Numerical simulation and HPC in Oil & Gas Industry
TOTAL Group

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TOTAL/DS

Calculs Parallèles et Applications – ASPROM- 1er Octobre 2014
TOTAL: POOL OF ENERGIES

- Heavy Oil production

- E.O.R. simulations
  - thermal
  - chemical

- Polymers

- Heavy Oil production

- ASPROM-TOTAL-2014-01-Oct-PhR

- Storage polysaccharides
  - Saccharose
  - Starch

- Structural polysaccharides
  - Celluloses
  - Hemicelluloses

- Simple degradation
  - Dilute acid
  - Amylase

- Complex degradation
  - Cellulase
  - Hemicellulase

- Glucose
- Fructose
- Xylose
- Arabinose
- C6
- C5
- C2
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:** Geology, Geomechanics, **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, ...
HPC allows Combination of

✓ More and more accurate physic modeling
✓ More and more performing numerical schema
✓ Stochastic methods, Robust optimization
SEA ICE MODELLING

Dynamics of an Assembly of Rigid Ice Floes

Sea Ice Floes

Towards an accurate continuum dynamical model for sea ice

Numerical simulation of ice performance of ships

Forecast of gas dispatch schedule from Arctic area
SEISMIC DATA

Conventional NAZ

WAZ Explo 2
Larger Xline offset

RAZ/Full WAZ
Development

Cost for ~200 km²

7-9 M$
30-70M$
50-110M$

Seismic and geological Data
unconventional

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HPC for Depth Imaging: 3 fundamental steps

1. Numerical analyst
   Numerical Methods

2. Geo-physics
   Maths for Physic Modeling

3. Embarrassingly Parallel approximation

HPC Computing
HPC implementation

100,000 Cores + Options GPU

Studies
WEST AFRICA
DEPTH IMAGING: AN ALGORITHM

\[(\nabla^2 - \frac{1}{c^2} \frac{\partial^2}{\partial t^2}) u(r, t) = 0.\] Wave Equation (hyperbolic)

\[u(r, t) = A(r)T(t).\] Approximation:
Helmholtz Equation (elliptic)

\[(\nabla^2 + k^2)A = 0.\]

Billions unknown variables,
Large solvers

Common Azimuth Migration: a brief description of the algorithm

Depth loop over \(Z\) sequential loop: dependence in \(Z\)
Frequency loop over \(\omega\) parallel loop: no dependence in \(\omega\)

Helmholtz Migration: massively parallel implementation

Data: 100 TBytes to 1 Pbytes
I/O Parallelization!

Link with computer science
FWI ALGORITHM

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

FWI is the best Approach today to determine reservoir properties.

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.

A data misfit results after several iterations, producing local and global minima depending on the starting models.
THE TOP500 LIST: TWENTY YEARS OF INSIGHT INTO HPC PERFORMANCE

Projected Performance Development  

Oil & Gas Companies

Oil & Gas Companies

TOTAL  
2.3 PF  2013 CPU

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, ...

**Challenge: Integrated Approach of Oil System :**

**interaction geology – geophysic :** foot hills, non conventional reservoirs, ...

**Same Roadmap in BP, Chevron**

**Absolute Need of multi skills Multidisciplinary teams**
HPC & Reservoir Modeling  From Pore to Darcy

Needs of new and efficient reservoir simulations

- Heavy oil: combining Maxwell law + Darcy law, simulating SAGD (evolution of the steam chamber)
- E.O.R. mechanisms requiring thermo-hydraulic modeling, chemical reaction simulation...
- CO2 project: simulation of storage (CO2 migration) and well integrity, predicting long term behavior

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

Multi Fluids including polymers, MultiPhase Flows, Multi Physics, including geomechanic, Chemistry, ...

Multi Scale, Different Physics at different scales
Upscaling laws from nanometer to meter

Essential for new fractured reservoirs, Shale Oil, Shale Gas

Matching performance needs by applying parallelism techniques at all levels
Maximization of Oil reservoir production, Oil recovery (EOR)

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

$$u_\beta = -k_\beta \frac{\partial p_\beta - \rho_\beta g}{\mu_\beta}$$

for each phase of each component

Where $\beta$ indicates the phase, $k_\beta$ 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 pressure is negative), and $\mu_\beta$ the viscosity in the phase.

