

**From granular media to suspensions.  
Taking contacts and close interactions into account.**

**XX Jacques-Louis Lions Spanish French School  
On Numerical Simulations in Physics and Engineering**

**Barcelona, Spain, 3 - 7 July 2023**

**Aline Lefebvre-Lepot**



# Granular media and suspensions.



Macroscopic, non-brownian grains  
Dry system or Stokes flow

# Rheology.

**Rheology** : ” the branch of physics concerned with the flow and change of shape of matter ”

[Collins English Dictionary]

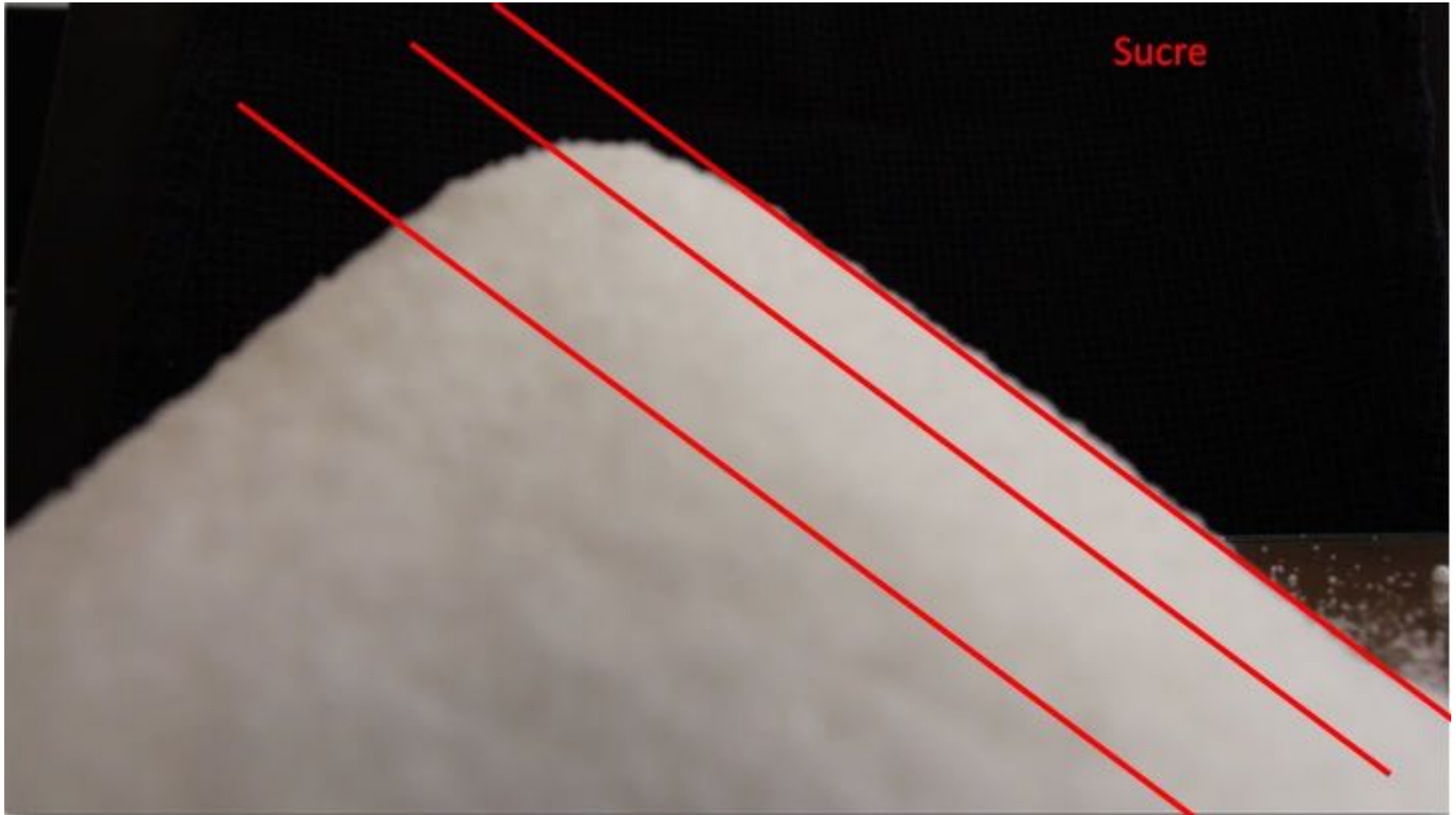
▶ flow, segregation, mixing, blocking, collapse...

***Macroscopic behaviour***

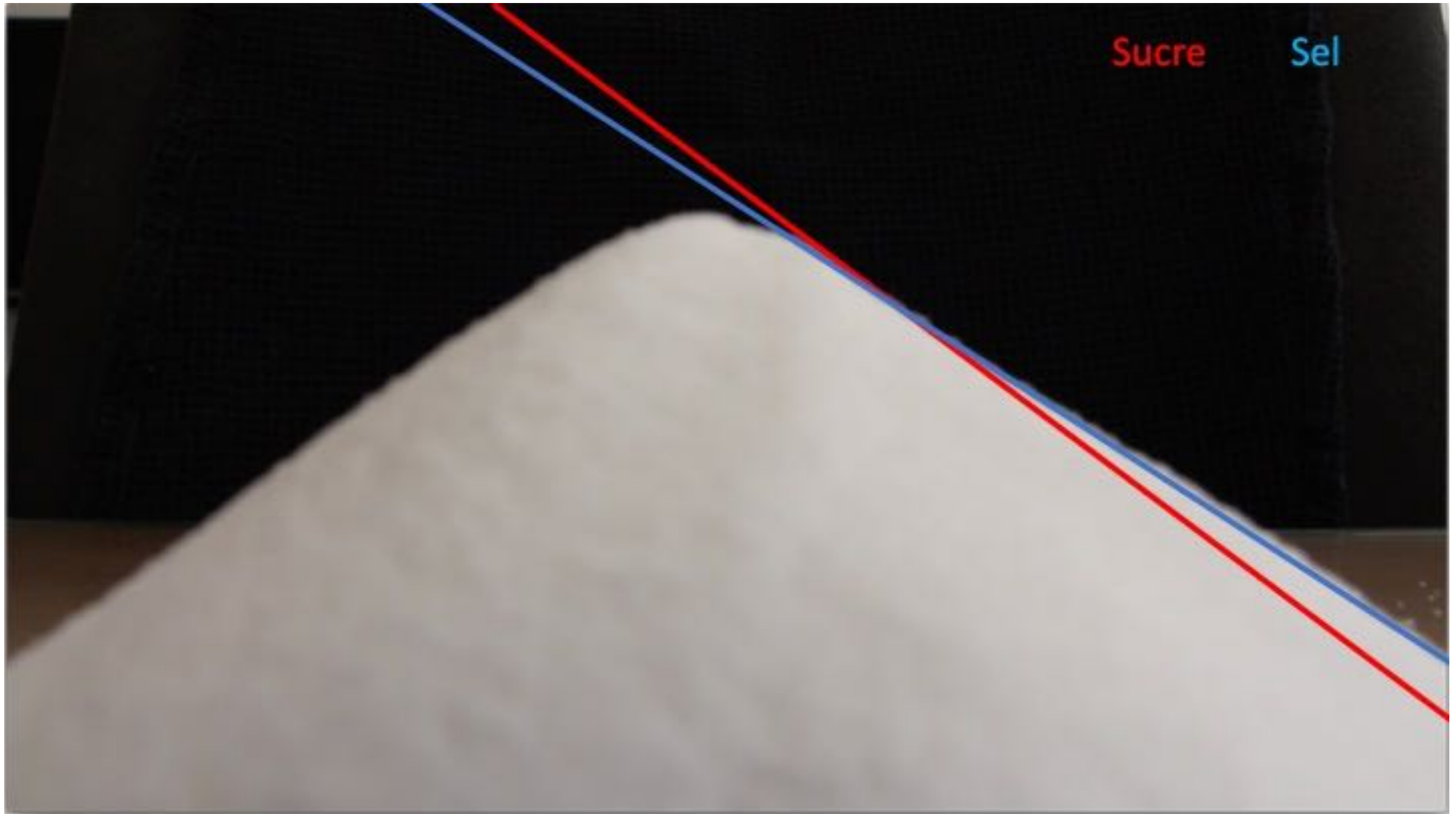
# Learning to swim?



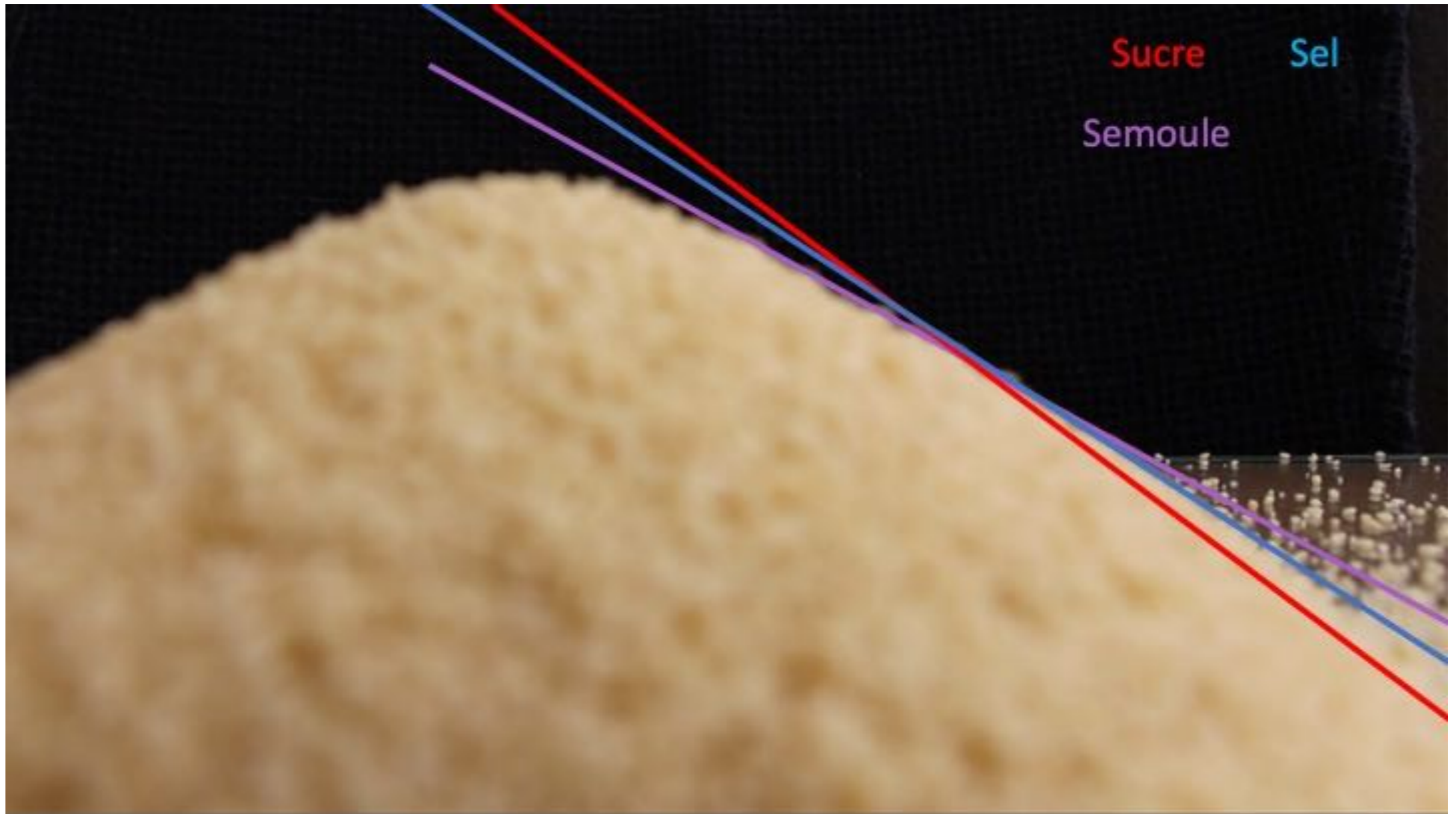
# A complex behavior: kitchen experiment...



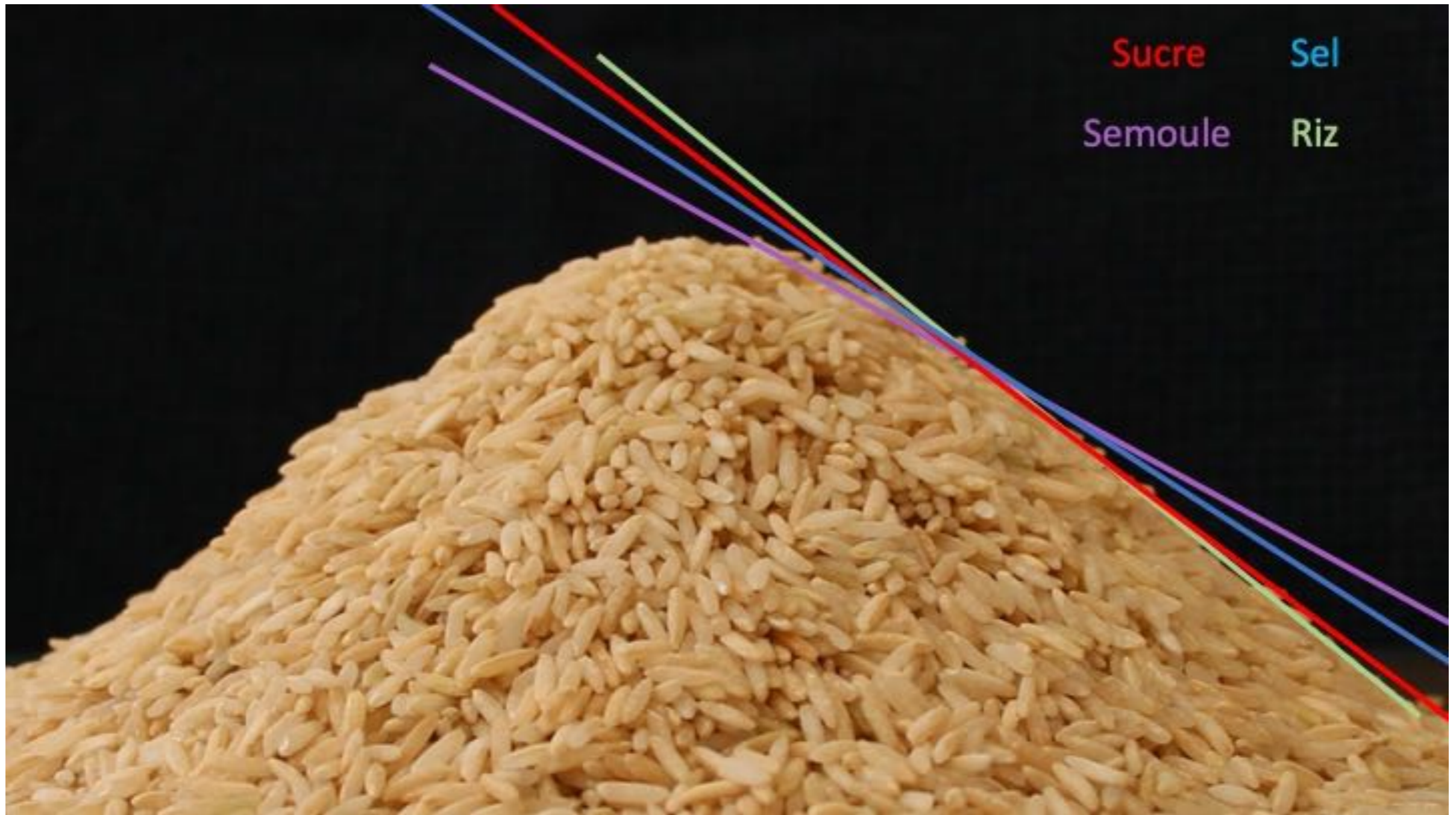
# A complex behavior: kitchen experiment...



# A complex behavior: kitchen experiment...



# A complex behavior: kitchen experiment...





# A complex behavior: solid, liquid or gaz?



Sandcastle / Solid



Hourglass / Liquid

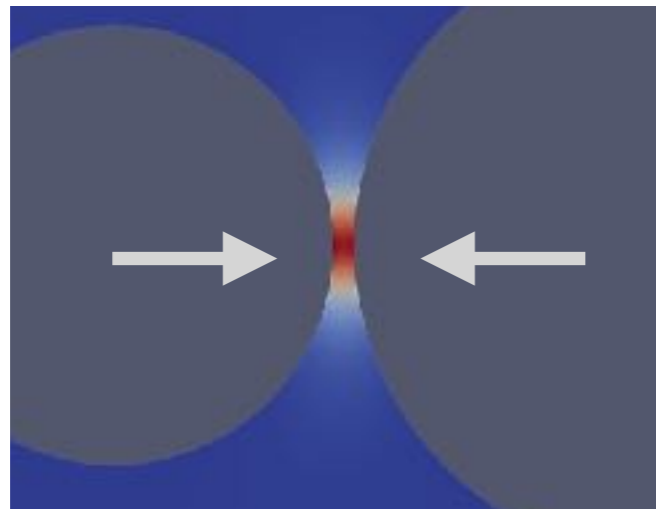


Sandstorm / Gaz

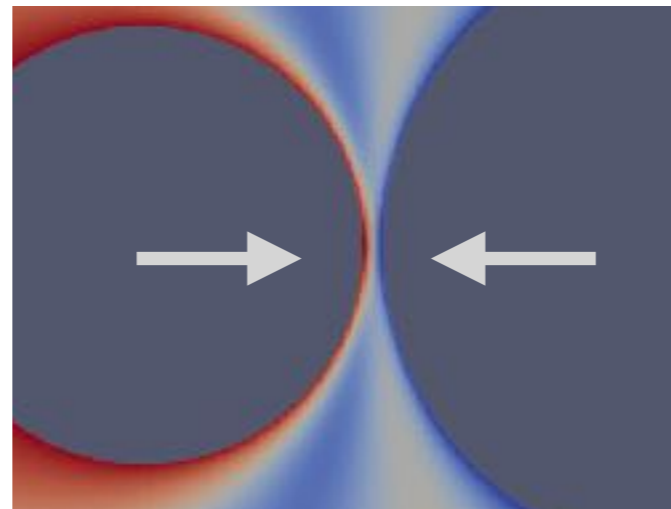


B. Andreotti, Y. Forterre, and O. Pouliquen.  
Granular media: between fluid and solid.  
Cambridge University Press, 2013

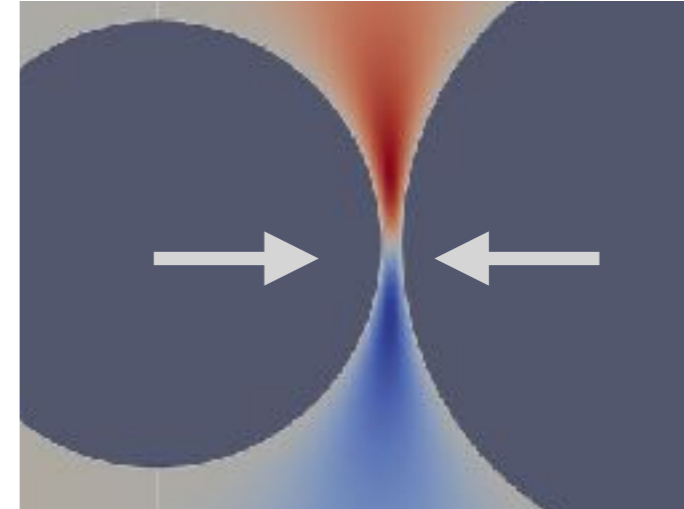
# A complex behavior: lubrication in suspensions



Pression

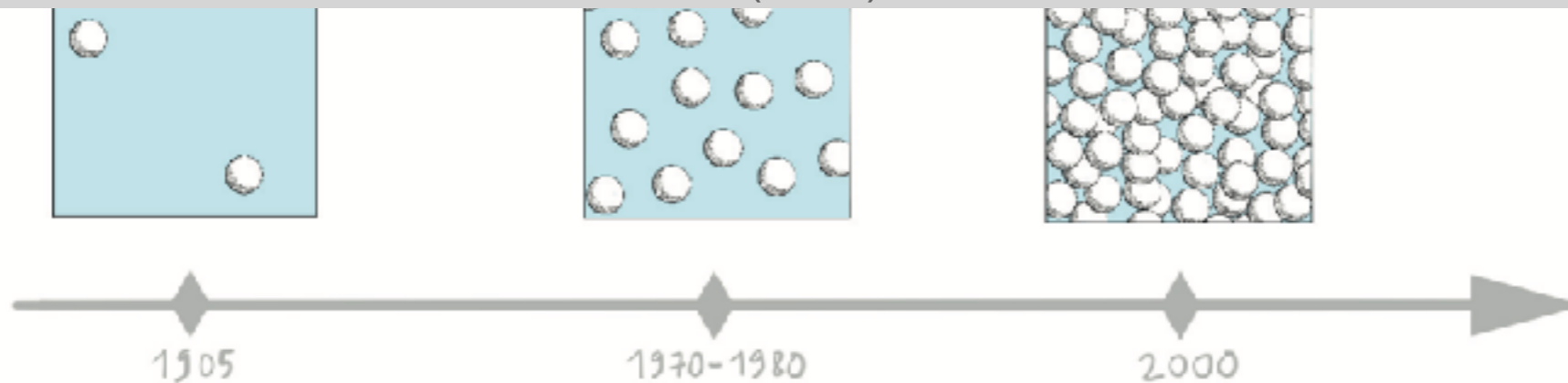


Vitesse horizontale



Vitesse verticale

E. Guazzelli and O. Pouliquen. "Rheology of dense granular suspensions".  
In: Journal of Fluid Mechanics 852 (2018)



# Methodology

## Microscopic phenomena

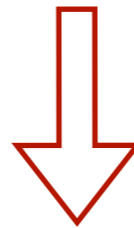
Local  
micro-structure

Non-local  
effects

Multi-particle  
interactions

Contact  
Friction

Shape of  
particles



***Macroscopic behavior***

# Methodology

## Microscopic phenomena

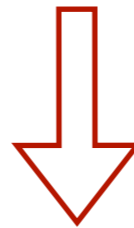
Local  
micro-structure

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effects

Multi-particle  
interactions

Contact  
Friction

Shape of  
particles



***Macroscopic behavior***



***Numerical simulations at the microscopic level***

# Numerical simulations. The difficulties.

▶ Macroscopic behaviour

⇒ Large number of particles

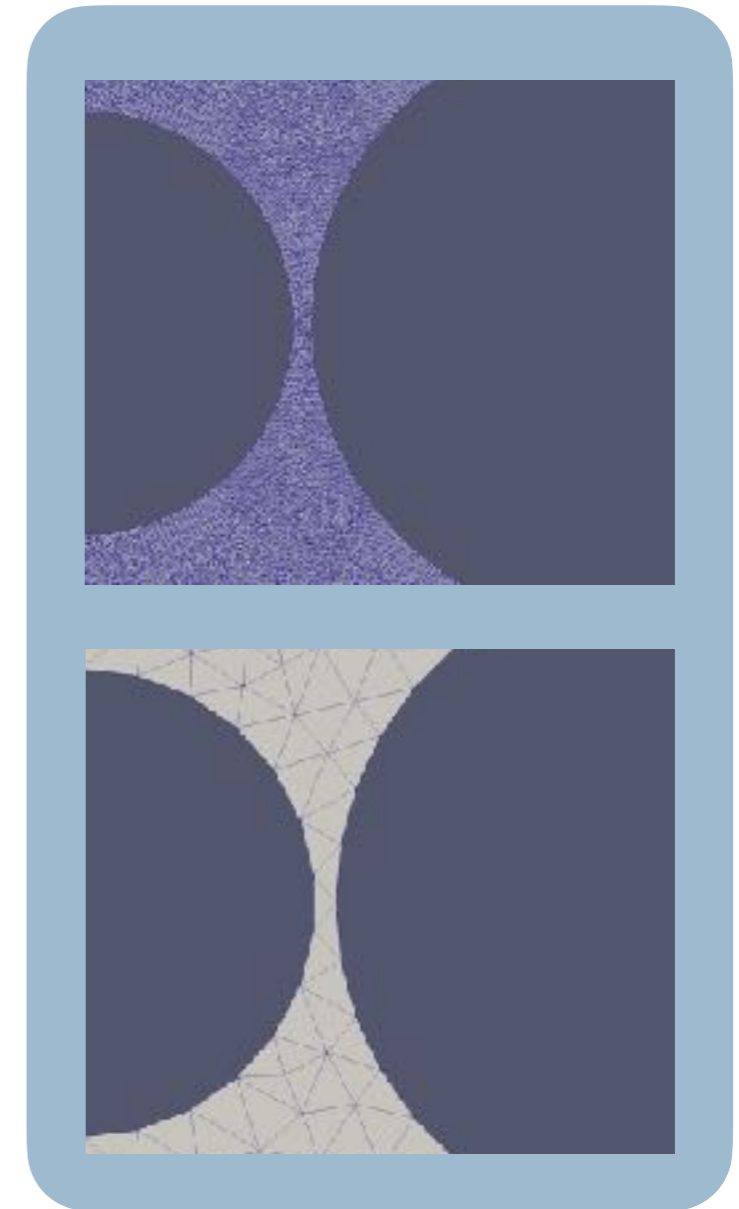
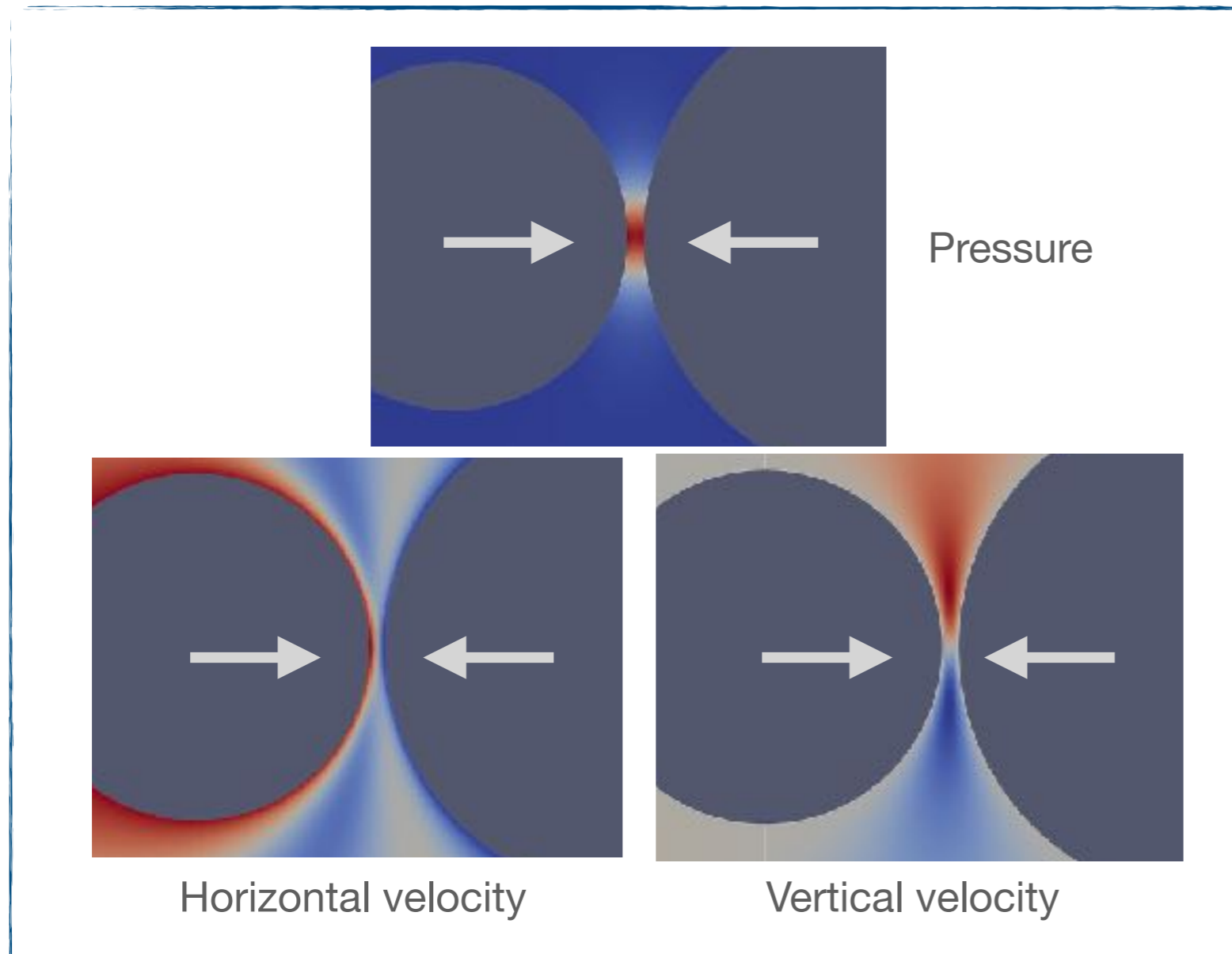
▶ Steady state and time average

⇒ Long time simulations

***Need for fast N-body computations***

# Numerical simulations. The difficulties.

► Dense suspensions  $\Rightarrow$  Close interactions due to the fluid

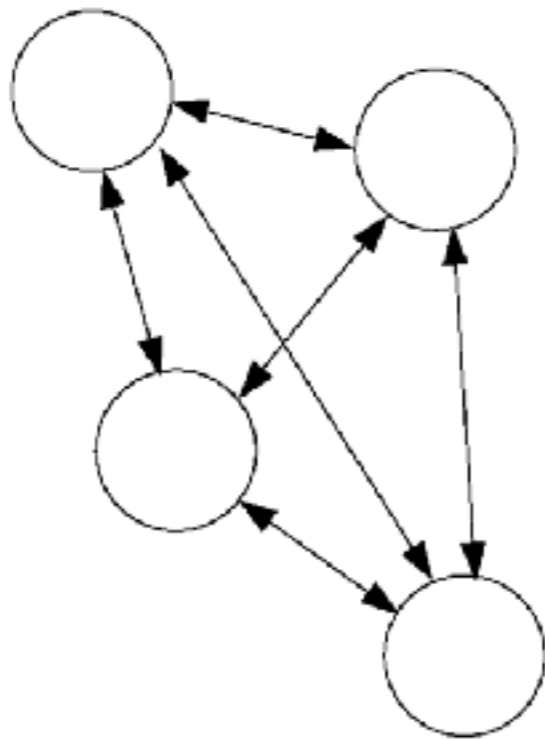


***Need for methods taking lubrication into account***

# Numerical simulations. The difficulties.

- ▶ Dense suspensions
- ▶ Granular media

⇒ Solid contacts between particles



$$m_i \frac{d\dot{\mathbf{x}}_i}{dt} = F_i^{ext} + \sum_{i < j} F_{ij}^{contact}, \quad i = 1 \dots N$$

- ▶ Multi-particle interactions
- ▶ Stiff interactions / non-continuous forces, depending on the model.

***Need for a stable algorithm to deal with contacts***

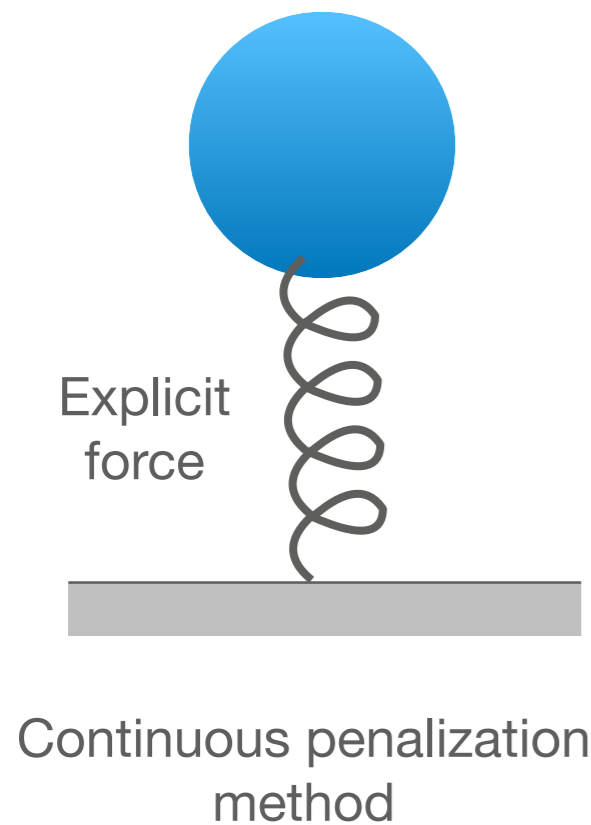
# Numerical simulations. The difficulties.

▶ Dense suspensions

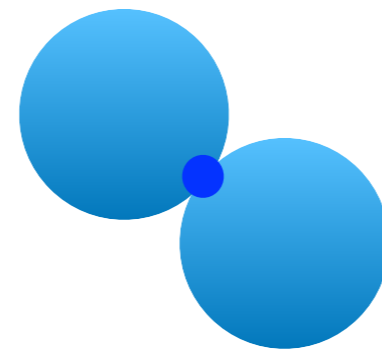
▶ Granular media

⇒ Solid contacts between particles

## Explicit penalty force



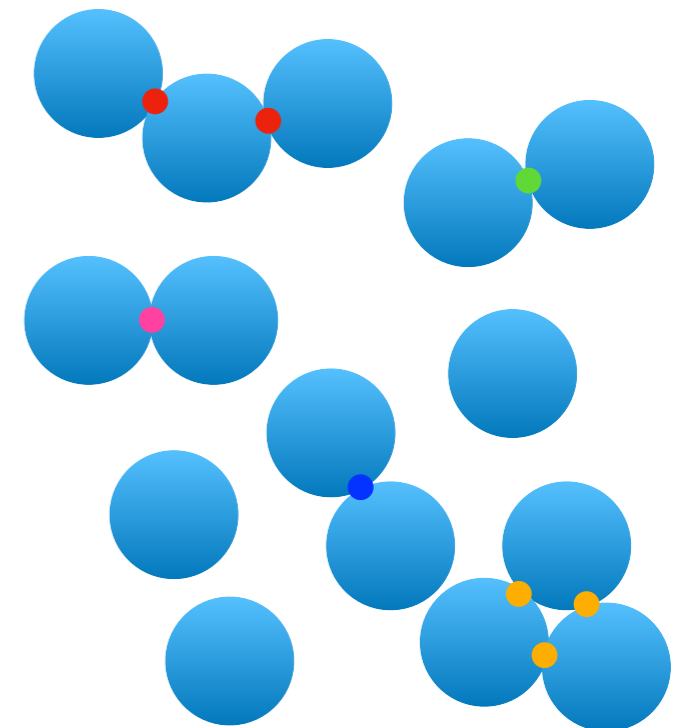
## Contact law



Inelastic contacts  
Coulomb friction law

Explicit solution for 2 particles

## Multi-contact problem



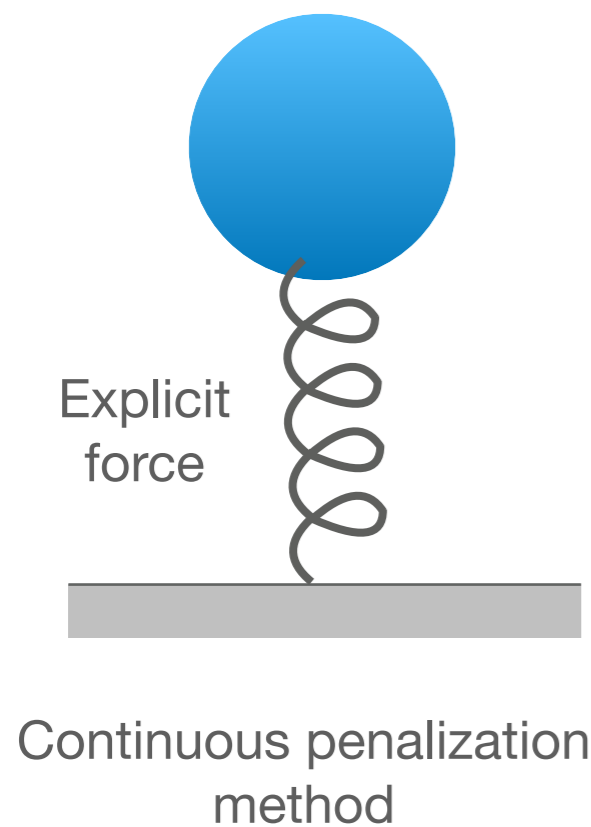


# Numerical simulations. The difficulties.

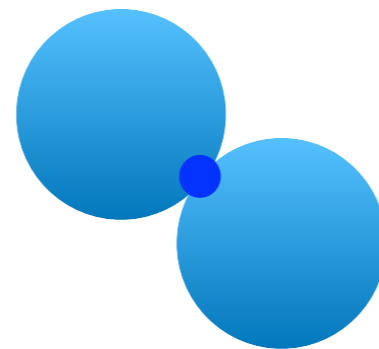
- ▶ Dense suspensions
- ▶ Granular media

