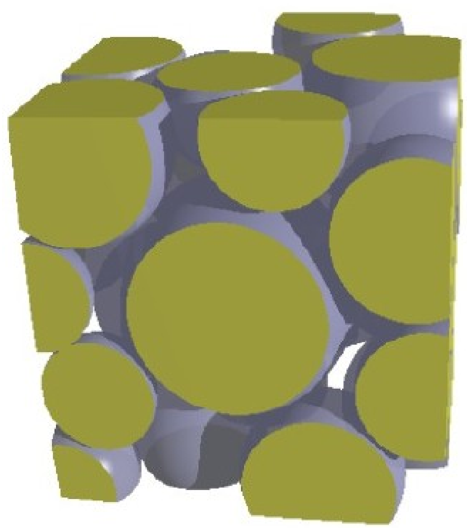
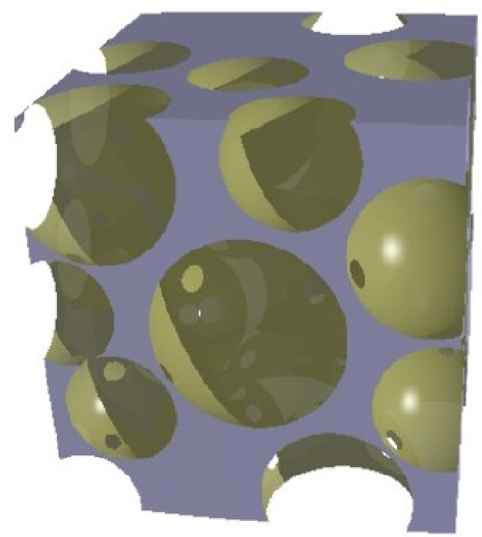
Discrete Element Modeling
Part2. One phase flow

Bruno Chareyre



Solid phase



Porosity

Numérique avancé – ENSE3 2017

Content

2.Fully resolved methods

Single-phase Navier-Stokes (FV, LBM, FEM...)
+ no-slip condition: $u_f = u_s$ on the solid phase
+ explicit integration of the drag forces in the DEM

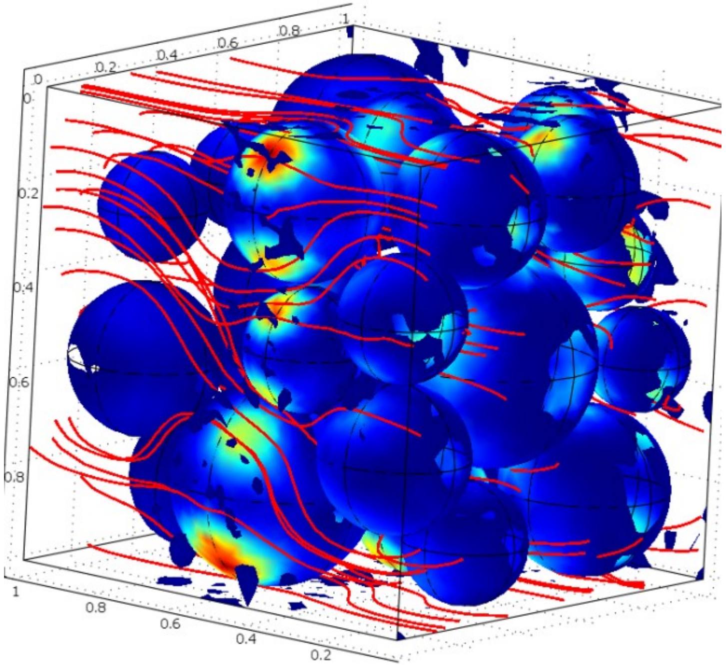
$$\rho_f \frac{\partial \mathbf{u}_f}{\partial t} + \rho_f (\mathbf{u}_f \cdot \nabla)\mathbf{u}_f = -\nabla p + \mu \nabla^2 \mathbf{u}_f \quad \text{in } \Omega_F,$$

$$\nabla \cdot \mathbf{u}_f = 0 \quad \text{in } \Omega_F,$$

$$\mathbf{u}_f = \mathbf{u}_\Gamma \quad \text{on } \Gamma,$$

$$\mathbf{u}_f = \mathbf{u}_p \quad \text{and} \quad \sigma \cdot \hat{\mathbf{n}} = t_{\Gamma_P} \quad \text{on } \Gamma_P,$$

$$\mathbf{u}_f(x, t=0) = \mathbf{u}_0(x) \quad \text{in } \Omega_F.$$



3. Averaged methods (1)

Two-phase Navier-Stokes

$$\frac{\partial \alpha_f}{\partial t} + \nabla \cdot (\alpha_f \mathbf{u}_f) = 0,$$

$$\frac{\partial (\alpha_f \mathbf{u}_f)}{\partial t} + \nabla \cdot (\alpha_f \mathbf{u}_f \mathbf{u}_f) = -\alpha_f \nabla \frac{p}{\rho_f} - \mathbf{R}_{pf} + \nabla \cdot \boldsymbol{\tau}.$$

Momentum exchange (a.k.a permeability or drag)

$$\mathbf{R}_{pf} = \mathbf{K}_{pf} (\mathbf{u}_f - \langle \mathbf{u}_p \rangle),$$

$$\mathbf{K}_{pf} = 150 \frac{(1-\alpha_f)^2 \nu_f}{\alpha_f d_p^2} + 1.75 \frac{(1-\alpha_f)\,|\mathbf{u}_f - \mathbf{u}_p|}{d_p}$$ (ex. Ergun)

+ averaging for granular quantities and discretization of the drag force

3. Averaged methods (2)

Two-phase Navier-Stokes

$$\frac{\partial \alpha_f}{\partial t} + \nabla \cdot (\alpha_f \mathbf{u}_f) = 0,$$

$$\frac{\partial (\alpha_f \mathbf{u}_f)}{\partial t} + \nabla \cdot (\alpha_f \mathbf{u}_f \mathbf{u}_f) = -\alpha_f \nabla \frac{p}{\rho_f} - \mathbf{R}_{pf} + \nabla \cdot \boldsymbol{\tau}.$$

$$\mathbf{R}_{pf} = \mathbf{K}_{pf} (\mathbf{u}_f - \langle \mathbf{u}_p \rangle),$$

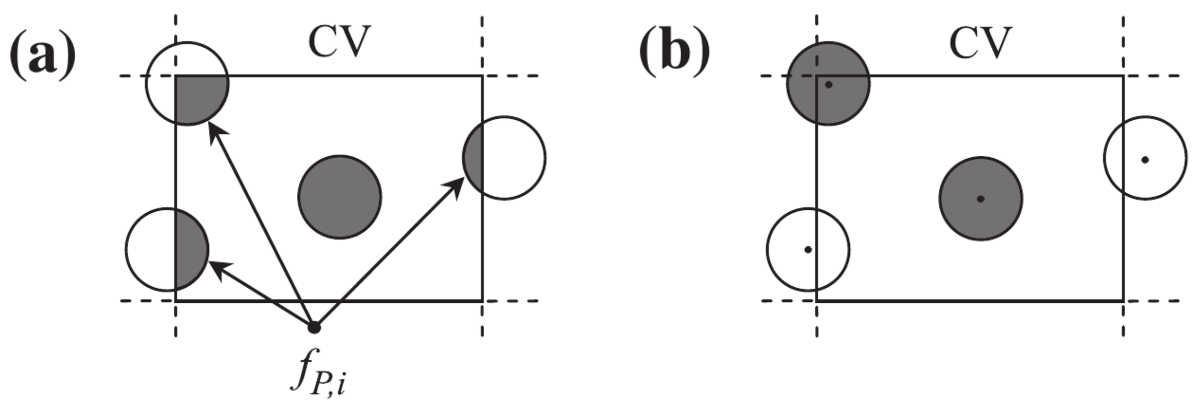
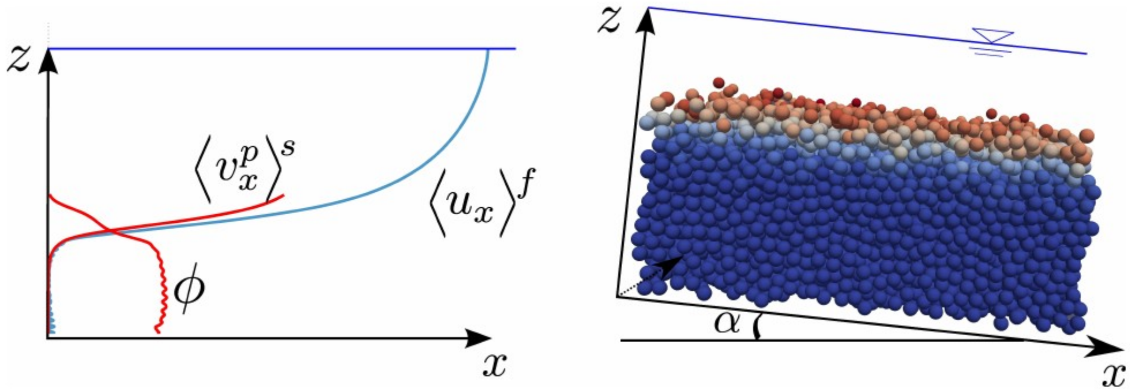


Fig. 2. Porosity determination: (a) exact method, and (b) particle centre method.