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

Observed data not at the same scale than models
RESERVOIR MODELLING: COMPLEXITY

- Reservoir: geostatistic fine representation of $K$ (permeability tensor), $\Phi$ (flows vector)
- Stochastic PDE: Uncertainties
- Homogenization on a meshing: $K$, $\Phi$ constant by mesh
- $kr(S)$, $Pc(S)$ by lithology (estimation from transport at pore level)
- Anisotropy: $K_{xy}/K_z$ 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 $\Delta t$
- Locally conservative schema in space
- Stability of multi phase transport (approx)
- Local Explicit schema for flows ($\Phi$) 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**

Large improvement on tasks schedule, reducing synchronization
Test:

Finite Volume on 1 Billion Cells
Uniform value of P by 1000 cells

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

Reservoir Modelling: Basis

Transport

Black Oil Model (o,g,w)
Compositional Model

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

Composition / chemistry / Thermodynamics

Transport

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

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

Multi-scale:
- Molecule (~1A)
- Assembly (~1 nm)
- Particle (~1 µm)
- Cell (~1 mm)
- Cluster Component (~1 cm)
- Apparatus (~10 m)
- Factory (~100 m, ~1000 m)

Multi-level:
- Product
- Process
- System

Bottleneck:
Multi-scale structure

Process Material

Petro Chemical Process
**MULTI SCALE CFD : FCC RISER / MULTI SCALE - HPC**

Snapshot of 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

**Experimental**

**Simulation**

**Fluid Catalytic Cracking**

**Multi Scale in FCC**
- Macro (m)
- Meso (cm³?)
- Micro (cata)

**Micro (cata) Meso (cm³?) Multi Scale in FCC Turbulence**
HPC AND SAFETY: MULTI SCALE IN EXPLOSIONS

Experiments
Performed by Gexcon

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

Simulation LES

Time: 1.0

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 field
Resolved
Modeled information
Modeled
LES filter
cutoff
DNS
RANS
LES

Navier-Stokes Equations for a compressible reactive flow:

\[
\begin{align*}
\frac{\partial \rho}{\partial t} & + \frac{\partial (\rho \tilde{u}_i)}{\partial x_i} = 0 \\
\frac{\partial \rho \tilde{E}}{\partial t} & + \frac{\partial (\rho \tilde{E} \tilde{u}_j)}{\partial x_j} + \frac{\partial \rho \tilde{u}_j}{\partial x_j} = \frac{\partial \tau_{ij}}{\partial x_j} - \frac{\partial q_i}{\partial x_j} \\
\end{align*}
\]

Unstationary terms
Non-Viscous terms
Viscous terms
Subgrid terms

Only the terms below grid size are modelled

Resolved
Subgrid

\[
f = \overline{f} + f'
\]
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
  \( p = 2 \rightarrow 1701 \text{ dofs} \)
  \( p = 3 \rightarrow 3888 \text{ dofs} \)
Molecular Simulation: Multiscale Modeling

Calculated properties:
- Mechanical
- Morphology
- Structure, Density, Diffusion
- Energetics, Spectroscopy, Chemical actions

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

Time

- $10^{-3}$ s
- $10^{-6}$ s
- $10^{-9}$ s
- $10^{-12}$ s

Interaction of Segments, $\chi$

Density of Segments

Molecular mechanics (Atoms)

Quantum mechanics (Electrons)

Mesoscale modeling (Segments)

Finite element analysis

Process simulation

Finite Element Analysis

Engineering design

Unit process design

Polymers Hut

Plating, Adhesion, Ato

MC, MD, CPMD

kMC

Thermo EP

MC, MD

Coarse Grain

QM/MM

10^{-12} m

10^{-8} m

10^{-6} m

10^{-4} m

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HPC IN TOTAL

128 quadricore Intel Nehalem, Westmere (512 Cores)

- RC homogeneous Catalyst polymer & Heterogeneous catalyst

- Atotech Adhesion Plating

- 1 Cluster

- 1 Cluster Atotech

+ Existing 4TF Cluster

+ IBM 4TF Cluster + 3 Clusters CdR Hutchinson

+ 1 Cluster M&S Located in CdR Hutchinson

+ 2 Clusters Labo Montpellier

- Model & development of Multifunctional solids

- 1 Cluster RC Linear Programming

+ Potential External Resources PRACE, INCITE, ...

- Hut TP + elastomer, Adhesion

- M&S Lubricant

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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

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

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

- **Specialties**
  - Compound Materials Deformation, Structure Calculations (Hutchinson)
    - *Meso Scale: Representative Volume 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)

All documents on EESI WP, WG Reports, All Final Reports
Roadmap, Vision & Recommendations
http://www.eesi-project.eu

D7.2
2014 Update
Vision & Recommendations

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