⇒ Solid contacts between particles

## Explicit penalty force



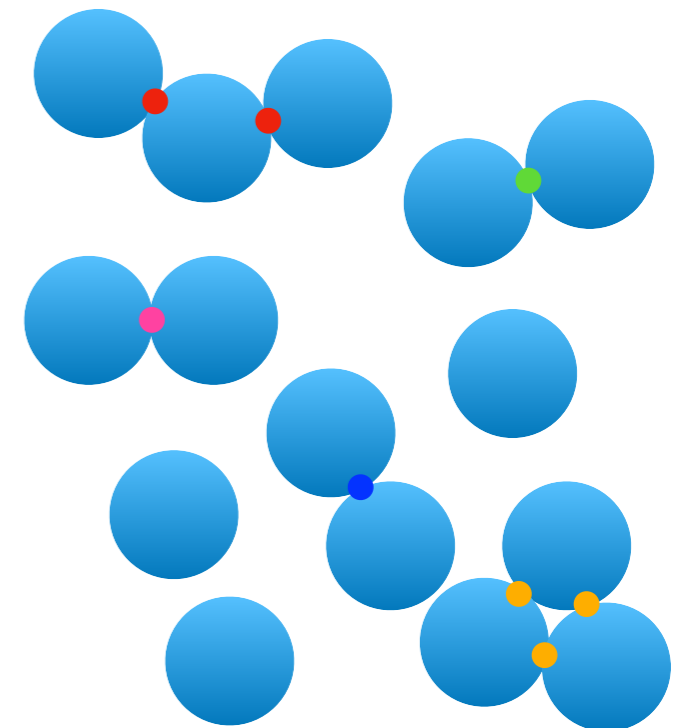
## Contact law



Inelastic contacts  
Coulomb friction law

Explicit solution for 2 particles

## Multi-contact problem



**Molecular Dynamics**

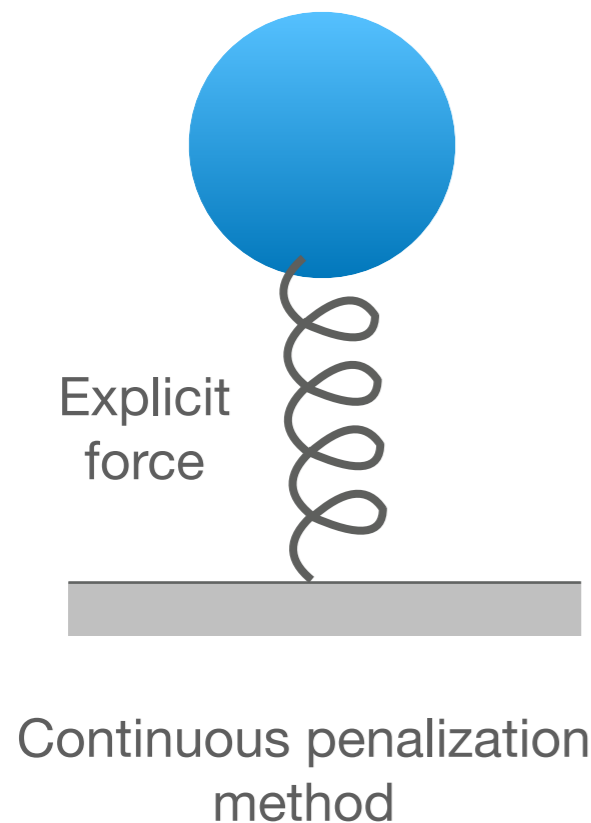
[Cundall, Strack, 1979]

# Numerical simulations. The difficulties.

- ▶ Dense suspensions
- ▶ Granular media

⇒ Solid contacts between particles

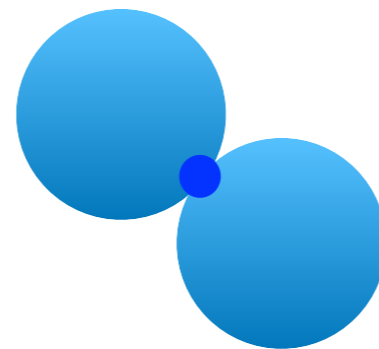
## Explicit penalty force



## Molecular Dynamics

[Cundall, Strack, 1979]

## Contact law



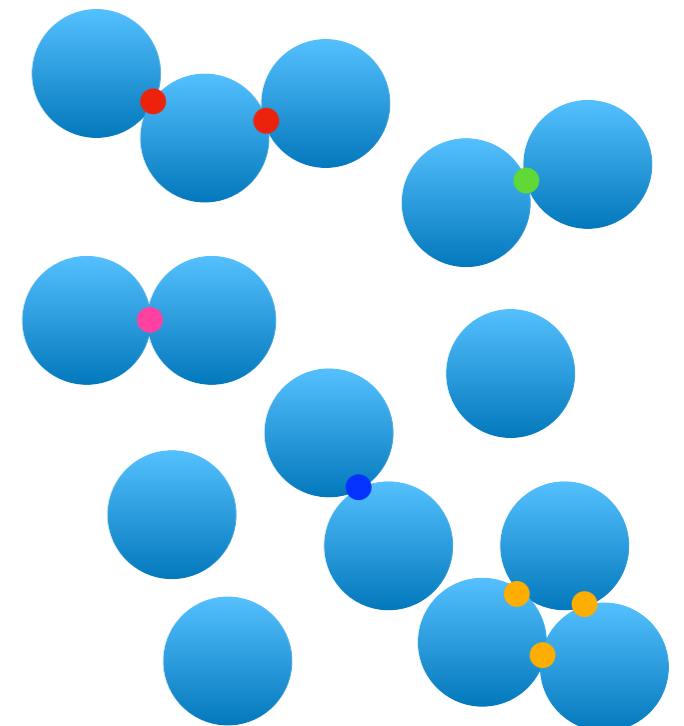
Inelastic contacts  
Coulomb friction law

Explicit solution for 2 particles

## Non-Smooth Contact Dynamics

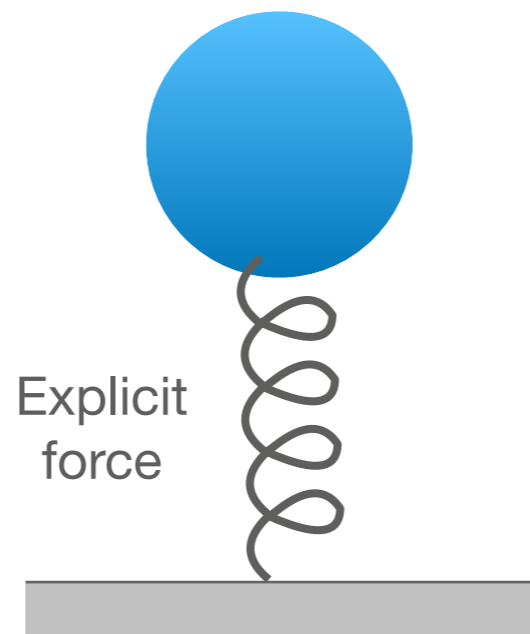
[Moreau, 1988] [Moreau, Jean, 1992]

## Multi-contact problem



# Frictionless Molecular Dynamics Models

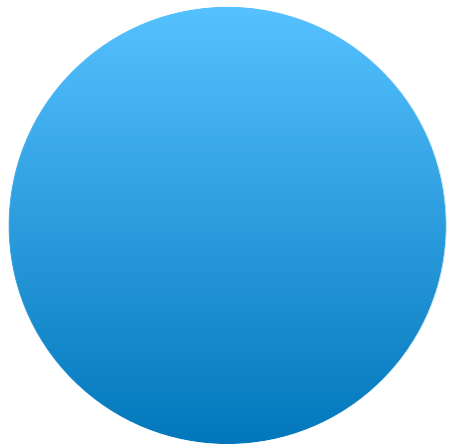
**Explicit penalty force**



Continuous penalization  
method

# An explicit contact force

$$m\ddot{q} = f^e + f^c$$



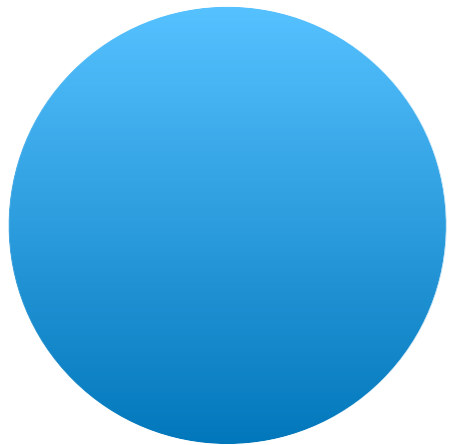
$q$



- ▶ Contact forces explicit
- ▶ Which choice for the contact model?

# An explicit contact force

$$m\ddot{q} = f^e + f^c$$



► Linear spring model

$$f^c(q) = 0 \quad \text{if } q \geq 0$$
$$= -k q \quad \text{if } q \leq 0$$

When  $k \approx$  grain rigidity  $\longrightarrow +\infty$

**Signorini conditions.**

$$q \geq 0, \quad f^c(q) \geq 0$$

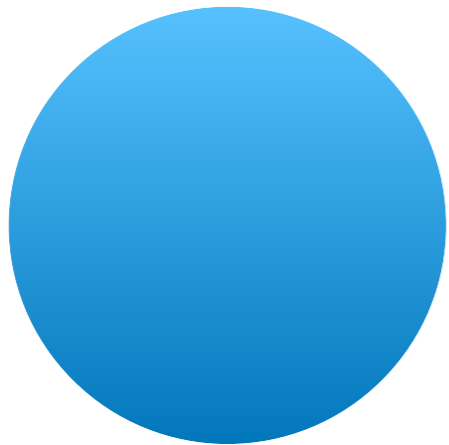
$$q f^c(q) = 0$$



**Negative contact force...  
Missing energy dissipation...**

# An explicit contact force

$$m\ddot{q} = f^e + f^c$$



► **Damped** linear spring model

$$f^c(q) = -k q - \gamma \frac{dq}{dt}$$

**Damped harmonic oscillator:**

$$\frac{d^2 q}{dt^2} = -\omega_0^2 (q - q_0) - 2\mu_0 \frac{dq}{dt}$$

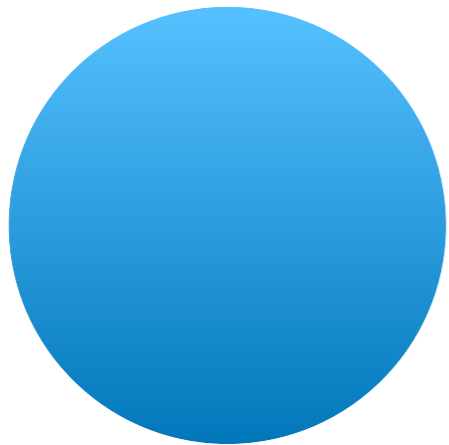
$$\omega_0 = \sqrt{\frac{k}{m}}, \quad \mu_0 = \frac{\gamma}{2m}, \quad q_0 = -\frac{mg}{k}$$



**Negative contact force...**  
**Fine tuning of parameters**

# An explicit contact force

$$m\ddot{q} = f^e + f^c$$



$q$

► Positive force

$$f^c(q) = 0 \quad \text{if } q \geq 0$$
$$= \max(0, \cdot) \quad \text{if } q \leq 0$$

► Many non-linear contact laws  
Ex: Hertz contact law

$$f^c(q) = \frac{E\sqrt{2r}}{3(1-\nu^2)} q^{3/2}$$

► Repulsive force, adhesion force,  
variable parameters ...

► Tangential force

# An explicit contact force

$$m\ddot{q} = f^e + f^c$$

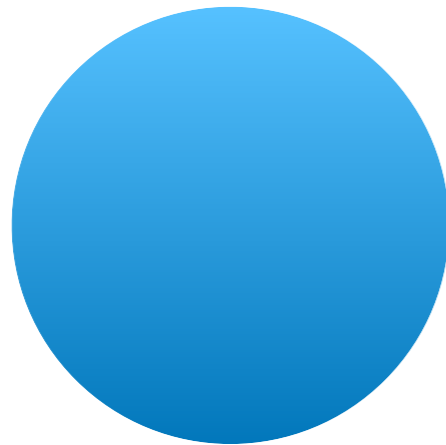


Table 1: Contact models described in Chapter 5

Contact model	Constitutive law	Hysteretic factor/damping coefficient
Hertz [11, 11]	$F_c = k \cdot \delta$	
Hertz [10]	$F_c = k \cdot \delta^{3/2}$	
Kelvin-Voigt [34]	$F_c = k \cdot \delta + D \cdot \dot{\delta}$	
Group 1: Models based on experimental data		
Ratno [82], Liu-Herrmann [83]	$F_c = k \cdot \delta^{3/2} + \gamma \cdot \delta^{3/2} \cdot \dot{\delta}$	Empirical
Nikolic et al. [193]	$F_c = k \cdot \delta^{3/2} + \gamma \cdot \dot{\delta}$	Empirical
Fukaya et al. [153]	$F_c = k \cdot \delta^{3/2} + \gamma \cdot \delta^{3/2} \cdot \dot{\delta}$	Empirical
Radice-Raposo [150]	$F_c = k \cdot \delta^{3/2} + \gamma \cdot \delta^{3/2} \cdot \dot{\delta}$	Empirical
Almstedt et al. [187]	$F_c = k \cdot \delta^{3/2} + \gamma \cdot \delta^{3/2} \cdot \dot{\delta}$	Empirical
Group 2: Models that propose an exact expression for determining $\gamma$		
Hertz-McWainall [158]	$F_c = k \cdot \delta^{3/2} + \gamma \cdot \delta^{3/2} \cdot \dot{\delta}$	$\gamma = \frac{10 \cdot \gamma_0}{100 - \gamma_0} \cdot \frac{F_c}{k \cdot \delta}$
Gupta et al. [167, 161]	$F_c = k \cdot \delta + \gamma \cdot \dot{\delta}$	$D = \frac{k \cdot \delta}{100 - \gamma_0}$ $\gamma_0 = \sqrt{\frac{2k \cdot \delta}{\rho \cdot v}}$ $\gamma = \gamma_0 \cdot \frac{1}{1 + \frac{100 - \gamma_0}{\gamma_0} \cdot \frac{F_c}{k \cdot \delta}}$
Guo et al. [90], Zhang-Liu [159]	$F_c = k \cdot \delta^{3/2} + \gamma \cdot \delta^{3/2} \cdot \dot{\delta}$	$\gamma = \frac{10 \cdot \gamma_0}{100 - \gamma_0} \cdot \frac{F_c}{k \cdot \delta}$
Fan-Guo [160]	$F_c = \left( \delta^{3/2} + 1 \right) \cdot \gamma \cdot \delta^{3/2} \cdot \dot{\delta}$	$\gamma = \frac{10 \cdot \gamma_0}{100 - \gamma_0} \cdot \frac{F_c}{k \cdot \delta}$
Kawachi et al. [69]	$F_c = k \cdot \delta^{3/2} + \gamma \cdot \delta^{3/2} \cdot \dot{\delta}$	$(1 - \epsilon) = \frac{\gamma}{100} \cdot k \cdot \frac{\delta^{3/2}}{F_c}$
Tan et al. [168]	$F_c = k \cdot \delta^{3/2} + \gamma \cdot \delta^{3/2} \cdot \dot{\delta}$	$\epsilon = \frac{\gamma}{100} \cdot \frac{F_c}{k \cdot \delta}$
$\epsilon = \begin{cases} 1 & 0 \leq \epsilon \leq 0.25 \\ 1.1968 \cdot \epsilon^2 - 2.5288 \cdot \epsilon + 0.9721 \cdot \epsilon_0 + 0.9100 & 0.25 < \epsilon < 0.28, 0.3 \\ 1.1968 \cdot \epsilon^2 - 2.4897 \cdot \epsilon + 0.9073 \cdot \epsilon_0 + 1.0117 & 0.28 < \epsilon < 0.4, 0.5 \\ 1.1968 \cdot \epsilon^2 - 1.3292 \cdot \epsilon - 0.3236 \cdot \epsilon_0 + 1.1472 & 0.4 < \epsilon < 0.6, 0.8 \\ 1.1968 \cdot \epsilon^2 - 0.9660 \cdot \epsilon - 0.8917 \cdot \epsilon_0 + 1.2848 & 0.6 < \epsilon < 0.8, 1 \end{cases}$		
Group 3: Models that consider a simple assumption to provide an explicit expression of the hysteretic factor		
Han-Cowley [138], Mentele-Gao [140]	$F_c = k \cdot \delta^{3/2} + \gamma \cdot \delta^{3/2} \cdot \dot{\delta}$	$\epsilon = \frac{10 \cdot \gamma_0}{100 - \gamma_0} \cdot \frac{F_c}{k \cdot \delta}$
Lee-Wang [89]	$F_c = k \cdot \delta^{3/2} + \gamma \cdot \delta^{3/2} \cdot \dot{\delta}$	$\epsilon = \frac{10 \cdot \gamma_0}{100 - \gamma_0} \cdot \frac{F_c}{k \cdot \delta}$
Kawachi-Kono [154]	$F_c = k \cdot \delta^{3/2} + \gamma \cdot \delta^{3/2} \cdot \dot{\delta}$	$\epsilon = 2 \cdot \frac{\gamma_0}{100 - \gamma_0}$
$\gamma = \frac{10 \cdot \gamma_0 \cdot \frac{F_c}{k \cdot \delta} + \frac{100 - \gamma_0}{100} \cdot \frac{F_c}{k \cdot \delta}}{1 + \frac{10 \cdot \gamma_0 \cdot \frac{F_c}{k \cdot \delta} + \frac{100 - \gamma_0}{100} \cdot \frac{F_c}{k \cdot \delta}}{100 - \gamma_0}}$		
Ambrósio [172]	$F_c = k \cdot \delta + D \cdot \dot{\delta}$	$D = 2 \cdot \gamma_0 \cdot \sqrt{k \cdot \delta}$ $\gamma_0 = \frac{10 \cdot \gamma_0}{100 - \gamma_0} \cdot \frac{F_c}{k \cdot \delta}$
Lazarus-Silvestri [194]	$F_c = k \cdot \delta^{3/2} + \gamma \cdot \delta^{3/2} \cdot \dot{\delta}$	$\epsilon = \frac{10 \cdot \gamma_0}{100 - \gamma_0} \cdot \frac{F_c}{k \cdot \delta}$
Tan et al. [170]	$F_c = k \cdot \delta^{3/2} + \gamma \cdot \delta^{3/2} \cdot \dot{\delta}$	$D = \gamma_0 \cdot \sqrt{k \cdot \delta} \cdot \frac{F_c}{k \cdot \delta}$
Billmore et al. [134]	$F_c = k \cdot \delta^{3/2} + \gamma \cdot \delta^{3/2} \cdot \dot{\delta}$	$\epsilon = \frac{1}{100} \cdot k \cdot \delta$
$k = \frac{10 \cdot \gamma_0 \cdot \frac{F_c}{k \cdot \delta} + \frac{100 - \gamma_0}{100} \cdot \frac{F_c}{k \cdot \delta}}{1 + \frac{10 \cdot \gamma_0 \cdot \frac{F_c}{k \cdot \delta} + \frac{100 - \gamma_0}{100} \cdot \frac{F_c}{k \cdot \delta}}{100 - \gamma_0}}$		
Zhang et al. [178]	$F_c = k \cdot \delta^{3/2} + \gamma \cdot \delta^{3/2} \cdot \dot{\delta}$	$\epsilon = 2 \cdot \frac{\gamma_0}{100 - \gamma_0} \cdot \frac{F_c}{k \cdot \delta}$
$\delta = \frac{10 \cdot \gamma_0 \cdot \frac{F_c}{k \cdot \delta} + \frac{100 - \gamma_0}{100} \cdot \frac{F_c}{k \cdot \delta}}{1 + \frac{10 \cdot \gamma_0 \cdot \frac{F_c}{k \cdot \delta} + \frac{100 - \gamma_0}{100} \cdot \frac{F_c}{k \cdot \delta}}{100 - \gamma_0}}$		

Table 2: continued

Contact model	Constitutive law	Hysteretic factor/damping coefficient
Bellmann et al. [195]	$F_c = k \cdot \delta^{3/2} + \gamma \cdot \delta^{3/2} \cdot \dot{\delta}$	$\epsilon = \frac{1}{100} \cdot k \cdot \delta$
$k = \frac{10 \cdot \gamma_0 \cdot \frac{F_c}{k \cdot \delta} + \frac{100 - \gamma_0}{100} \cdot \frac{F_c}{k \cdot \delta}}{1 + \frac{10 \cdot \gamma_0 \cdot \frac{F_c}{k \cdot \delta} + \frac{100 - \gamma_0}{100} \cdot \frac{F_c}{k \cdot \delta}}{100 - \gamma_0}}$		
Isaković [187, 191]	$F_c = \begin{cases} k \cdot \delta^{3/2} + \gamma \cdot \delta^{3/2} \cdot \dot{\delta} & \delta > 0 \\ k \cdot \delta^{3/2} & \delta \leq 0 \end{cases}$	$\epsilon = 2 \cdot \frac{\gamma_0}{100} \cdot \sqrt{k \cdot \delta}$ $\gamma_0 = \sqrt{2 \cdot \frac{10 \cdot \gamma_0}{100 - \gamma_0}}$
Özbingölç [163]	$F_c = k \cdot \delta^{3/2} + \gamma \cdot \delta^{3/2} \cdot \dot{\delta}$	$\epsilon = \frac{10 \cdot \gamma_0 \cdot \frac{F_c}{k \cdot \delta} + \frac{100 - \gamma_0}{100} \cdot \frac{F_c}{k \cdot \delta}}{100 - \gamma_0}$
Chao-Ikarić [107]	$F_c = k \cdot \delta^{3/2} + \gamma \cdot \delta^{3/2} \cdot \dot{\delta}$	$\epsilon = \frac{10 \cdot \gamma_0}{100 - \gamma_0} \cdot \frac{F_c}{k \cdot \delta}$
Wang et al. [185]	$F_c = k \cdot \delta^{3/2} + \gamma \cdot \delta^{3/2} \cdot \dot{\delta}$	$\epsilon = \frac{10 \cdot \gamma_0}{100 - \gamma_0} \cdot \frac{F_c}{k \cdot \delta}$ $\gamma_0 = 1 - \frac{1.26 \cdot k \cdot \delta^{3/2}}{F_c}$
$\epsilon^* = \begin{cases} \frac{\epsilon_1}{\epsilon_1 + \epsilon_2} & \epsilon_1 \geq 0.5 \epsilon \\ \frac{\epsilon_2}{\epsilon_1 + \epsilon_2} & \epsilon_1 < 0.5 \epsilon \end{cases}$		
Group 4: Models that consider an expression to relate the hysteretic factor and the hysteretic damping coefficient, obtaining an explicit expression of the coefficient of restitution and the hysteretic damping factor		
Ye et al. [166], Flores et al. [91]	$F_c = k \cdot \delta^{3/2} + \gamma \cdot \delta^{3/2} \cdot \dot{\delta}$	$\epsilon = \frac{10 \cdot \gamma_0}{100 - \gamma_0} \cdot \frac{F_c}{k \cdot \delta}$
Yu-Guo [169]	$F_c = k \cdot \delta^{3/2} + \gamma \cdot \delta^{3/2} \cdot \dot{\delta}$	$\epsilon = \frac{10 \cdot \gamma_0}{100 - \gamma_0} \cdot \frac{F_c}{k \cdot \delta}$
Wang et al. [93]	$F_c = k \cdot \delta^{3/2} + \gamma \cdot \delta^{3/2} \cdot \dot{\delta}$	$\epsilon = \frac{10 \cdot \gamma_0}{100 - \gamma_0} \cdot \frac{F_c}{k \cdot \delta}$
Suhubi-Friedlander [151]	$F_c = k \cdot \delta^{3/2} + \gamma \cdot \delta^{3/2} \cdot \dot{\delta}$	$\epsilon = \frac{10 \cdot \gamma_0}{100 - \gamma_0} \cdot \frac{F_c}{k \cdot \delta}$
Group 5: Models and constitutive laws that are proposed as a function of the hysteretic factor		
Moreau [133]	$F_c = \begin{cases} k \cdot \delta^{3/2} & 0 \leq \delta \leq \delta_c \\ k \cdot \delta^{3/2} + \gamma \cdot \delta^{3/2} \cdot \dot{\delta} & \delta_c < \delta \leq \delta_m \\ k \cdot \delta^{3/2} & \delta > \delta_m \end{cases}$	static recovery
Choi et al. [88]	$F_c = \max[k \cdot \delta^{3/2}, \gamma \cdot \delta^{3/2} \cdot \dot{\delta}]$	$\epsilon = \frac{10 \cdot \gamma_0}{100 - \gamma_0}$
Nigh et al. [196]	$F_c = \begin{cases} k \cdot \delta^{3/2} & \delta \leq \delta_c \\ k \cdot \delta^{3/2} + \gamma \cdot \delta^{3/2} \cdot \dot{\delta} & \delta_c < \delta \leq \delta_m \\ k \cdot \delta^{3/2} & \delta > \delta_m \end{cases}$	static recovery
Lee-Centeno [171]	$F_c = \frac{k \cdot \delta^{3/2}}{1 + \frac{\gamma \cdot \delta^{3/2} \cdot \dot{\delta}}{k \cdot \delta^{3/2}}}$	
Ning et al. [152]	$\epsilon = \max\left\{ \frac{10 \cdot \gamma_0}{100 - \gamma_0}, \frac{10 \cdot \gamma_0}{100 - \gamma_0} \cdot \frac{F_c}{k \cdot \delta} \right\}$	
Liu et al. [80]	$F_c = F_{c,static} + F_{c,dynamic}$	
$F_{c,static} = \frac{10 \cdot \gamma_0 \cdot \frac{F_c}{k \cdot \delta} + \frac{100 - \gamma_0}{100} \cdot \frac{F_c}{k \cdot \delta}}{1 + \frac{10 \cdot \gamma_0 \cdot \frac{F_c}{k \cdot \delta} + \frac{100 - \gamma_0}{100} \cdot \frac{F_c}{k \cdot \delta}}{100 - \gamma_0}}$		
$F_{c,dynamic} = \frac{10 \cdot \gamma_0 \cdot \frac{F_c}{k \cdot \delta} + \frac{100 - \gamma_0}{100} \cdot \frac{F_c}{k \cdot \delta}}{1 + \frac{10 \cdot \gamma_0 \cdot \frac{F_c}{k \cdot \delta} + \frac{100 - \gamma_0}{100} \cdot \frac{F_c}{k \cdot \delta}}{100 - \gamma_0}} \cdot \sqrt{k \cdot \delta^{3/2}} \cdot \cos\left(\frac{F_c}{k \cdot \delta^{3/2}}\right)$		

[E. Corral, R.G. Moreno, M.J.G. Garcia, and C. Castejon. Nonlinear phenomena of contact in multibody systems dynamics: a review. Nonlinear Dynamics, 2021.]



# Further extensions

## ▶ Multi-particle case

- Obvious extension of the model
- Need for neighbour search algorithms
- Need for additional dissipation to dampen long waves

## ▶ Non-spherical particles

- Composed of assemblies of spheres
- Polygons (various contact scenarios)

# Time discretization

- ▶ Stiff second order ODE to solve
- ▶ The forces are not time-derivable
  - No high-order scheme
- ▶ Mainly used numerical schemes:
  - Leap-frog scheme
  - Predictor/corrector schemes

# Summary

▶ Stiff explicit second order ODE model

## Pros

- Easy to implement
- Many contact models available

## Cons

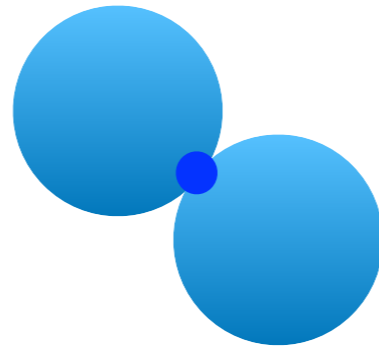
- Fine tuning of parameters
- Small time steps
- Interpreting the results can be difficult

# Bibliography

- P.A. Cundall and O.D.L. Strack. A discrete numerical model for granular assemblies. *Geotechnique*, 29(1):47–65, 1979. Publisher: ICE Publishing.
- S. Luding. Introduction to discrete element methods. *European Journal of Environmental and Civil Engineering*, 12(7-8):785–826, 2008
- E. Corral, R.G. Moreno, M.J.G. Garcia, and C. Castejon. Nonlinear phenomena of contact in multibody systems dynamics: a review. *Nonlinear Dynamics*, 2021.
- F. Radjai, F. Dubois (2011), *Discrete-element modeling of granular materials*, (Wiley-Iste, Berlin), 425 pages, ISBN 978-1-84821-260-2

# Frictionless Contact Dynamics Models

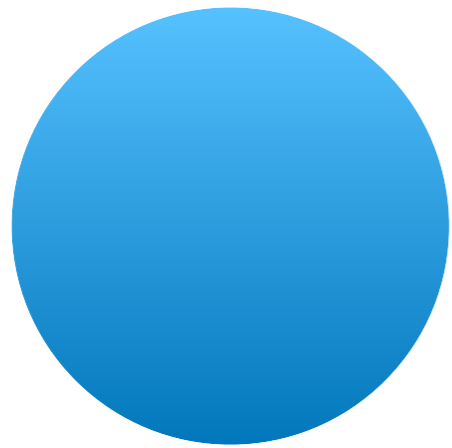
Contact law



Inelastic contacts

# An implicit contact force, a constrained problem

$$m\ddot{q} = f^e + \lambda$$



$q$

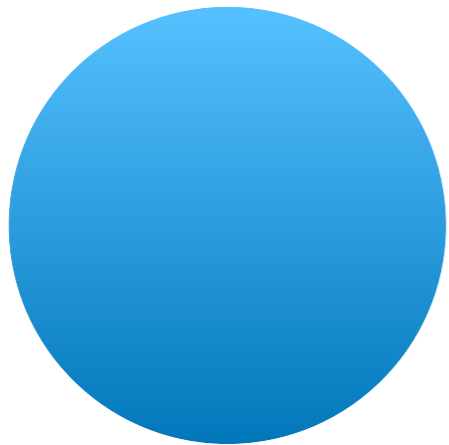


► Contact forces implicit

► How to determine  $\lambda$ ?

# An implicit contact force, a constrained problem

$$m\ddot{q} = f^e + \lambda$$



$q$

$$m\ddot{q} = f^e + \lambda$$

$$\text{supp}(\lambda) \subset \{t / q(t) = 0\}$$

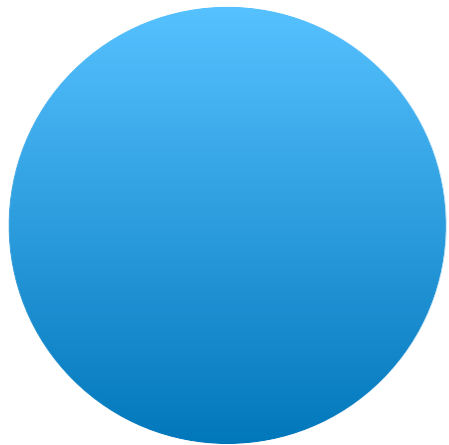
$$q \geq 0, \quad \lambda \geq 0$$

$$\dot{q}^+ = P_{C_q}(\dot{q}^-)$$

$$C_q = \{v \in \mathbb{R} / v \geq 0 \text{ if } q = 0\}$$

# An implicit contact force, a constrained problem

$$m\ddot{q} = f^e + \lambda$$



$q$

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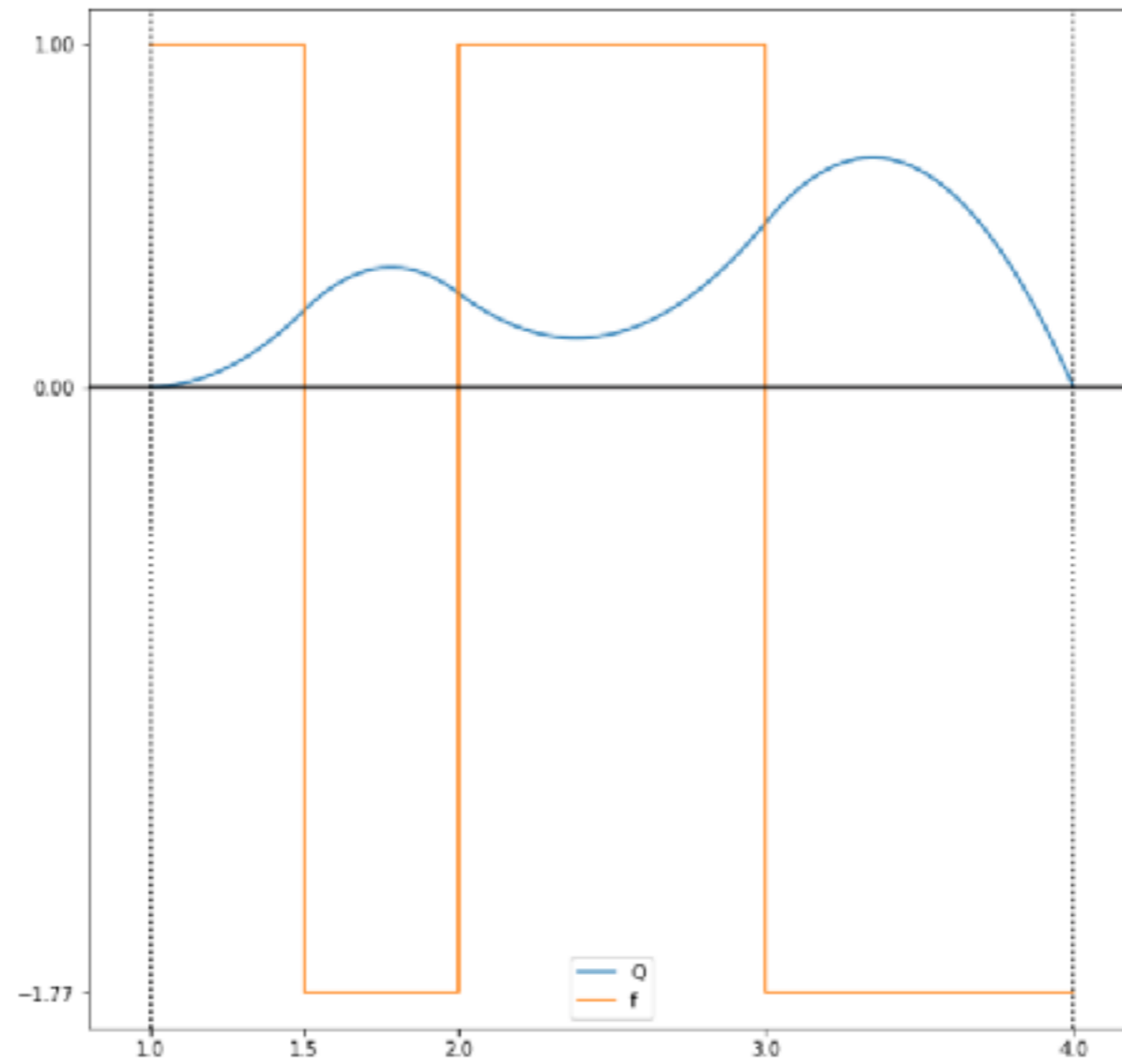
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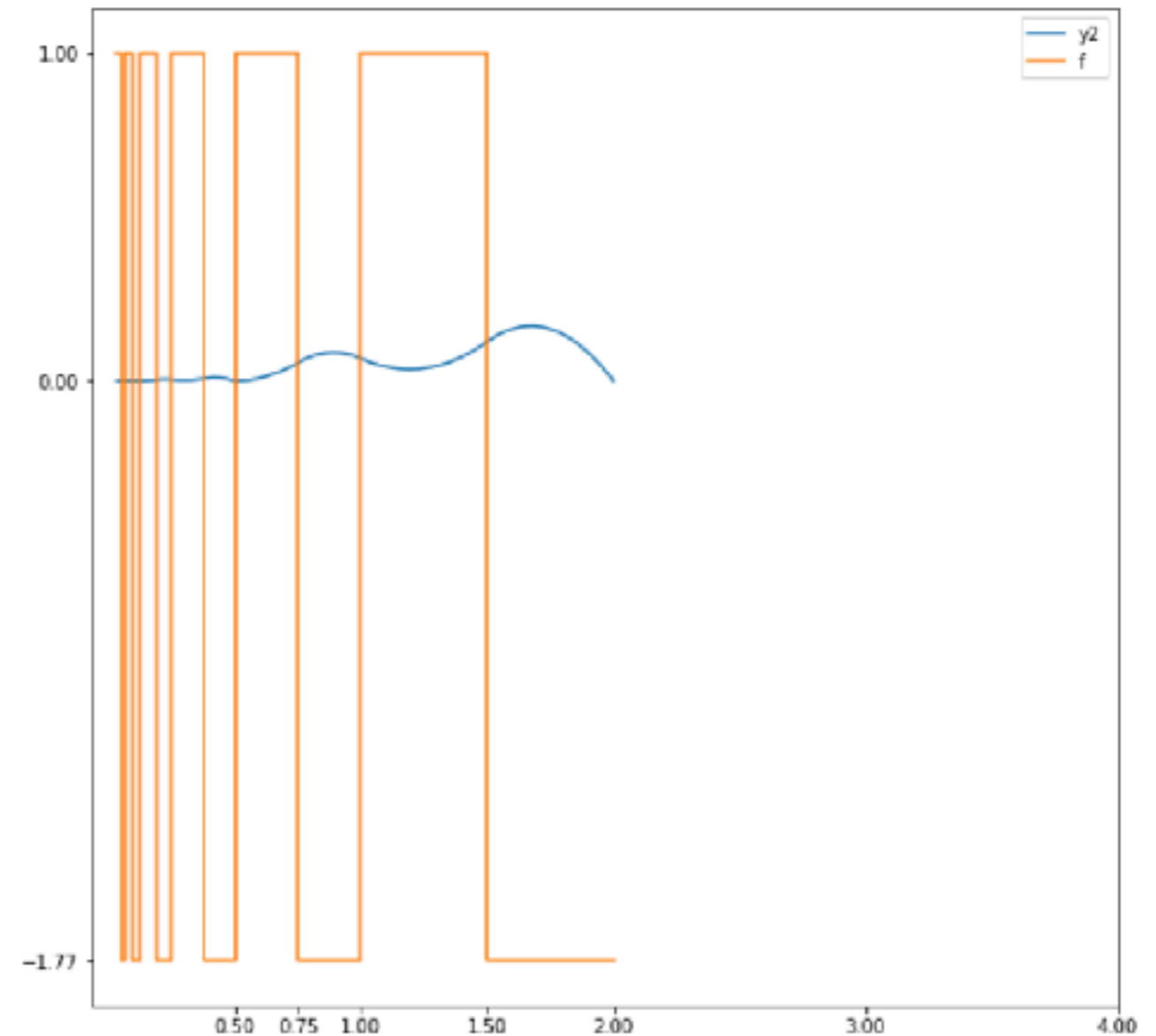
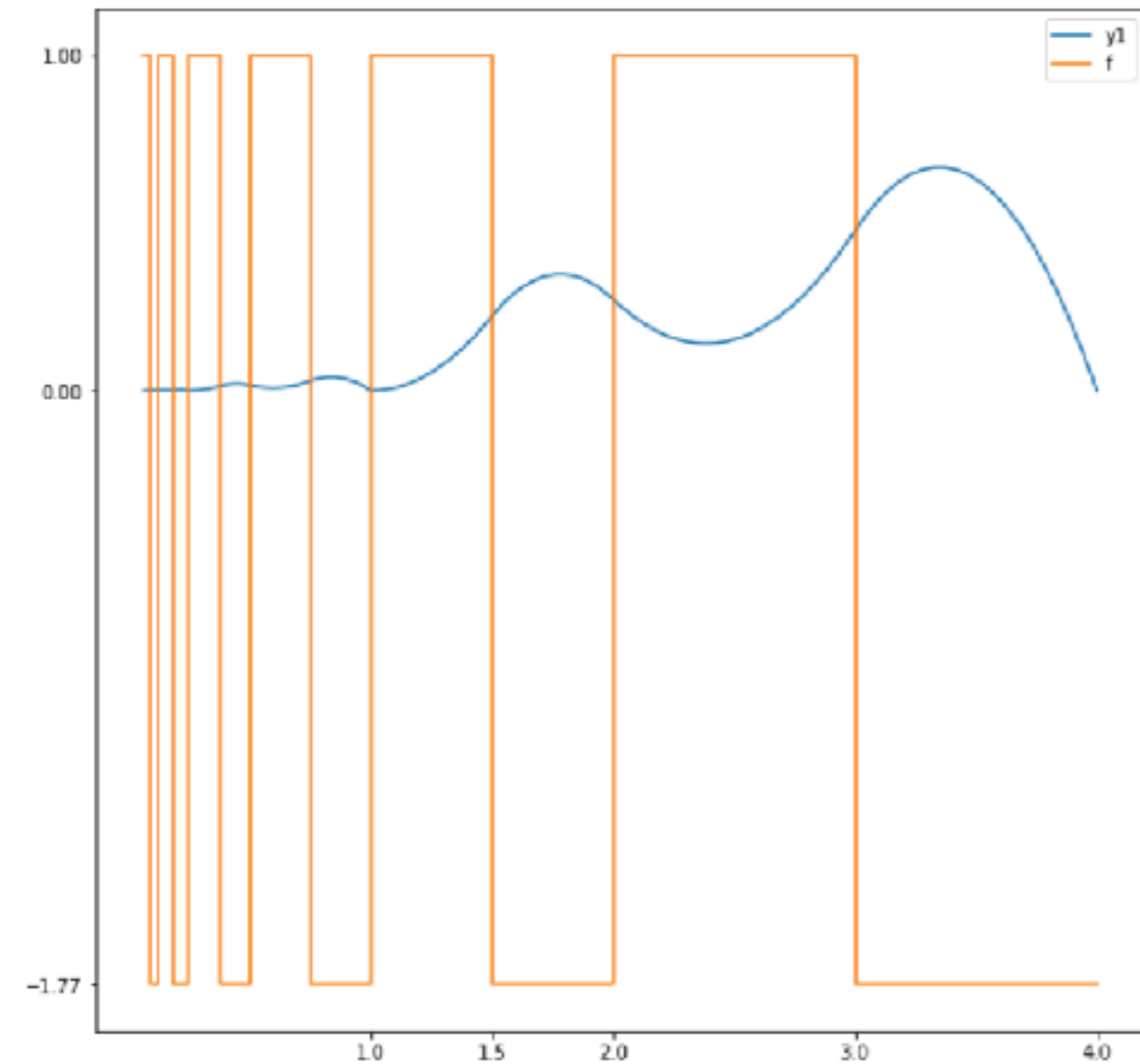
$$q \in W^{1,\infty}, \quad \dot{q} \in BV, \quad \lambda \in \mathcal{M}$$



# Non-uniqueness



# Non-uniqueness



► Need for analytic forces to obtain uniqueness

- Schatzman, Michelle. "A class of nonlinear differential equations of second order in time." *Nonlinear Analysis: Theory, Methods and Applications* 2.3 (1978): 355-373.
- Ballard, Patrick. "The dynamics of discrete mechanical systems with perfect unilateral constraints." *Archive for Rational Mechanics and Analysis* 154 (2000): 199-274.

