Institut de Recherche en Génie Civil et Mécanique
UMR CNRS 6183

UNIVERSITÉ DE NANTES

Centrale Nantes

Grenoble, June 27th – July 1st, 2011

Modelling fluid-grain interactions in two phase materials
Discrete element–lattice Boltzmann coupled methods

Olek Zienkiewicz Course 2011
Discrete Mechanics of Geomaterials

Luc Sibille, Franck Lominé
Philippe Poullain, Didier Marot
GeM Laboratory – Nantes University – ECN – CNRS

Région PAYS DE LA LOIRE

I. Introdution

Warning!

This presentation does not aim to give a state of the art about the lattice Boltzmann method and its coupling with DEM.

This presentation just gives an insight into a such approach and it is based on a development work still in progress, mistakes certainly exist and possibilities of improvements are great!

Consequently, if you want to go further please refer to reference books and litterature:

- Master teaching book on statistical physics for background (Boltzmann equation, Chapman-Enskog expansion ...)
  Ngô C. & Ngô H. "Physique Statistique Introduction". Dunod, 2008 (in French ☹)

- *Succi S. "The Lattice Boltzmann Equation for Fluid Dynamics and Beyond". Oxford University Press, 2001,* for the Lattice Boltzmann method.

- Many articles in the fields of physics and numerical methods in fluids.

I. Introdution

Coupled numerical method

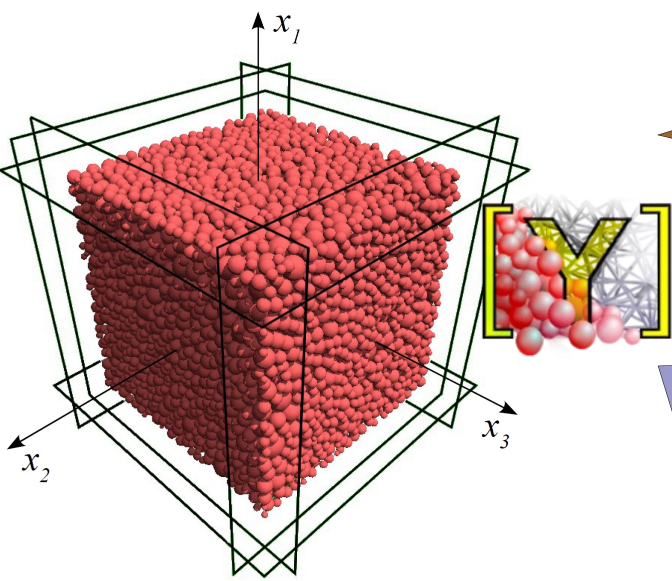
- **Description of the solid phase at the particle scale**
- **Description of the fluid dynamic in the inter-particle space**

Solid phase: Discrete Element Method
DEM, *Yade Software*

- Contact stiffnesses
- Contact friction angle
- Contact adhesion

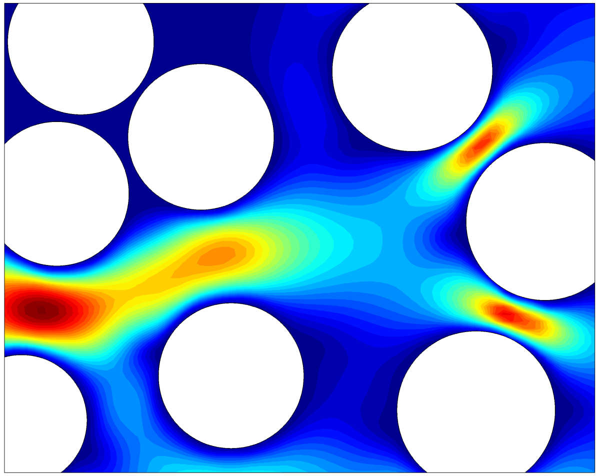
Fluid phase
Lattice Boltzmann Method (LBM)

- Fluid viscosity
- position of each solid particle explicitely described



Particle positions and velocities

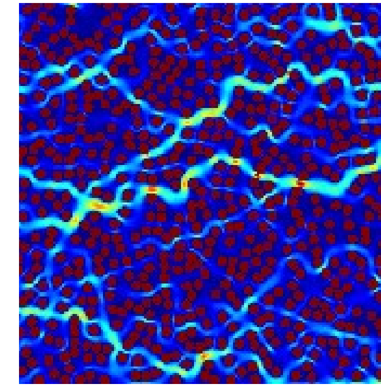
hydro-dynamic forces



No assumption on fluid/solid interactions: permeability, drag forces, etc... result from the coupling.

I. Introdution

LBM, why?



- Description quite easy of moving boundaries with complicated geometrical shape 👍
- Nice numerical implementation (iterative process as for the DEM) 👍
- Versatile method for future development (surface tension and multiphase flows, thermal flow, reactive flow ...) 👍

- Need of a fine lattice (many nodes) to describe interstitial fluid flow 👎
(a minimum of about 10 lattice nodes in a particle diameter seems to be required, but possibility of parallelization)
- Indirect description of the pressure field (related to fluid density), consequently only low pressure variations can be simulated 👎
- Space discretization (lattice) depends on velocity of the fluid flow 👎

⇒ DEM-LBM coupled method should be applied on a small domain (REV ...)

⇒ Should be use essentially to improve the qualitative understanding of physical phenomenon (quantitative approach seems tricky).

Outline

I. Introduction (what? why?)

II. Lattice Boltzmann Method (very few words about background)

III. Practical use of the LBM (main steps to be considered)

IV. DEM-LBM coupling (exchange of information and time step)

V. Application to piping erosion.

II. Lattice Boltzmann Method

II-1 Boltzmann equation

Established by Ludwig Boltzmann (1872):

- The Boltzmann Equation aims initially to describe the statistical distribution of one particle (or molecule) in rarefied gas.
- This equation is the cornerstone of the kinetic theory (branch of the statistical physics) dealing with the dynamics of non-equilibrium processes and their relaxation to thermodynamic equilibrium.

> **Ex:** heat up a pan of water, stop the heating: water temperature decreases with time until reaching the temperature of the outside environment and there is thermal equilibrium.

- Originally developed in the framework of dilute gas systems, this equation is now applied in many physics area: interactions in two phase fluids, electron transport in semiconductors...

⇒ Central object of kinetic theory and Boltzmann Equation: the probability density or distribution function $f(\vec{x}, \vec{p}, t)$**.**

$f(\vec{x}, \vec{p}, t)$ is the probability of finding a molecule (or particle) around position $\vec{x}$ at time t with momentum $\vec{p}$ (with $\vec{p} = m\vec{v}$).

II. Lattice Boltzmann Method

II-2 BGK collision operator

The Boltzmann Equation is a non-linear integro-differential equation:

$$\underbrace{\frac{\partial f}{\partial t} + \vec{v}.\frac{\partial f}{\partial \vec{x}} + \frac{\vec{F}^{ext}}{m}.\frac{\partial f}{\partial \vec{v}}}_{\equiv \text{ Newton single-particle dynamics}} = \underbrace{\iint (f' f'_1 - f f_1) v_{rel} \sigma(\Omega') \, d\Omega' d\vec{v}_1}_{\text{Collision between particles}}$$

≡ Newton single-particle dynamics

Collision between particles

⇒ Bhatnagar-Gross-Krook simplified collision operator (1954, BGK operator); can be seen as a “linearised” collision operator:

$$f(\vec{x},t) - \frac{1}{\tau}\left[f(\vec{x},t) - f^{eq}(\vec{x},t)\right]$$

$f^{eq}(\vec{x},t)$ is an equilibrium distribution function parametrized by macroscopic quantities, density ρ, speed $\vec{u}$ and temperature T.

τ is a typical time-scale associated with relaxation towards the equilibrium distribution function.

II. Lattice Boltzmann Method

II-3 Discretization (LGCA)

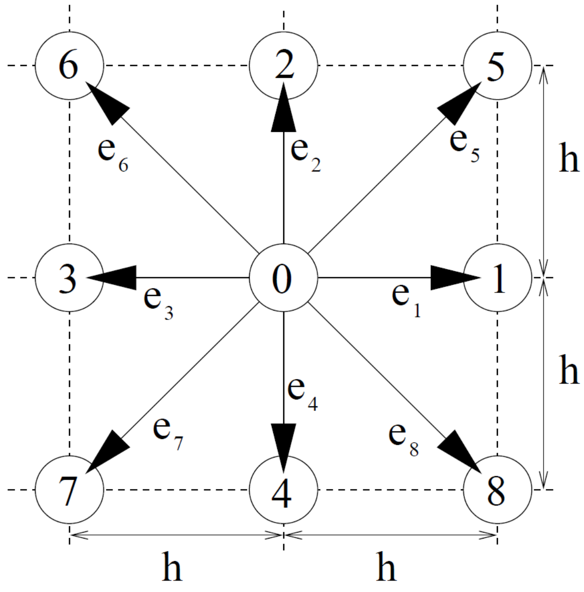
⇒ Discretization of space, time, and particle velocities (based on Lattice Gas Cellular Automata (LGCA; Hardy et coll., 1973) ⇒ Lattice Boltzmann Equation:

$$\underbrace{f_i(\vec{x}+\vec{e_i}\mathrm{d}t, t+\mathrm{d}t)}_{\text{Propagation}} = \underbrace{f_i(\vec{x},t) - \frac{1}{\tau}\left[f_i(\vec{x},t) - f_i^{eq}(\vec{x},t)\right]}_{\text{Collision}}$$

i represents a discrete space direction.

$\vec{e}_i$ is a discrete velocity of propagation in direction ***i*** of the distribution function f_i

D2Q9 model



⇒ At each node of the lattice (the discretized space) macroscopic properties are deduced from:

<u>density</u>:

$$\rho = \sum_{i=0}^{8} f_i$$

<u>velocity</u> :

$$\vec{v} = \frac{1}{\rho}\sum_{i=0}^{8} f_i\vec{e_i}$$

<u>pressure</u>: $p = C_s^2\rho$ *with* $C_s = C/\sqrt{3}$ *where* C *is the lattice speed* $C = h/dt$

II-4 Derivation of Navier-Stokes Equations

⇒ Derivation of incompressible Navier-Stokes Equations based on the Chapman-Enskog Expansion:

- This procedure is based on a double Taylor series expansion from a spatial and temporal point of view, involving a multi-scale representation of space and time variables.