3. Averaged methods (3)

An example in 1D (Maurin et al. 2015)



$$\langle \mathbf{u}^f \rangle = \langle u_x^f \rangle (z)\ \mathbf{e}_x$$

Coupling

3D Discrete Element Method $\Longleftrightarrow$ Mean fluid resolution (1D)

3D Discrete Element Method	Mean fluid resolution (1D)
Describe each particle *Newton's law*	*Volume-averaged mom. balance* *Steady uniform :* 1D
Open-source code YADE Spring-dashpot contact law	Clear Newtonian fluid Mixing length closure

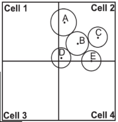
Drag and buoyancy
Dallavalle (1943) + Richardson Zaki (1954)

Maurin, Chauchat, Chareyre and Frey. A minimal coupled fluid-discrete element model for bedload transport. Physics of Fluids, 27(11), 2015.

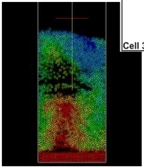
The art of compromise (part 2)

A variety of methods are being developed to couple the DEM with fluid flow models. Two main groups of methods emerge (review paper: Zhu et al. (2007)):

- Macro-continuum scale for the fluid (CFD-DEM)
- Sub-particle scale for the fluid (DNS-DEM, LB-DEM, SPH-DEM,...)

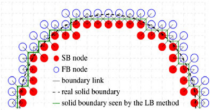


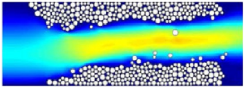
Zhao (2013)



Chen (2009), YADE+OpenFOAM

Equivalent continuum scale

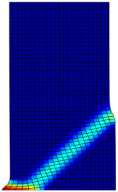




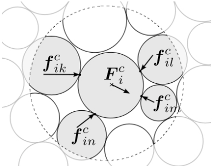
Lomine, Scholtes, Sibille, Poulain (2011), YADE+LBM

Continuum scale

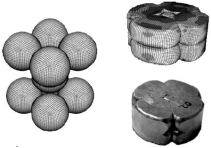
The art of compromise (part 2)



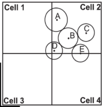
Equivalent continuum scale



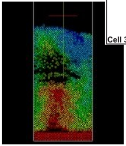
DEM



Continuum scale (Harthong et al. (2012))



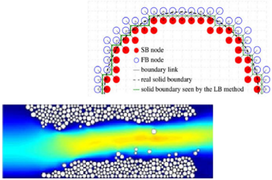
Zhao (2013)



Chen (2009), YADE+OpenFOAM

Equivalent continuum scale

Intermediate scale?



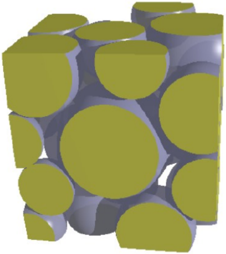
Lomine, Scholtes, Sibille, Poulain (2011), YADE+LBM

Continuum scale

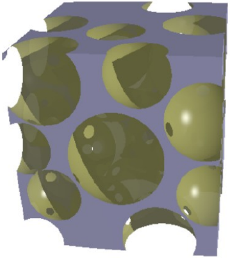
Pore Scale Finite Volumes

DEM-PFV: length scale for the fluid of the order of the particles sizes, aiming at:

- A compromise in terms of computational cost vs. accuracy
- An efficient integration scheme for strong poromechanical couplings



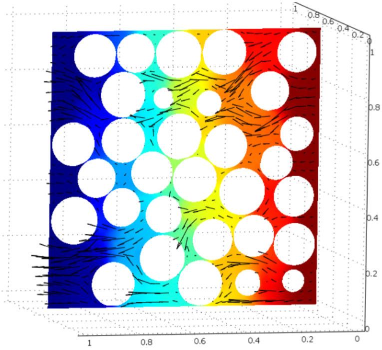
Solid phase



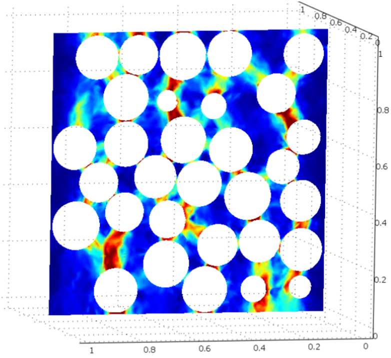
Porosity

A closer look at how the fluid flows

The pressure drop along the flow path is highly localized.



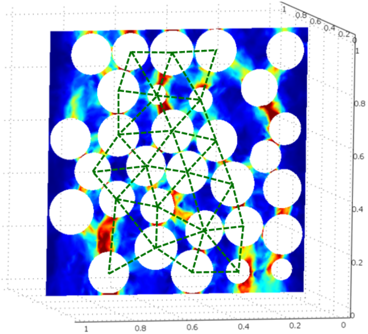
(d) Pressure field + velocity



(e) Pressure gradient

PFV: partitionning the pore space

A *pore* is that part of the void space enclosed in the cell of a triangulation, in which pressure is approximately constant.

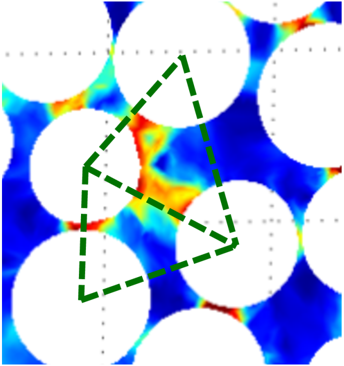


- Side note: it is of the upmost importance to employ a suitable type of triangulation. Delaunay triangulation would be irrelevant for polydispersed packings. *regular triangulation* (Pion and Teillaud, 2006) is a solution.

Incompressible Stokes Flow

Governing equations & num. scheme

- Stokes flow:
  $\int_{f_{ij}} \vec{u}_w^* \cdot \vec{n} ds = q_{ij}^* = k_{ij}(P_j - P_i)$
  (u_w^*: relative velocity)
- Continuity:
  $\int_{\partial\Omega} \vec{u}_w \cdot \vec{n} ds = 0$ (incompressible)
  or: $\int_{\partial\Omega} (\vec{u}_w^* + \vec{u}_s) \cdot \vec{n} dS = 0$
  linking fluid velocity and deformation rate:
  $\int_{\partial\Omega} \vec{u}_w^* \cdot \vec{n} ds = \dot{V}_i$
- implicit dependency of P on particles velocity:
  $\sum_{j=1}^{4} k_{ij}(P_j - P_i) = \dot{V}_i$
- P solution of the linear system:
  $\mathbf{K}\,\mathbf{P} = \mathbf{E}\dot{\mathbf{X}} + \mathbf{Q}_{BC}$
- Forces on the particles function of P:
  $\mathbf{F}_w = \mathbf{S}\mathbf{K}^{-1}(\mathbf{E}\dot{\mathbf{X}} + \mathbf{Q}_{BC})$



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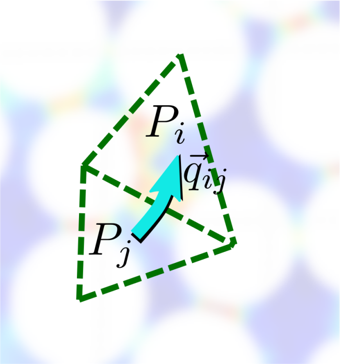

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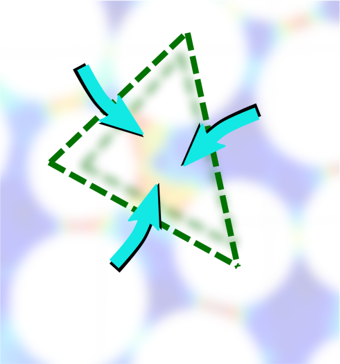

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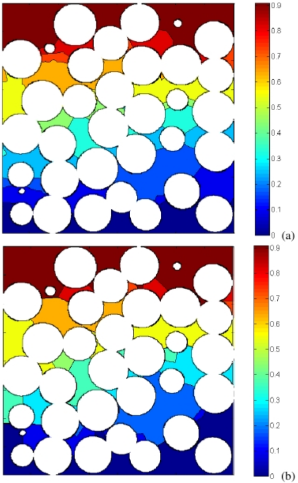

Solution DNS (a) and PFV (b)

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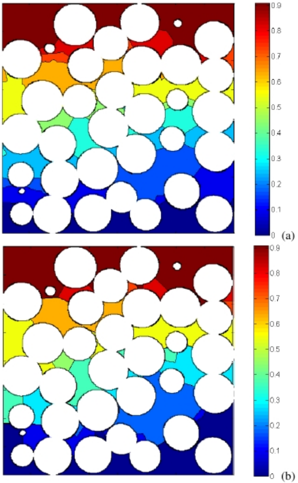


Solution DNS (a) and PFV (b)

Poromechanical coupling

We end up with a discrete analog of the equations of continuum (Biot's) poromechanics for incompressible phases (Catalano et al. (2013)).