# Existence

$$\dot{q}^+ = P_{C_q}(\dot{q}^-)$$
$$C_q = \{v \in \mathbb{R} / v \geq 0 \text{ if } q = 0\}$$

► Proofs = time discretization + compactness results

$q^n, u^n$  given

$$1) \quad \bar{u}^{n+1} = u^n + \frac{\Delta t}{m} f^e(t^n, q^n)$$

$$2) \quad u^{n+1} = P_{m, C_{q^n}}(\bar{u}^{n+1})$$

$$C_{q^n} = \{v \in \mathbb{R} / v \geq 0 \text{ if } q^n = 0\}$$

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- Paoli, Laetitia, and Michelle Schatzman. "A numerical scheme for impact problems I: The one-dimensional case." *SIAM Journal on Numerical Analysis* 40.2 (2002): 702-733.
- Marques, Manuel DP Monteiro, and Laetitia Paoli. "An existence result in non-smooth dynamics." *Nonsmooth Mechanics and Analysis: Theoretical and Numerical Advances*. Springer US, 2006.

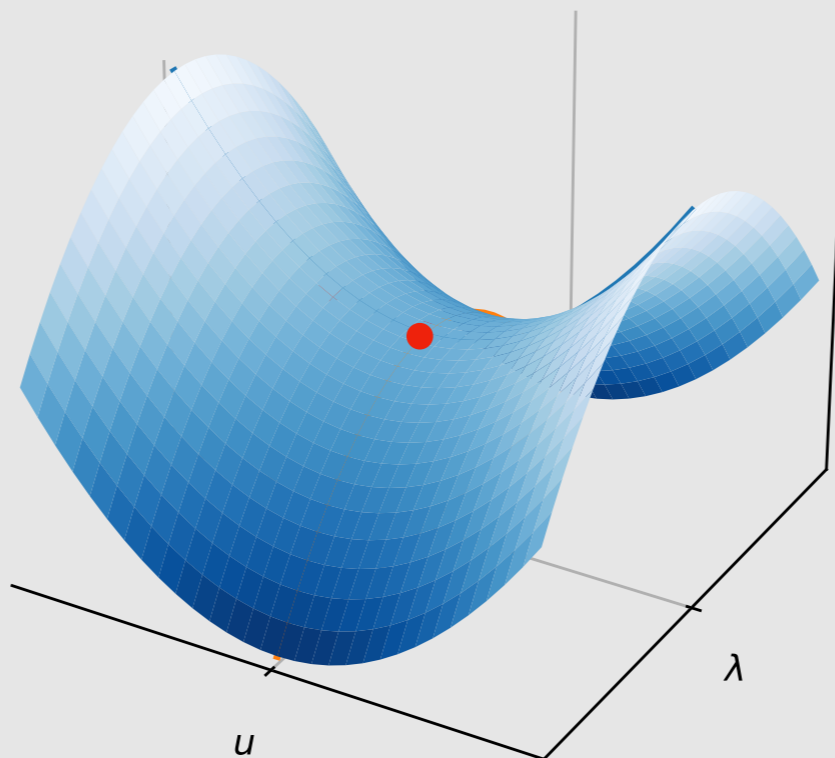


# Saddle-points, constrained optimization and duality

$$\mathcal{L} : \mathbf{U} \times \mathbf{\Lambda} \mapsto \mathbb{R} \quad \mathbf{U} \subset \mathbb{R}^N \quad \mathbf{\Lambda} \subset \mathbb{R}^m$$

$(u, \lambda) \in \mathbf{U} \times \mathbf{\Lambda}$  is a saddle point of  $\mathcal{L}$  if and only if

$$\mathcal{L}(u, \mu) \leq \mathcal{L}(u, \lambda) \leq \mathcal{L}(v, \lambda) \quad \forall v \in \mathbf{U}, \mu \in \mathbf{\Lambda}$$



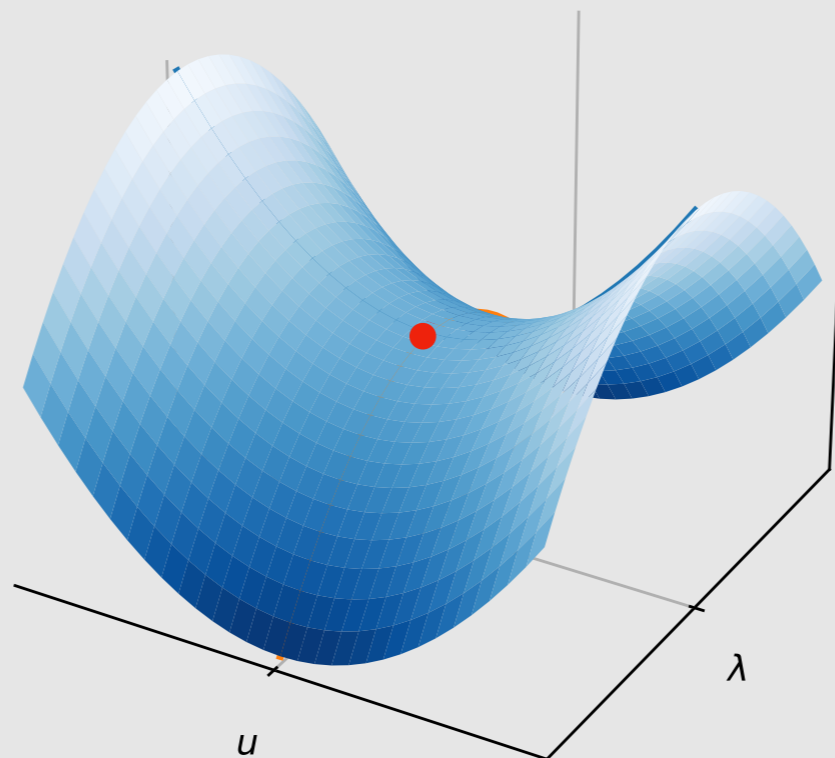


# Saddle-points, constrained optimization and duality

$$\mathcal{L} : \mathbf{U} \times \mathbf{\Lambda} \mapsto \mathbb{R} \quad \mathbf{U} \subset \mathbb{R}^N \quad \mathbf{\Lambda} \subset \mathbb{R}^m$$

$(u, \lambda) \in \mathbf{U} \times \mathbf{\Lambda}$  is a saddle point of  $\mathcal{L}$  if and only if

$$\min_{v \in \mathbf{U}} \sup_{\mu \in \mathbf{\Lambda}} \mathcal{L}(v, \mu) = \max_{\mu \in \mathbf{\Lambda}} \inf_{v \in \mathbf{U}} \mathcal{L}(v, \mu)$$





# Saddle-points, constrained optimization and duality

$$\left| \begin{array}{l} u \in K \\ J(u) = \min_{v \in K} J(v) \end{array} \right.$$

where

$$K = \{v \in \mathbb{R}^N, g(v) \leq 0\}$$

$$J : \mathbb{R}^N \mapsto \mathbb{R}$$

$$J(v) = \frac{1}{2}a(v, v) - l(v)$$

$$g : \mathbb{R}^N \mapsto \mathbb{R}$$

$g$  affine



# Saddle-points, constrained optimization and duality

$$\left| \begin{array}{l} u \in K \\ J(u) = \min_{v \in K} J(v) \end{array} \right.$$

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$$J(v) = \frac{1}{2}a(v, v) - l(v)$$

$$g : \mathbb{R}^N \mapsto \mathbb{R}$$

$g$  affine

Lagrangian of the optimization problem:

$$\mathcal{L} : \mathbb{R}^N \times \mathbb{R}_+ \mapsto \mathbb{R}$$

$$\mathcal{L}(v, \mu) = J(v) + \mu g(v)$$

$$\sup_{\mu \in \mathbb{R}^+} \mathcal{L}(v, \mu) = \left| \begin{array}{ll} J(v) & \text{if } v \in K \\ +\infty & \text{else} \end{array} \right.$$



# Saddle-points, constrained optimization and duality

$$\left| \begin{array}{l} u \in K \\ J(u) = \min_{v \in K} J(v) \end{array} \right.$$

where

$$K = \{v \in \mathbb{R}^N, g(v) \leq 0\}$$

$$(u, \lambda) \in \mathbb{R}^N \times \mathbb{R}_+$$

$(u, \lambda)$  saddle-point of  $\mathcal{L}$

[if constraints qualified...]  $\exists \lambda$  s.t.





# Saddle-points, constrained optimization and duality

$$\left| \begin{array}{l} u \in K \\ J(u) = \min_{v \in K} J(v) \end{array} \right.$$

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$(u, \lambda)$  saddle-point of  $\mathcal{L}$

[if constraints qualified...]  $\exists \lambda$  s.t.

$$\min_{v \in \mathbb{R}^N} \sup_{\mu \in \mathbb{R}_+} \mathcal{L}(v, \mu)$$

**Primal problem**



# Saddle-points, constrained optimization and duality

$$\left| \begin{array}{l} u \in K \\ J(u) = \min_{v \in K} J(v) \end{array} \right.$$

where

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[if constraints qualified...]  $\exists \lambda$  s.t.

$$\min_{v \in \mathbb{R}^N} \sup_{\mu \in \mathbb{R}_+} \mathcal{L}(v, \mu)$$

Primal problem

$$\max_{\mu \in \mathbb{R}_+} \inf_{v \in \mathbb{R}^N} \mathcal{L}(v, \mu)$$

Dual problem



# Saddle-points, constrained optimization and duality

$$\left| \begin{array}{l} u \in K \\ J(u) = \min_{v \in K} J(v) \end{array} \right.$$

where

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$(u, \lambda)$  saddle-point of  $\mathcal{L}$

[if constraints qualified...]  $\exists \lambda$  s.t.

$$\min_{v \in \mathbb{R}^N} \sup_{\mu \in \mathbb{R}_+} \mathcal{L}(v, \mu)$$

Primal problem

$$\max_{\mu \in \mathbb{R}_+} \inf_{v \in \mathbb{R}^N} \mathcal{L}(v, \mu)$$

Dual problem

$$\nabla J(u) = -\lambda \nabla g(u)$$

$$g(u) \leq 0, \quad \lambda \geq 0$$

$$g(u)\lambda = 0$$

Optimality conditions

# Existence

$$\dot{q}^+ = P_{C_q}(\dot{q}^-)$$
$$C_q = \{v \in \mathbb{R} / v \geq 0 \text{ if } q = 0\}$$

► Proofs = time discretization + compactness results

$q^n, u^n$  given

$$1) \quad \bar{u}^{n+1} = u^n + \frac{\Delta t}{m} f^e(t^n, q^n)$$

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$$3) \quad q^{n+1} = q^n + \Delta t u^{n+1}$$

$$\nabla J(u) = -\lambda \nabla g(u)$$

Optimality conditions

$$\exists \lambda^{n+1} \geq 0 \text{ s.t. } m \frac{u^{n+1} - u^n}{\Delta t} = f^e(t^n, q^n) + \lambda^{n+1}$$

# Numerical schemes

► Algorithms based on the discretization used to prove existence

- **Explicit** admissible velocity space

$$C_{q^n} = \{v \in \mathbb{R} / v \geq 0 \text{ if } q^n \leq 0\}$$

- **Implicit** contact forces

$$\text{Find } (u^{n+1}, \lambda^{n+1}) \text{ with } m \frac{u^{n+1} - u^n}{\Delta t} = f^e(t^n, q^n) + \lambda^{n+1}$$

► Can lead to non-admissible configurations (overlapping)

# Numerical schemes

$$\begin{cases} u \in K \\ J(u) = \min_{v \in K} J(v) \end{cases}$$

Optimization problem

## ► Fully implicit algorithms

- **Implicit** admissible velocity space

$$C_{q^n} = \{v \in \mathbb{R} / q^{n+1} = q^n + \Delta t v \geq 0\}$$

- **Implicit** contact forces

$$\text{Find } (u^{n+1}, \lambda^{n+1}) \text{ with } m \frac{u^{n+1} - u^n}{\Delta t} = f^e(t^n, q^n) + \lambda^{n+1}$$

## ► Admissible configurations, large time-steps

- Anitescu, M., & Hart, G. D. (2004). A constraint-stabilized time-stepping approach for rigid multibody dynamics with joints, contact and friction. *International Journal for Numerical Methods in Engineering*, 60(14), 2335-2371.
- B. Maury. A time-stepping scheme for inelastic collisions. *Numerische Mathematik*, 102(4):649-679, 2006.

# Numerical schemes

$$\nabla J(u) = -\lambda \nabla g(u)$$

$$g(u) \leq 0, \quad \lambda \geq 0$$

$$g(u)\lambda = 0$$

Optimality conditions

► Fully implicit algorithms - Convergence result

## Model

$$m\ddot{q} = f^e + \lambda$$

$$q \geq 0, \quad \lambda \geq 0$$

$$\text{supp}(\lambda) \subset \{t / q(t) = 0\}$$

$$\dot{q}^+ = P_{C_q}(\dot{q}^-)$$

$$C_q = \{v \in \mathbb{R} / v \geq 0 \text{ if } q = 0\}$$

## Algorithm

$$m \frac{u^{n+1} - u^n}{\Delta t} = f^e(t^n, q^n) + \lambda^{n+1}$$

$$q^n + \Delta t u^{n+1} \geq 0, \quad \lambda^{n+1} \geq 0$$

$$(q^n + \Delta t u^{n+1}) \lambda^{n+1} = 0$$

$$u^{n+1} = P_{m, C_{q^n}}(\bar{u}^{n+1})$$

$$C_{q^n} = \{v \in \mathbb{R} / q^{n+1} = q^n + \Delta t v \geq 0\}$$



# Numerical schemes

► Fully implicit algorithms - Dual problem

$$\max_{\mu \in \mathbb{R}_+} \inf_{v \in \mathbb{R}^N} \mathcal{L}(v, \mu)$$

Dual problem

# Numerical schemes

$$\max_{\mu \in \mathbb{R}^+} \inf_{v \in \mathbb{R}^N} \mathcal{L}(v, \mu)$$

Dual problem

► Fully implicit algorithms - Dual problem

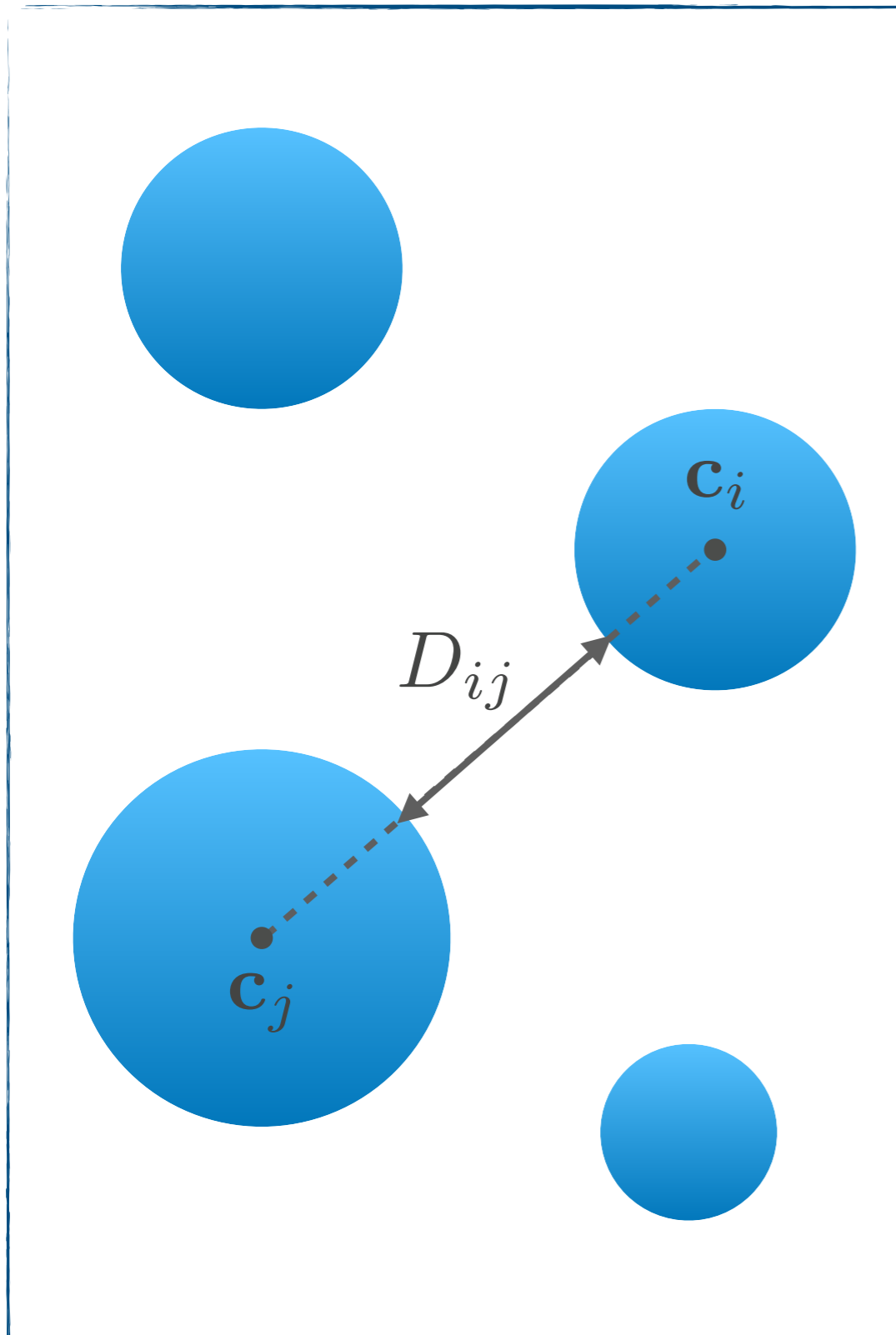
$$\min_{\mu \in \mathbb{R}^+} \mu \left( q^n + \Delta t \frac{u_\mu + \bar{u}^{n+1}}{2} \right)$$

where

$$m \frac{u_\mu - u^n}{\Delta t} = f^e(t^n, q^n) + \mu$$

- On convex numerical schemes for inelastic contacts with friction, with H. Bloch, Proceeding SMAI2021, Accepted for publication
- M. Frémond. Non-Smooth Thermomechanics. Springer Berlin Heidelberg, Berlin, Heidelberg, 2002

# The multi particle case



$$\mathbf{c} = (\mathbf{c}_1, \dots, \mathbf{c}_N) \in \mathbb{R}^{3N} \quad \mathbf{v} = \dot{\mathbf{c}}$$

$$M\ddot{\mathbf{x}} = \mathbf{f}^e + \sum_{i < j} \lambda_{ij} \nabla D_{ij}(\mathbf{c})$$

$$\text{supp}(\lambda_{ij}) \subset \{t / D_{ij}(\mathbf{c}(t)) = 0\}$$

$$D_{ij}(\mathbf{c}(t)) \geq 0, \quad \lambda_{ij} \geq 0$$

$$\dot{\mathbf{c}}^+ = P_{C_{\mathbf{c}}}(\dot{\mathbf{c}}^-)$$

$$C_{\mathbf{c}} = \{ \mathbf{v} \in \mathbb{R}^{3N} / \forall i < j,$$

$$\nabla D_{ij} \cdot \mathbf{v} \geq 0 \text{ if } D_{ij}(\mathbf{c}) = 0 \}$$

# The multi particle case

► Fully implicit algorithm

$\mathbf{c}^n, \mathbf{v}^n$  given

$$1) \quad \bar{\mathbf{v}}^{n+1} = \mathbf{v}^n + \Delta t M^{-1} \mathbf{f}^e(t^n, \mathbf{c}^n)$$

$$2) \quad \mathbf{v}^{n+1} = P_{M, C^n}(\bar{\mathbf{v}}^{n+1})$$

$$C^n = \left\{ \mathbf{v} \in \mathbb{R}^{3N} / \forall i < j, \right. \\ \left. D_{ij}(\mathbf{c}^n) + \Delta t \nabla D_{ij}(\mathbf{c}^n) \cdot \mathbf{v} \geq 0 \right\}$$

$$3) \quad q^{n+1} = q^n + \Delta t u^{n+1}$$

# The multi particle case

► Fully implicit algorithm

$\mathbf{c}^n, \mathbf{v}^n$  given

$$1) \quad \bar{\mathbf{v}}^{n+1} = \mathbf{v}^n + \Delta t M^{-1} \mathbf{f}^e(t^n, \mathbf{c}^n)$$

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$$C^n = \{ \mathbf{v} \in \mathbb{R}^{3N} / \forall i < j,$$

$$D_{ij}(\mathbf{c}^n) + \Delta t \nabla D_{ij}(\mathbf{c}^n) \cdot \mathbf{v} \geq 0 \}$$

$$3) \quad q^{n+1} = q^n + \Delta t u^{n+1}$$

$$\nabla J(\mathbf{v}) = - \sum_{i < j} \lambda_{ij} \nabla g_{ij}(\mathbf{v})$$

Optimality conditions

$$\exists \lambda_{ij} \geq 0 \text{ s.t. } M \frac{\mathbf{v}^{n+1} - \mathbf{v}^n}{\Delta t} = \mathbf{f}^e(t^n, \mathbf{c}^n) + \sum_{i < j} \lambda_{ij} \nabla D_{ij}(\mathbf{c}^n)$$

# The multi particle case

► Fully implicit algorithm

$\mathbf{c}^n, \mathbf{v}^n$  given

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- B. Maury. A time-stepping scheme for inelastic collisions. *Numerische Mathematik*, 102(4):649–679, 2006.
- Bernicot, F., & Lefebvre-Lepot, A. (2010). Existence results for nonsmooth second-order differential inclusions, convergence result for a numerical scheme and application to the modeling of inelastic collisions. *Confluentes Mathematici*, 2(04), 445-471.

# The multi particle case

► Fully implicit algorithm - the corresponding dual problem

$$\min_{\lambda_{ij} \in \mathbb{R}^+} \sum_{i < j} \lambda_{ij} \left[ D_{ij}(\mathbf{c}^n) + \Delta t \mathbf{n}_{ij} \cdot \mathbf{A}_{ij} \left( \frac{\mathbf{v}_\lambda + \bar{\mathbf{v}}^{n+1}}{2} \right) \right]$$

$$\text{where } M \frac{\mathbf{v}_\lambda - \mathbf{v}^n}{\Delta t} = \mathbf{f}^e(t^n, \mathbf{c}^n) + \sum_{i < j} \lambda_{ij} \nabla D_{ij}(\mathbf{c}^n)$$

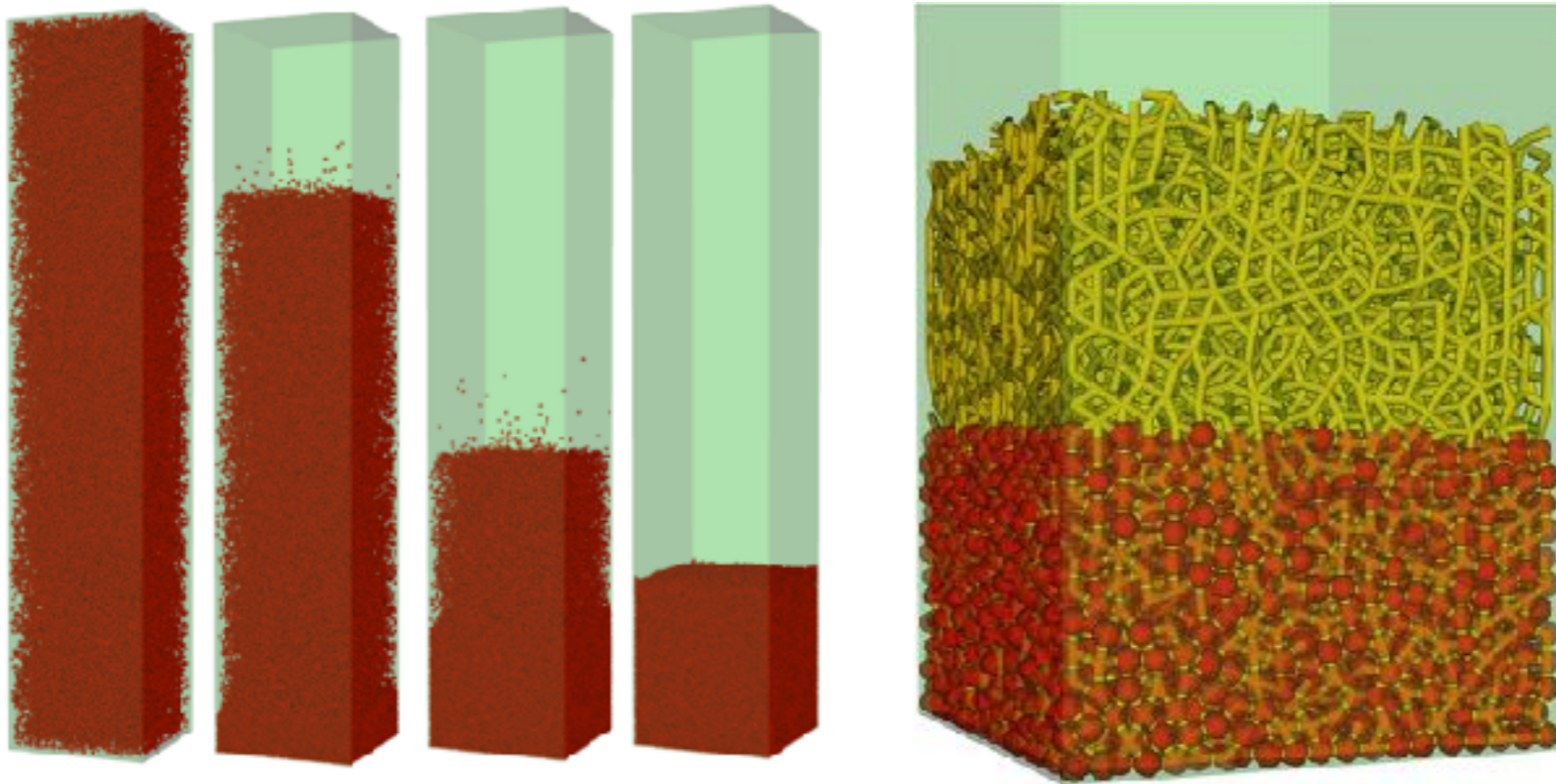
► Can be solved using Projected Gradient Algorithms

# Application: random packing of non-convex particles

► Inelastic contacts

► SCoPI

► Validation for spheres



Random packing:

$63.7 \pm 0.2\%$

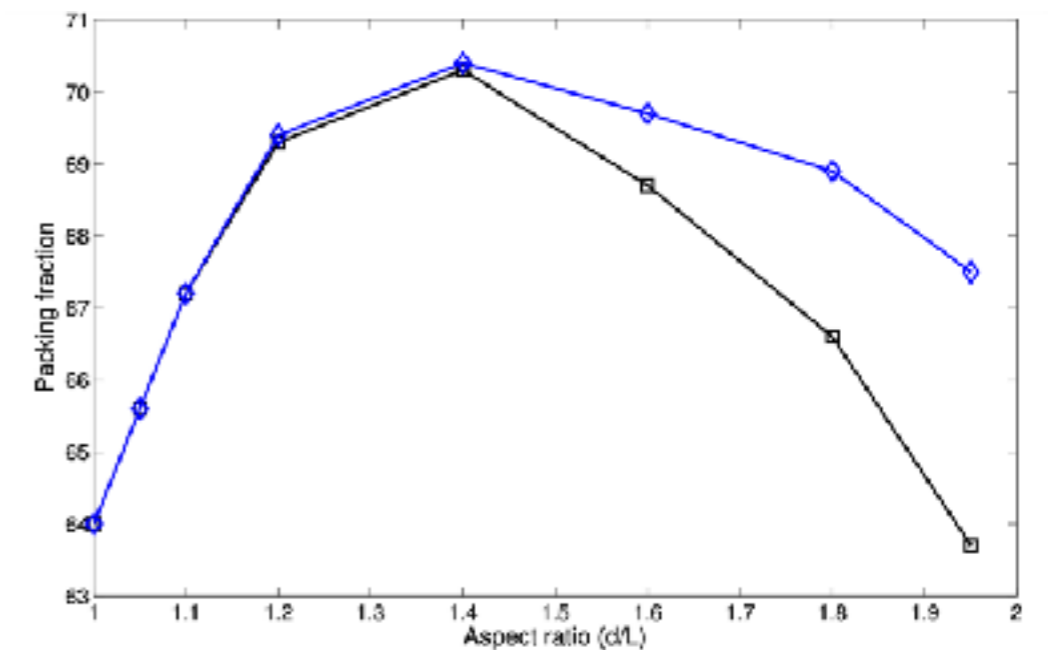
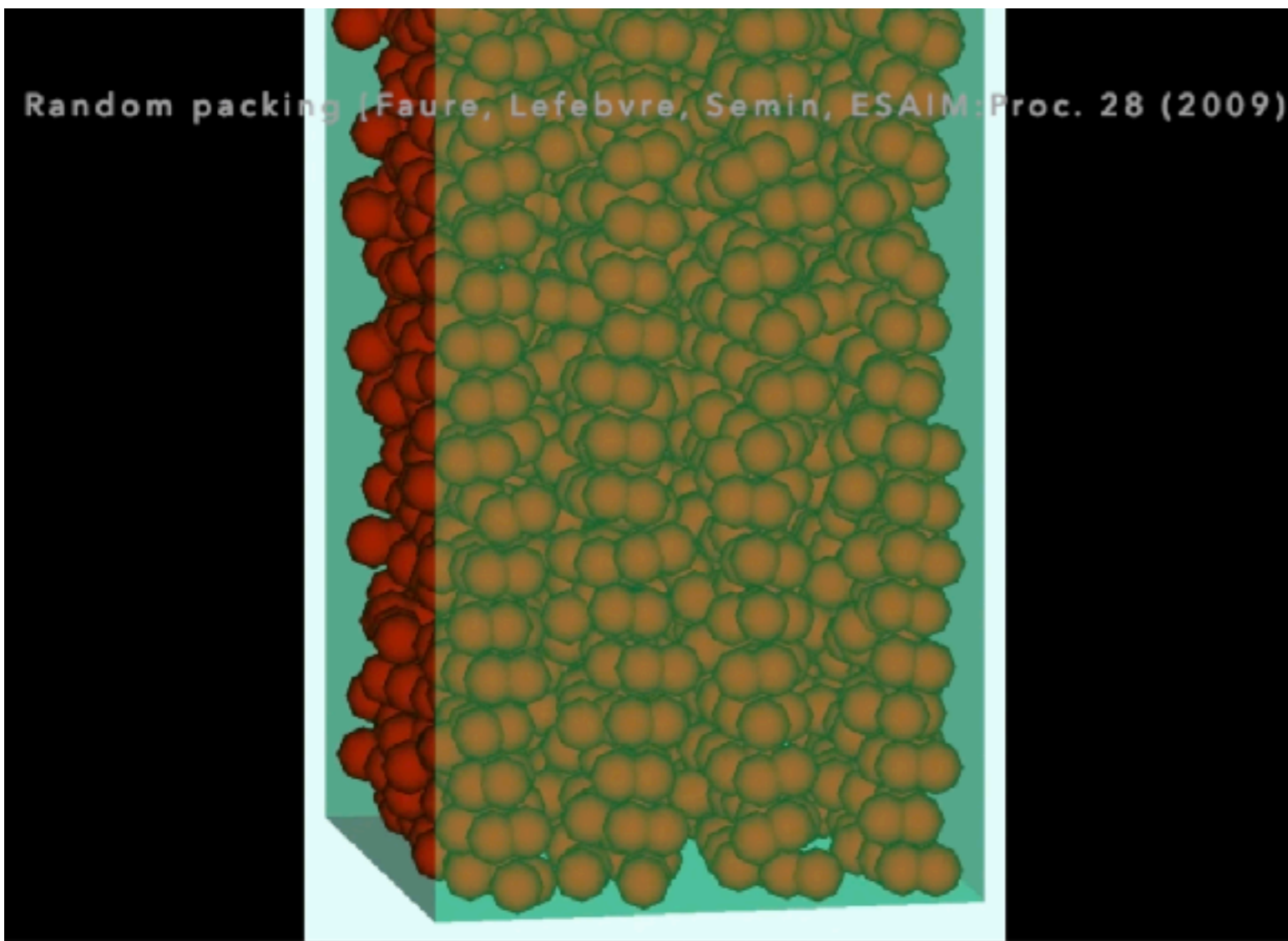
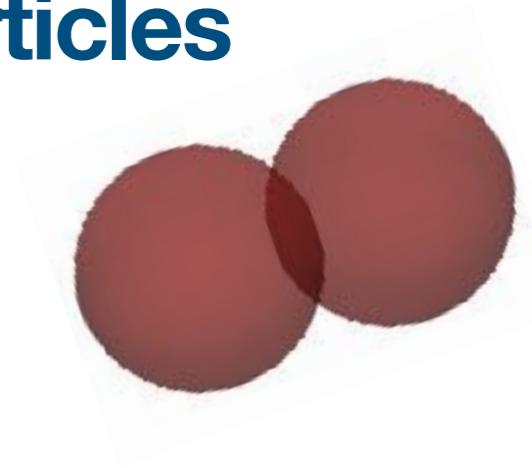


# Application: random packing of non-convex particles

► Inelastic contacts

► SCoPI

► Case of non-convex particles

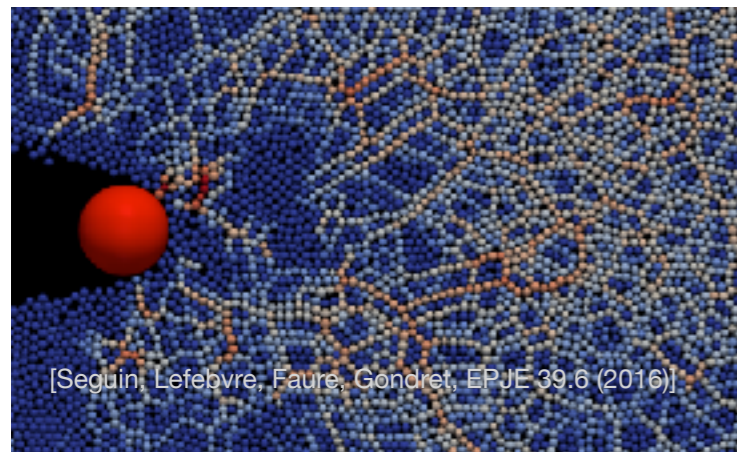
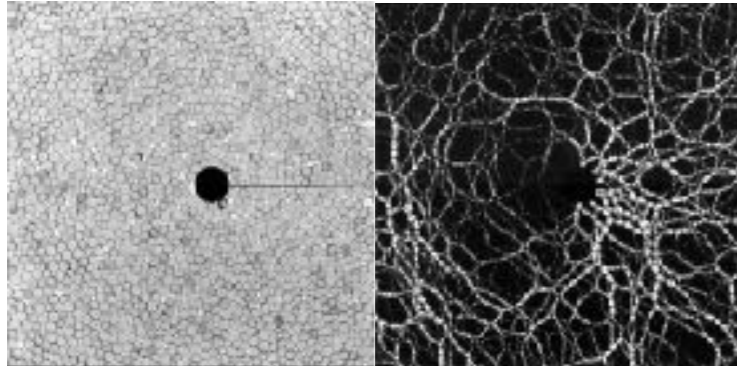