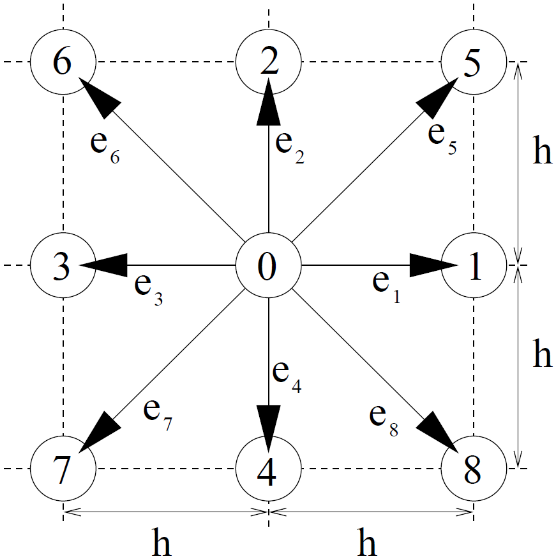
- Conservation of momentum, mass and energy at macroscopic scale are found for:

- a small Mach number $M = \frac{v_{max}}{C}$
- small density variations (in classical LBM the fluid is slightly compressible)
- an equilibrium distribution function writing:

$$f_i^{eq} = w_i \rho \left(1 + \frac{3}{C^2}\vec{e_i}.\vec{v} + \frac{9}{2C^4}(\vec{e_i}.\vec{v})^2 - \frac{3}{2C^2}\vec{v}.\vec{v}\right)$$

with $w_0 = 4/9;\ w_{1,2,3,4} = 1/9$ *and* $w_{5,6,7,8} = 1/36$ for the D2Q9 model.

D2Q9 model



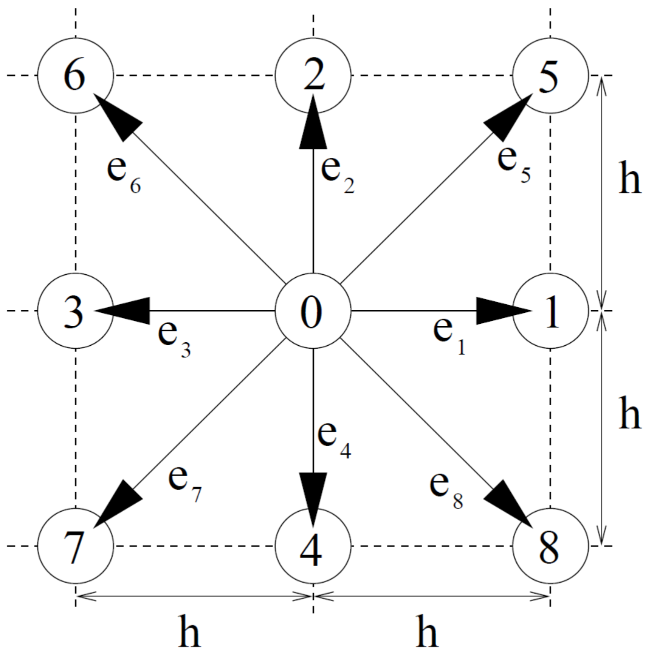
- Identification of the relation between τ and the kinematic viscosity ν :

$$\nu = \frac{1}{3}\left(\tau - \frac{1}{2}\right) Ch$$

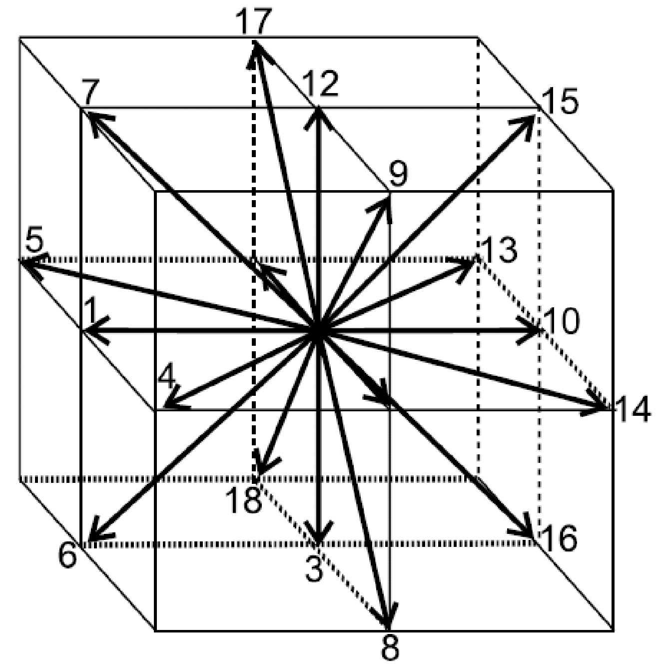
($\tau > 0.5$ for $\upsilon > 0$)

III-1 Space discretization model

D2Q9 model

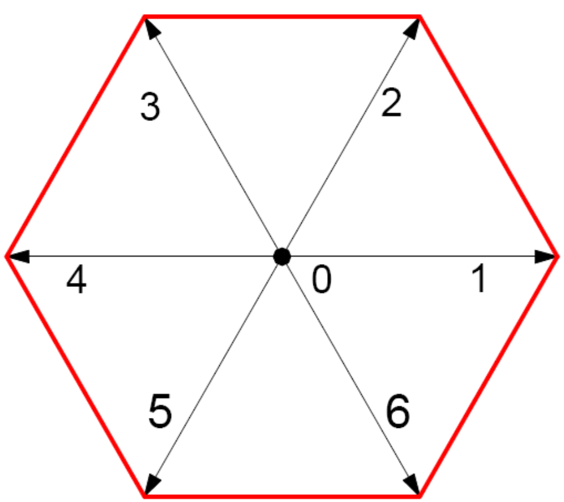


D3Q19 model (Mansouri et al., 2009)



D3Q15
D3Q27
...

D2Q7 model



Some space discretization models are unable to recover Navier-Stokes!

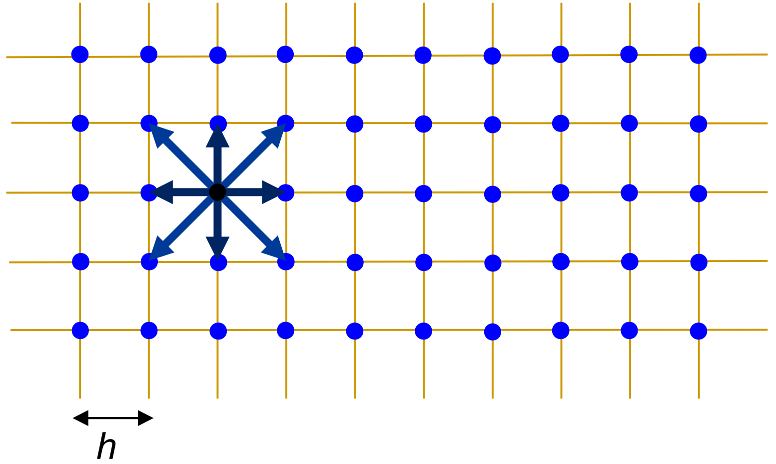
III. Practical use of the LBM

III-1 Space discretization model

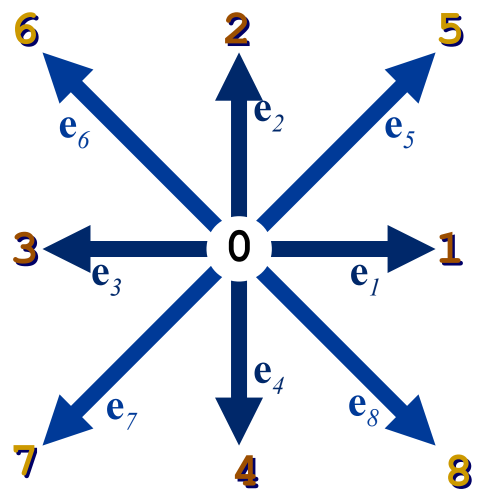
D2Q9 model

- fixed lattice : h
- time step : dt

$$C = h/dt$$



- for each node, we define:
  - 9 directions: i
  - 9 discrete velocities: $\vec{e}_i$
  - 9 distribution functions: f_i



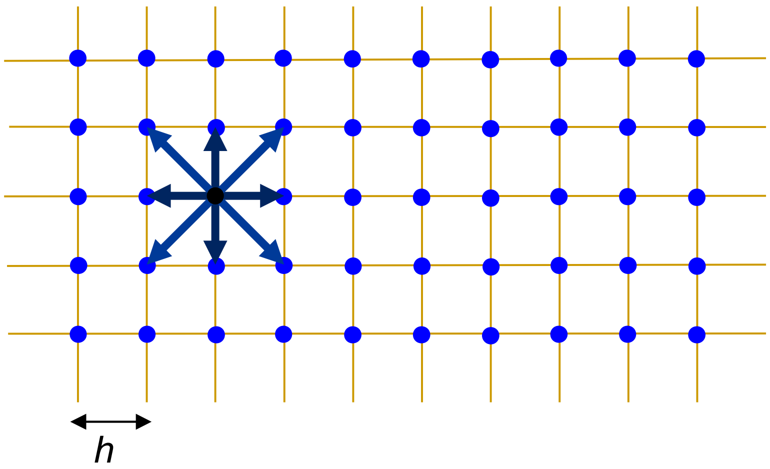
$$\vec{e}_i = \begin{cases} (0,0) & \text{if } i = 0 \\ C\left(\cos\left(\frac{\pi(i-1)}{2}\right), \sin\left(\frac{\pi(i-1)}{2}\right)\right) & \text{for } i = 1,\dots,4 \\ C\left(\cos\left(\frac{\pi(2i-9)}{4}\right), \sin\left(\frac{\pi(2i-9)}{4}\right)\right) & \text{for } i = 5,\dots,8 \end{cases}$$

