates the phase, $k_{r\beta}$ is the relative permeability (between 0 and 1) for the phase, and

$p_\beta = p + p_{c\beta}$ is the fluid pressure in the phase, which is the sum of the pressure in a reference phase (usually the gas phase) and the capillary pressure (capillary $p_{c\beta}$ pressure is negative), and μ_β the viscosity in the phase.

Estimation of macro parameters such as relative permeability fundamental for reservoir simulation

Many sources

- **Many scales (10^{-5} to 10^8cm)**
- **Sparse**
- **Not always reliable**



Observed data not at the same scale than models

RESERVOIR MODELLING: COMPLEXITY

- Reservoir: geostatistic fine representation of K *(permeability tensor)* , Φ *(flows vector)*
- • Stochastic PDE: Uncertainties
- • Homogenization on a meshing : K, Φ constant by mesh
- • kr(S), Pc(S) by lithology (estimation from transport at pore level)
- • Anisotropy: Kxy/Kz from 1 to 10, K based on the principal slopes

❖ **Coupled equations : Elliptic/Parabolic in Pressure and Hyperbolic/Parabolic non linear degenerate in saturations/compositions**

❖ **Non linear Closure laws (kr, Pc, densities, viscosities, thermodynamic equilibrium)**

❖ **Coupled Resolution in P-S (c_a) :**

  - **Local conservation equations for compressible**
  - **Transport-thermodynamics coupling**

❖ **Implicit discretization in time**

  - **Large Δt**

❖ **Locally conservative schema in space**

❖ **Stability of multi phase transport (approx)**

❖ **Local Explicit schema for flows (Φ) depending on variables of neighbor mesh of the ridge**

  - **Cost on implicit way**

❖ **Best Extract of physics : Discrete conservation law**

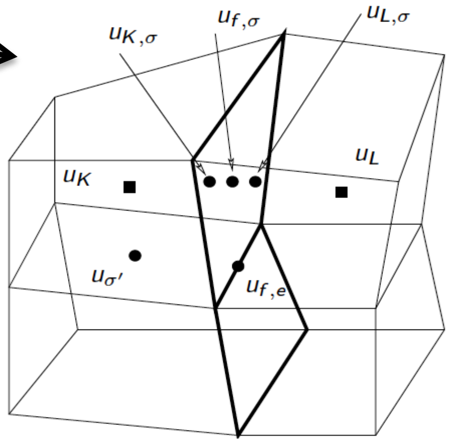
  - **Physical acceptable solution on «rough» meshing**
  - **Homogenization**

RESERVOIR MODELING: PERSPECTIVES

Darcy stochastic EDP→ Difficult ways to parallelization (few hundreds cores, <3000 in history matching)

Future: **Many cores (up to 100 000 cores) application**

- ✓ Refined meshing (close to wells) → **Adaptive Intelligent Mesh**
- ✓ Improvement of Domain decomposition methods
  - ❖ **Time domain decomposition / Parallelization of time**
- ✓ Hybrid numerical schema for fractured reservoir
  - ❖ **Discontinuous Galerkin**

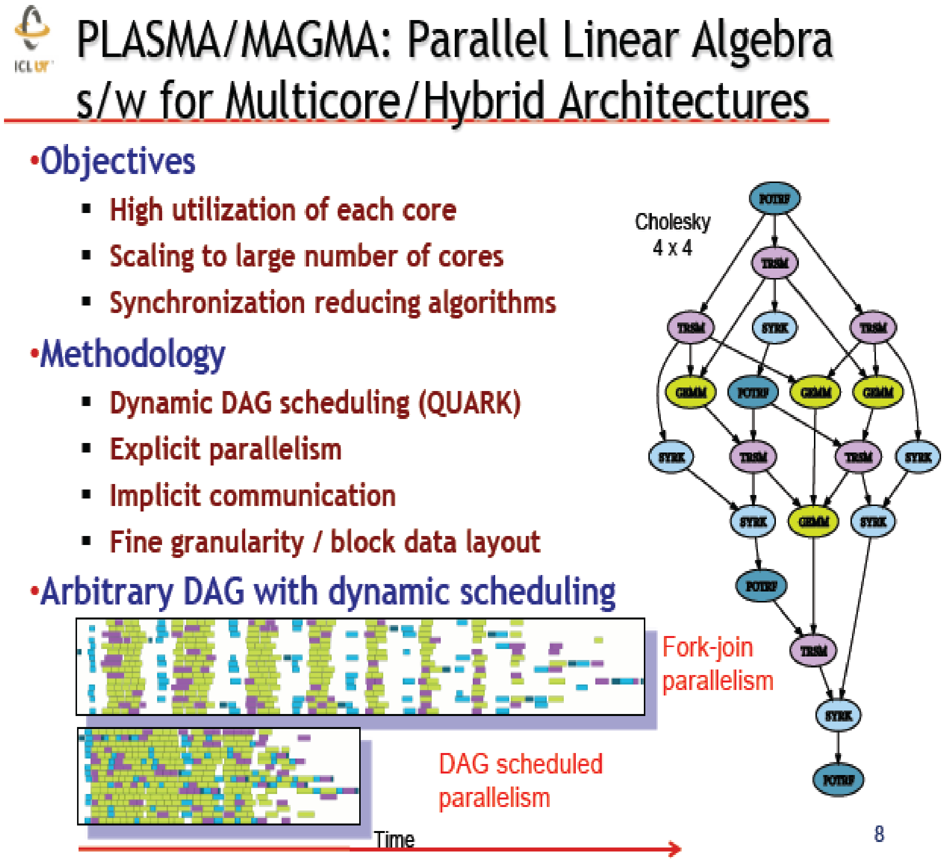


- ✓ Fine Discretization, CFL limit (IMPRES), … > Billons meshes
- ✓ New linear algebra:
  - ❖ Factorization, Directed Acyclic Graphs (DAG)
  - ❖ **Communication Avoiding Algorithms**
  - ❖ Performing Embedded iterative solvers (Modified Newton)
  - ❖ **Disruptive new non linear new algebra, Qualitative Computing**
- ✓ Physics coupling: Thermal, Thermodynamic, chemistry, transport

  …..