# Application: clustering and flow around an intruder

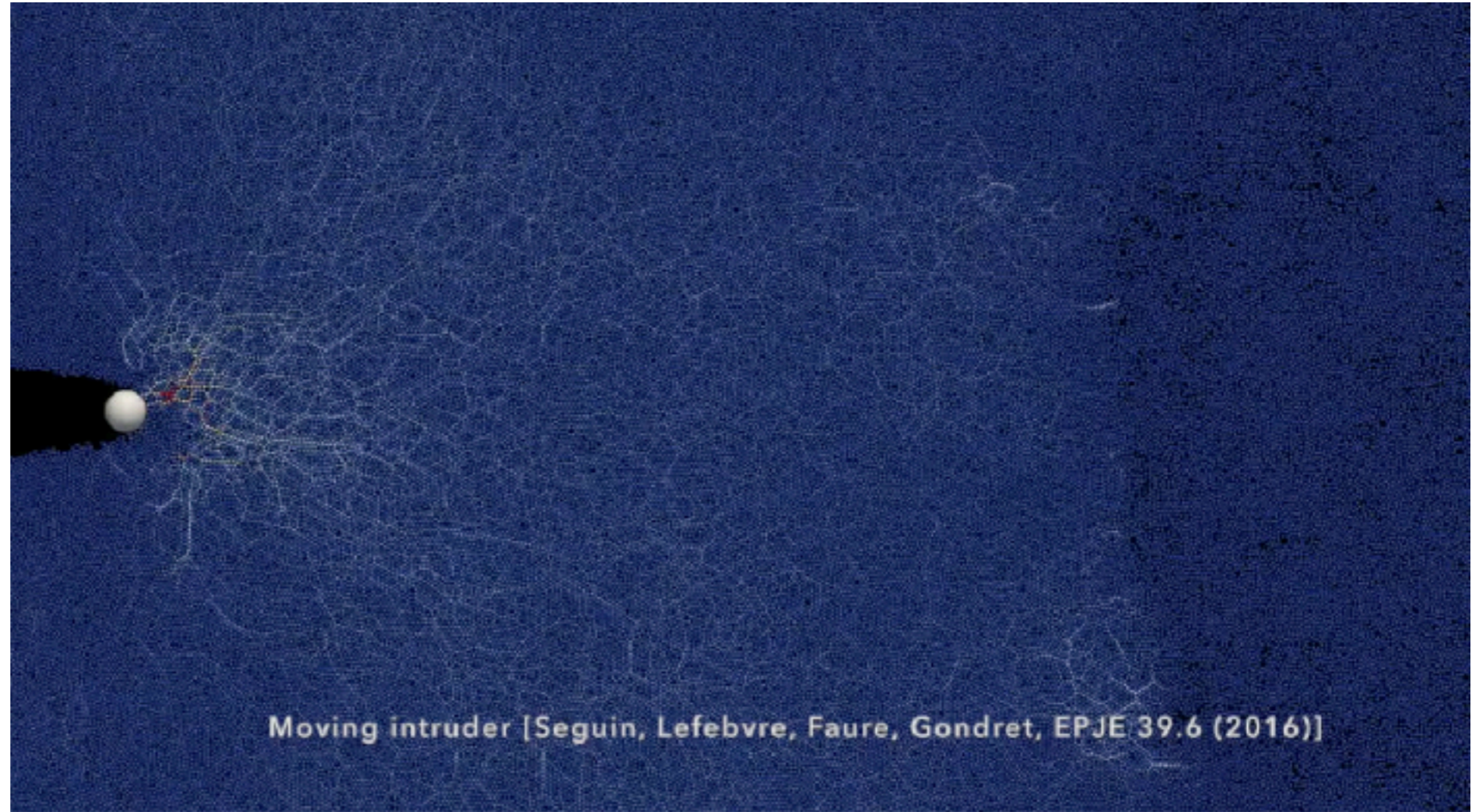
► Inelastic contacts

► Spherical particles

► SCoPI

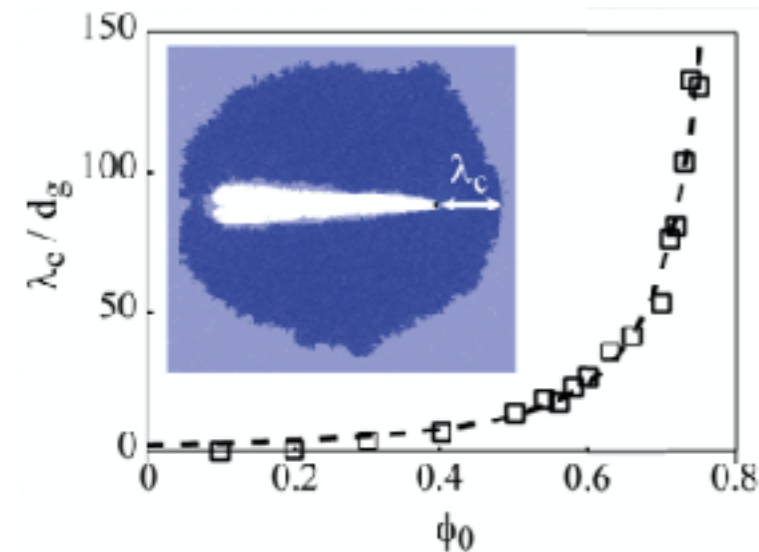


[Seguin, Lefebvre, Faure, Gondret, EPJE 39.6 (2016)]



► Rheology

► Chains of forces

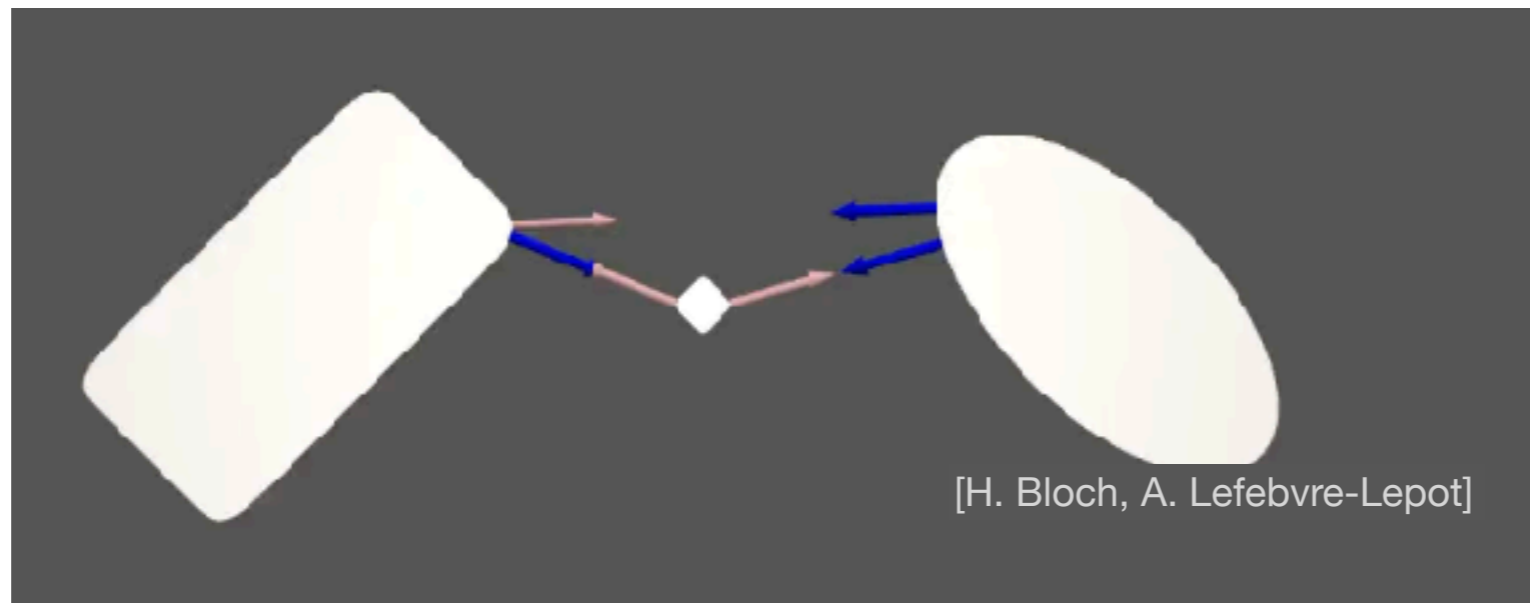


# Extension to non-spherical particles.

▶ Non-spherical particles

▶ H el ene Bloch [CMAP]

▶ SCoPI

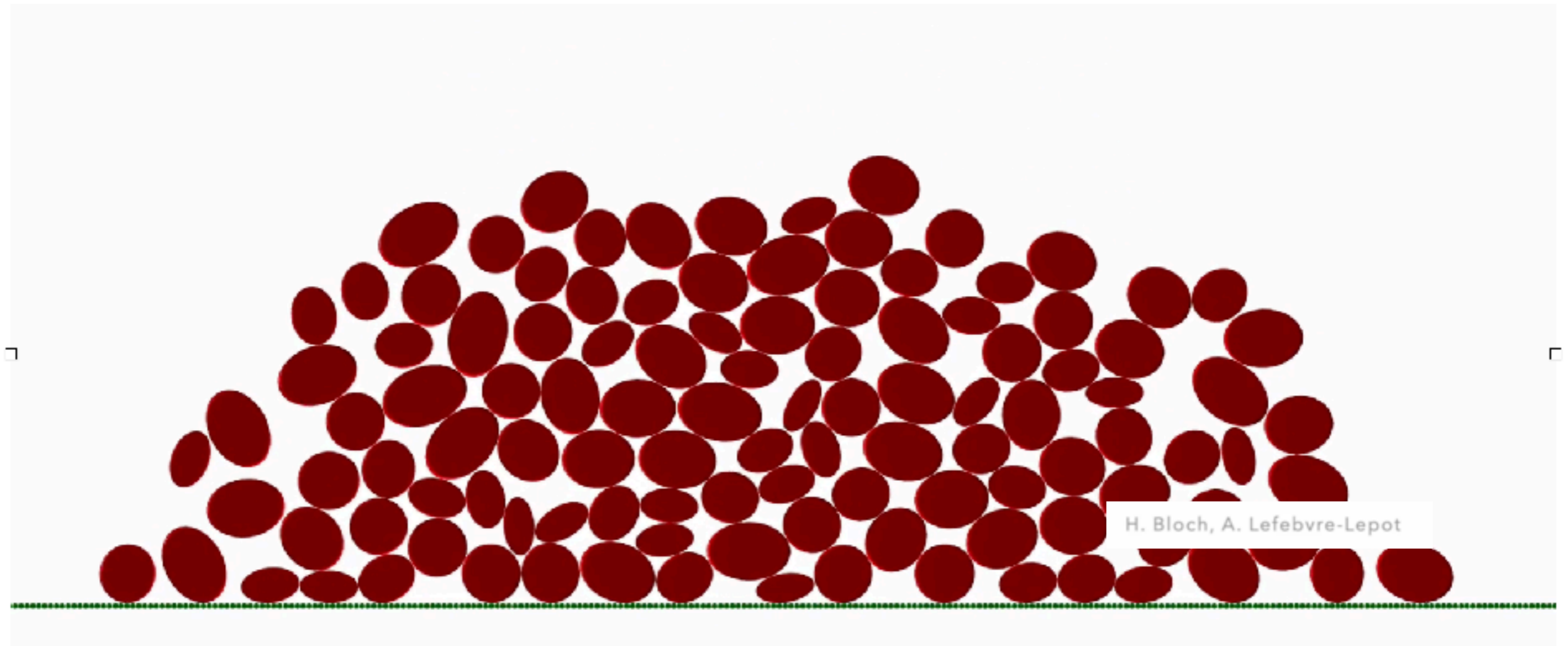


# Stable and convex contact algorithms.

▶ Non-spherical particles

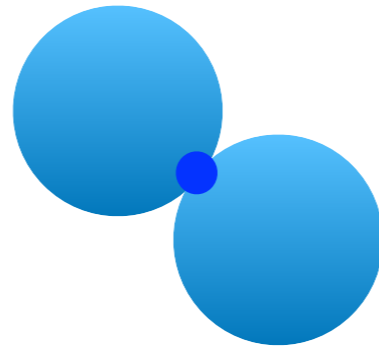
▶ H el ene Bloch [CMAP]

▶ SCoPI



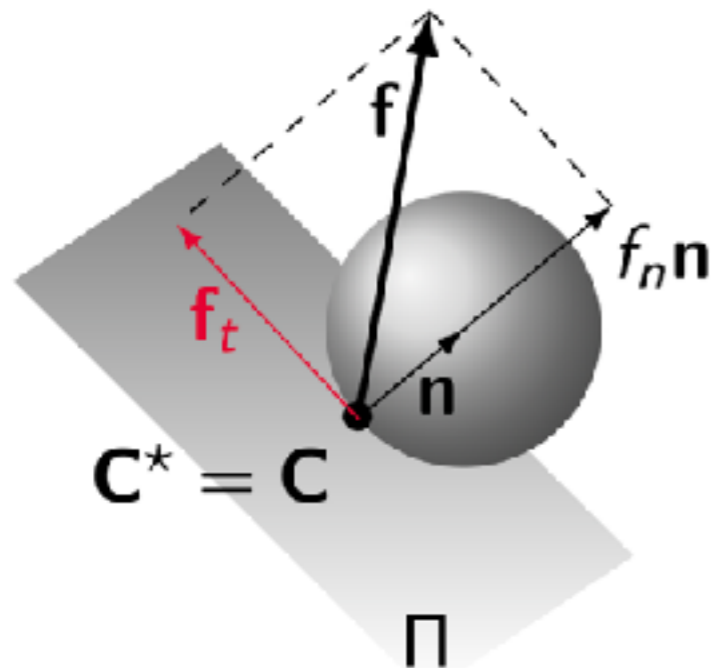
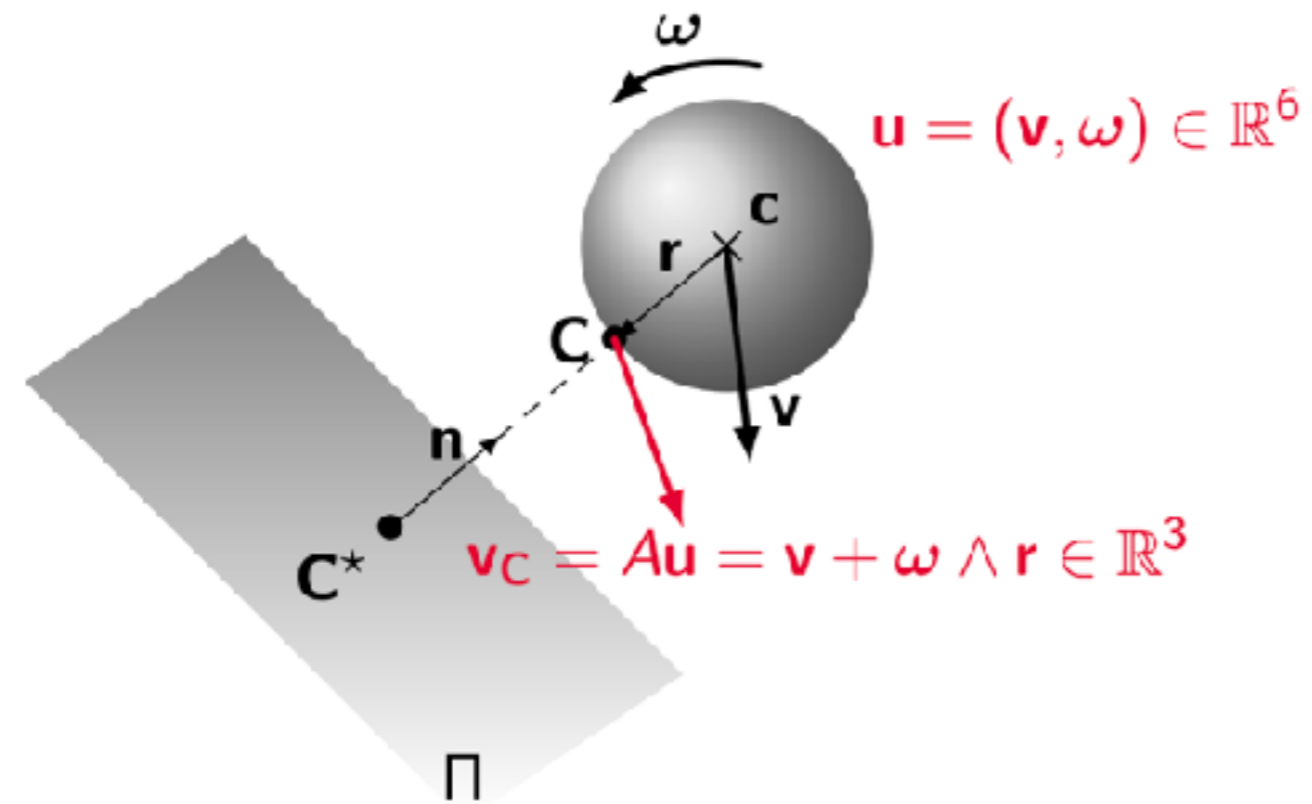
# Contact Dynamics Models including friction

Contact law



Inelastic contacts  
Coulomb friction law

# Modeling friction.



► Contact force

$$\mathbf{f} = f_n \mathbf{n} + \mathbf{f}_t$$

► If  $P\mathbf{v}_C^+ = 0$  (no slip)

$$|\mathbf{f}_t| \leq \mu f_n$$

► If  $P\mathbf{v}_C^+ \neq 0$  (sliding motion)

$$\mathbf{f}_t = -\mu f_n \frac{P\mathbf{v}_C^+}{|P\mathbf{v}_C^+|}$$

# Modeling friction.

$$M \frac{d\mathbf{u}}{dt} = \mathbf{f}^e + A^T (f_n \mathbf{n} + \mathbf{f}_t) \quad (\text{FPD})$$

$$D(\mathbf{c}) \geq 0, \quad f_n \geq 0, \quad D(\mathbf{c})f_n = 0 \quad (\text{Norm. Cont.})$$

$$\mathbf{u}^+ = P_{C_c} \mathbf{u}^-$$

$$\text{If } PA\mathbf{u}^+ = 0 \text{ (no slip), } |\mathbf{f}_t| \leq \mu f_n \quad (\text{Tang. Cont.})$$

$$\text{If } PA\mathbf{u}^+ \neq 0 \text{ (sliding motion), } \mathbf{f}_t = -\mu f_n \frac{PA\mathbf{u}^+}{|PA\mathbf{u}^+|}$$

$$[\mathbf{u} = (\mathbf{v}, \boldsymbol{\omega}), \quad A\mathbf{u} = \mathbf{v} + \boldsymbol{\omega} \wedge \mathbf{r}, \quad A^T \mathbf{f} = (\mathbf{f}, \mathbf{r} \wedge \mathbf{f}) \in \mathbb{R}^6]$$

# Founding NSCD algorithms

$$M \frac{\mathbf{u}^{n+1} - \mathbf{u}^n}{\Delta t} = \mathbf{f}^e + A^{n,T} (f_n \mathbf{n}^n + \mathbf{f}_t) \quad (\text{FPD})$$

$$f_n \geq 0 \quad (\text{Norm. Cont.})$$

$$D^n + \Delta t \nabla_{\mathbf{c}} D^n \cdot \mathbf{v}^{n+1} \geq 0$$

$$(D^n + \Delta t \nabla_{\mathbf{c}} D^n \cdot \mathbf{v}^{n+1}) f_n = 0$$

$$\text{If } P^n A^n \mathbf{u}^{n+1} = 0 \quad |\mathbf{f}_t| \leq \mu f_n \quad (\text{Tang. Cont.})$$

$$\text{If } P^n A^n \mathbf{u}^{n+1} \neq 0 \quad \mathbf{f}_t = -\mu f_n \frac{P^n A^n \mathbf{u}^{n+1}}{|P^n A^n \mathbf{u}^{n+1}|}$$

- Jean, M. (1999). The non-smooth contact dynamics method. *Computer methods in applied mechanics and engineering*, 177(3-4), 235-257.
- Dubois, F., & Jean, M. (2006). The non smooth contact dynamic method: recent LMGC90 software developments and application. *Analysis and simulation of contact problems*, 375-378.



# Convex optimization for friction?

## Lagrange multipliers

$$\left| \begin{array}{l} u \in K \\ J(u) = \min_{v \in K} J(v) \end{array} \right.$$

$$K = \{v \in \mathbb{R}^N, g(v) \leq 0\}$$

Under qualification conditions,

$\exists \lambda \in \mathbb{R}$  such that

$$\nabla J(u) = -\lambda \nabla g(u)$$

$$g(u) \leq 0, \quad \lambda \geq 0$$

$$g(u)\lambda = 0$$

Optimality conditions

$$M \frac{d\mathbf{u}}{dt} = \mathbf{f}^e + A^T (f_n \mathbf{n} + \mathbf{f}_t)$$

$$D(\mathbf{c}) \geq 0, \quad f_n \geq 0, \quad D(\mathbf{c})f_n = 0$$

$$\mathbf{u}^+ = P_{C_c} \mathbf{u}^-$$

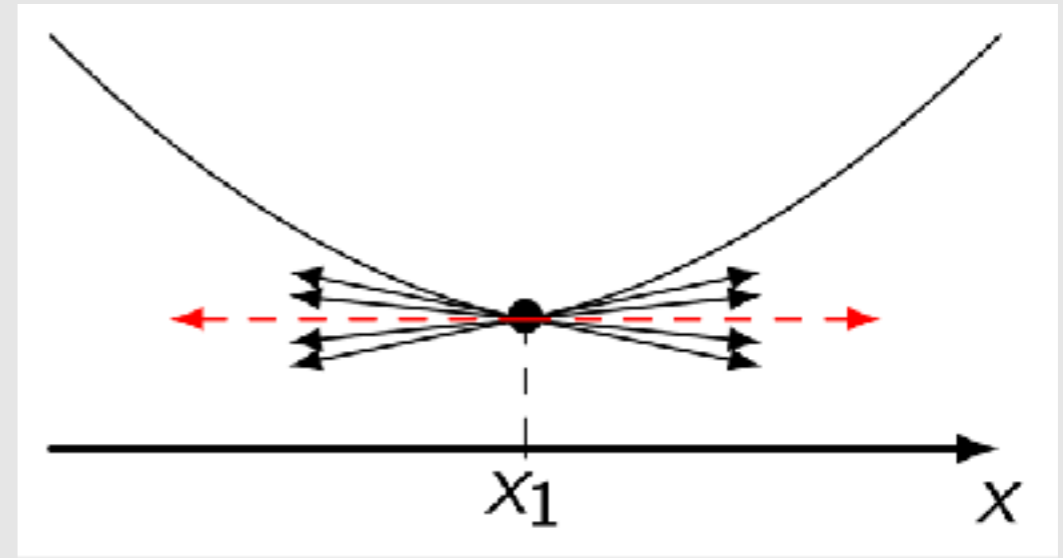
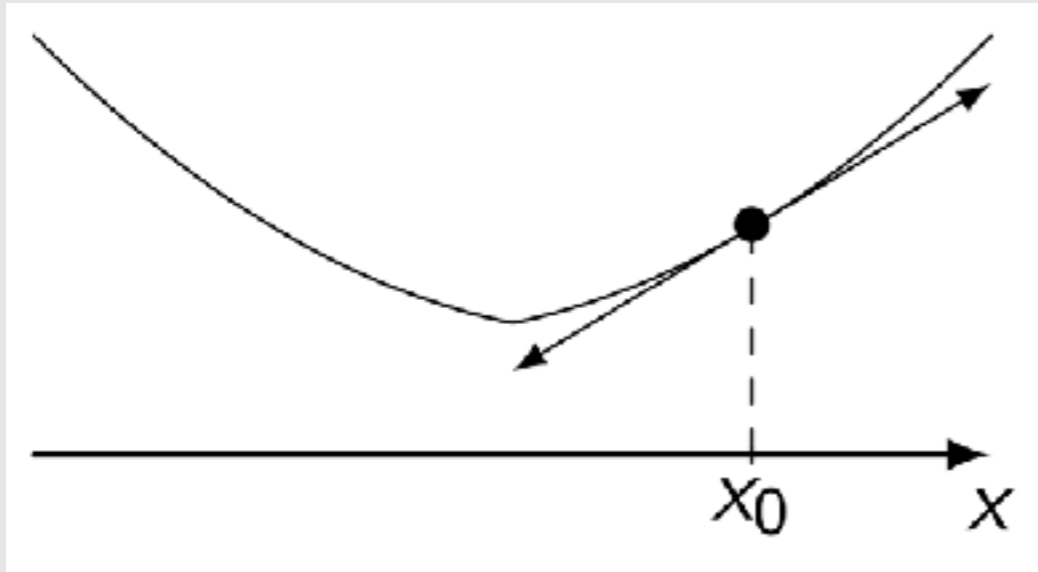
$$PA\mathbf{u}^+ \neq 0 \quad \mathbf{f}_t = -\mu f_n \frac{PA\mathbf{u}^+}{|PA\mathbf{u}^+|}$$

$$PA\mathbf{u}^+ = 0 \quad |\mathbf{f}_t| \leq \mu f_n$$

$\Rightarrow$  Need for non-derivable  $g$



# Notion of sub-differential



## Sub-differential of a convex function

$\Phi : \mathbb{R}^n \rightarrow \mathbb{R}$ , convex function

$$\partial\Phi[\mathbf{x}] = \{ \mathbf{y} \in \mathbb{R}^n / \forall \hat{\mathbf{x}} \in \mathbb{R}^n, \Phi(\hat{\mathbf{x}}) \geq \Phi(\mathbf{x}) + \mathbf{y} \cdot (\hat{\mathbf{x}} - \mathbf{x}) \}$$

Optimality condition:  $\mathbf{x}$  minimum of  $\Phi \iff 0 \in \partial\Phi[\mathbf{x}]$



# Notion of sub-differential

► Lagrange multiplier

$$\left| \begin{array}{l} u \in K \\ J(u) = \min_{v \in K} J(v) \end{array} \right. \quad K = \{v \in \mathbb{R}^N, g(v) \leq 0\}$$

Under qualification conditions,  $\exists \lambda \in \mathbb{R}$  such that

$$\nabla J(u) \in -\lambda \partial g[u]$$

$$g(u) \leq 0, \quad \lambda \geq 0$$

$$g(u)\lambda = 0$$

**Optimality conditions**

# Convex optimization for friction?

## Lagrange multipliers

$$\left| \begin{array}{l} u \in K \\ J(u) = \min_{v \in K} J(v) \end{array} \right.$$

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$$D(\mathbf{c}) \geq 0, \quad f_n \geq 0, \quad D(\mathbf{c})f_n = 0$$

$$\mathbf{u}^+ = P_{C_c} \mathbf{u}^-$$

$$PA\mathbf{u}^+ \neq 0 \quad \mathbf{f}_t = -\mu f_n \frac{PA\mathbf{u}^+}{|PA\mathbf{u}^+|}$$

$$PA\mathbf{u}^+ = 0 \quad |\mathbf{f}_t| \leq \mu f_n$$

$\Rightarrow$  Need for non-derivable  $g$

# Convex optimization for friction?

► Fully implicit algorithm

$\mathbf{c}^n, \mathbf{u}^n$  given

$$1) \quad \bar{\mathbf{u}}^{n+1} = \mathbf{u}^n + \Delta t M^{-1} \mathbf{f}^e(t^n, \mathbf{c}^n)$$

$$2) \quad \mathbf{u}^{n+1} = P_{M, C_\mu^n}(\bar{\mathbf{u}}^{n+1})$$

$$C_\mu^n = \{ \mathbf{v} \in \mathbb{R}^6 / D(\mathbf{c}^n) + \Delta t \nabla D(\mathbf{c}^n) \cdot \mathbf{v} \geq \mu \Delta t |P^n A^n \mathbf{u}| \}$$

$$3) \quad \mathbf{c}^{n+1} = \mathbf{c}^n + \Delta t \mathbf{v}^{n+1}$$

# Convex optimization for friction?

► Fully implicit algorithm

$$M \frac{\mathbf{u}^{n+1} - \mathbf{u}^n}{\Delta t} = \mathbf{f}^e + A^{n,T} (f_n \mathbf{n}^n + \mathbf{f}_t) \quad (\text{FPD})$$

$$f_n \geq 0 \quad (\text{Norm. Cont.})$$

$$D^n + \Delta t \nabla_{\mathbf{c}} D^n \cdot \mathbf{v}^{n+1} \geq \mu \Delta t |P^n A^n \mathbf{u}^{n+1}|$$

$$(D^n + \Delta t \nabla_{\mathbf{c}} D^n \cdot \mathbf{v}^{n+1} - \mu \Delta t |P^n A^n \mathbf{u}^{n+1}|) f_n = 0$$

$$\text{If } P^n A^n \mathbf{u}^{n+1} = 0 \quad |\mathbf{f}_t| \leq \mu f_n \quad (\text{Tang. Cont.})$$

$$\text{If } P^n A^n \mathbf{u}^{n+1} \neq 0 \quad \mathbf{f}_t = -\mu f_n \frac{P^n A^n \mathbf{u}^{n+1}}{|P^n A^n \mathbf{u}^{n+1}|}$$

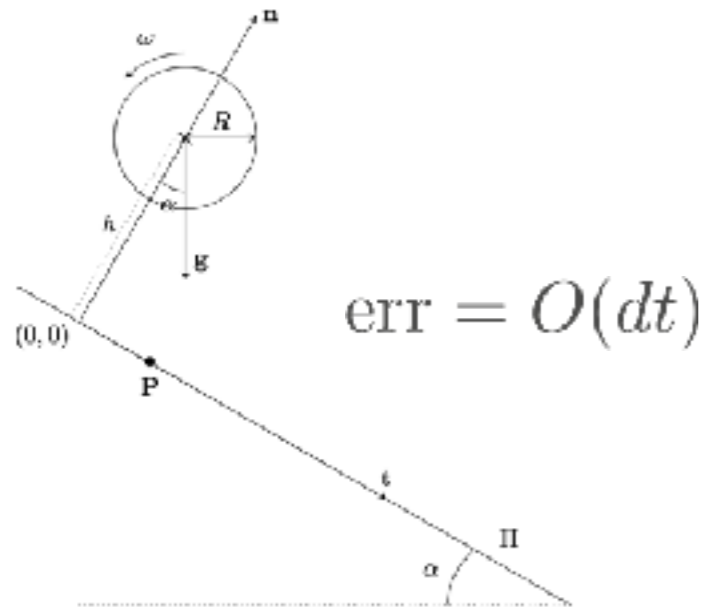
- Anitescu, M. (2006). Optimization-based simulation of nonsmooth rigid multibody dynamics. *Mathematical Programming*, 105, 113-143.
- On convex numerical schemes for inelastic contacts with friction, with H. Bloch, Proceeding SMAI2021, Accepted for publication

# Convex optimization for friction?

► Fully implicit algorithm

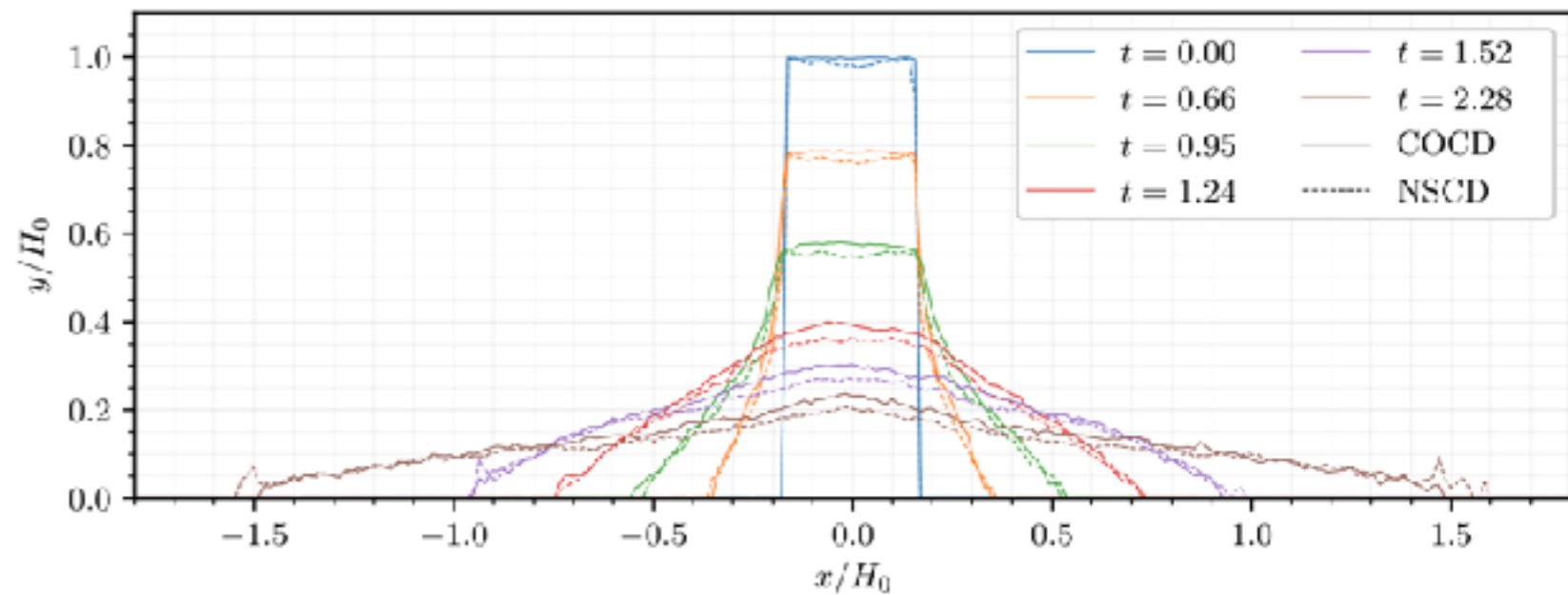
► Order of convergence?

Numerical study:



► Influence of convexification?