III-1 Space discretization model

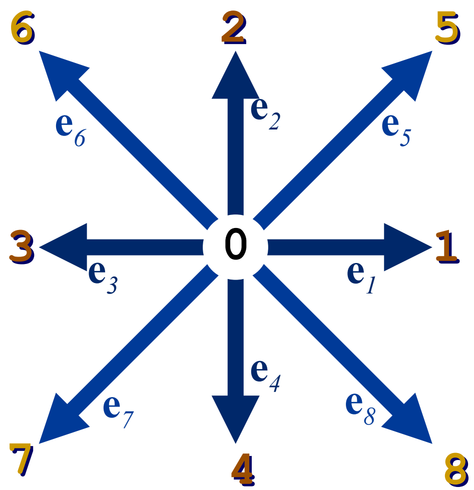
D2Q9 model

- fixed lattice : h
- time step : dt

$$C = h/dt$$



- for each node, we define:
  - 9 directions: i
  - 9 discrete velocities: $\vec{e}_i$
  - 9 distribution functions: f_i



- macroscopic properties:

density:

$$\rho = \sum_{i=0}^{8} f_i$$

velocity :

$$\vec{v} = \frac{1}{\rho} \sum_{i=0}^{8} f_i \vec{e_i}$$

pressure: $p = C_s^2 \rho$ *with* $C_s = C/\sqrt{3}$

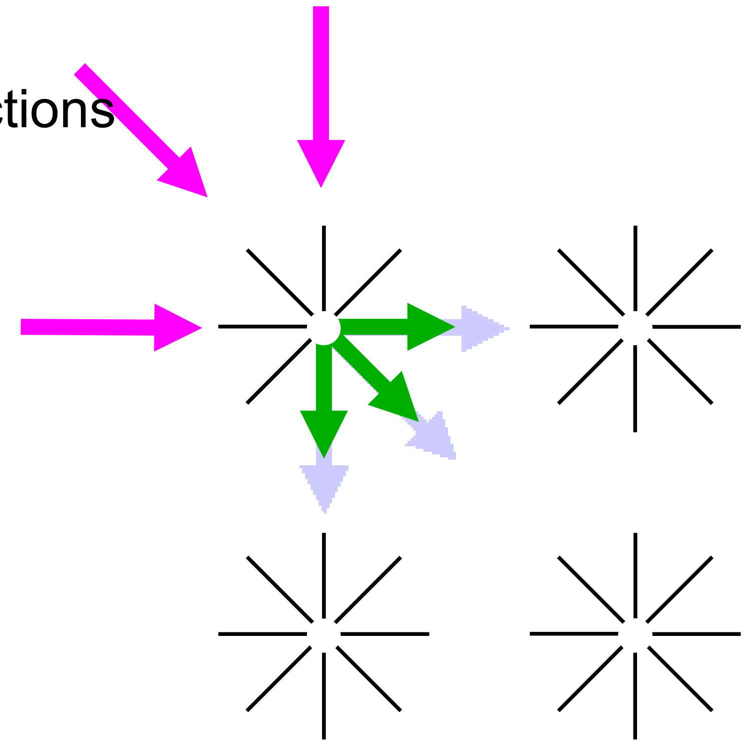
III. Practical use of the LBM

III-2 A two steps iterative process

LB method in 2 steps: collisions and propagation

- consider 3 distributions functions arriving on a node

- **collisions:** relaxation towards equilibrium functions



$$f_i(\vec{x}, t^+) = f_i(\vec{x}, t) - \frac{1}{\tau}\left[f_i(\vec{x}, t) - f_i^{eq}(\vec{x}, t)\right]$$

$$\begin{cases} f_i^{eq} = w_i \rho \left(1 + \frac{3}{C^2}\vec{e_i}.\vec{v} + \frac{9}{2C^4}(\vec{e_i}.\vec{v})^2 - \frac{3}{2C^2}\vec{v}.\vec{v}\right) \\ (i = 1, ..., 8) \qquad \Delta t = \left(\tau - \frac{1}{2}\right)\frac{h^2}{3\nu} \end{cases}$$

- **propagation** along each direction

$$f_i(\vec{x} + \vec{e_i}\mathrm{d}t, t + \mathrm{d}t) = f_i(\vec{x}, t^+)$$

III. Practical use of the LBM

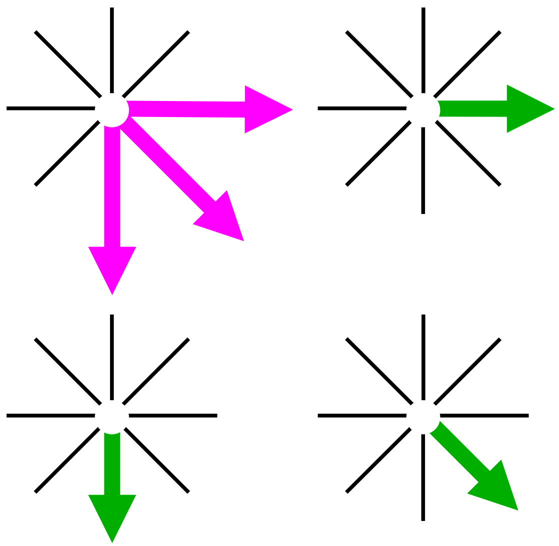
III-2 A two steps iterative process

LB method in 2 steps: collisions and propagation

- consider 3 distributions functions arriving on a node

- **collisions:** relaxation towards equilibrium functions

$$f_i(\vec{x}, t^+) = f_i(\vec{x}, t) - \frac{1}{\tau}\left[f_i(\vec{x}, t) - f_i^{eq}(\vec{x}, t)\right]$$



$$\begin{cases} f_i^{eq} = w_i \rho \left(1 + \frac{3}{C^2}\vec{e_i}.\vec{v} + \frac{9}{2C^4}(\vec{e_i}.\vec{v})^2 - \frac{3}{2C^2}\vec{v}.\vec{v}\right) \\ (i = 1, ..., 8) \qquad \Delta t = \left(\tau - \frac{1}{2}\right)\frac{h^2}{3\nu} \end{cases}$$

- **propagation** along each direction

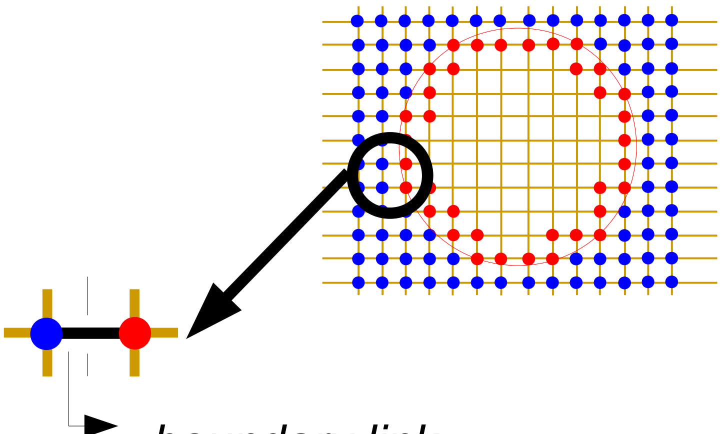
$$f_i(\vec{x} + \vec{e_i}\mathrm{d}t, t + \mathrm{d}t) = f_i(\vec{x}, t^+)$$

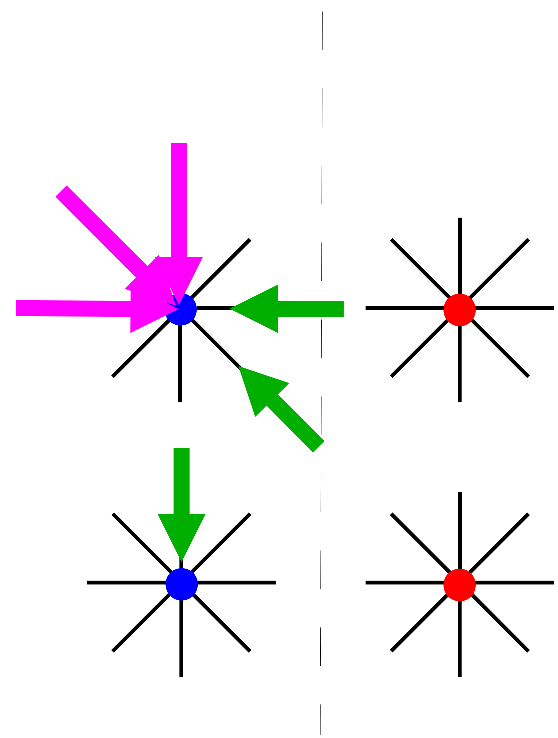
III. Practical use of the LBM

III-3 No slip condition on solid obstacle boundary

- discretize the obstacles
- differentiate « fluid » nodes and « solid » nodes
- bounce back on each boundary link:

$$f_{-\sigma i}(\vec{x}_{FB}, t + \mathrm{d}t) = f_{\sigma i}(\vec{x}_{FB}, t^{+})$$

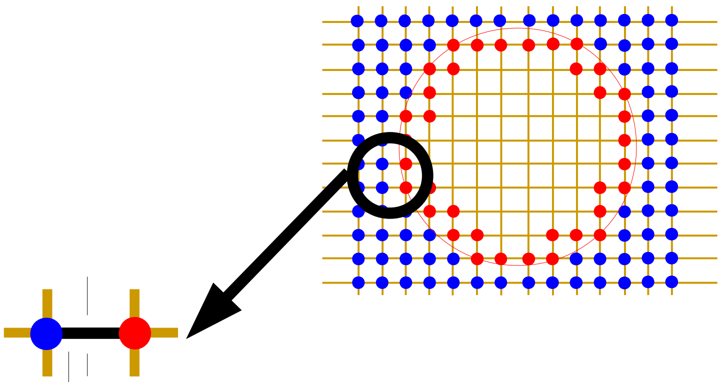




⇒ Vanishing of the macroscopic fluid velocity at the point where distribution functions are reflected.

⇒ For the LBM, the solid boundary is halfway between solid and fluid nodes.

