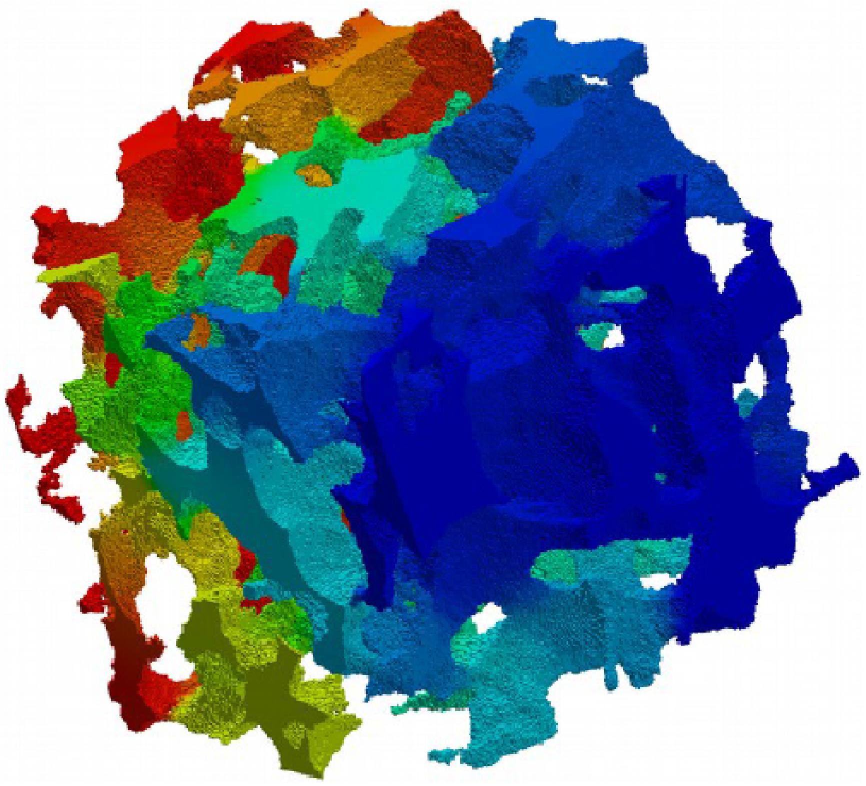
# SIMULATION TECHNIQUES TO MODEL FLOW AND TRANSPORT AT THE PORE-SCALE

4TH CARGESE SUMMER SCHOOL

CARGESE, JULY 4, 2018

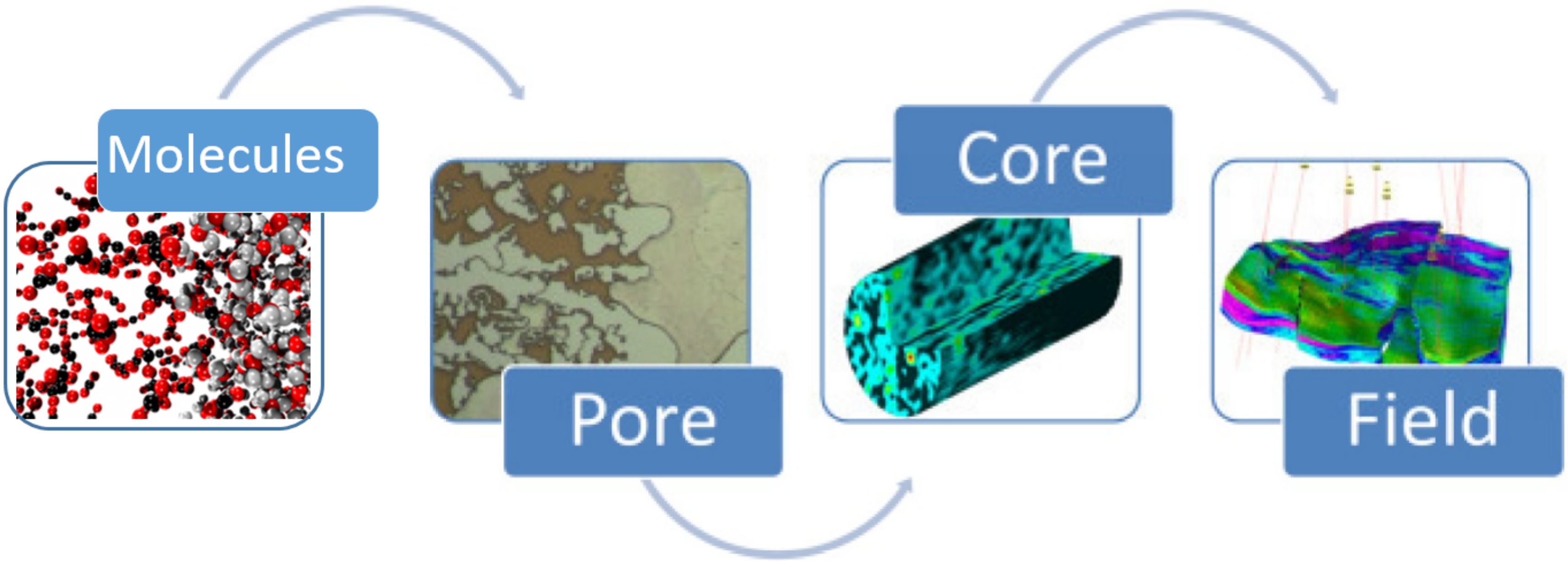


Cyprien Soulaine

# Outline

- Pore-scale modeling,
- Derivation of Navier-Stokes equations,
- Properties of Navier-Stokes equations,
- Numerical approaches to solve the flow at the pore-scale,
- Simulation examples,
- Two-phase flow at the pore-scale.

# Multi-scale modeling




Statistical mechanics

Continuum mechanics

Navier-Stokes

Darcy

(Adapted from Buchgraber 2012)