Granular column collapse:



- An optimization-based model for dry granular flows: application to granular collapse on erodible beds, with H. Martin, A. Mangeney, Y. Maday, B. Maury, Submitted, hal-03790427
- On convex numerical schemes for inelastic contacts with friction, with H. Bloch, Proceeding SMAI2021, Accepted for publication

# Convex optimization for friction?

► Fully implicit algorithm - the corresponding dual problem

$$\min_{|\mathbf{f}_t| \leq \mu f_n} f_n \left[ D^n + \Delta t \mathbf{n}^n \cdot A^n \left( \frac{\mathbf{u}_f + \bar{\mathbf{u}}^{n+1}}{2} \right) \right] + \left\langle \mathbf{f}_t, \Delta t P^n A^n \left( \frac{\mathbf{u}_f + \bar{\mathbf{u}}^{n+1}}{2} \right) \right\rangle$$

► Can be solved using Projected Gradient Algorithms

- Melanz, D., Fang, L., Jayakumar, P., & Negrut, D. (2017). A comparison of numerical methods for solving multibody dynamics problems with frictional contact modeled via differential variational inequalities. *Computer Methods in Applied Mechanics and Engineering*, 320, 668-693.
- Corona, E., Gorsich, D., Jayakumar, P., & Veerapaneni, S. (2019). Tensor train accelerated solvers for nonsmooth rigid body dynamics. *Applied Mechanics Reviews*, 71(5), 050804.
- On convex numerical schemes for inelastic contacts with friction, with H. Bloch, Proceeding SMAI2021, Accepted for publication

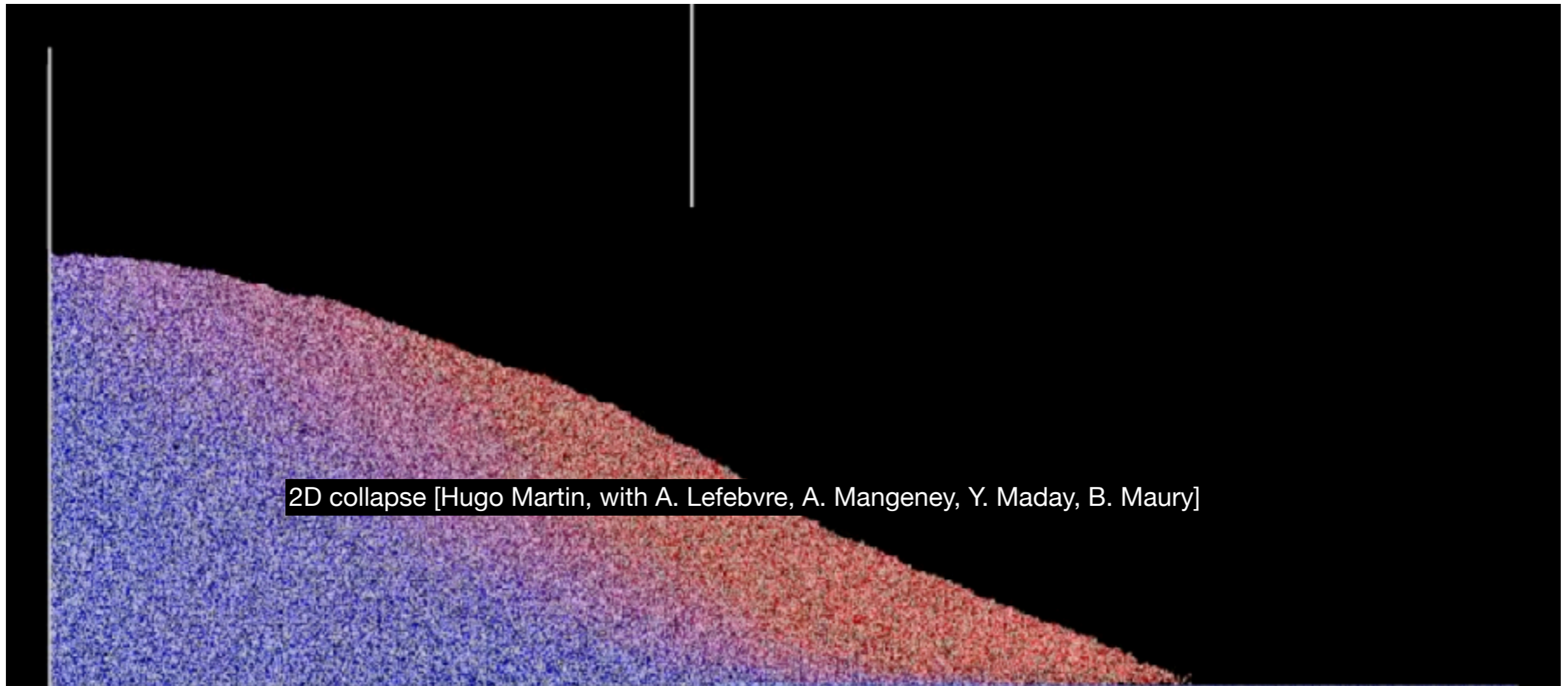


# Application: granular collapse

► Friction

► Spherical particles

► Hugo Martin [LJLL, IPGP]



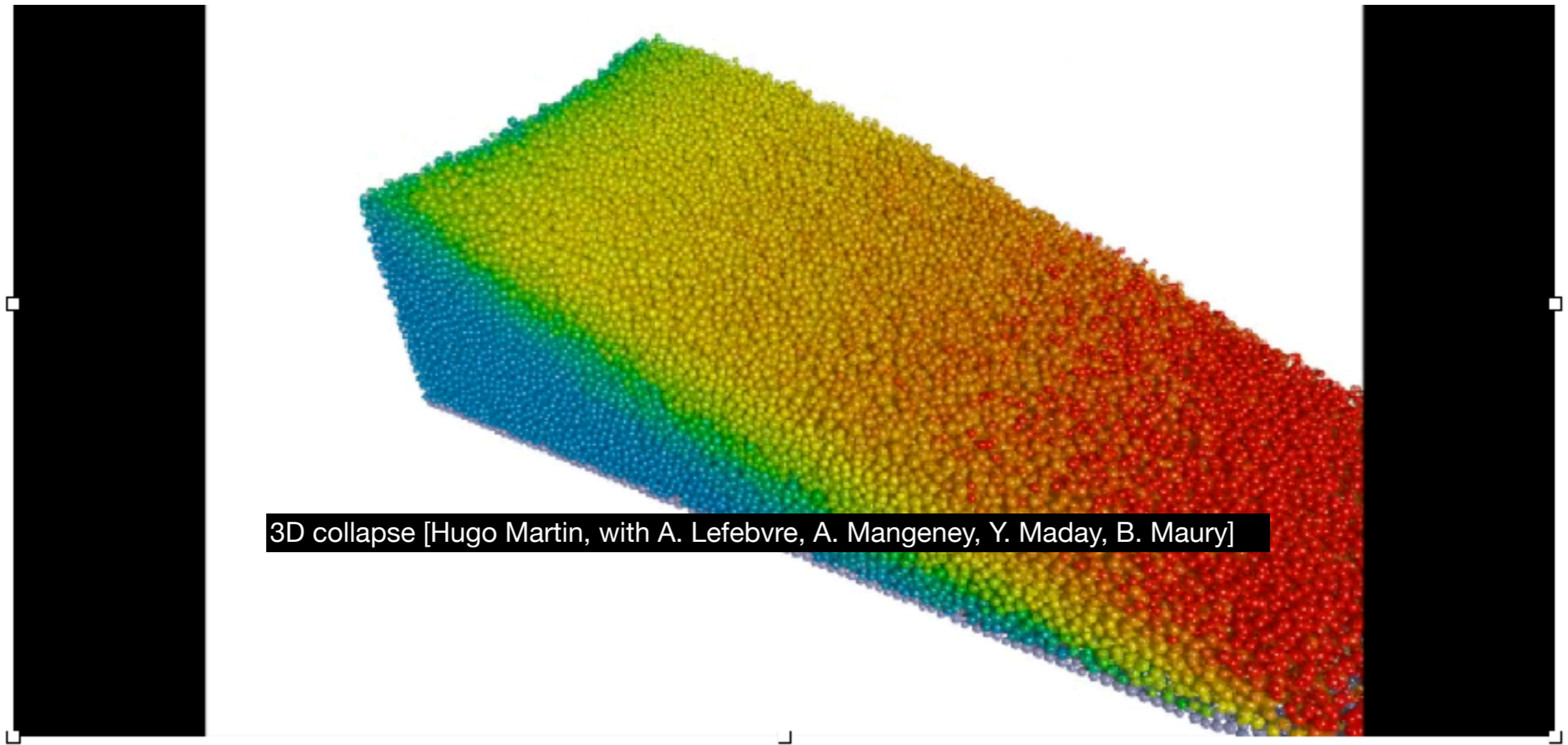
- An optimization-based model for dry granular flows: application to granular collapse on erodible beds, with H. Martin, A. Mangeney, Y. Maday, B. Maury, Submitted, hal-03790427

# Application: granular collapse

► Friction

► Spherical particles

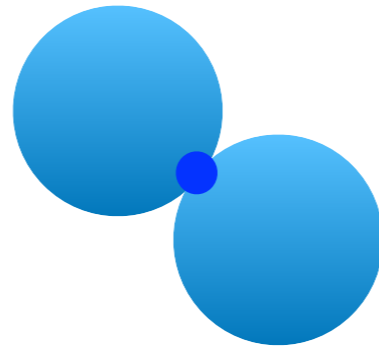
► Hugo Martin [LJLL, IPGP]



3D collapse [Hugo Martin, with A. Lefebvre, A. Mangeney, Y. Maday, B. Maury]

# Contact Dynamics Model including lubrication in suspensions

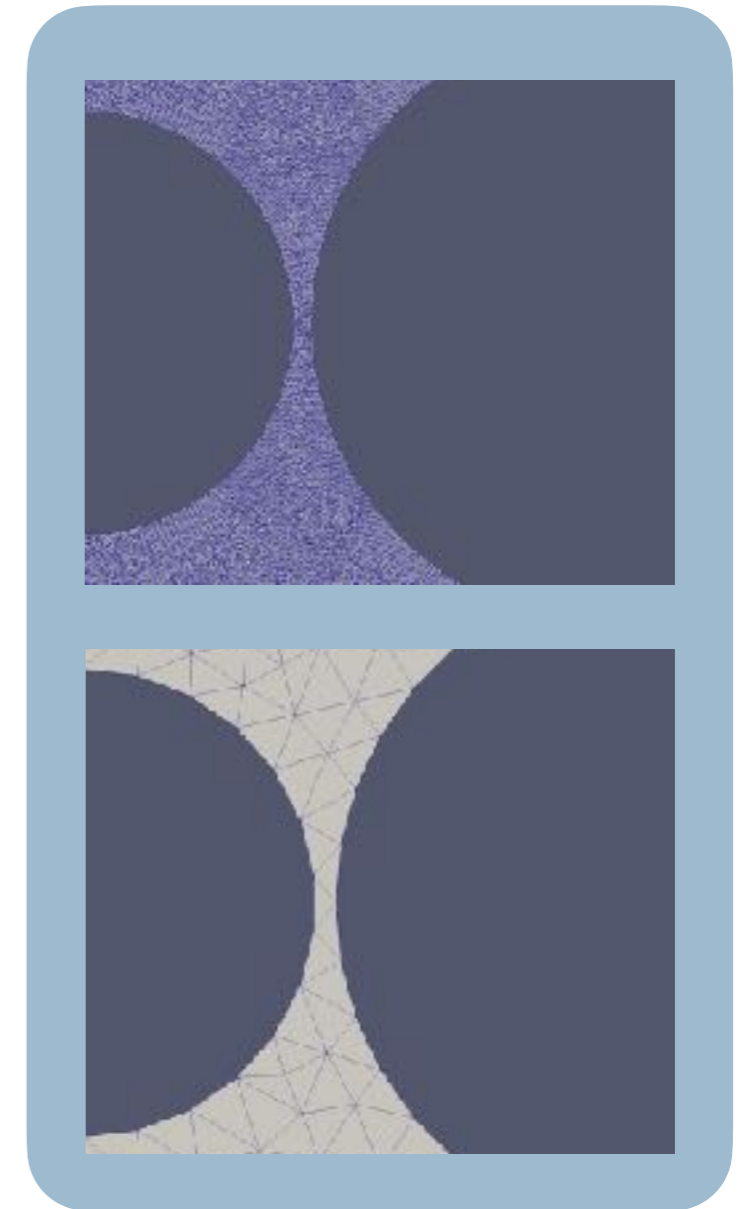
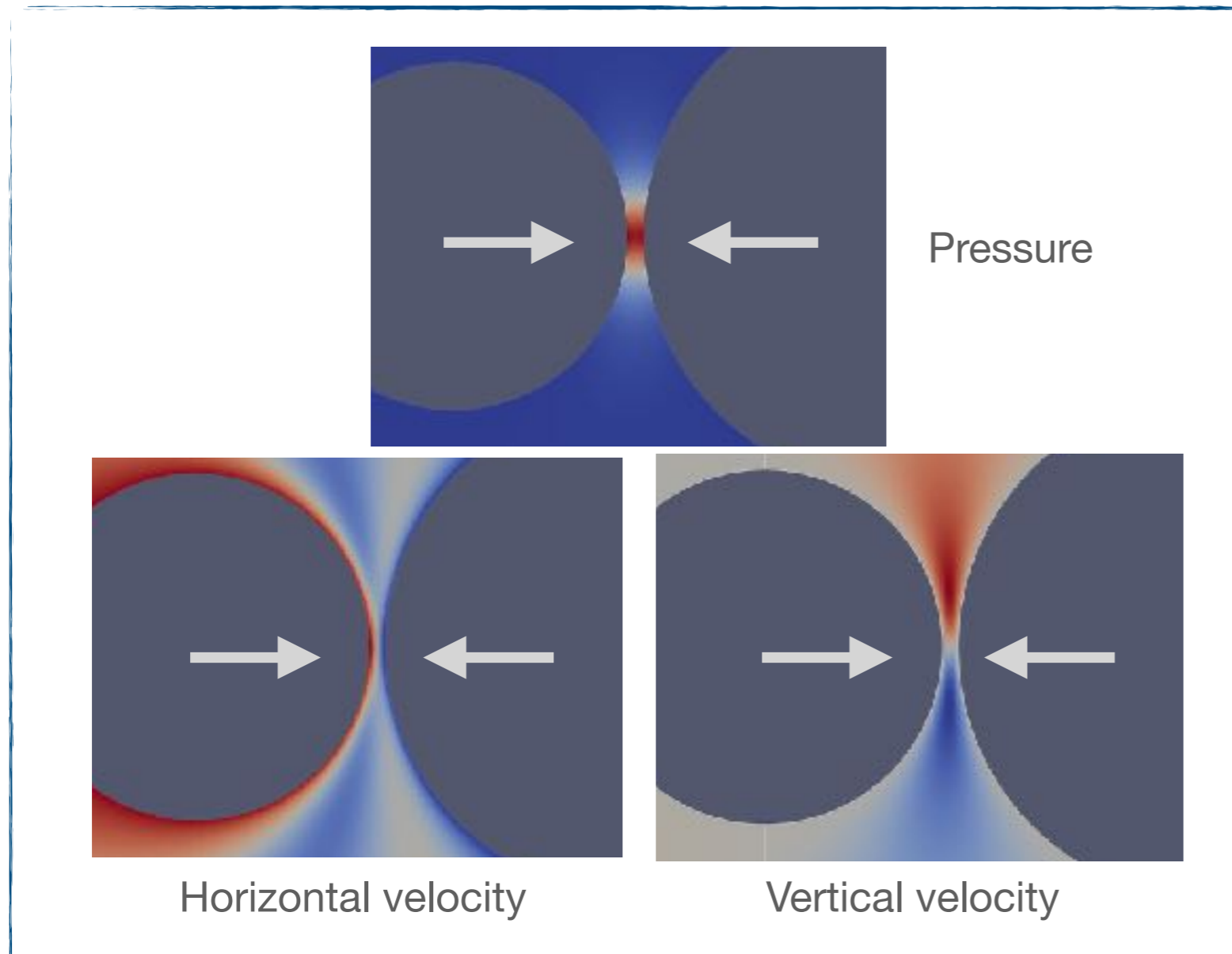
Contact law



Gluey contact model

# Lubrication and Numerical simulations.

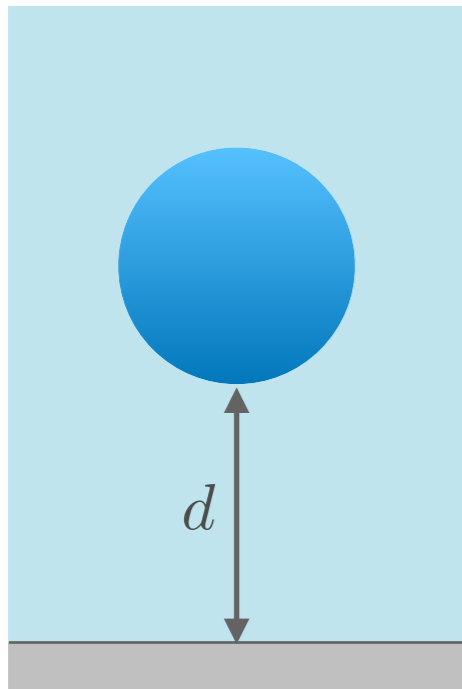
► Dense suspensions  $\Rightarrow$  Close interactions due to the fluid



***Need for methods taking lubrication into account***

# A stiff problem.

Lubrication force



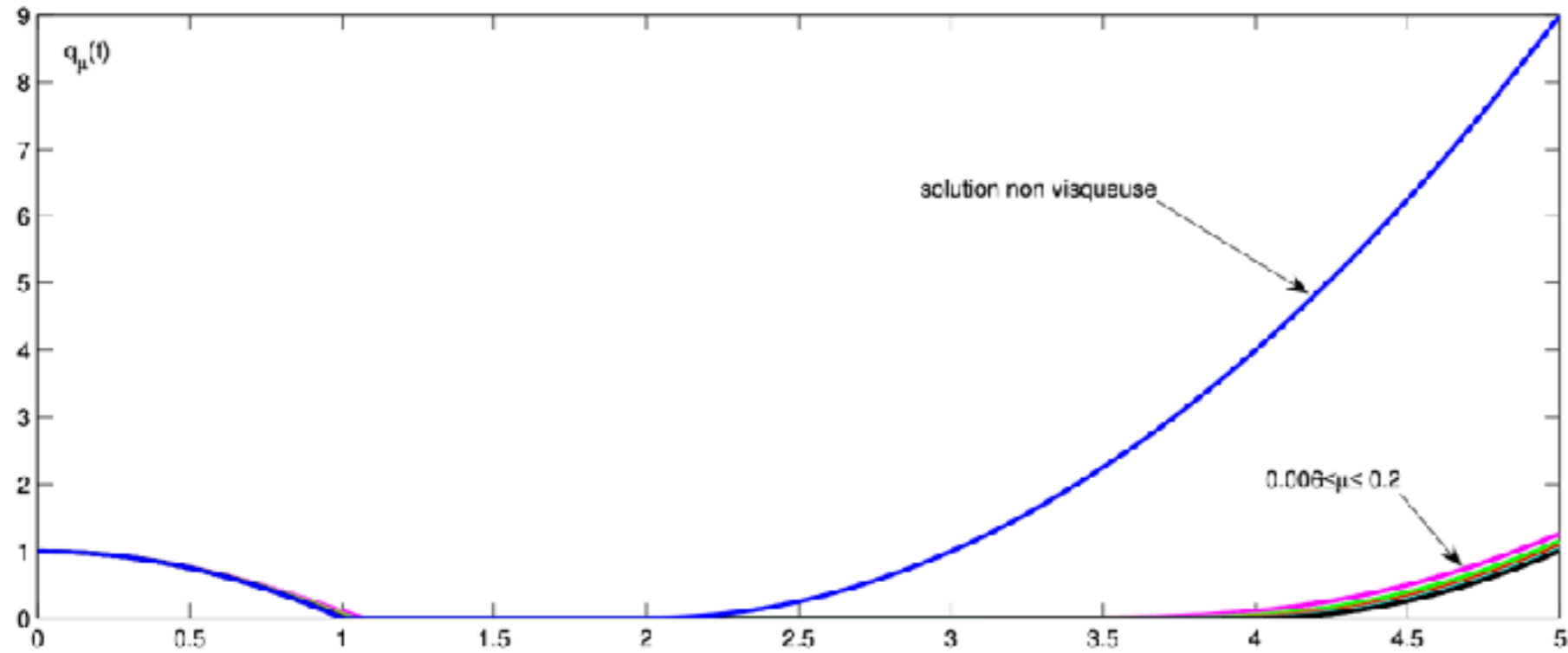
$$F_{lub}(d) = -6\pi\mu r^2 \frac{\dot{d}}{d}$$

[Cox, 1974]

$$m\ddot{q} = -6\pi\mu r^2 \frac{\dot{q}}{q} + m f_y$$

- $q(t) > 0$  for any  $t$
- BUT very small...

# Modeling lubrication: the gluey contact model.

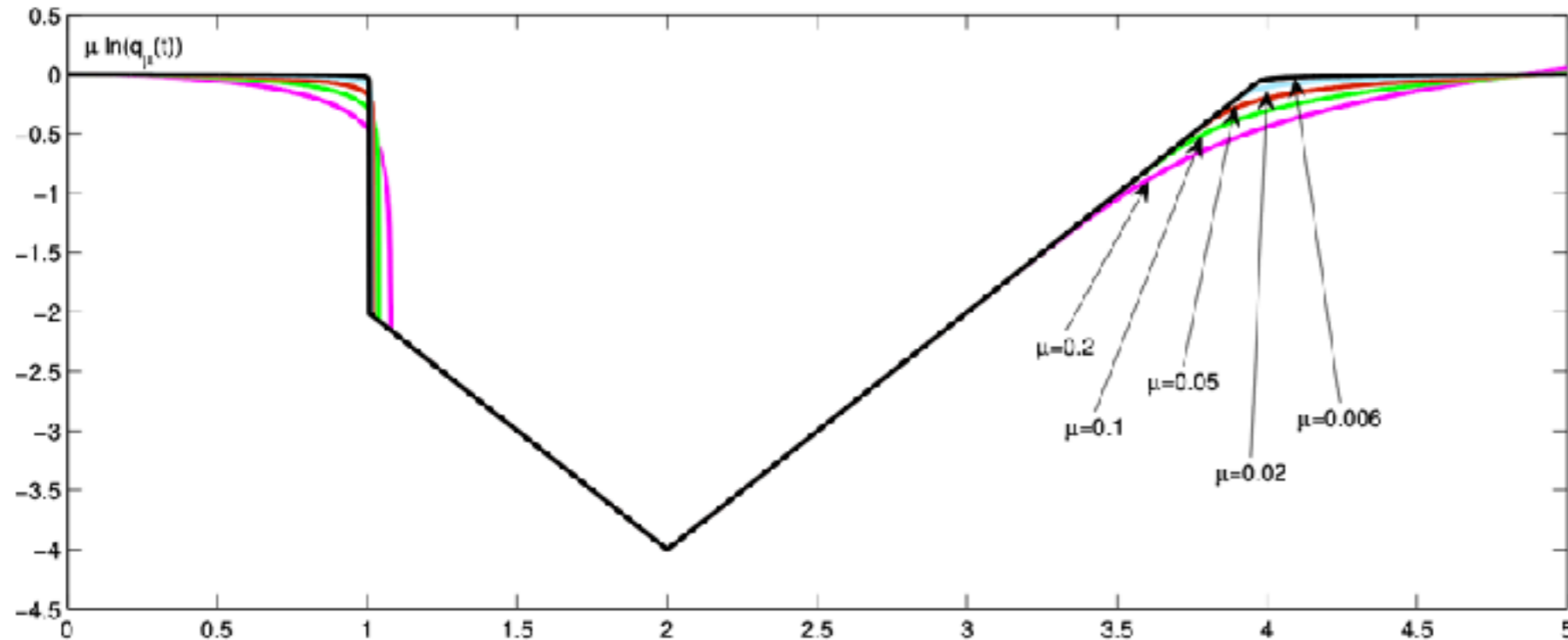


$$f_y = -2 \mathbf{1}_{[0,2]} + 2 \mathbf{1}_{[2,+\infty]}$$

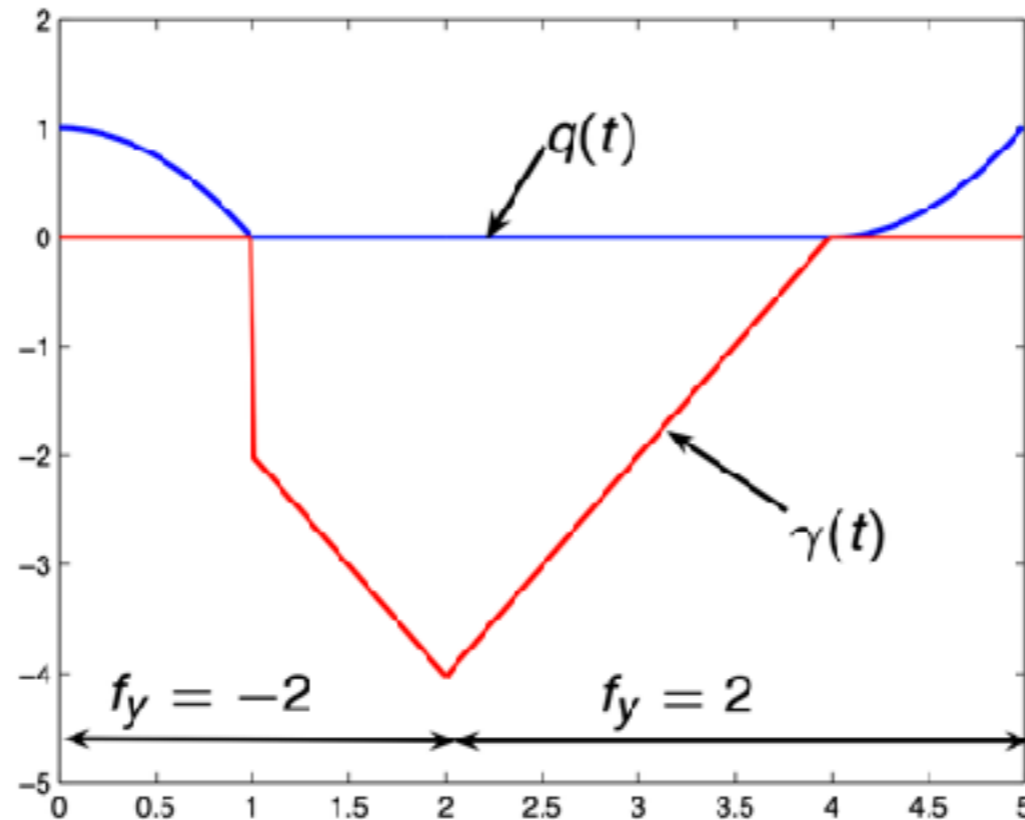
$$\ddot{q}_\mu = -\mu \frac{\dot{q}_\mu}{q_\mu} + f_y$$

$$\dot{q}_\mu(0) = 0$$

$$q_\mu(0) = 1$$



# Modeling lubrication: the gluey contact model.



$$\dot{q}^+ = P_{C_{q,\gamma}} \dot{q}^-$$

$$m\ddot{q} = m f_y + \lambda$$

$$\text{supp}(\lambda) \subset \{t, q(t) = 0\}$$

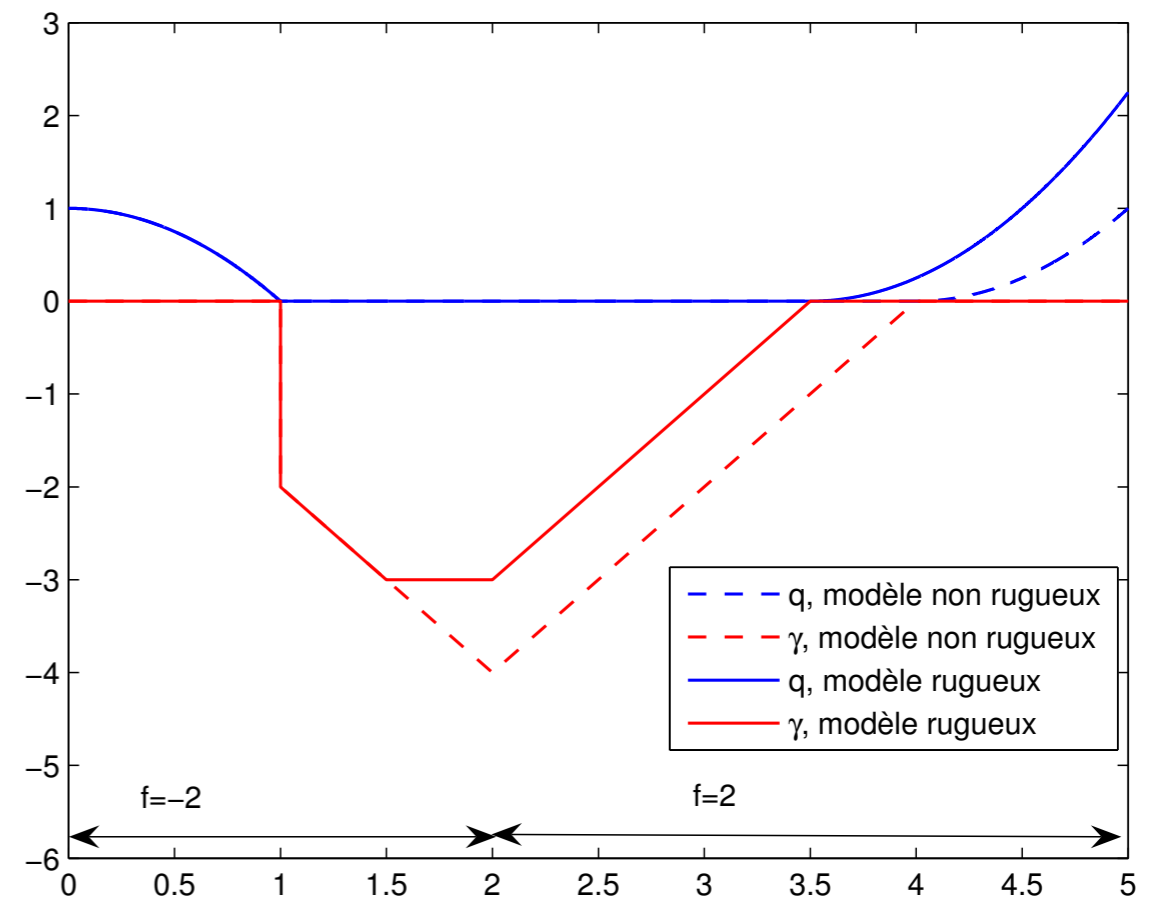
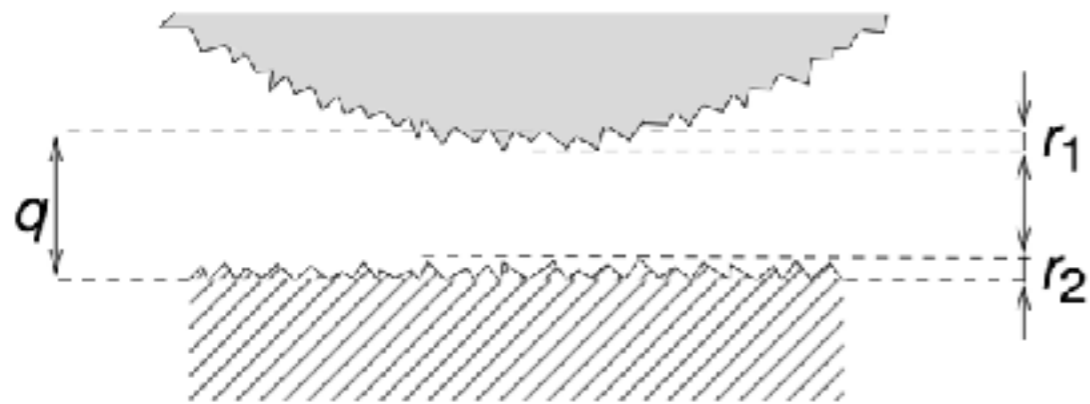
$$\dot{\gamma} = -\lambda$$

$$q \geq 0, \gamma \leq 0$$

$$C_{q,\gamma} = \begin{cases} \{0\} & \text{si } \gamma^- < 0 \\ \mathbb{R}^+ & \text{si } \gamma^- = 0 \\ & q = 0 \\ \mathbb{R} & \text{sinon} \end{cases}$$

- B. Maury, A gluey particle model, ESAIM Proceedings, July 2007, Vol.18, 133-142
- A. Lefebvre, Numerical simulation of gluey particles, M2AN, 43:53-80 (2009)

# Modeling lubrication: the gluey contact model.

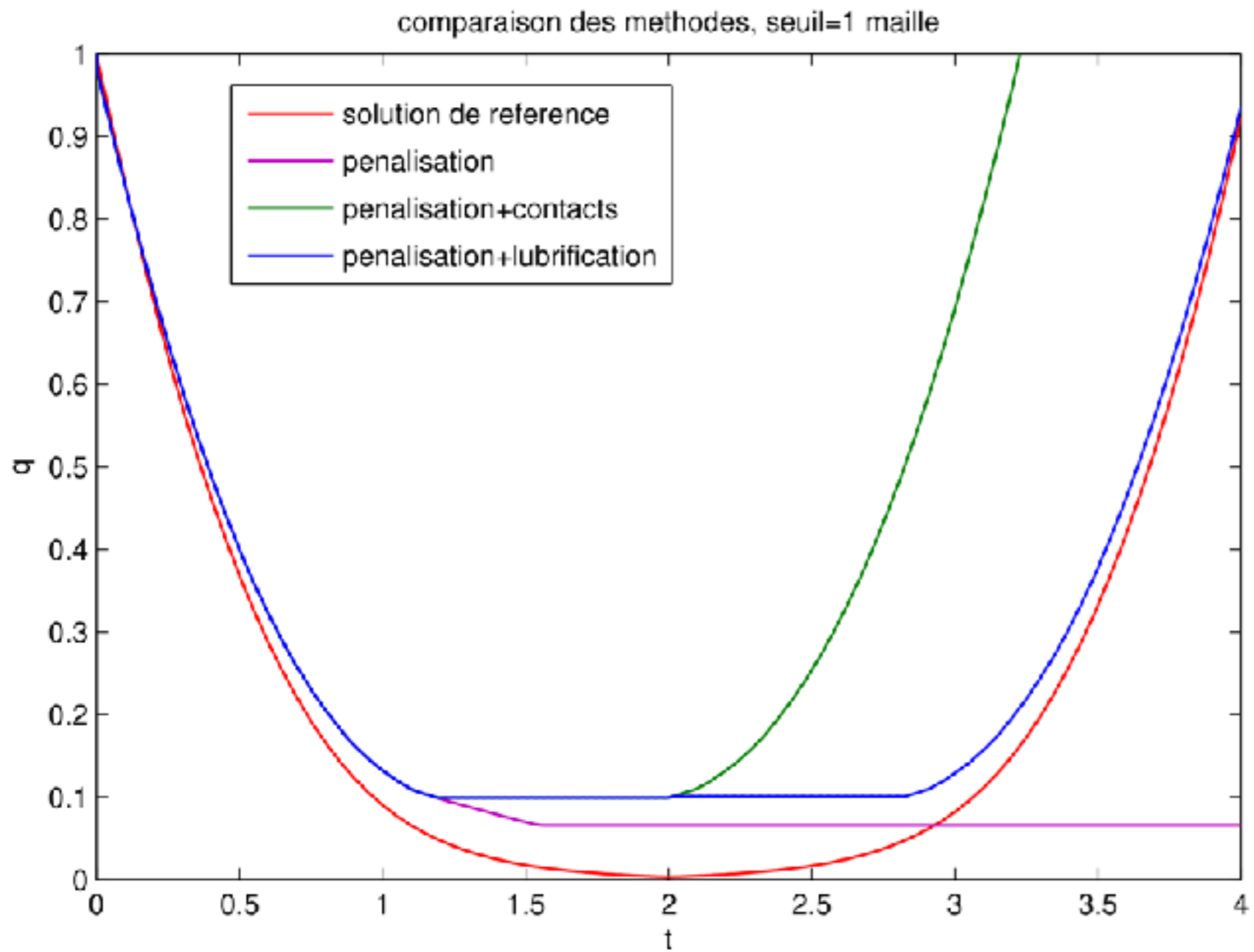


- Roughness  $\implies$  contact
- Model : contact for  $q = r_1 + r_2$

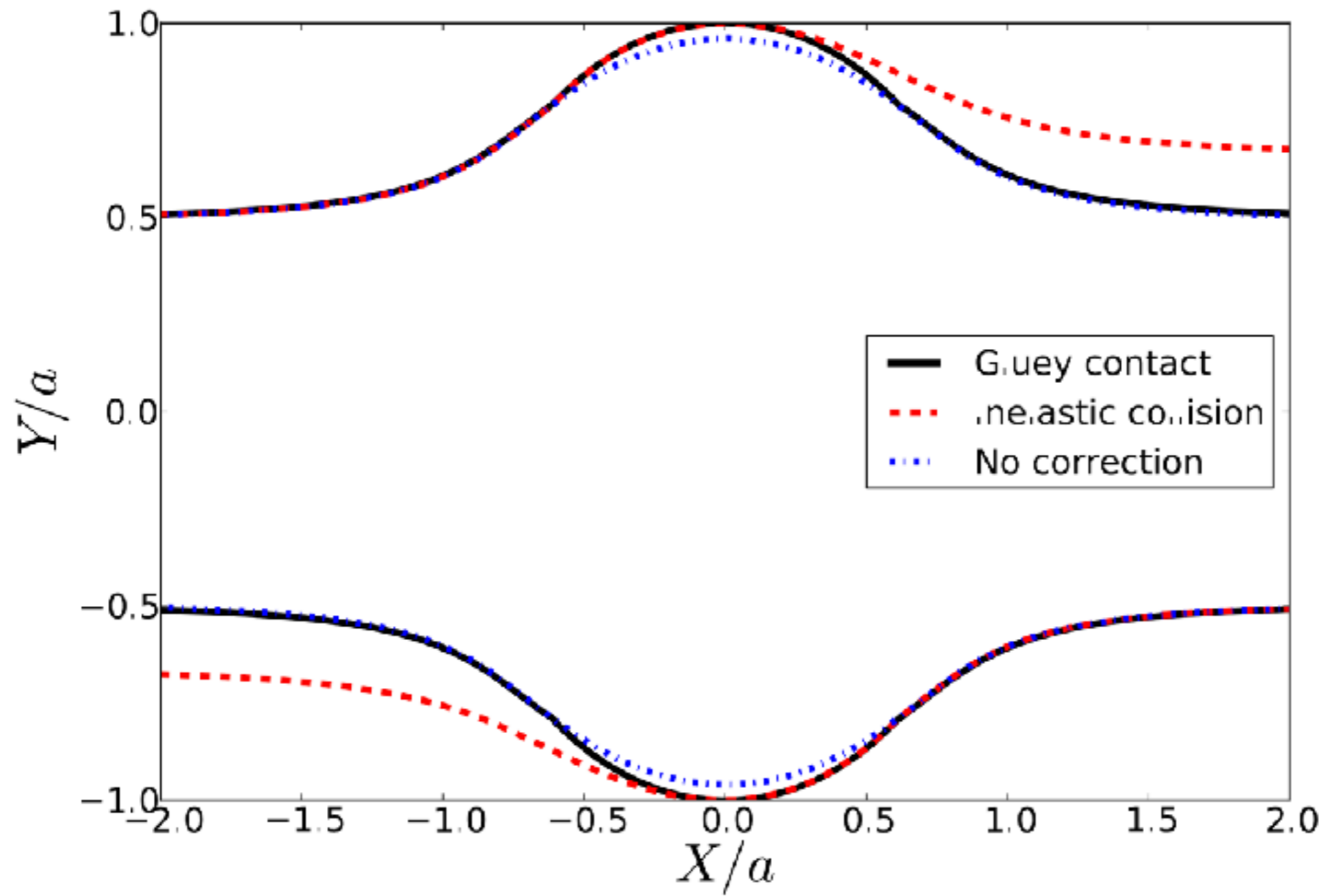
$\implies$  Threshold for  $\gamma$  :  $\gamma \geq \gamma_{min} = \mu \ln(r_1 + r_2)$



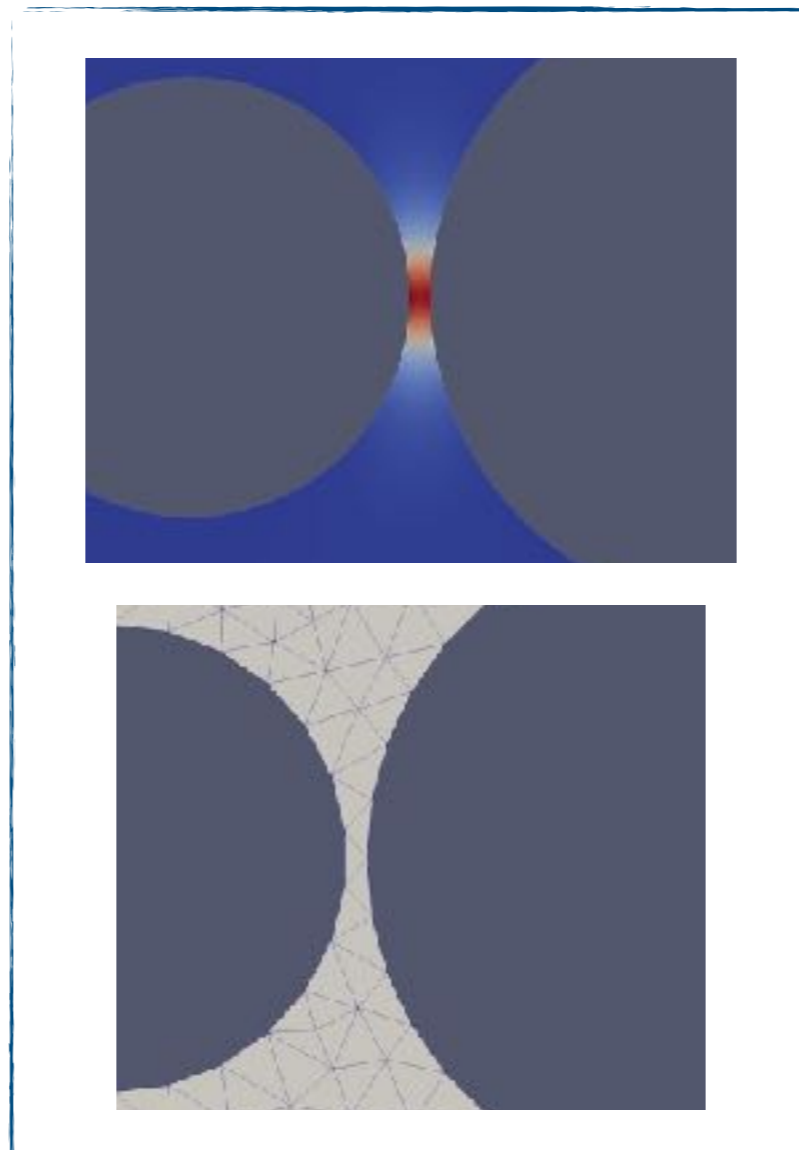
# Coupling lubrication model and fluid solver



