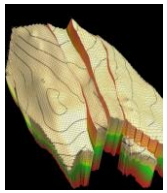
TOTAL
COMMITTED TO BETTER ENERGY

Multiple applications of HPC and Numerical Simulations in TOTAL Group

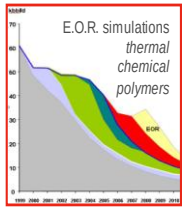
Philippe Ricoux

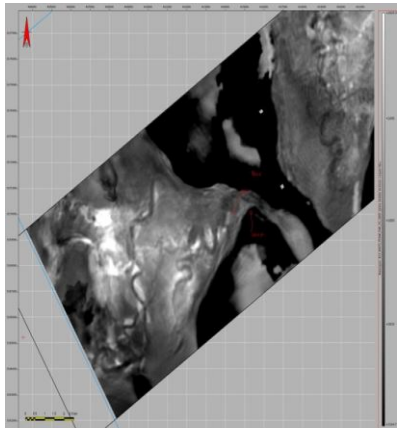
DG/DS

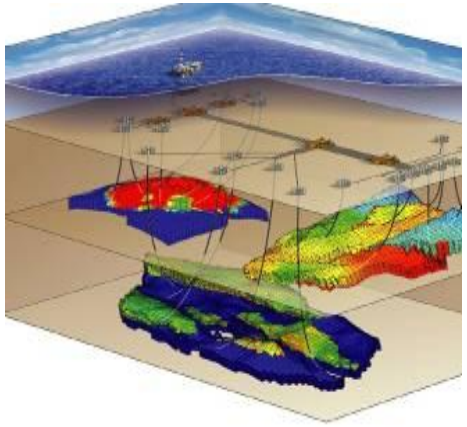
TOTAL: POOL OF ENERGIES , STRATEGIC CHOICES

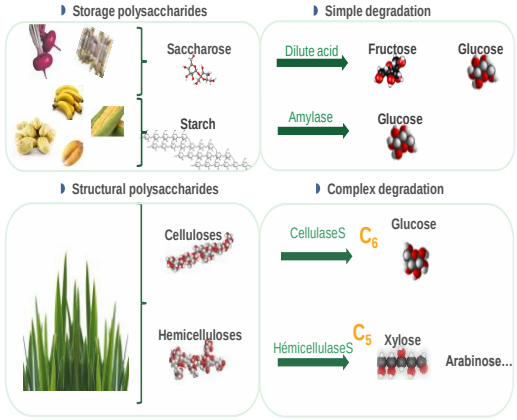


Heavy Oil production









New TOTAL BRANCH

Electricity Provider & Integrator

Generation, Storage, Smart Energy

+ CO2, Preparing deployment of CCS

+ Gas , H2

A WORLD OF PROMISING ADVANCED TECHNOLOGIES

Facing energy future: implications for R&D strategy

- IT Technologies
- Material sciences
- Biotechnologies
- Nanotechnologies
- New analytical techniques
- New Energies
- Energy Efficiency
- …

VERY IMPORTANT for TOTAL which has no « National Resources » and has to be selected by other NOC (National Oil Companies) to be alive.

→ TOTAL at the TOP at least for some technologies

- **Numerical Simulation / Advanced Computing**
  - ✓ **Major implications at present**
  - ✓ **Solutions for the future**

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, …***

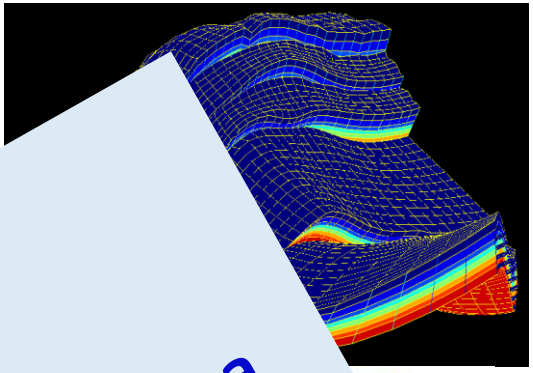
Benefits of Numerical Simulation :

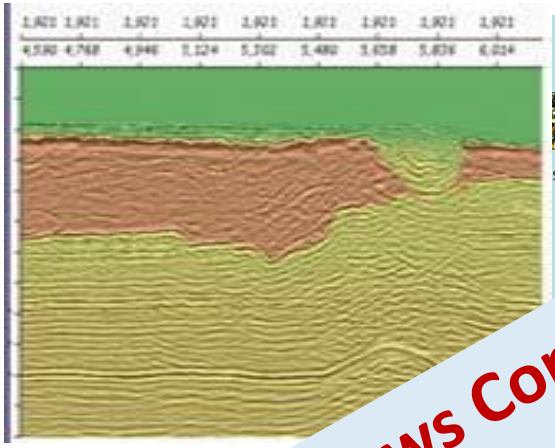
- **Better Understanding with a** ***huge reduction of errors and risks***
- **Increase range of parameters variation (closer limits)** ***with reduction of dangerous or expansive experiments***
- **Large «time saving» of development phases, before pilot**

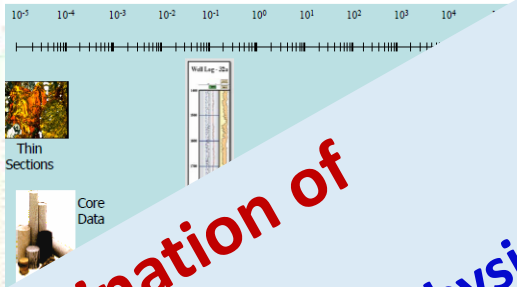
Necessary way to go further: Work together

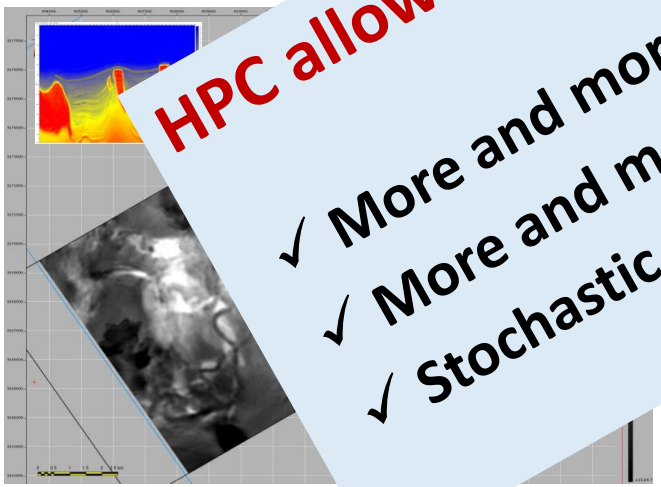
- **Collaboration, Multi disciplinary teams**: ***Share tools and algorithms, merge skill, …***
- **Multi domains** ***Team Building , workgroup : Maths, Computer Science, Applicative experts, Engineers, …***

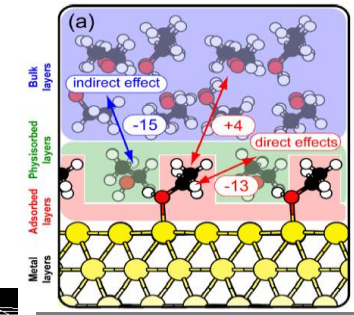
TOTAL
NUMERICAL SIMULATION AND HPC

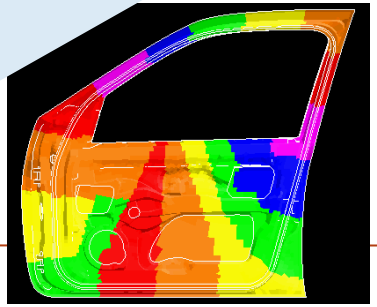


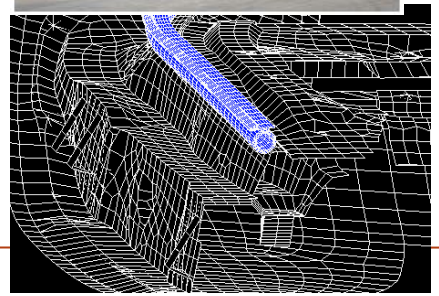


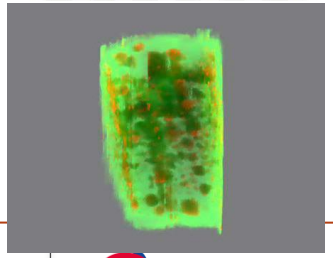










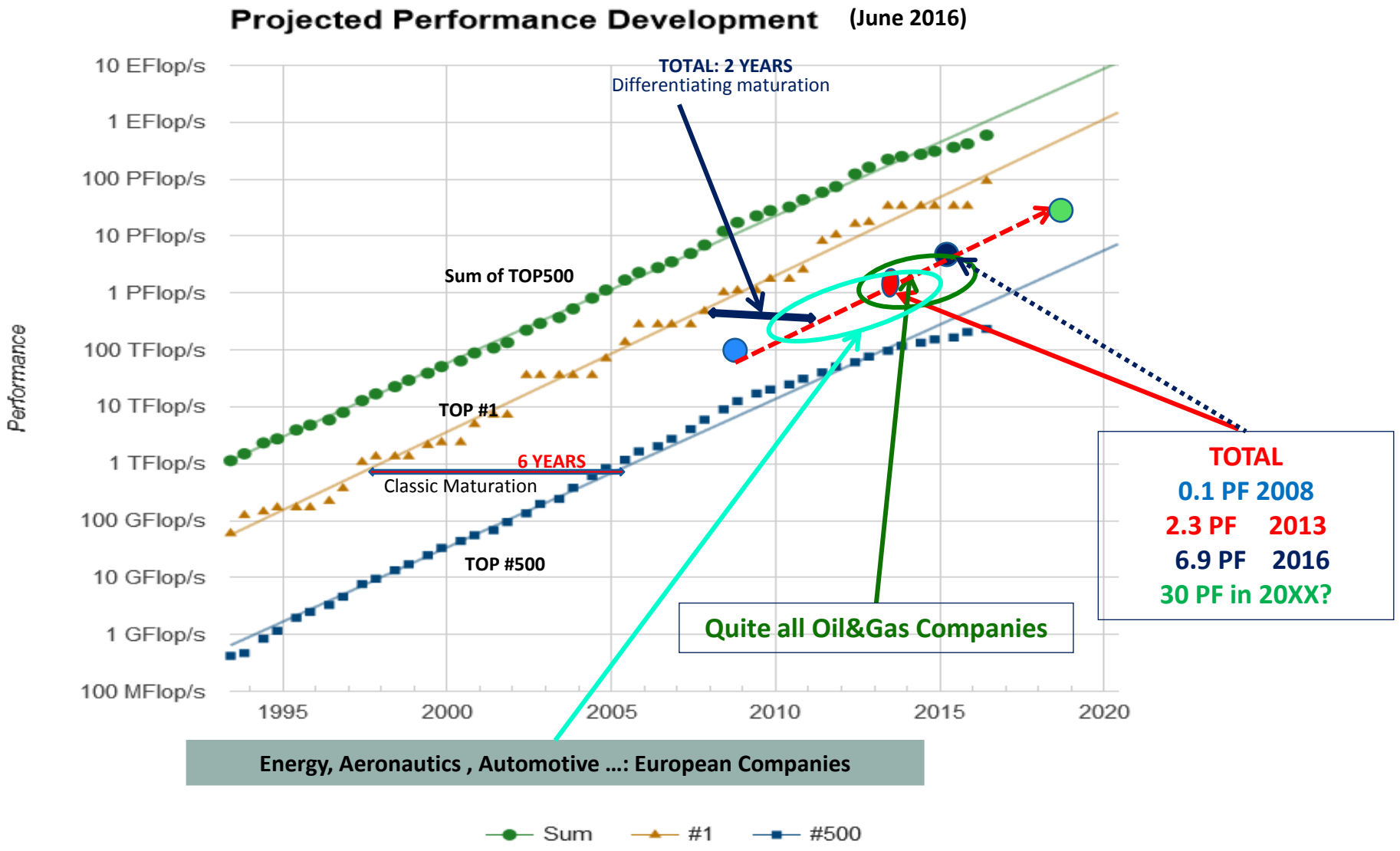


HPC allows Combination of

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

TOTAL

TOTAL well placed into HPC Performance (TOP 500)



SOME SUPER COMPUTERS

Tianhe-2 , China, 33.86 PF , CPU (Ivy Intel)

Titan , Oak Rigde, 17.59 PF, CRAY , CPU/GPU

Pangea ,TOTAL , 6.9 PF, SGI, CPU

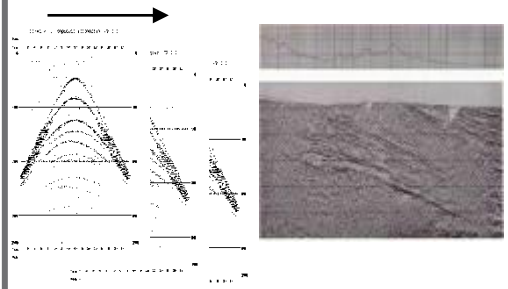
Sequoia , LLNL , 16.32 PF, IBM, CPU

CONTENT

DIVERSE NUMERICAL METHODS

- APPLICATION TO SEISMICS
- APPLICATION TO MULTI FLUIDS MULTI SCALE REACTORS
- APPLICATION TO MECHANICAL MATERIALS
- MESH, MESHLESS, ISOGEOMETRY
- IN SITU DATA PROCESSING

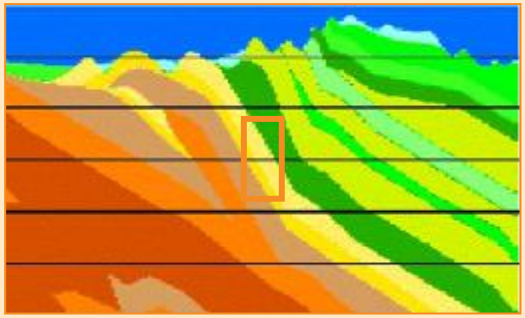
TOTAL APPLICATIONS: EXPLORATION / DEPTH IMAGING

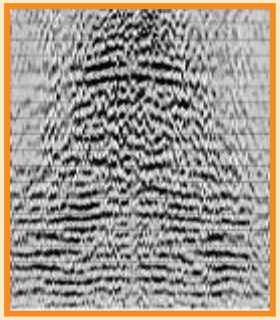


Seismic and geological Data

A – Data Acquisition

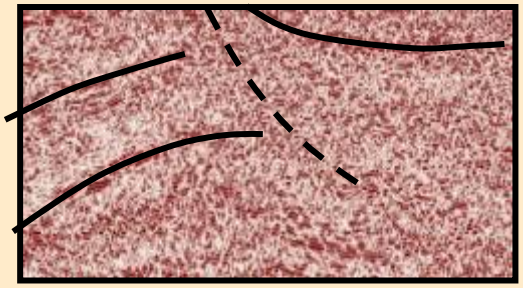
B – Seismic Depth Imaging

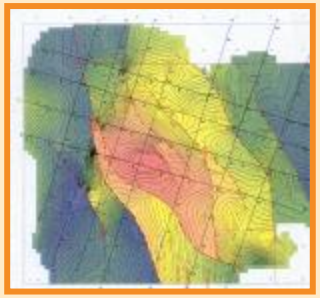




Velocity Model ~ Snap Shot

C - Structure Interpretation



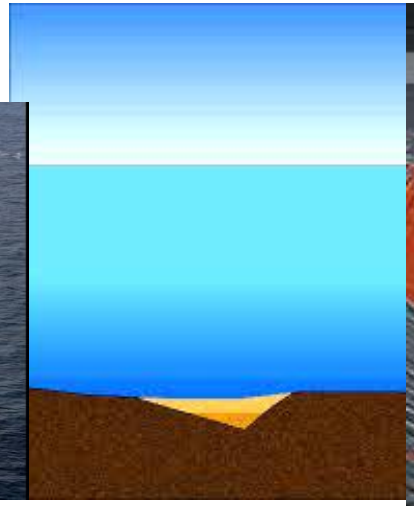


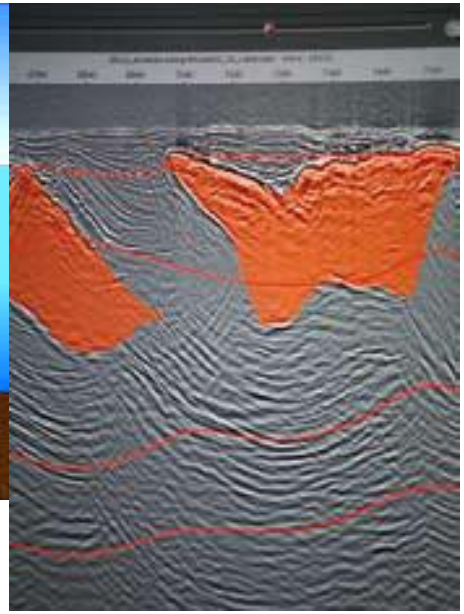
Seismic interpretation ~ Geological Study

TOTAL EP/EXPLO
TOTAL EP/R&D/NUMET
TOTAL DS + Academics

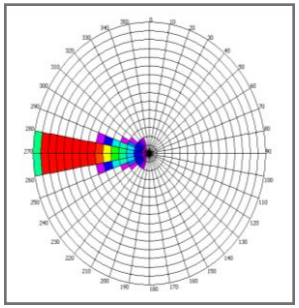
MULTIDISCIPLINARY with HPC

OFFSHORE SEISMIC DATA



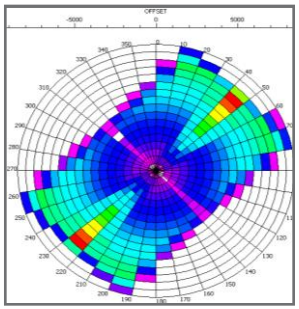


Conventional NAZ



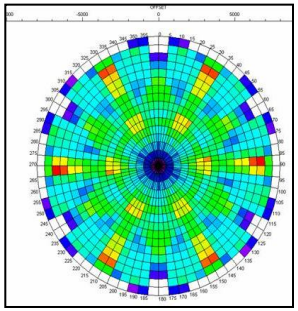
7-9 M$

WAZ Explo 2
Larger Xline offset



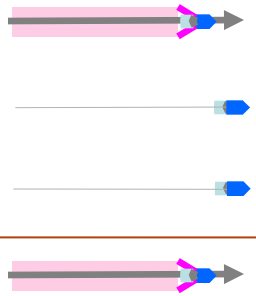
30-70M$

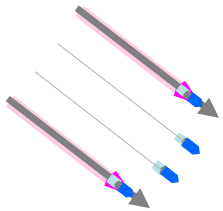
RAZ/Full WAZ
Development

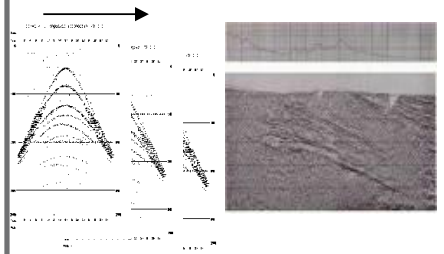


50-110M$

Cost for ~200 km²







Seismic and geological Data

unconventional

Seismic Data Matrix in Frequency Domain

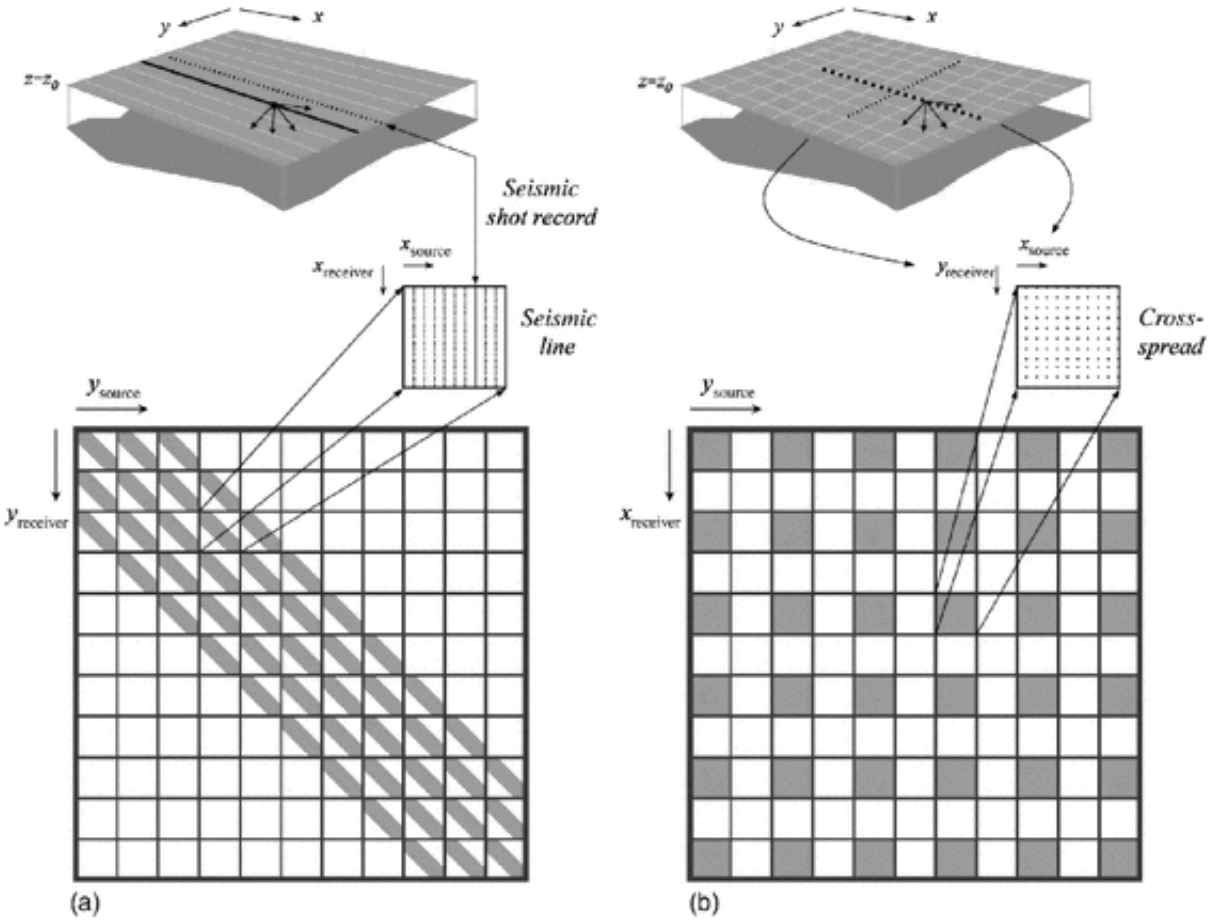


FIGURE 1 The data matrix for 3D seismic measurements. In multi-streamer marine data (**a**), one column represents one shot record (in this example five streamers are shown). In multi-cross-spread land data (**b**), one submatrix represents the data of a single cross-spread (in this example 36 cross-spreads are shown).

RTM REVERSE TIME MIGRATION

Migration: Conversion time-depth of the vertical scale to pass from image by sensors in time in a "real" image of the basement.

Traditional wave equation migrations (WEM) use one-way downward continuation and this is why turning ray is not incorporated into these algorithms.

The reverse time migration (RTM) combines both benefits of one-way wave equation migration for the multi-arrivals and Kirchhoff migration for steep and overturned reflectors. The other advantage of the reverse time migration is the amplitude handling compared to the previously mentioned methods. It provides correct amplitude and phase information at reflectors.