- ✓ Multi Scale methods
  - ➢ Different time scale: split chemistry (saturation, low scale) and transport (large macro scale)
  - ➢ ***Upscaling laws* from pore network modeling**

DENSE LINEAR ALGEBRA, PLASMA *(CF. JACK DONGARRA)*

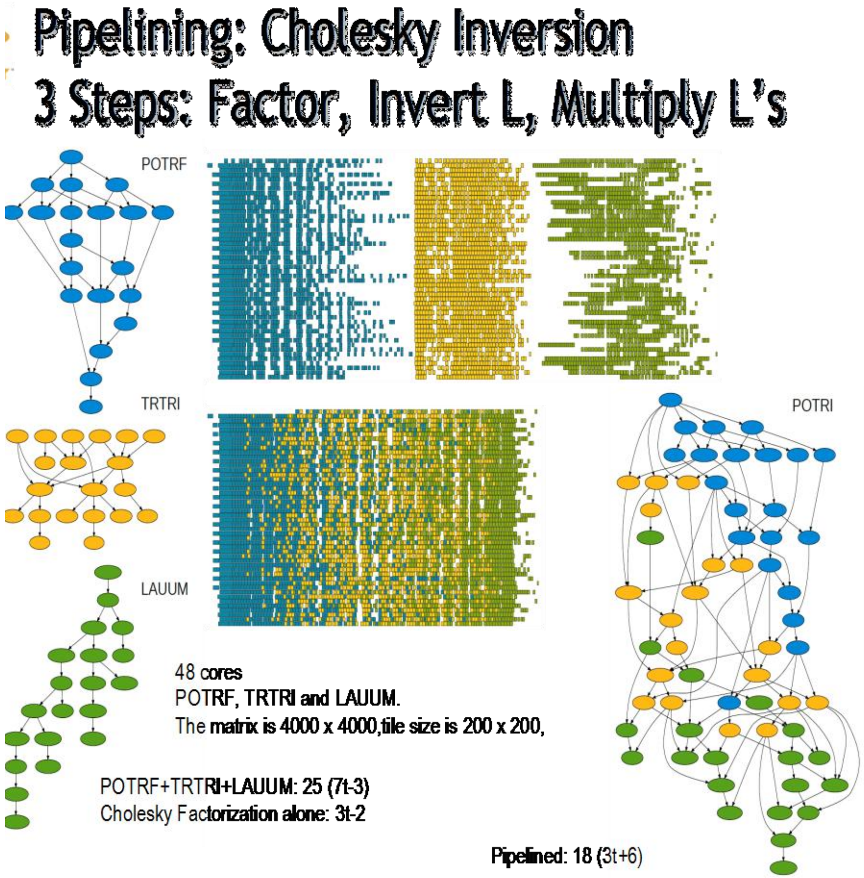


PLASMA/MAGMA: Parallel Linear Algebra s/w for Multicore/Hybrid Architectures

- Objectives
  - High utilization of each core
  - Scaling to large number of cores
  - Synchronization reducing algorithms
- Methodology
  - Dynamic DAG scheduling (QUARK)
  - Explicit parallelism
  - Implicit communication
  - Fine granularity / block data layout
- Arbitrary DAG with dynamic scheduling

Fork-join parallelism

DAG scheduled parallelism



Pipelining: Cholesky Inversion
3 Steps: Factor, Invert L, Multiply L's

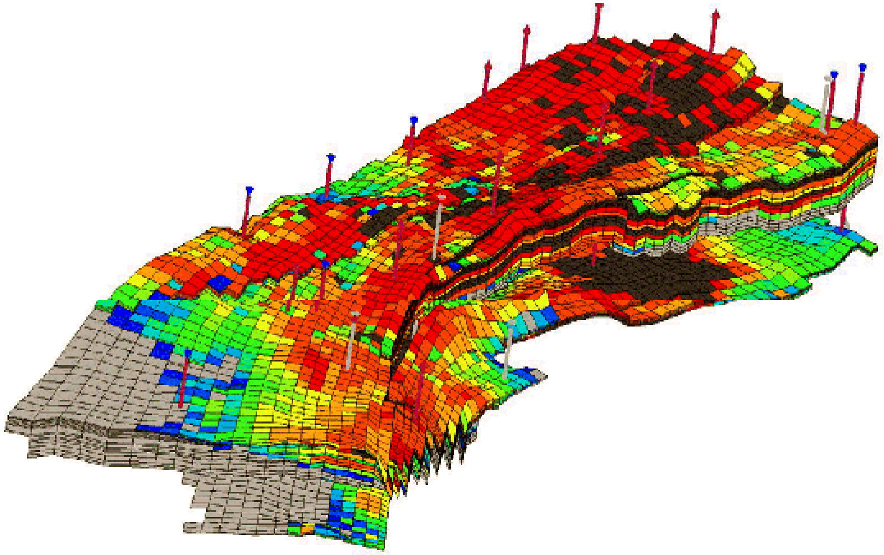
48 cores
POTRF, TRTRI and LAUUM.
The matrix is 4000 x 4000,tile size is 200 x 200,

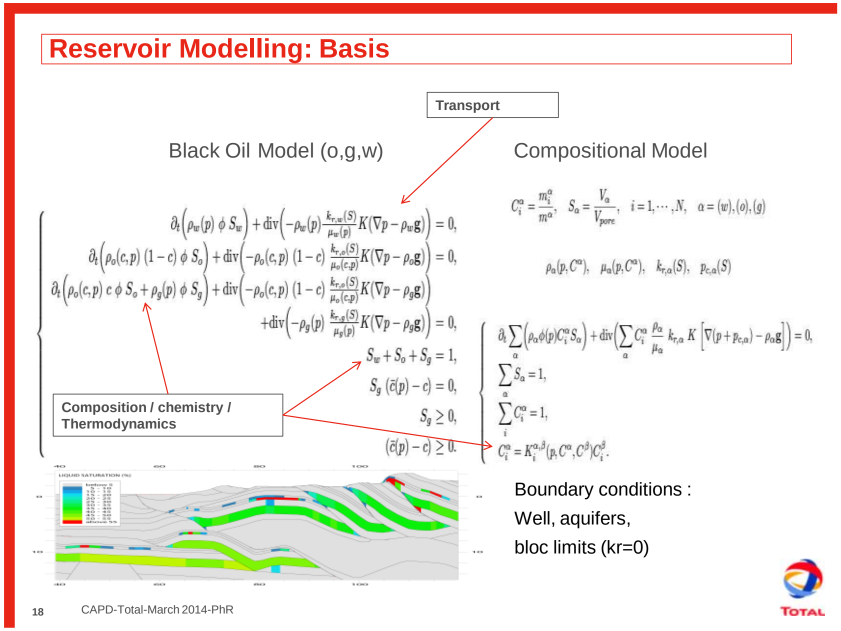
POTRF+TRTRI+LAUUM: 25 (7t-3)
Cholesky Factorization alone: 3t-2

Pipelined: 18 (3t+6)