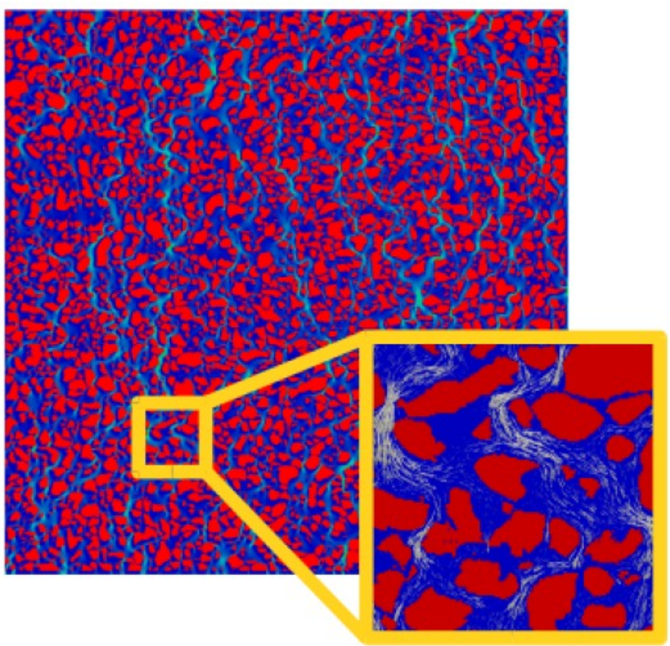
# Discret vs continuum

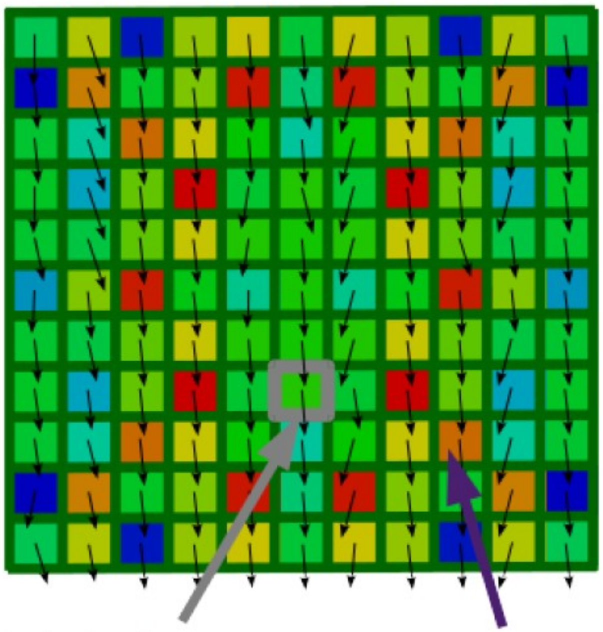
direct modeling

continuum modeling

$p_\beta$

$\mathbf{v}_\beta$






$\langle p_\beta \rangle^\beta$

$\langle \mathbf{v}_\beta \rangle$

for every point of the domain

fluid OR solid

fluid AND solid

# Digital Rock Physics

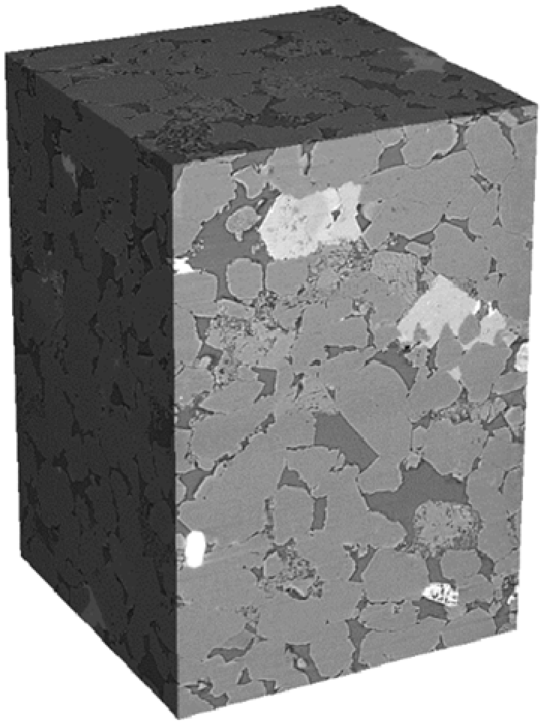
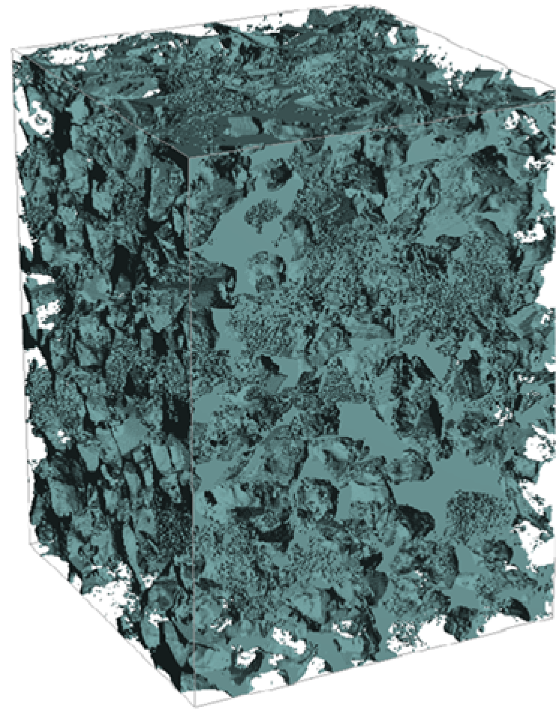
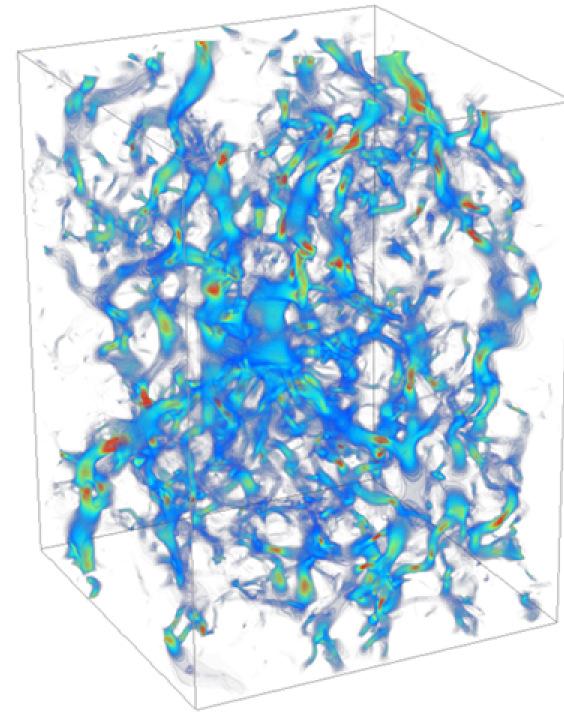


Image of core, plug or cutting



Segmented pores/minerals in image



Computation of rock properties

(source: GeoDict)

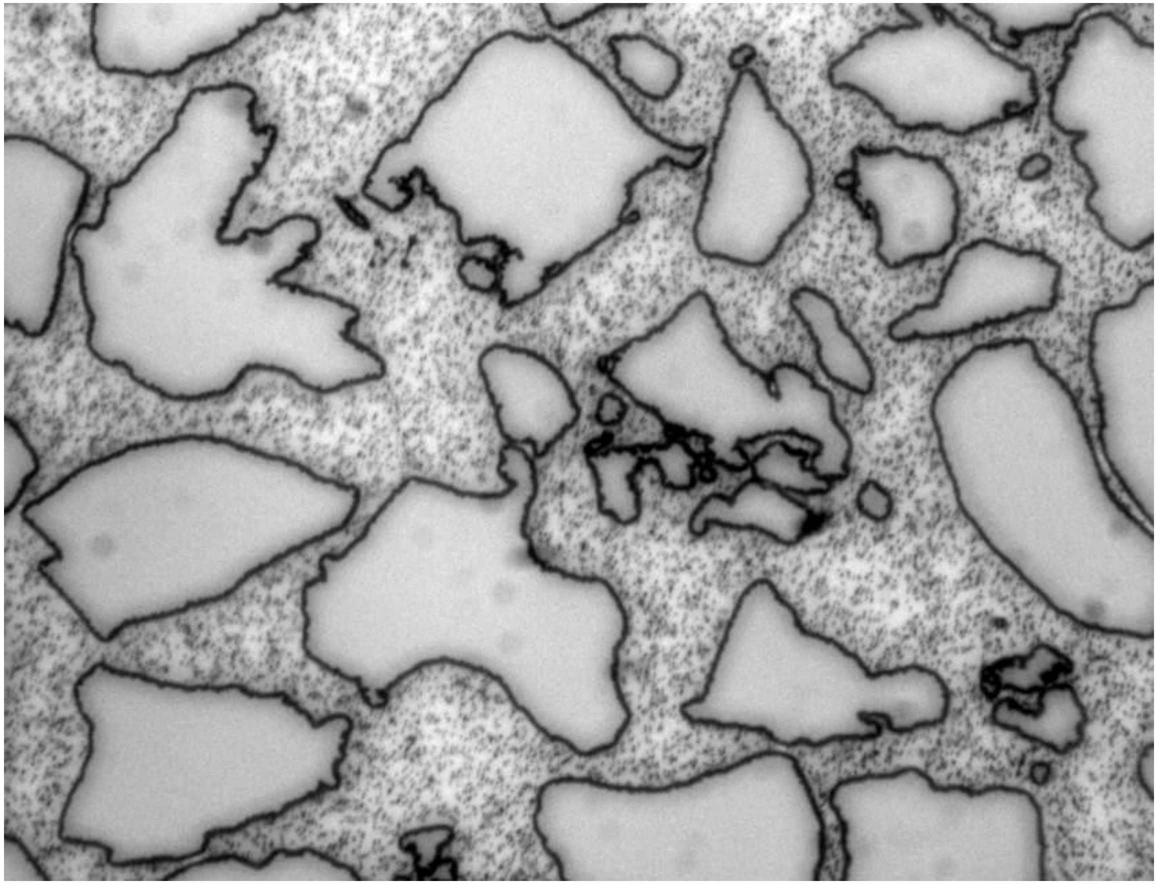
**Geometrical parameters**
- Porosity
- Percolation
- Surface area
- Tortuosity

