DIGITAL ROCK PHYSICS: OBJECTIVES AND CHALLENGES

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Background: porous media modeling

Target:

- Understand and model complex physics of flow and transport in reservoirs (geothermal energy, nuclear wast storage, water resources, oil and gas recovery, CO₂ 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



Discret vs continuum



Why working at the pore-scale?





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 mascroscale properties

Pre-processing

- Image segmentation
- Gridding

Reach a REV

- High Performance Computing
- Efficient time-stepping

Direct Numerical Simulation techniques



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



- 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).

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



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...

¹Heath et al., *Pore Networks in continental and marine mudstones: Characteristics and controls on sealing behavior* Geosphere, 2011, 7, 429 – 454 ²Falk et al., *Effect of Chain Length and Pore Accessibility on Alkane Adsorption in Kerogen*, Energy & Fuels, 2015, 29, 7889-7896

Darcy-Brinkman-Stokes equation

control volume, V





¹Brinkman *A Calculation of The Viscous Force Exerted by a Flowing Fluid on a Dense Swarm of Particles* Appl. Sci. Res. (1947) ²Neale and Nader *Practical significance of Brinkman's extension of Darcy's law: coupled parallel flows within a channel and a bounding porous medium*. (1974) ³Soulaine and Tchelepi *Micro-continuum approach for pore-scale simulation of subsurface processes* Transport in Porous Media (2016)

Impact of sub-voxel porosity in microtomography images¹

Cube 300 x 300 x 300



dark grey : macropores blue : microporous phase

Sub-grid model:

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



913

804

673

(+97%)

¹Soulaine et al. *The impact of sub-resolution porosity of X-ray microtomography images on the permeability* Transport in Porous Media (2016)

K+ (mD)

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

Landrot, G., J. B. Ajo-Franklin, L. Yang, S. Cabrini, and C. I. Steefel (2012). Measurement of accessible reactive surface area in a sandstone, with application to CO₂ mineralization. Chemical Geology 318, 113–125.

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 ($\epsilon_0 = 0.1 \pm 3\%$ and $k_0 = 10^{-11} \text{ m}^2 \pm 10 \%$)



Daccord and Lenormand (1987)

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

(N/m)

• Contact line dynamics at the solid surface

<u>Surface tension</u> is the elastic tendency of a fluid surface which makes it acquire the least surface area possible



Sophie Roman (Univ of Orléans, FR)

The <u>contact angle</u> 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

0	0	0	0	0	0
0	0	0	0	0	0
0	0.2	0.1	0	0	0.1
0.6	1	0.8	0.4	0.1	0.6
1	1	1	1	1	1
1	1	1	1	1	1

Color function

Single-field variables

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

$$\boldsymbol{v} = \alpha \boldsymbol{v}_1 + (1 - \alpha) \, \boldsymbol{v}_2$$
$$p = \alpha p_1 + (1 - \alpha) \, p_2$$
$$\rho = \alpha \rho_1 + (1 - \alpha) \, \rho_2$$
$$\mu = \alpha \mu_1 + (1 - \alpha) \, \mu_2$$

Single-field equations¹

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

$$\nabla \boldsymbol{.} \boldsymbol{v} = 0$$

$$\overline{\frac{\partial \alpha}{\partial t} + \boldsymbol{v} \cdot \nabla \alpha = 0}$$

Continuum Surface Force (CSF)²

$$\boldsymbol{F}_{c} = \sigma \nabla \cdot \left(\frac{\nabla \alpha}{\|\nabla \alpha\|} \right) \nabla \alpha$$



Graveleau et al. 2017

¹Hirt, C. & Nichols, B. *Volume of fluid (VOF) method for the dynamics of free boundaries* Journal of Computational Physics, 1981, 39, 201 - 225 ²Brackbill 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!

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