Coupling equations of poromechanics in the quasi-static regime:

$$k\nabla^2 p = -\nabla \cdot \dot{u}_s$$

$$\nabla \cdot \boldsymbol{\sigma'} - \nabla p + (1-n)(\rho^s - \rho^f)\mathbf{g} = 0$$

Our discrete form, locally:

$$\sum_{j=1}^{4} k_{ij}(P_j - P_i) = \dot{V}_i \qquad \text{(for a pore } i\text{)}$$

$$\sum_k \mathbf{f}^c_{nk} + \mathbf{F}_{w,n} + \mathbf{W}_n = 0 \qquad \text{(for a particle } n\text{)}$$

For the whole system:

$$\mathbf{K}\,\mathbf{P} = \mathbf{E}\dot{\mathbf{X}} + \mathbf{Q}_{BC}$$

$$\mathbf{F}_c + \mathbf{S}\mathbf{K}^{-1}(\mathbf{E}\dot{\mathbf{X}} + \mathbf{Q}_{BC}) + \mathbf{W} = 0$$

Benchmark tests

Permeability predictions:
Experiments on mixtures of two-sized glass beads compared to PFV and empirical/semi-empirical relations (Tong et al., 2012).

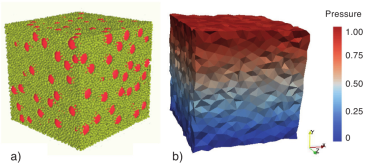
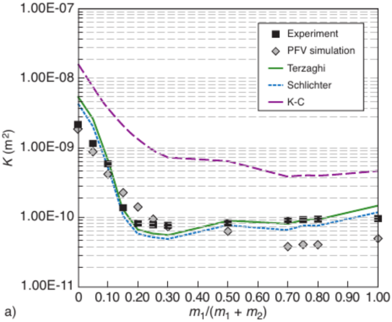


Figure 8

a) A typical numerical sample for $m_1 / (m_1 + m_2) = 0.5$;
b) pressure field in simulated permeameter.



Benchmark tests

Consolidation problem:
Time evolution of a saturated medium under external load

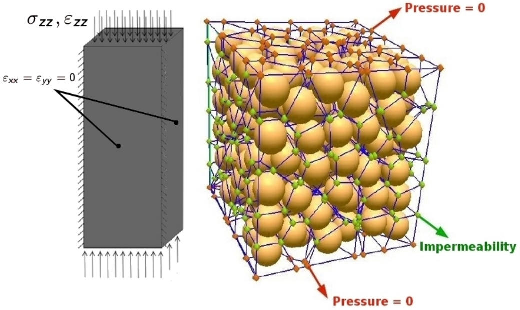
Terzaghi's theory of consolidation

Coefficient of consolidation:

$$C_v = \frac{kE_{oed}}{\gamma} \quad (1)$$

Consolidation time:

$$T_v = \frac{C_v t}{H^2} \quad (2)$$



SOLID BOUNDARY CONDITIONS

FLUID BOUNDARY CONDITIONS

Benchmark tests

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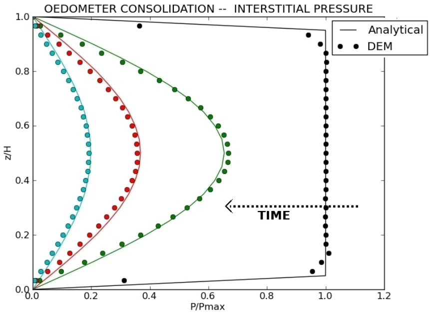
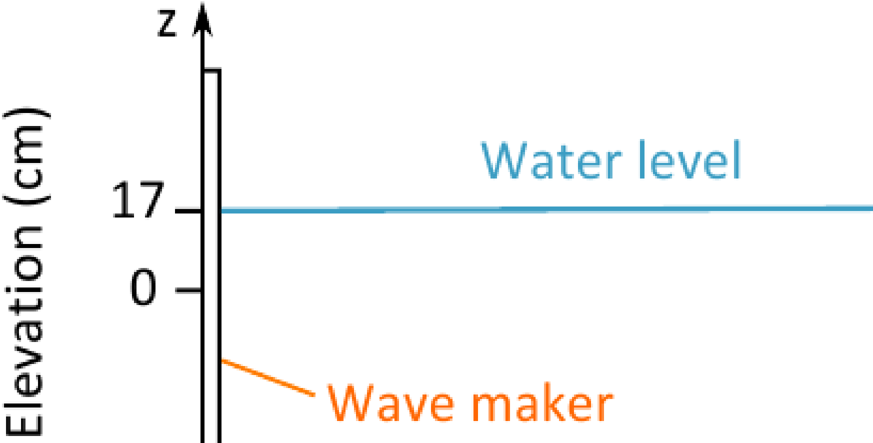
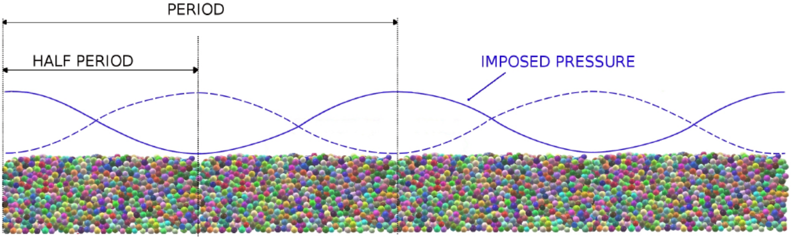


Sediment under stationary waves

Physical model at LEGI, Grenoble
(Michallet et al. (2012), Project C2D2-Hydrofond)



Sediment under stationary waves



Flow regime inside the sediment

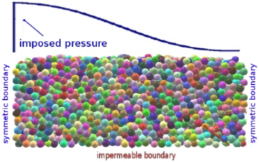
Typical values of dimensionless numbers:

- Particles Reynolds number: $R_e \approx 10^{-8}$
- Stokes number: $Stk \to \infty$ (if relevant)
- Mach number: $M \approx 10^{-8}$ (numerical model: $M = 0$)

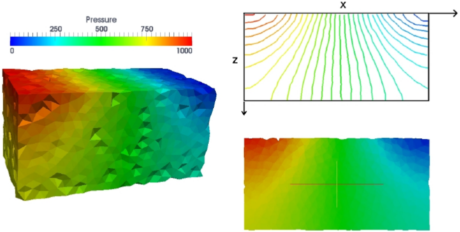
Steady incompressible viscous flow is a rather good approximation.

Simulation

DEM-PFV modeling of the sediment (Catalano et al., 2011)



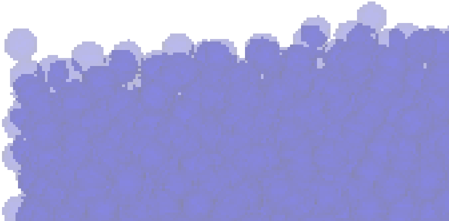
(f) Geometry and loading



(g) Pressure field in a stable system

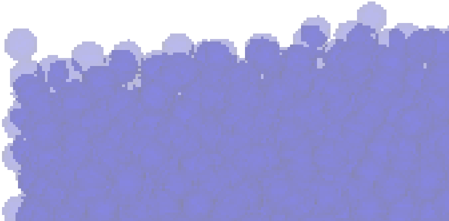
Simulation

Particles velocity and fluid pressure



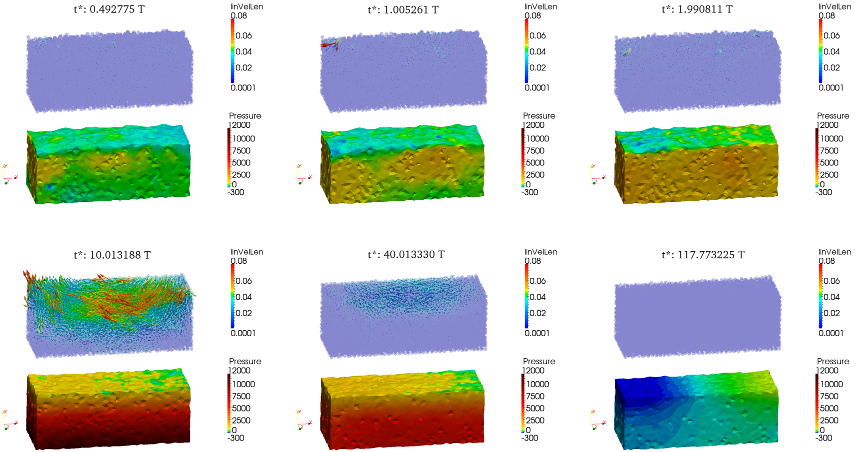
Simulation

Particles velocity and fluid pressure (1 image per period)



