Numerical Modelling of Granular Flows

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Model (hard spheres, non elastic collisions)

Strategies

A stable method to handle non elastic collisions

Numerical tests

Theoretical framework and analysis of the scheme

Gluey particle model (with A. Lefebvre)

N rigid spheres in $\mathbb{R}^d$ (with $d = 3$, 2, or 1), radii $(r_i)_{1 \leq i \leq N}$, mass 1 .

$$Q = \{\mathbf{q} = (\mathbf{q}_1, \mathbf{q}_2, \cdots, \mathbf{q}_N) \in \mathbb{R}^{dN}\}$$

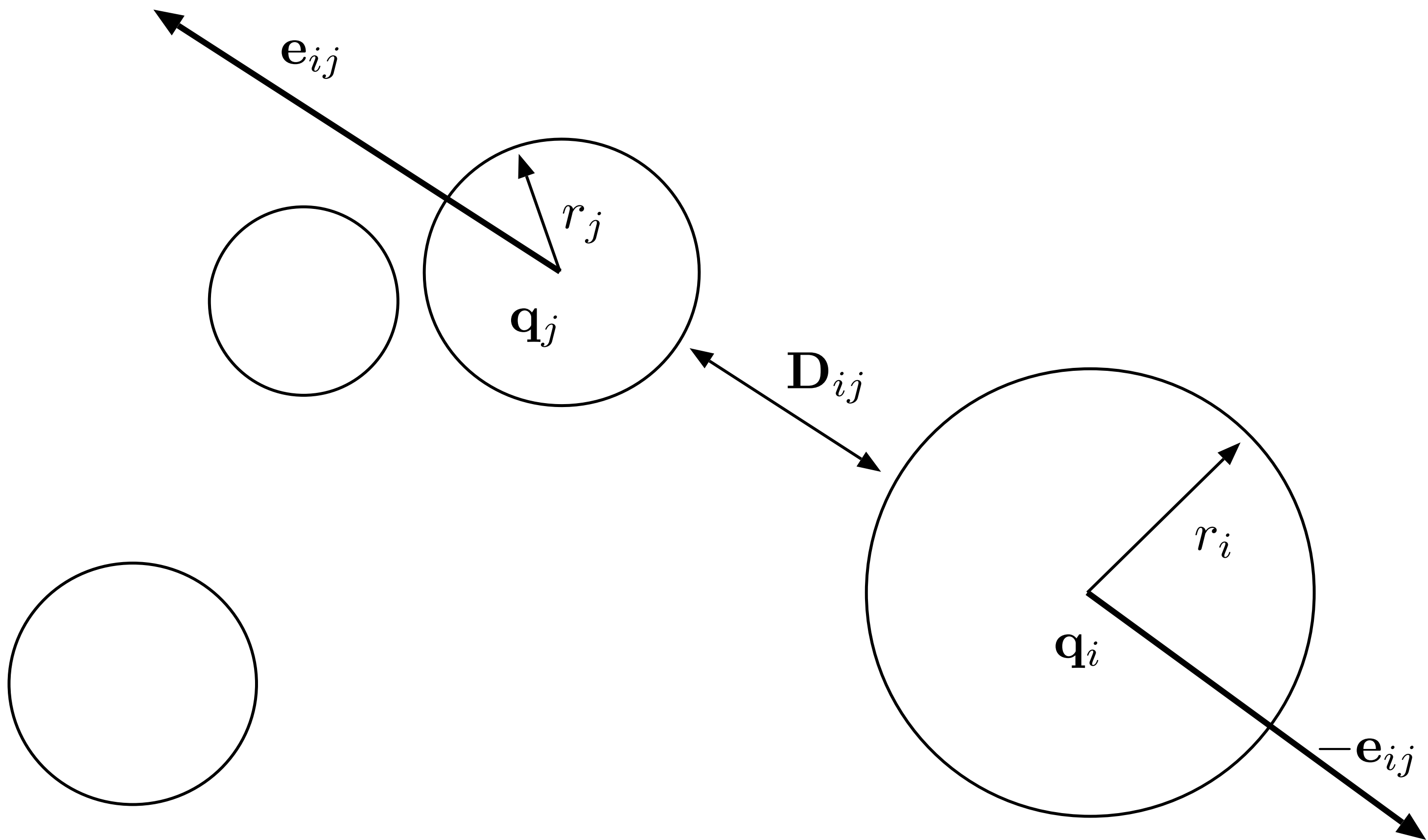
Feasible set :

$$Q_0 = \{\mathbf{q} \in Q, D_{ij}(\mathbf{q}) \geq 0 \quad \forall i, j \;, \;\; 1 \leq i < j \leq N\}$$

where $D_{ij}(\mathbf{q}) = |\mathbf{q}_i - \mathbf{q}_j| - (r_i + r_j)$

(Rk. : Obstacle treated in the same way: $D_{ik}(\mathbf{q}) \geq 0$)

N.B.: D_{ij} may be negative, and it is smooth in a neighbourhood of Q_0 (for finite size particles).