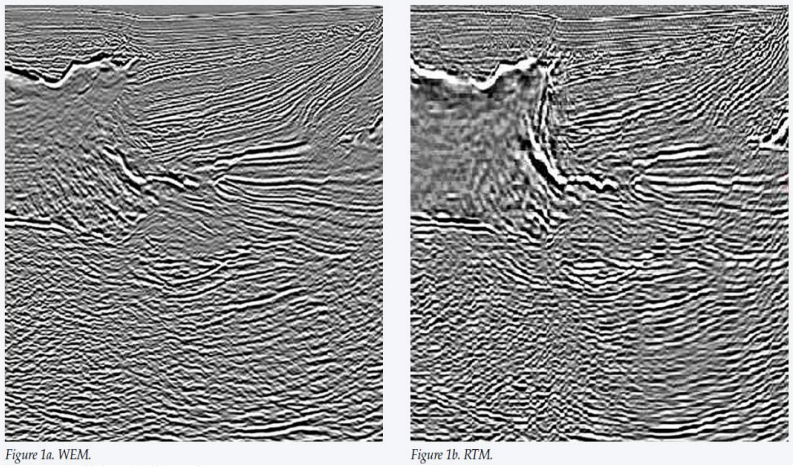
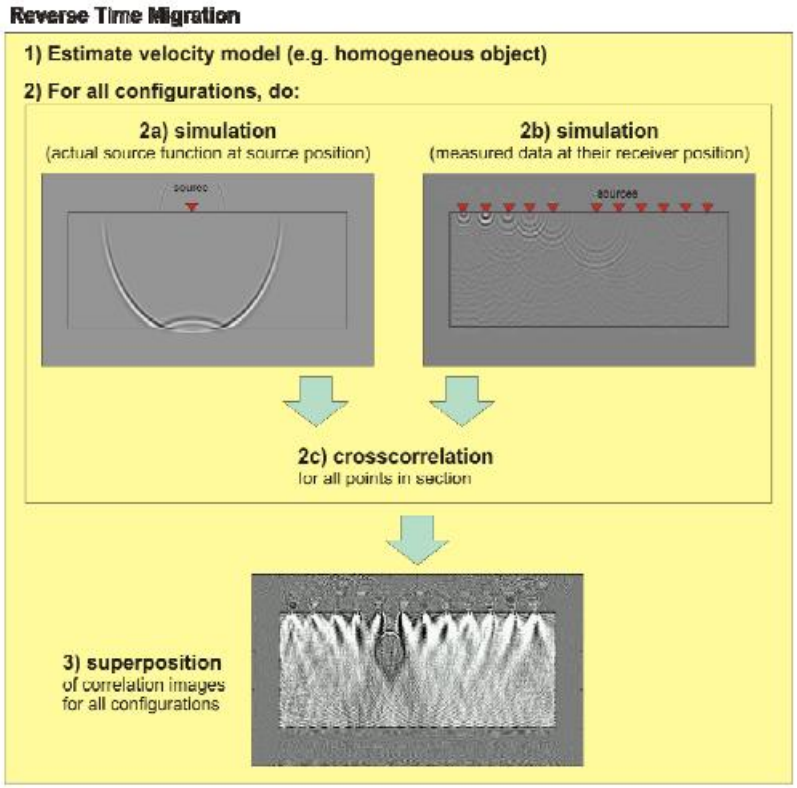


Figure 1a. WEM. *Figure 1b. RTM.*



RTM is the adjoint of an idealised modelling algorithm ,
Finite Difference Method
Based on solutions of the full wave-equation

- **Forward simulate the actual experiment, save the 4D wavefield**
- **Inject and back propagate the data**
- **At each imaging step, correlate the source and receiver wavefields**
- **The sum of all correlations gives an image estimate**

REVERSE TIME MIGRATION

First step: to forward propagate a shot wavefield from the shot point to out past all the reflecting horizons of interest using equation (1).

Next step: to propagate the recorded wavefield backward to the positions of the reflectors using the same equation (1).

$$\frac{\partial^2 U}{\partial t^2} = v(x,z)\left[\frac{\partial}{\partial x}v(x,z)\frac{\partial U}{\partial x} + \frac{\partial}{\partial z}v(x,z)\frac{\partial U}{\partial z}\right] \qquad (1)$$

At each time step where the shot wavefield and the recorded wavefield overlap are the places for reflecting interfaces.

Finally the zero-lag value of cross-correlation of the two wavefields is taken to obtain the positions of the reflectors. The imaging condition for pre-stack reverse time migration can be expressed as:

$$I(x,z,h) = \int_0^T S(x-h,z,t)R(x+h,z,T-t)dt$$

Velocity model building using two-way wave-equation migration

Model building is an essential part to achieve the best possible velocities (expensive). Salt geometry determination is one of the most critical steps towards the final outcome.

Reverse time migration has the benefit of accurately imaging salt flanks, being multi-arrival, and capable of producing models to aid, validate, and interpret the velocity model.

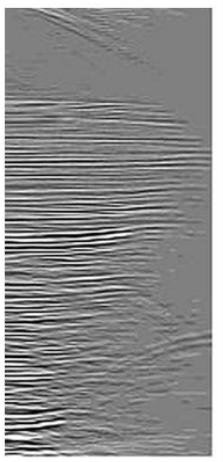


Figure 4a. One-way gather.

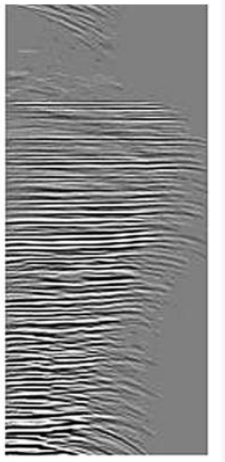


Figure 4b. Two-way gather.

DEPTH IMAGING: AN PARALLEL ALGORITHM

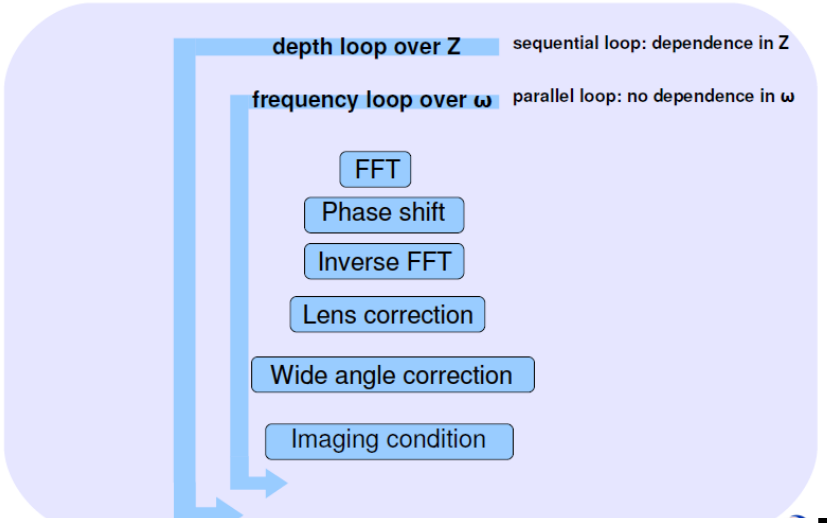
$$\left(\nabla^2 - \frac{1}{c^2}\frac{\partial^2}{\partial t^2}\right) u(\mathbf{r},t) = 0.$$ **Wave Equation (hyperbolic)**

$$u(\mathbf{r},t) = A(\mathbf{r})T(t).$$
$$(\nabla^2 + k^2)A = 0$$

Approximation :
Helmholtz Equation (elliptic)

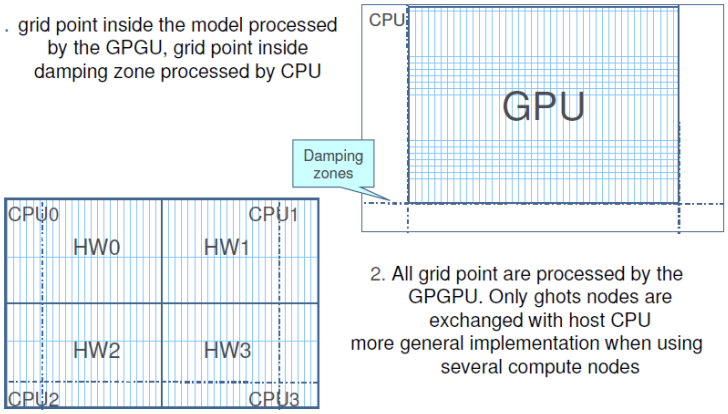
Billions unknown variables ,
Large solvers

Common Azimuth Migration: a brief description of the algorithm



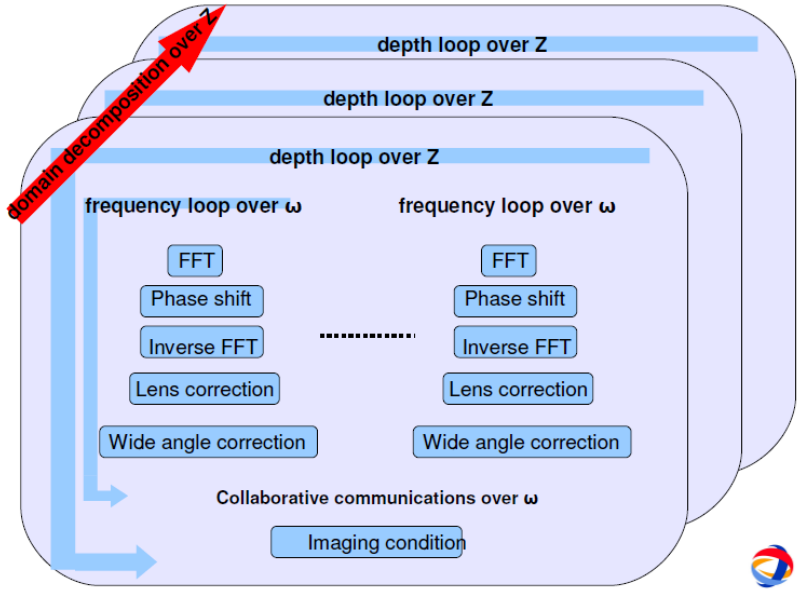
2D acoustic Wave Equation Finite difference implementation on GPGPU

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



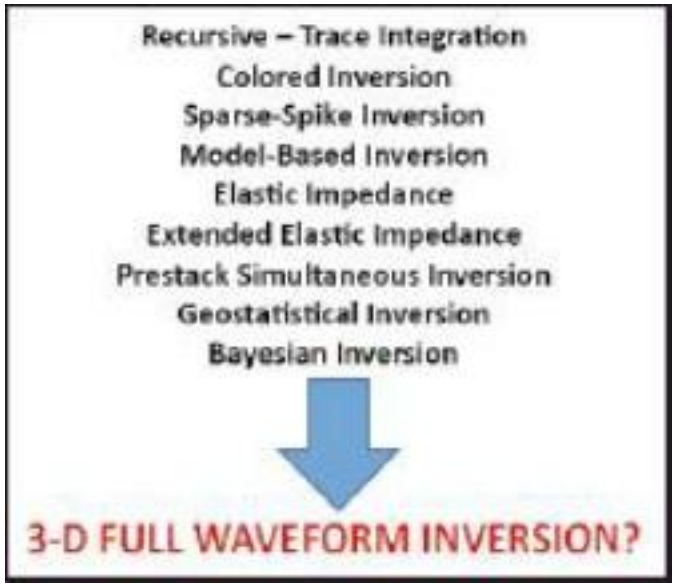
2. All grid point are processed by the GPGPU. Only ghots nodes are exchanged with host CPU
more general implementation when using several compute nodes

Common Azimuth Migration: massively parallel implementation

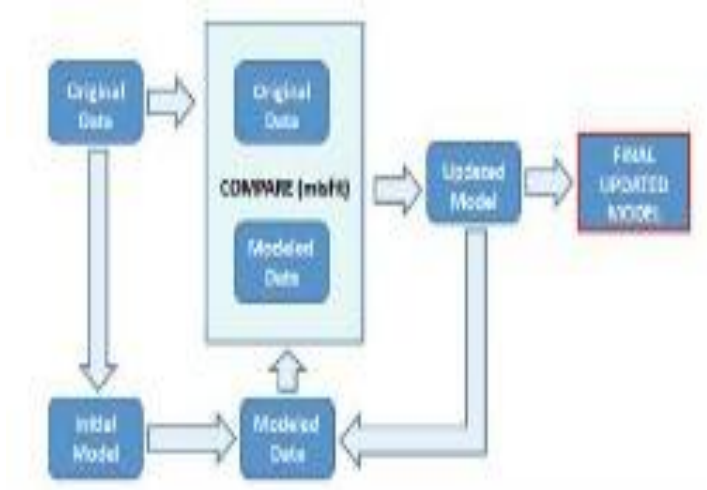


Link with computer science

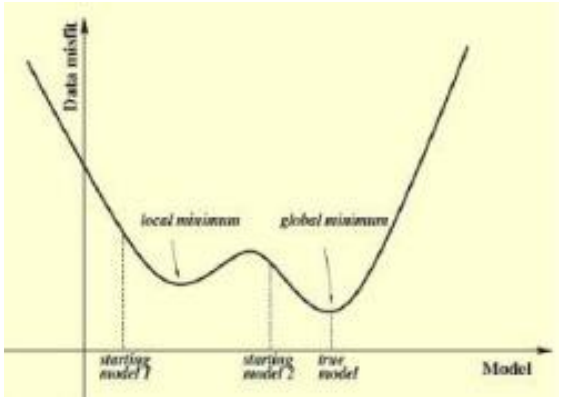
FULL WAVEFORM INVERSION: FWI ALGORITHM



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.



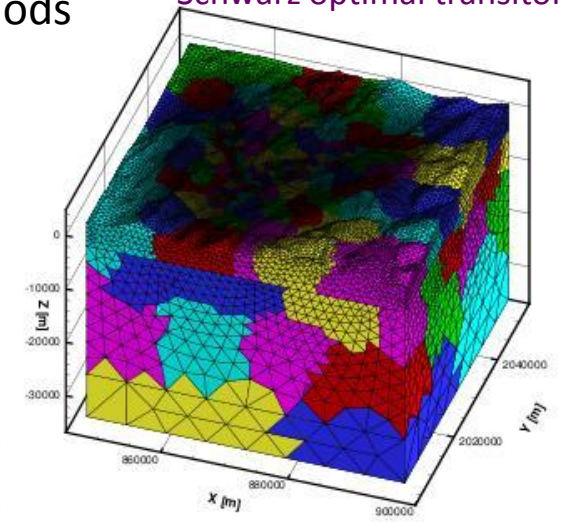
A data misfit results after several iterations, producing local and global minima depending on the starting models.

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

HPC for Depth Imaging : 3 fundamental steps

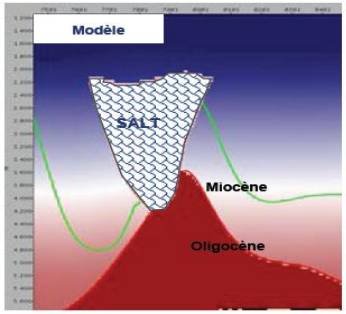
Numerical analyst
Numerical Methods

Schwarz optimal transitory

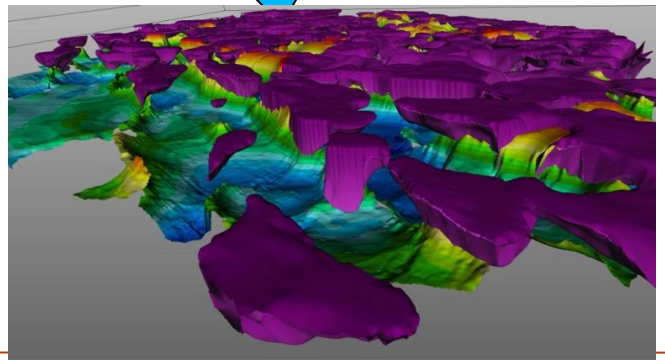


HPC Computing
HPC implementation

100 000
Cores
+
Options
GPU



Studies

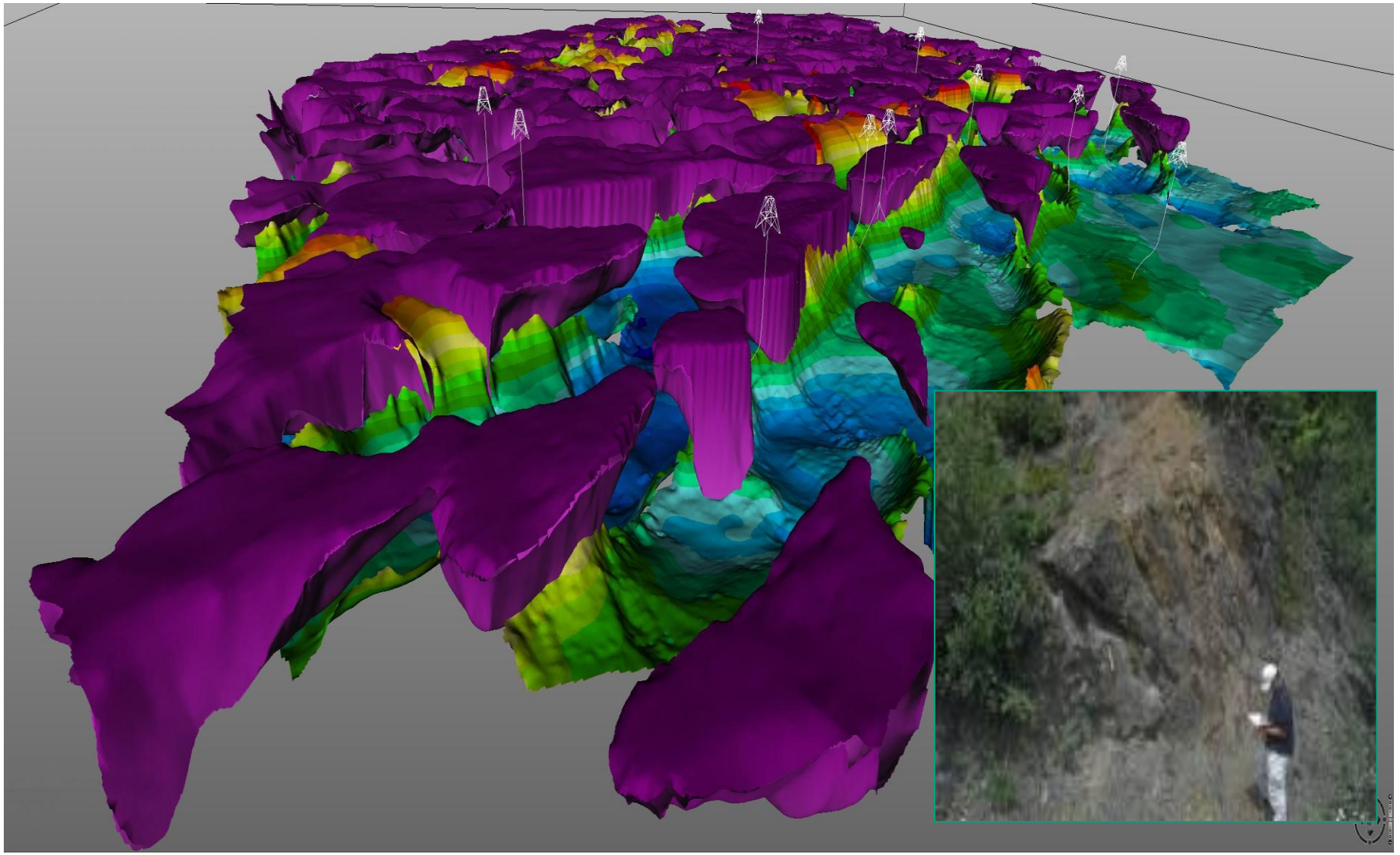


Geo-physics
Maths for Physic Modeling

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

Embarrassingly Parallel approximation

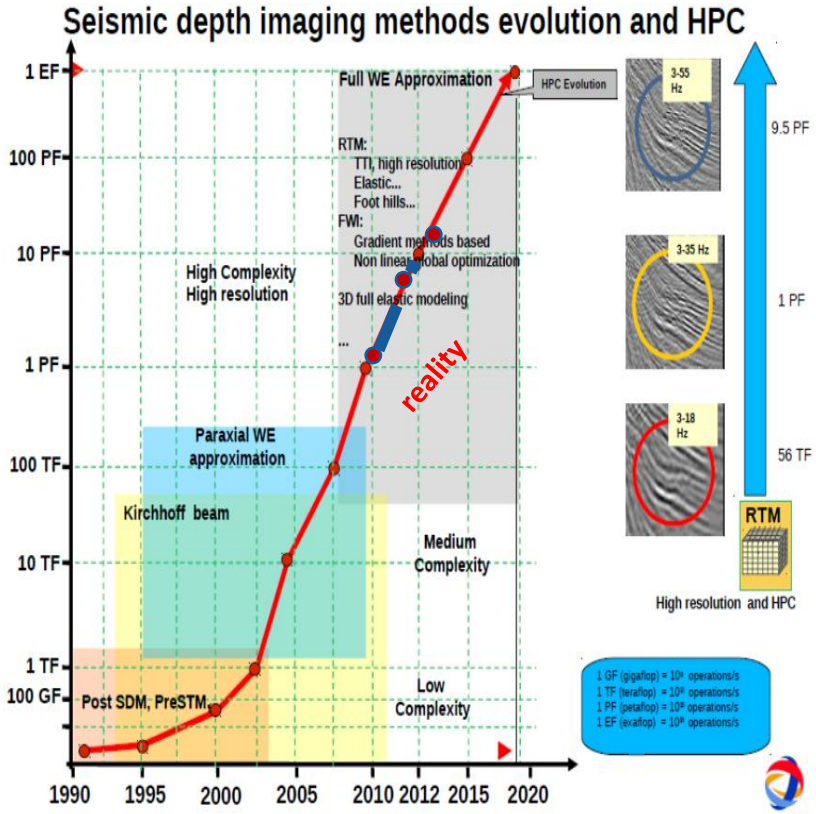
WEST AFRICA



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, …



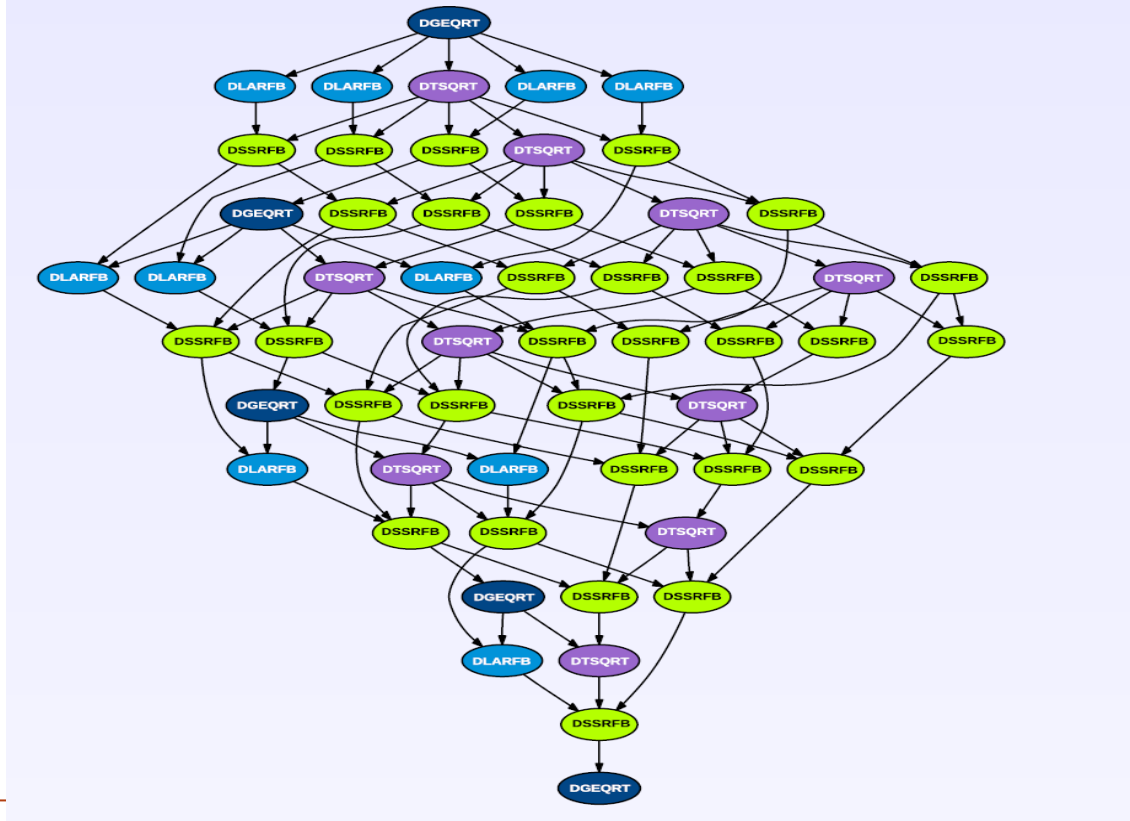
Same Roadmap in BP , Chevron

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

Absolute Need of multi skills Multidisciplinary teams

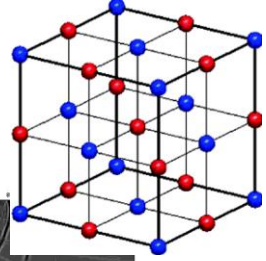
TASK PROGRAMMING MODEL, DEFINITION

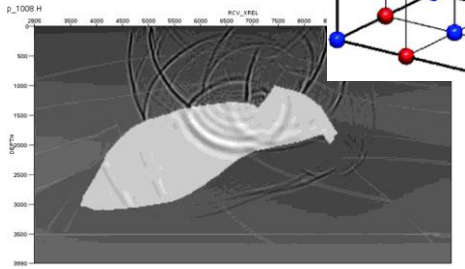
- Task programming model definition:
  - **Describe an algorithm as a graph of tasks**
  - **Manage task dependencies**
  - **Optimize asynchronous task execution**
  - **DAG: Direct Acyclic Graph**