Simulation

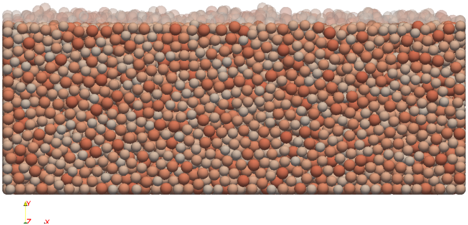
Progressive build-up of pore pressure

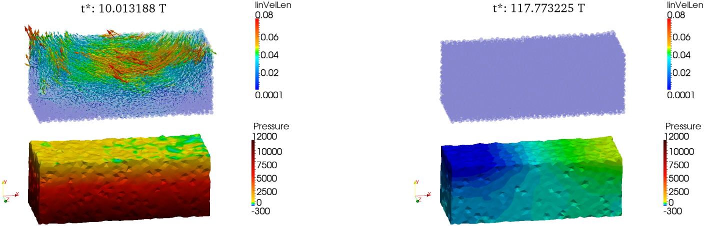


Simulation

Transient liquefaction comes with a slow *consolidation* process

we recall: $\mathbf{M}\ddot{\mathbf{X}} = \mathbf{F}_c + \mathbf{W} + \mathbf{S}\mathbf{K}^{-1}(\mathbf{E}\dot{\mathbf{X}} + \mathbf{Q}_{BC})$

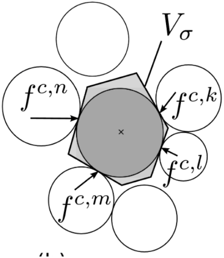


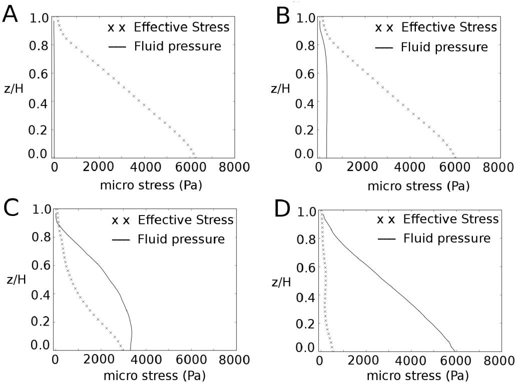


Simulation

Effective stress vanishes (*liquefaction*)

$$\sigma' = \frac{1}{V_\sigma} \sum_k \mathbf{f}_k^c \otimes \mathbf{x}_k$$





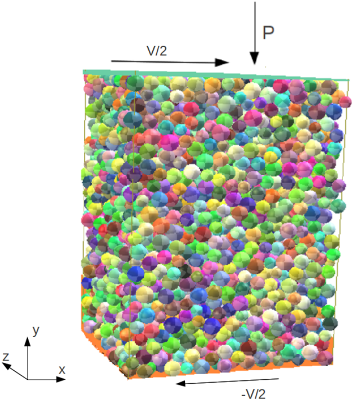
Dense supensions

Something is missing. Coupling equation:

$\sum_{j=1}^{4} k_{ij}(P_j - P_i) = \dot{V}_i$

or in conventional geomechanics (also in CFD-DEM couplings):

$k\nabla^2 p = -\nabla \cdot \dot{u}_s$



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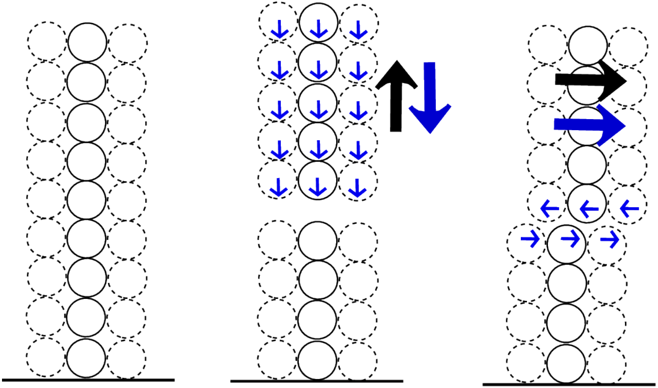
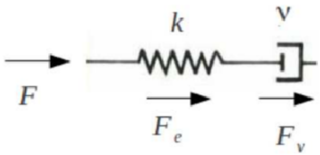


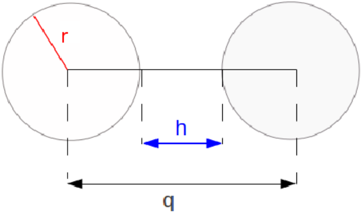
Dense supensions

Stokesian dynamics turns fluid mechanics into pair interactions, convenient in a DEM framework

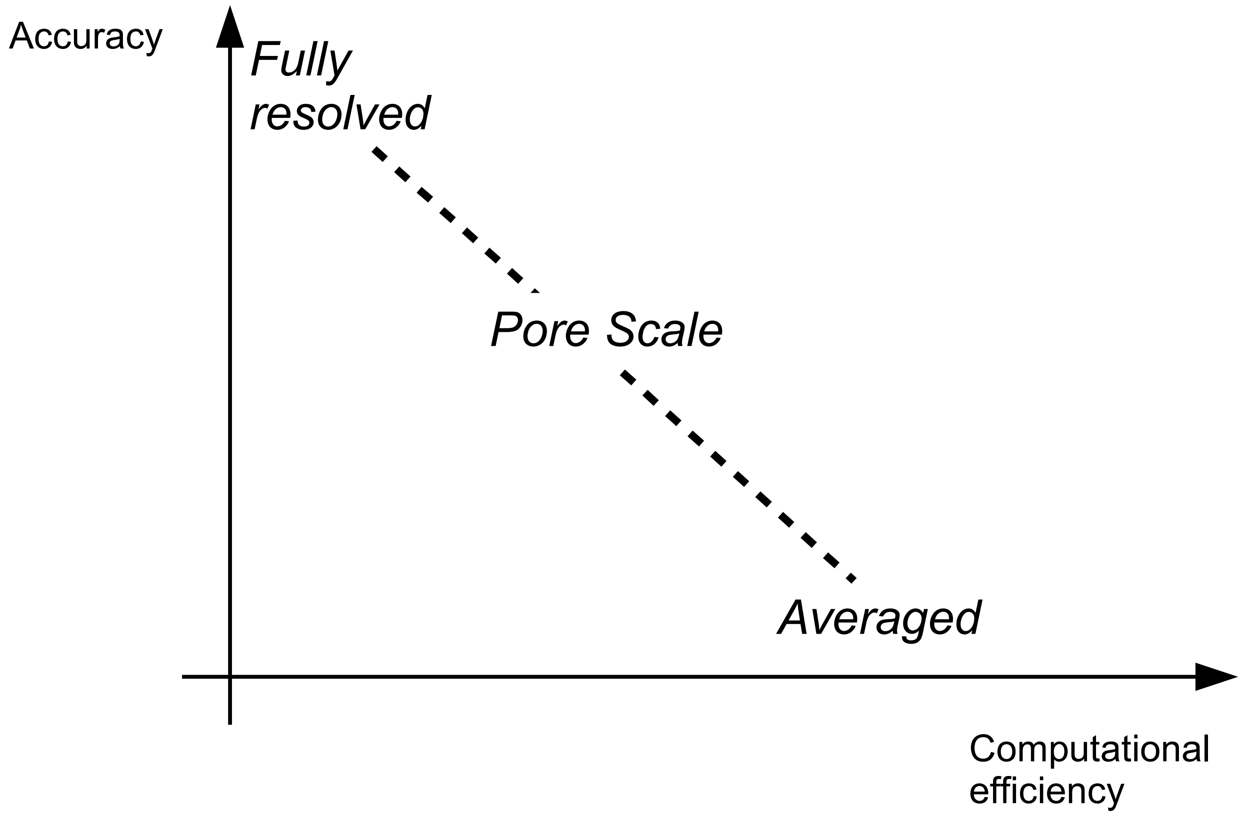
Lubrications forces have been introduced as a first step.

$$F^{lub}_{shear} = \frac{\pi\mu}{2}(-2r + q ln(\frac{q}{h}))v_t \qquad and \qquad F^{lub}_{normal} = \frac{3}{2}\pi\mu\frac{r^2}{h}v_n$$