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$\mathbf{G}_{ij} = \nabla D_{ij} \in T_Q = \mathbb{R}^{dN}$: gradient of the distance between spheres i and j:

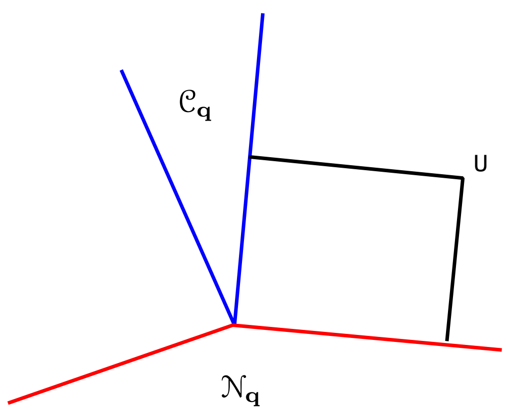
$$\mathbf{G}_{ij} = (\cdots, 0, -\mathbf{e}_{ij}, 0, \cdots, 0, \mathbf{e}_{ij}, 0, \cdots), \quad \mathbf{e}_{ij} = \frac{\mathbf{q}_j - \mathbf{q}_i}{|\mathbf{q}_j - \mathbf{q}_i|},$$

$\mathcal{C}_{\mathbf{q}}$: set of feasible directions at $\mathbf{q} \in Q_0$,

$$\mathcal{C}_{\mathbf{q}} = \{\mathbf{v} \in \mathrm{T}_Q \ , \quad \mathbf{G}_{ij} \cdot \mathbf{v} \geq 0 \quad \text{as soon as} \ \ D_{ij}(\mathbf{q}) = 0\} \ ,$$

Outward normal cone to Q_0 at $\mathbf{q}$ (polar cone of $\mathcal{C}_{\mathbf{q}}$):

$$\begin{aligned} \mathcal{N}_{\mathbf{q}} &= \mathcal{C}_{\mathbf{q}}^{\circ} = \{\mathbf{h} \in \mathrm{T}_Q \ , \quad \mathbf{h} \cdot \mathbf{v} \leq 0 \quad \forall \mathbf{v} \in \mathcal{C}_{\mathbf{q}}\} \\ &= \{-\sum_{i<j} \mu_{ij} \mathbf{G}_{ij}(\mathbf{q}) \ , \ \ \mu_{ij} \geq 0 \ , \ \ D_{ij}(\mathbf{q}) \mu_{ij} = 0\} \quad \text{(Farkas Lemma)} \end{aligned}$$



$$I_d = P_{\mathcal{C}_{\mathbf{q}}} + P_{\mathcal{N}_{\mathbf{q}}} \ \text{(Moreau)}$$

Find $t \longmapsto \mathbf{q}(t) \in Q_0$, $\mathbf{u} = \dot{\mathbf{q}}$,

$$\left\{ \begin{array}{rcl} \dfrac{d\mathbf{u}}{dt} & = & \mathbf{f}(\mathbf{q},t) + \displaystyle\sum_{i<j} \lambda_{ij} \mathbf{G}_{ij} \\ \lambda_{ij} \in \mathcal{M}^+(I)\ ,\ \ \mathrm{supp}(\lambda_{ij}) & \subset & \{t\ ,\ \ D_{ij}(\mathbf{q}(t)) = 0\}, \\ \mathbf{u}^+ & = & P_{\mathcal{C}_\mathbf{q}} \mathbf{u}^-, \end{array} \right.$$

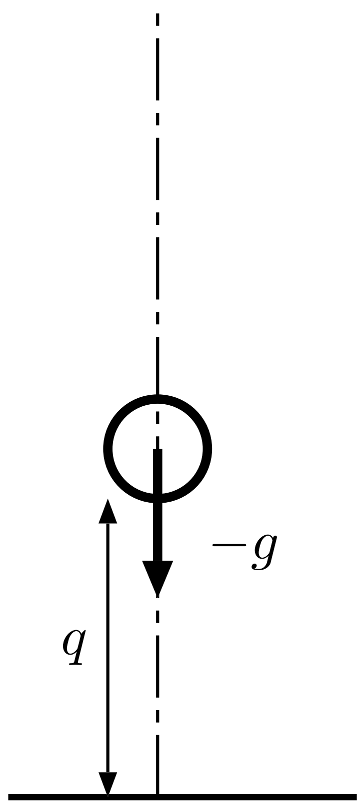
$$\mathcal{C}_\mathbf{q} = \{\mathbf{v} \in \mathrm{T}_Q\ ,\ \ \mathbf{G}_{ij} \cdot \mathbf{v} \geq 0 \quad \text{as soon as}\ \ D_{ij}(\mathbf{q}) = 0\}\,,$$