**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

# Single-phase flows at the pore-scale

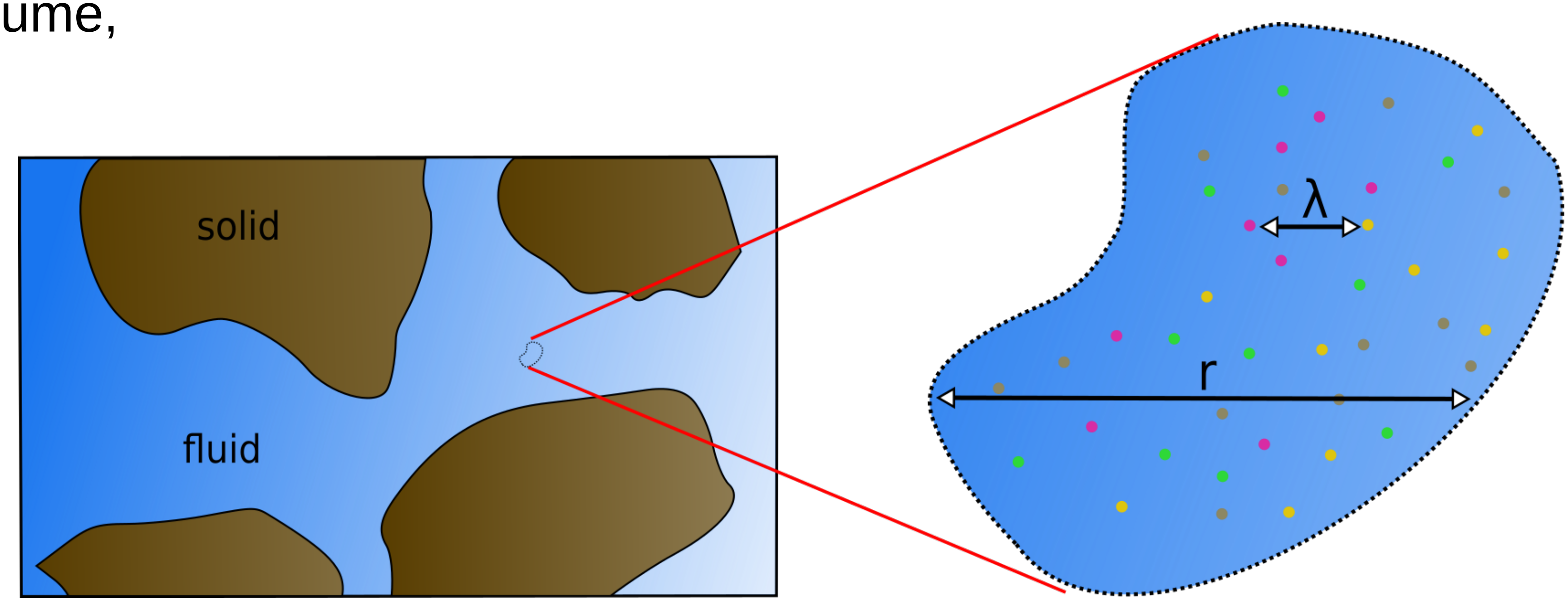


- Water seeded with micro-particles to visualize the flow in the pore-space*,
- The particle trajectories are not random and are deterministic.

* Roman et al. *Particle velocimetry analysis of immiscible two-phase flow in micromodels*, Advances in Water Resources *2016*

# The Navier-Stokes equations

- The flow motion obeys the continuum mechanics conservation laws for fluid,
- These laws are derived from mass and momentum balance in a control volume,

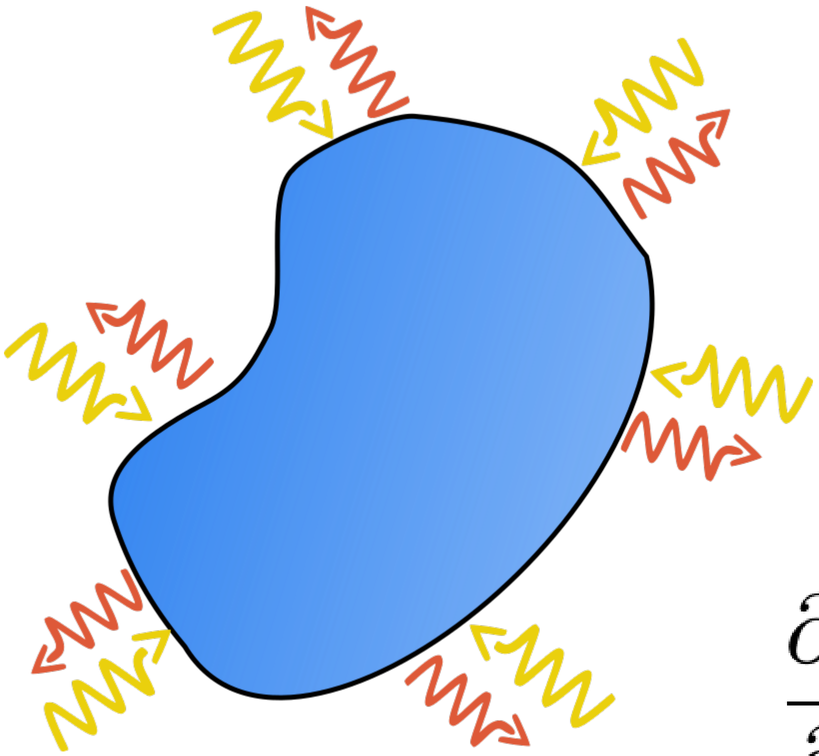



- The Navier-Stokes equations are made of:
  - A continuity equation,
  - A momentum equation,
  - Boundary conditions at the solid surface.

$\lambda$ = mean free path

$\lambda \ll r$

# Mass balance equation



$\rho$ = fluid density = $\frac{\text{mass of fluid}}{\text{control volume}}$

$$\frac{\partial \rho}{\partial t} + \nabla . (\rho \boldsymbol{v}) = 0$$

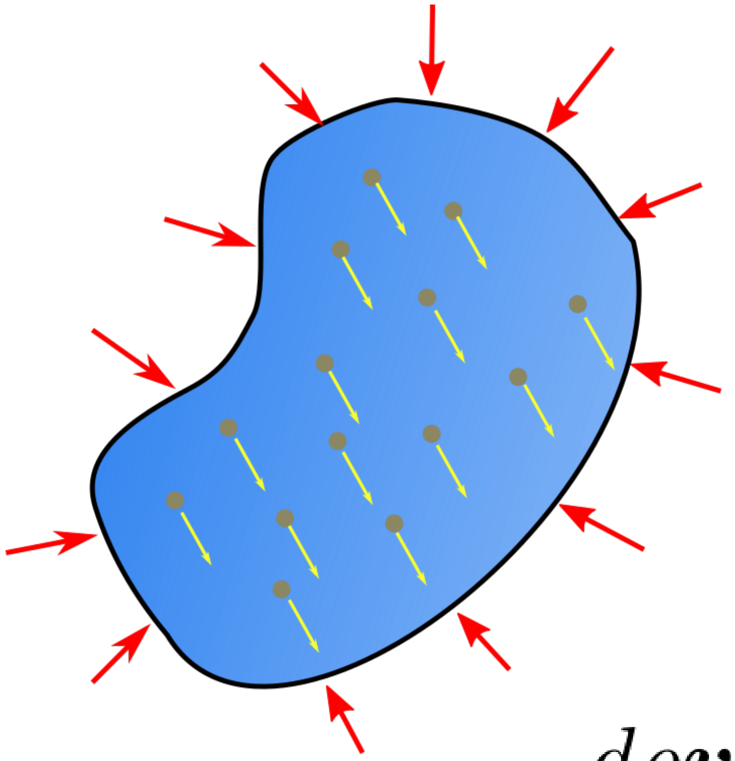
Variation of mass in the control volume

Mass fluxes coming and going out the control volume

For an incompressible fluid (most of the liquids):

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

# Cauchy momentum equation



$\rho\boldsymbol{v}$ = fluid momentum

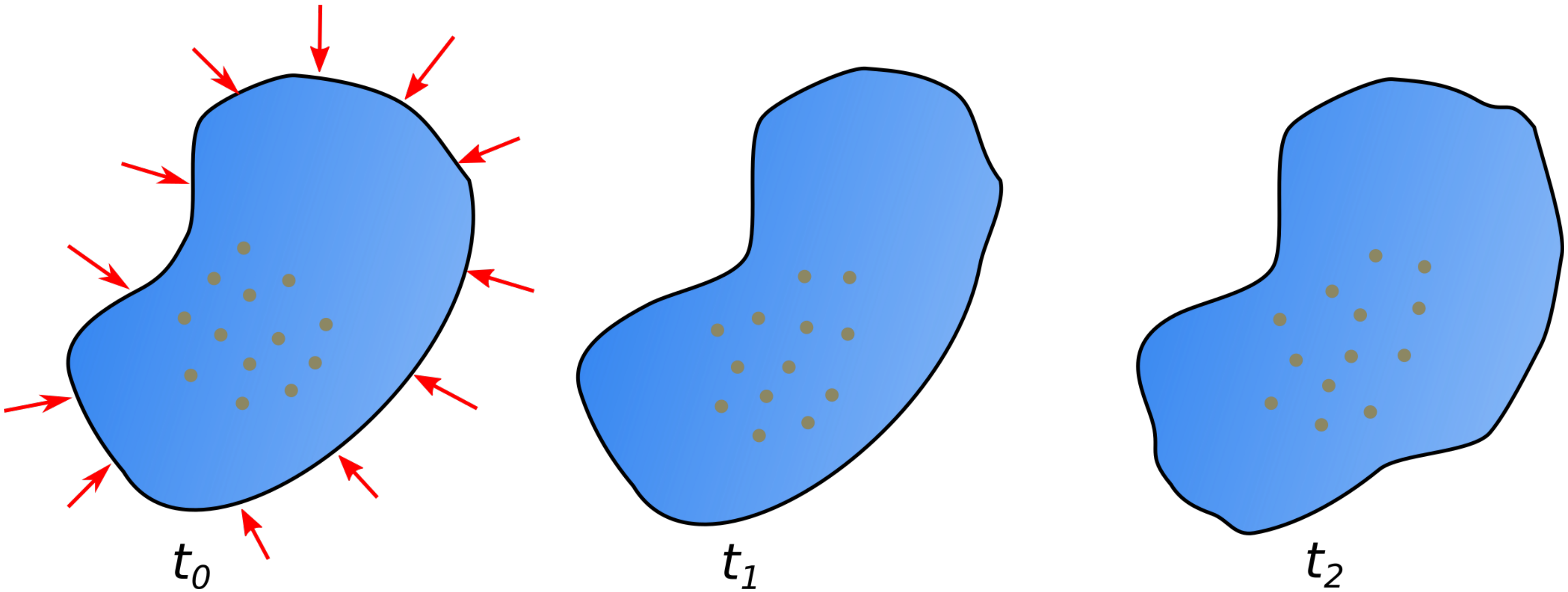
Conservation of momentum obtained from Newton’s second law of motion (the variation of momentum and the sum of forces balance each other):

$$\frac{d\rho\boldsymbol{v}}{dt} = \underbrace{\nabla.\sigma}_{\text{surface forces}} + \underbrace{\rho\boldsymbol{f}}_{\text{body forces}}$$