Numerical Methods

NUMERICAL METHODS WORK PROGRAM





- Advanced methods for PDEs:

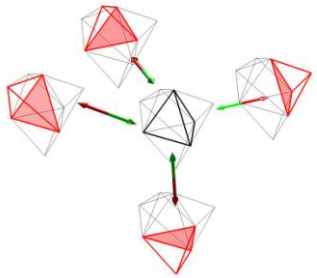
Numerical methods for Wave Equation propagators

- **Finite difference operators**
  - **2015: Extend 2D-3D isotropic elastic formulation to TTI elastic formulation:**
    - **Provide direct , adjoint states and parameter operator derivatives**
    - **Provide normalized API to GYQ for integration**
    - **Optimized implementation on different the different hardware targets explored by the HPC team**
    - **TRL 3-4**
  - 2016: Optimization of actual method: combining staggered grid and lebedev grid ➔ FD acoustic-elastic

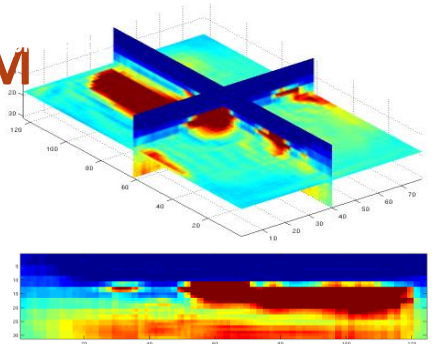
✓ **Discontinuous Galerkin Finite Element WE**

- **2015:**
  - **acoustic, elastic, TTI elastic propagators (DIP-INRIA)**
  - **Provide API and code structure to GYQ for Seismic Depth Imaging algorithms**
  - **TRL2-3**
  - **Collaboration (DIP-INRIA, GMIG)**

- **2016:**
  - **hp-refinement, local time stepping**
  - **Adjoint formulation**
  - **Hybrid tetrahedron-hexahedron discretization**
  - **Collaborations (DIP-INRIA,GMIG)**



NUMERICAL METHODS WORK PROGRAM



- Optimization:

  - **Stability, convergence criteria for inverse problem**
    - ❖ **2015-2016**
      - ➢ **Mesh deformation et regularization (M de Hoop GMIG follow up, F Peyrusse, TRL 2-3)**
      - ➢ **Local multi scale refinement and model compression (PhD F Faucher ,TRL 2-3)**
      - ➢ **Model reduction technics: (PhD F Faucher, M de Hoop)**

  - **Gradient free optimization**
    - ❖ **2015-2016**
      - ➢ **Collaboration with CERFACS: Nacer Soualmi PhD follow up (TRL1-2), application to log inversion?**
      - ➢ **Global search technics integrated with local non linear integration (M de Hoop, F Faucher, R Hewett, TRL 2-3)**

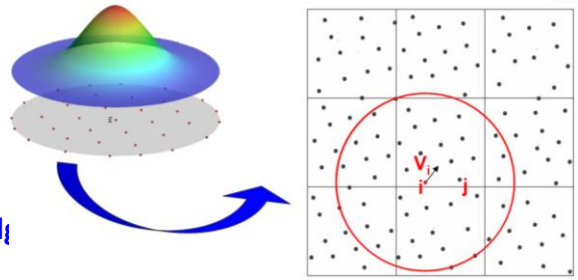
CHALLENGES AND OBJECTIVES

- Scalable Optimized Solver
  - **Define optimal solver for Wave Equation simulation:**
    - **In time space domain**
      - Irregular topography
      - Acoustic-Elastic coupling
      - Regular and irregular meshes
      - High order integration in time and space
      - Local time step
      - Highly scalable implementation
    - **In Complex Frequency Domain**
      - Irregular topography,
      - Acoustic-elastic coupling
      - Regular irregular meshes
      - High order space approximation
      - Highly scalable solver (direct or Hybrid) for large matrices.

NUMERICAL METHODS WORK PROGRAM

- Advanced methods for PDEs:
  - ✓ **Smoothed Particle methods**
    - ❖ **2015, 2016**
      - ➢ **Follow up MIT project: provide support to VIS**
      - ➢ **Understand numerical methods**

  - ➢ **Leda Flow**
    - ❖ **2015, 2016**
      - ➢ **Get a better understanding of the methods, Slug Regime flows (// al**
      - ➢ **Speed lab laboratory ?**



  - ✓ **Beyond grid based methods**
    - ❖ **2015-2016**
      - ➢ **Explore new technology for solving WE operators**
      - ➢ **Provide a review of the new trends**
      - ➢ **Recommendation and work program for 2017 and after**

- Large Sparse Linear Algebra:
  - **CA ALGO, EGMRES,**
  - **Reservoir simulation (*Talk P Henon*), CEMRACS Project**
  - **Depth Imaging (Works of Hussam & Laura), Multi RHS**

CHALLENGE IN GETTING SCALABLE SOLVERS

WORKS OF HUSSAM AL DAAS, LAURA GRIGORI

A Krylov solver finds a solution x_k from $x_0 + K_k(A, r_0)$, where

$$K_k(A, r_0) = span\{r_0, A\,r_0, \ldots, A^{k-1} r_0\}$$

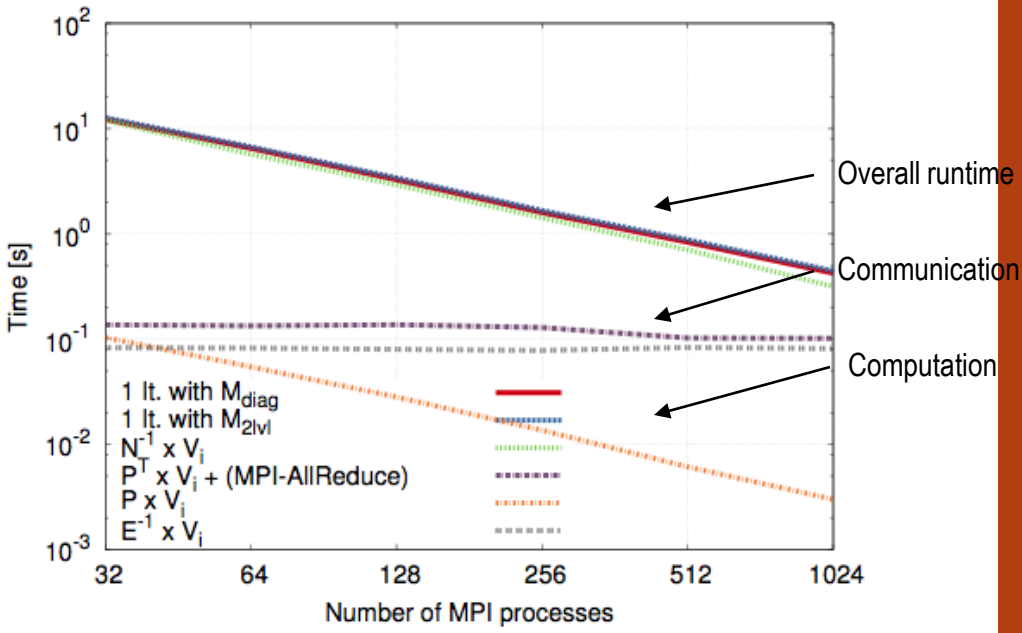
Each iteration requires

Sparse matrix vector product

-> point to point communication

Dot products for the orthogonalization process

-> global synchronization



Map making, with R. Stompor, M. Szydlarski

Results obtained on Hopper, Cray XE6

Our goal:

- Decrease the number of iterations to decrease the number of global communications
- Increase arithmetic intensity

ENLARGED KRYLOV SUBSPACE SOLVERS *(CF. HUSSAM SLIDE)*

- Partition the matrix into t domains
- At k-th iteration,
  - split the residual r_{k-1} into t vectors corresponding to the t domains,

$$r_{k-1} \rightarrow T(r_{k-1}) = \begin{bmatrix} * & 0 & & 0 \\ \vdots & \vdots & & \vdots \\ * & 0 & & 0 \\ 0 & * & & 0 \\ \vdots & \vdots & & \vdots \\ 0 & * & & 0 \\ & & \ddots & \\ 0 & 0 & & * \\ \vdots & \vdots & & \vdots \\ 0 & 0 & & * \end{bmatrix}, T_s(r_{k-1}) = \{T(r_{k-1})(:,1), \ldots T(r_{k-1})(:,t)$$

  - generate t new basis vectors, obtain an enlarged Krylov subspace

$$\mathscr{K}_{t,k}(A, r_0) = span\{T_s(r_0), AT_s(r_0), A^2 T_s(r0), ..., A^{k-1} T_s(r_0)\}$$

  - search for the solution of the system $Ax = b$ in $\mathscr{K}_{t,k}(A, r_0)$

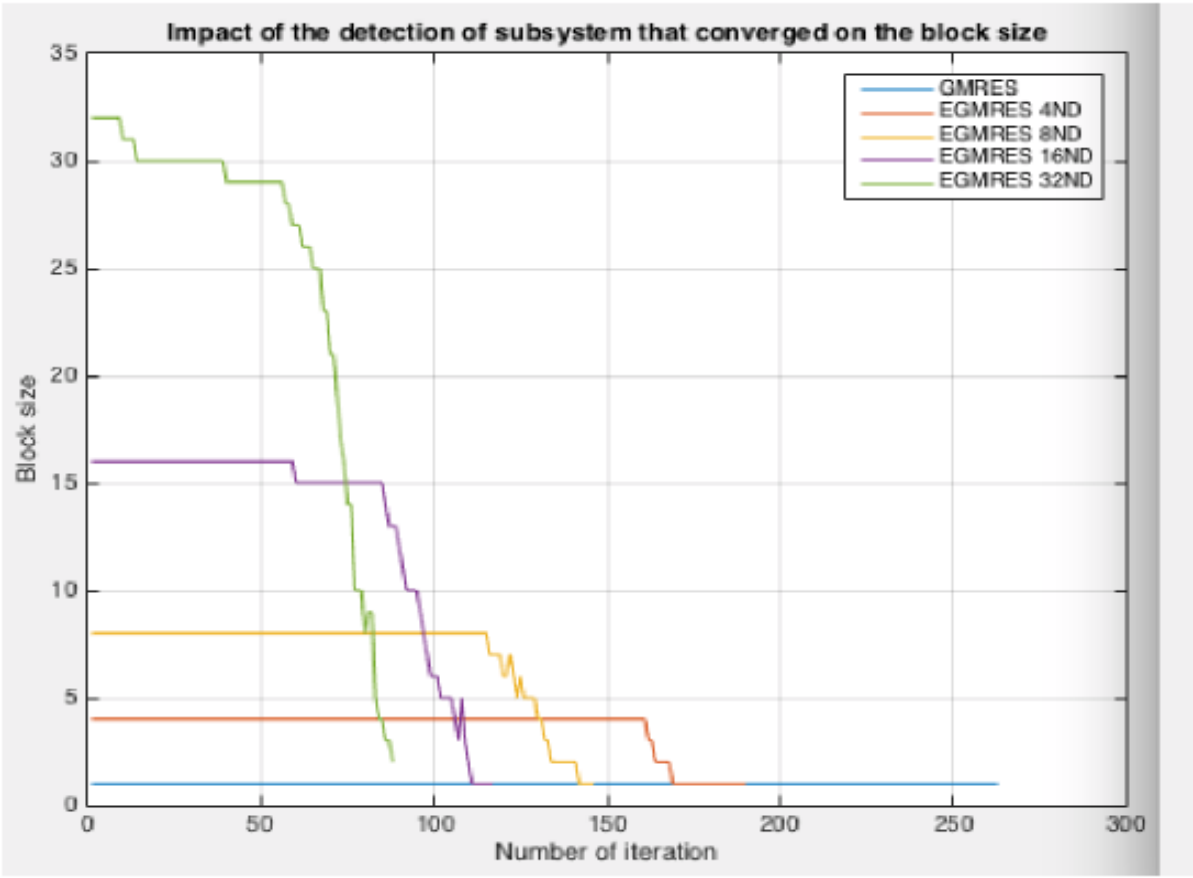
EGMRES

Properties

- Capability of using BLAS3.
- Capability of using TSQR.
- Faster convergence than GMRES.
- Restarted and deflated variant is possible.

Matrix name	Type	*N*	*NnZ*	Real	Symmetric	SPD
BIGCO24	Saturation	752283	5495556	yes	no	no
P-BIGCO24	Pressure	83587	539605	yes	no	no
BIGP1	Saturation	169328	2469485	yes	no	no
P-BIGP1	Pressure	42332	275946	yes	no	no
Seismic3	Seismic imaging	123414	613600	no	no	no

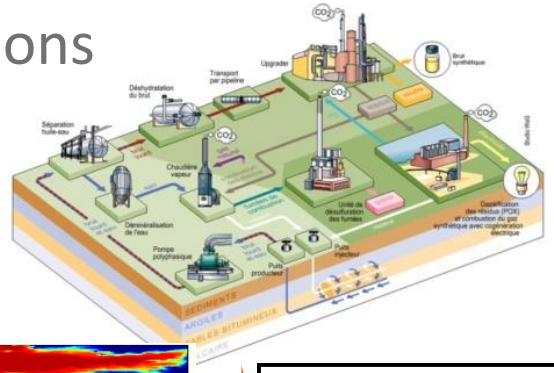
Table: Matrices used for tests. *N* is the size of the matrix, *NnZ* is the number of nonzero elements



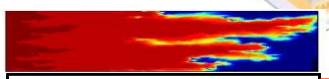
Matrix	*Np*	*ItBGS*	*RelErr*	*ND*	*ItEG*	*RelErr*
LS3 *tol* = 1e ¯8	1	1114	1e-7	4	407	6e-8
				8	248	3e-8
				16	153	1e-8
				32	100	6e-9
	4	424	5e-8	4	157	1e-8
				8	102	6e-9

TOTAL APPLICATION: PRODUCTION / RESERVOIR MODELING

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
- **Structure of reservoir:** Nano-porosity, Geomechanical and Geochemical structure and behavior of the rocks.
- **Pore Network Modeling**:
  - Modeling mechanisms at pore scale
  - Processing requirements could result in resources comparable to seismic imaging.

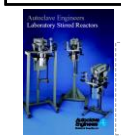


Chess & Hytec

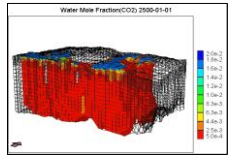
Select main geochemical reactions at a local scale

GEM

Activate main reactions for global reservoir/geochemistry simulation

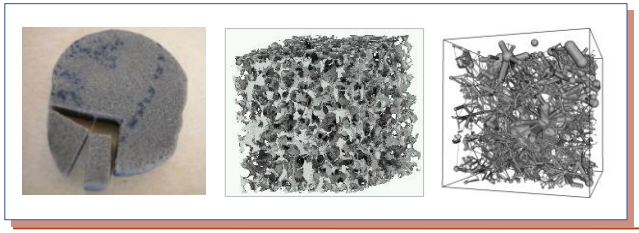


Lab experiment for calibration and matching



Matching performance needs by applying parallelism techniques at all levels

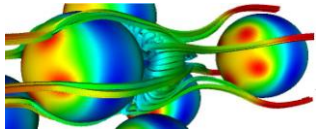
Essential for new fractured reservoirs, Shale Oil, Shale Gas



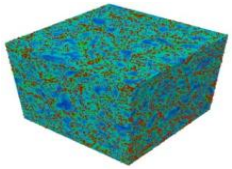
TOTAL EP/DSO/GIS
TOTAL EP/R&D/NUMET
TOTAL DS + Academics

- **MULTI FLUIDS FLOWS**

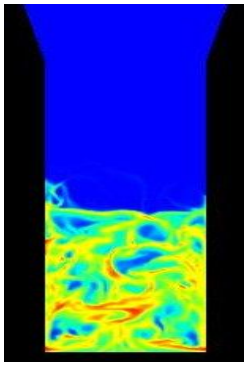
MULTI SCALE CFD : FCC RISER / MULTI SCALE - HPC



Micro (cata)



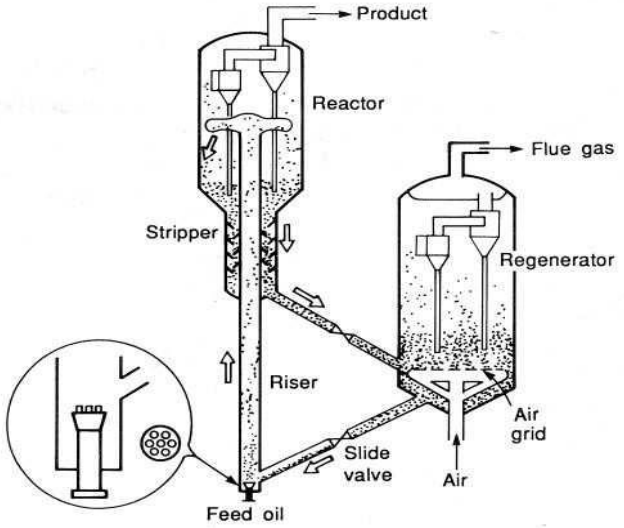
Meso (cm^3?)

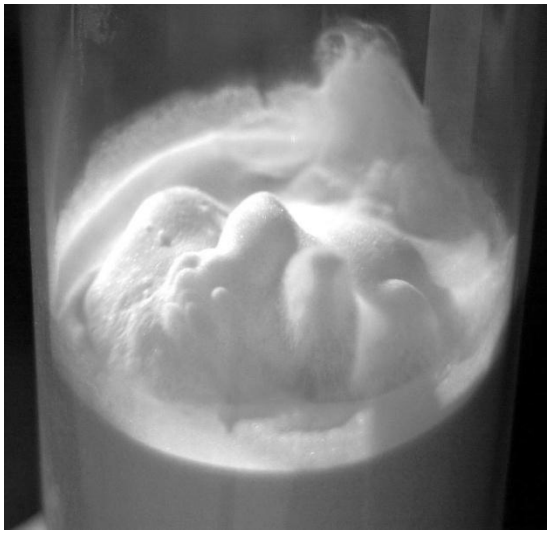


Macro (m)

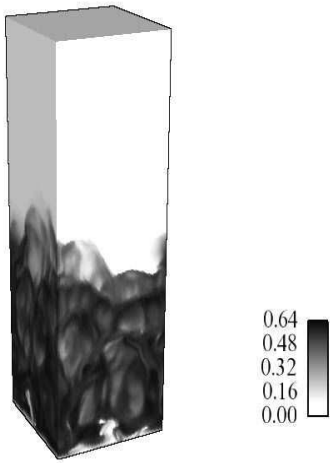
Multi Scale in FCC Turbulence

Fluid Catalytic Cracking





Experimental



Simulation

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

Neptune Many cores Runs

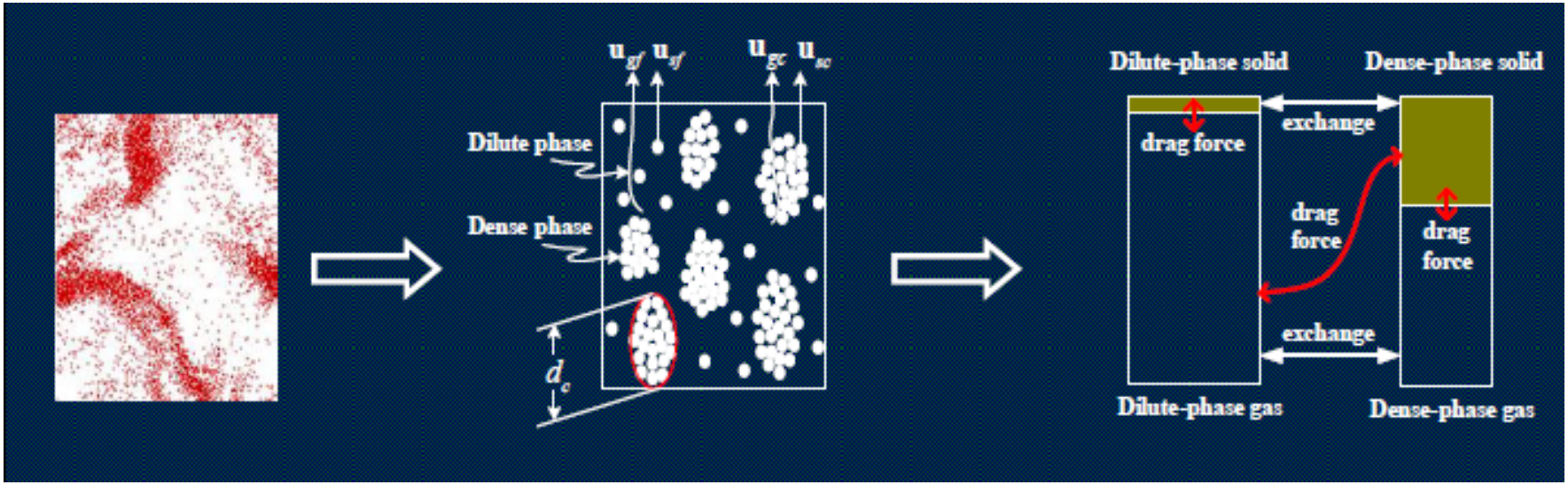
Scalability proven up to 4096 cores

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

But :

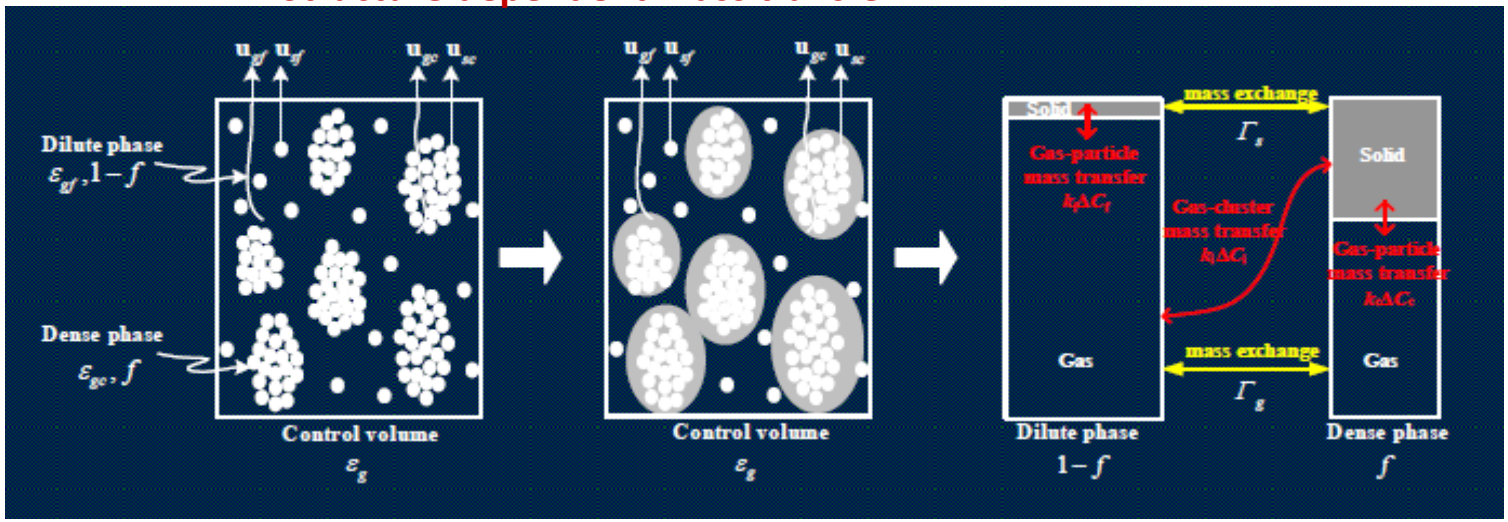
- **Need much more cores to simulate 3D industrial scale Riser experimental**
- **Multi Scale need HPC**