Large improvement on tasks schedule, reducing synchronization

LARGE SCALE RESERVOIR MODELLING → BIG DATA





Reservoir Modelling: Basis

Transport

Black Oil Model (o,g,w)

$$\begin{cases} \partial_t\Big(\rho_w(p)\ \phi\ S_w\Big) + \mathrm{div}\Big(-\rho_w(p)\frac{k_{r,w}(S)}{\mu_w(p)}K(\nabla p - \rho_w \mathbf{g})\Big) = 0, \\ \partial_t\Big(\rho_o(c,p)\ (1-c)\ \phi\ S_o\Big) + \mathrm{div}\Big(-\rho_o(c,p)\ (1-c)\ \frac{k_{r,o}(S)}{\mu_o(c,p)}K(\nabla p - \rho_o \mathbf{g})\Big) = 0, \\ \partial_t\Big(\rho_o(c,p)\ c\ \phi\ S_o + \rho_g(p)\ \phi\ S_g\Big) + \mathrm{div}\Big(-\rho_o(c,p)\ (1-c)\ \frac{k_{r,o}(S)}{\mu_o(c,p)}K(\nabla p - \rho_g \mathbf{g})\Big) \\ \qquad + \mathrm{div}\Big(-\rho_g(p)\ \frac{k_{r,g}(S)}{\mu_g(p)}K(\nabla p - \rho_g \mathbf{g})\Big) = 0, \\ S_w + S_o + S_g = 1, \\ S_g\ (\bar{c}(p) - c) = 0, \\ S_g \geq 0, \\ (\bar{c}(p) - c) \geq 0. \end{cases}$$

Composition / chemistry / Thermodynamics

Compositional Model

$$C_i^\alpha = \frac{m_i^\alpha}{m^\alpha}, \quad S_\alpha = \frac{V_\alpha}{V_{\text{pore}}}, \quad i = 1, \cdots, N, \quad \alpha = (w), (o), (g)$$

$$\rho_\alpha(p, C^\alpha), \quad \mu_\alpha(p, C^\alpha), \quad k_{r,\alpha}(S), \quad p_{c,\alpha}(S)$$

$$\begin{cases} \partial_t \sum_\alpha \Big(\rho_\alpha \phi(p) C_i^\alpha S_\alpha\Big) + \mathrm{div}\Big(\sum_\alpha C_i^\alpha \frac{\rho_\alpha}{\mu_\alpha} k_{r,\alpha}\ K\ \big[\nabla(p + p_{c,\alpha}) - \rho_\alpha \mathbf{g}\big]\Big) = 0, \\ \sum_\alpha S_\alpha = 1, \\ \sum_i C_i^\alpha = 1, \\ C_i^\alpha = K_i^{\alpha,\beta}(p, C^\alpha, C^\beta) C_i^\beta. \end{cases}$$

LIQUID SATURATION (%)

Boundary conditions :
Well, aquifers,
bloc limits (kr=0)

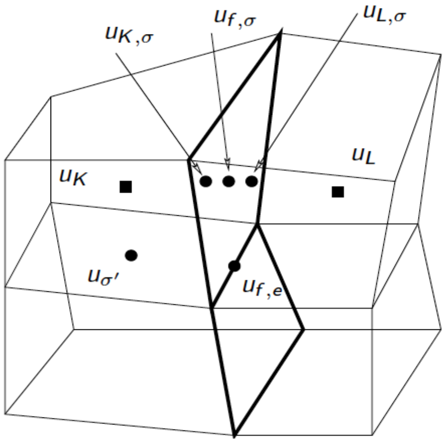
18 CAPD-Total-March 2014-PhR

Test:

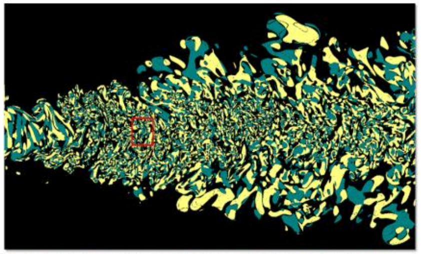
Finite Volume on 1 Billion Cells

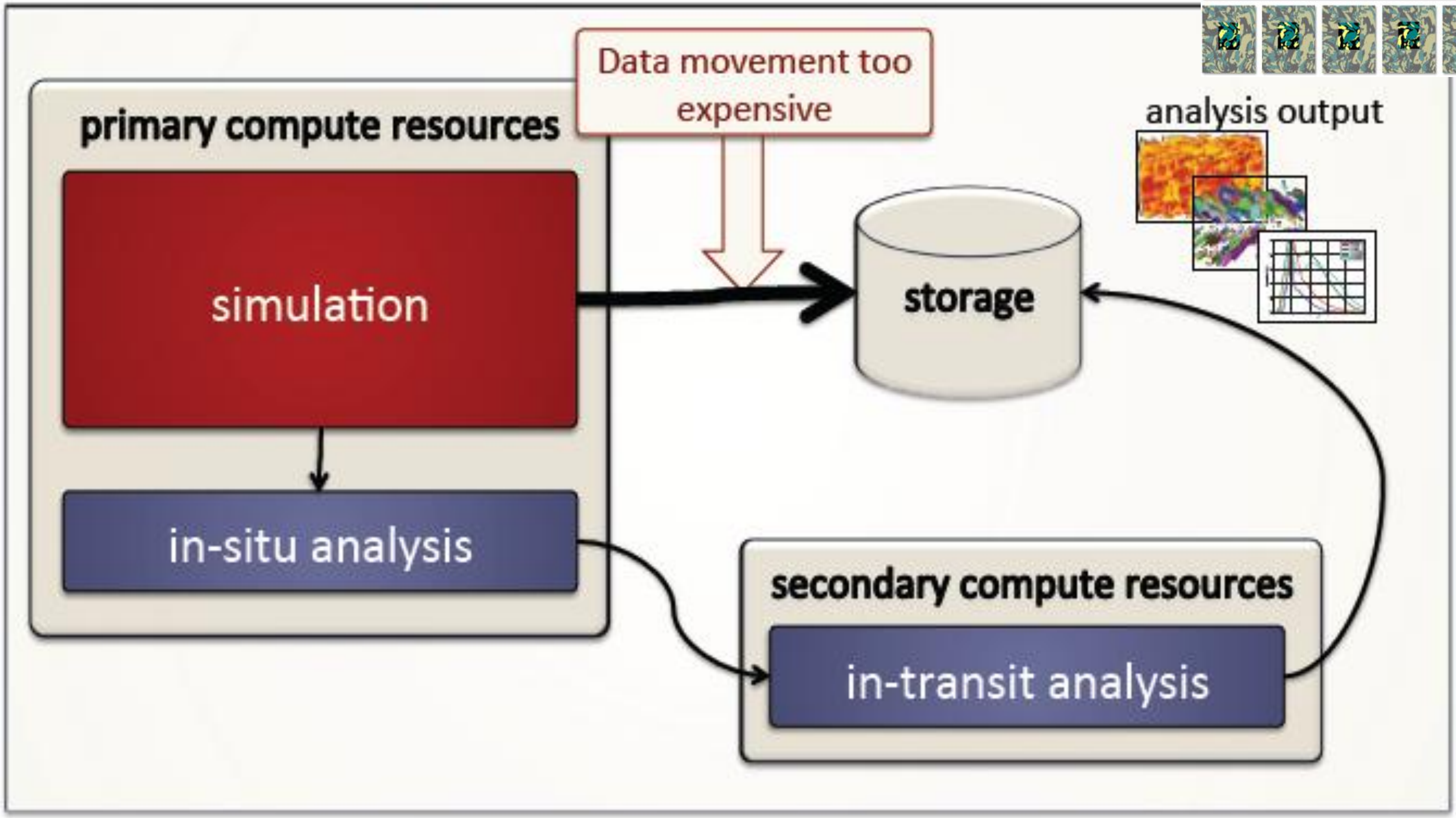
Uniform value of P by 1000 cells

Generation of 350 TB by Run
Storage?? Post processing??? Restart??