III-3 No slip condition on solid obstacle boundary

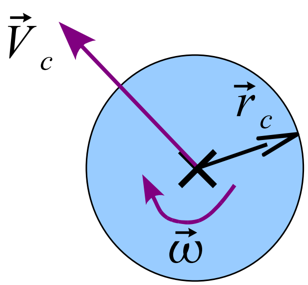


Case of moving solid obstacles:

$$f_{-\sigma i}(\vec{x}_{FB}, t + \mathrm{d}t) = f_{\sigma i}(\vec{x}_{FB}, t^{+}) - 2\alpha_i \vec{V_b}.\vec{e_i}$$

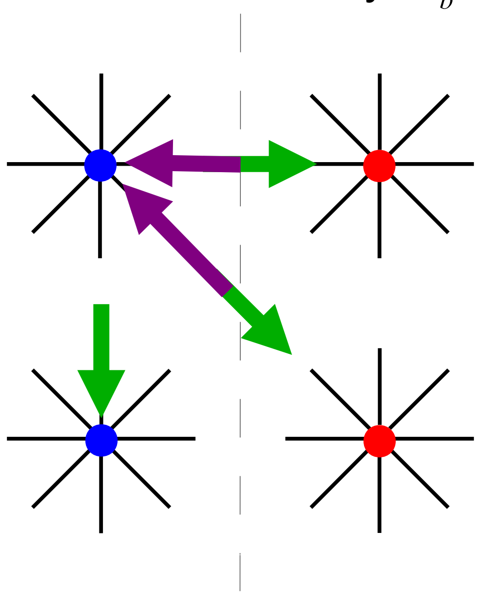
$$\alpha_i = 3 w_i \rho C^2$$

$\vec{V}_b$ is the solid velocity at the middle of the boundary link, for a circular solid particle:



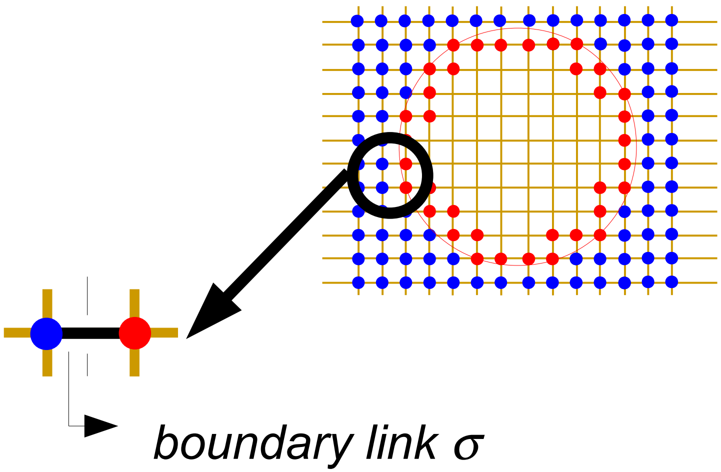
$$\vec{V_b} = \vec{V_c} + \vec{w} \wedge \vec{r_c}$$

Obstacle boundary, $V_b \neq 0$



III. Practical use of the LBM

III-3 No slip condition on solid obstacle boundary



Force applied by fluid on solid obstacles:

• Force (and then torque) is obtained by derivation of the momentum exchange with respect to time:

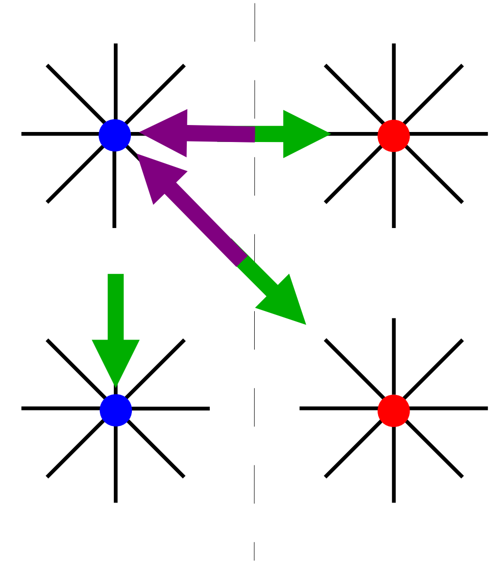
$$\vec{F}_\sigma(\vec{x}, t + \frac{1}{2}\mathrm{d}t) = 2\frac{\Omega}{\mathrm{d}t}\left[f_{\sigma i}(\vec{x}, t^+) - \alpha_i \vec{V}_b.\vec{e}_i\right]\vec{e}_{\sigma i}$$

$$\vec{T}_\sigma(\vec{x}, t + \frac{1}{2}\mathrm{d}t) = \vec{r}_c \times \vec{F}_\sigma(\vec{x}, t + \frac{1}{2}\mathrm{d}t)$$

• For the whole solid boundary:

$$\vec{F}_h(t + \frac{1}{2}\mathrm{d}t) = \sum_\sigma \vec{F}_\sigma(\vec{x}, t + \frac{1}{2}\mathrm{d}t)$$

Obstacle boundary, $V_b \neq 0$



III. Practical use of the LBM

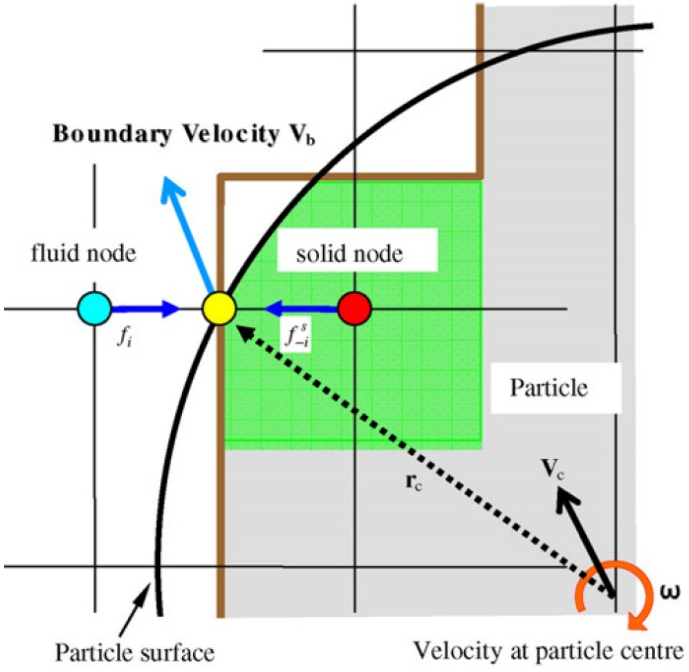
III-3 No slip condition on solid obstacle boundary

⇒ **The bounce back rule presented here is one of the simplest (and rough) way to deal with interactions between fluid and moving solid boundaries.**

⇒ **More complex scheme exist such as the immerse boundary scheme where the LB equation is weighted by the solid/fluid surface ratio at the vicinity of the node considered.**

⇒ **The classical bounce back rule limit the computation cost and is satisfactory as a first approximation.**

Han et al, 2007



III-4 Pressure boundary condition

The distribution function $f_i(\vec{x}, t)$ is the only object handled with the LBM.

⇒ Pressure and velocity boundary conditions cannot be imposed directly.

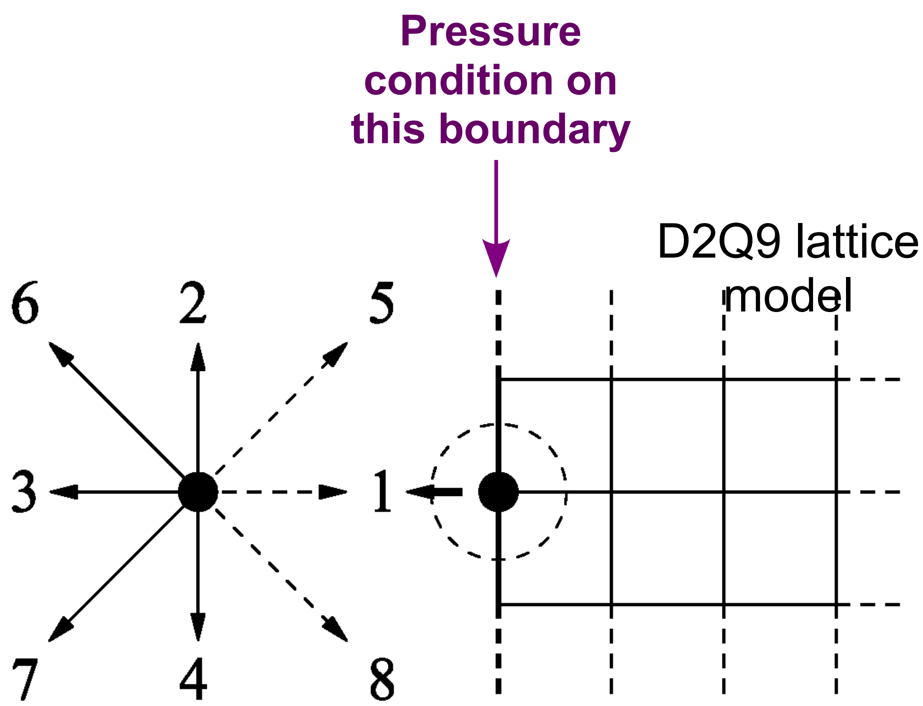
⇒ Distribution functions have to be defined to match the desired boundary condition (see work of Zou & He, 1997; Succi 2001).

Case of a pressure limit condition

For the considered node and after the propagation step:

- $f_{2,3,4,6,7}$ are known,
- $f_{1,5,8}$ are unknown.

⇒ Need of three equations where unknown distribution functions are expressed with respect to the macroscopic pressure and velocity.