Body forces = gravity, magnetic of electric fields…

Surface forces = forces responsible for the deformation of the control volume

# Shear stress for Newtonian fluids




Cauchy stress tensor quantifies the change in shape and/or size of the control volume,

$$\underbrace{\sigma}_{\text{Cauchy stress tensor}} = \underbrace{-p\mathsf{I}}_{\text{pressure forces}} + \underbrace{\tau}_{\text{viscous stress tensor}}$$

For Newtonian fluid, the viscous stress is proportional to the strain rate (the rate at which the fluid is being deformed),

$$\tau = \mu \left( \nabla \boldsymbol{v} +^{t} \nabla \boldsymbol{v} \right)$$

# Navier-Stokes momentum equation

In an Eulerian frame, the combination of Cauchy's law and Cauchy stress tensor gives the Navier-Stokes momentum equation,

$$\underbrace{\rho \frac{\partial \boldsymbol{v}}{\partial t} + \rho \boldsymbol{v}.\nabla \boldsymbol{v}}_{\text{inertia}} = \underbrace{-\nabla p}_{\text{pressure gradient}} + \underbrace{\rho \boldsymbol{g}}_{\text{gravity}} + \underbrace{\mu \nabla^2 \boldsymbol{v}}_{\text{viscous force}}$$

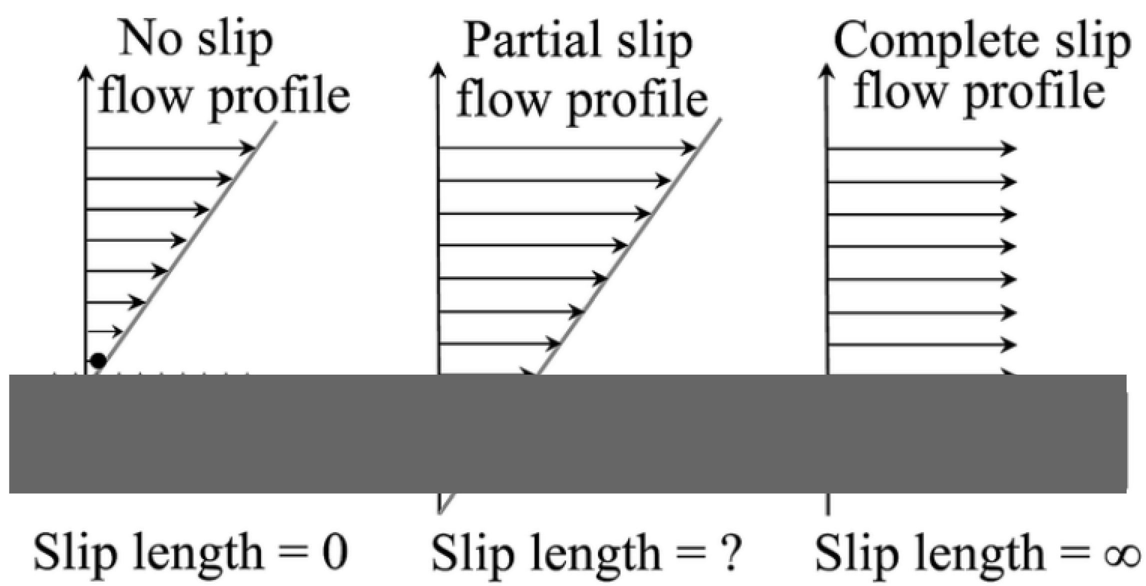
For slow flow, the inertial term is negligible compared with the dissipative viscous force and Navier-Stokes becomes the Stokes equation,

$$0 = -\nabla p + \rho \boldsymbol{g} + \mu \nabla^2 \boldsymbol{v}$$

Stokes is a particular case of Navier-Stokes, which means that all Navier-Stokes solvers are also valid for Stokes without any modification!

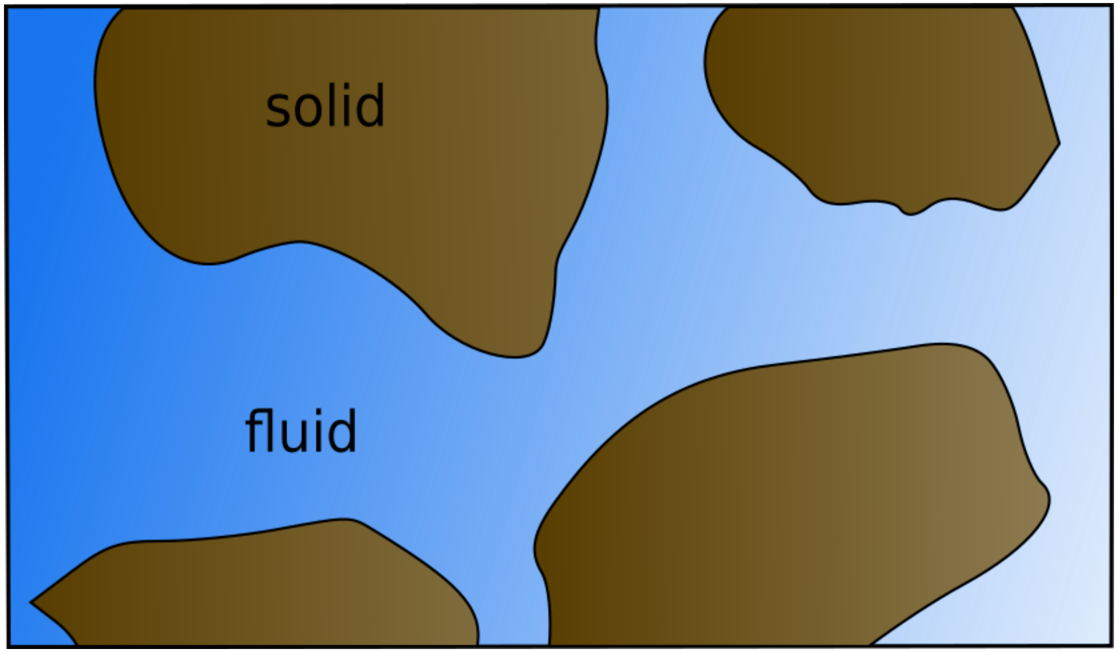
# Boundary conditions at the solid surface

$$\boldsymbol{v} = \underbrace{\boldsymbol{v}_\perp}_{\text{normal component}} + \underbrace{\boldsymbol{v}_\parallel}_{\text{tangential component}}$$




$$\boldsymbol{v} = 0 \qquad v = \beta \frac{\partial v}{\partial n} \qquad \frac{\partial v}{\partial n} = 0$$

# The Navier-Stokes equations: summary




- Mass balance equation,

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

- Momentum balance equation,

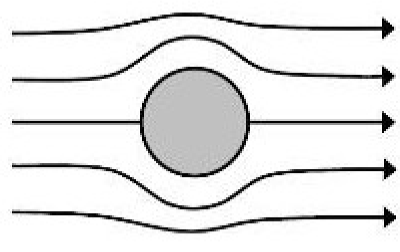
$$\rho \frac{\partial \boldsymbol{v}}{\partial t} + \rho \boldsymbol{v} . \nabla \boldsymbol{v} = -\nabla p + \rho \boldsymbol{g} + \mu \nabla^2 \boldsymbol{v}$$

- No slip condition at the solid surface,

$$\boldsymbol{v} = 0$$

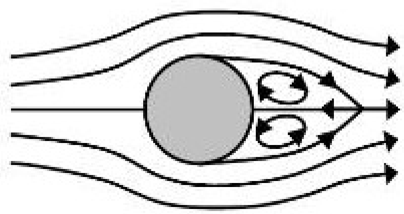
# Different flow regimes (past a cylinder)

$$Re = \frac{\rho U_0 L_0}{\mu}$$



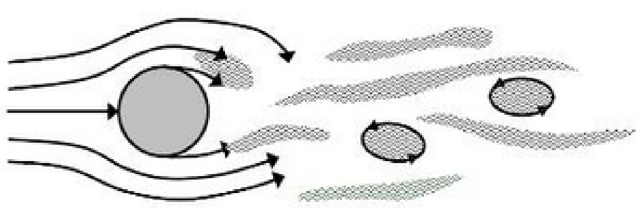
a

Creeping flow regime (Re<1): the flow is governed by the viscous effects only and the streamlines embrace the solid structure. The flow is modeled by the Stokes equations. Most of the time, we are in this situation.