MULTI SCALE APPROACH: TO BE CONSISTENT WITH STRUCTURE



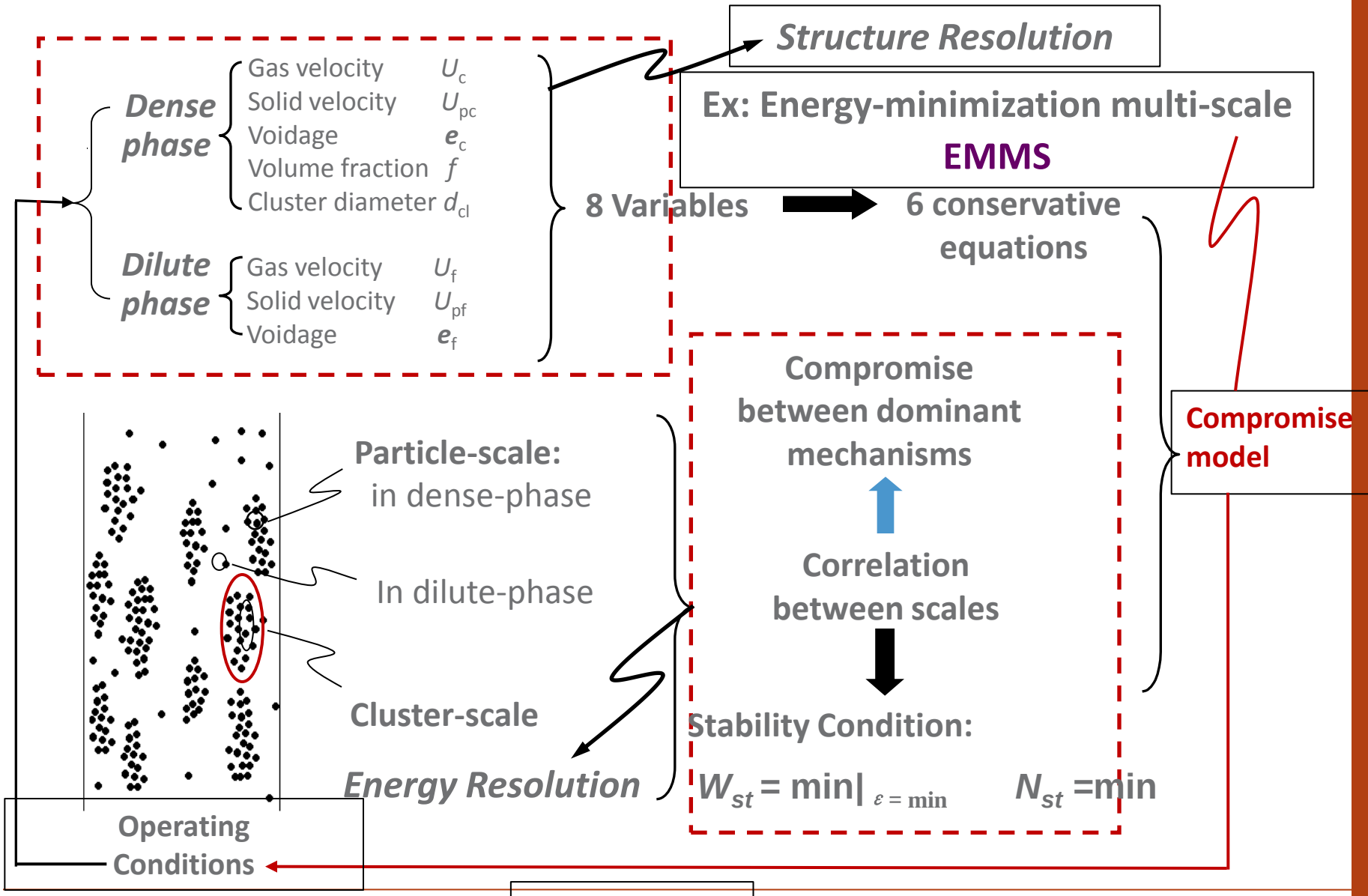
Real Structure **Dilute-dense meso scale structure** **SFM (Structure dependent multi Fluid Model)**

Structure dependent mass transfer



Dilute Dense meso **Heterogeneous mass transfer** **SFM/Mass Transfer**

MULTI SCALE APPROACH WITH ENERGY COMPROMISE

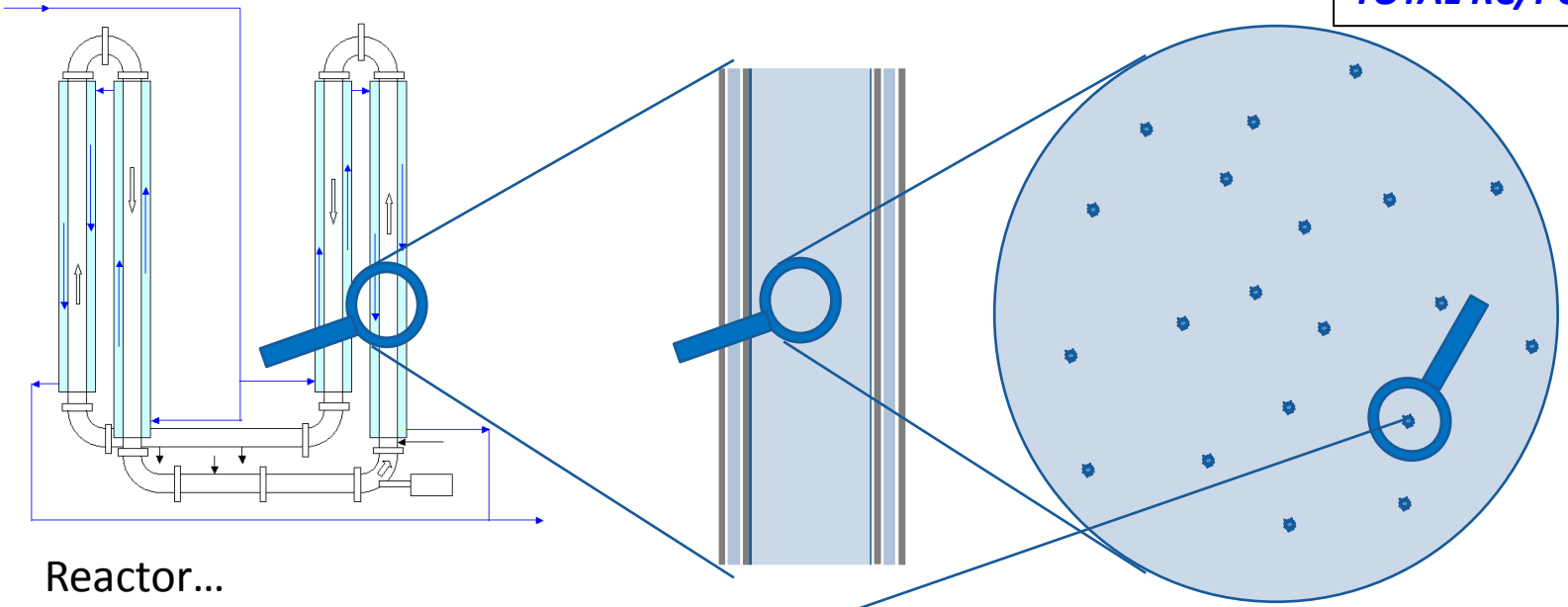


(*Li & Kwauk, 1989*)

TOTAL APPLICATION: LIQUID – SOLID (HIGH RATIO) REACTOR

- Polyethylene production in a slurry-loop reactor

TOTAL DS
TOTAL RC/POL

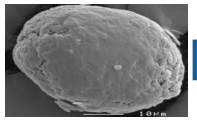


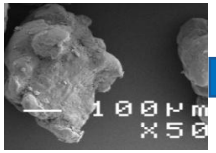
Reactor…

…full of liquid…

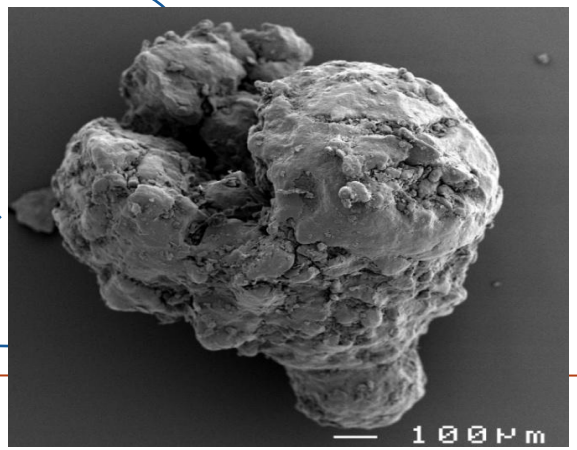
…containing tiny catalyst grains.

Catalyst grain
10µ





Reaction process

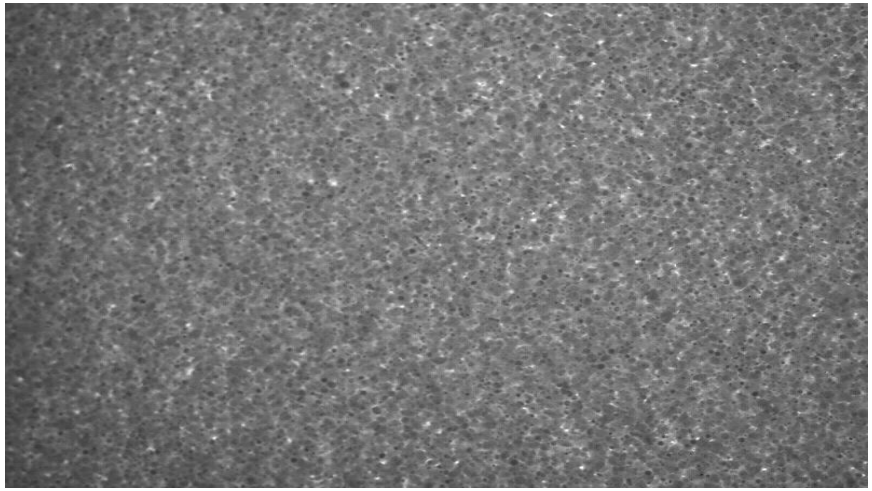


? ? ? ? ? ? ?

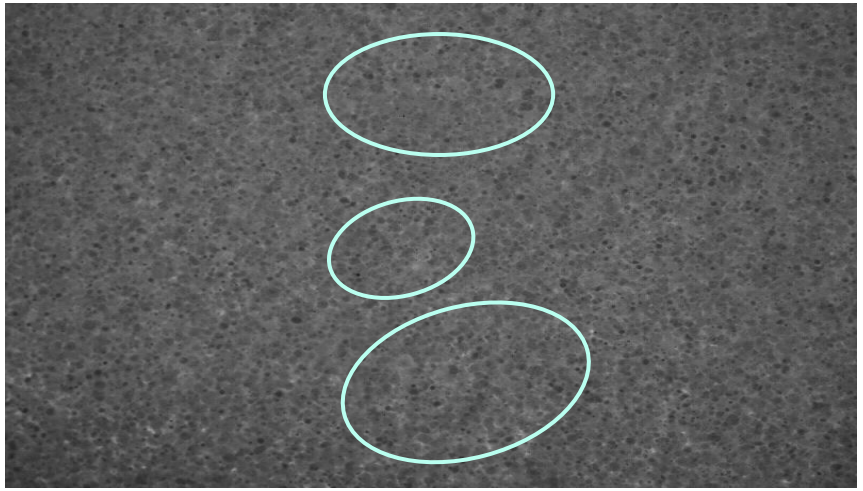
High concentration slurry

TOTAL

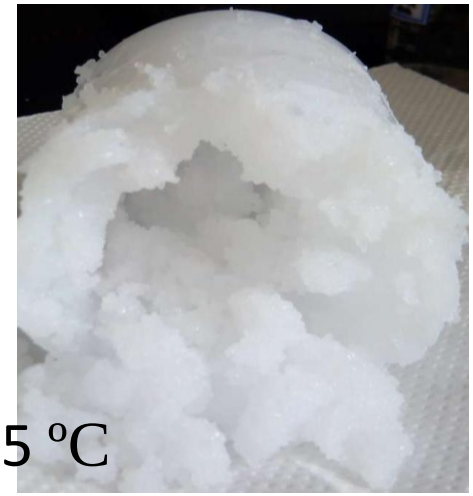
LIQUID SOLID FLOWS EXPERIMENTS 40 WT% CASES



T=35 °C



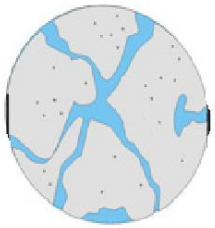
T=55 °C



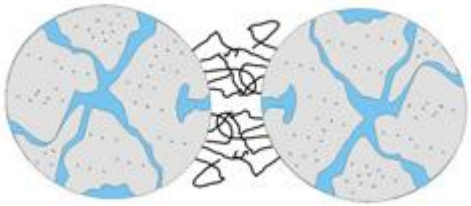
T=85 °C

Models that describe the swelling systems

Physical phenomena



Swelling particles,



Aggregation between swelling particles?

Theory basis

- **Linear and nonlinear mass transfer rate models**
- **Force balance model for natural aggregation**

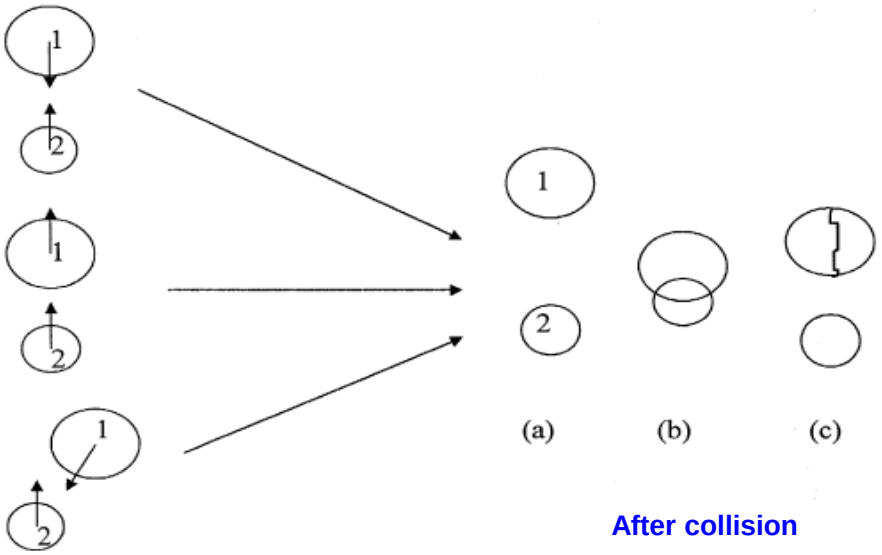
Research in collaboration with IPE, CAS, Beijing, China

Models that describe the swelling systems

- **Force balance model for natural aggregation**

Zhou et al.(2007) proposed a aggregation model based on force balance of particles for vertical gas-solid flows, when van der Waals forces are the main interparticle forces.

$$F_{drag} + F_{collision} = F_{gravity} + F_{vander\_waals} \qquad (1)$$

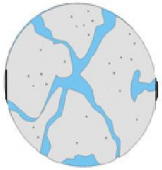


Schematic of the model of agglomerate collision
(Zhou and Li, Powder Technol., 111, 60 (2000))

- **If the equation has solution, it means that two agglomerates would separate after collision.**
- **If the equation has no solution, it means that the two agglomerates may agglomerate after collision.**

Swelling dependent Two-Fluid model

Physical background



A mixture phase of
oil and solid matrix

Model assumption

Solid phase is assumed as a mixture phase and the mass transfer due to swelling is considered in the new model.

Governing equations

Continuity equations:

$$\frac{\partial(\varepsilon_l \rho_l)}{\partial t} + \nabla \cdot (\varepsilon_l \rho_l \mathbf{u}_l) = m_{ls}$$

$$\frac{\partial(\varepsilon_s \rho_s)}{\partial t} + \nabla \cdot (\varepsilon_s \rho_s \mathbf{u}_s) = m_{sl}$$

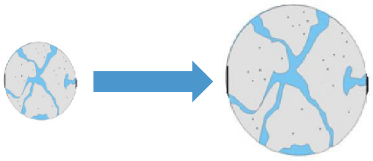
Momentum balance equations:

$$\frac{\partial(\varepsilon_l \rho_l \mathbf{u}_l)}{\partial t} + \nabla \cdot (\varepsilon_l \rho_l \mathbf{u}_l \mathbf{u}_l) = -\varepsilon_l \nabla P + \mu_{l,eff}\, \varepsilon_l \left[\nabla \mathbf{u}_l + (\nabla \mathbf{u}_l)^T\right] + \varepsilon_l \rho_l \mathbf{g} + \mathbf{F}_{ls}^D + m_{ls}\, \mathbf{u}_l$$

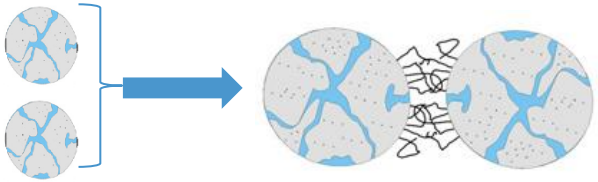
$$\frac{\partial(\varepsilon_s \rho_s \mathbf{u}_s)}{\partial t} + \nabla \cdot (\varepsilon_s \rho_s \mathbf{u}_s \mathbf{u}_s) = -\varepsilon_s \nabla P - \nabla P_s + \mu_{s,eff}\, \varepsilon_s \left[\nabla \mathbf{u}_s + (\nabla \mathbf{u}_s)^T\right] + \varepsilon_s \rho_s \mathbf{g} + \mathbf{F}_{sl}^D + m_{sl}\, \mathbf{u}_s$$

Swelling dependent Two-Fluid model

Physical background



growth



Aggregation

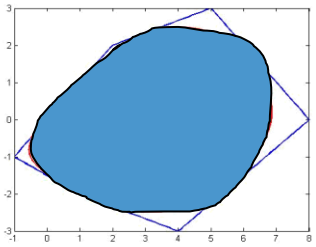
Model modification

- The growth of particle size due to mass transfer is calculated via **population balance model (PBM).**
- Swelling-induced aggregation is also considered via the **aggregation term** in population balance equations.

Population balance equations

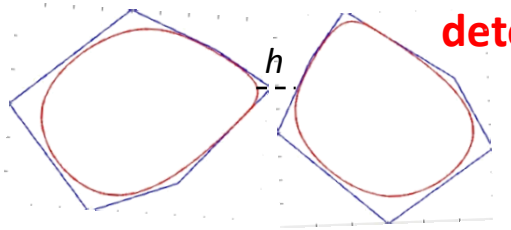
$$\frac{\partial[n(L;\mathbf{x},t)]}{\partial t}+\nabla\cdot[\vec{u}\cdot n(L;\mathbf{x},t)]=-\frac{\partial[G(L)n(L;\mathbf{x},t)]}{\partial L}+B_{ag}(L;\mathbf{x},t)+D_{ag}(L;\mathbf{x},t)$$

NURBS-BASED DEM IMPLEMENTATION



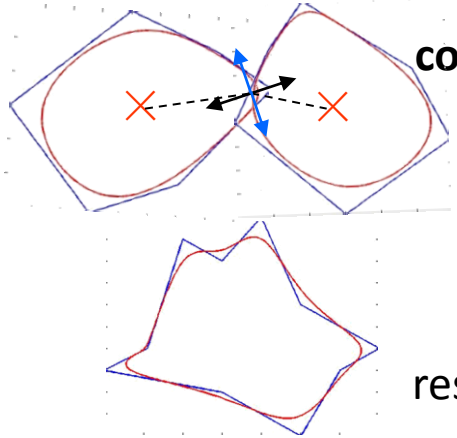
integration on the entire body

$$M = \iiint_{VOL} m dv$$



detection of the collision

$$h = \left\{ \left| C_1(u_1) - C_2(u_2) \right| \right\}\Big|_{\min}$$

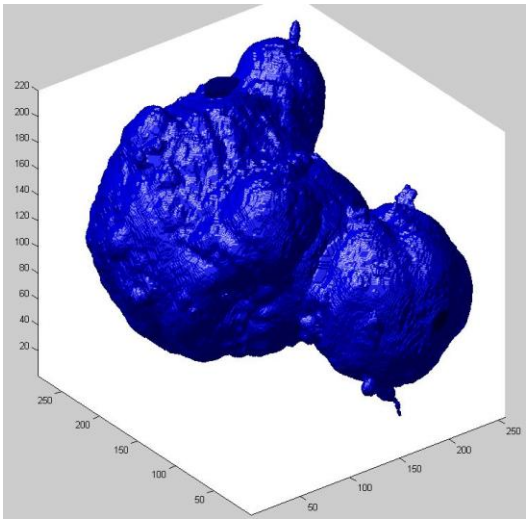


computation of the collision

$$\vec{\mathbf{f}} = f\left(\Delta vol,\ \overrightarrow{\Delta \mathbf{u}},\ \overrightarrow{\Delta \boldsymbol{\omega}};\ C_1, C_2\right)$$

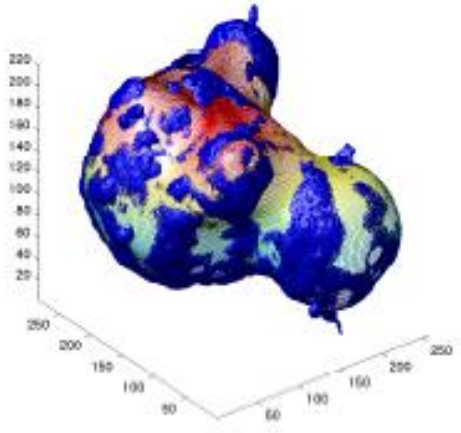
$$\vec{\boldsymbol{\tau}} = \vec{\mathbf{f}} \times \vec{\mathbf{r}}$$

resistance of deformation



PE particle

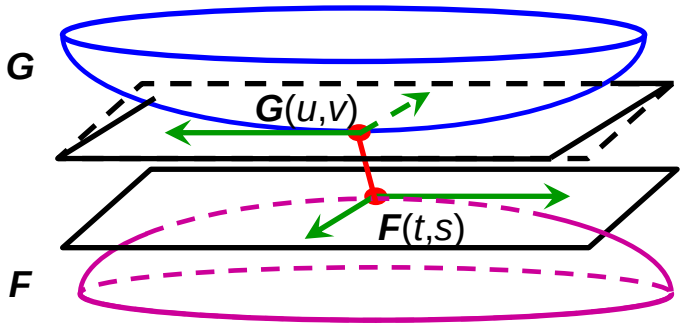
NURBS Representaion



Criterion of minimum distance

Minimum distance line must perpendicular to each two normal vectors of tangent planes at each surface, which are two first-order partial derivatives at minimum distance point.