# Coupling lubrication model and fluid solver

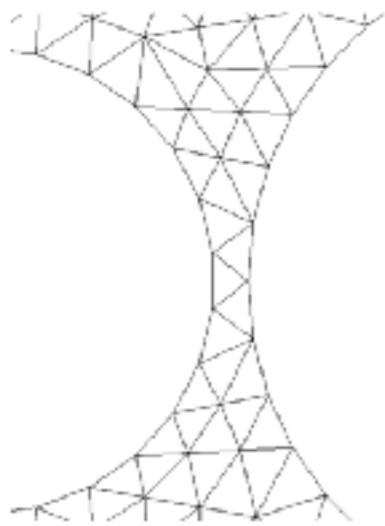


# Taking lubrication into account when using direct fluid/particle solvers

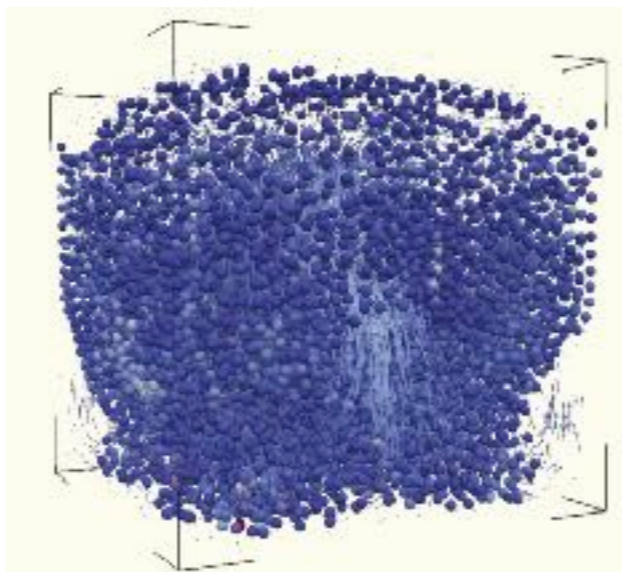


# Direct numerical simulations

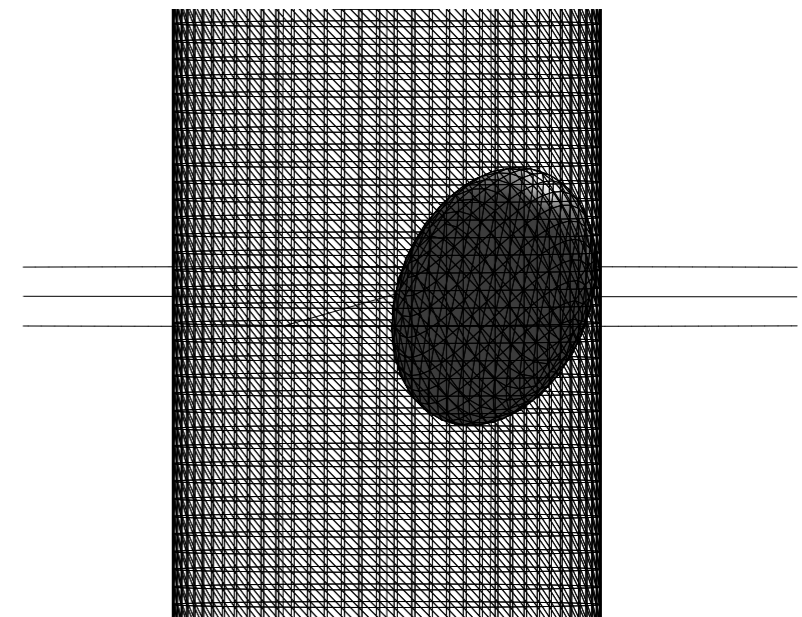
- ▶ Solving the fluid-particles PDE model
- ▶ **Approximation of the velocity and pressure fields**
- ▶ Underlying mesh
- ▶ Converging results



Freefem++

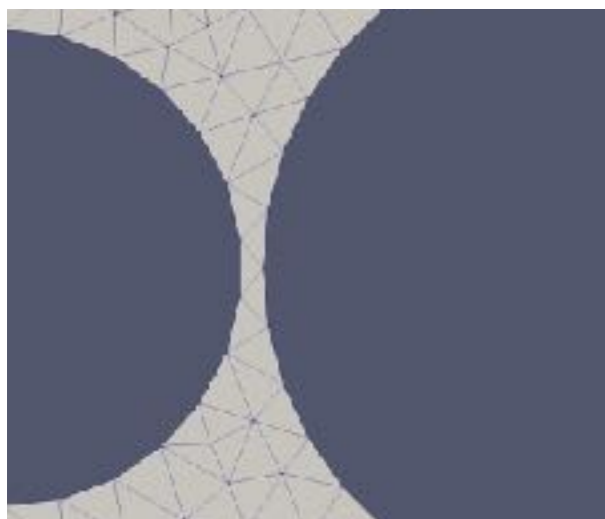
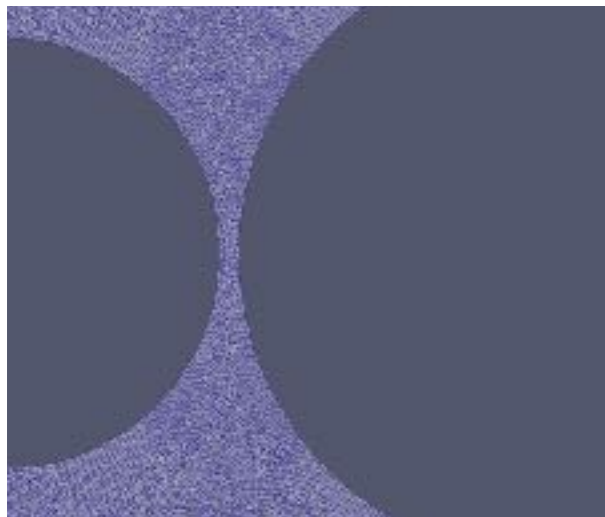
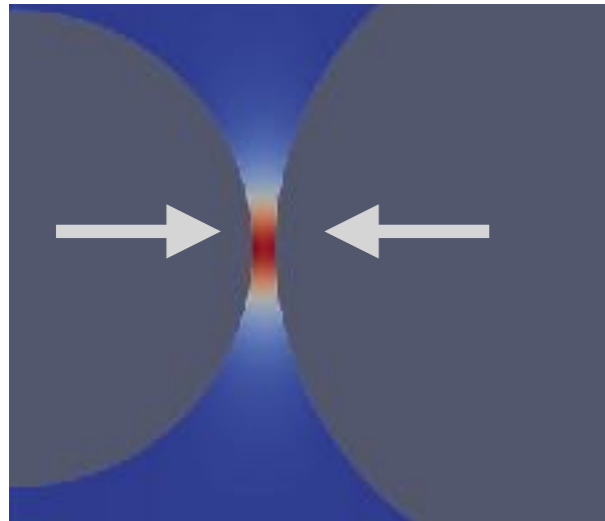


CAFES (CMAP-LMO)



MyBEM (CMAP)

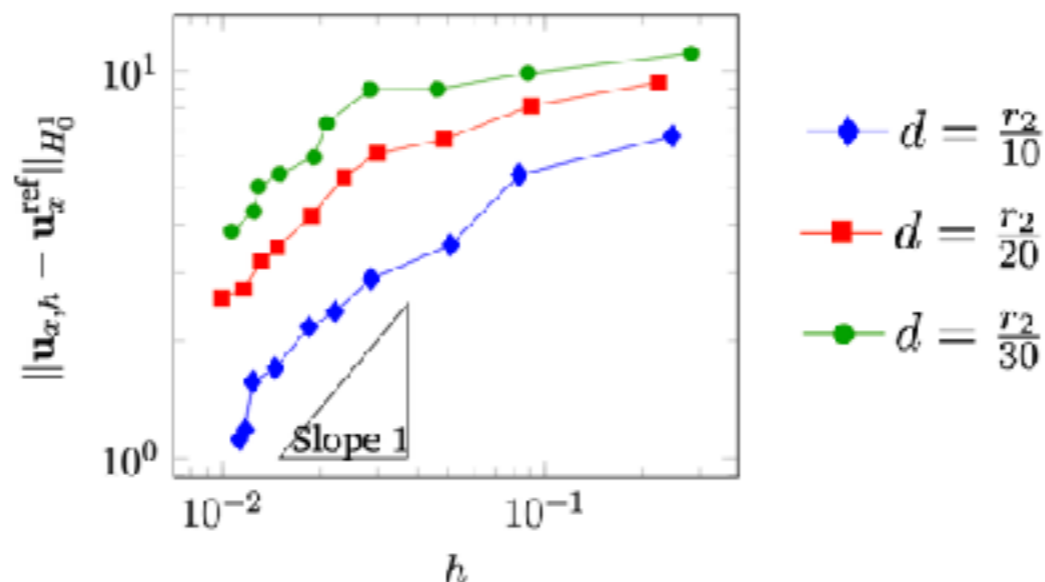
# Lubrication phenomenon



▶ Numerical resolution of a singular problem...

$$\begin{aligned} -\mu\Delta\mathbf{u} + \nabla p &= 0 & \text{in } \mathcal{F} \\ \nabla \cdot \mathbf{u} &= 0 & \text{in } \mathcal{F} \\ \mathbf{u} &= \mathbf{u}^* & \text{on } \partial B \end{aligned}$$

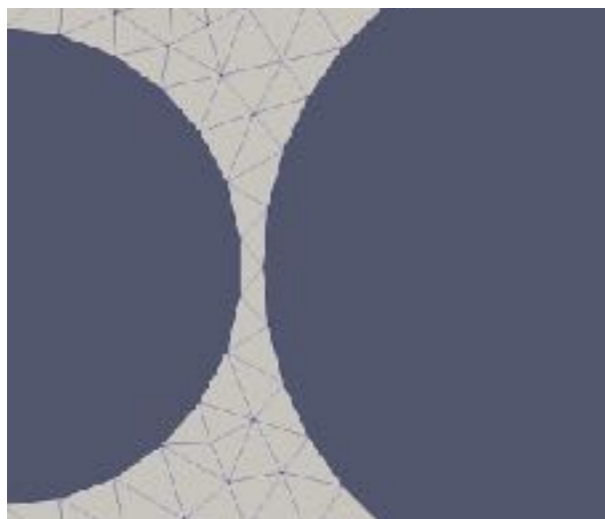
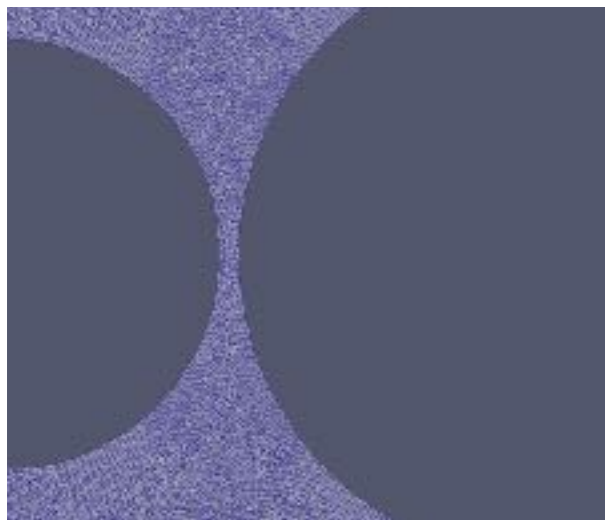
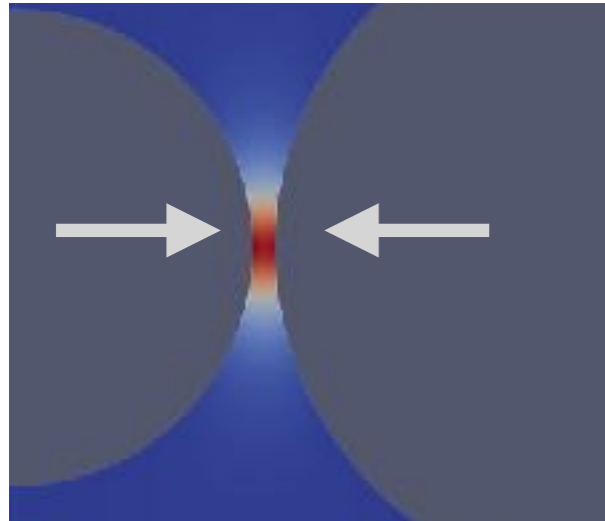
$$\|\mathbf{u} - \mathbf{u}_h\| \leq C \|(\mathbf{u}, p)\| h^\alpha$$



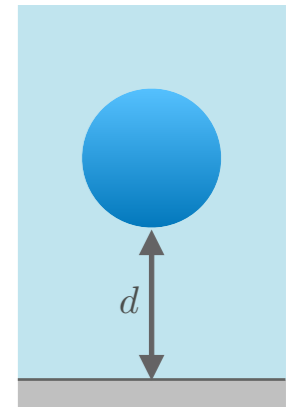
Blows up  
when the distance  
goes to zero...

***Need for methods taking lubrication into account***

# An explicit asymptotic expansion



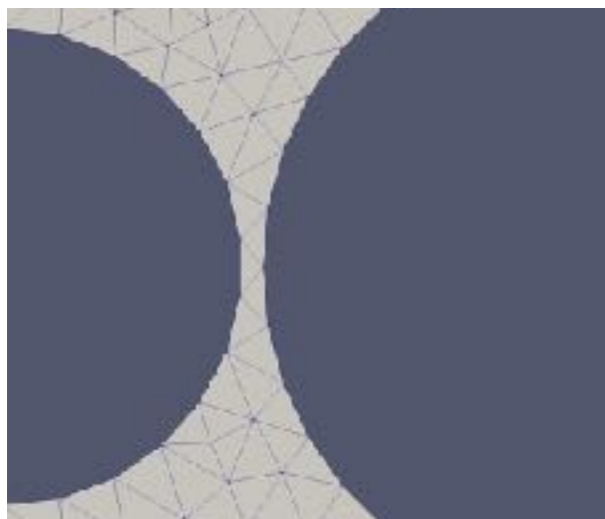
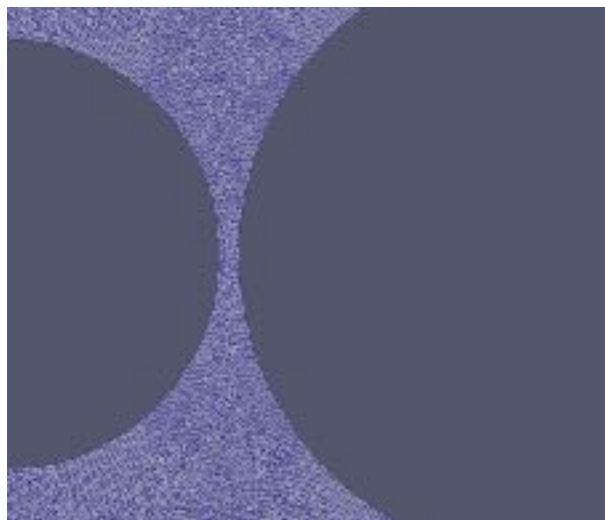
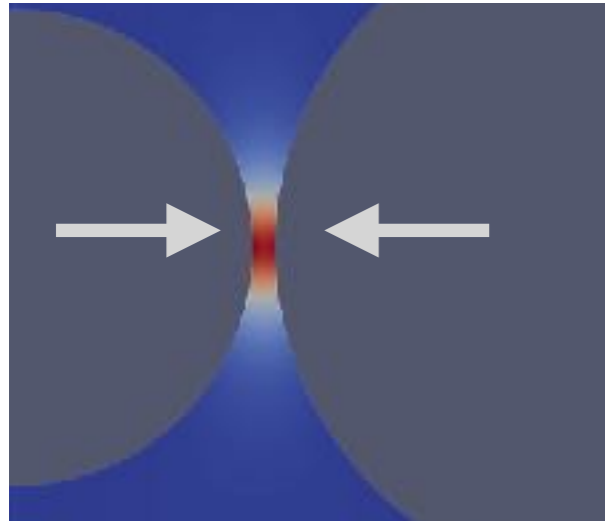
Lubrication force



$$F_{lub}(d) = -6\pi\mu r^2 \frac{\dot{d}}{d}$$

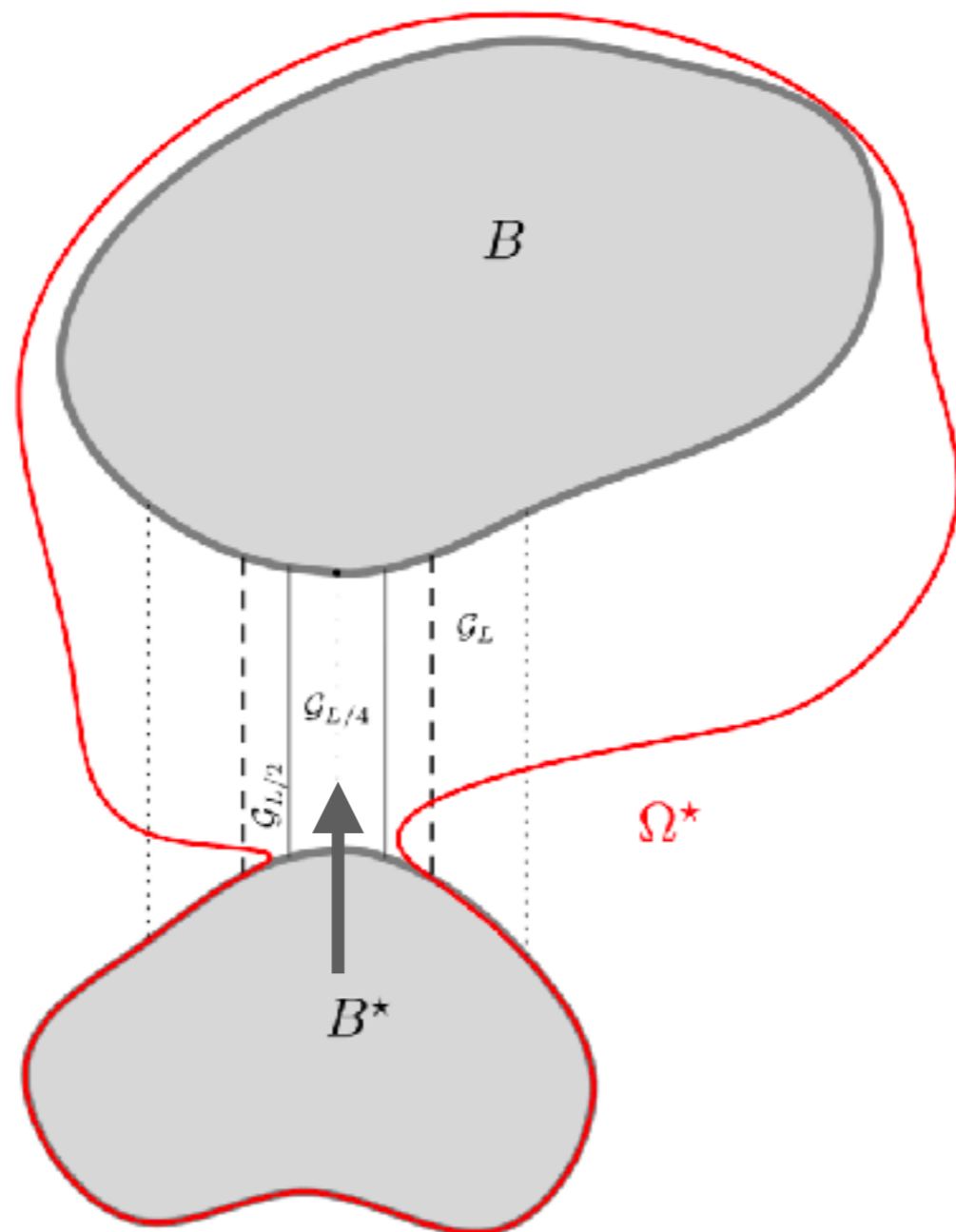
[Cox, 1974]

# An explicit asymptotic expansion

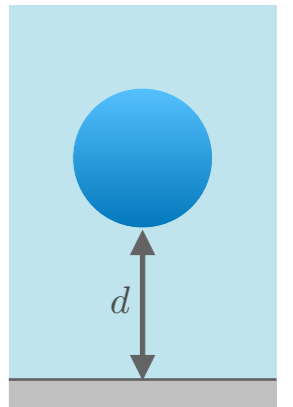


Explicit asymptotic expansion  
[Hillairet, Kelai, 2015]

$$(\mathbf{u}, p) = (\mathbf{u}^{\text{sing}}, p^{\text{sing}}) + (\mathbf{u}^{\text{reg}}, p^{\text{reg}})$$



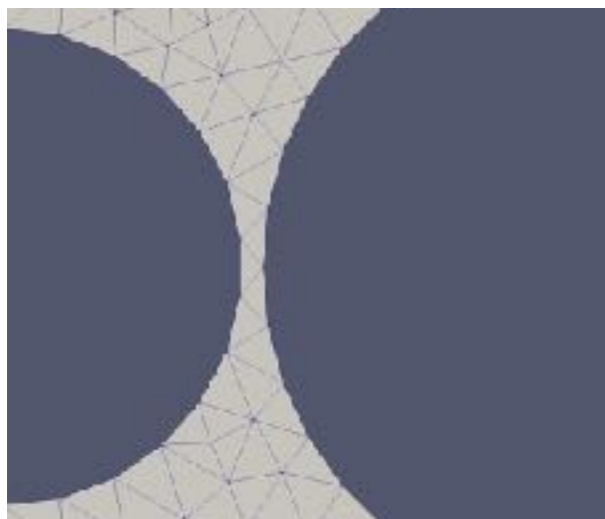
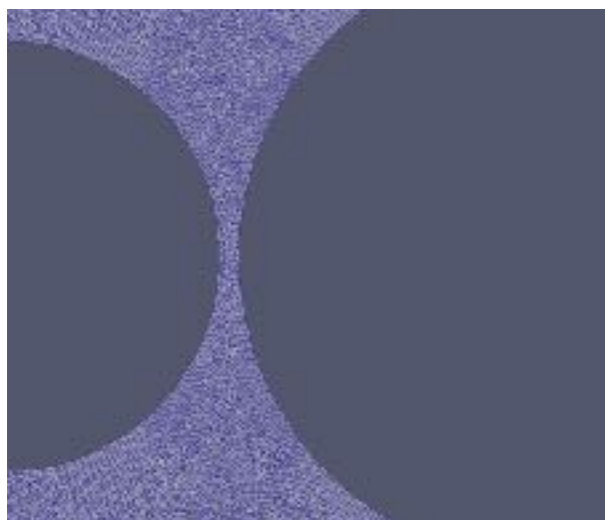
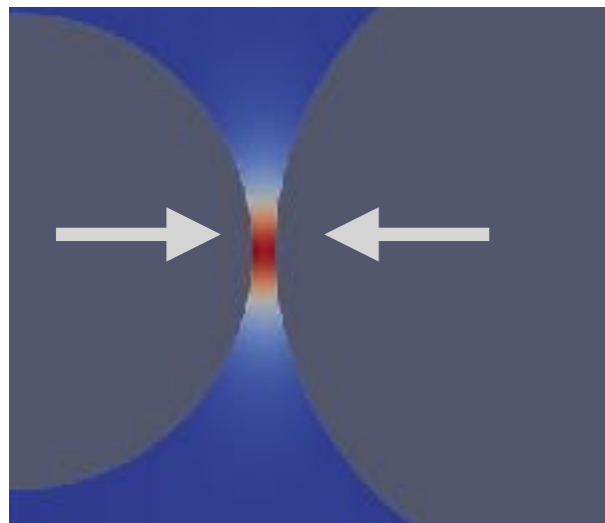
Lubrication force



$$F_{\text{lub}}(d) = -6\pi\mu r^2 \frac{\dot{d}}{d}$$

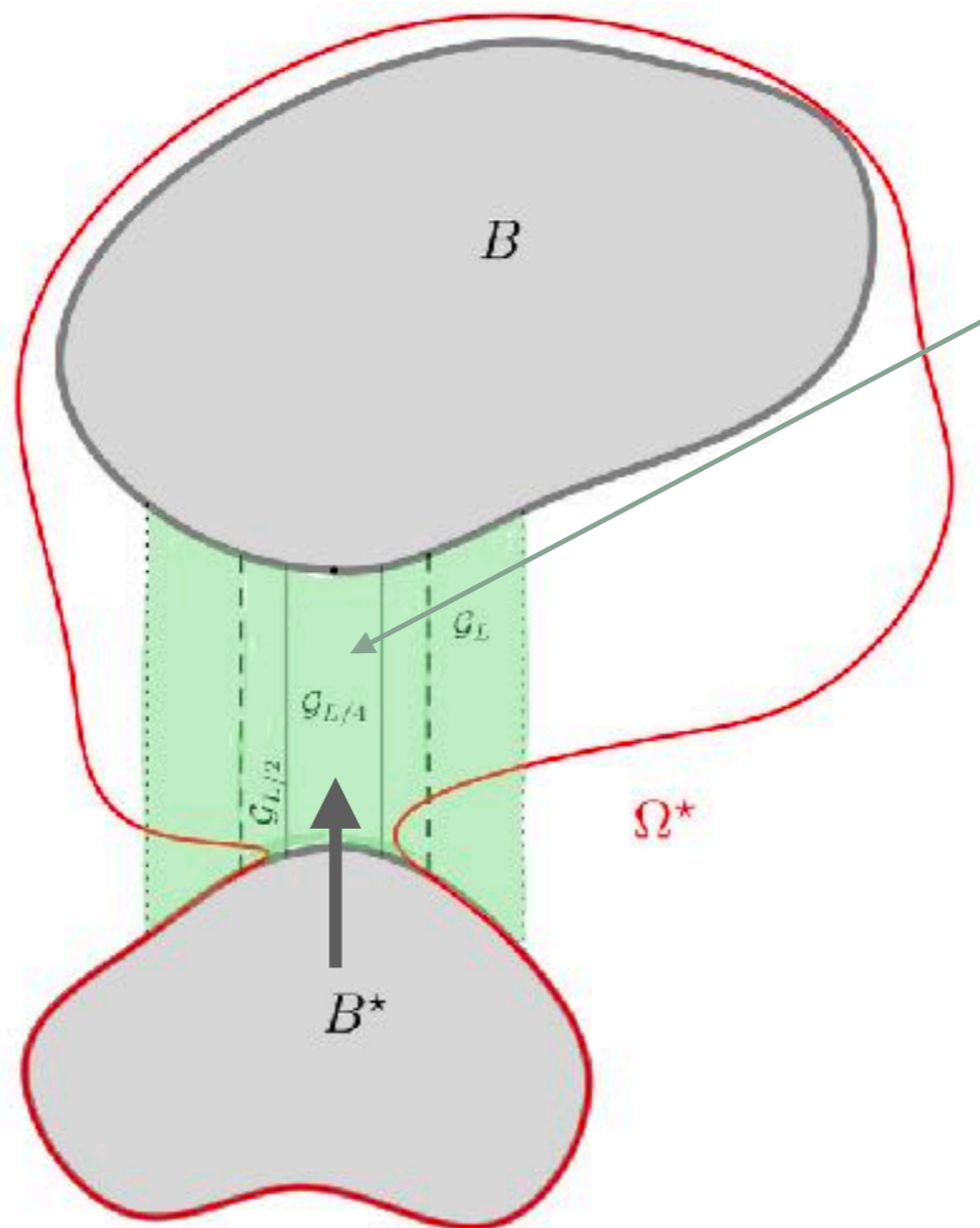
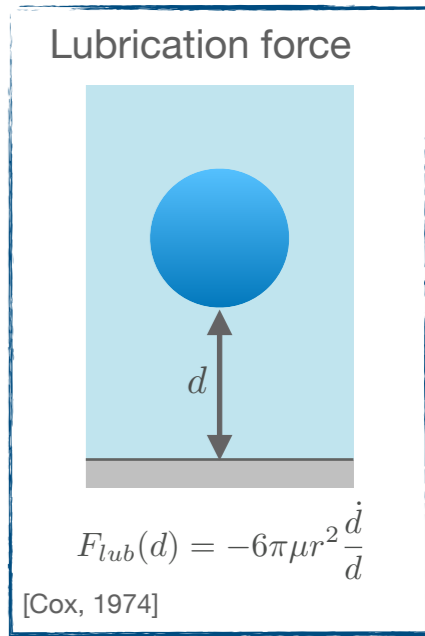
[Cox, 1974]

# An explicit asymptotic expansion



Explicit asymptotic expansion  
[Hillairet, Kelai, 2015]

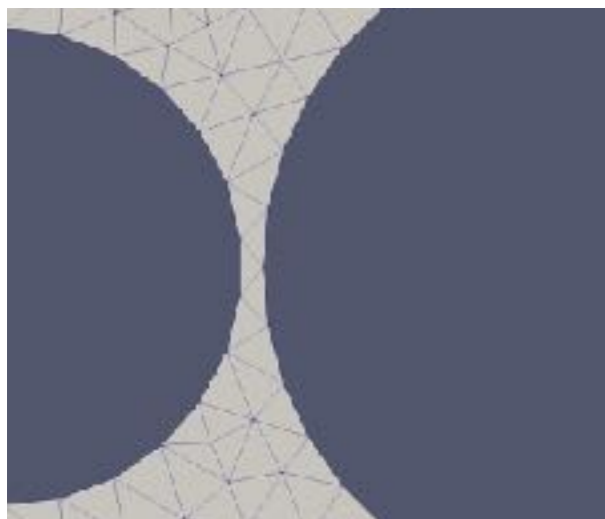
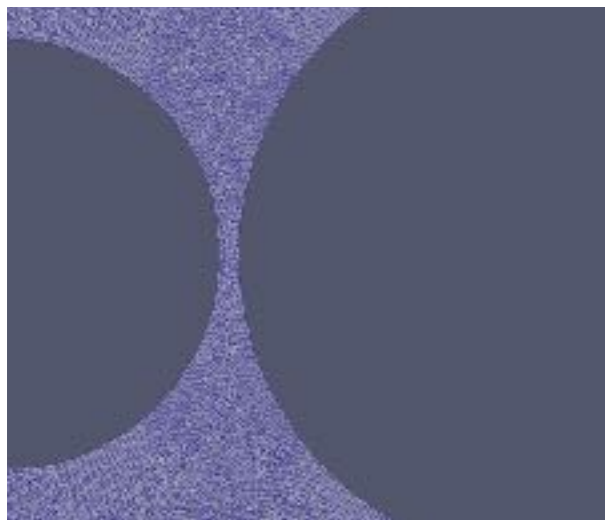
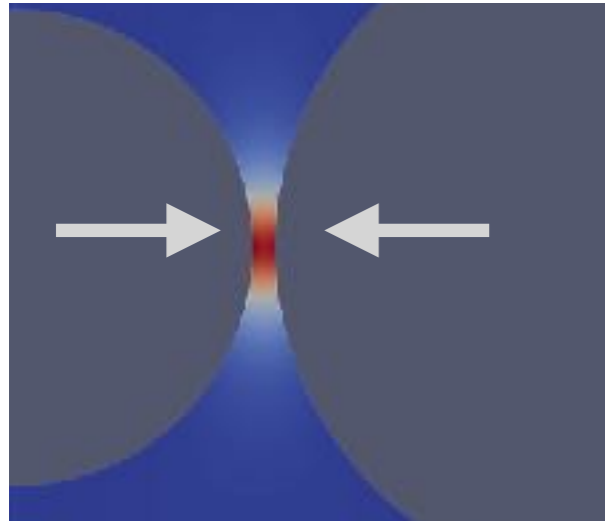
$$(\mathbf{u}, p) = (\mathbf{u}^{\text{sing}}, p^{\text{sing}}) + (\mathbf{u}^{\text{reg}}, p^{\text{reg}})$$



Divergence free explicit expansion

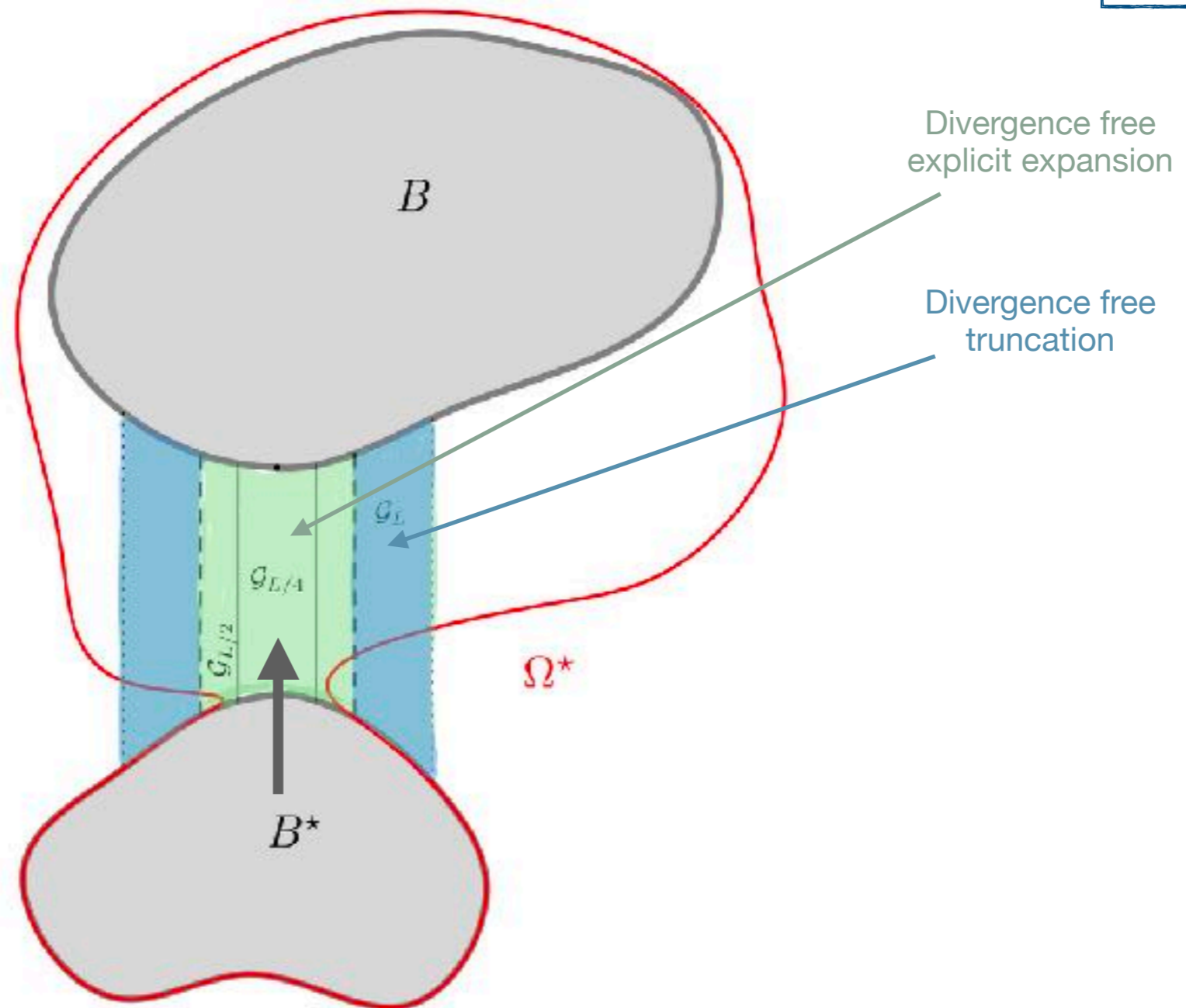
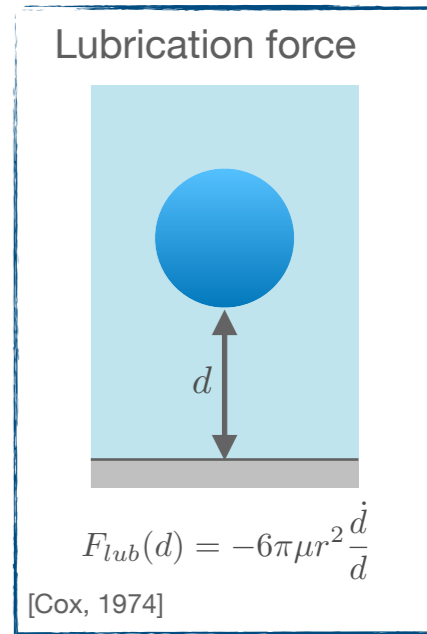


# An explicit asymptotic expansion

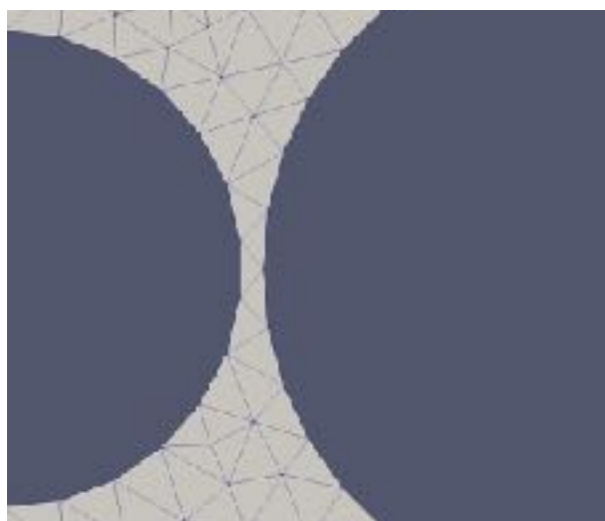
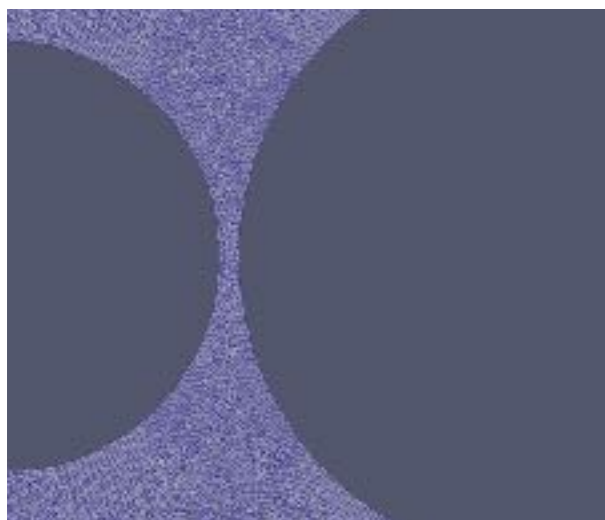
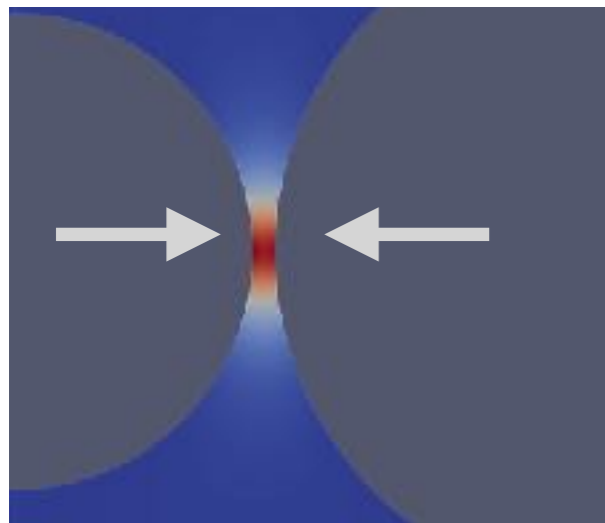