III. Practical use of the LBM

III-4 Pressure boundary condition

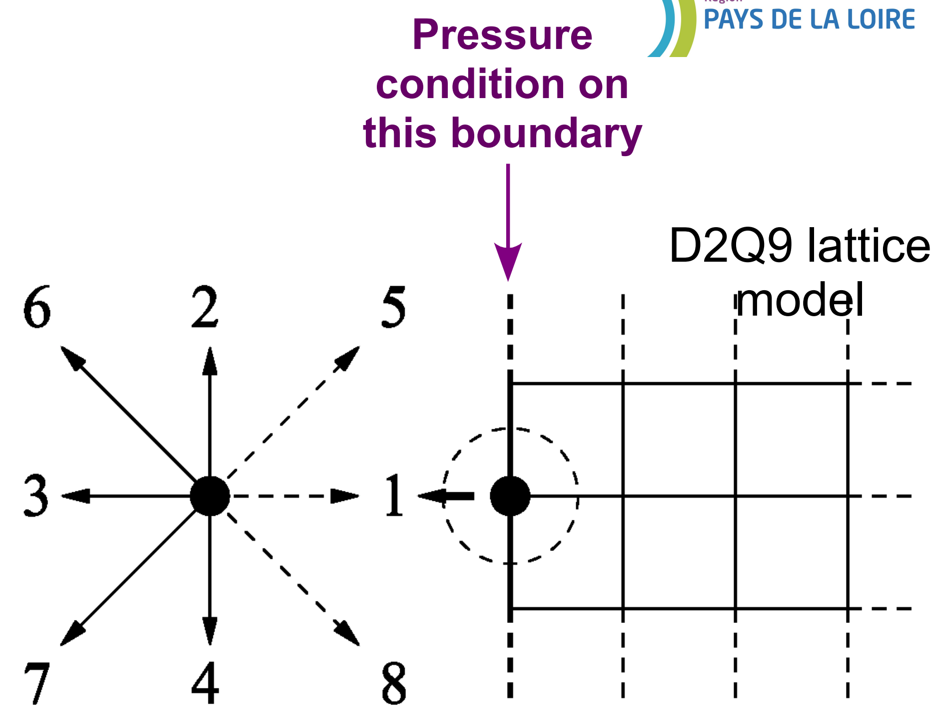
$$\vec{v} = \frac{1}{\rho}\sum_{i=0}^{8} f_i \vec{e_i}$$

Projection on the two space directions

$$\begin{cases} \bar{f}_1 + \bar{f}_5 + \bar{f}_8 & = \bar{\rho}\bar{v}_x + \bar{f}_3 + \bar{f}_6 + \bar{f}_7 \\ \bar{f}_5 - \bar{f}_8 & = \bar{\rho}\bar{v}_y + (-\bar{f}_2 + \bar{f}_4 - \bar{f}_6 + \bar{f}_7) \end{cases}$$

$$\rho = \sum_{i=0}^{8} f_i$$

$$\bar{f}_1 + \bar{f}_5 + \bar{f}_8 = \bar{\rho} - (\bar{f}_0 + \bar{f}_2 + \bar{f}_3 + \bar{f}_4 + \bar{f}_6 + \bar{f}_7)$$



III. Practical use of the LBM

III-4 Pressure boundary condition

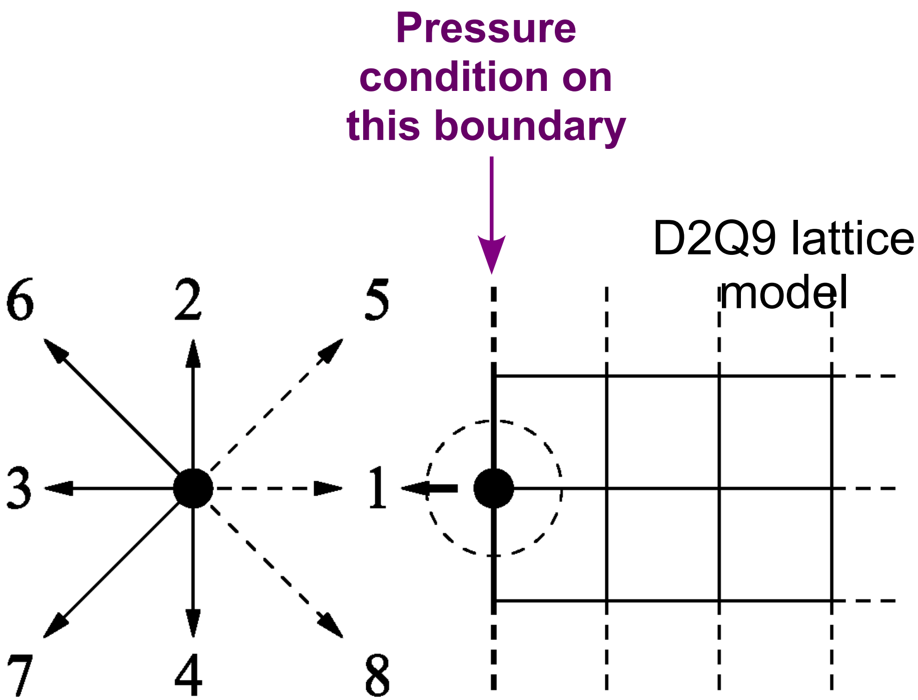
$\Rightarrow$ ρ ? v_x ? v_y ?

- Pressure condition $\equiv$ density condition $p = C_s^2 \rho$
- Assumption: tangential velocity to the boundary is nil, $v_y = 0$
- Additional equation: bounce back rule for the non-equilibrium part of the distribution functions normal to the boundary (Zou & He, 1997).

$$f_1 - f_1^{eq} = f_3 - f_3^{eq}$$

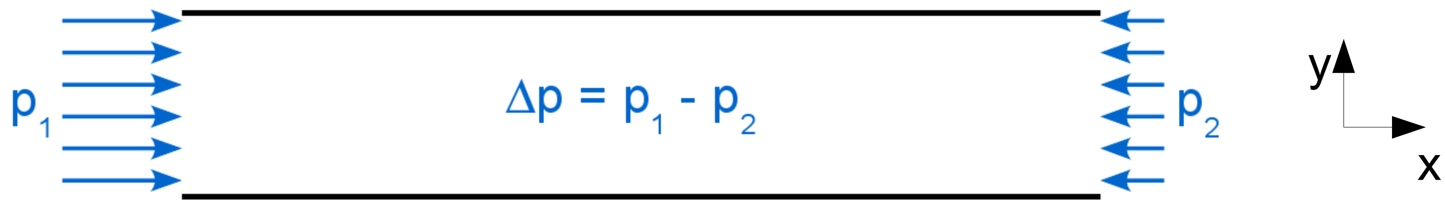
By developing the equilibrium functions

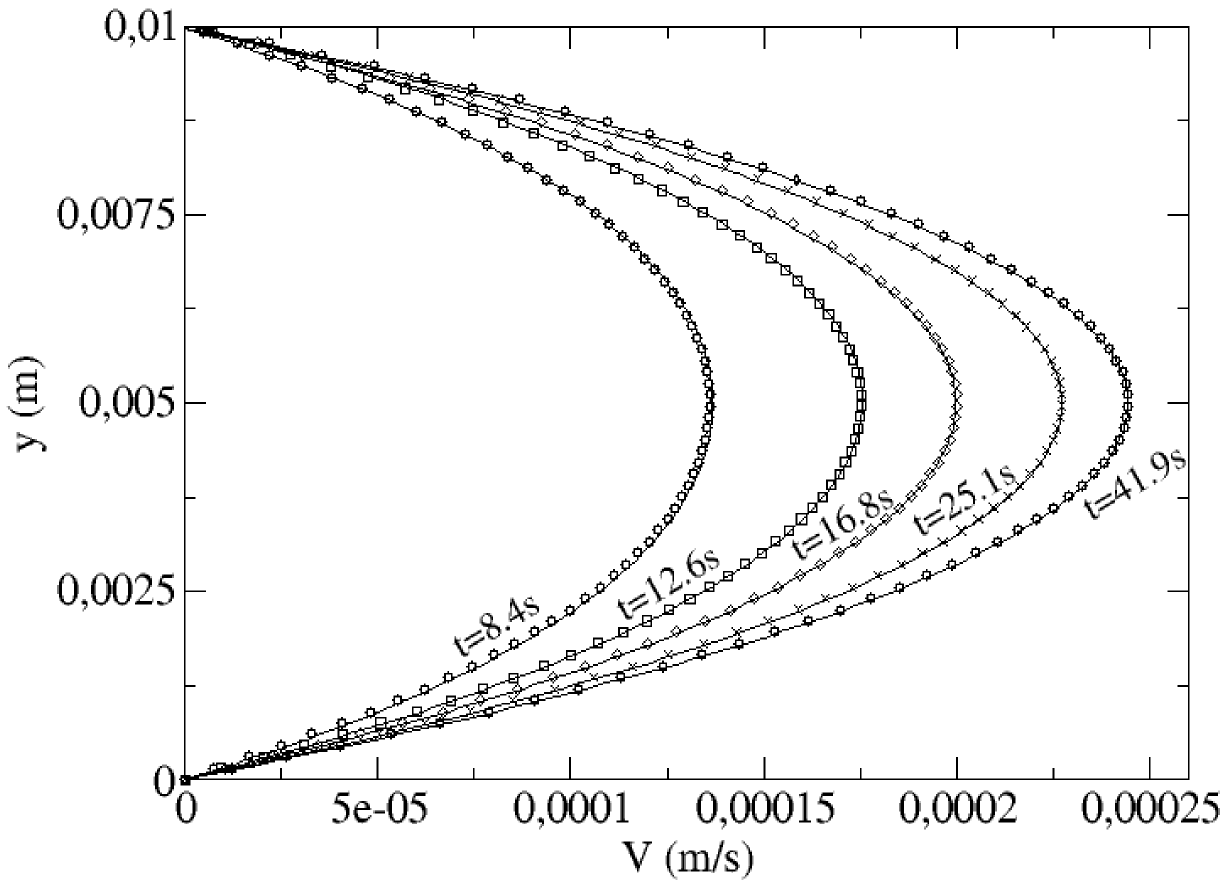
$$\bar{f}_1 = \bar{f}_3 + \frac{2}{3}\bar{\rho}\bar{v}_x$$



III-5 Validation on simple flow cases

Poiseuille flow





⇒ agreement with serie solutions for transient and stationnary solutions

(Lominé et al, AGS'10, 2010)