G(*u*,*v*), ***F***(*t*,*s*) present two minimum distance points. Four vertical relation



Newton-Raphson iteration

Multidimensional Newton-Raphson equation

$$\mathbf{X}_{i+1} - \mathbf{X}_i = -\left[J(F(\mathbf{X}_i))\right]^{-1} F(\mathbf{X}_i)$$

Let **X**=[*u*, *v*, *t*, *s*]', *F*(**X**)=[*gu*, *gv*, *ft*, *fs*]', the iterator equation is

$$\begin{bmatrix} u_{i+1} \\ v_{i+1} \\ t_{i+1} \\ s_{i+1} \end{bmatrix} - \begin{bmatrix} u_i \\ v_i \\ t_i \\ s_i \end{bmatrix} = - \begin{bmatrix} \partial gu/\partial u & \partial gv/\partial u & \partial ft/\partial u & \partial fs/\partial u \\ \partial gu/\partial v & \partial gv/\partial v & \partial ft/\partial v & \partial fs/\partial v \\ \partial gu/\partial t & \partial gv/\partial t & \partial ft/\partial t & \partial fs/\partial t \\ \partial gu/\partial s & \partial gv/\partial s & \partial ft/\partial s & \partial fs/\partial s \end{bmatrix}^{-1} \begin{bmatrix} gu \\ gv \\ ft \\ fs \end{bmatrix}$$

Iteration solving for [*u*, *v*, *t*, *s*]' of this quaternion matrix equation

The minimum distance is |*G*(*u*,*v*)-*F*(*t*,*s*) |

$$gu(u,v,t,s) = (\mathbf{G}(u,v) - \mathbf{F}(t,s)) \frac{\partial \mathbf{G}(u,v)}{\partial u}$$

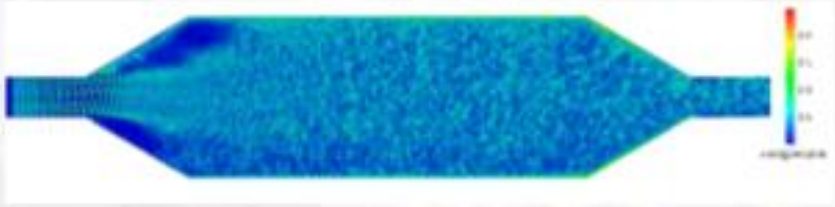
$$gv(u,v,t,s) = (\mathbf{G}(u,v) - \mathbf{F}(t,s)) \frac{\partial \mathbf{G}(u,v)}{\partial v}$$

$$ft(u,v,t,s) = (\mathbf{F}(t,s) - \mathbf{G}(u,v)) \frac{\partial \mathbf{F}(t,s)}{\partial t}$$

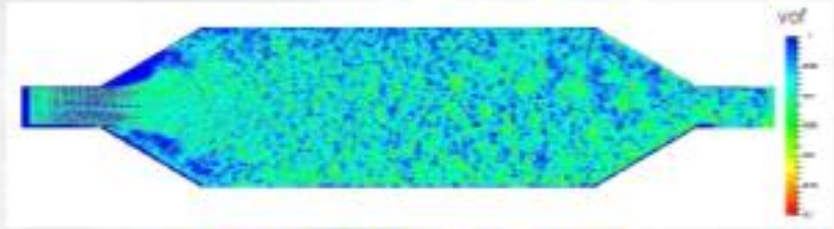
$$fs(u,v,t,s) = (\mathbf{F}(t,s) - \mathbf{G}(u,v)) \frac{\partial \mathbf{F}(t,s)}{\partial s}$$

Contour of time averaged liquid volume fraction

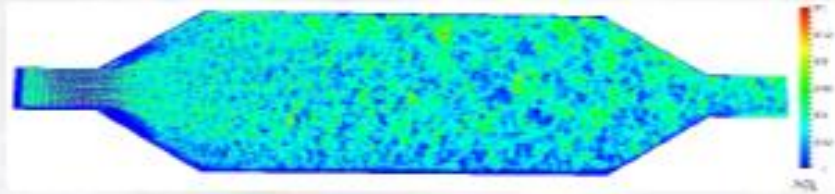
A = 0



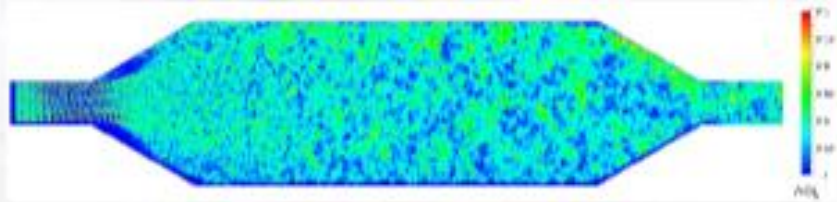
A = 2.1e-19



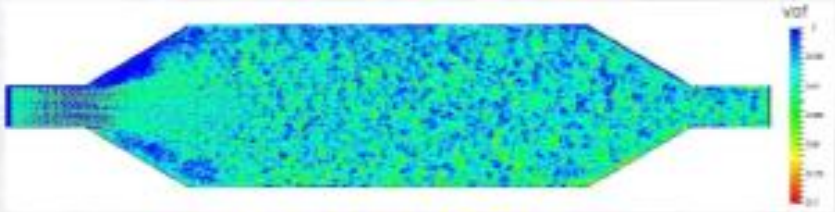
A = 2.1e-14



A = 2.1e-13

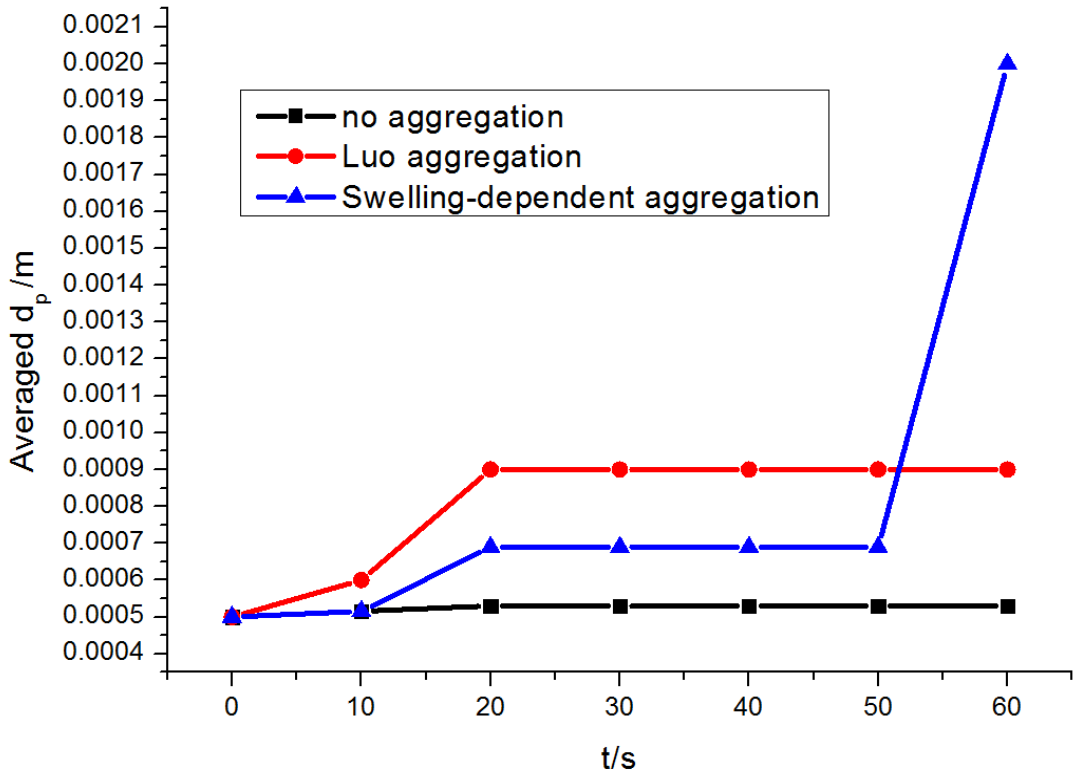


A = 2.1e-10



Results and discussion

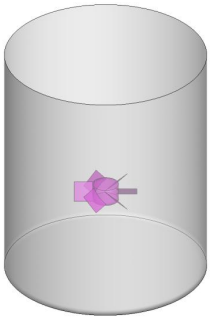
- **Averaged diameter using different models**

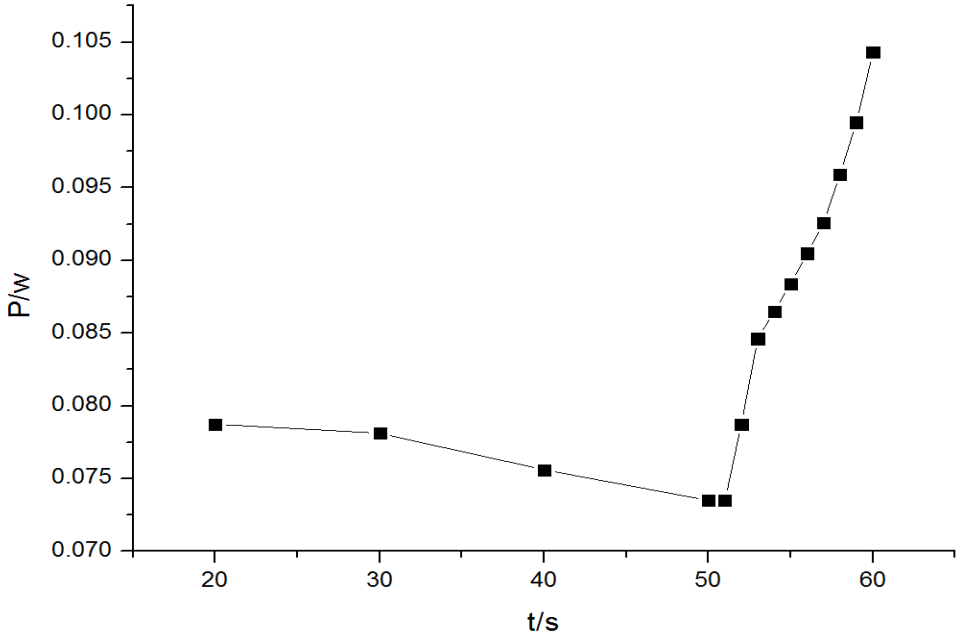


- **No aggregation considered, the increase of averaged diameter is not obvious.**
- **Using traditional aggregation model, the diameter increases a lot but finally attains a steady state.**
- **Using swelling-dependent aggregation model, a sharp jump of the averaged diameter appears around t=50 s, which indicates that when swelling attains a higher level, the aggregation will be accelerated.**

Results and discussion

- **Power consumption**





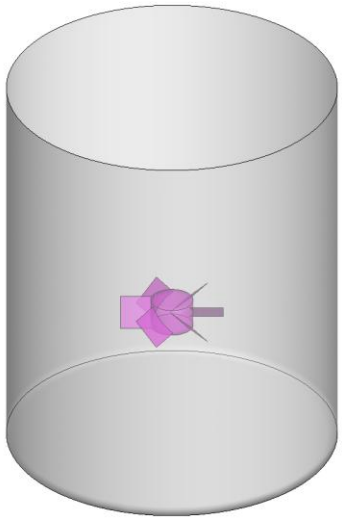
- **The result indicates that the sudden acceleration of aggregation induces a sharp jump of the impeller power. Physically, it can be seen as a sudden increase of the suspension viscosity.**

The new TFM equations coupled with PBM predicts a sharp jump of both the averaged diameter and power consumption.
The current concept model can at least qualitatively reflect the effect of swelling behavior.
This is consistent with the experimental observations.

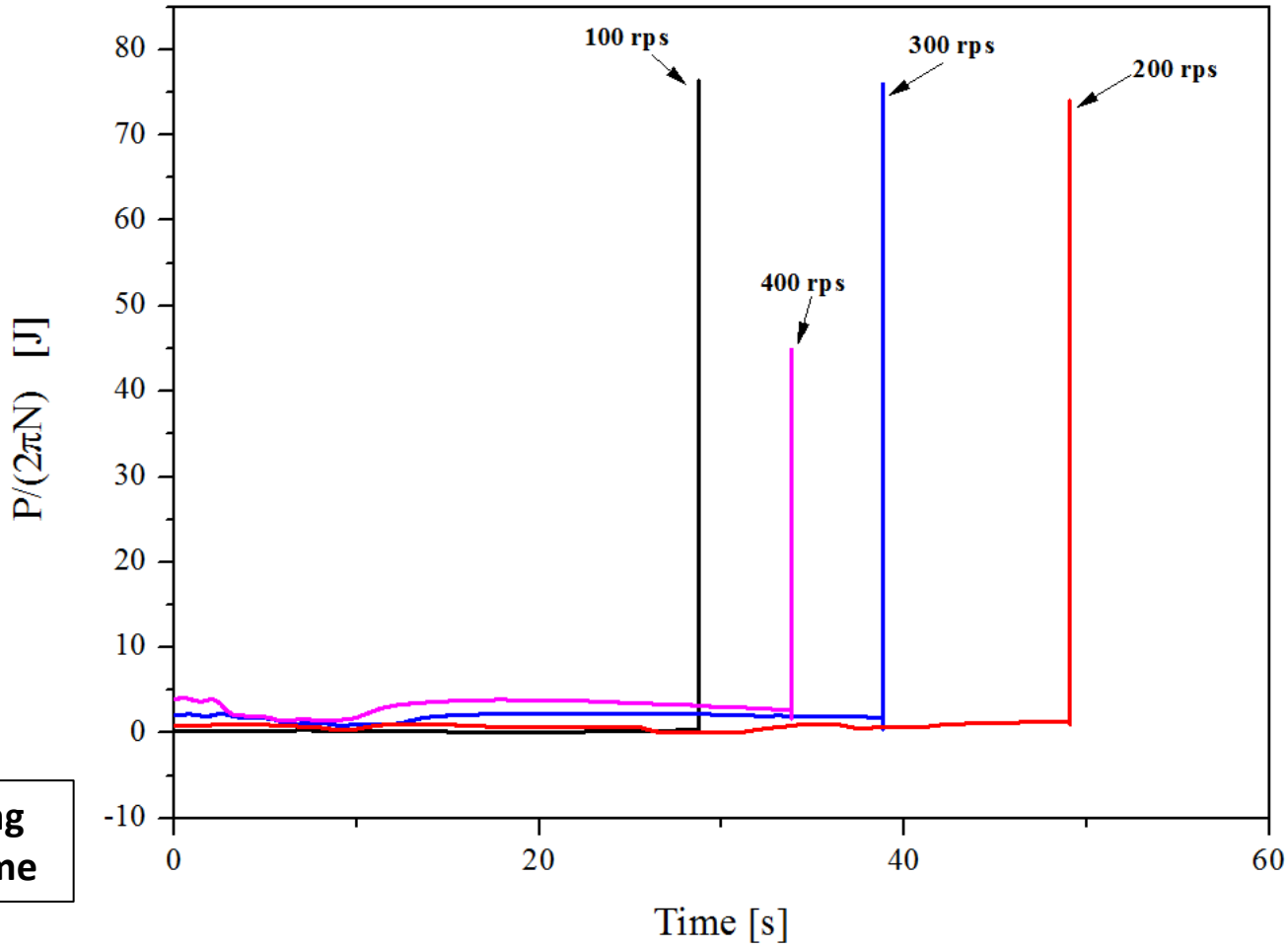
Research continues in collaboration with IPE, CAS, Beijing, China

Model application I

Case 1



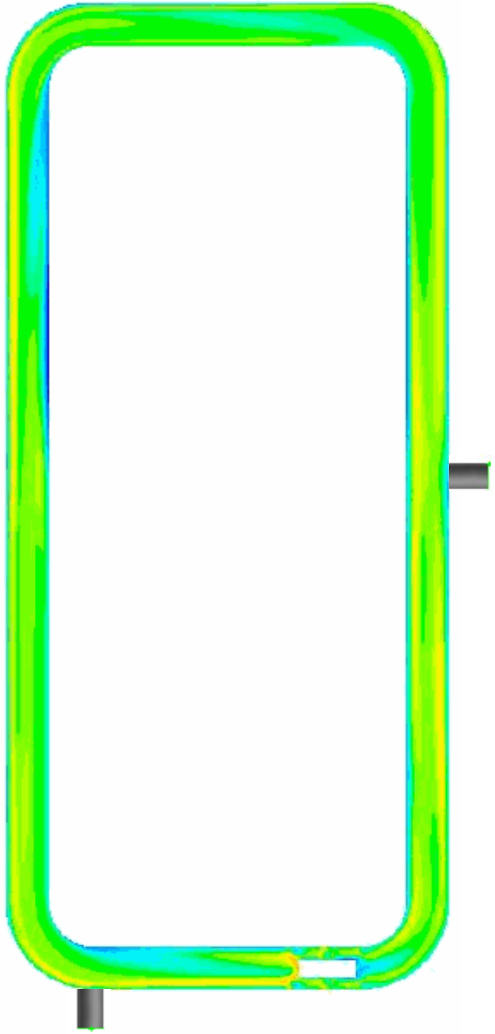
- Two phase flow: PE-dodecane flow
- Initial liquid level: 0.28 m
- Initial solid concentration: 40 vol. %
- Initial solid diameter: 500 µm
- Impeller speed: 100 rps



Large swelling apparition time

Test of secondary flow

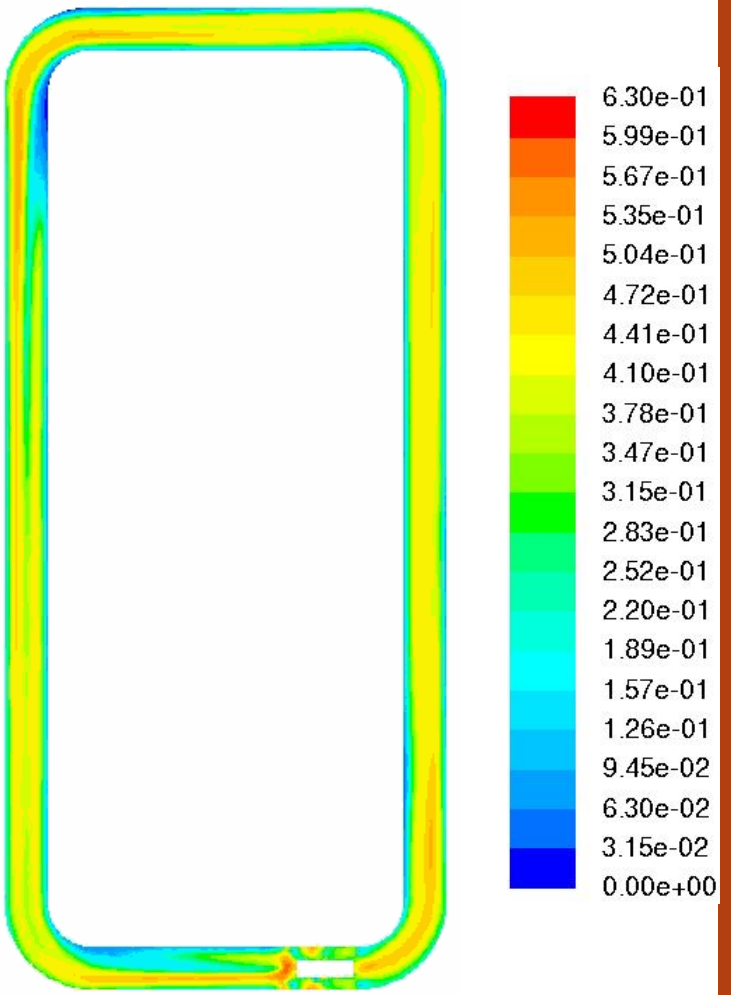
With secondary flow



(Time=3.5000e+01)

- **With secondary flow, the blockage due to swelling was reduced from t=53 s, and then appeared again from t=78 s.**
- **Without secondary flow, the blockage cannot be reduced, and that's why the sharp increase of the power consumption appeared faster.**

Without secondary flow



(Time=2.1000e+01)

TOTAL

- **MATERIALS**

HPC & Numerical Simulation in Hutchinson Material Structure & Acoustics compounds

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

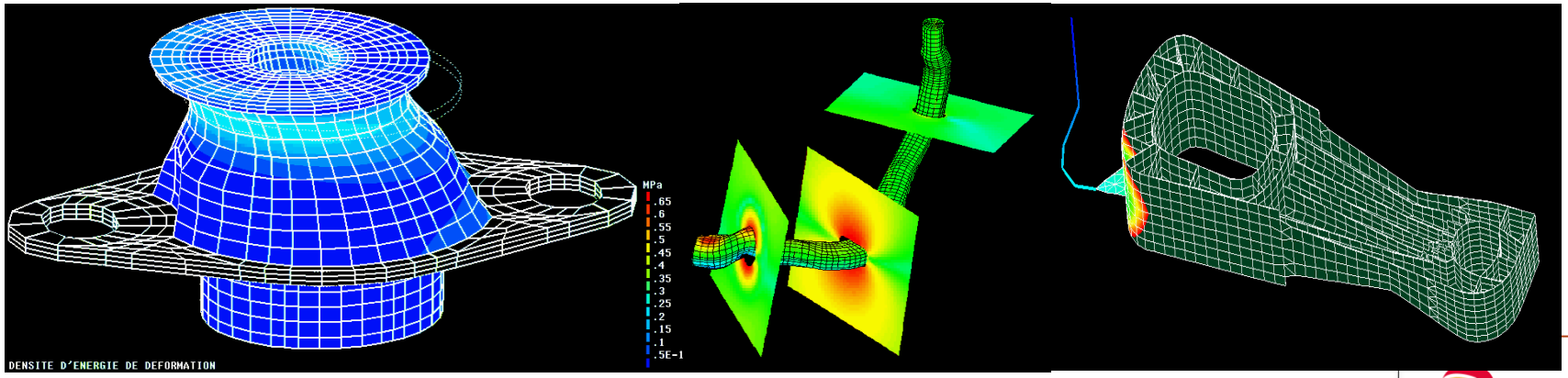
Permitted Source : Hutchinson

New Products Development Assistance

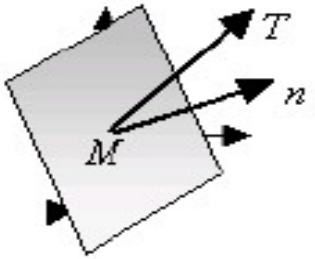
- Performances forecast (static & dynamic stress, acoustic, …)
- Length of life warranty (constraints, distortions, ...)
- Optimization

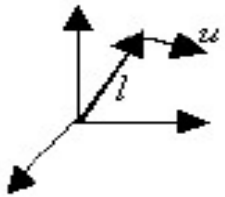
Process Implementation Assistance : Injection, Extrusion ..

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



DEFORMATION MATERIAU





Description de l'État Mécanique Local

Contrainte		Déformation
$\overrightarrow{T}(M,\overrightarrow{n}) = \overline{\overline{\sigma}}\,\overrightarrow{n}$	Définition	$\overrightarrow{u}(M,\overrightarrow{l}) = \overline{\overline{\varepsilon}}\,\overrightarrow{l}$
$\sigma_{ij} = \sigma_{ji}$	Symétrie	$\varepsilon_{ij} = \varepsilon_{ji}$

Principe Fondamental de la Dynamique

$$\mathbf{Div}\overline{\overline{\sigma}} + \rho\overrightarrow{X} = \rho\overrightarrow{\gamma}$$

$$\frac{\partial \sigma_{ij}}{\partial x_j} + \rho X_i = \rho\gamma_i$$

Relation Déformation - Déplacement

$$2\overline{\overline{\varepsilon}} = \mathbf{Grad}\,\overrightarrow{u} + {}^t\mathbf{Grad}\,\overrightarrow{u}$$

$$\frac{dV}{V} = \mathbf{Tr}\overline{\overline{\varepsilon}} = \mathbf{div}\,\overrightarrow{u}$$

Conditions aux Limites

$$\overline{\overline{\sigma}}(M)\,\overrightarrow{n} = \overrightarrow{f}$$

Conservation de la Masse

$$\mathbf{Inc}_{ij}(\overline{\overline{\varepsilon}}) = \delta_{ipq}\delta_{jrs}\frac{\partial^2 \varepsilon_{pr}}{\partial x_q \partial x_s}$$

Description Indépendante du Comportement du Matériau

Equation d'État du Matériau

$$\mathcal{F}\{\overline{\overline{\sigma}}, \frac{d\overline{\overline{\sigma}}}{dt}, \ldots, \overline{\overline{\varepsilon}}, \frac{d\overline{\overline{\varepsilon}}}{dt}, \ldots\} = 0$$

Description du Comportement du Matériau en σ et ε vraies.