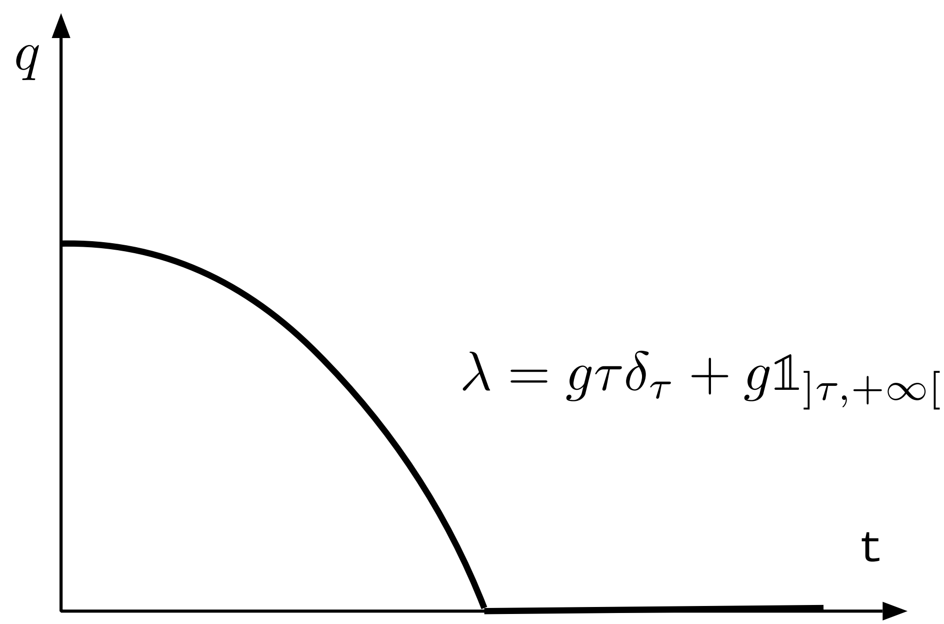
Extended collision model (with $e \in [0,1]$: restitution coefficient):

$$\mathbf{u}^+ = \mathbf{u}^- - (1+e) P_{\mathcal{N}_\mathbf{q}} \mathbf{u}^-,$$

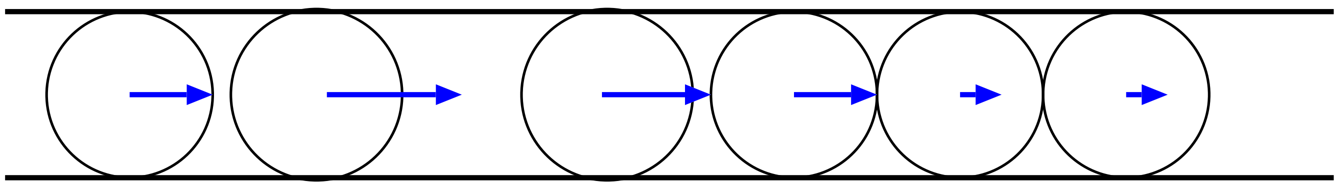
$$\text{Differential inclusion formulation :}\ \frac{d^2\mathbf{q}}{dt^2} + \mathcal{N}_\mathbf{q} \ni \mathbf{f}$$

1D example





$1D$ problems : Q_0 defined as a connected component of the set of all configurations $\mathbf{q}$ with no overlapping.



In this case,

$$Q_0 = \{\mathbf{q} = (q_1, \ldots, q_N) \in \mathbb{R}^N \ , \ \ q_{i+1} - q_i \geq r_{i+1} + r_i\}$$

is closed and convex, and $\mathcal{N}_\mathbf{q}$ is with the subdifferential of the indicatrix of Q_0:

$$\mathcal{N}_\mathbf{q} = \partial I_{Q_0}(\mathbf{q}) \text{ with } I_{Q_0}(\mathbf{q}) = \left| \begin{array}{rcl} 0 & \text{if} & \mathbf{q} \in Q_0 \\ +\infty & \text{if} & \mathbf{q} \notin Q_0 \end{array} \right.$$

and hence $\mathbf{q} \longmapsto \mathcal{N}_\mathbf{q}$ is a maximal monotone operator.

In general, Q_0 is prox-regular (see Federer [10], Edmont-Thibault [8]).

Theoretical analysis

Schatzmann [22], Ballard [1], Moreau, Buttazzo [5].

Only analiticity ensures uniqueness.

Numerical simulation

Molecular Dynamics: slight overlapping allowed, short-range repulsive force with local damping (Glowinski [11], Luding [13], Richefeu).

Contact Dynamics: (1) Prediction of the violated constraints, then succession of single contact problems, with relaxation (Moreau and coworkers in Montpellier [21])

(2) Linearization of the constraints, global handling of contacts (Stewart [23], Maury [17]).