The curse of too much data is causing a shift to concurrent analysis workflows





Data movement too expensive

primary compute resources

simulation

in-situ analysis

storage

analysis output

secondary compute resources

in-transit analysis

Post-Moore’s law scaling: compute power increasing faster than I/O

IN SITU TECHNIQUES AND METHODS

Data Reduction

The transform by itself is reversible, and does not compress the data

Subsample, Single precision or double precision, Direct scalar quantization, Adaptive scalar quantization, Vector quantization (VQ) or block quantization (Linde-Buzo-Gray (LBG) algorithm similar to the K-means method in data clustering)

Transform-based compression: FT, Discrete Cosine Transform DCT, Wavelet Transform

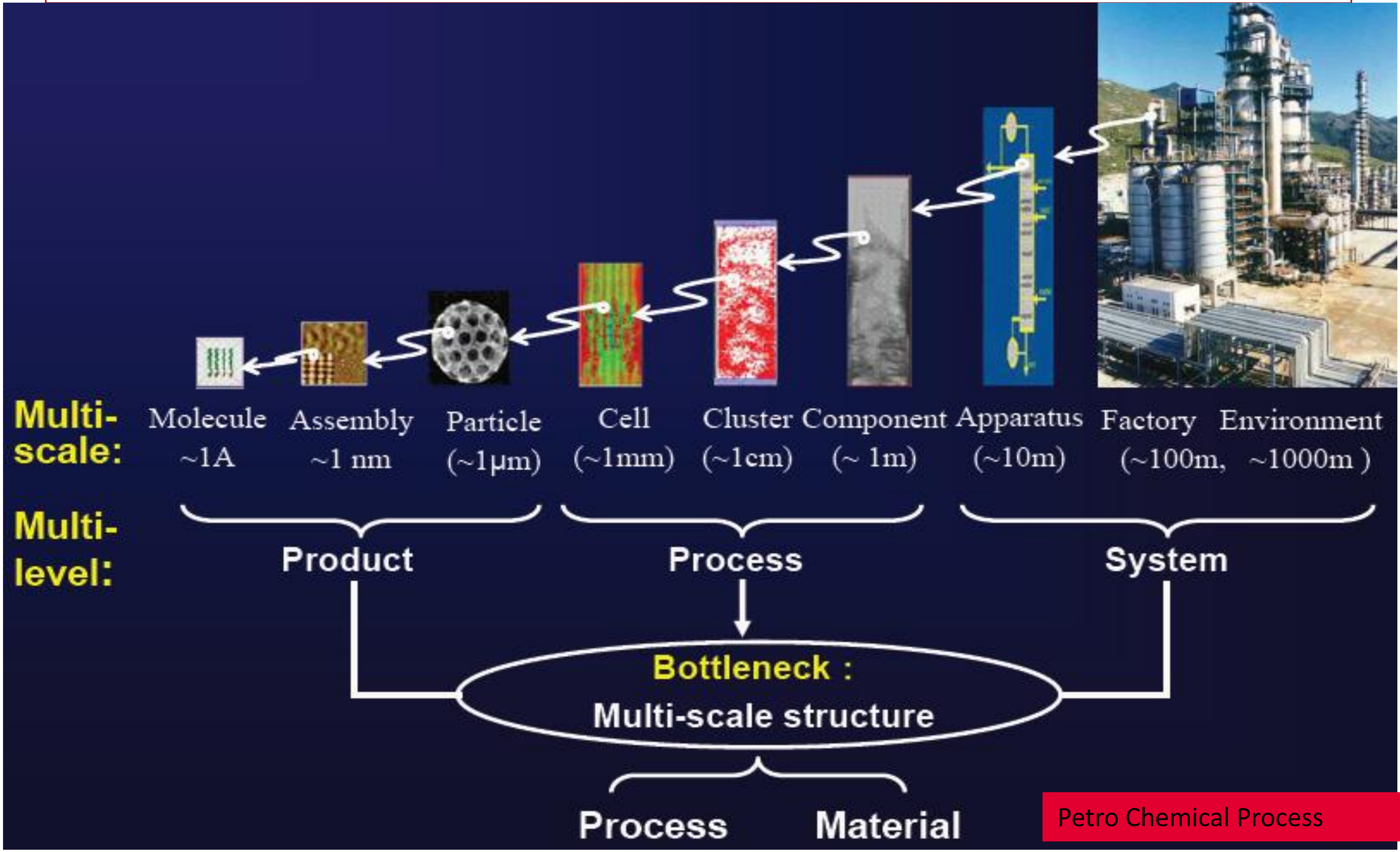
Feature Extraction

Large-scale scientific simulations generate massive amounts of data that must be validated and analyzed for understanding and possibly new discovery.

Quality Assessment

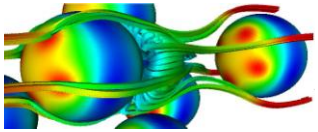
Issues In Situ Visualization

HPC FOR INDUSTRIAL MULTI SCALE PROBLEMS

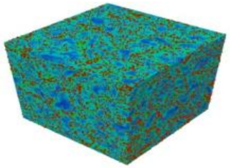


Petro Chemical Process

MULTI SCALE CFD : FCC RISER / MULTI SCALE - HPC



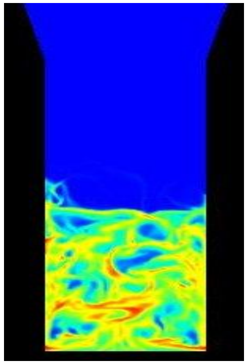
Micro (cata)



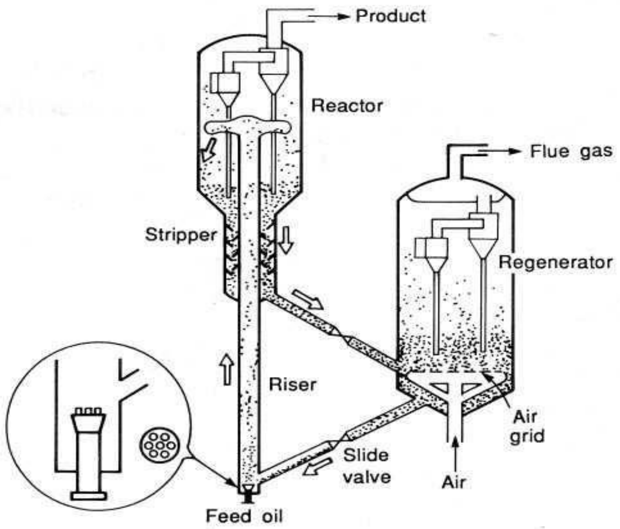
Meso (cm^3?)

