DIGITAL ROCK PHYSICS: OBJECTIVES AND CHALLENGES

29ème JOURNÉE CASCIMODOT
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Cyprien Soulaine, BRGM
Background: porous media modeling

**Target:**
- Understand and model complex physics of flow and transport in reservoirs (geothermal energy, nuclear waste storage, water resources, oil and gas recovery, CO$_2$ sequestration, ...),
- Replace/complement lab-scale experiments (permeability...)

**Challenges:**
- Multi-scale problem,
- Multiphase flow,
- Fractured/damaged media,
- Thermal processes,
- Phase change,
- Bio-geochemistry,
- Evolution of the pore structure,
- Mechanics,
- ...
Multi-scale modeling

Molecules

Pore

Core

Field

Statistical mechanics

Continuum mechanics

Navier-Stokes

Darcy

(Adapted from Buchgraber 2012)
Discret vs continuum

for every point of the domain

fluid OR solid

$$\rho \frac{\partial \mathbf{v}}{\partial t} + \mathbf{\rho v} \cdot \nabla \mathbf{v} = -\nabla p + \mathbf{\rho g} + \mu \nabla^2 \mathbf{v}$$

fluid AND solid

$$\mathbf{V} = -\frac{K}{\mu} \cdot (\nabla P - \rho_f \mathbf{g})$$
Why working at the pore-scale?

- Understand
- Characterize
- Upscale
Digital Rock Physics

Image of core, plug or cutting

Segmented pores/minerals in image

Computation of rock properties

(source: GeoDict)

**Geometrical parameters**
- Porosity
- Percolation
- Surface area
- Tortuosity

**Flow Parameters**
- Permeability
- Multi-scale/phase flow
- Capillary pressure curve

**Electrical parameters**
- Formation factor
- Resistivity index
- Saturation exponent
- Cementation exponent

**Mechanical parameters**
- Elastic moduli
- Stiffness
- In-Situ conditions
Advantages of using digital experiments

- Non-destructive,
- Sensitivity analysis,
- Laboratory hazards such as leaks or temperature variations are simply removed,
- Can reach pressure and temperature conditions that are difficult to consider in the lab without the use of dedicated equipment,
- Moreover, the information resulting from these simulations is spatialized (distribution of phases, velocities or stresses) which gives a greater flexibility of post-treatment whereas the classical petrophysical experiments only give access to macroscopic data.
Challenges

Solve the physics:
- Define correct models
- Develop solution algorithm
- Model validation

Interpret the results:
- Link with macroscale properties

Pre-processing
- Image segmentation
- Gridding

Reach a REV
- High Performance Computing
- Efficient time-stepping
Direct Numerical Simulation techniques

Direct modeling

Navier-Stokes on Eulerian grids (CFD)
- Solve Navier-Stokes equations on a Eulerian grid,
- Differential operators discretized with FVM, FDM or FEM,
- Nowadays, all the CFD softwares are efficient, robust and parallelized.

Lattice Boltzmann Method (LBM)
- Solve the discrete Boltzmann equation instead of Navier-Stokes,
- The nature of the lattice determines the degree of freedom for the particle movement,
- Easy to program, massively parallel,
- No limitation due to Knudsen number.

Smoothed-Particle Hydrodynamics (SPH)
- Mesh-free technique,
- Fluid is divided into a set of discrete particles,
- To represent continuous variables, a kernel defined the sphere of influence of a particle,
- Particles are tracked in time as they move in the pore-space using a Lagrangian framework.

- Directly deal with the real pore structure geometry,
- Can be used to investigate the physics
- More computationally expensive than PNM,
- Efficient multiphase solver are still in development.
Application: compute the permeability of a sandstone

\[ K_{ij} = \mu \langle v_i \rangle \left( \frac{\Delta P}{L} \right)^{-1} \quad i = x, y, z \]

- Digital rock obtained from microtomography imaging,
- Grid the pore-space,
- In CFD simulations, the results may be very sensitive to the grid quality. At least 10 cells are required in each pore-throat,
- The grid quality is even more important when dealing with multiphase flow (refinement near the walls),
- Solve steady-state Stokes equations (SIMPLE algorithm with OpenFOAM).
Challenge 1: How to account for sub-voxel porosity?

... for example when imaging a source rock including micro-cracks and nanoporosity

- At the SEM scale, only the larger pores are captured
- The nanoporosity is not resolved in the image,
- But hydrocarbon molecules are transported through the nanoporosity...