Numerical Scheme

$$\mathbf{f}_h^{n+1}(\mathbf{q}) = \int_{t^n}^{t^{n+1}} \mathbf{f}(\mathbf{q}, t).$$

1. Initialization

$$(\mathbf{q}_h^0, \mathbf{u}_h^0) = (\mathbf{q}_0, \mathbf{u}_0).$$

2. Compute $\mathbf{u}_h^{n+1}$ as the solution to the constrained minimization problem

$$\min_{\mathbf{u} \in \mathrm{C}_h(\mathbf{q}_h^n)} \frac{1}{2} \left| \mathbf{u} - \mathbf{u}_h^n - h \mathbf{f}_h^{n+1}(\mathbf{q}_h^n) \right|^2$$

with

$$\mathrm{C}_h(\mathbf{q}_h^n) = \{\mathbf{u} \in \mathrm{T}_Q, \underbrace{D_{ij}(\mathbf{q}_h^n) + h\mathbf{G}_{ij}(\mathbf{q}_h^n) \cdot \mathbf{u}}_{\approx D_{ij}(\mathbf{q}_h^n + h\mathbf{u})} \geq 0\}.$$

3. Update the positions

$$\mathbf{q}_h^{n+1} = \mathbf{q}_h^n + h\mathbf{u}_h^{n+1}.$$

Interpretation of the scheme

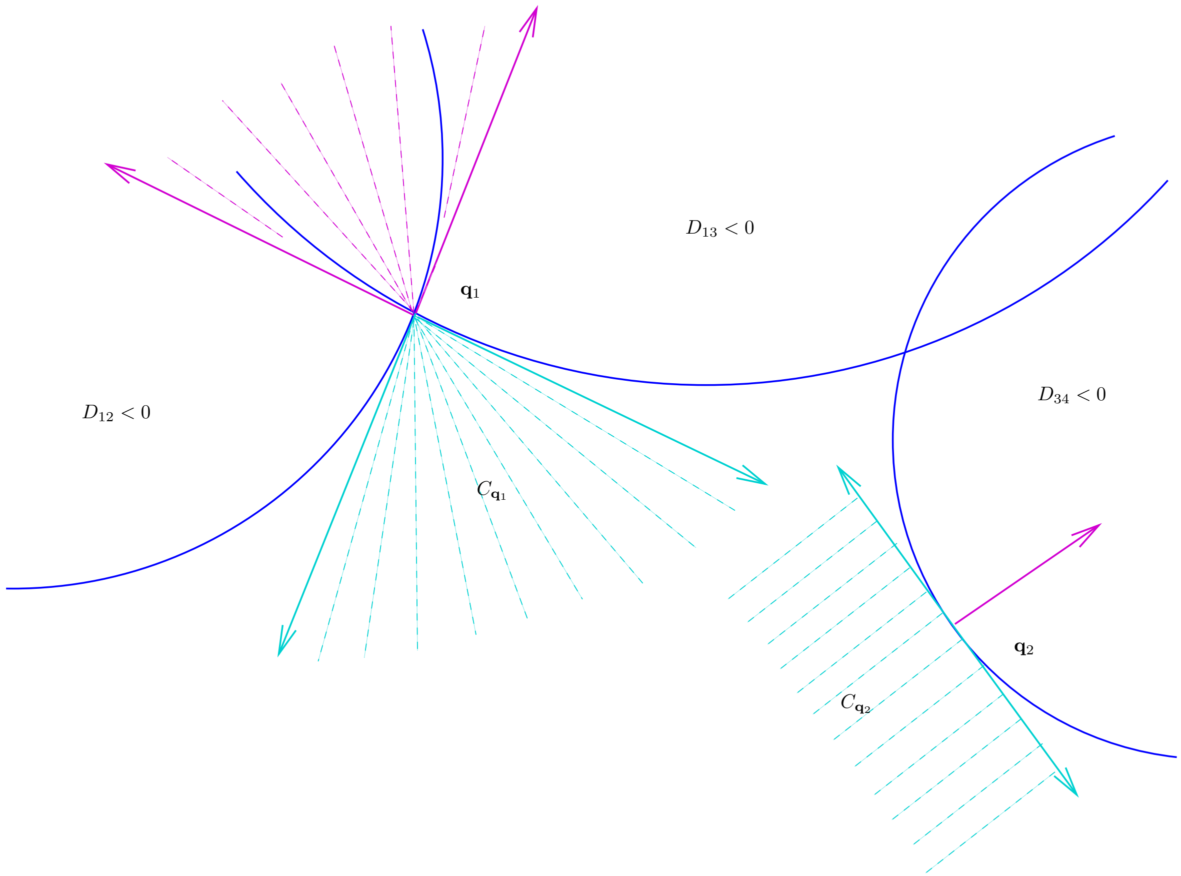
$$\mathbf{u}_h^{n+1} = P_{\mathrm{C}_h(\mathbf{q}_h^n)}(\mathbf{u}_h^n + h\mathbf{f}_h^{n+1}(\mathbf{q}_h^n))$$

equivalent to say that

$$\mathbf{u}_h^n + h\mathbf{f}_h^{n+1}(\mathbf{q}_h^n) - \mathbf{u}_h^{n+1} \in \partial I_{\mathrm{C}_h(\mathbf{q}_h^n)}(\mathbf{u}_h^{n+1}).$$

where

$$\partial\varphi(x) = \{v, \varphi(x)+(v,h) \leq \varphi(x+h) \quad \forall h\}\ , \quad I_K(v) = \left| \begin{array}{rcc} 0 & \text{if} & v \in K \\ +\infty & \text{if} & v \notin K \end{array} \right.$$