b

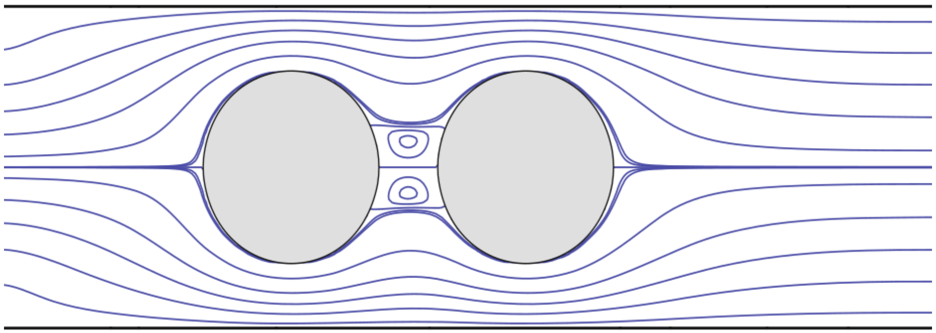
The inertia effects distort the streamlines and flow recirculations are generated downstream the obstacles. The flow is modeled by the laminar Navier-Stokes equations.



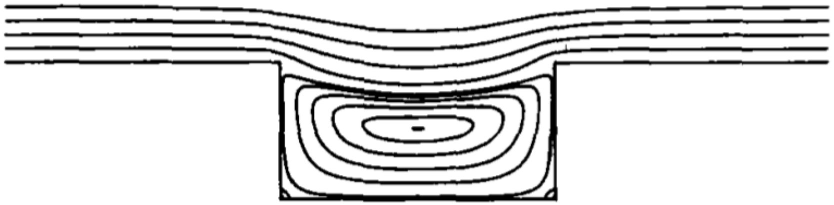
At very high Reynolds numbers, turbulence effects emerge. The flow is modeled by turbulent Navier-Stokes equations (RANS, LES...)

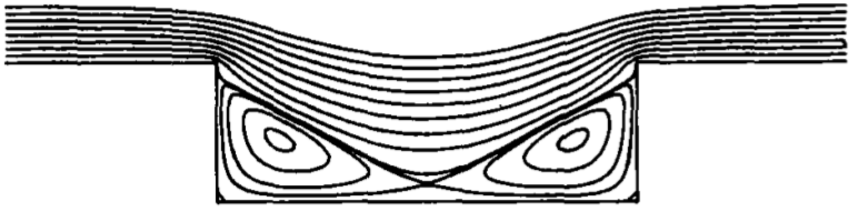
# Recirculating motion in Stokes flows

- Space between two grains[1]



- Cavities/ Roughness[2]

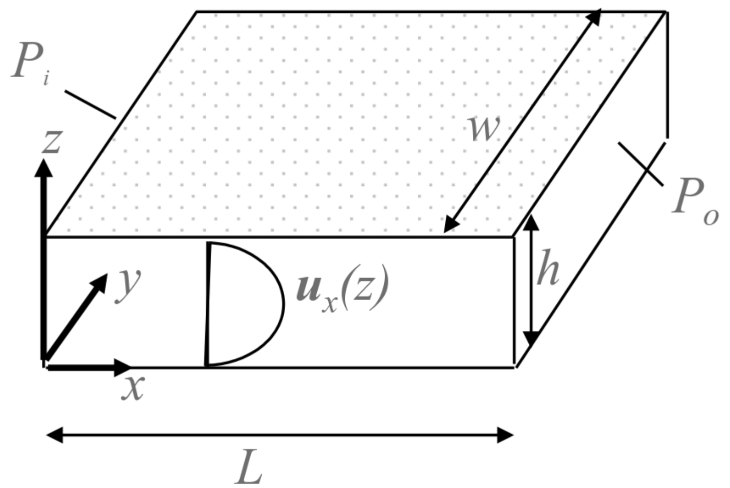




[1]Caltagirone, *Physique des écoulements continus*, 2013

[2]Higdon, *Stokes flow in arbitrary two-dimensional domains: shear flow over ridges and cavities*, Journal of Fluid Mechanics, 1985, 159, 195-226

# Analytical solution: flow between two parallel plates




W and L assume to be large enough so

$$\boldsymbol{v} = v_x(z)\boldsymbol{e}_x$$

$$\nabla p = \frac{\Delta P}{L}\mathbf{e}_x.$$

The Stokes problem in Cartesian coordinates reads

$$\begin{cases} \mu \dfrac{\partial^2 v_x}{\partial z^2} = \dfrac{\Delta P}{L} \\ v_x\left(z = \pm\dfrac{h}{2}\right) = 0. \end{cases}$$

Parabolic profile

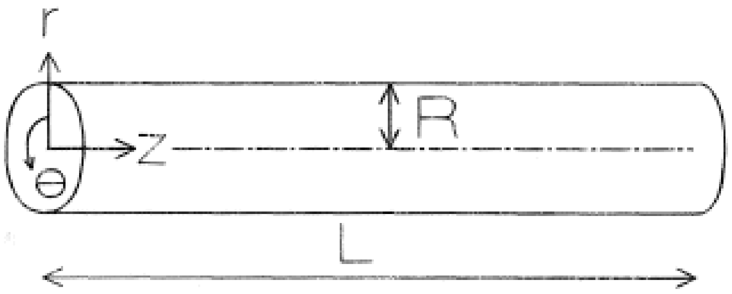
$$v_x(z) = \frac{1}{\mu}\frac{h^2}{8}\frac{\Delta P}{L}\left[1 - \left(\frac{2z}{h}\right)^2\right]$$

When volume averaging the velocity profile:

$$\bar{v}_x^f = \frac{1}{h}\int_{-\frac{h}{2}}^{\frac{h}{2}} v_x(z)\,dz = \frac{h^2}{12\mu}\frac{\Delta P}{L}$$

Hele-Shaw equation

# Analytical solution: flow in a micro-tube




Due to the geometry, it is natural to use cylindrical coordinates.

L assumes to be long enough so the flow does not depend on *z*. Moreover, it is invariant by rotation and is carried by z only:

$$\boldsymbol{v} = v_z\left(r\right)\boldsymbol{e}_z \qquad \nabla p = \frac{\Delta P}{L}\mathbf{e}_z$$

The Stokes problem in cylindrical coordinates reads

$$\begin{cases} \mu \dfrac{1}{r}\dfrac{\partial}{\partial r}\left(r\dfrac{\partial v_z}{\partial r}\right) = \dfrac{\Delta P}{L} \\ v_z(r = R) = 0. \end{cases} \Rightarrow \quad v_z(r) = \frac{R^2}{4\mu}\left(1 - \left(\frac{r}{R}\right)^2\right)\frac{\Delta P}{L}$$

Parabolic profile

When volume averaging the velocity profile:

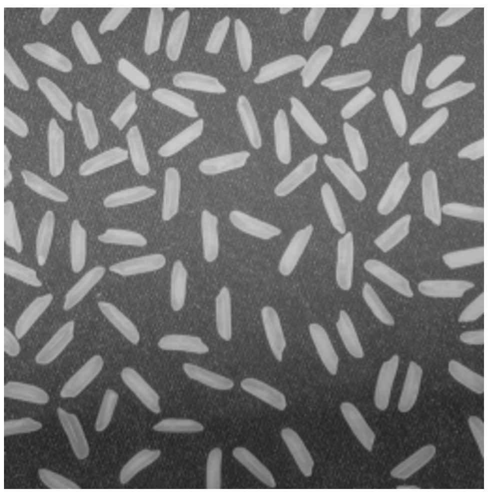
$$\bar{v}_z^f = \frac{2}{R^2}\int_0^R v_z\left(r\right) r dr = \frac{R^2}{8\mu}\frac{\Delta P}{L}$$

Hagen-Poiseuille law:

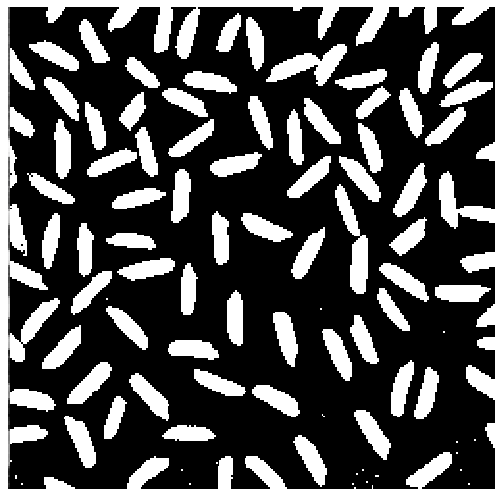
$$Q^f = \rho \bar{v}_z^f S = \frac{\pi R^4}{8\mu}\frac{\Delta P}{L}$$