Multi Scale in FCC Turbulence

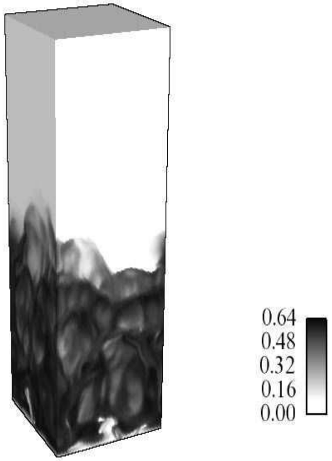
Macro (m)



Fluid Catalytic Cracking



Experimental



Simulation

Snapshot of a the particle volume fraction field
In the three-dimensional fluidized bed.

Neptune Many cores Runs

Scalability proven up to 4096 cores

- **3D Validation**
- **Pilot scale validation**
- **Validation in dilute area (TDH, transport disengagement height).**
- **Mesh up to 3 M cells on bubble / laminar / turbulent regime**
- **Mesh sensitivity**
- **Neptune optimum = 10 000 cells/core**

But : imental

- **Need much more cores to simulate 3D industrial scale Riser experimental**
- **Multi Scale need HPC**

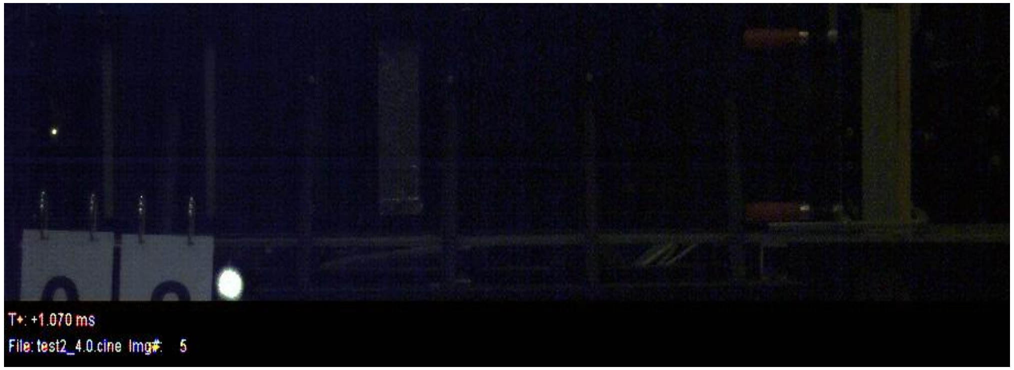
HPC AND SAFETY: MULTI SCALE IN EXPLOSIONS


Buncefield 2007

Experiments

Performed by

cmr Gexcon

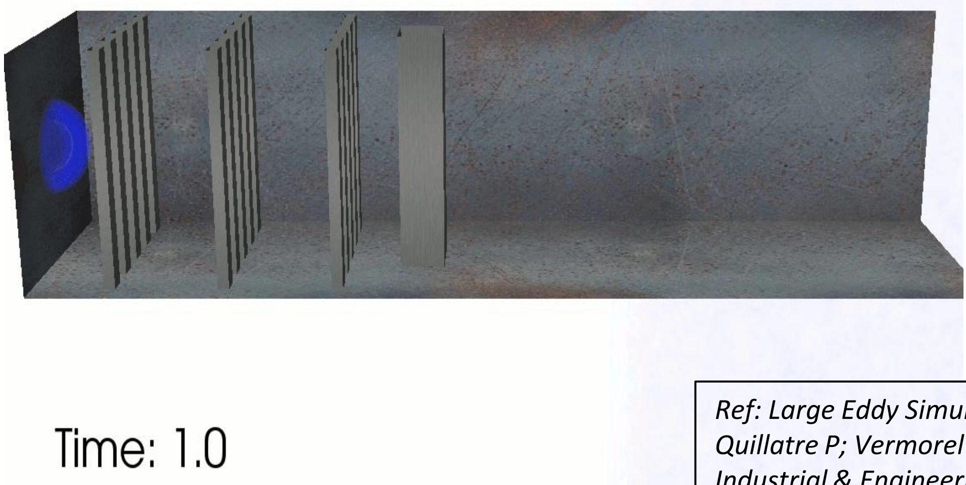


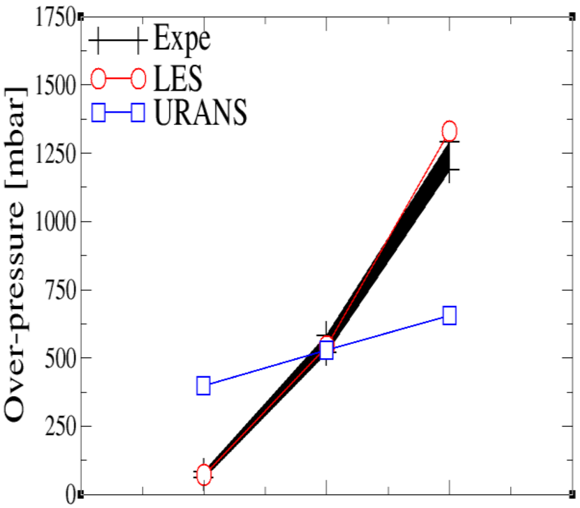
Understanding for safety

Integration in “on using” codes of danger studies

(large economical issue)

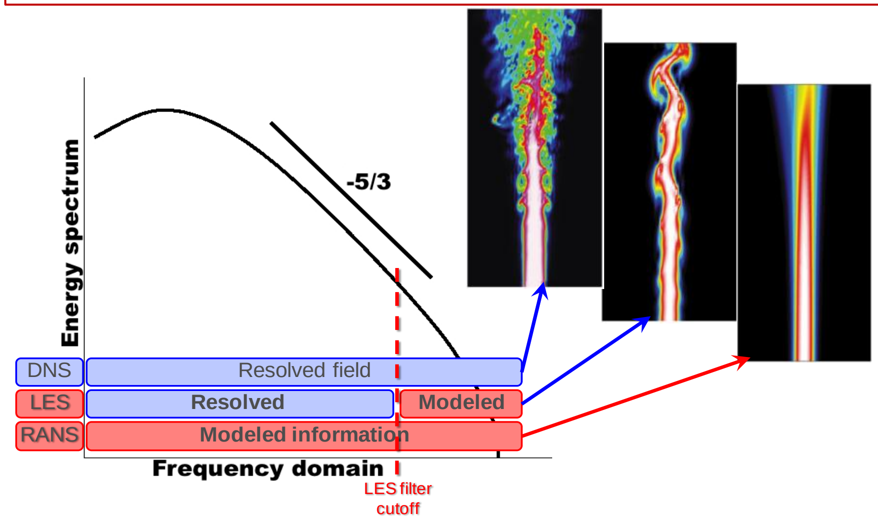
Simulation
LES





Ref: Large Eddy Simulation of Vented Deflagration
Quillatre P; Vermorel O; Poinsot T; Ricoux Ph
Industrial & Engineering Chemistry Research , Feb.2013