As a consequence, the scheme can be written

$$\frac{\mathbf{u}_h^{n+1} - \mathbf{u}_h^n}{h} + \partial I_{\mathrm{C}_h(\mathbf{q}_h^n)}\left(\mathbf{u}_h^{n+1}\right) \ni \mathbf{f}_h^{n+1}(\mathbf{q}_h^n)$$

$$\frac{\mathbf{u}_h^{n+1} - \mathbf{u}_h^n}{h} + \partial I_{\mathrm{C}_h(\mathbf{q}_h^n)}\left(\mathbf{u}_h^{n+1}\right) \ni \mathbf{f}_h^{n+1}(\mathbf{q}_h^n) \qquad (\star)$$

For any $\mathbf{q} \in Q_0$, $\mathcal{N}_{\mathbf{q}}$ is the convex closure of half lines $-\mathbb{R}_+\mathbf{G}_{ij}$ for indices verifying $D_{ij}(\mathbf{q}) = 0$, and $\partial I_{\mathrm{C}_h(\mathbf{q})}(\mathbf{u})$ can be written as the same sum for indices i and j such that

$$D_{ij}(\mathbf{q}) + h\mathbf{G}_{ij} \cdot \mathbf{u} = 0.$$

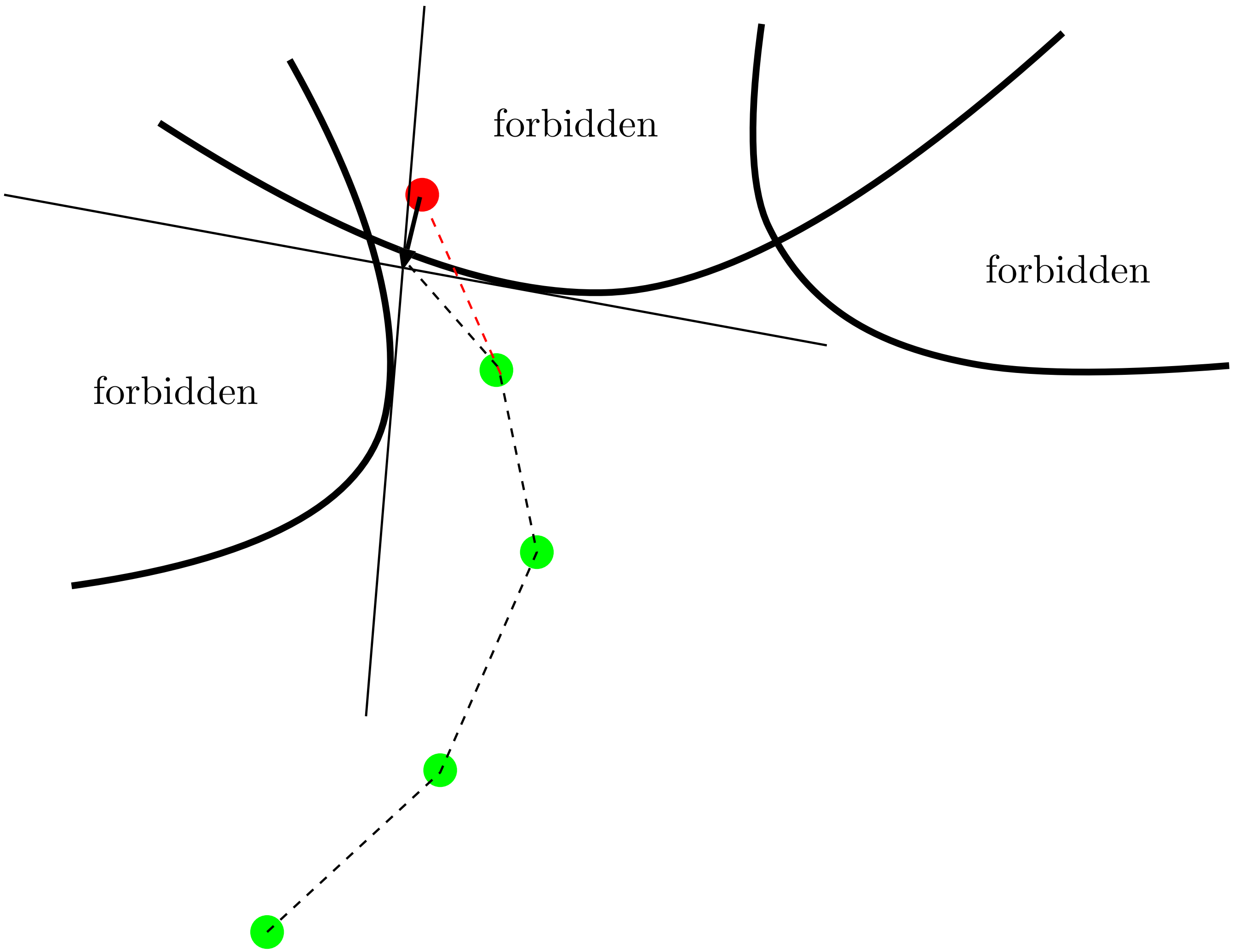
Left-hand side: Taylor expansion of $D_{ij}(\mathbf{q} + h\mathbf{u})$

$\longrightarrow$ the set $\partial I_{\mathrm{C}_h(\mathbf{q}_h^n)}(\mathbf{u}_h^{n+1})$ can be seen as a prediction of $\mathcal{N}_{\mathbf{q}_h^{n+1}}$.