ELASTICITE

Loi de Hooke

$$E\overline{\overline{\varepsilon}} = -\eta \mathbf{Tr}(\overline{\overline{\sigma}})\overline{\overline{\delta}} + (1+\eta)\overline{\overline{\sigma}} \quad \text{Young} \quad E\varepsilon_{ij} = -\eta\sigma_{kk}\delta_{ij} + (1+\eta)\sigma_{ij}$$
$$\sigma = \lambda \mathbf{Tr}(\overline{\overline{\varepsilon}})\overline{\overline{\delta}} + 2\mu\overline{\overline{\varepsilon}} \quad \text{Lame} \quad \sigma_{ij} = \lambda\varepsilon_{kk}\delta_{ij} + 2\mu\varepsilon_{ij}$$
$$\overline{\overline{S}}_\sigma = 3K\overline{\overline{S}}_\varepsilon \quad \text{Hooke} \quad \overline{\overline{D}}_\sigma = 2\mu\overline{\overline{D}}_\varepsilon \quad \overline{\overline{\pi}}_\sigma = \overline{\overline{\pi}}_\varepsilon$$

Équation de Lamé en déplacement

$$(\lambda+\mu)\mathbf{Grad}(\mathbf{Div}\,\overrightarrow{u}) + \mu\Delta\overrightarrow{u} + \rho\overrightarrow{X} = \rho\frac{d^2\overrightarrow{u}}{dt^2}$$
$$(\lambda+\mu)\mathbf{Rot}(\mathbf{Rot}\,\overrightarrow{u}) + (\lambda+2\mu)\Delta\overrightarrow{u} + \rho\overrightarrow{X} = \rho\frac{d^2\overrightarrow{u}}{dt^2}$$
$$\frac{1}{1-2\eta}\mathbf{Grad}(\mathbf{Div}\,\overrightarrow{u}) + \Delta\overrightarrow{u} + \frac{\rho}{\mu}\overrightarrow{X} = \frac{\rho}{\mu}\frac{d^2\overrightarrow{u}}{dt^2}$$

Relations entre les modules élastiques

$$\lambda = \frac{\eta E}{(1+\eta)(1-2\eta)} \quad G = \mu = \frac{E}{2(1+\eta)}$$
$$E = \frac{\mu(3\lambda+2\mu)}{\lambda+\mu} \quad \eta = \frac{\lambda}{2(\lambda+\mu)}$$
$$K = \frac{E}{3(1-2\eta)} \quad K = \lambda + \frac{2}{3}\mu$$

Potentiel d'élasticité et énergie élastique

Le travail de déformation W s'écrit soit en terme de forces externes, soit en terme de forces internes :

$$W = \int_V \mathbf{Tr}(\overline{\overline{\sigma\varepsilon}})dV = \int_V \overrightarrow{f}\,\overrightarrow{u}\,dV + \int_S \overrightarrow{T}\,\overrightarrow{u}\,dS$$

En l'absence de forces de volume, l'énergie élastique stockée s'écrit :

$$\Rightarrow \quad \text{élasticité linéaire}$$
$$\frac{dU^E}{dV} = \int_0^{\overline{\overline{\varepsilon}}} \mathbf{Tr}(\overline{\overline{\sigma}}d\overline{\overline{\varepsilon}}) \qquad \frac{dU^E}{dV} = \frac{1}{2}\mathbf{Tr}(\overline{\overline{\sigma\varepsilon}})$$
$$U^E = \int_V \frac{dU^E}{dV}dV = \int_S \overrightarrow{T}\,d\overrightarrow{u}\,dS \qquad U^E = \frac{1}{2}\int_S \overrightarrow{T}\,\overrightarrow{u}\,dS$$

HUTCHINSON APPROACH

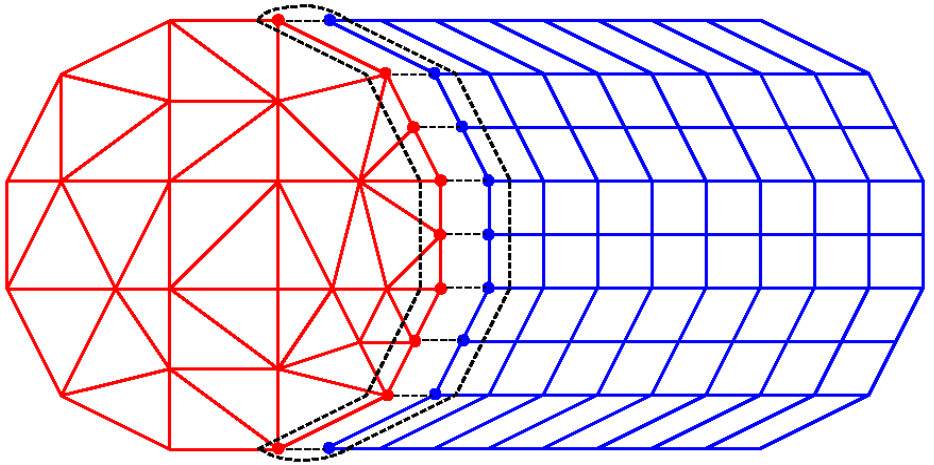
- Finite element on structured or unstructured meshes
- Non overlapping domain decomposition methods
- Schur complement, FETI, FETI-H, FETI-2LM
- Implementation in NUMEA

LOCAL CONDENSATION : SCHUR COMPLEMENT METHOD *(FX ROUX)*

- Interface unknown: $x_3 = x_3^{(1)} = x_3^{(2)}$

- Solution of internal equations in subdomains

$$K_{11}\, x_1 = b_1 - K_{13}\, x_3$$
$$K_{22}\, x_2 = b_2 - K_{23}\, x_3$$



- Equilibrium condition on interface => definition of residual

$$K_{31}\, x_1 + K_{32}\, x_2 + K_{33}\, x_3 - b_3 =$$
$$\left(K_{33} - K_{31}K_{11}^{-1}K_{13} - K_{32}K_{22}^{-1}K_{23}\right)x_3 - \left(b_3 - K_{31}K_{11}^{-1}b_1 - K_{32}K_{22}^{-1}b_2\right)$$

IMPLEMENTATION *(FX ROUX)*

- Solution of local system via a direct method (Gauss, Cholesky)

$$K_{11}\,x_1 = b_1 - K_{13}\,x_3 \qquad K_{22}\,x_2 = b_2 - K_{23}\,x_3$$

- Local contribution to interface residual

$$\begin{pmatrix} K_{11} & K_{13} \\ K_{31} & K_{33}^{(1)} \end{pmatrix} \begin{pmatrix} x_1 \\ x_3 \end{pmatrix} - \begin{pmatrix} b_1 \\ b_3^{(1)} \end{pmatrix} = \begin{pmatrix} 0 \\ \left(K_{33}^{(1)} - K_{31}K_{11}^{-1}K_{13}\right)x_3 - \left(b_3^{(1)} - K_{31}K_{11}^{-1}b_1\right) \end{pmatrix}$$

$$\begin{pmatrix} K_{22} & K_{23} \\ K_{32} & K_{33}^{(2)} \end{pmatrix} \begin{pmatrix} x_2 \\ x_3 \end{pmatrix} - \begin{pmatrix} b_2 \\ b_3^{(2)} \end{pmatrix} = \begin{pmatrix} 0 \\ \left(K_{33}^{(2)} - K_{32}K_{22}^{-1}K_{23}\right)x_3 - \left(b_3^{(2)} - K_{32}K_{22}^{-1}b_2\right) \end{pmatrix}$$

- Global interface residual obtained by assembling local contributions

$$\left(K_{33}^{(1)} - K_{31}K_{11}^{-1}K_{13}\right)x_3 - \left(b_3^{(1)} - K_{31}K_{11}^{-1}b_1\right) + \left(K_{33}^{(2)} - K_{32}K_{22}^{-1}K_{23}\right)x_3 - \left(b_3^{(2)} - K_{32}K_{22}^{-1}b_2\right)$$
$$= \left(S_3^{(1)} + S_3^{(2)}\right)x_3 - \left(c_3^{(1)} + c_3^{(2)}\right)$$

FETI *(FX ROUX)*

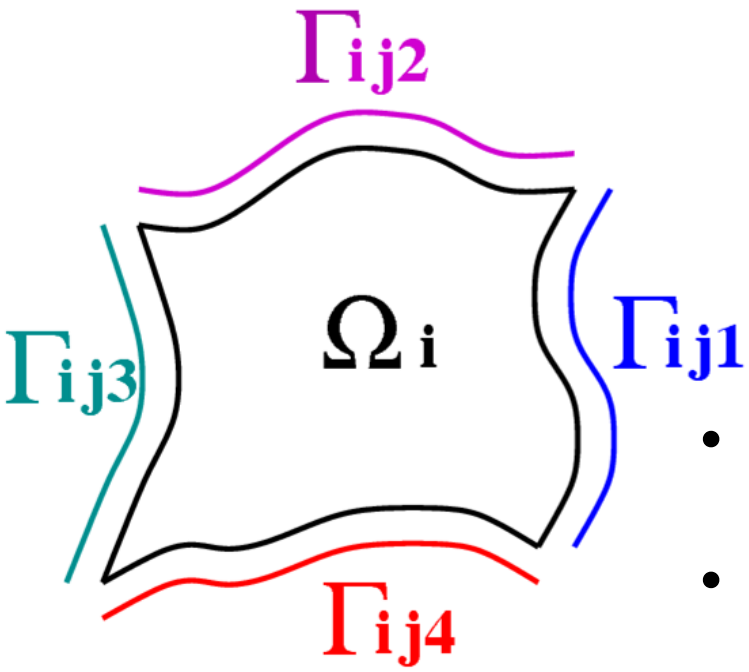
- Interface unknown : $\lambda = \lambda_1 = -\lambda_2$
- Local problems :

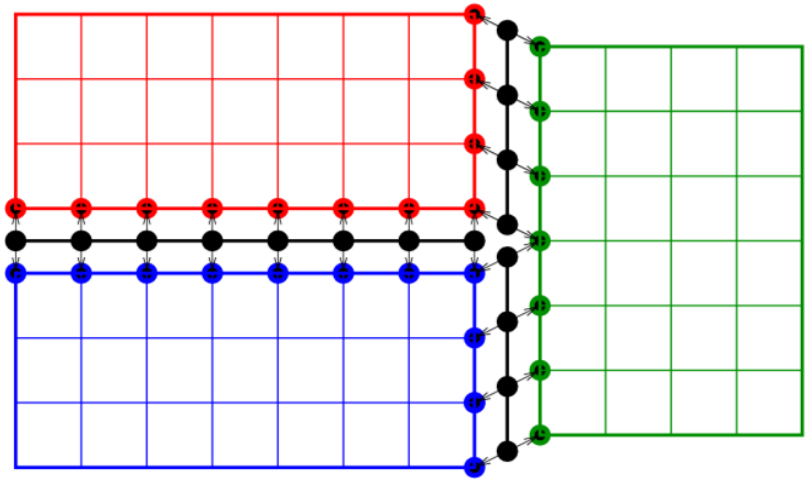
$$\begin{pmatrix} K_{11} & K_{13} \\ K_{31} & K_{33}^{(1)} \end{pmatrix} \begin{pmatrix} x_1 \\ x_3^{(1)} \end{pmatrix} = \begin{pmatrix} b_1 \\ b_3^{(1)} + \lambda \end{pmatrix} \quad \begin{pmatrix} K_{22} & K_{23} \\ K_{32} & K_{33}^{(2)} \end{pmatrix} \begin{pmatrix} x_2 \\ x_3^{(2)} \end{pmatrix} = \begin{pmatrix} b_2 \\ b_3^{(2)} - \lambda \end{pmatrix}$$

- Interface residual : $x_3^{(1)} - x_3^{(2)}$
- Use CG to converge to the solution of the implicit condensed interface problem

EASY INTERFACE MANAGEMENT

- No multiple interface unknowns

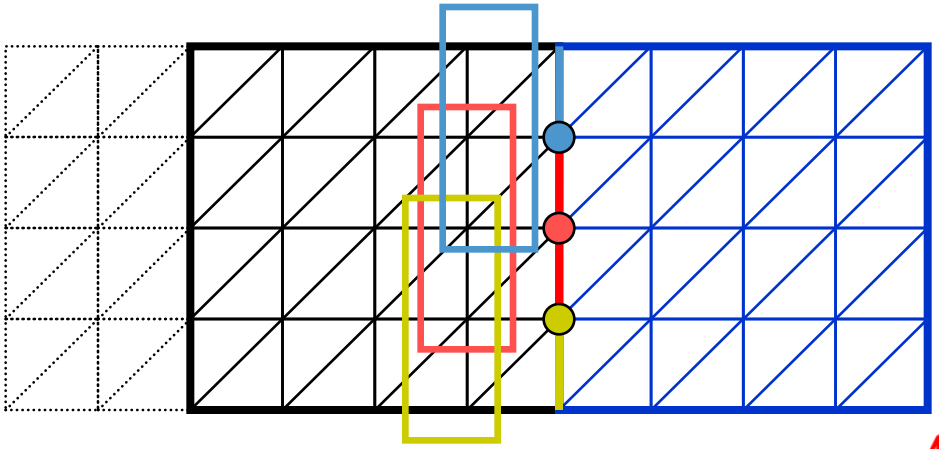


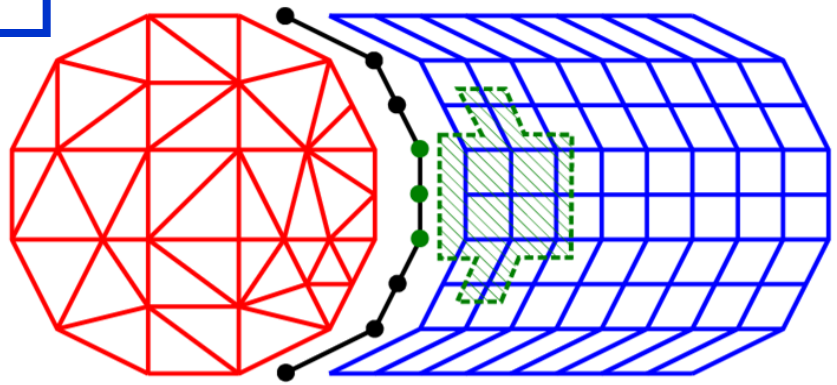


- Uncoupled computation of jump of interface displacements
- Very simple implementation in message passing programming environment
- Same implementation for 2 or *N* subdomains

SPARSE APPROXIMATION OF SCHUR COMPLEMENT

- Local condensation on small patches
- Weighted assembling





- Purely algebraic approach
- Black box implementation
- Works for any kind of element
- Very fast convergence for highly heterogeneous problems

INTERFACE AT ELEMENT LEVEL

- One MPI process per subdomain
- Each process computes only elemental contributions for its own element (coloring, color = subdomain number)
- Interface between finite element code and DDSolv

  symbolic phase : list of DOFs in each element, list of DOFs for essential boundary conditions, list of DOFs in each multi-point constraint

  numeric phase : element matrices, MPCs coefficients

  solution phase : right hand side, essential BC values, MPCs values
- Global numbering
- Non element based information can be global
- **Computation of element contributions parallelized without any modification of existing code except color testing**

DDSOLV : CONCLUSION

- Finite Element methods for structural analysis and linear algebra are different businesses
- Keep both in different libraries
- Solver parallelization through domain decomposition methods with very limited impact on the original code (except deletion of linear algebra part)
- The most complex issue : how to deal with non element based models (MPCs, rigid bodies, contact…)
- Future development : non conforming interfaces, multi-domain contact

« Dissection » implemented in Open Source FreeFM, developed by F. Hecht (LJLL,UPMC),

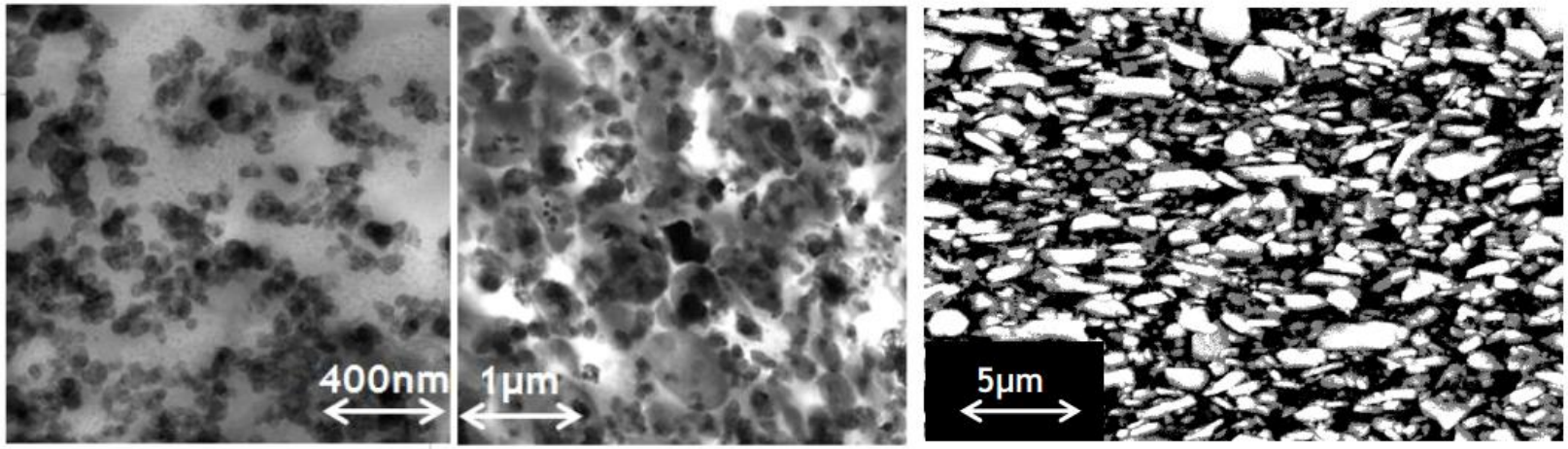
A dissection solver with kernel detection for symmetric finite element matrices on shared memory computers; Suzuki, Atsushi; Roux, François-Xavier, International Journal for Numerical Methods in Engineering, (2014)

Cf . Francois Xavier Roux Talk

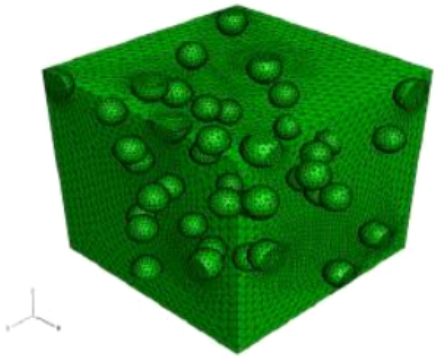
BENEFITS WITH THIS METHODOLOGY

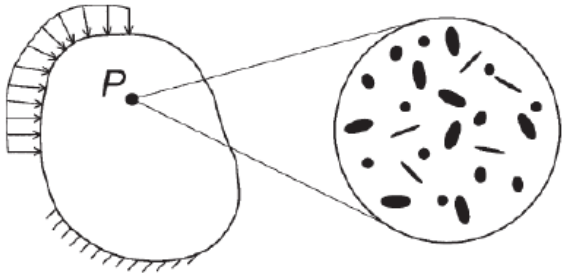
- Each library uses its own data structure and even its own language
- Data exchanged via simple arrays
- FE2FETI can manage MPI
- The finite element code does not perform any linear algebra computation
- **The FE2FETI interface can be adapted to any FE code (and not the opposite)**
- Co-development
- Interface with available sparse matrix solvers : MUMPS, PARDISO, BCS, … + skyline solver for small global problems and testing

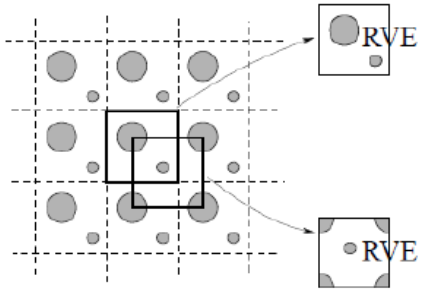
MULTI SCALE MATERIALS



Composite materials with inclusions

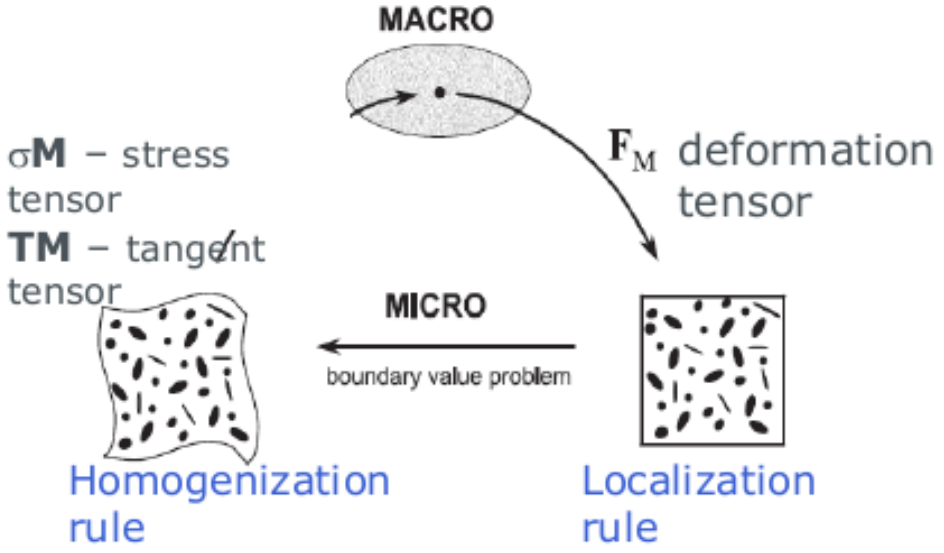






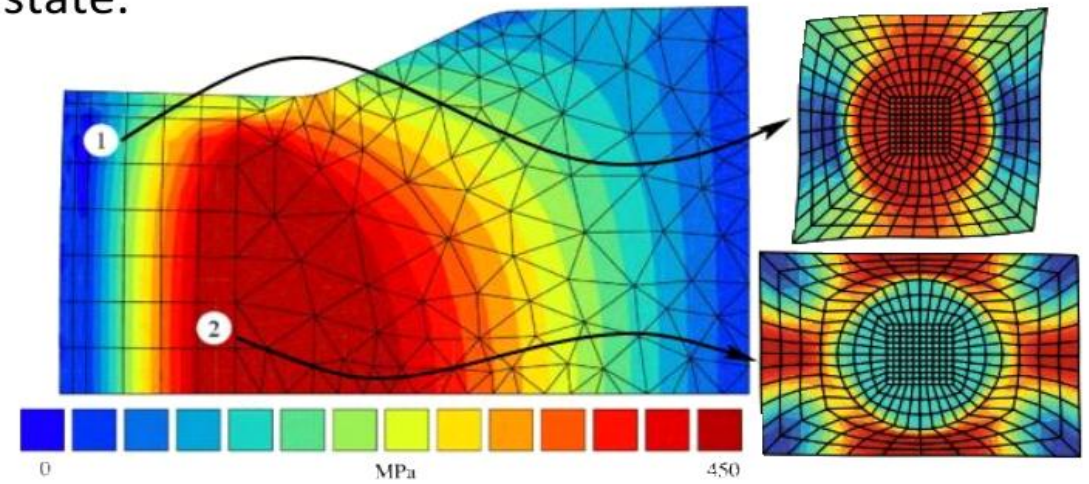
Direct micro-macro methods

- For overcoming the RVE method limitations direct micro-macro approac has been proposed.
- This approach does not lead to an overall material description valid for the whole macroscopic piece of material, but estimates the relevant stress-strain relationship at a macroscopic point by performing separate calculations on the RVE, assigned to that macroscopic point.
- The analysis on the RVE level is done using the finite element method.