# How to solve flows in complex porous structures?

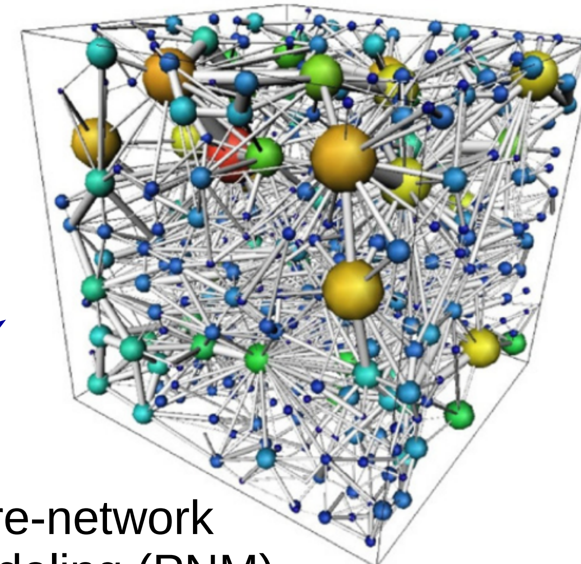
Source: Blunt et al. (2013)



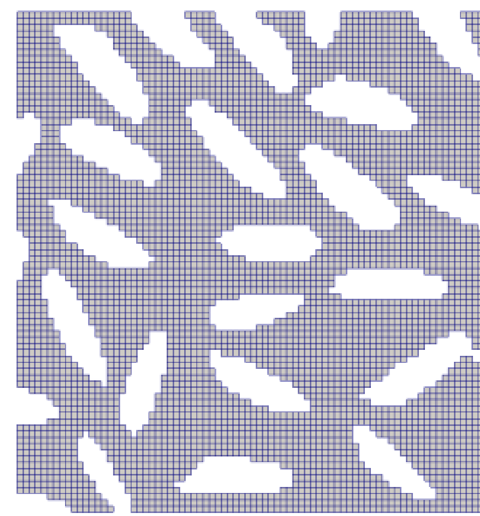
Acquisition of the image (micro-CT ...)



Segmentation in fluid and solid

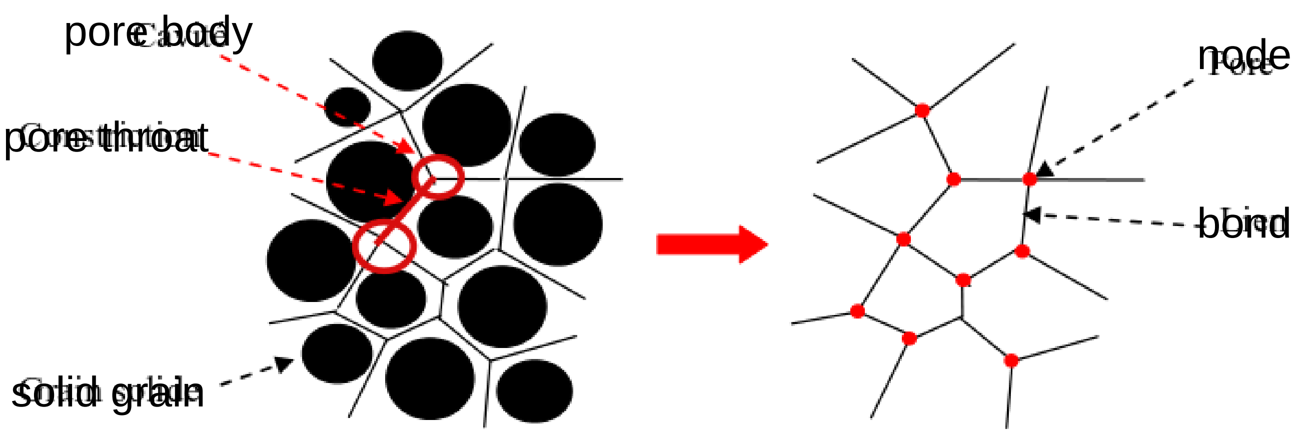


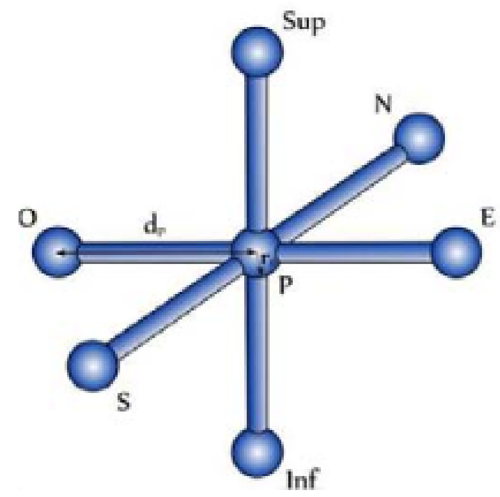
Pore-network modeling (PNM)



Direct Numerical Simulation (DNS)

# Pore Network Modeling




For a cylindrical bond of radius $r_i$ and length $L_i$ that relates the nodes P and i, the mass flow rate is

$$Q_{ij} = g_{ij}\left(P_i - P_j\right) \quad \text{with} \quad g_{ij} = \frac{\rho \pi r_{ij}^4}{8 \mu L_{ij}}$$

(cf. Poiseuille flow in a microtube)

Due to the mass conservation, for all pores P:

$$\sum_j Q_{ij} = 0 \quad \rightarrow \quad \boxed{\sum_j g_{ij}\left(P_i - P_j\right) = 0}$$

- Very easy to program
- Can compute relatively large domains (up to cm)

- Need more sophisticated models to be more representative of the actual geometry (bonds are not always cylindrical).
- It is not a tool to investigate the physics, the results will depend on the input…
- Still needs some research to the extension for multiphase

# 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.

# Some popular CFD softwares

ANSYS Fluent is a CFD software using the finite volume method.

Another commercial CFD software.

COMSOL Multiphysics is a finite element package for various physics and engineering application, especially coupled phenomena or multiphysics.

OpenFOAM is a general purpose open-source CFD code. OpenFOAM is written in C++ and uses an object oriented approach which makes it easy to extend. The package includes modules for a wide range of applications. It uses the finite volume method.

https://www.cypriensoulaine.com/openfoam

# Pressure-velocity coupling with projection algorithms

- Two equations, two unknowns (pressure and velocity) but no equation for the pressure field.

$$\nabla . \boldsymbol{v} \quad = \quad 0 \qquad \text{and} \qquad \rho \frac{\partial \boldsymbol{v}}{\partial t} + \rho \boldsymbol{v}.\nabla \boldsymbol{v} = -\nabla p + \rho \boldsymbol{g} + \mu \nabla^2 \boldsymbol{v}$$

- A pressure equation can be derived by taking the divergence of the momentum equation.

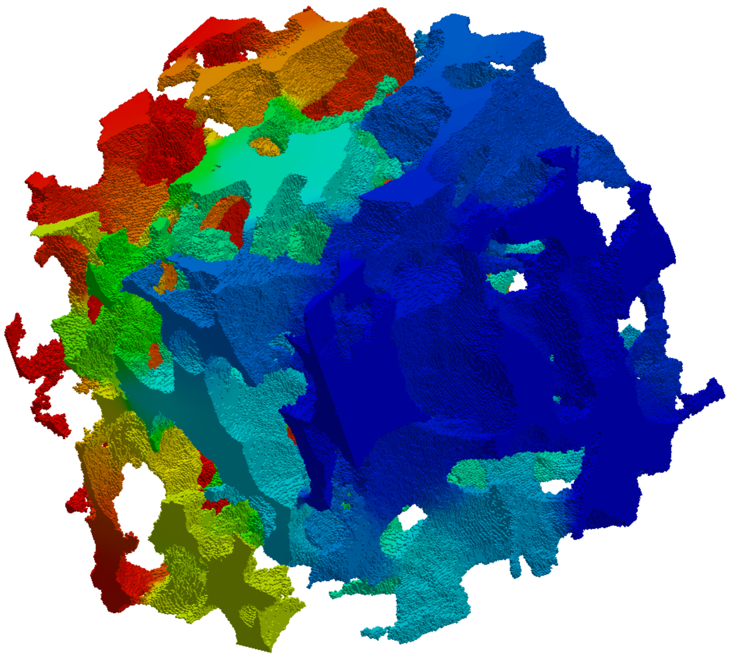
- The pressure and velocity equations are solved in a sequential manner using predictor-corrector projection algorithms. In OpenFOAM®, you have to choose between PISO and SIMPLE:

| algorithm | transient | Steady -state | comments | OpenFOAM solver |
|---|---|---|---|---|
| PISO* PIMPLE | YES | YES | Can be used to find the stationary solution by solving all the time steps | **icoFoam**, pisoFoam, pimpleFoam, interFoam, twoPhaseEulerFoam, rhoPimpleFoam... |
| SIMPLE** | NO | YES | Faster than PISO to converge to the steady state | **simpleFoam**, rhoSimpleFoam... |