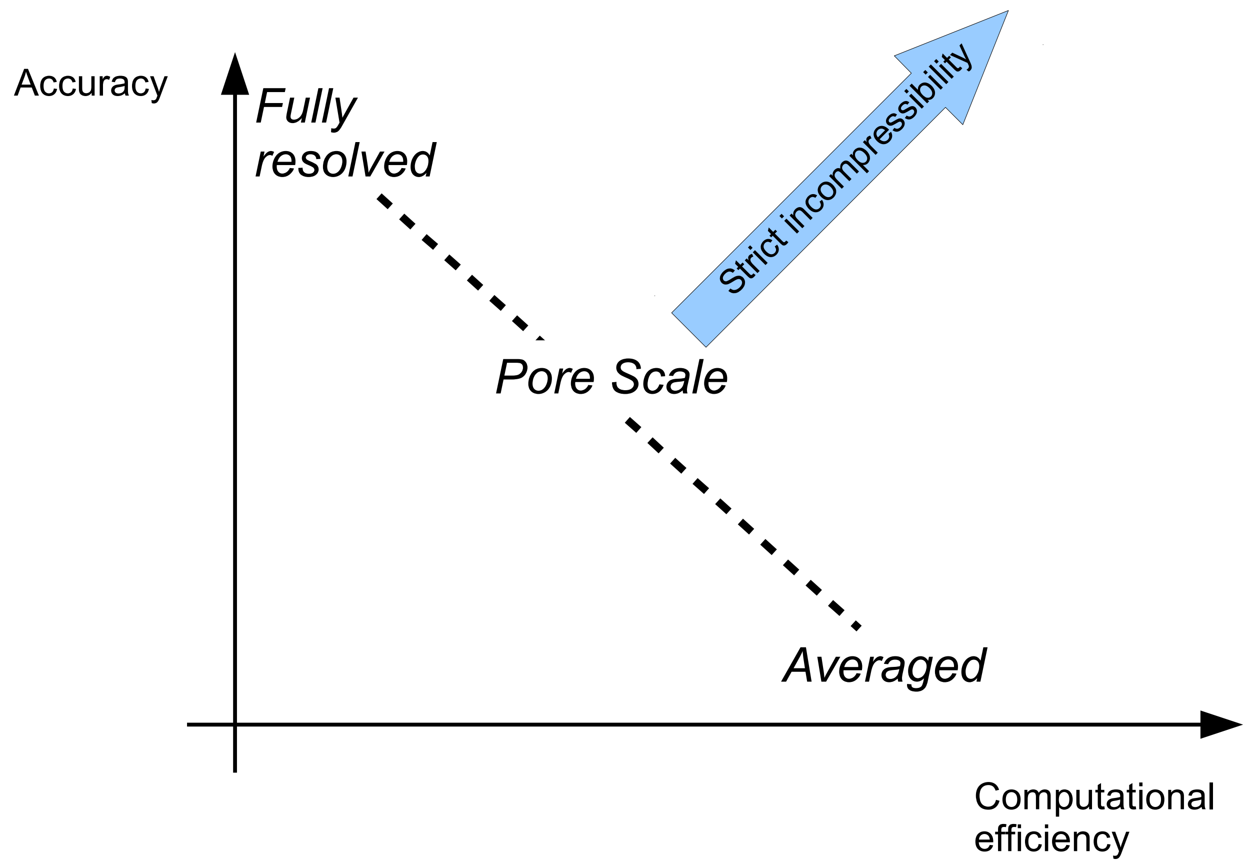




Summary


Accuracy
Fully
resolved
Pore Scale
Averaged
Computational
efficiency

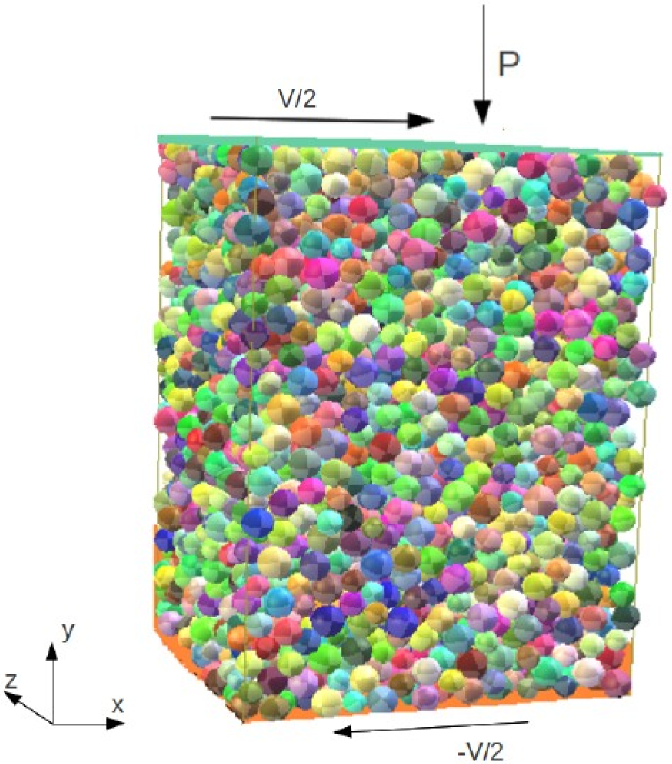
Summary


Accuracy
Fully
resolved
Strict incompressibility
Pore Scale
Averaged
Computational
efficiency

5. Lubrication

Something is missing. Coupling equation:

$\sum_{j=1}^{4} k_{ij}(P_j - P_i) = \dot{V}_i$
or in conventional geomechanics (also in CFD-DEM couplings):
$k\nabla^2 p = -\nabla \cdot \dot{u}_s$



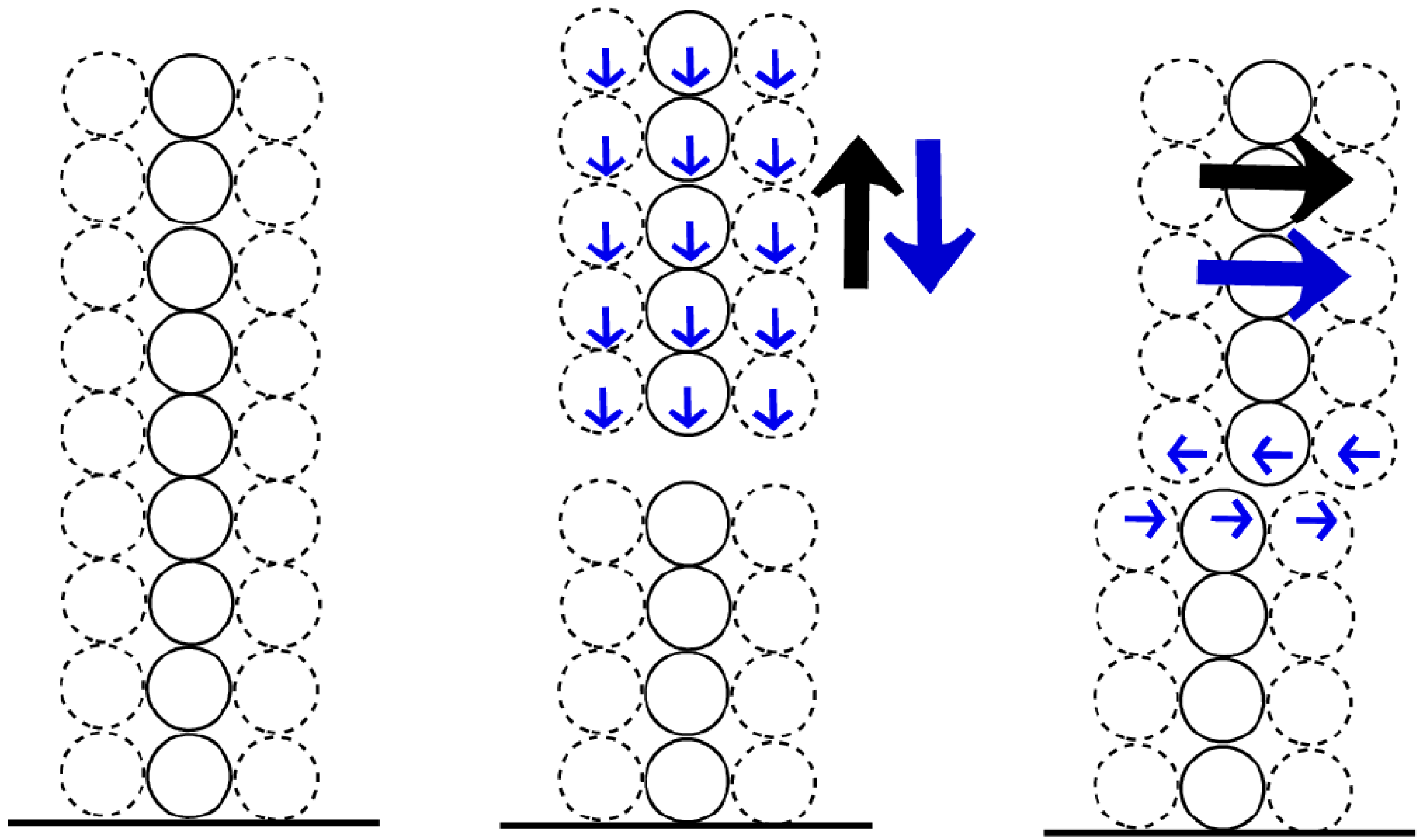
5. Lubrication

Coupling equation:

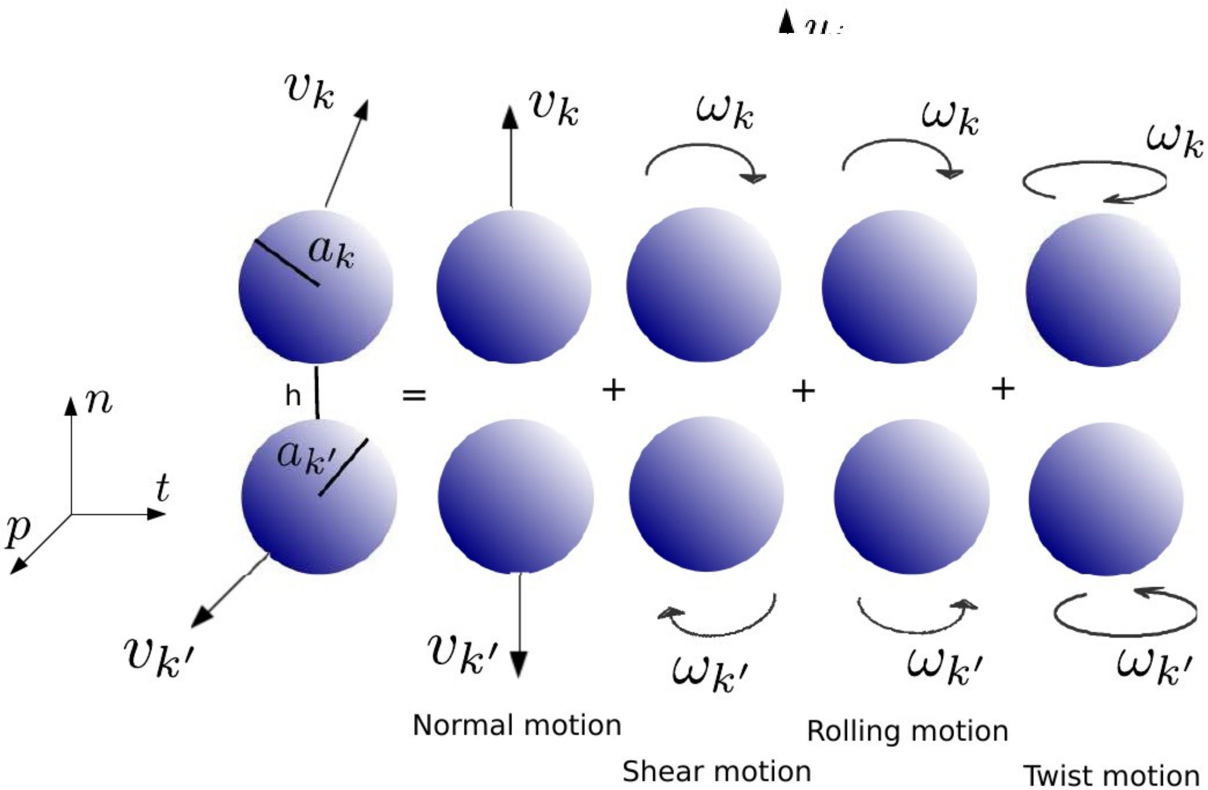
$\sum_{j=1}^{4} k_{ij}(P_j - P_i) = \dot{V}_i$

or in continuum mechanics (also in CFD-DEM couplings):

$k\nabla^2 p = -\nabla \cdot \dot{u}_s$

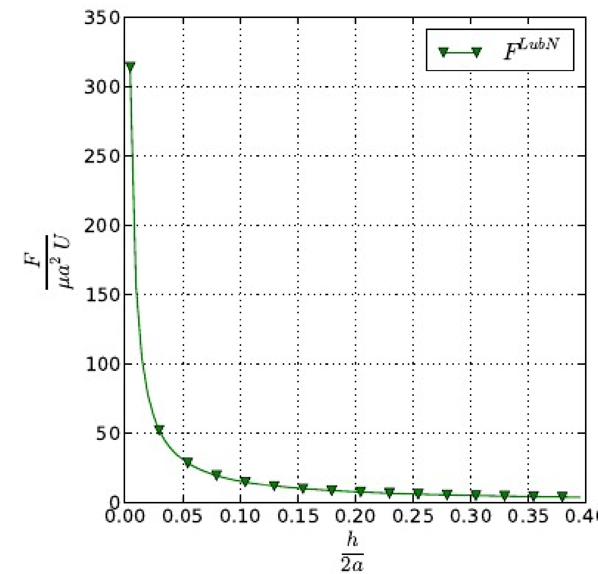


5. Lubrication



$$F_n^L = \frac{3}{2}\,\pi\,\mu\,\frac{r^2}{h}\,\dot{h}$$

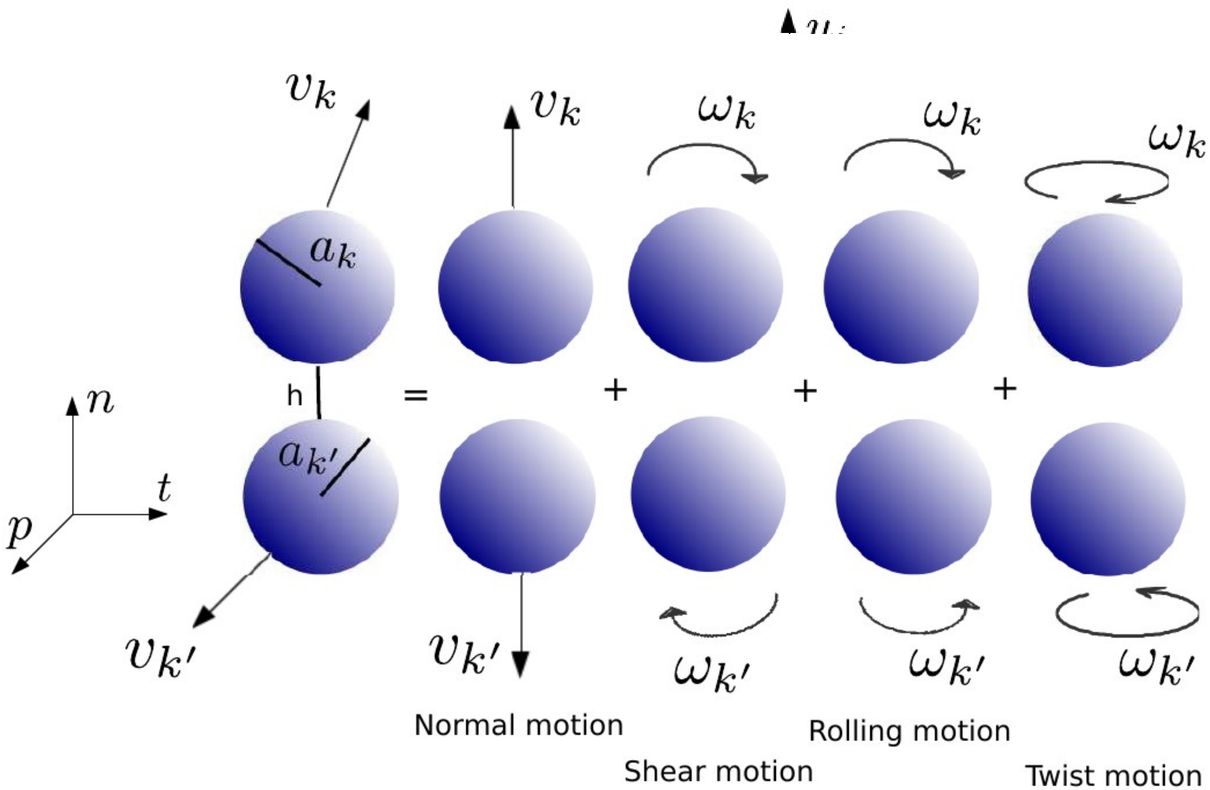
(*no additional parameter*)



See Marzougui et al. *Granular Matter* (2015).