Direct micro-macro methods: FE^2

- This class of models is often called "FE^2" because it requires the simultaneous computation of the mechanical response at two different scales: macro and micro.
- FE^2 models are constructed using three main ingredients:
  - Modeling of the mechanical behavior at the lower scale (the RVE);
  - Localization rule which determines the local solutions inside the unit cell, for any given overall strain;
  - Homogenization rule giving the macroscopic stress tensor, knowing the micromechanical stress state.



F. Feyel (1999), Multiscale FE2 elastoviscoplastic analysis of composite structures, Computational Materials Science, 344-354.

Block Low-Rank multifrontal solver

Block **L**ow-**R**ank approximations to improve sparse multifrontal solvers

Works with MUMPS Consortium

Multifrontal solver

- direct solver for large linear systems
- objective: $A = LU$

Low-rank approximations

- compression and flop reduction
- accuracy controlled by a numerical parameter

(⟶ can also be used as a preconditionner)

Many representations: Recursive H, H^2 [Bebendof, Börm, Hackbush, Grasedyck,. ..], HSS/SSS [Chandrasekaran, Dewilde, Gu, Li, Xia,. ..], Flat block low-rank (BLR) …

- **Geometry Library / Isogeometry**

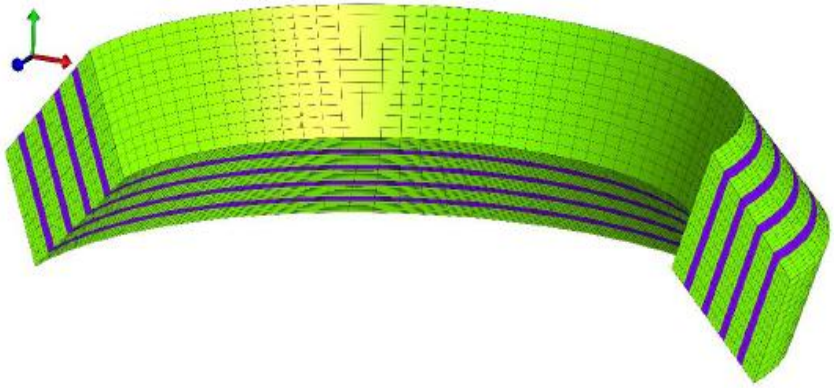
NEW FEM approach : Iso geometry (IGA) : FEM vs IGA mesh

Objective: New Efficient Mechanical Structure Simulation Method

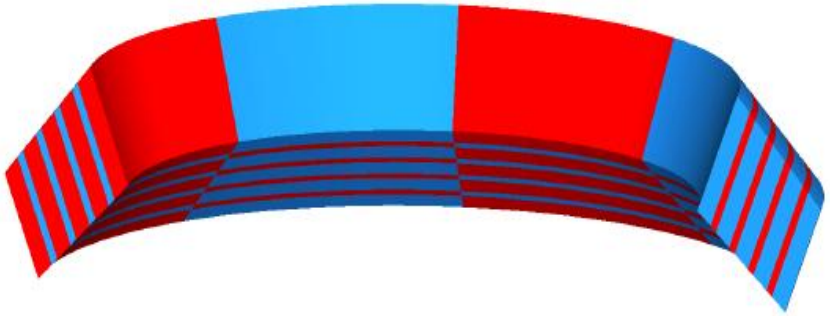
CADs (like IRIT) use NURBS (non-uniform rational B-splines)

IGA use NURBS for the PDE solver

Works with Annalisa Buffa, Gershon Elber, FX Roux

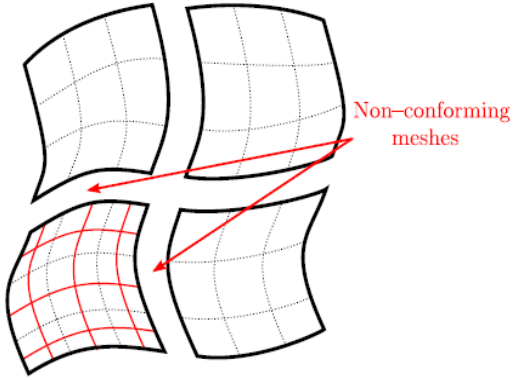


19800 elements
67626 dofs



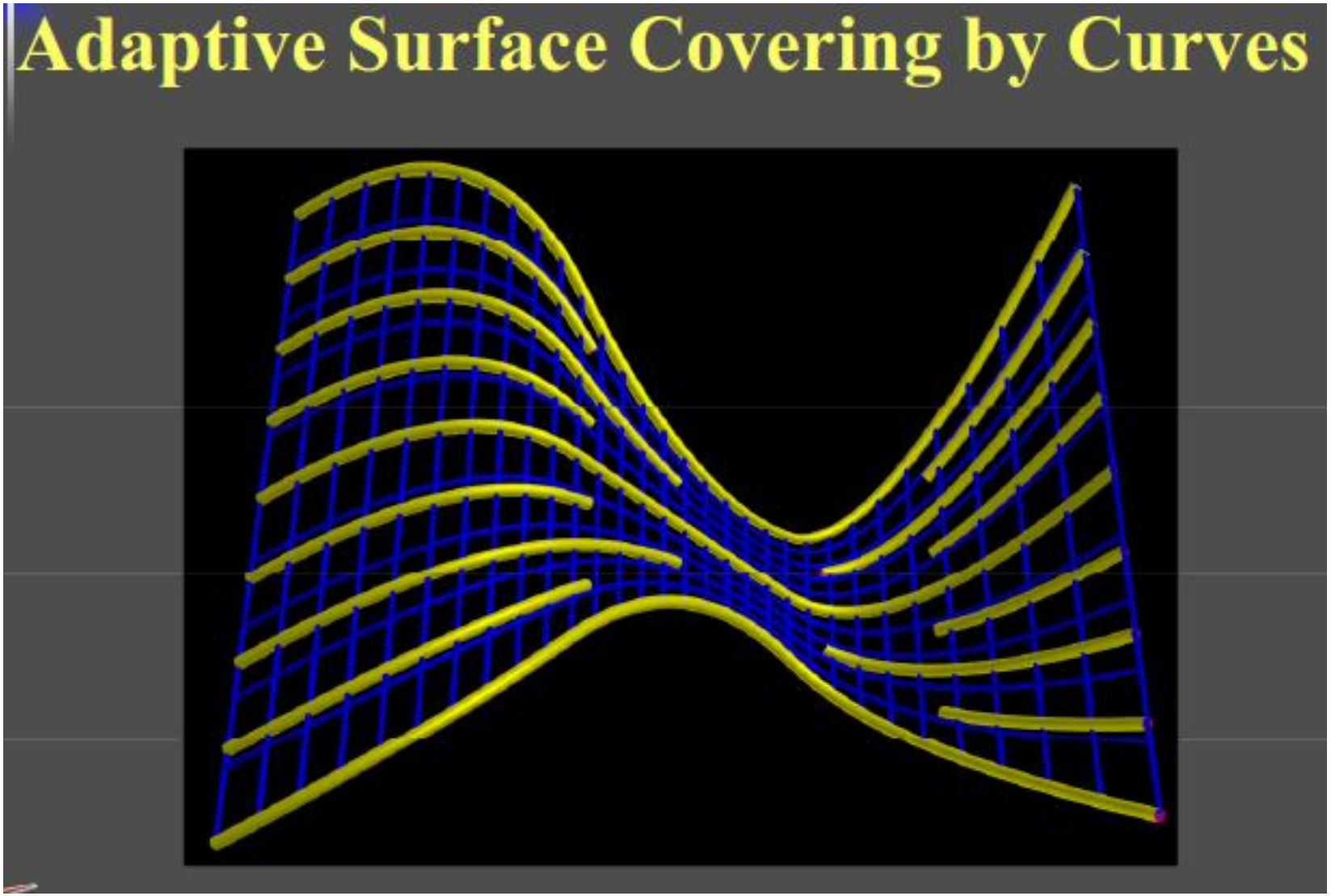
36 elements

$p = 2 \rightarrow$ 1701 dofs
$p = 3 \rightarrow$ 3888 dofs



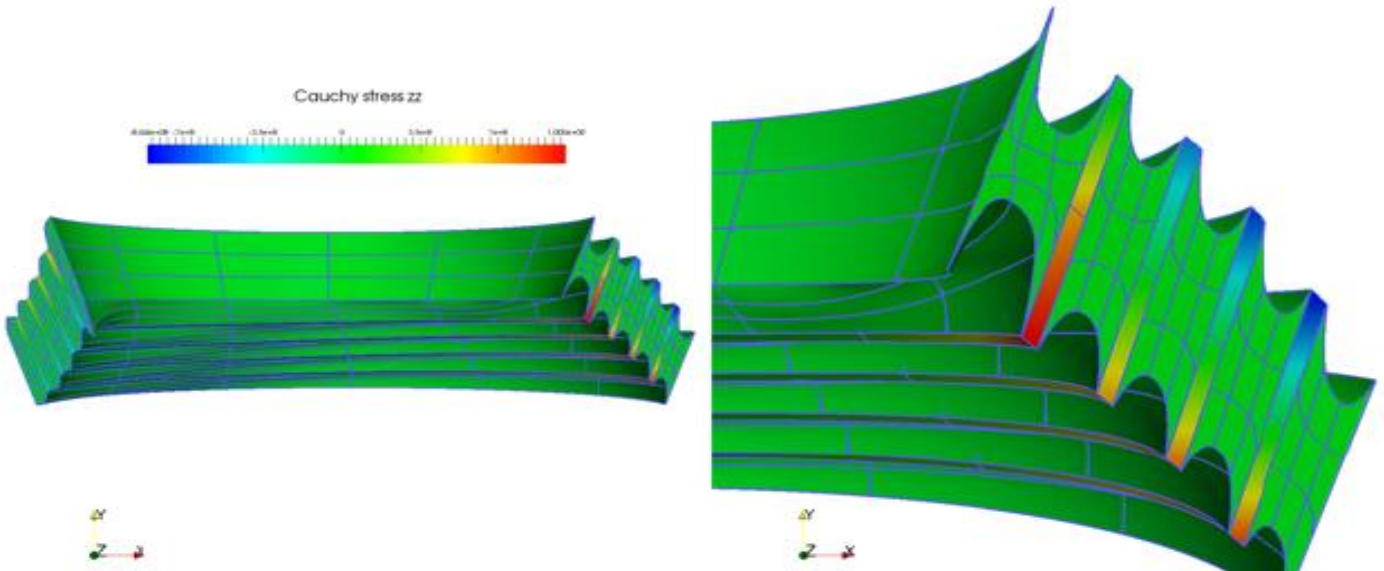
CHALLENGE: treatment of non-matching patch interfaces, regular gluing when possible.

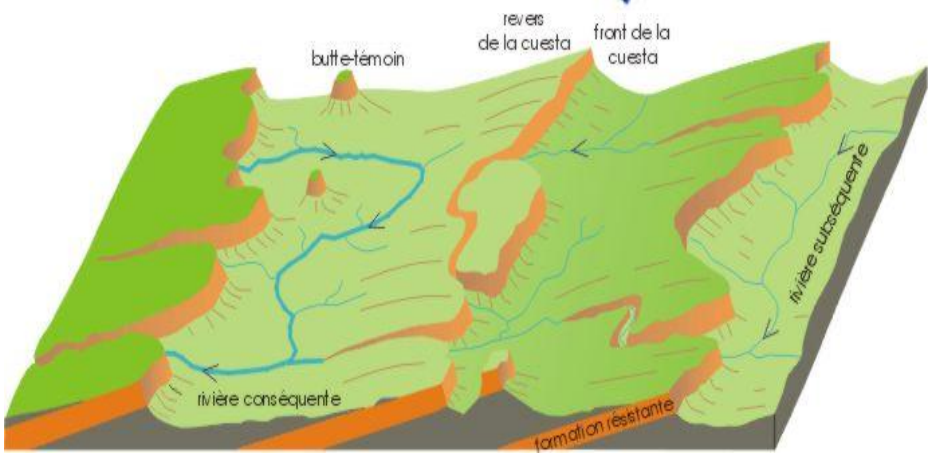
GOEMETRY LIBRARY / ISOGEOMETRY



GOEMETRY LIBRARY / ISOGEOMETRY

Stress zz component:

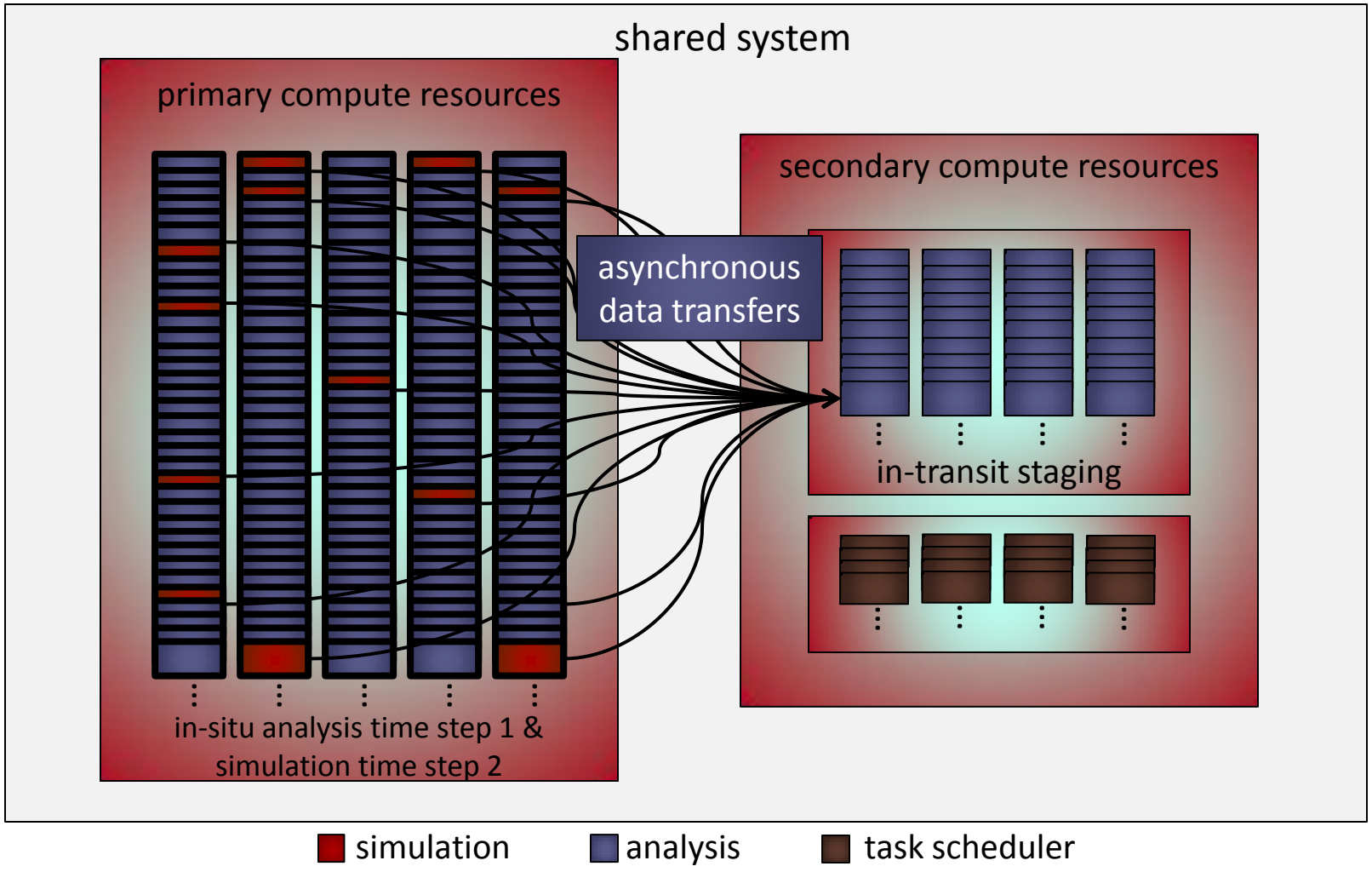




TRANSFERT OF THIS METHODOLOGY TO BASSIN MODELING

- **NEXT HPC**

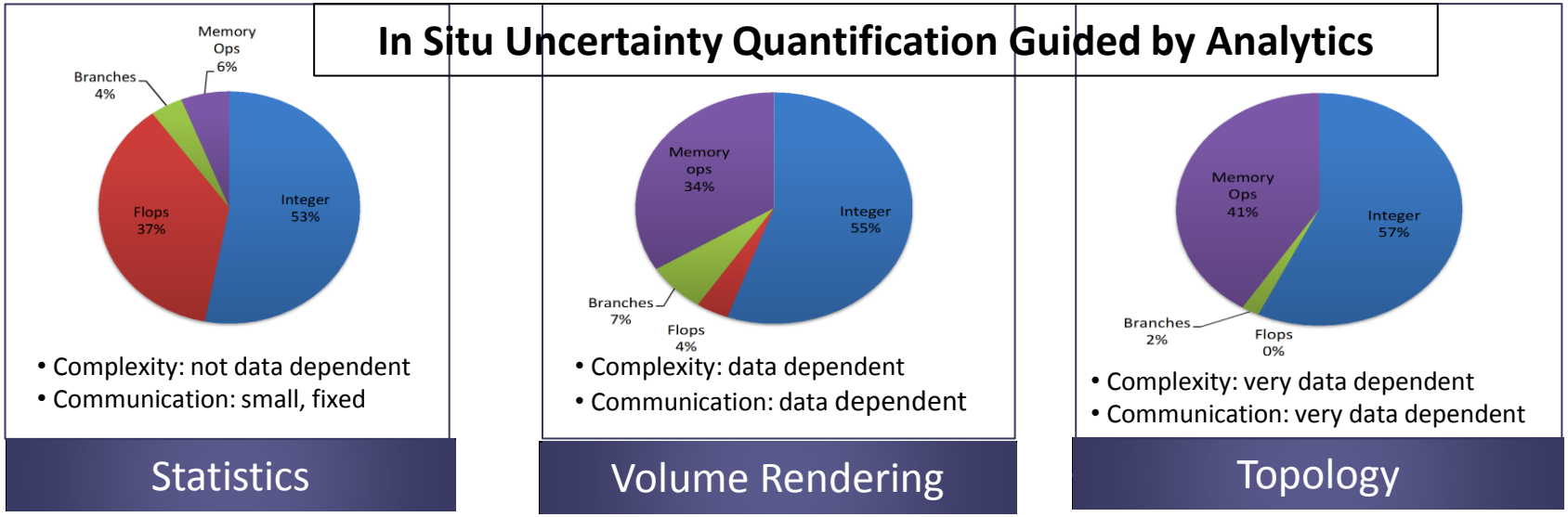
Exploring the design space of workflows: Temporally multiplexed hybrid in-situ + in-transit workflow



EFFICIENT IN SITU DATA PROCESSING: COUPLING 3 ALGORITHMS WITH DIFFERENT CHARACTERISTICS

Works with Julien Tierny, Jackie Chen

In Situ Uncertainty Quantification Guided by Analytics



Statistics

- Debugging and Analysis, Filtering and averaging (spatial and temporal)
- Statistical moments (conditional)
  - In-situ local moments & aggregation
  - In-situ local moments + in-transit aggregation
- Statistical dimensionality reduction
- Spectra (scalar, velocity, coherency)

Volume Rendering

- Qualitative visual depiction of data
- Local data: partial images via image compositing
- In-situ down-sampling + in-transit rendering & compositing

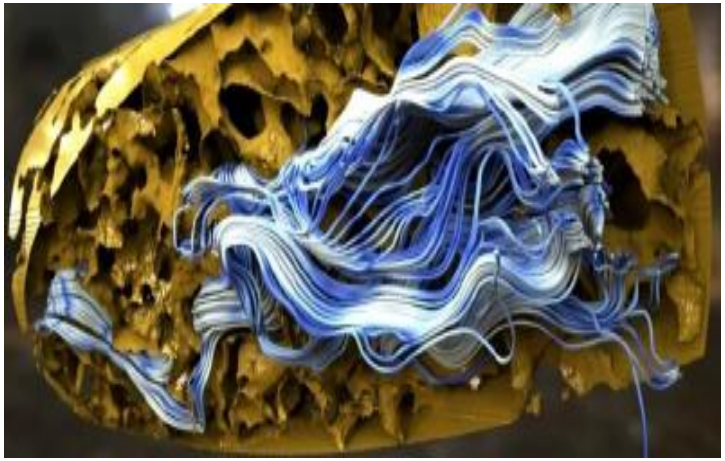
Topological Segmentation and Tracking

- Distance field (level set)
- Compute local merge trees
- Integrate to resolve features spanning multiple cores
- Adjust local merge trees

IN-SITU VISUALIZATION

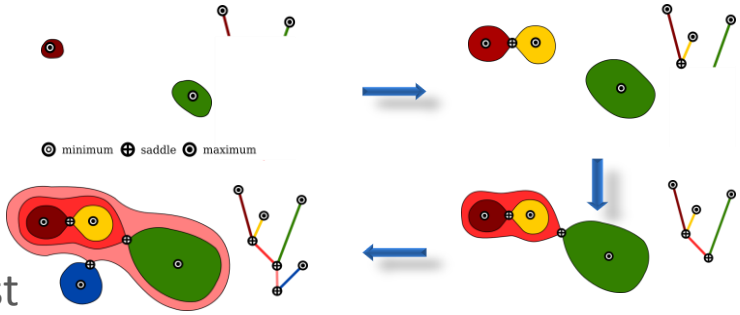
Parallel volume rendering

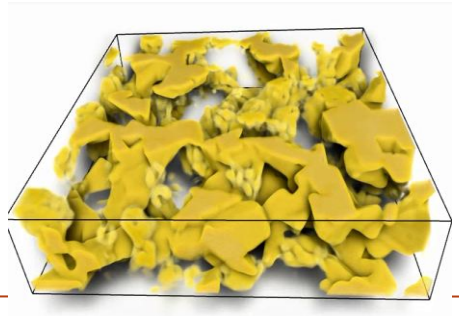
- Design grid adaptor mechanism
- Visualization directly takes data regions from grid adaptor
- Highly scalable parallel volume rendering, particle rendering and image compositing
- **Down sampling**

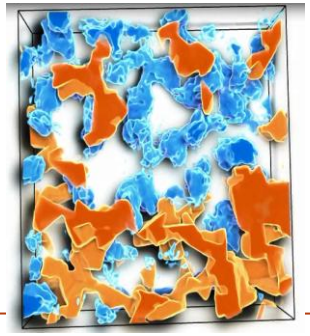


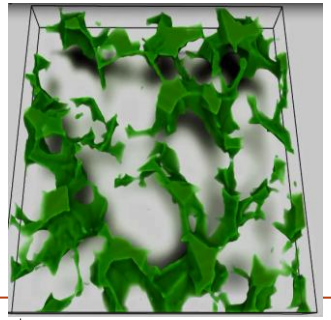
Reduced topology computation

- Complete characterization of **level-set** behavior of simulation variables
- Used to define features of interest
- Compute local merge trees
- Integrate to resolve features spanning multiple cores
- Adjust local merge trees









TOTAL

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, Polymers

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 (Hutchinson, Atotech)
  - Molecular Simulation for interface definition of adhesives, polymer compounds, …

Safety / Explosion
Turbulence, Flame speed, detonation, …

CONCLUSIONS

Numerous and Diverse Numerical simulations / Modeling in the group

Numerical Analysis not on the same level

Large number of potential improvements by transverse sharing or exchange

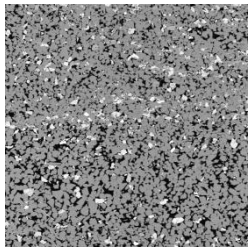
- **Mesh / Adaptive / Intelligent**
- **FE, FV, FD ….**
- **Mesh less methods**
- **Sparse solvers**
- **CA algo.**