MULTI SCALE IN EXPLOSIONS: LES FILTERING – NS EQUATIONS



Resolved **Subgrid**

$$f = \boxed{\overline{f}} + \boxed{f'}$$

Navier-Stokes Equations for a compressible reactive flow:

$$\begin{aligned}
\frac{\partial \overline{\rho}}{\partial t} &+ \frac{\partial(\overline{\rho}\widetilde{u}_i)}{\partial x_i} = 0 \\
\frac{\partial(\overline{\rho}\widetilde{u}_i)}{\partial t} &+ \frac{\partial(\overline{\rho}\widetilde{u}_i\widetilde{u}_j)}{\partial x_j} + \frac{\partial \overline{p}}{\partial x_i} = \frac{\partial \overline{\tau}_{ij}}{\partial x_j} + \frac{\partial \overline{\tau}^t_{ij}}{\partial x_j} \\
\underbrace{\frac{\partial \overline{\rho}\widetilde{E}}{\partial t}}_{Unstationnary\ terms} &+ \underbrace{\frac{\partial \overline{\rho}\widetilde{E}\widetilde{u}_j}{\partial x_j} + \frac{\partial \overline{pu_j}}{\partial x_j}}_{Non-Viscous\ terms} = \underbrace{\frac{\partial \overline{\tau}_{ij}\widetilde{u}_i}{\partial x_j} - \frac{\partial \overline{q}_i}{\partial x_i}}_{Viscous\ terms} + \underbrace{\frac{\partial \overline{\tau}^t_{ij}\widetilde{u}_i}{\partial x_j} - \frac{\partial \overline{q}^t_i}{\partial x_i}}_{Subgrid\ terms} + \underbrace{\boxed{\overline{\dot{\omega}_T}} + \boxed{\overline{\dot{\omega}_T}^t}}_{Chemical\ Source\ terms}
\end{aligned}$$

Only the terms below grid size are modelled

Resolved **Modelled**

HPC & Numerical Simulation in Hutchinson
Material Structure & Acoustics compounds

« One of key technologies contributing to be a world Leader »

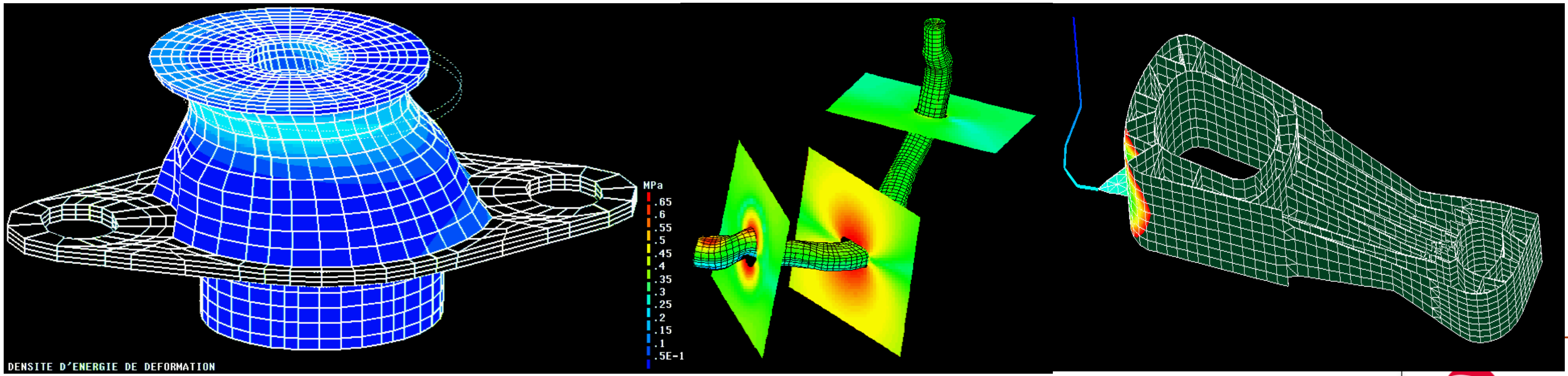
Permitted Source : Hutchinson

New Products Development Assistance

- Performances forecast (static & dynamic stress, acoustic, …)
- Length of life warranty (constraints, distortions, ...)
- Optimization

Process Implementation Assistance : Injection, Extrusion ..

- Equipment Conception (molds, tools,..)
- Global Process Monitoring , optimization and Control : extrusion, injection, vulcanisation, pressing,…

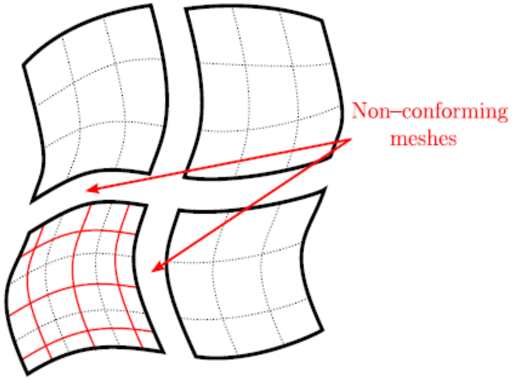


NEW FEM approach : Iso geometry (IGA) : FEM vs IGA mesh

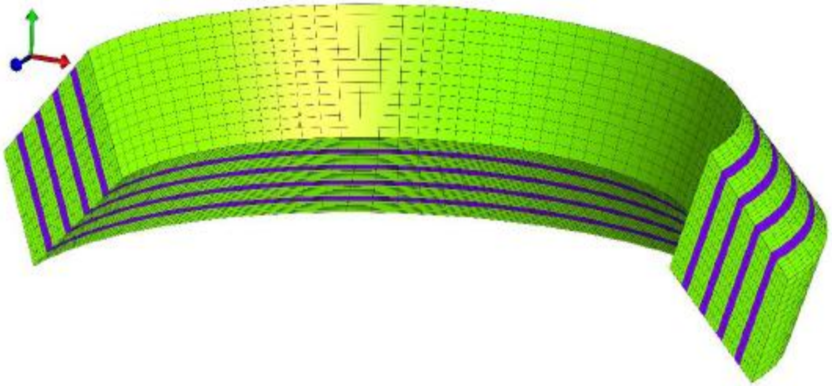
Objective: New Efficient Mechanical Structure Simulation Method