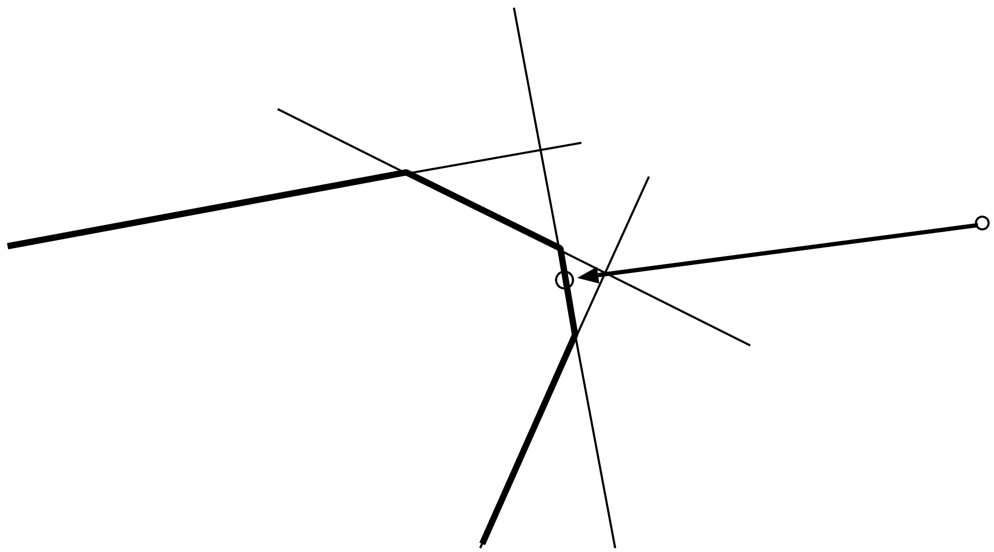
To sum up : $(\star)$ is a semi-implicit time discretization of inclusion

$$\frac{d\mathbf{u}}{dt} + \mathcal{N}_{\mathbf{q}} \ni \mathbf{f}(\mathbf{q}).$$

Interpretation in terms of positions



Projection step (independent from the scheme itself)



$$\text{Find } \mathbf{u} = \arg\min_K \frac{1}{2} \left|\mathbf{u} - \mathbf{U}\right|^2 \ , \quad K = \{\mathbf{v} \ , \ \ B\mathbf{v} \leq \mathbf{D}\}$$

with $B \in \mathcal{M}_{r,2N}(\mathbb{R})$ ($r = N(N-1)/2 =$ number of constraints).

Dual formulation: Find $(\mathbf{u}, \boldsymbol{\lambda}) \in \mathbb{R}^{2N} \times \mathbb{R}^r_+$ saddle point of

$$\mathcal{L}(\mathbf{v}, \boldsymbol{\mu}) = \frac{1}{2}|\mathbf{v} - \mathbf{U}|^2 + (B\mathbf{v} - \mathbf{D}, \boldsymbol{\mu}),$$

$$\mathcal{L}(\mathbf{u}, \boldsymbol{\mu}) \leq \mathcal{L}(\mathbf{u}, \boldsymbol{\lambda}) \leq \mathcal{L}(\mathbf{v}, \boldsymbol{\lambda}), \quad \forall \mathbf{v} \in \mathrm{T}_Q \ , \quad \boldsymbol{\mu} \in \mathbb{R}^r_+.$$

Equivalently:

$$\begin{cases} \mathbf{u} + B^\star \boldsymbol{\lambda} & = & \mathbf{U} \\ B\mathbf{u} & \leq & \mathbf{D} \\ (B\mathbf{u} - \mathbf{D}, \boldsymbol{\lambda}) & = & 0. \end{cases}$$

with $\mathbf{U}$ predicted velocity, $\mathbf{u}$ actual velocity.

Uzawa algorithm:

$$\boldsymbol{\lambda}^{k+1} = \Pi_+ \left(\boldsymbol{\lambda}^k + \rho \left(B(\mathbf{U} - B^\star \boldsymbol{\lambda}^k) - \mathbf{D} \right) \right)$$

Back to our problem:

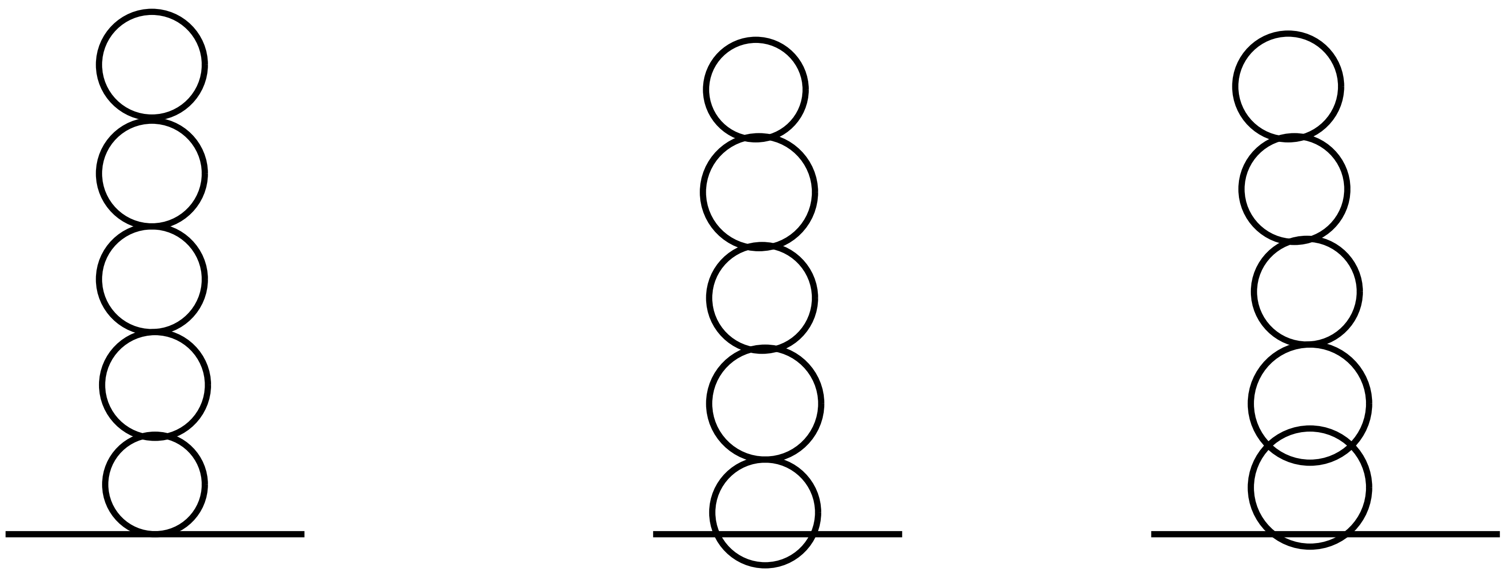
$$\mathbf{U} = \mathbf{u}_h^n + h\mathbf{f}_h^{n+1}(\mathbf{q}_h^n)\ , \quad B\mathbf{v} = (-h\mathbf{G}_{ij}\cdot\mathbf{v})_{i<j}\ , \quad \mathbf{D} = (\mathrm{D}_{ij}(\mathbf{q}_h^n))_{i<j},$$

so that $\mathbf{u}_h^{n+1}$ and $\boldsymbol{\lambda}_h^{n+1} = (\lambda_{ij}^{n+1})_{1\leq i<j\leq r}$ are related by

$$\frac{\mathbf{u}_h^{n+1} - \mathbf{u}_h^n}{h} = \mathbf{f}_h^{n+1}(\mathbf{q}_h^n) + \sum_{i<j} \lambda_{ij}^{n+1}\mathbf{G}_{ij}(\mathbf{q}_h^n).$$