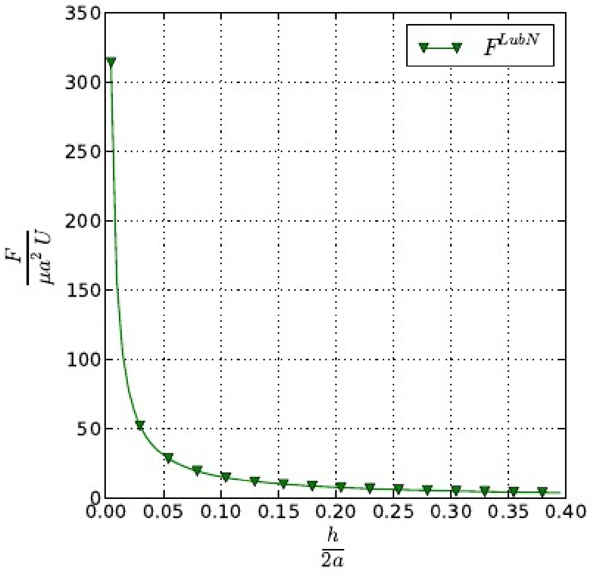
5. Lubrication

Never "fully" resolved



$$F_n^L = \frac{3}{2}\,\pi\,\mu\,\frac{r^2}{h}\,\dot{h}$$

(*no additional parameter*)

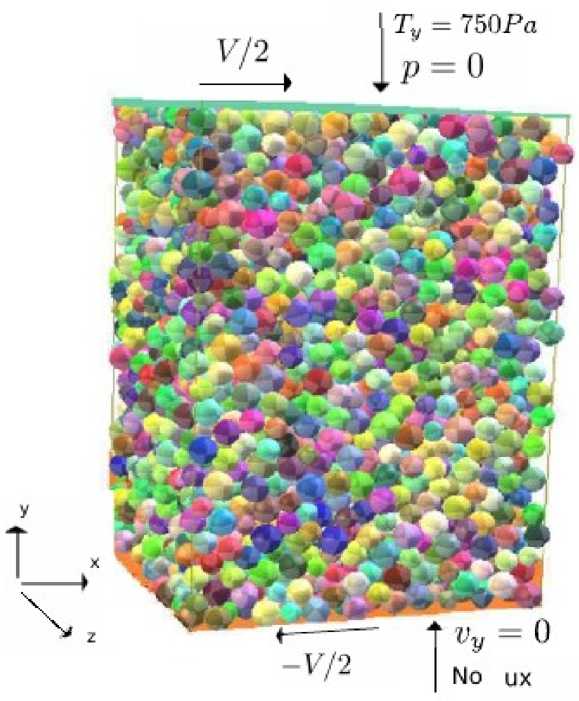


See Marzougui et al. *Granular Matter* (2015).

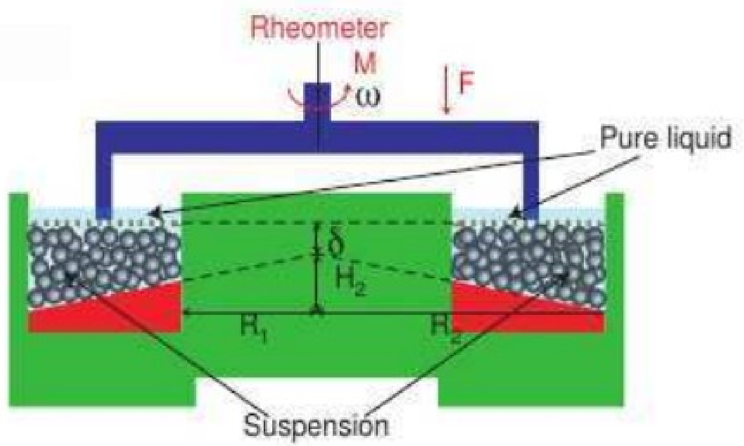
5. Lubrication

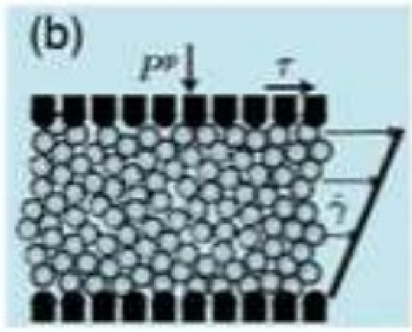
Numerical configuration

shearFlow



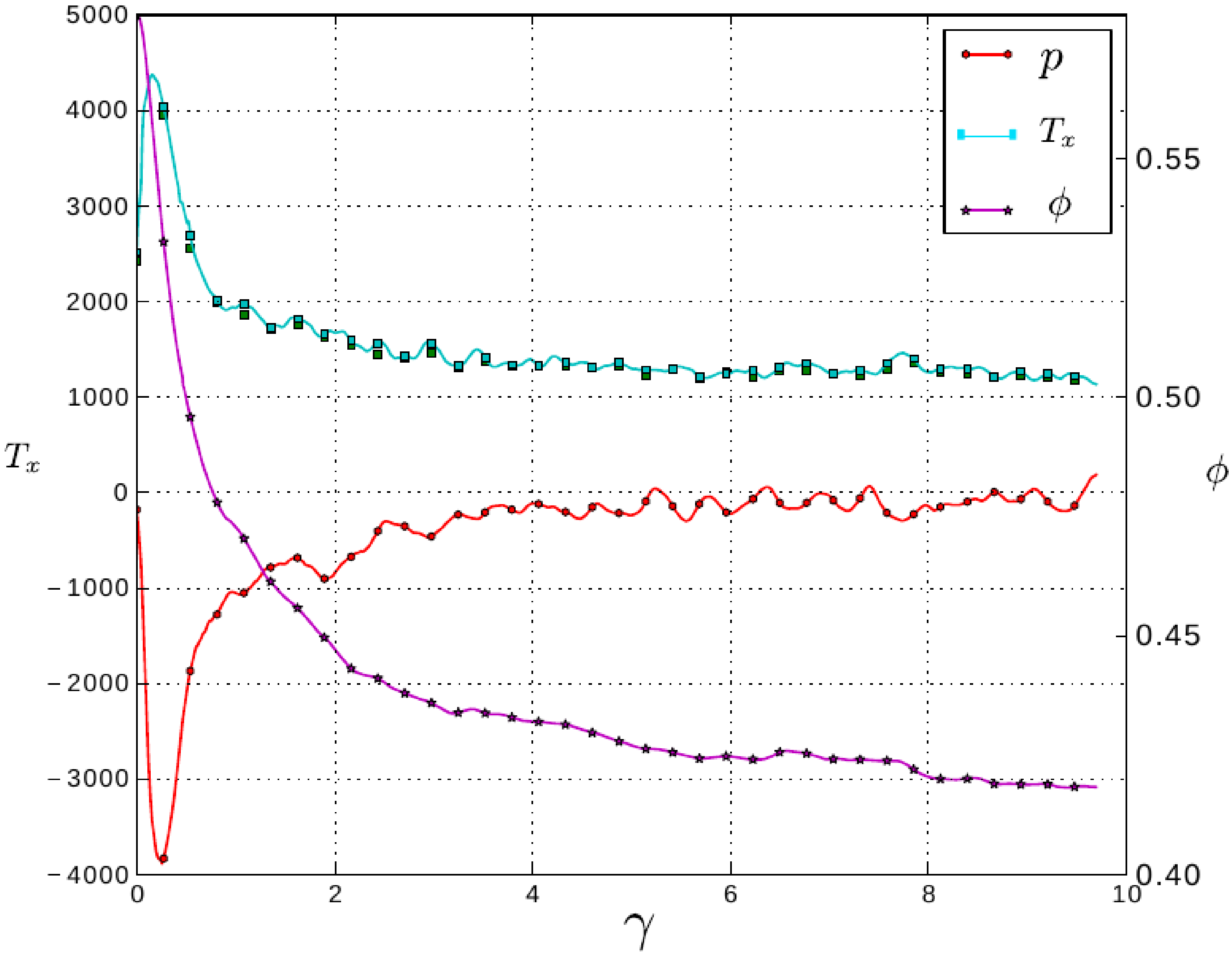
Experimental configuration of Boyer et al





Boyer et al, Physical Review Letters (2011)