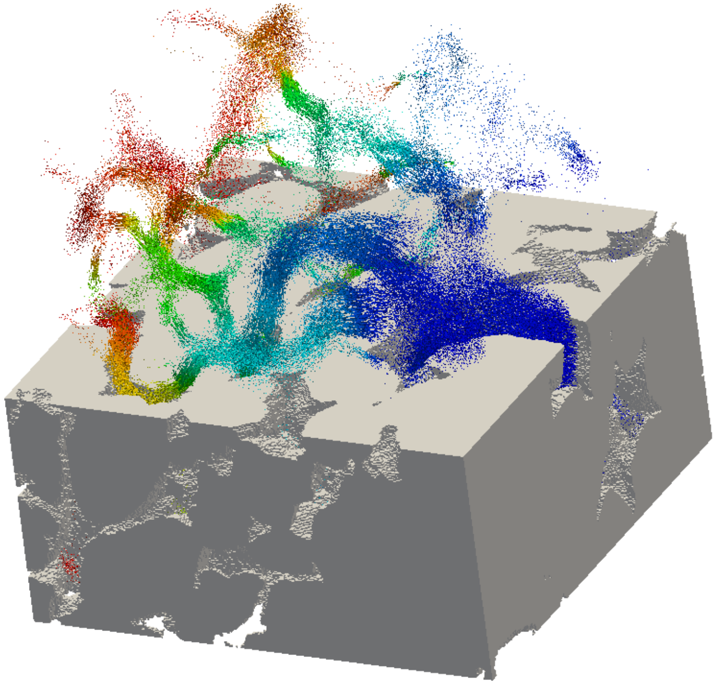
- PISO is not unconditionally stable and the time step is limited by a CFL condition.
- SIMPLE is an iterative procedure that under-relaxes the pressure field and velocity matrix at each iteration.
- To allow larger time steps, a combination of both algorithm is sometime proposed (PIMPLE).
- Multiphase Navier-Stokes equations are solved in the framework of the PISO solution procedure.
- Stokes momentum equation does not involve transient terms and can be solved with SIMPLE.

* Issa. *Solution of the Implicitly Discretised Fluid Flow Equations by Operator-Splitting.* Journal of Computational Physics, 62:40-65, 1985.
** Patankar. *Numerical Heat Transfer And Fluid Flow,* Taylor & Francis, 1980

# Application: compute the permeability of a sandstone



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



- 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).

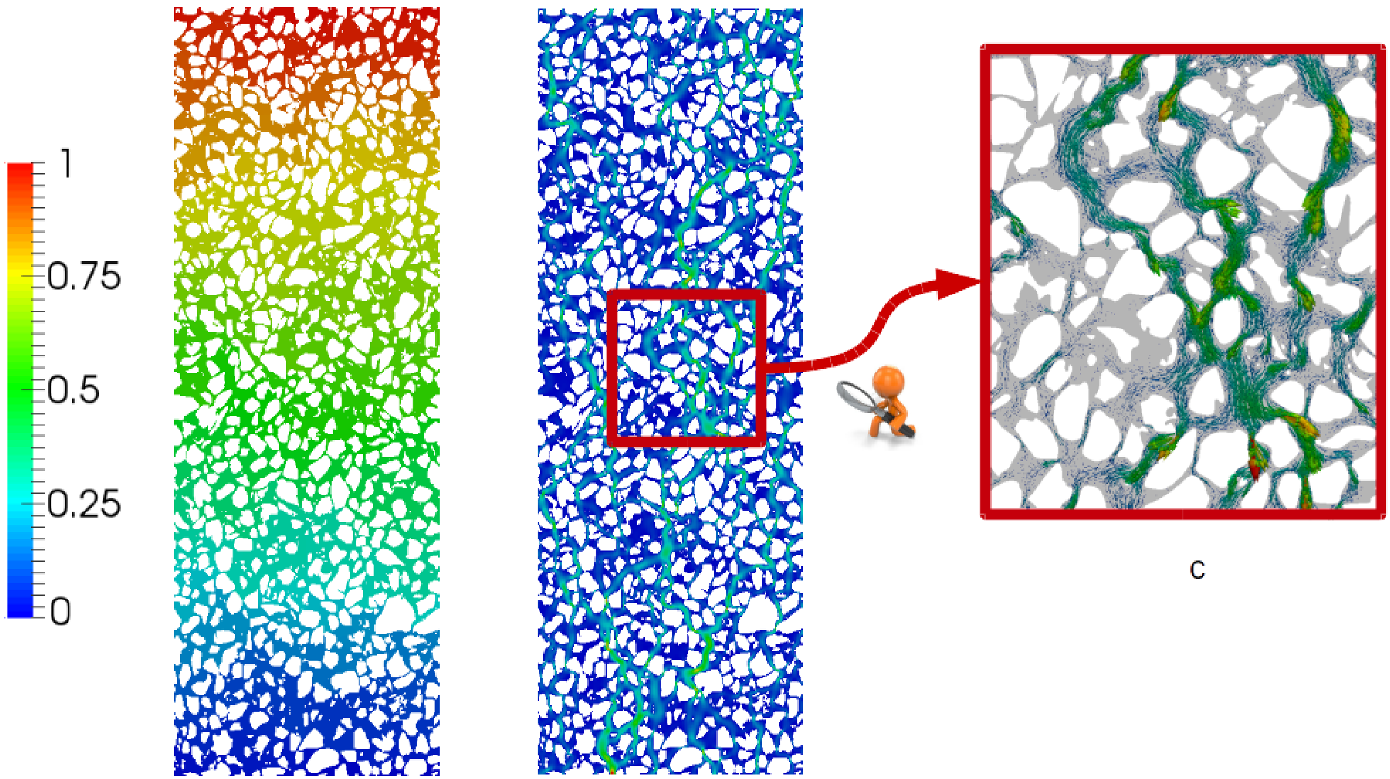
# Simulations in “2.5D” micromodels

The simulation is 2D. The 3D effects are included assuming a Poiseuille profile in the depth of the micromodels and then considering Stokes flow equations averaged over the thickness, i.e. adding an Hele-Shaw correction term.

$$0 = -\nabla p + \mu \nabla^2 \boldsymbol{v} - \mu \frac{12}{h^2} \boldsymbol{v}$$

Hele-Shaw correction term

Pressure Velocity

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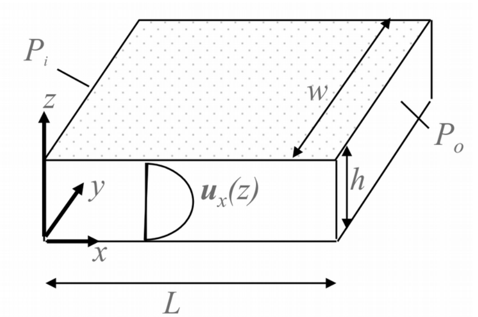
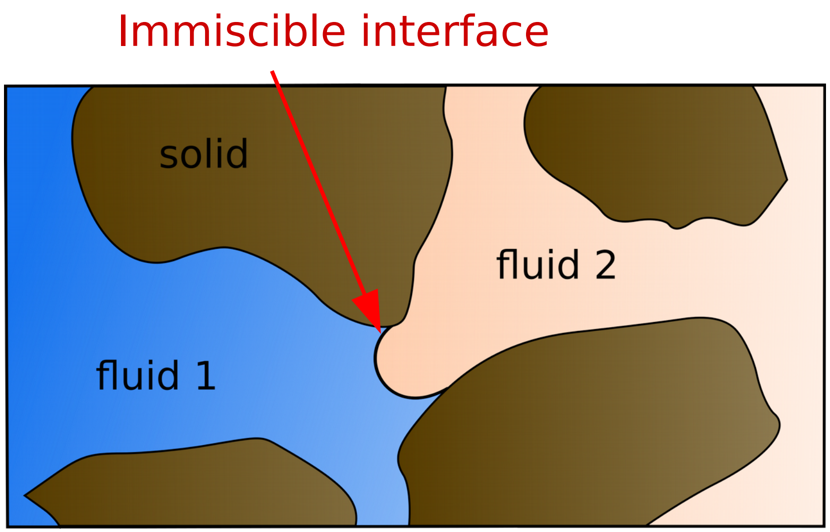



* Roman et al. *Particle velocimetry analysis of immiscible two-phase flow in micromodels*, Advances in Water Resources *2016*

# Physics of two-phase flow in porous media at the pore-scale




## Particularity of multi-phase flow

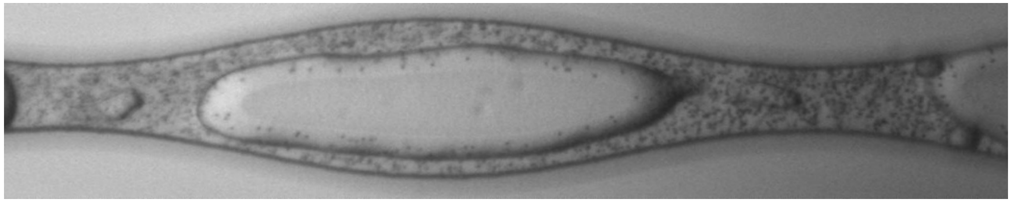
- Navier-Stokes equation in each phases
- Continuity of the tangential component of the velocity at the fluid/fluid interface
- Laplace law for a surface at the equilibrium