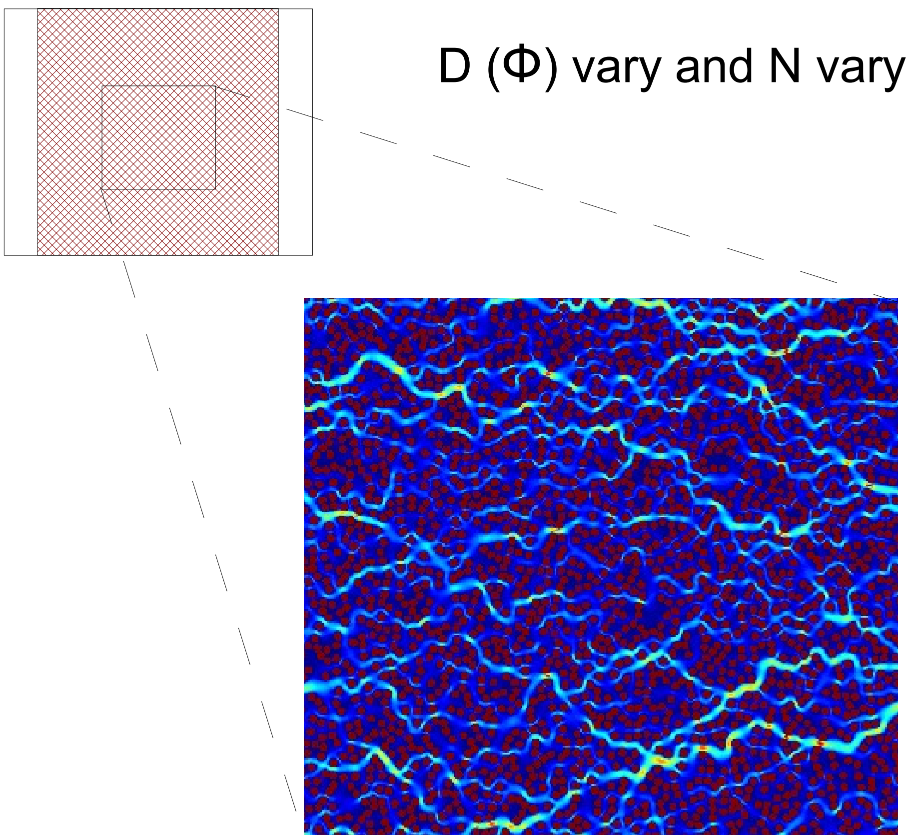
III. Practical use of the LBM

III-5 Validation on simple flow cases

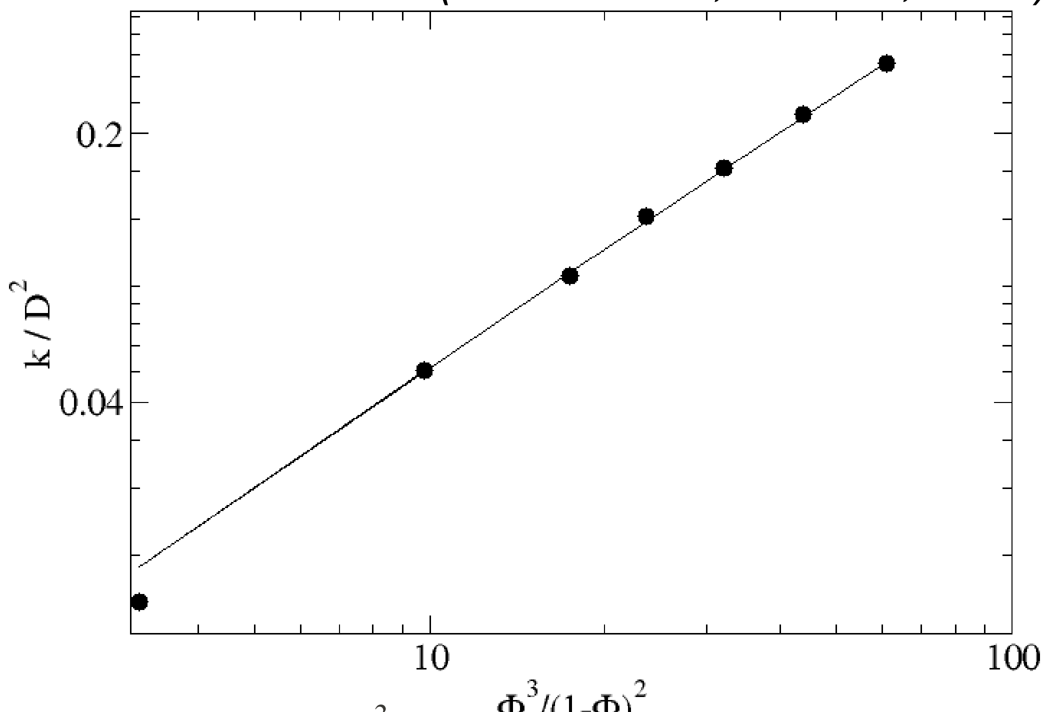
Fluid flow in porous media

We consider bi-dimensional porous media with porosity Φ,made with spherical particles of diameter D.

D (Φ) vary and N vary from ~3000 to ~5000 particles



(Lominé et al, AGS'10, 2010)



⇒ we retrieve the Kozeny-Carman relation: $\frac{k}{D^2} \propto \frac{\Phi^3}{(1-\Phi)^2}$

IV. DEM-LBM coupling

IV-1 Subcycle

- DEM time step is limited for stability condition by a critical time step: $dt_{DE} < dt_{DE}^{cr} = 2\pi\sqrt{m/k}$
- LBM time step given by: $\mathrm{d}t = \frac{1}{3\nu}\left(\tau - \frac{1}{2}\right)h^2$

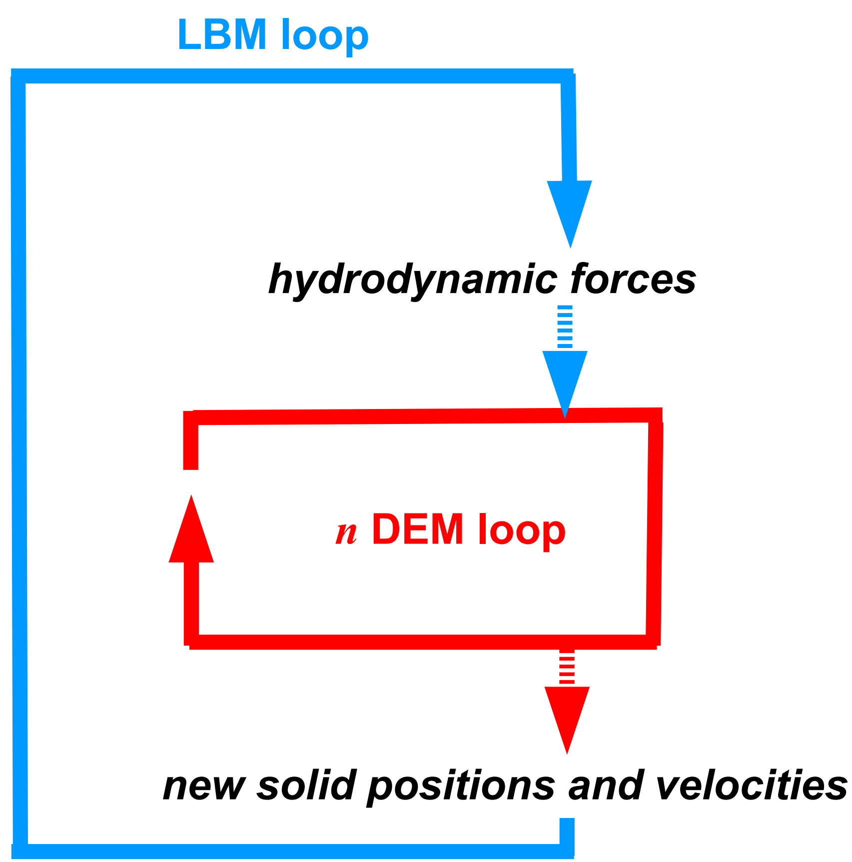
⇒ For usual material parameters (contact stiffness, solid density, fluid density and viscosity): DEM time step < LBM time step.

⇒ The DEM loop is considered as a subcycle of the LBM loop (Feng et al., 2007)

- The DEM time step is adjusted such as an integer number n of DEM loop can be performed in one LBM loop: $dt = n\, dt_{DE}$

- Same value of F_h applied on solid particles during the n DEM loop

  (*smooth solid particle motion required during the n DEM loop*)



IV. DEM-LBM coupling

IV-2 Hydrodynamic forces and Newton's law

Action of fluid on solid particles is simply taken into account in Newton's law:

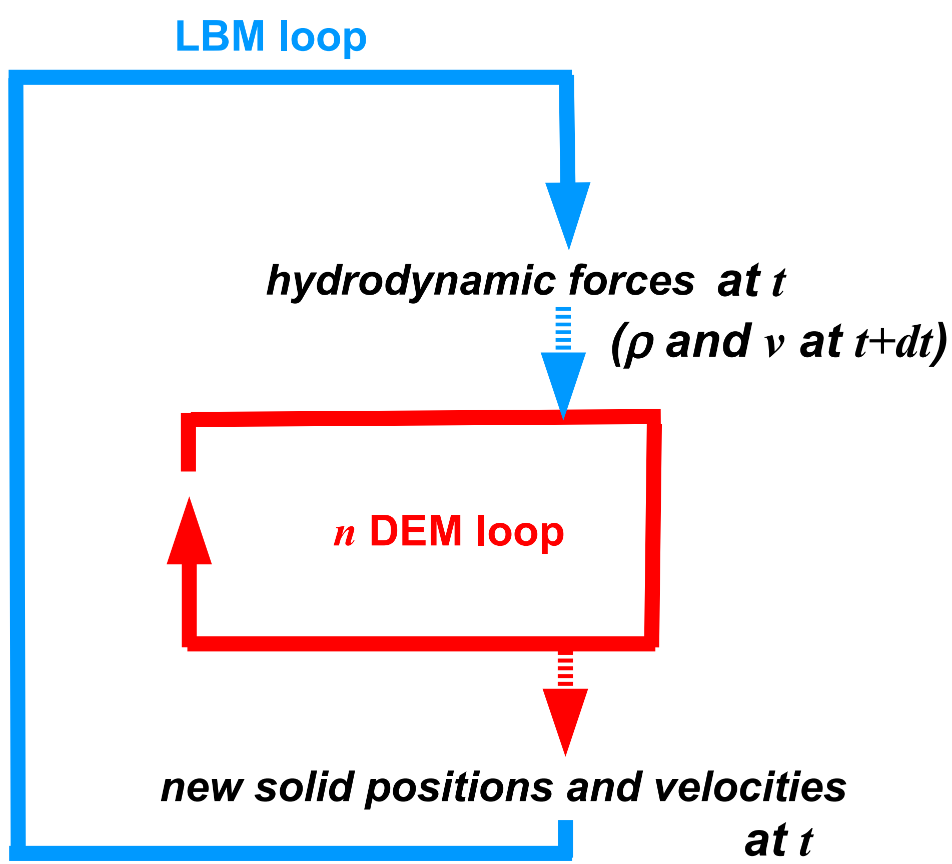
Contacts (DE method)

$$m\,\vec{\gamma} = \vec{F}_c + \vec{F}_h$$

$$J\,\dot{\vec{\omega}} = \vec{T}_c + \vec{T}_h$$

Fluid (LB method)

.