Explicit asymptotic expansion  
[Hillairet, Kelai, 2015]

$$(\mathbf{u}, p) = (\mathbf{u}^{\text{sing}}, p^{\text{sing}}) + (\mathbf{u}^{\text{reg}}, p^{\text{reg}})$$

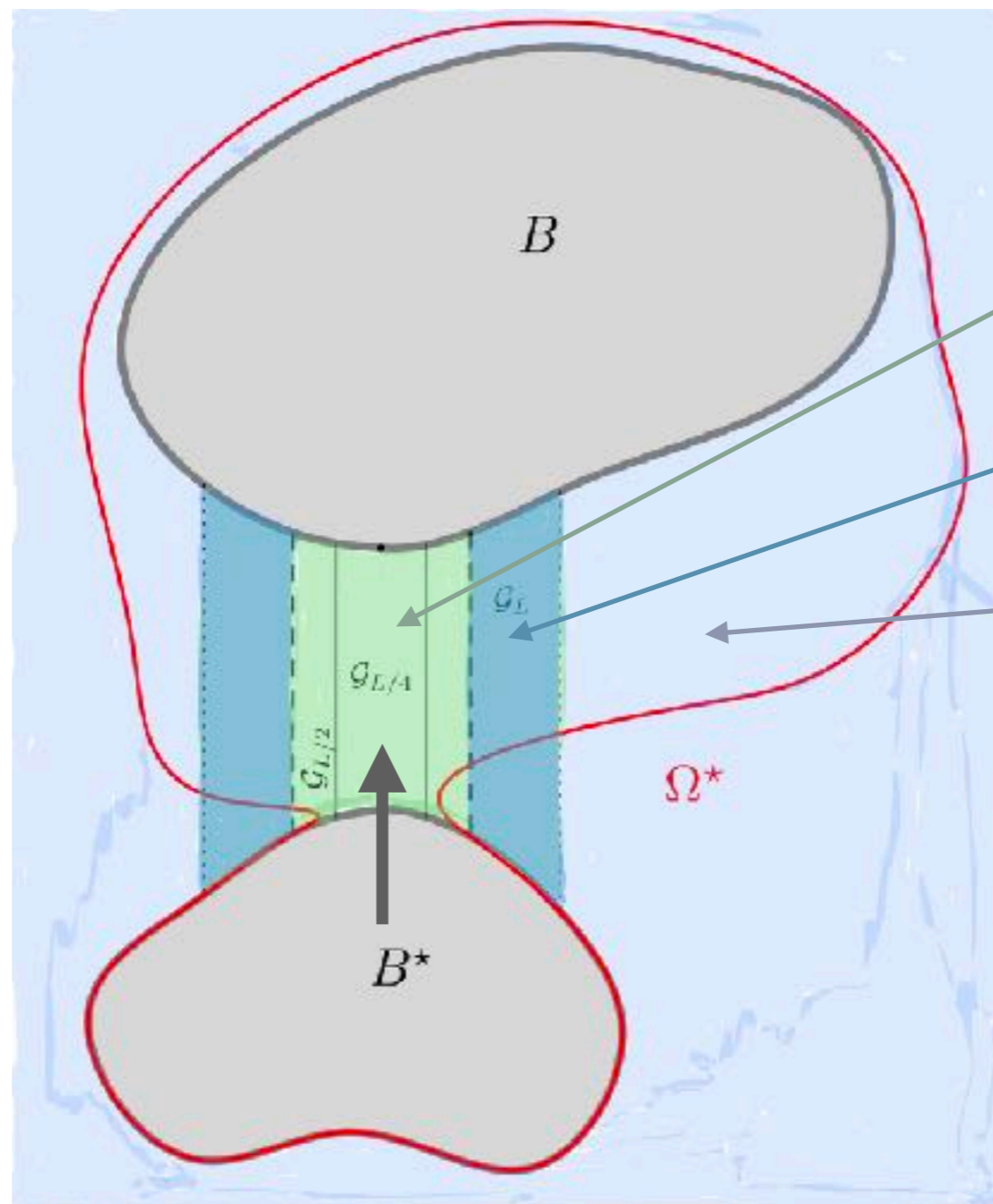
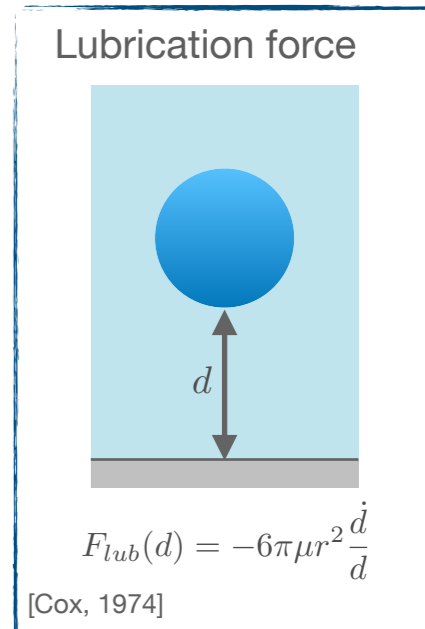


# An explicit asymptotic expansion



Explicit asymptotic expansion  
[Hillairet, Kelai, 2015]

$$(\mathbf{u}, p) = (\mathbf{u}^{\text{sing}}, p^{\text{sing}}) + (\mathbf{u}^{\text{reg}}, p^{\text{reg}})$$

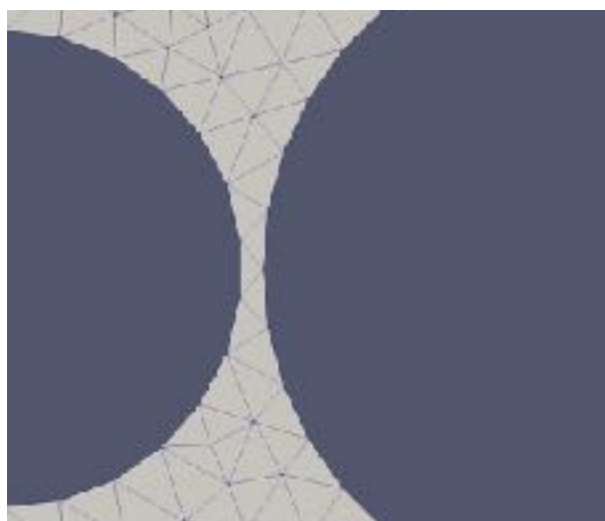
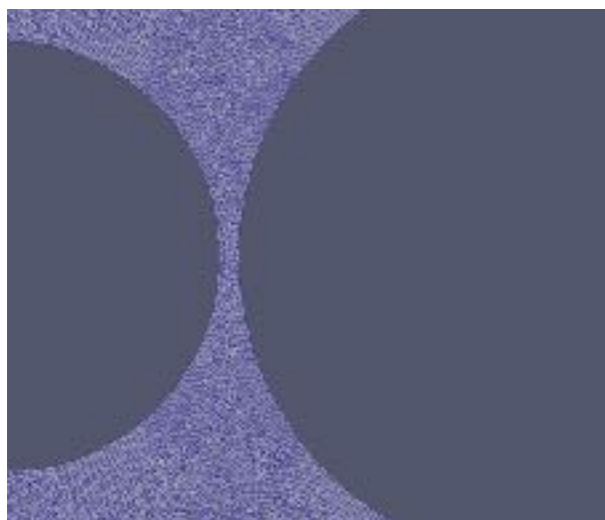
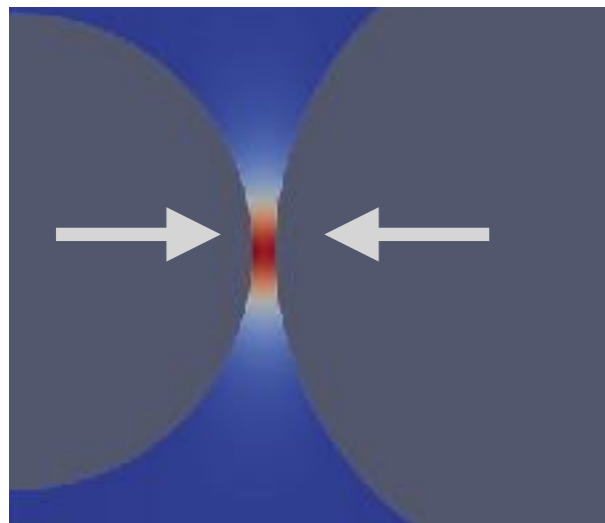


Divergence free explicit expansion

Divergence free truncation

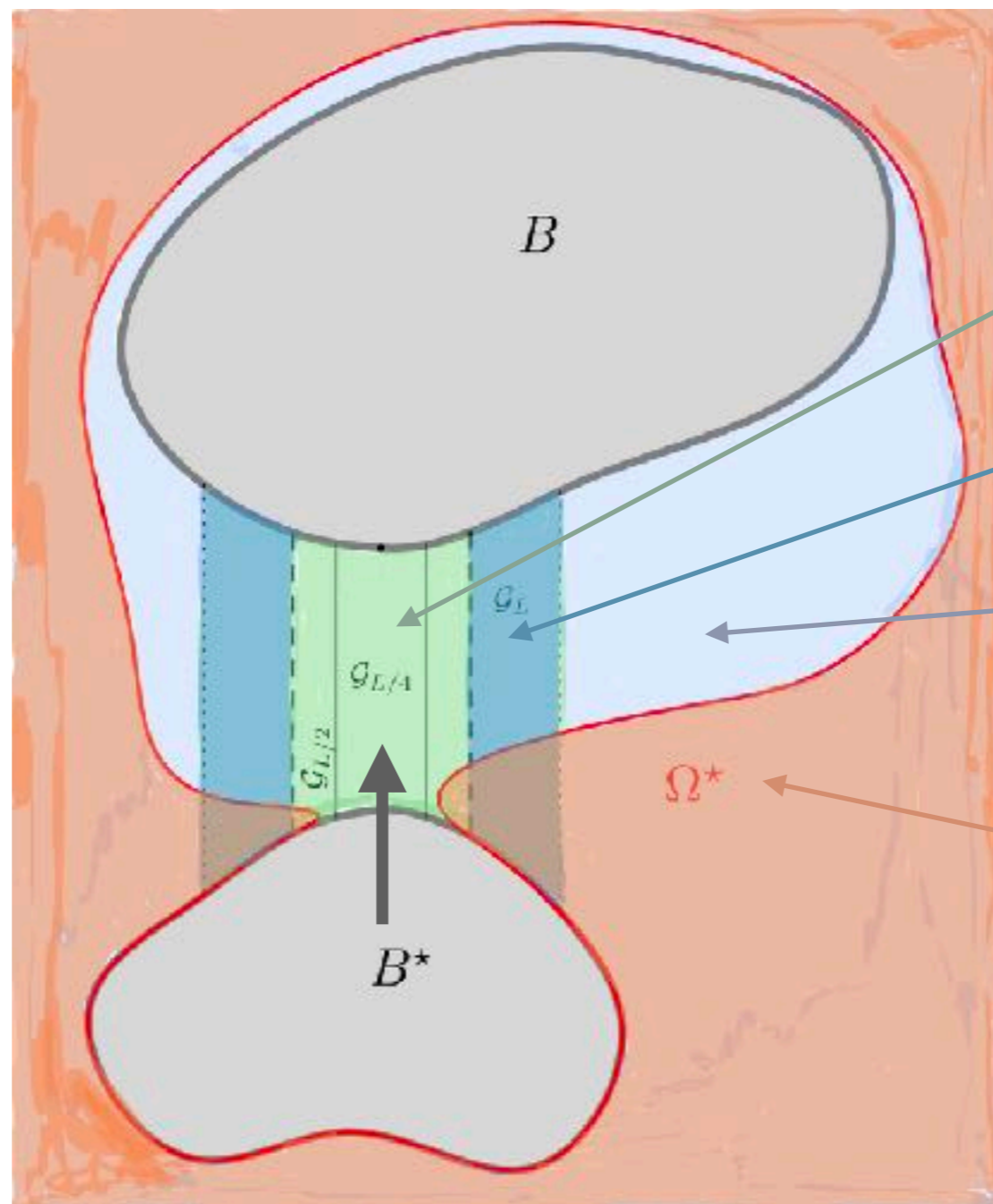
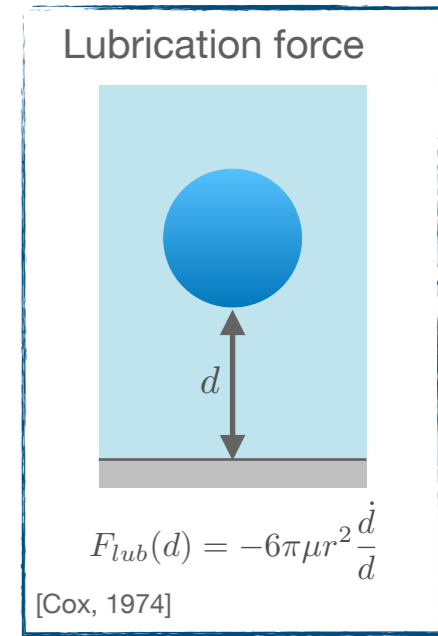
Vanishing extension

# An explicit asymptotic expansion



Explicit asymptotic expansion  
[Hillairet, Kelai, 2015]

$$(\mathbf{u}, p) = (\mathbf{u}^{\text{sing}}, p^{\text{sing}}) + (\mathbf{u}^{\text{reg}}, p^{\text{reg}})$$



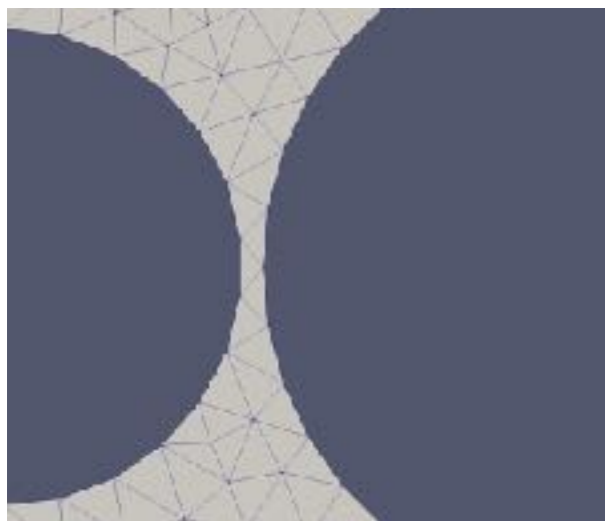
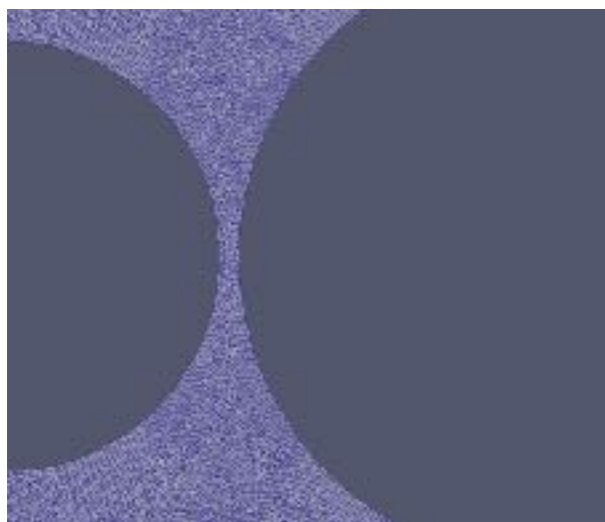
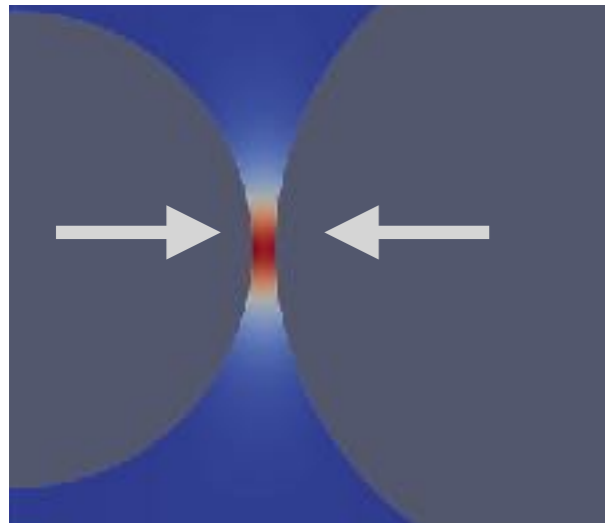
Divergence free explicit expansion

Divergence free truncation

Vanishing extension

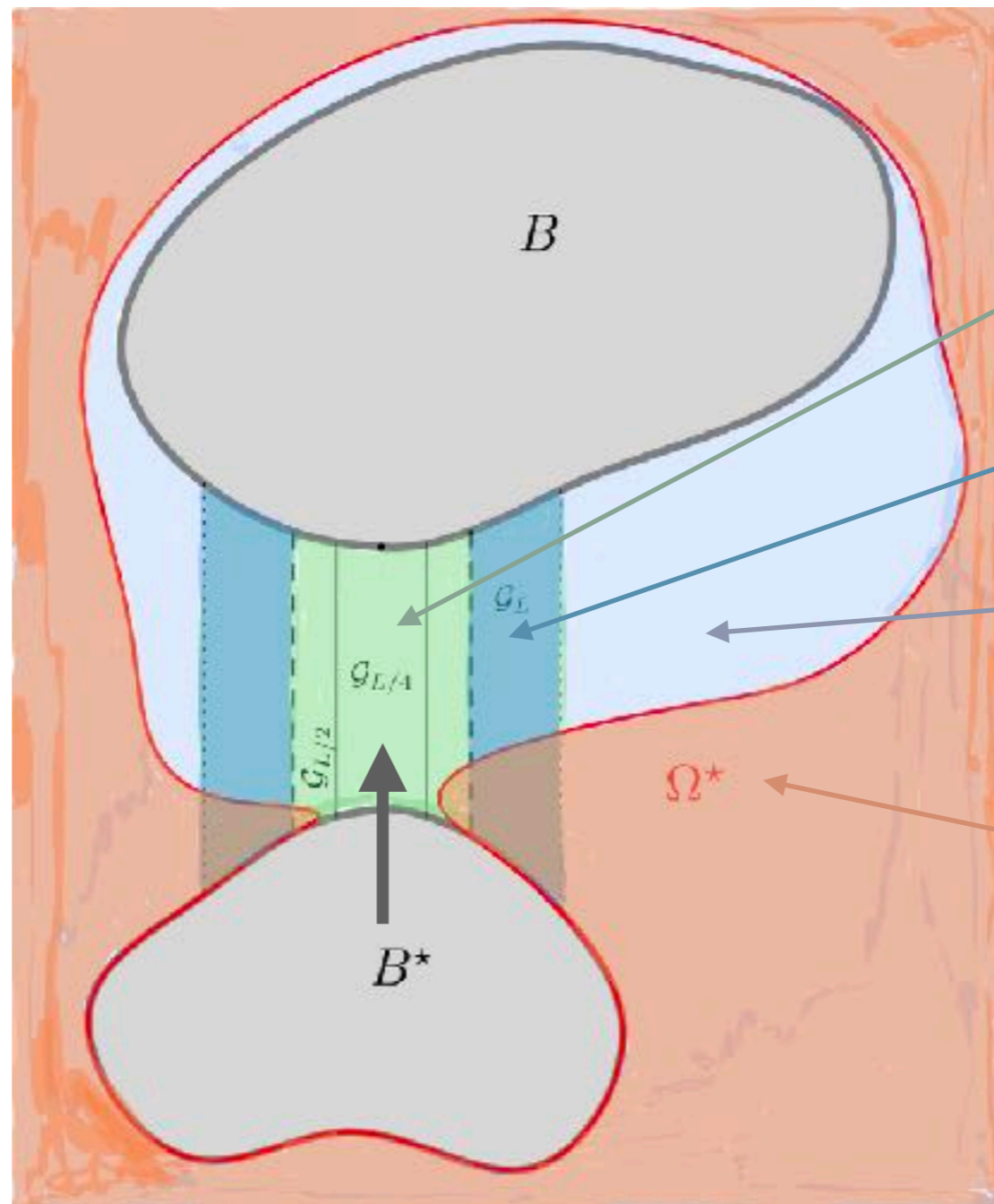
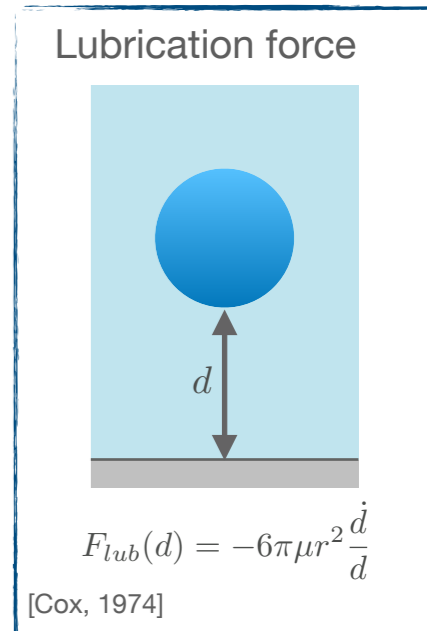
Divergence free modification to match boundary conditions

# An explicit asymptotic expansion



Explicit asymptotic expansion  
[Hillairet, Kelai, 2015]

$$(\mathbf{u}, p) = (\mathbf{u}^{\text{sing}}, p^{\text{sing}}) + (\mathbf{u}^{\text{reg}}, p^{\text{reg}})$$



Divergence free explicit expansion

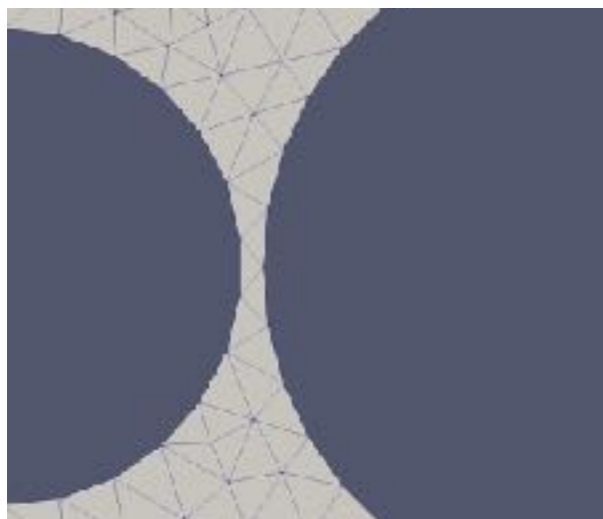
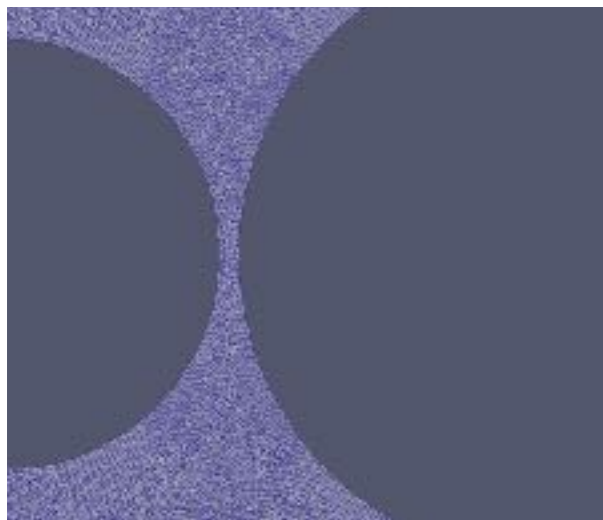
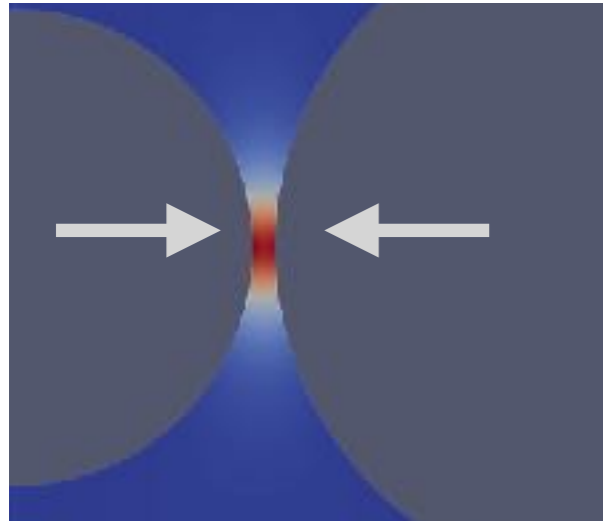
Divergence free truncation

Vanishing extension

Divergence free modification to match boundary conditions

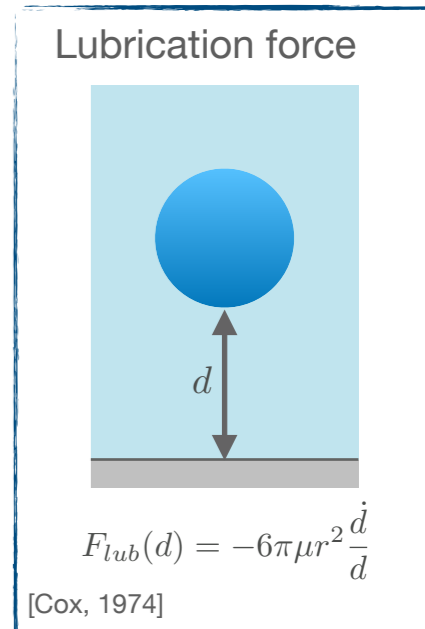
$\Omega^*$  must be independent of the distance

# An explicit asymptotic expansion



Explicit asymptotic expansion  
[Hillairet, Kelai, 2015]

$$(\mathbf{u}, p) = (\mathbf{u}^{\text{sing}}, p^{\text{sing}}) + (\mathbf{u}^{\text{reg}}, p^{\text{reg}})$$



$(\mathbf{u}^{\text{reg}}, p^{\text{reg}})$  solution to

$$-\mu\Delta\mathbf{u}^{\text{reg}} + \nabla p^{\text{reg}} = \mu\Delta\mathbf{u}^{\text{sing}} - \nabla p^{\text{sing}} \quad \text{in } \mathcal{F}$$

$$\nabla \cdot \mathbf{u}^{\text{reg}} = -\nabla \cdot \mathbf{u}^{\text{sing}} \quad \text{in } \mathcal{F}$$

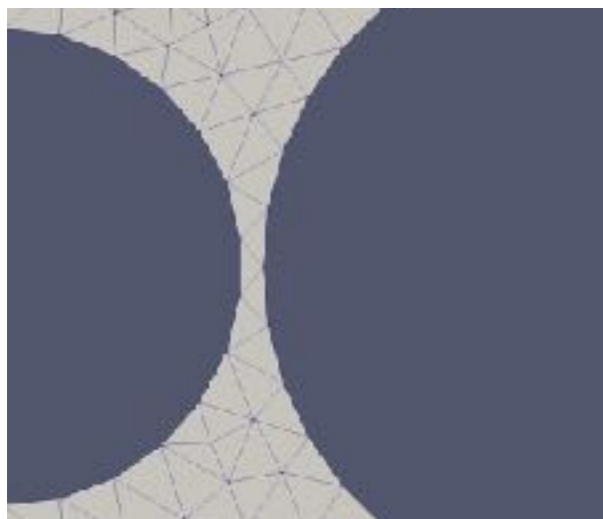
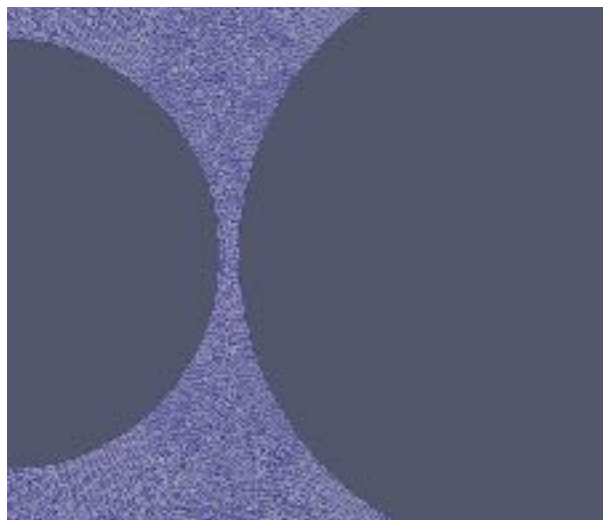
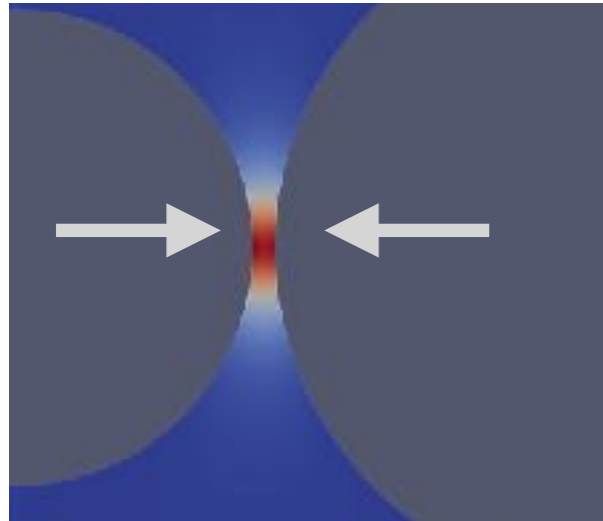
$$\mathbf{u}^{\text{reg}} = \mathbf{u}^* - \mathbf{u}^{\text{sing}} \quad \text{on } \partial B$$

in  $\mathcal{F}$

in  $\mathcal{F}$

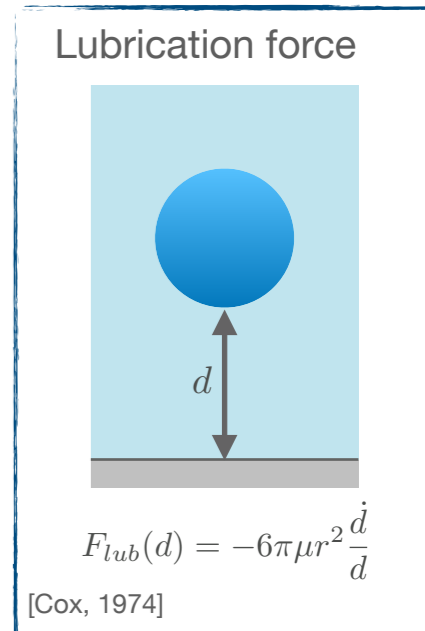
on  $\partial B$

# An explicit asymptotic expansion



Explicit asymptotic expansion  
[Hillairet, Kelai, 2015]

$$(\mathbf{u}, p) = (\mathbf{u}^{\text{sing}}, p^{\text{sing}}) + (\mathbf{u}^{\text{reg}}, p^{\text{reg}})$$



$(\mathbf{u}^{\text{reg}}, p^{\text{reg}})$  solution to

$$\begin{aligned} -\mu\Delta\mathbf{u}^{\text{reg}} + \nabla p^{\text{reg}} &= \mu\Delta\mathbf{u}^{\text{sing}} - \nabla p^{\text{sing}} && \text{in } \mathcal{F} \\ \nabla \cdot \mathbf{u}^{\text{reg}} &= -\nabla \cdot \mathbf{u}^{\text{sing}} && \text{in } \mathcal{F} \\ \mathbf{u}^{\text{reg}} &= \mathbf{u}^* - \mathbf{u}^{\text{sing}} && \text{on } \partial B \end{aligned}$$

► [M. Hillairet, T. Kelai, 2015]

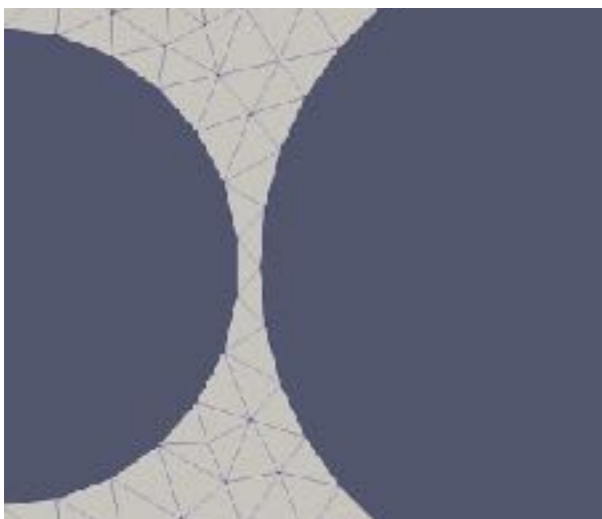
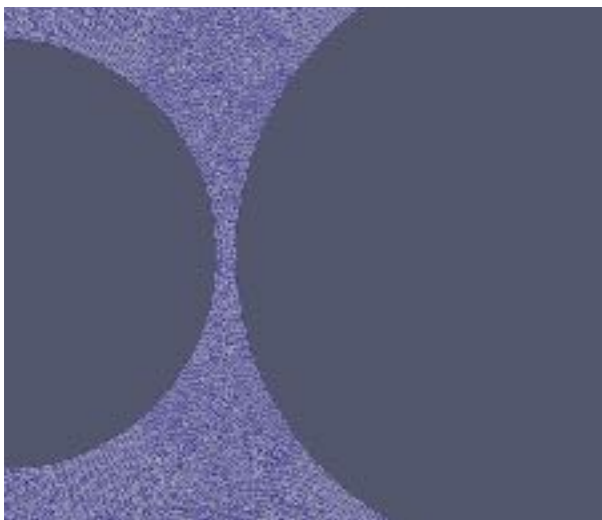
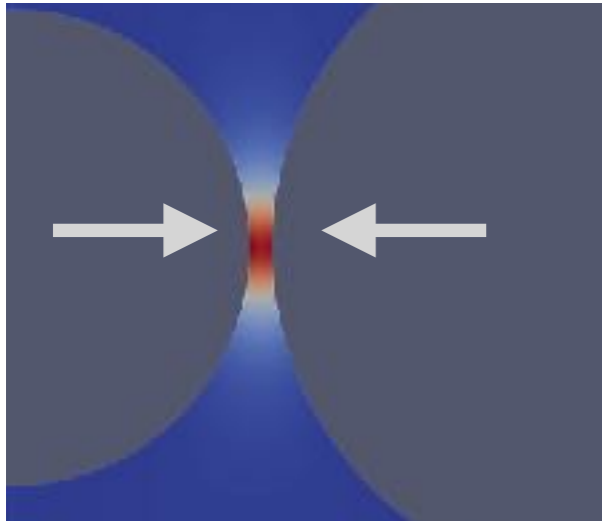
$$\|(\mathbf{u}^{\text{reg}}, p^{\text{reg}})\| \leq C$$

with  $C$  independent of the distance

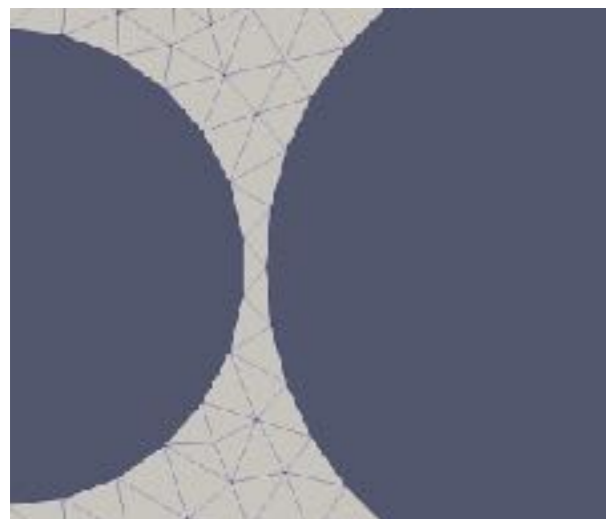
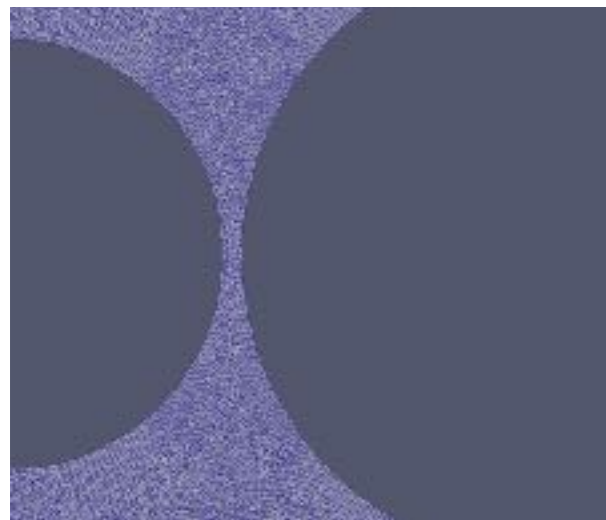
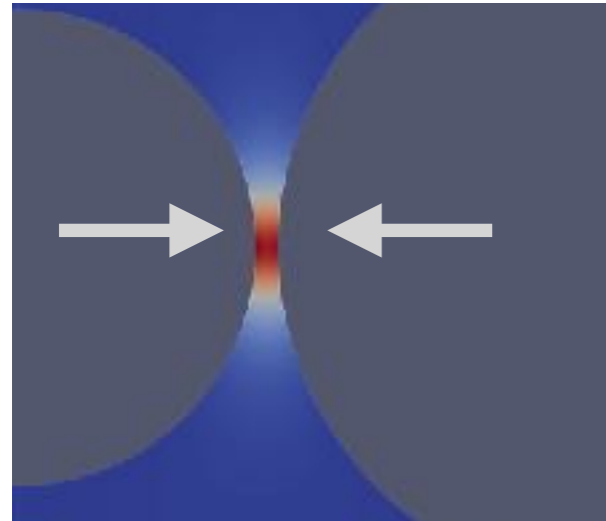
# Taking lubrication into account in the fluid solver.