1 Heath et al., *Pore Networks in continental and marine mudstones: Characteristics and controls on sealing behavior* Geosphere, 2011, 7, 429 – 454
2 Falk et al., *Effect of Chain Length and Pore Accessibility on Alkane Adsorption in Kerogen*, Energy & Fuels, 2015, 29, 7889-7896
The Darcy-Brinkman-Stokes\textsuperscript{1,2,3} equation allows a single domain formulation

\[
0 = -\nabla \tilde{p}_f + \frac{\mu_f}{\varepsilon_f} \nabla^2 \tilde{v}_f - \mu_f k^{-1} \tilde{v}_f
\]

Vanishes in the void space
Dominant in the porous region

\textsuperscript{1}Brinkman A Calculation of The Viscous Force Exerted by a Flowing Fluid on a Dense Swarm of Particles Appl. Sci. Res. (1947)

\textsuperscript{2}Neale and Nader Practical significance of Brinkman's extension of Darcy's law: coupled parallel flows within a channel and a bounding porous medium. (1974)

\textsuperscript{3}Soulaine and Tchelepi Micro-continuum approach for pore-scale simulation of subsurface processes Transport in Porous Media (2016)
Impact of sub-voxel porosity in microtomography images

**Cube 300 x 300 x 300**

- dark grey: macropores
- blue: microporous phase

3.16 µm = synchrotron resolution

**Sub-grid model:**

- Sub-voxel porosity from the grayscale,
- Local permeability from Kozeny-Carman combined with the image resolution,

<table>
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<th>sample</th>
<th>1</th>
<th>2</th>
<th>3</th>
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<tbody>
<tr>
<td>K (mD)</td>
<td>518</td>
<td>534</td>
<td>341</td>
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<tr>
<td>K- (mD)</td>
<td>211 (-59%)</td>
<td>475</td>
<td>305</td>
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<tr>
<td>K+ (mD)</td>
<td>913</td>
<td>804</td>
<td>673 (+97%)</td>
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1Soulaine et al. *The impact of sub-resolution porosity of X-ray microtomography images on the permeability* Transport in Porous Media (2016)
Challenge 2: hydro-geochemical coupling

- Darcy scale = averaged equations with averaged properties (permeability, surface area...)
- How does the permeability evolves when the pore-structure changes due to the dissolution/precipitation?
- What is the surface area accessible to the acid component? Complex interplay of diffusion, convection, reaction

Calcite dissolution: Simulation vs Experiment

- Dissolution of a calcite crystal in a micro-channel (Sophie Roman, Wen Song and Tony Kovscek, Stanford University),

- Acquisition of a high resolution dataset to compare with numerical simulations.

Dissolution at the core-scale

- Core-scale model (Darcy formulation)
- Diffuse Interface Model (DIM)
- Now the porous region has porosity and permeability
  \( \varepsilon_0 = 0.1 \pm 3\% \) and \( k_0 = 10^{-11} \text{ m}^2 \pm 10\% \)

\[\text{Soulaine and Tchelepi} \quad \text{Micro-continuum approach for pore-scale simulation of subsurface processes} \quad \text{Transport in Porous Media (2016)}\]

Challenge 3: two-phase flow in porous media

Particularity of multi-phase flow
- Navier-Stokes equation in each phases
- Continuity of the tangential component of the velocity at the fluid/fluid interface
- Laplace law for a surface at the equilibrium

\[ \Delta p = \sigma \left( \frac{1}{R_1} + \frac{1}{R_2} \right) \]

Surface tension is the elastic tendency of a fluid surface which makes it acquire the least surface area possible.

The contact angle quantifies the wettability affinity of a solid surface by a liquid.

The displacement of a wetting fluid by a non-wetting fluid (drainage) is different than the displacement of a non-wetting fluid by a wetting fluid (imbibition).
The Volume of Fluid (VOF) technique

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Color function

\[
\alpha = \begin{cases} 
0 & \text{in phase 2} \\
0 < \alpha < 1 & \text{on the interface} \\
1 & \text{in phase 1}
\end{cases}
\]

Single-field variables

\[
\begin{align*}
\mathbf{v} &= \alpha \mathbf{v}_1 + (1 - \alpha) \mathbf{v}_2 \\
p &= \alpha p_1 + (1 - \alpha) p_2 \\
\rho &= \alpha \rho_1 + (1 - \alpha) \rho_2 \\
\mu &= \alpha \mu_1 + (1 - \alpha) \mu_2
\end{align*}
\]

Single-field equations\(^1\)

\[
\rho \frac{\partial \mathbf{v}}{\partial t} + \rho \mathbf{v} \cdot \nabla \mathbf{v} = -\nabla p + \rho \mathbf{g} + \nabla \cdot \mu \left( \nabla \mathbf{v} + \nabla^t \mathbf{v} \right) + \mathbf{F}_c
\]

\[
\nabla \cdot \mathbf{v} = 0
\]

\[
\frac{\partial \alpha}{\partial t} + \mathbf{v} \cdot \nabla \alpha = 0
\]

Continuum Surface Force (CSF)\(^2\)

\[
\mathbf{F}_c = \sigma \nabla \cdot \left( \frac{\nabla \alpha}{\|\nabla \alpha\|} \right) \nabla \alpha
\]

\(^1\)Hirt, C. & Nichols, B. *Volume of fluid (VOF) method for the dynamics of free boundaries* Journal of Computational Physics, 1981, 39, 201 - 225

\(^2\)Brackbill et al. *A continuum method for modeling surface tension* Journal of Computational Physics, 1992, 100, 335 - 354
Summary

• An on-going revolution in the porous media community!

• Digital Rock Physics technologies aim at replacing or at least complement standard petrophysical experiments

• Still a lot of interesting challenges to solve (coupled physics, solution algorithm efficiency, HPC....)
Thank you for your attention!

www.cypriensoulaire.com