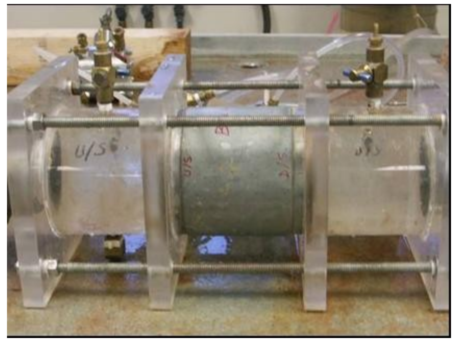
V. Application to piping erosion

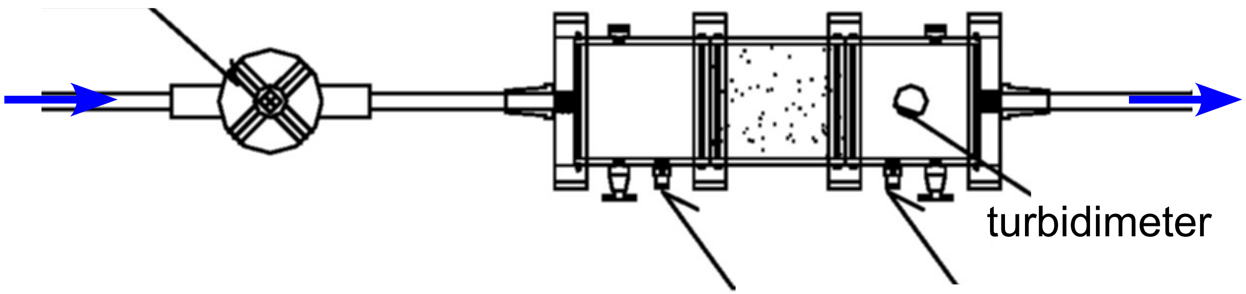
V-1 Characterization of soil erodability

- Laboratory test: Hole Erosion Test (HET)

(Regazzoni, 2009)

(Pham, 2008)

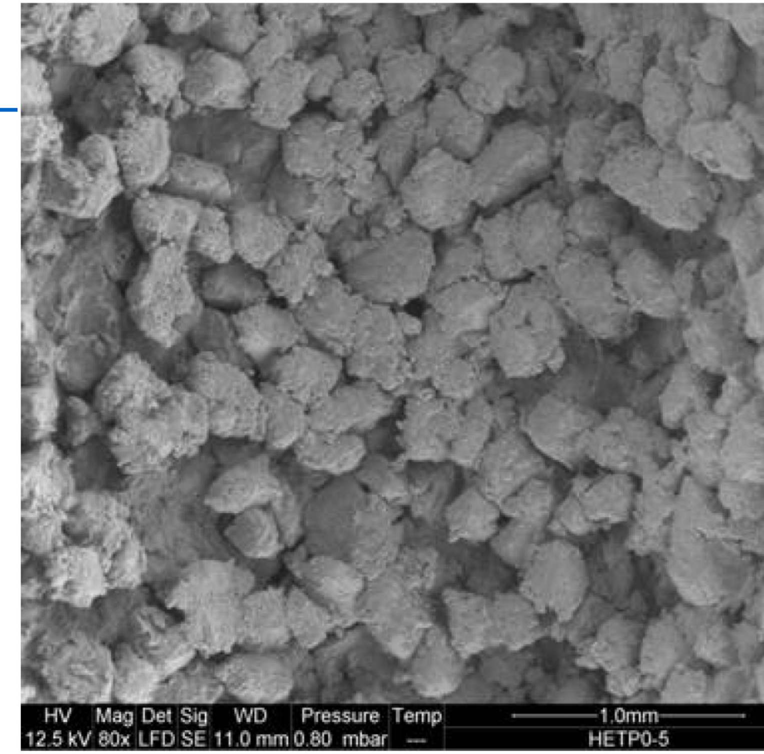




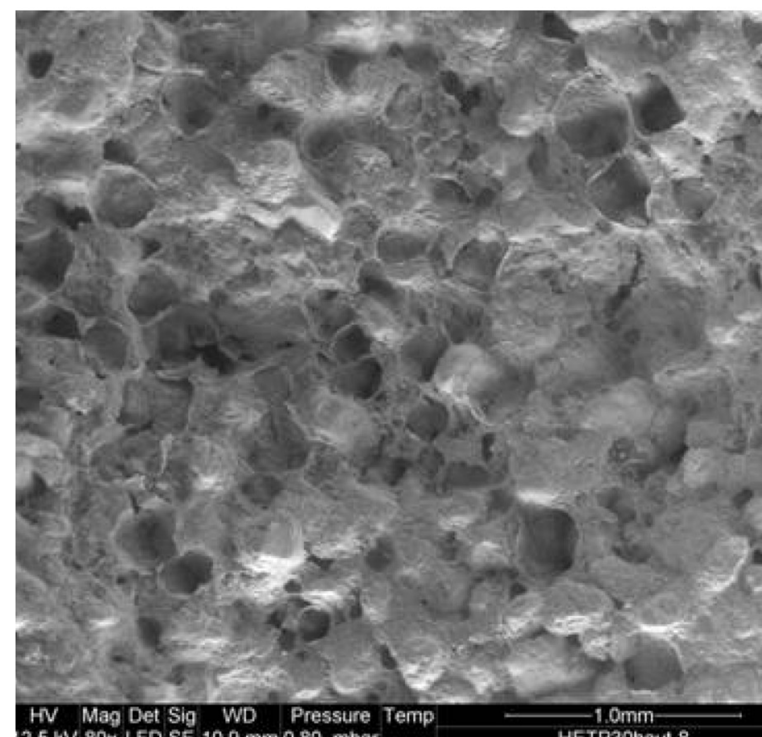
- Characterisation of particle detachments under hydro-mechanical loadings

→ Description of mechanisms involved at microscopic scale.

→ Identification of relevant parameters related to the solid and fluid phase



(Pham, 2008: sand and clay mix)



V. Application to piping erosion

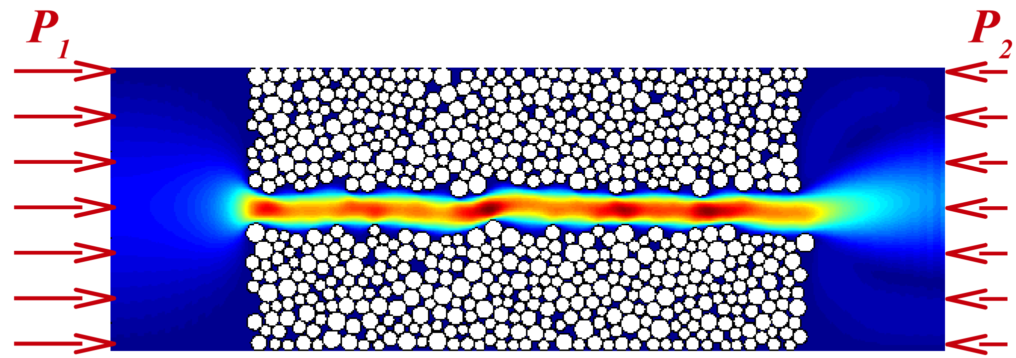
V-2 Model description

⇒ Simplified 2D Hole Erosion Test (HET):

- Cohesive frictional granular assembly:

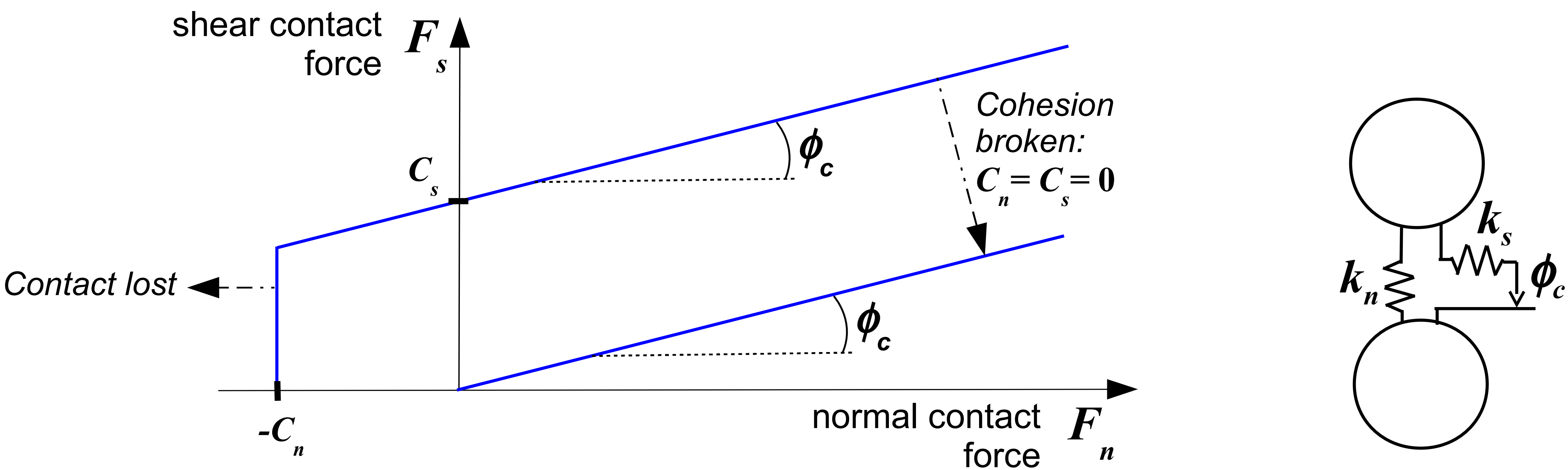
$$\phi_C = 20° \qquad C = -C_n = C_s$$

- Initial hole drilled in the granular assembly,
- Water flow under constant pressure gradient: $\Delta P = P_1 - P_2$.