5. Lubrication

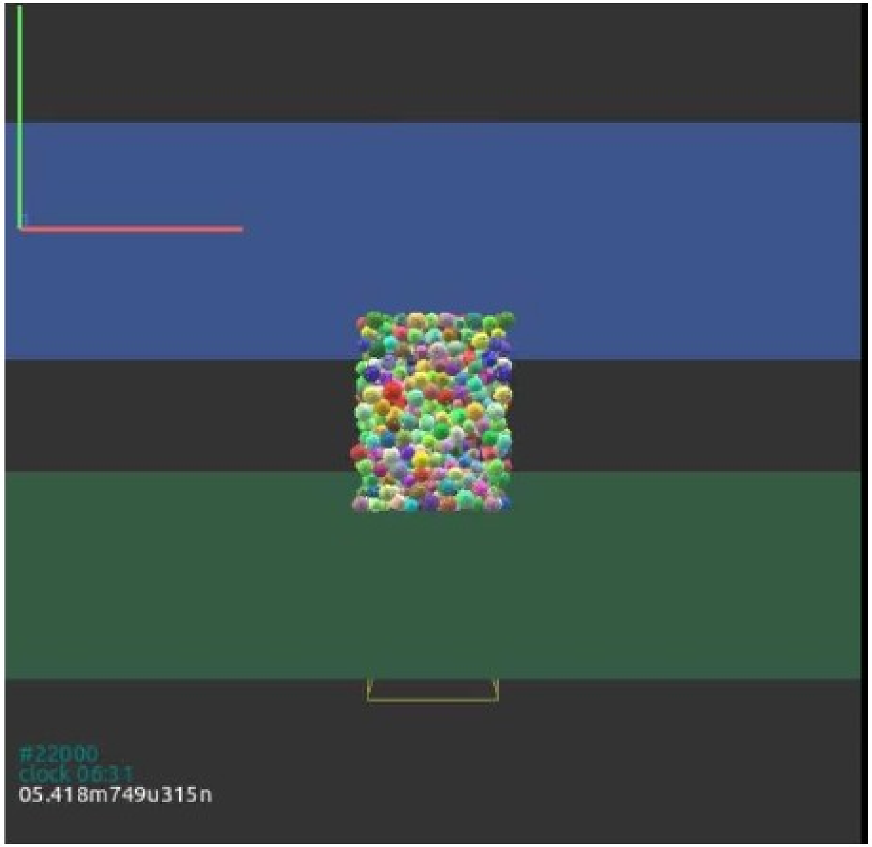


$$I_v = 0.223$$

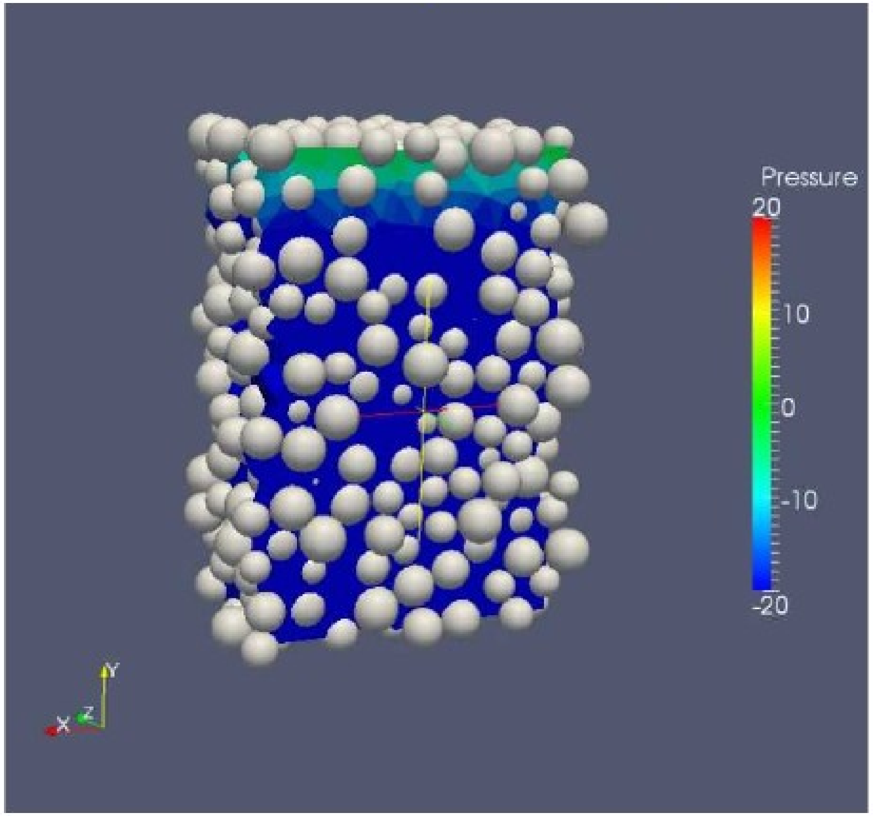
$$T_x = \frac{F_x}{S}$$

5. Lubrication

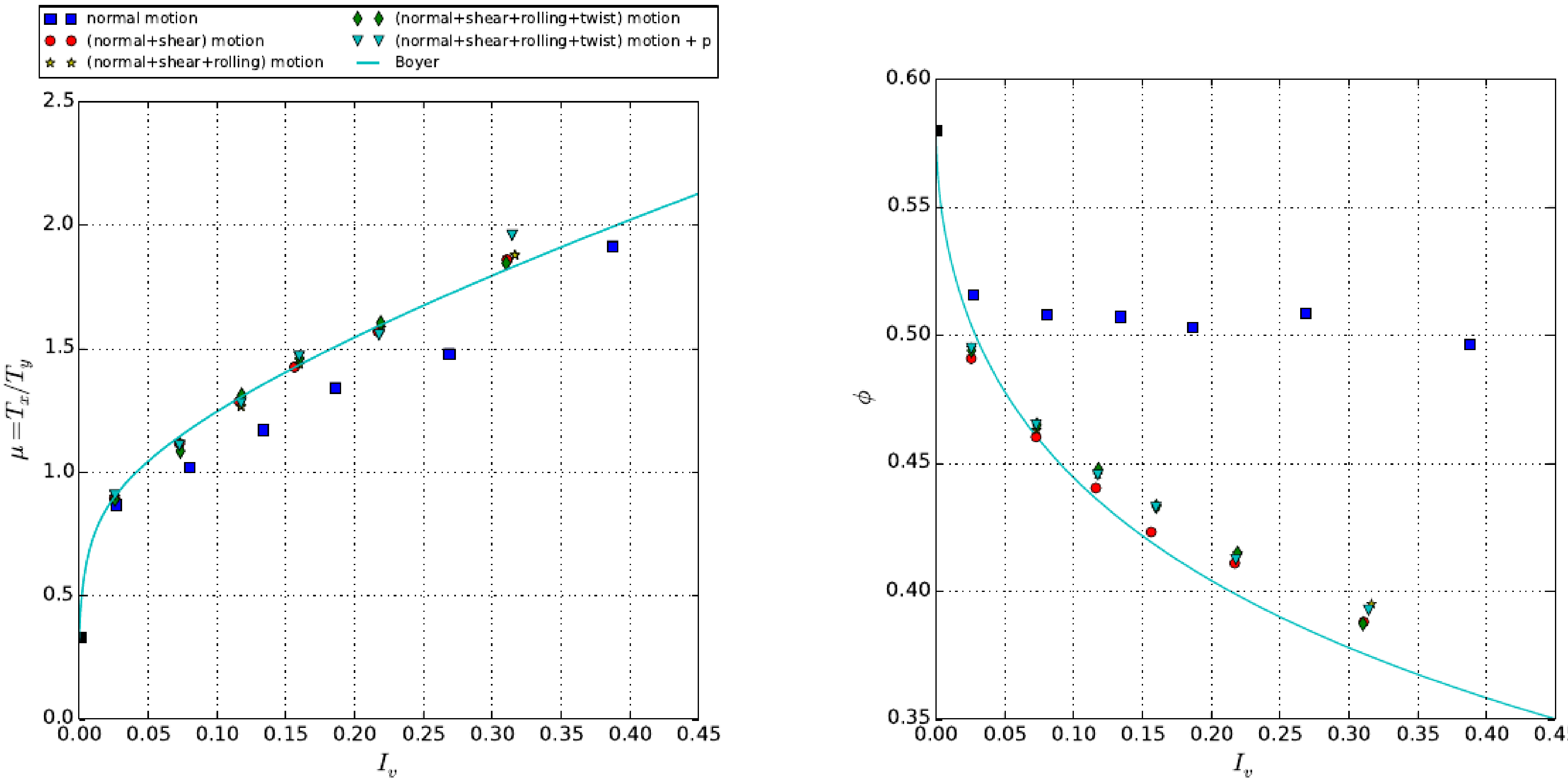
shearFlow



Pressure



5. Lubrication



Conclusion

- A variety of methods for solving the fluid problem, with three different modeling scales: micro-continuum, pore-scale, macro-continuum (and the corresponding assumptions / computational cost).

- Not all methods handle strict incompressibility efficiently, which may be a problem for strong poro-mechanical coupling.

- None of them will capture the lubrication forces, which dominates the rheology of fluid-grain mixtures. They need to be introduced in addition to the resolved drag forces (possibly with some cut-off).