CADs (like IRIT) use NURBS (non-uniform rational B-splines)

IGA use NURBS for the PDE solver

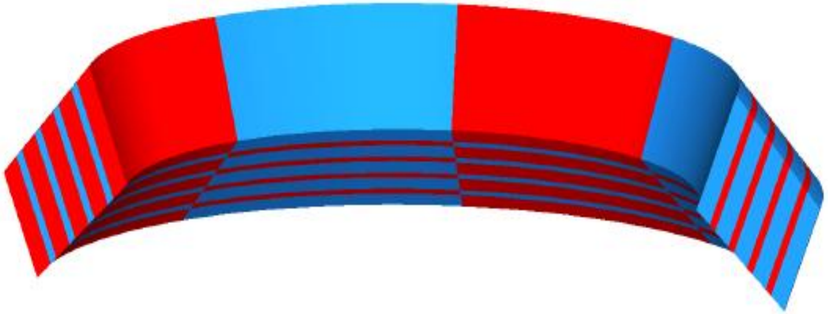


CHALLENGE: treatment of non-matching patch interfaces, regular gluing when possible.



19800 elements

67626 dofs

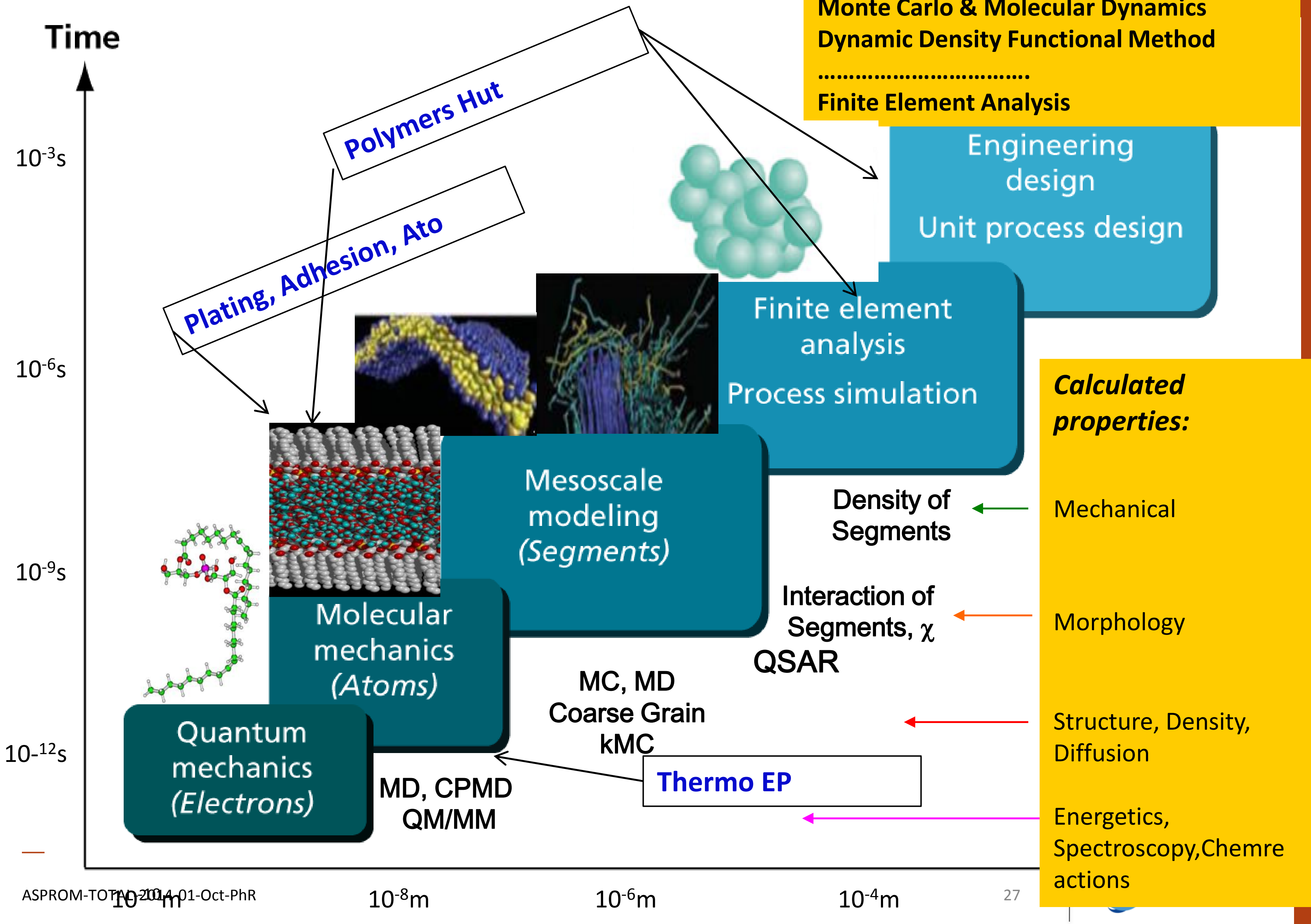


36 elements

$p = 2 \rightarrow$ 1701 dofs

$p = 3 \rightarrow$ 3888 dofs

Molecular Simulation: Multiscale Modeling



Computational Tools:
Density Functional Theory
Monte Carlo & Molecular Dynamics
Dynamic Density Functional Method
……………………………
Finite Element Analysis

Calculated properties:

Mechanical

Morphology

Structure, Density, Diffusion

Energetics, Spectroscopy,Chemreactions

HPC IN TOTAL

3 PF

+ Potential
External Resources
PRACE, INCITE, …

+

RC homogeneous
Catalyst polymer
& Heterogeneous
catyalyst

1 Cluster

IBM 4TF Cluster +
3 Clusters
CdR Hutchinson

Hut
TP +
elastomer,
Adhesion

1 Cluster M&S
Located in CdR
Hutchinson

M&S
Lubricant

128 quadricore Intel
Nehalem, Westmere
(512 Cores)

Atotech
Adhesion
Plating

1 Cluster
Atotech

+ Existing 4TF Cluster

2 Clusters
Labo Montpellier
Modeling & development of
Multifunctional solids

1 Cluster
RC Linear Programming

TOTAL NUMERICAL SIMULATION & HPC APPLICATIONS

- ☐ **Oil & Gas (E&P)**
  - ➢ **Seismic, Reservoir, Wells, …**
  - ➢ **Pipes, Risers, complex fluids transport**
  - ➢ **Separation, Hydro cyclone (Oil Sands), FPSO, …**
  - ➢ **Molecular Simulation for Thermodynamics**