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

Surface tension (N/m)

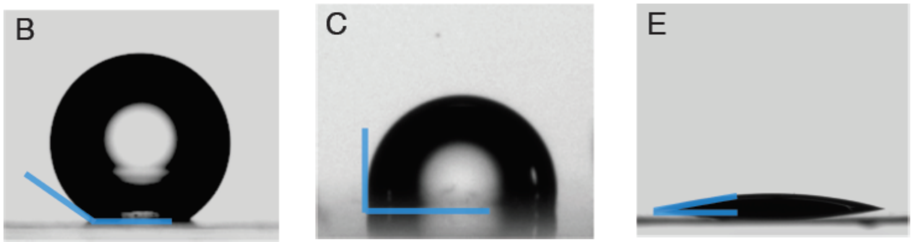
- Contact line dynamics at the solid surface

<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




θ=150° non-wetting

θ=90°

θ=7° wetting

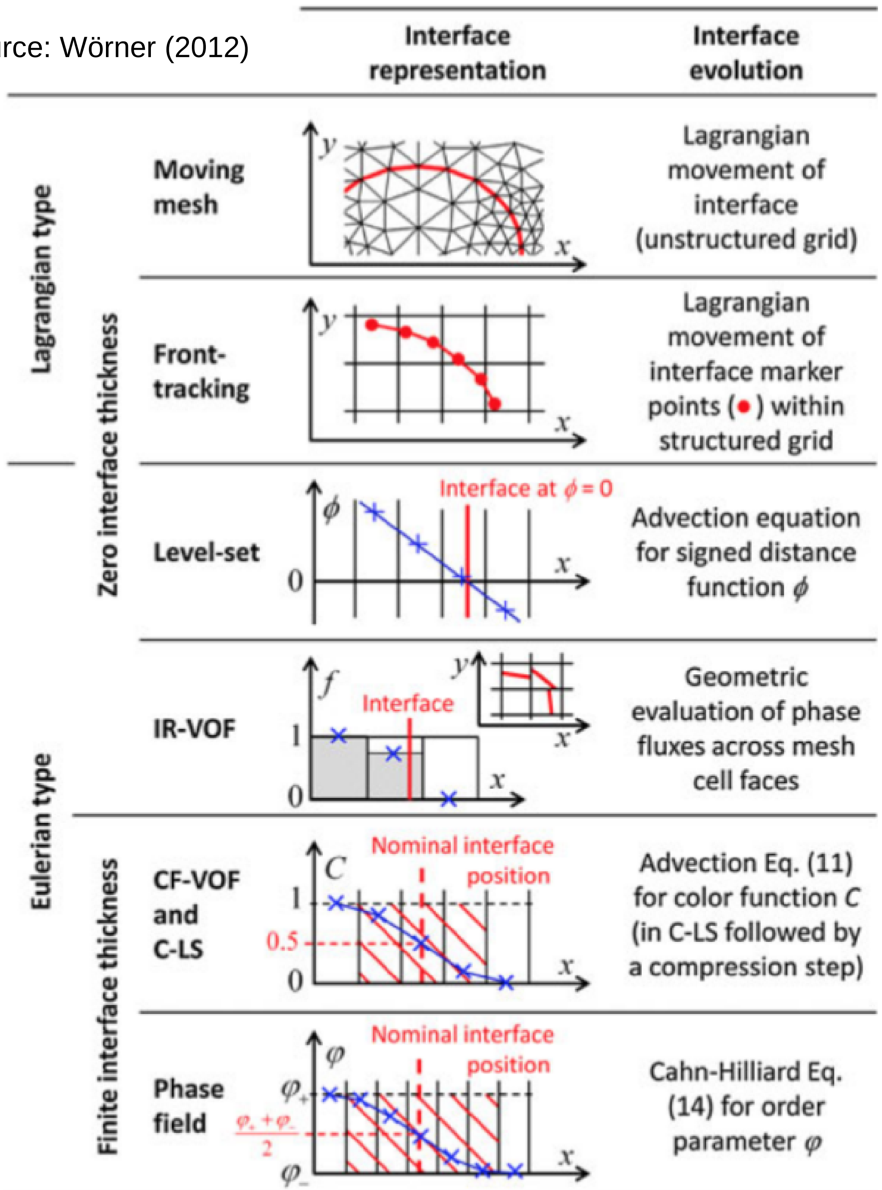
Zhao et al. (2016), PNAS

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)

# CFD for two-phase flow

## Simulation methods

Source: Wörner (2012)

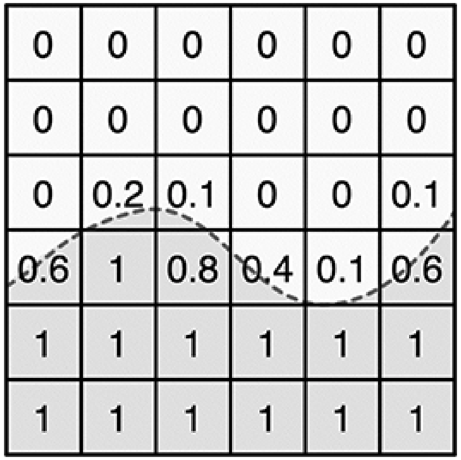



## Challenges

- The state-of-the-art simulations **can not** go below Ca=$10^{-5}$. Otherwise spurious currents can pollute and even drive the interface propagation
- The physics of contact line dynamics is still poorly understood and can have an order one impact on the flow (Constant contact angle? Cox-Voinov model? Lubrication theory for thin film? ).
- Solve the flow on large and complex domains.
- How to validate this numerical models?

Wörner, *Numerical modeling of multiphase flows in microfluidics and micro process engineering: a review of methods and applications*, Microfluidics and Nanofluidics *2012*

# The Volume of Fluid (VOF) technique




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

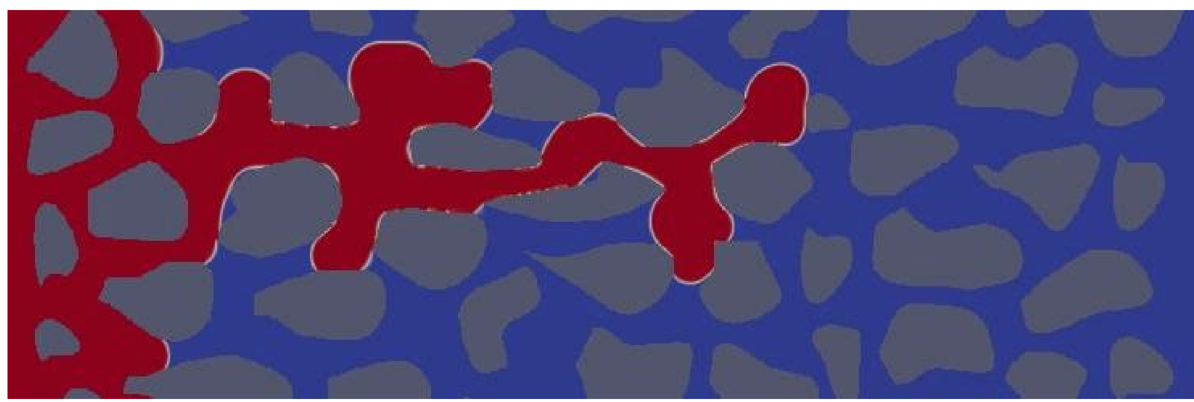
$$\boldsymbol{v} = \alpha \boldsymbol{v}_1 + (1-\alpha)\, \boldsymbol{v}_2$$
$$p = \alpha p_1 + (1-\alpha)\, p_2$$
$$\rho = \alpha \rho_1 + (1-\alpha)\, \rho_2$$
$$\mu = \alpha \mu_1 + (1-\alpha)\, \mu_2$$

Single-field equations[1]

$$\rho \frac{\partial \boldsymbol{v}}{\partial t} + \rho \boldsymbol{v}.\nabla \boldsymbol{v} = -\nabla p + \rho \boldsymbol{g} + \nabla.\mu \left( \nabla \boldsymbol{v} + {}^t \nabla \boldsymbol{v} \right) + \boldsymbol{F}_c$$
$$\nabla.\boldsymbol{v} = 0$$
$$\frac{\partial \alpha}{\partial t} + \boldsymbol{v}.\nabla \alpha = 0$$

Continuum Surface Force (CSF)[2]

$$\boldsymbol{F}_c = \sigma \nabla. \left( \frac{\nabla \alpha}{\|\nabla \alpha\|} \right) \nabla \alpha$$



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[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

Thank you for your attention!

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