Adapted explicit asymptotic expansion

$$(\mathbf{u}_h^{\text{new}}, p_h^{\text{new}}) = (\tilde{\mathbf{u}}^{\text{sing}}, \tilde{p}^{\text{sing}}) + (\tilde{\mathbf{u}}_h^{\text{reg}}, \tilde{p}_h^{\text{reg}})$$

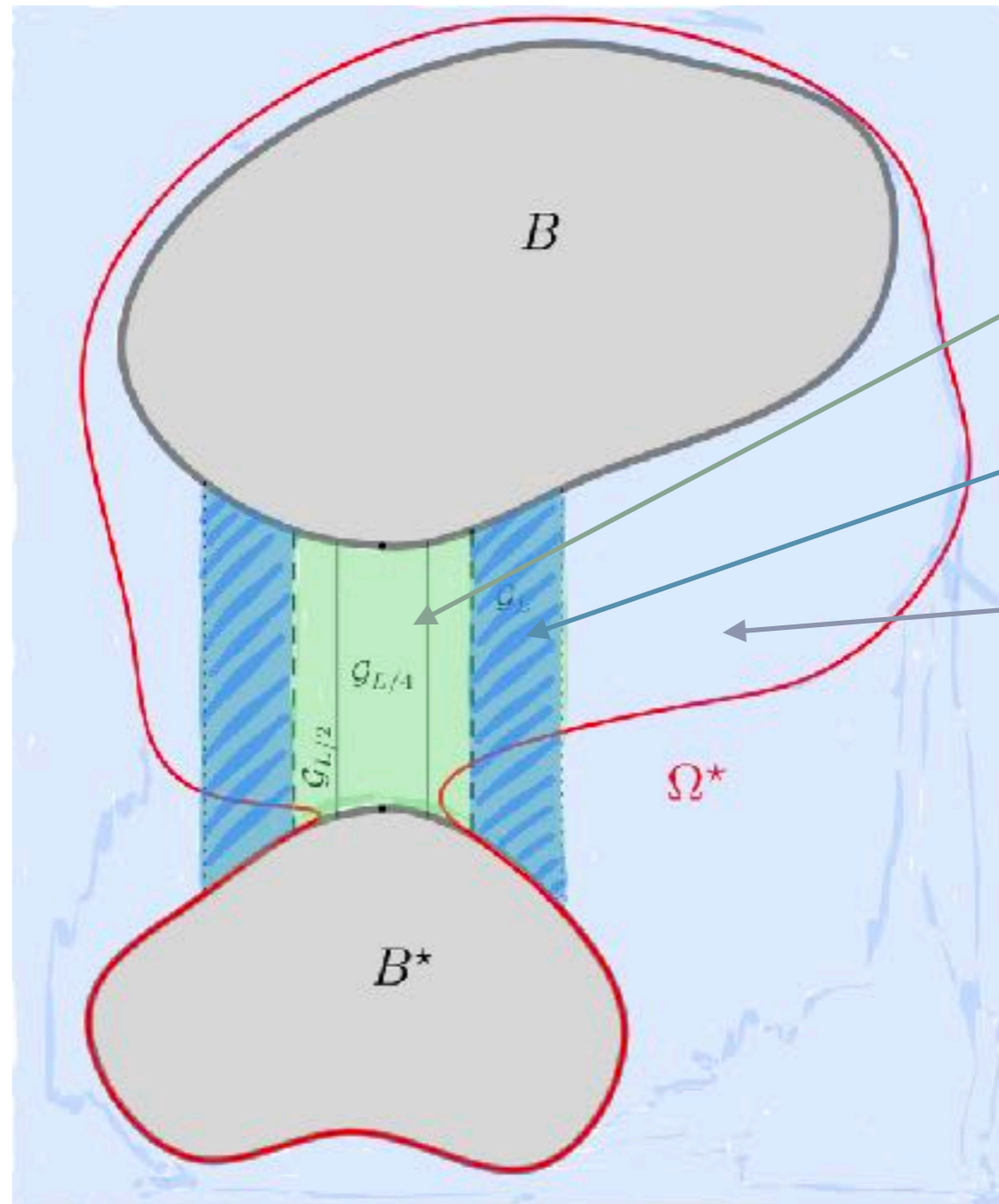


# Taking lubrication into account in the fluid solver.



Adapted explicit asymptotic expansion

$$(\mathbf{u}_h^{\text{new}}, p_h^{\text{new}}) = (\tilde{\mathbf{u}}^{\text{sing}}, \tilde{p}^{\text{sing}}) + (\tilde{\mathbf{u}}_h^{\text{reg}}, \tilde{p}_h^{\text{reg}})$$



Divergence free explicit expansion

Modified non-divergence free truncation

Vanishing extension



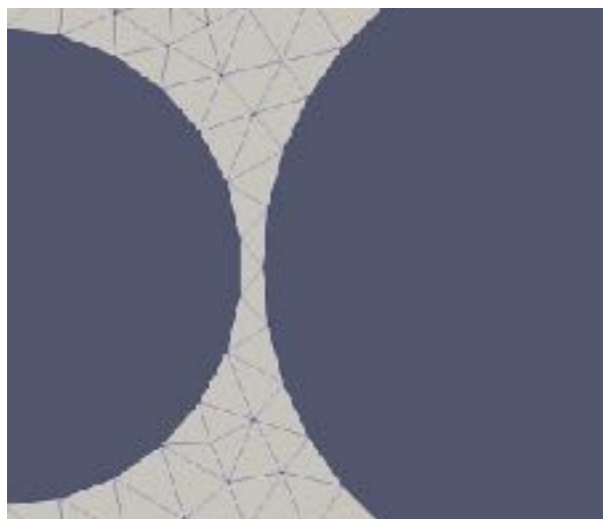
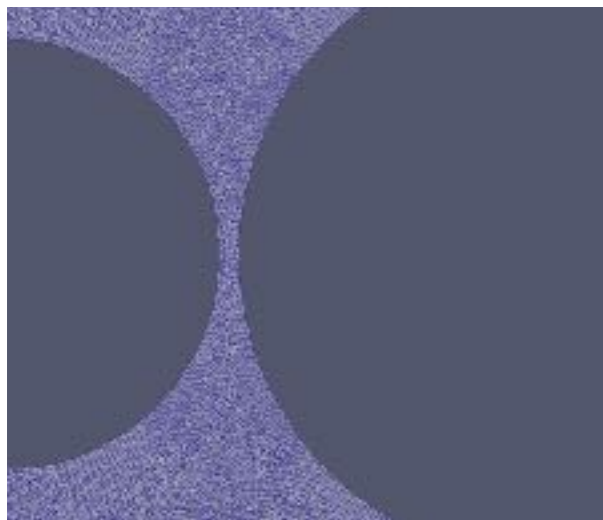
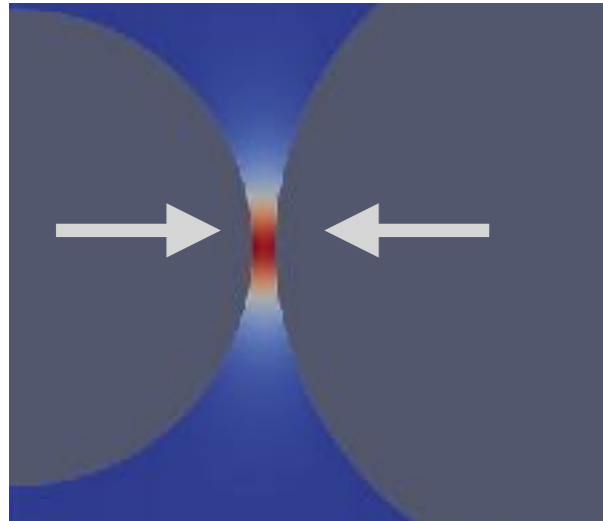
# Taking lubrication into account in the fluid solver.

Adapted explicit asymptotic expansion

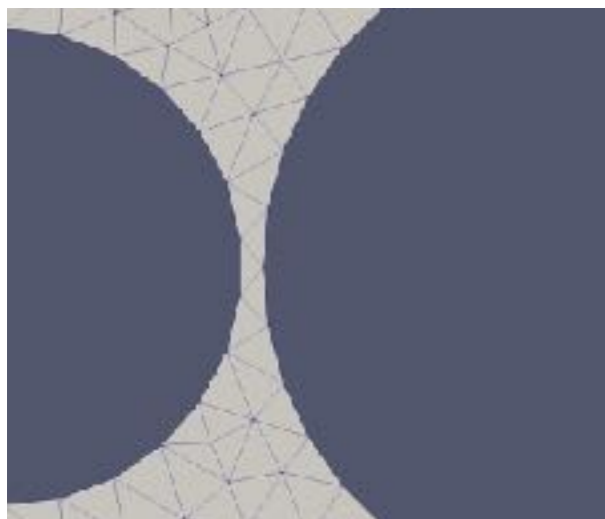
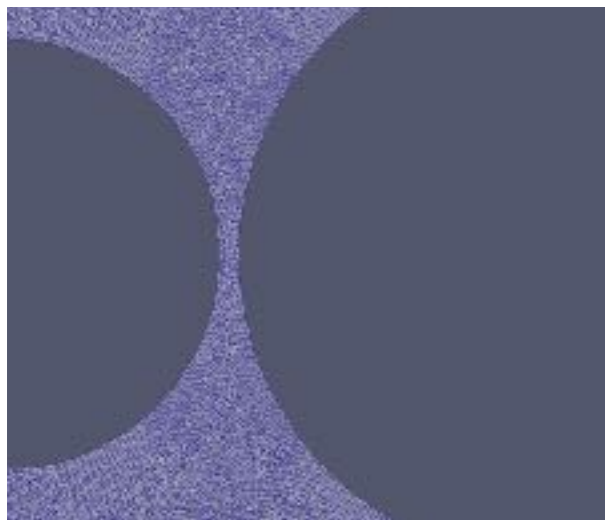
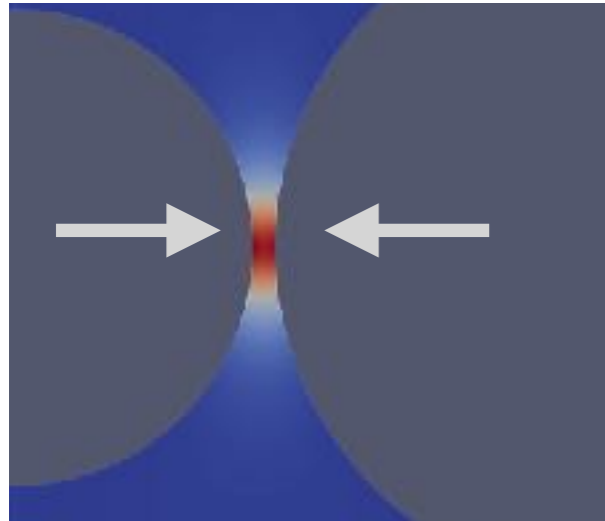
$$(\mathbf{u}_h^{\text{new}}, p_h^{\text{new}}) = (\tilde{\mathbf{u}}^{\text{sing}}, \tilde{p}^{\text{sing}}) + (\tilde{\mathbf{u}}_h^{\text{reg}}, \tilde{p}_h^{\text{reg}})$$

$(\tilde{\mathbf{u}}_h^{\text{reg}}, \tilde{p}_h^{\text{reg}})$  numerical solution to

$$\begin{aligned} -\mu\Delta\tilde{\mathbf{u}}_h^{\text{reg}} + \nabla\tilde{p}_h^{\text{reg}} &= \mu\Delta\tilde{\mathbf{u}}^{\text{sing}} - \nabla\tilde{p}^{\text{sing}} && \text{in } \mathcal{F} \\ \nabla\cdot\tilde{\mathbf{u}}_h^{\text{reg}} &= -\nabla\cdot\tilde{\mathbf{u}}^{\text{sing}} && \text{in } \mathcal{F} \\ \tilde{\mathbf{u}}_h^{\text{reg}} &= \mathbf{u}^* - \tilde{\mathbf{u}}^{\text{sing}} && \text{on } \partial B \end{aligned}$$



# Taking lubrication into account in the fluid solver.



Adapted explicit asymptotic expansion

$$(\mathbf{u}_h^{\text{new}}, p_h^{\text{new}}) = (\tilde{\mathbf{u}}^{\text{sing}}, \tilde{p}^{\text{sing}}) + (\tilde{\mathbf{u}}_h^{\text{reg}}, \tilde{p}_h^{\text{reg}})$$

$(\tilde{\mathbf{u}}_h^{\text{reg}}, \tilde{p}_h^{\text{reg}})$  numerical solution to

$$\begin{aligned} -\mu\Delta\tilde{\mathbf{u}}_h^{\text{reg}} + \nabla\tilde{p}_h^{\text{reg}} &= \mu\Delta\tilde{\mathbf{u}}^{\text{sing}} - \nabla\tilde{p}^{\text{sing}} && \text{in } \mathcal{F} \\ \nabla\cdot\tilde{\mathbf{u}}_h^{\text{reg}} &= -\nabla\cdot\tilde{\mathbf{u}}^{\text{sing}} && \text{in } \mathcal{F} \\ \tilde{\mathbf{u}}_h^{\text{reg}} &= \mathbf{u}^* - \tilde{\mathbf{u}}^{\text{sing}} && \text{on } \partial B \end{aligned}$$

$$\|\mathbf{u} - \mathbf{u}_h^{\text{new}}\| \leq C \|(\tilde{\mathbf{u}}^{\text{reg}}, \tilde{p}^{\text{reg}})\| h^\alpha$$

Bounded independently of the distance

# Taking lubrication into account in the fluid solver.

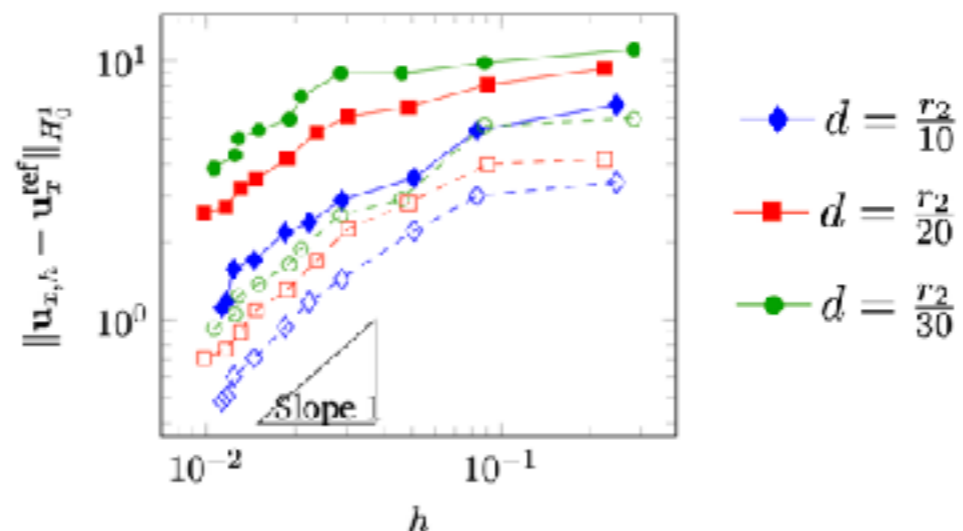
Adapted explicit asymptotic expansion

$$(\mathbf{u}_h^{\text{new}}, p_h^{\text{new}}) = (\tilde{\mathbf{u}}^{\text{sing}}, \tilde{p}^{\text{sing}}) + (\tilde{\mathbf{u}}_h^{\text{reg}}, \tilde{p}_h^{\text{reg}})$$

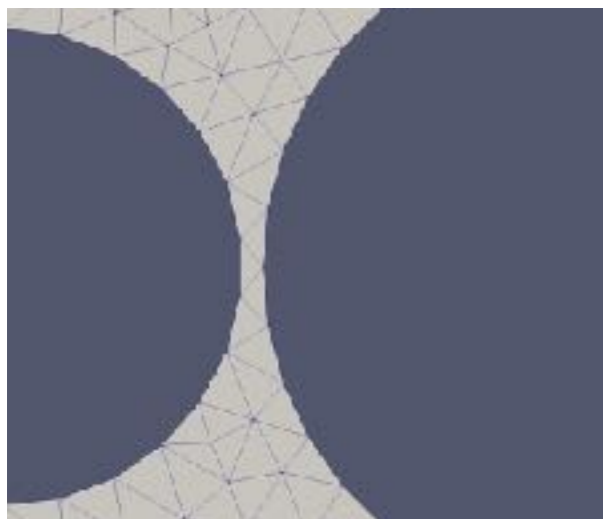
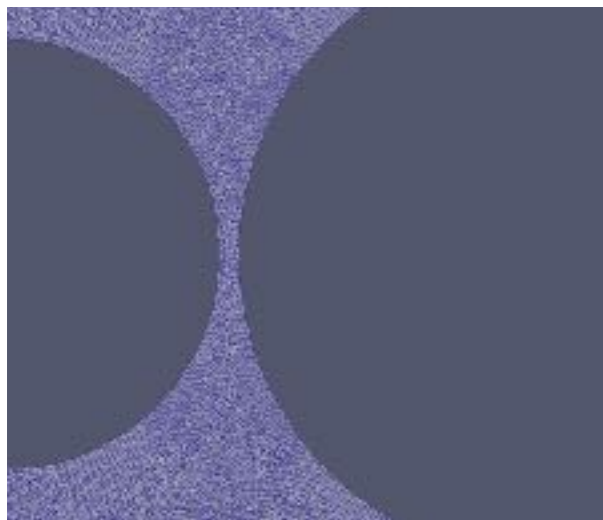
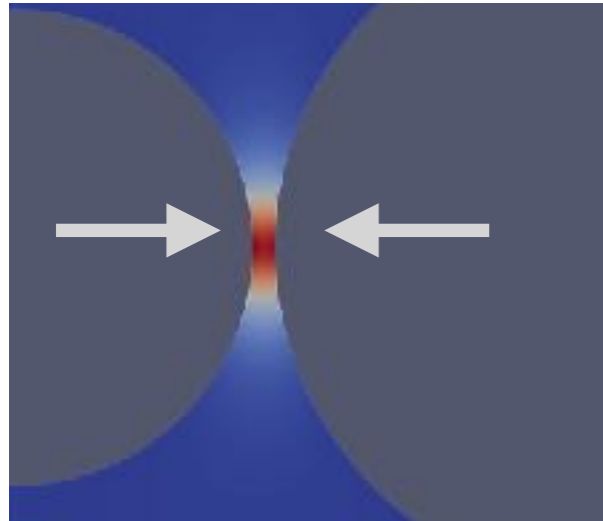
$(\tilde{\mathbf{u}}_h^{\text{reg}}, \tilde{p}_h^{\text{reg}})$  numerical solution to

$$\begin{aligned} -\mu\Delta\tilde{\mathbf{u}}_h^{\text{reg}} + \nabla\tilde{p}_h^{\text{reg}} &= \mu\Delta\tilde{\mathbf{u}}^{\text{sing}} - \nabla\tilde{p}^{\text{sing}} && \text{in } \mathcal{F} \\ \nabla\cdot\tilde{\mathbf{u}}_h^{\text{reg}} &= -\nabla\cdot\tilde{\mathbf{u}}^{\text{sing}} && \text{in } \mathcal{F} \\ \tilde{\mathbf{u}}_h^{\text{reg}} &= \mathbf{u}^* - \tilde{\mathbf{u}}^{\text{sing}} && \text{on } \partial B \end{aligned}$$

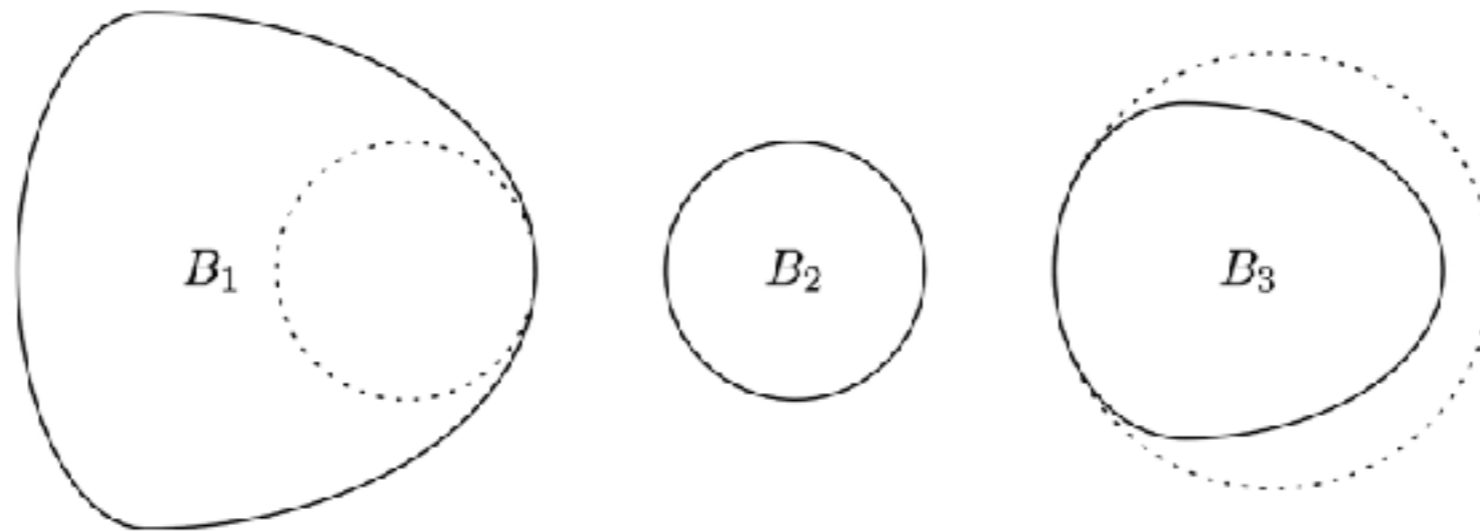
$$\|\mathbf{u} - \mathbf{u}_h^{\text{new}}\| \leq C \|(\tilde{\mathbf{u}}^{\text{reg}}, \tilde{p}^{\text{reg}})\| h^\alpha$$



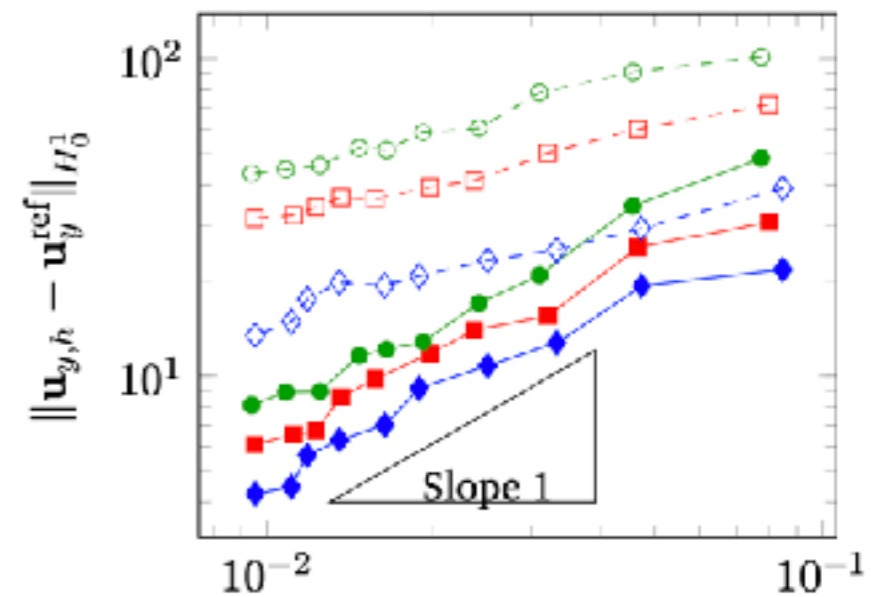
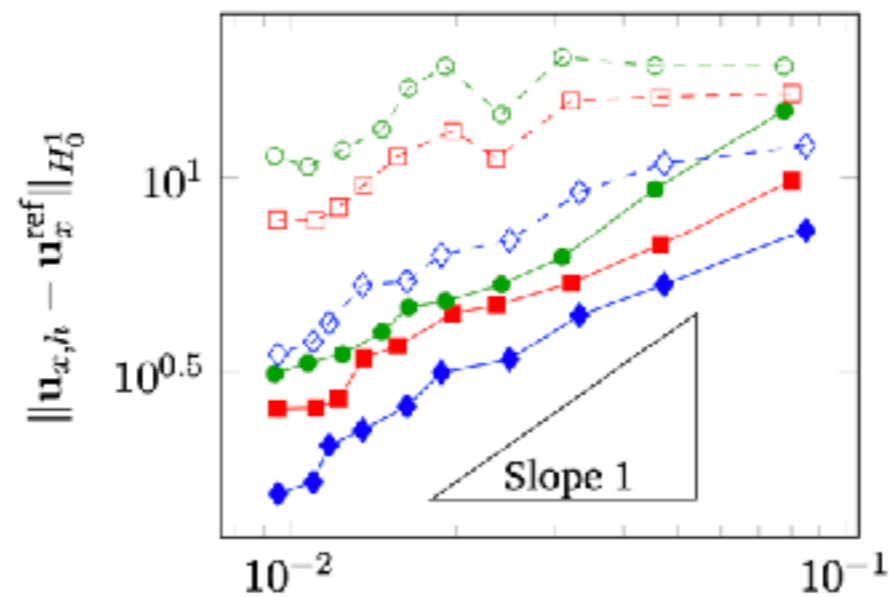
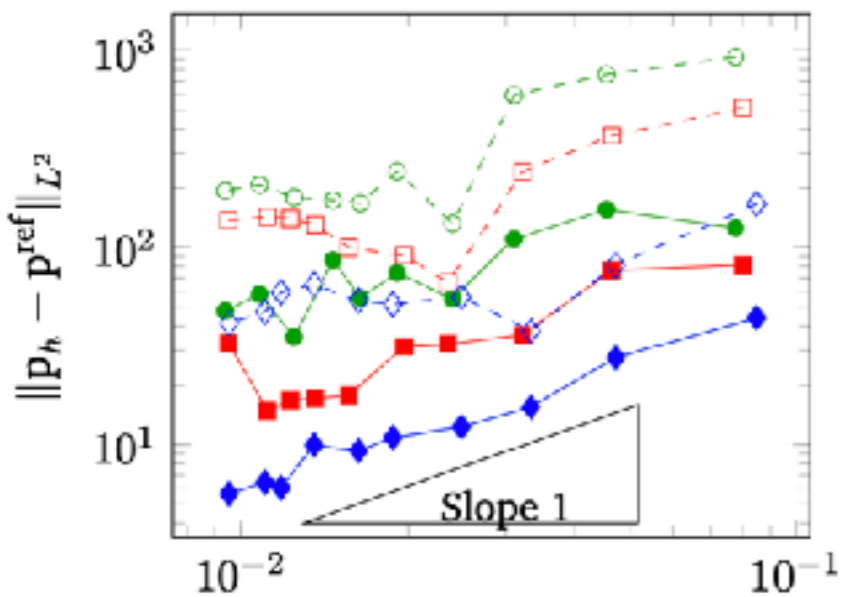
Bounded independently of the distance



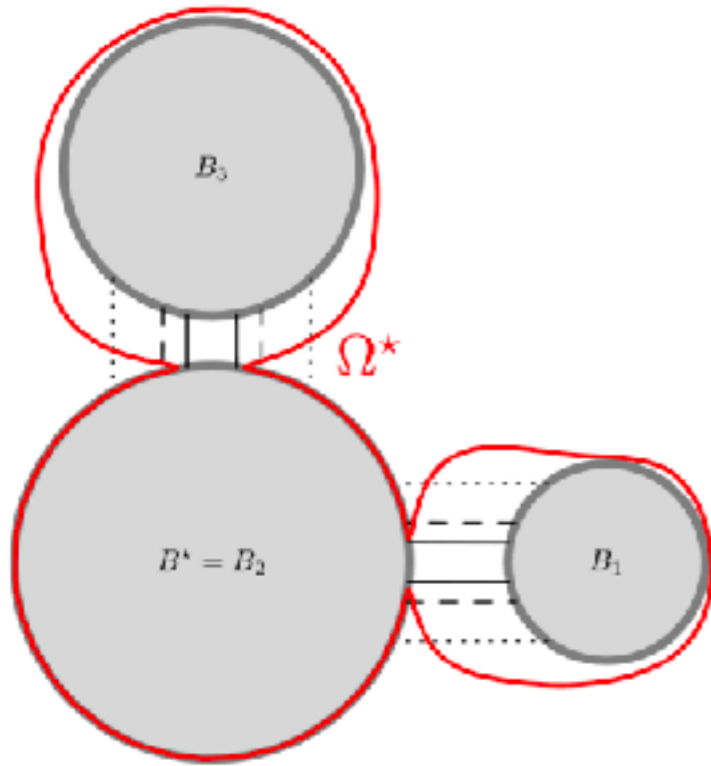
# 3 non-spherical particles with general rigid motion



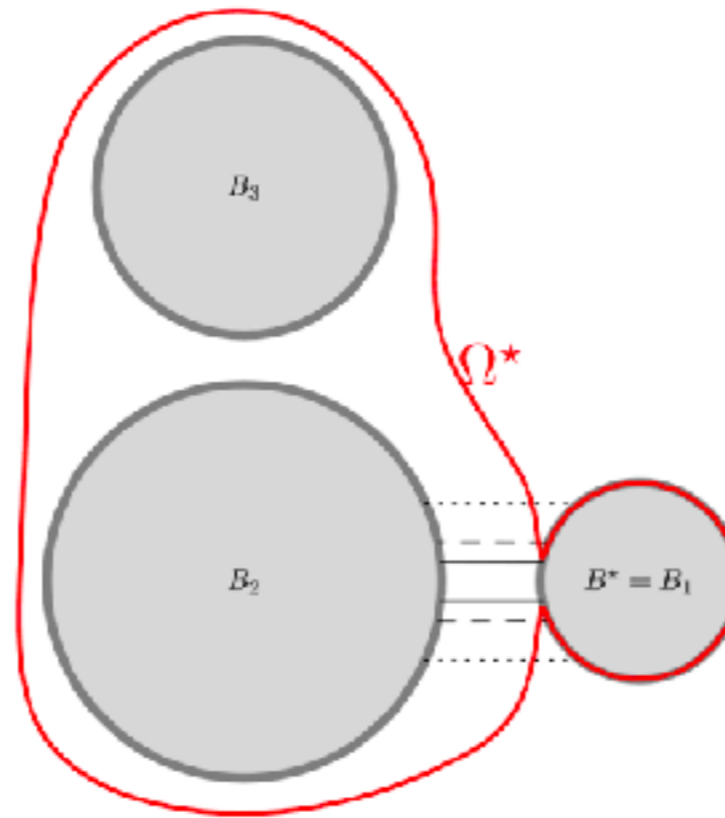
$$\mathbf{V}_1 = (1, 5), \mathbf{V}_2 = (-1, -2), \mathbf{V}_3 = (1.5, -5), \mathbf{w}_1 = 3, \mathbf{w}_2 = 5, \mathbf{w}_3 = 10$$



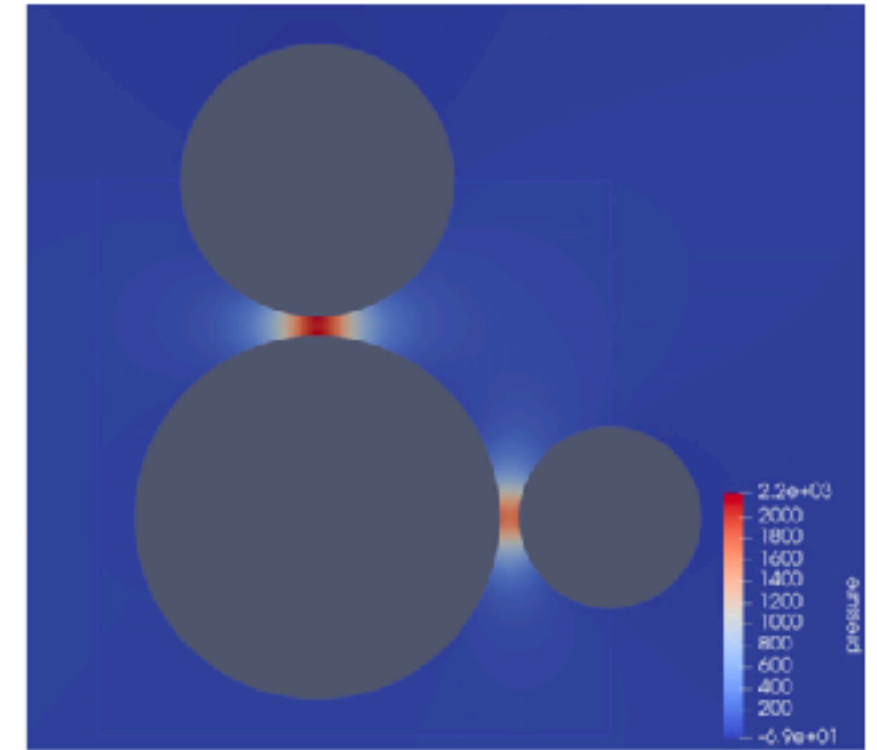
# Limitation in dimension 2



(A) Choice for  $\Omega^*$  when  $B_2$  is moving (2 singularities)

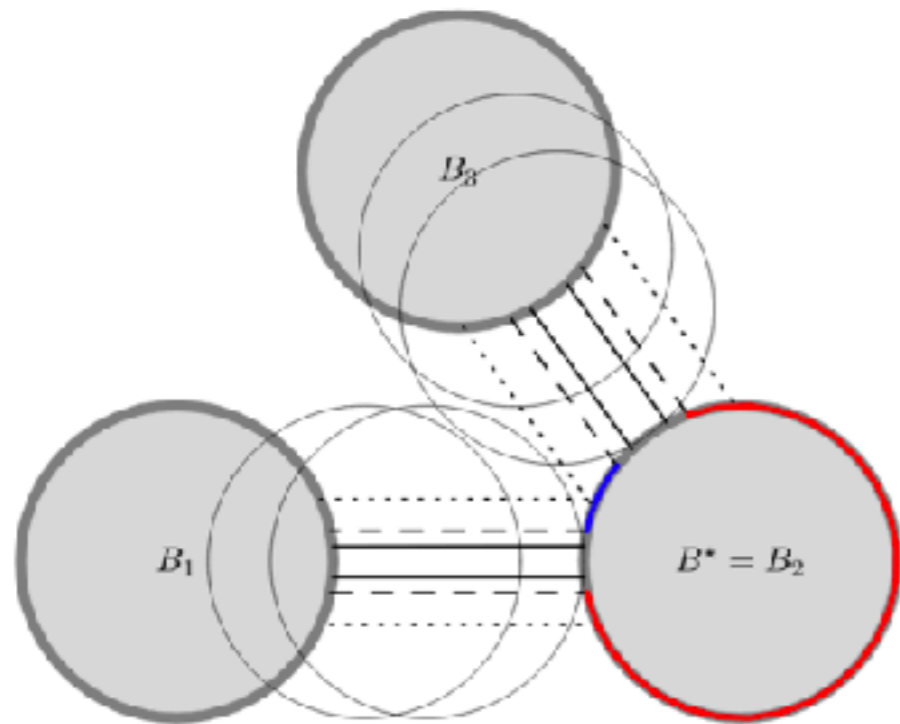


(B) Choice for  $\Omega^*$  when  $B_1$  is moving (1 singularity)

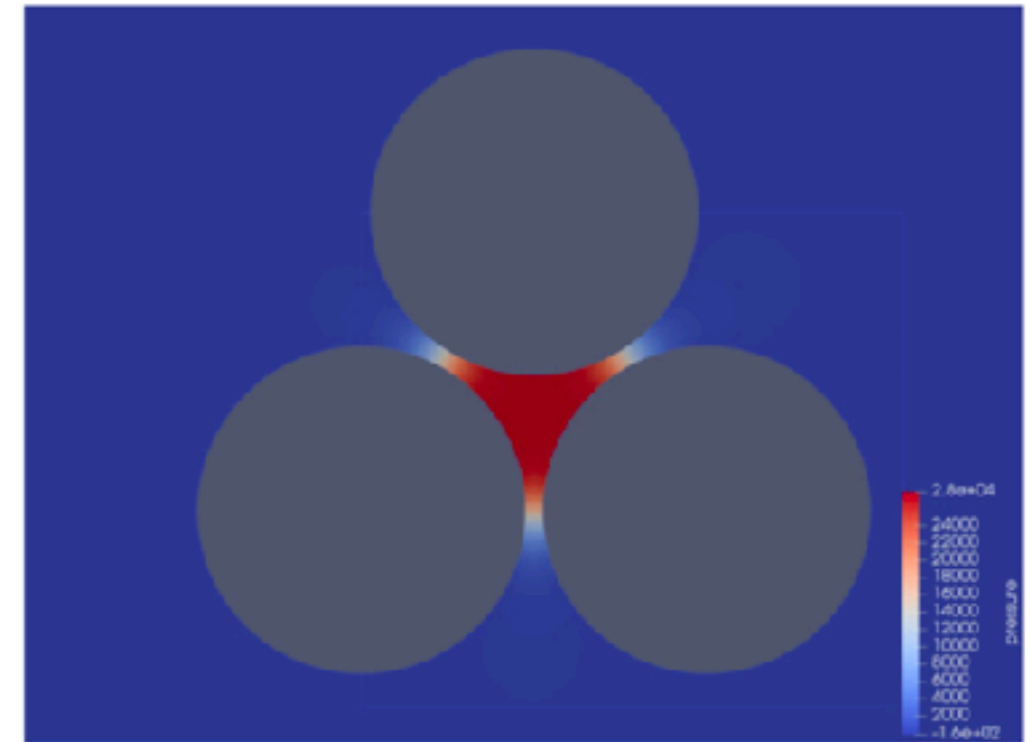


(C) Pressure field solution to the problem

# Limitation in dimension 2



(A) Evolution of the configuration when the distance goes to zero



(B) Pressure field solution to the problem