800 solid particles; fluid lattice of 335 000 nodes

⇒ Brittle cohesive inter-particle contacts:

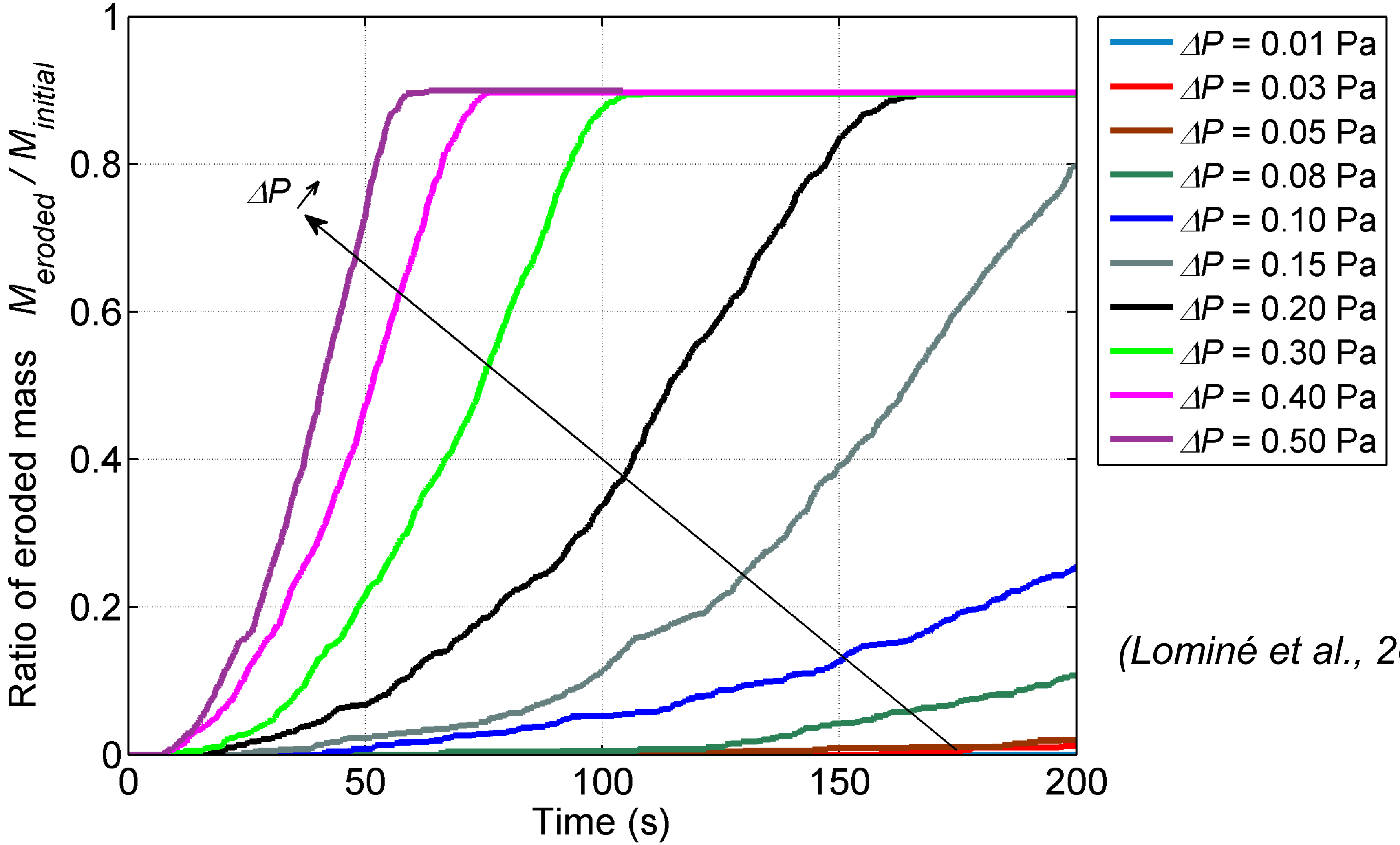


Lominé F., Sibille L., Marot D. (2011). *"A coupled discrete element – lattice Boltzmann method to investigate internal erosion in soil", In Proc. 2nd Int. Symp. on Computational Geomechanics COMGEOII, Dubrovnik, 27-29 avril 2011*

V. Application to piping erosion

V-3 Numerical results

⇒ **Ratio of eroded mass for a cohesion** $C/d = 0.506$ **N/m**



(Lominé et al., 2011)

→ No erosion for $\Delta P = 0.01$ Pa.

→ Acceleration of kinetic of erosion when ΔP increases.

V. Application to piping erosion

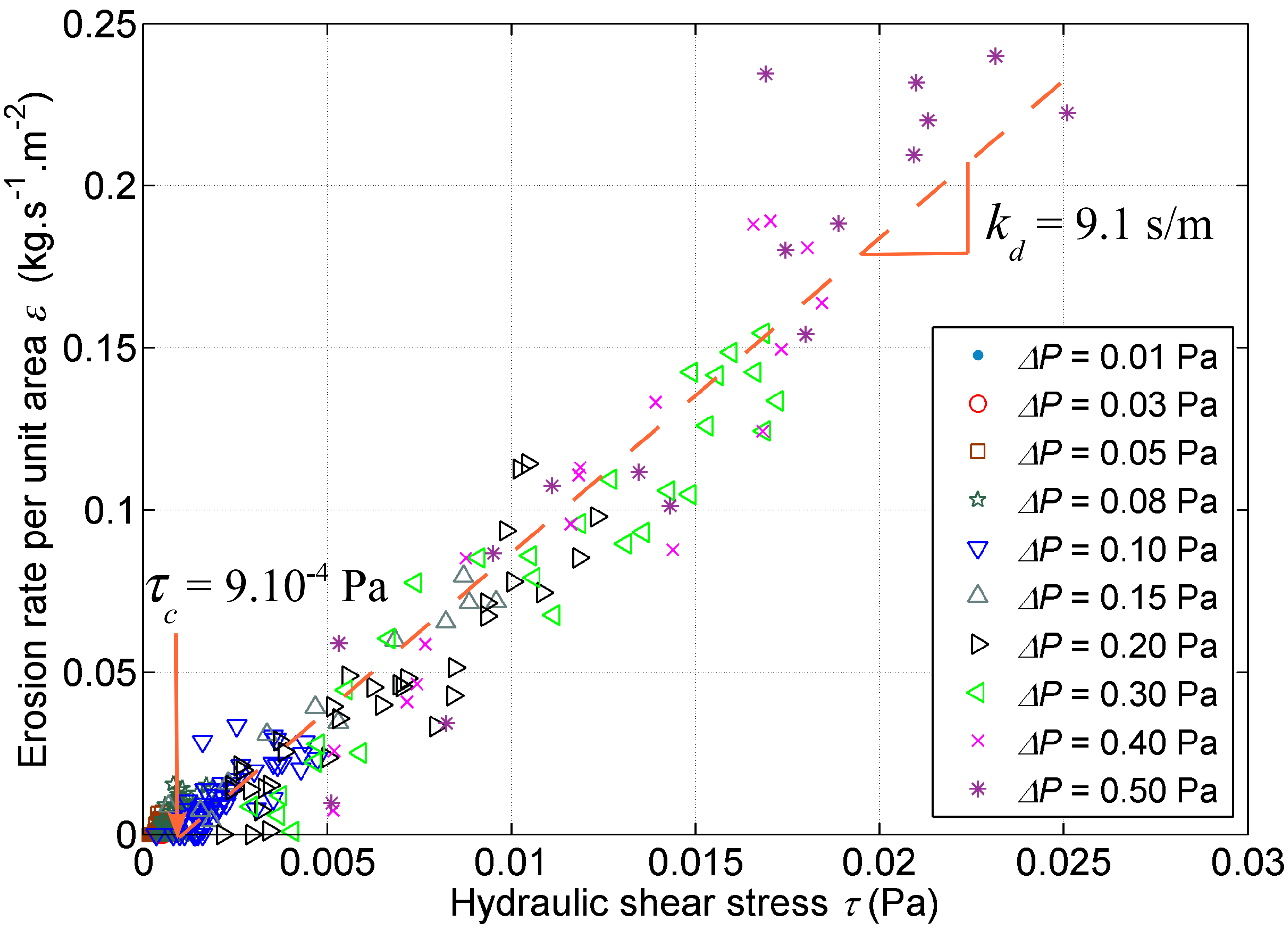
V-3 Numerical results

⇒ Classical interpretation with respect to the hydraulic shear stress τ :

$$\dot{\epsilon} = k_d\,(\tau - \tau_c) \text{ if } \tau > \tau_c$$ (Shields 1936, Wan & Fell 2002)

τ_c : critical shear stress

k_d : erosion rate .



→ Hydraulic shear stress computed along the hole border:

$$\tau = \nu \rho_0 \frac{\mathrm{d}V_x}{\mathrm{d}y}$$

(Lominé et al., 2011)