THANK YOU FOR ATTENTION

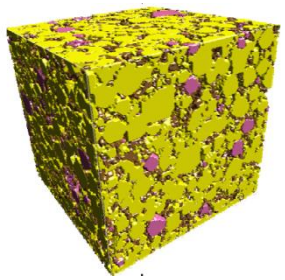
Q/A

CONSTRUCTION OF THE NUMERICAL ROCK

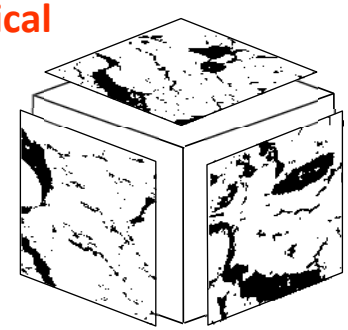
(a) Process- or physics-based



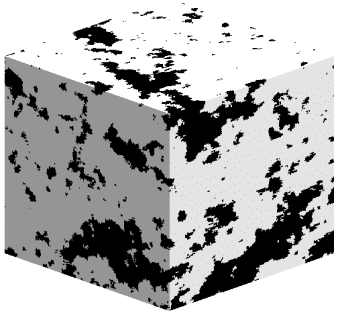
Thin section analysis and geological modelling



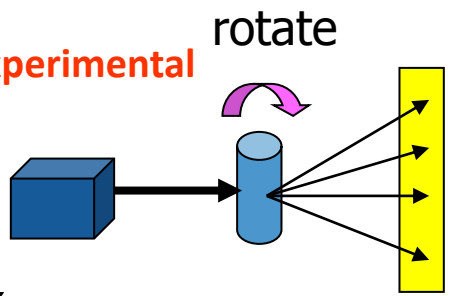
(b) Statistical

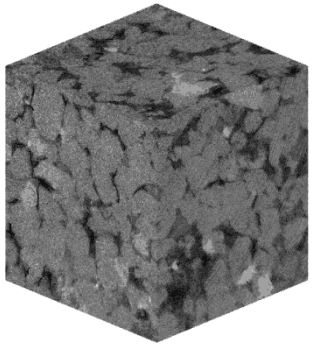


2D thin section



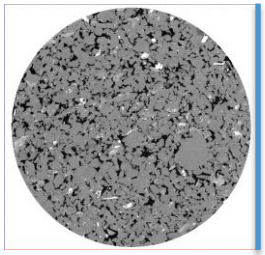
(c) Experimental





μ-Tomography Image

Typical Simulation domain



8 mm

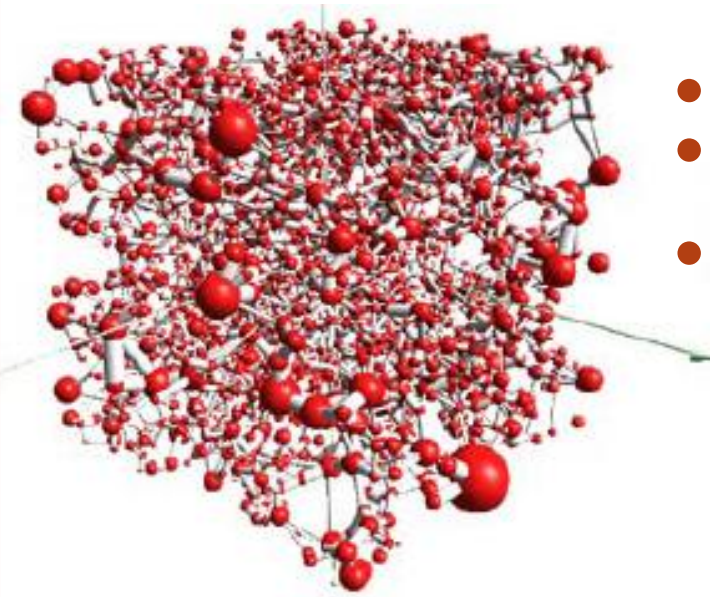
Method (c) includes FIB/SEM

TOTAL

MULTI-PHASE FLOW PROPERTIES: NETWORKS VS IMAGES

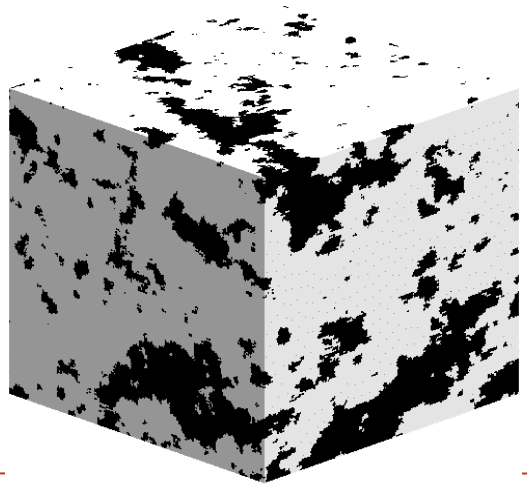
- Once 3D imaging is done, images can be used for simulation in two ways:

1. Either a simplified pore network model (PNM) is non-uniquely extracted from the image



- Fast computation
- Bigger: up to core scale
- Most known physics can be included in a semi-analytical way

2. Or the 3D imaged is used directly



- Slower computation
- Smaller volume: only few mm^3
- Complex physics more difficult to reproduce

Pore network extraction: outstanding challenges

Topological considerations

- Main flow paths that are relevant to multiphase flow – topology preservation

Geometrical considerations

- Merging of pores / throats / parallel throats e.t.c
- Definition of pore / throat lengths and the volume assigned to them
- Shape factor estimation

Reality:

- **Differences in geometrical characterisation will always result in different predicted single phase and multiphase results**

Absolute permeability

- Differences in pore and throat length definitions / estimations
- Differences in skeletonization methods

Relative permeabilty curves

- Differences in the topology (main flow path) and geometrical characterisation of network elements

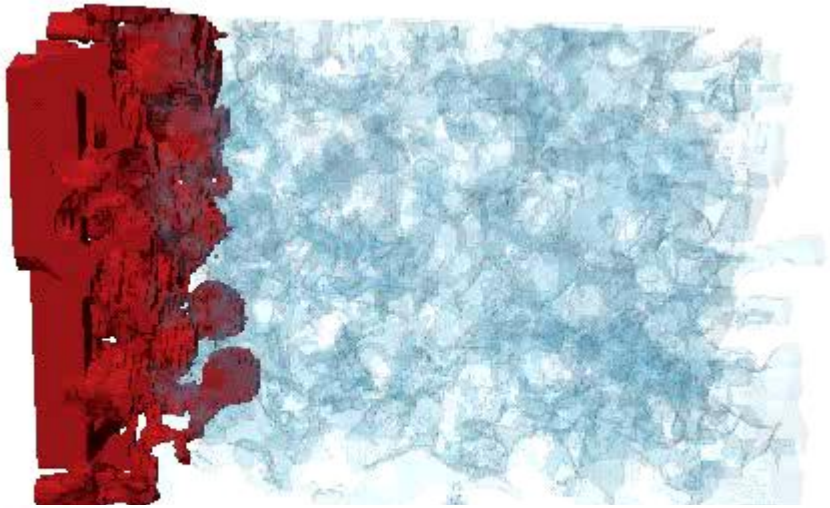
- **Wettability trend**
  - The % of total pore volume allocated to throats has a major impact on both the rel perm and rel perm wettability sensitivity trend

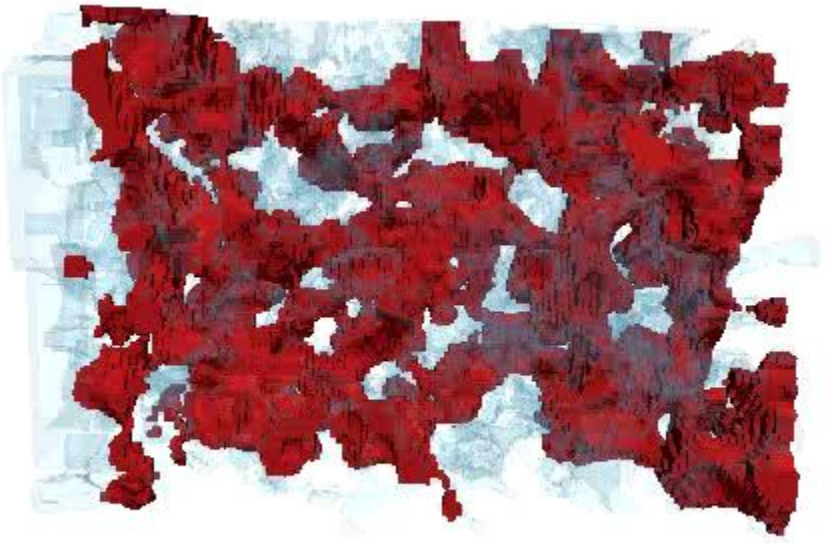
- **Geometrical characterisation of network elements has considerable impacts on computed petrophysical and multiphase properties**

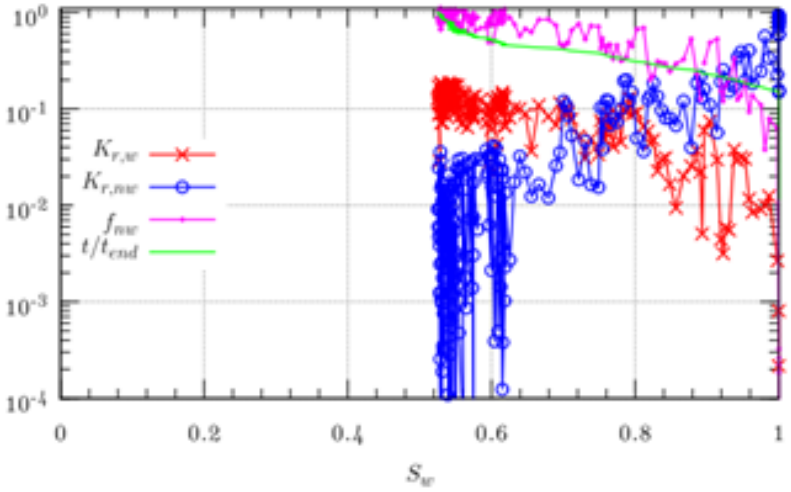
DIRECT SIMULATION IN 3D IMAGE: NAVIER-STOKES EQUATIONS (VOF, LEVEL SET, DIFFUSE INTERFACE…..)

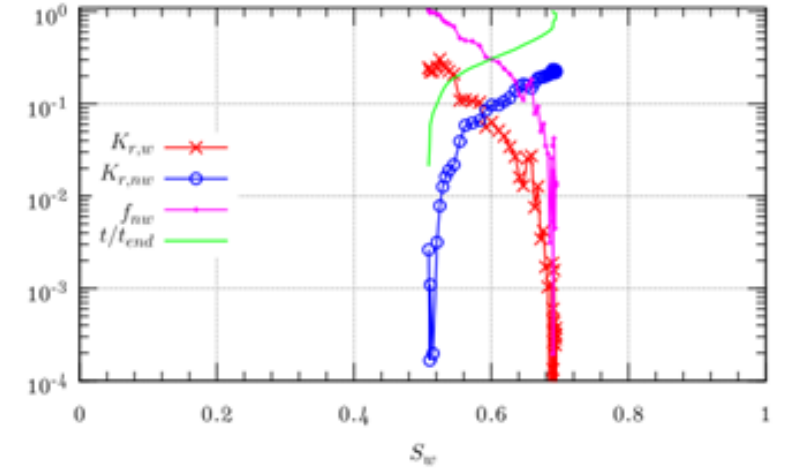
- Solving NS with methods such as finite difference systems in a complex pore space is far from simple, especially where more than one fluid phase is present in the pore space.
  - The no slip boundary condition has to be satisfied on an extremely intricate boundary surface—the pore/solid interface—which results in a very large system of equations to be numerically solved.
  - Moreover, in the case of multiple fluid phases, the moving fluid-fluid interface has to be incorporated and appropriate balances have to be satisfied on this boundary.
  - VOF or finite element methods, based on multigrid solvers will have difficulties to converge for porous media in which there are many obstacles.

DIRECT SIMULATION IN 3D IMAGE: NAVIER-STOKES EQUATIONS + VOF









From Ali Reini, Imperial College, 2013

SIMULATION AT PORE LEVEL BY LATTICE-BOLTZMANN METHOD

- Lattice-Boltzmann Method, CFD method
  - High parallel computing potential
  - Easy to deal with the complex geometry, such as porous media in our case
  - Easy boundary conditions and no need for meshing

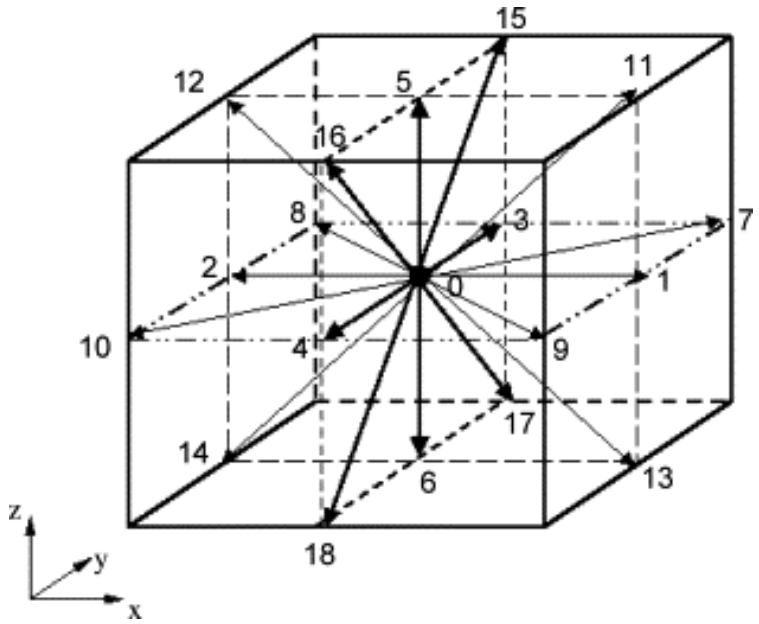
- The method uses “pseudo-particles” to discretize the flow.
  - These fluid particles are mesoscale, which is between the macro scale and atomic scale.

- Lattice Gas model derives from the Cellular Automaton (CA) which gives every fluid particle a state that could be changed by the neighborhood states at the next time step

D3Q19 MODEL

- **Lattice-Boltzmann Method (LBM) could use several model to describe the fluids: D2Q5, D2Q9, D3Q15, D3Q19, D3Q27.**

- **Each node has its own properties:**



Density: $$\rho = \sum_{0}^{N} N_i(\vec{x}, t)$$

Velocity: $$\vec{u}(\vec{x}, t) = \frac{\sum_0^N c_i N_i(\vec{x}, t)}{\sum_0^N N_i(\vec{x}, t)}$$

Where c_s **is the a lattice constant (sound speed, in BGK lattice D3Q19**

$$c_s^2 = 1/3$$

In D3Q19 model, for the distribution in node 0 (at rest) at time t:19 possible velocity vector

0	1	-1	0	0	0	0	1	-1	1	-1	1	-1	1	-1	0	0	0	0
0	0	0	1	-1	0	0	1	1	-1	-1	0	0	0	0	1	-1	1	-1
0	0	0	0	0	1	-1	0	0	0	0	1	1	-1	-1	1	1	-1	-1

TWO MAIN STEPS IN LBM NUMERICAL SIMULATION

- **Free steaming**
  - When the position and momenta are known at a particular time t, we could determine at a future time t+Δt:

$$N_i(\vec{x} + c_i\Delta t, t + \Delta t) = N_i(\vec{x}, t)$$

- **Collision**
  - When several fluid particles reach the same node, here comes a collision which is symbolized by a 'collision operator' :

$$N_i^{new}(\vec{x} + c_i\Delta t, t + \Delta t) - N_i^{old}(\vec{x}, t) = \Delta t\Omega_i$$

- When external force is added, we get the Lattice-Boltzmann equation

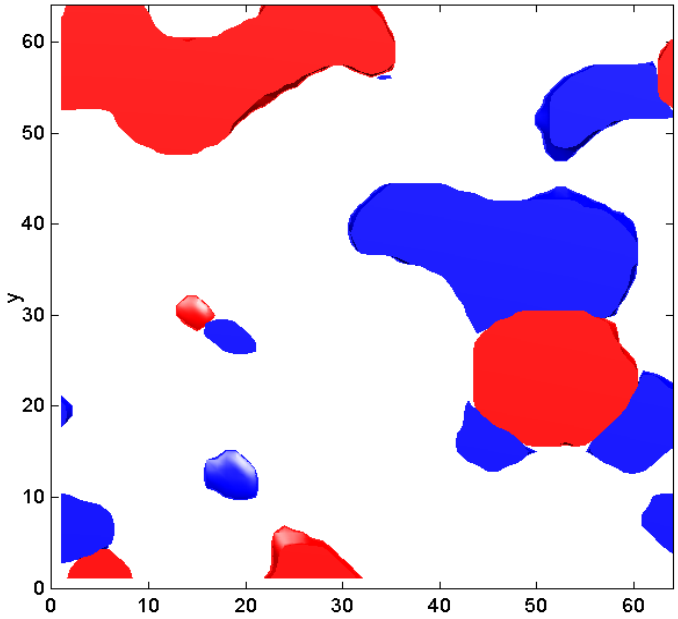
$$N_i^{new}(\vec{x} + c_i\Delta t, t + \Delta t) - N_i^{old}(\vec{x}, t) = \Delta t\Omega_i + \Delta t F_i$$

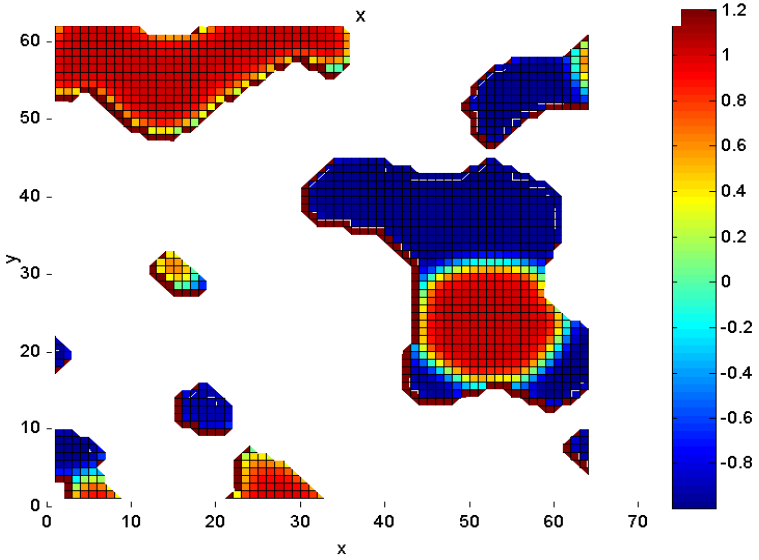
$N_i(\vec{x}, t)$ – *one particle distribution function ,*

X *– position,* c_i *– particle velocity,* ***t*** *– time,*

F *– external force,* Ω_i *– collision operator*

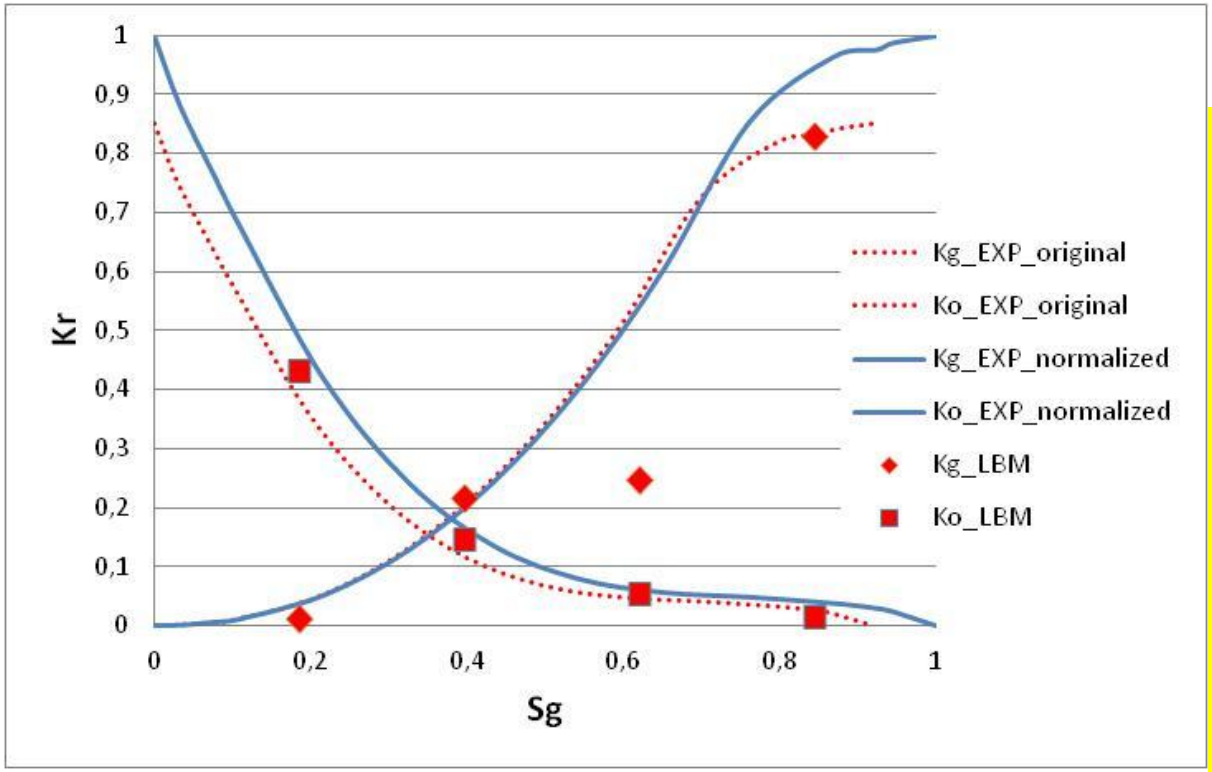
FOR TWO IMMISCIBLE FLUIDS





1. Each fluid treated explicitly with its properties
2. $Ni = Ni_{blue} + Ni_{red}$
3. The two phases have a tendency of demix (effect of surface tension)
4. Separation of the interface is obtained through a “color gradient”
5. Surface tension through a local perturbation of the particle distribution

COMPARISON WITH EXPERIMENT



- ~500days of cumulative CPU time
- 32 cores used (4 Cluster Nodes)
- 1 node x simulation
- 18 days (using TOTAL's Geoscience Research Centre HPC facilities, Aberdeen)

1. It took 6 months of work to put in place the simulation procedure
2. Only 1 real-case situation could be simulated: the result is promising

DRP / LATTICE-BOLTZMANN: CONSIDERATIONS

- Now fair internal experience: can get meaningful results for simple Kr problems if enough «human time» and CPUs are available.
- **Dynamic and unsteady state in nature.**
- Simulates directly in images on voxelized image (no meshing).
- The LBM solver is very dependent on **1) flow rates, 2) porosity, 3) scales, 4) densities and 5) viscosities 6) small/large contact angles/saturations.** Computation feasibility cannot be as certained without knowing which case or which sample has to be solved.
- **Very little literature for Kr application**.
- **Parallel hardware needed and high times for computation (=Sufficient volume of rock required (representative element volume))**
- Microporosity modelling out of reach (as well as high resolution features)
- **Important numerical instabilities**
- Probably the only mesh free method to address Pore Multiphase Flows issues

LBM shares many issues with more traditional CFD methods: but it is faster.

But Research on LBM and other methods continues in order to

- ✓ **improve really the knowledge of Multi Fluids Flows at pore level (see several talks in this conference)**
- ✓ **Achieve accurate multi scale modeling from the pore to Darcy**