Safety / Explosion

Turbulence, Flame speed, detonation, …

- ☐ **Refining**
  - ➢ **Fluidized Bed Reactors : FCC, DHC, …**
  - ➢ **Combustion, Engine combustion, …**
  - ➢ **Hydro conversion of heavy hydrocarbons, Fischer-Tropsch Reactors**
  - ➢ **Molecular Simulation for new lubricant & tribology**

Safety / Explosion

Turbulence, Flame speed, detonation, …

- ☐ **Chemical Plants**
  - ➢ **Slurry Loop, Polymerization, Swelling (PE*)***
  - ➢ **Multiphase Catalytic Reactors**
  - ➢ **Molecular Simulation for Catalyst**

Safety / Explosion

Turbulence, Flame speed, detonation, …

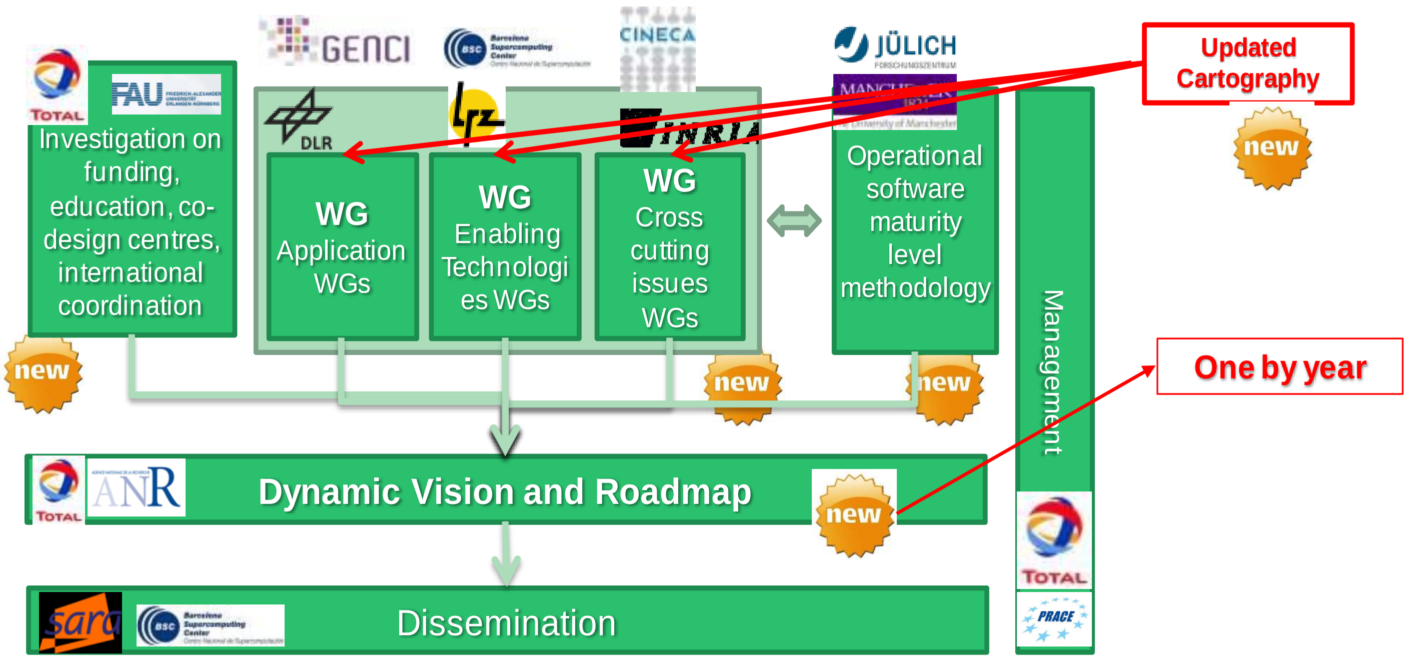
- ☐ **Specialties**
  - ➢ **Compound Materials Deformation, Structure Calculations (Hutchinson)**
    - ➢ ***Meso Scale: RepresentativeVolume Element (RVE)***
  - ➢ **Acoustics in compound materials (Hutchinson)**
  - ➢ **Coating in micro electronics (Atotech)**
  - ➢ **Adhesive (Bostik)**
  - ➢ **Molecular Simulation for interface definition of adhesives, polymer compounds, …**

Safety / Explosion

Turbulence, Flame speed, detonation, …

TOTAL IS THE LEADER OF THE EXASCALE EUROPEAN SOFTWARE INITIATIVE (EESI)

European Exascale Software Initiative 2



Investigation on funding, education, co-design centres, international coordination

WG Application WGs

WG Enabling Technologies WGs

WG Cross cutting issues WGs

Operational software maturity level methodology

Management

Updated Cartography

One by year

Dynamic Vision and Roadmap

Dissemination

All documents on EESI

WP, WG Reports, All Final Reports

Roadmap, Vision & Recommendations

http://www.eesi-project.eu

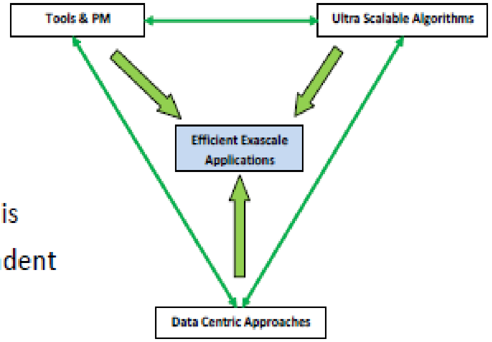
D7.2
2014 Update
Vision & Recommendations

CONTRACT NO EESI2 312478
INSTRUMENT CSA (Support and Collaborative Action)
THEMATIC INFRASTRUCTURE

Due date of deliverable:
Actual submission date: 30th July 2014
Publication date:
Start date of project: 1 September 2012 Duration: 34 months
Name of lead contractor for this deliverable: TOTAL SA, Philippe RICOUX

The roadmap towards the implementation of efficient Exascale applications and the consecutive recommendations are gathered in three large pillars:

- Tools & Programming Models
- Ultra Scalable Algorithms
- Data Centric Approaches



Note that the Data Centric vision is very new in Europe but is essential for approaching the ultra complex and interdependent challenges of Extreme Computing and Extreme Data.

CONCLUSIONS

Numerical Simulation, HPC, Real Time data processing, are for TOTAL group **unavoidable transverse technologies for facing challenges of oil industry**

More and More Heavy Oil Prospection and Production, Deep Conversion Unit,, Asset Maximization, Leadership on some markets (Specialties, Petrochemical) , Energy Consumption Reduction, Global Warming

Explore and develop New Trends, New Methods, New Computer Science

Optimize Coupling Architecture/Algorithm/Application
Computing/Numerical/Physic (or chemical)

Thanks to HPC, internal teams must be Multidisciplinary

GeoPhysics, Physics, Chemistry… , Maths, Numerics, Computer Sciences, ...

Working with external Research Partnership (academic & suppliers)

THANK YOU FOR ATTENTION

Q/A