$$\frac{d\mathbf{u}}{dt} = \mathbf{f} + \sum_{i<j}\lambda_{ij}\mathbf{G}_{ij}$$

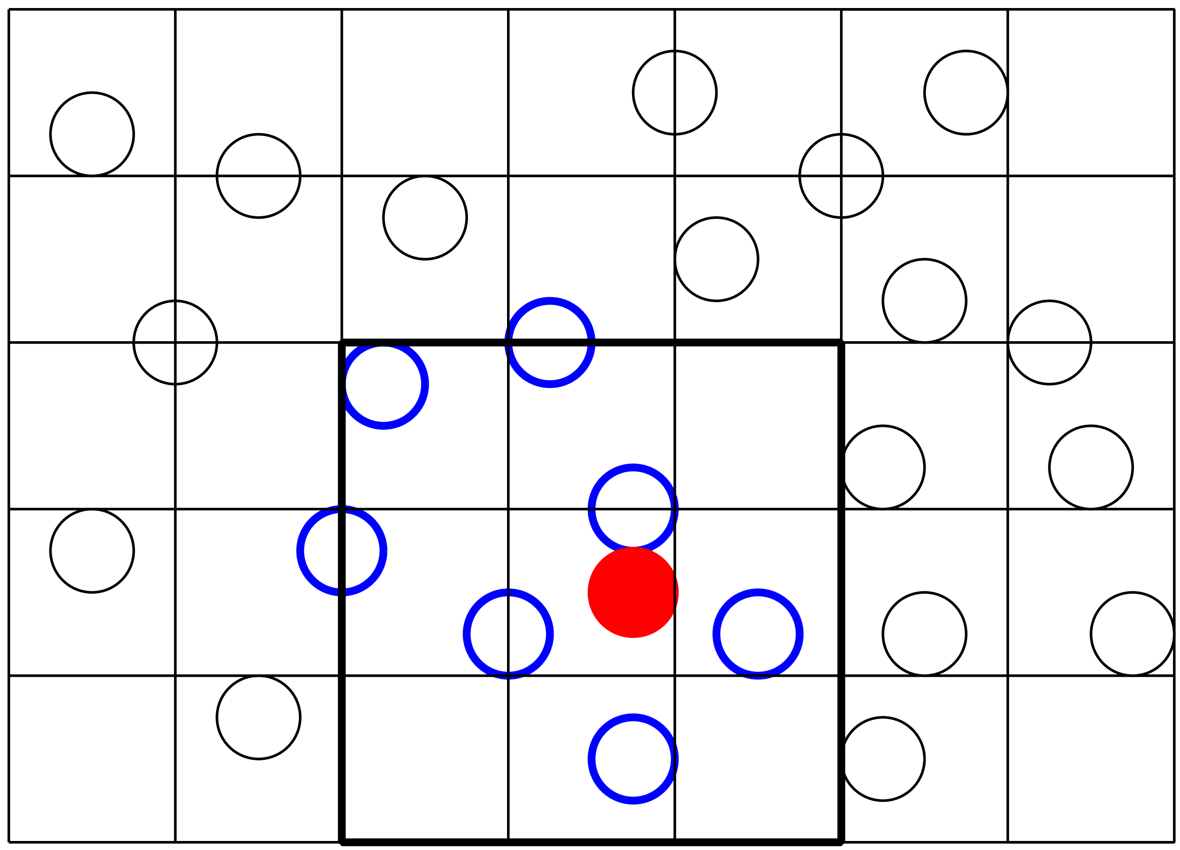
Behaviour of uzawa algorithm



Cost reduction

Number of constraints $r = N(N-1)/2$ can be reduced to $\mathcal{O}(N)$.

Bucket sorting:



NUMERICAL TESTS

Behaviour of the scheme in the case of huge time steps

Confrontation to a case of non-uniqueness

Many-body problem with large time steps

Stochastic forcing

Various animations

1D problem, spheres in a row, non elastic chock

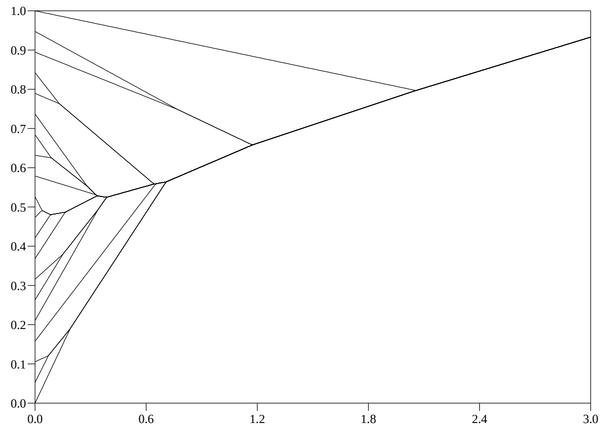
Discrete version of pressureless gas models

See Brenier [4] (sticky particles) for punctual particles

$$\begin{aligned}
\partial_t \rho + \partial_x(\rho u) &= 0, \\
\partial_t(\rho u) + \partial_x(\rho u^2) &= 0.
\end{aligned}$$

or Berthelin [2] (sticky blocks) for finite size particule

$$\begin{aligned}
\partial_t \rho + \partial_x(\rho u) &= 0, \\
\partial_t(\rho u) + \partial_x(\rho u^2) + \partial_x p &= 0. \\
\rho &\leq 1 \\
(1-\rho)p &= 0.
\end{aligned}$$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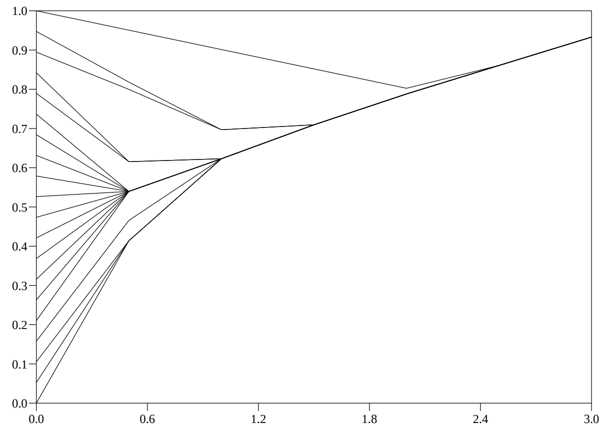
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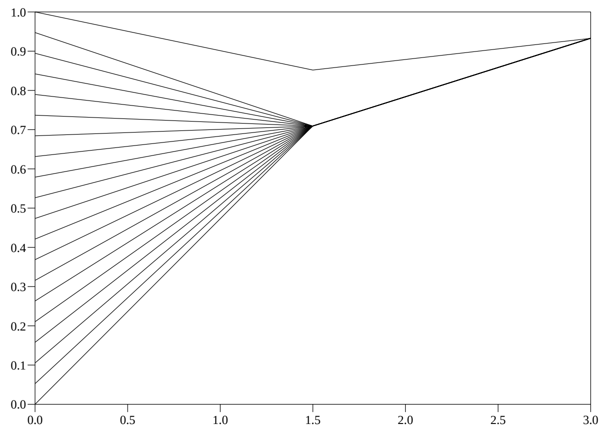
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Non uniqueness

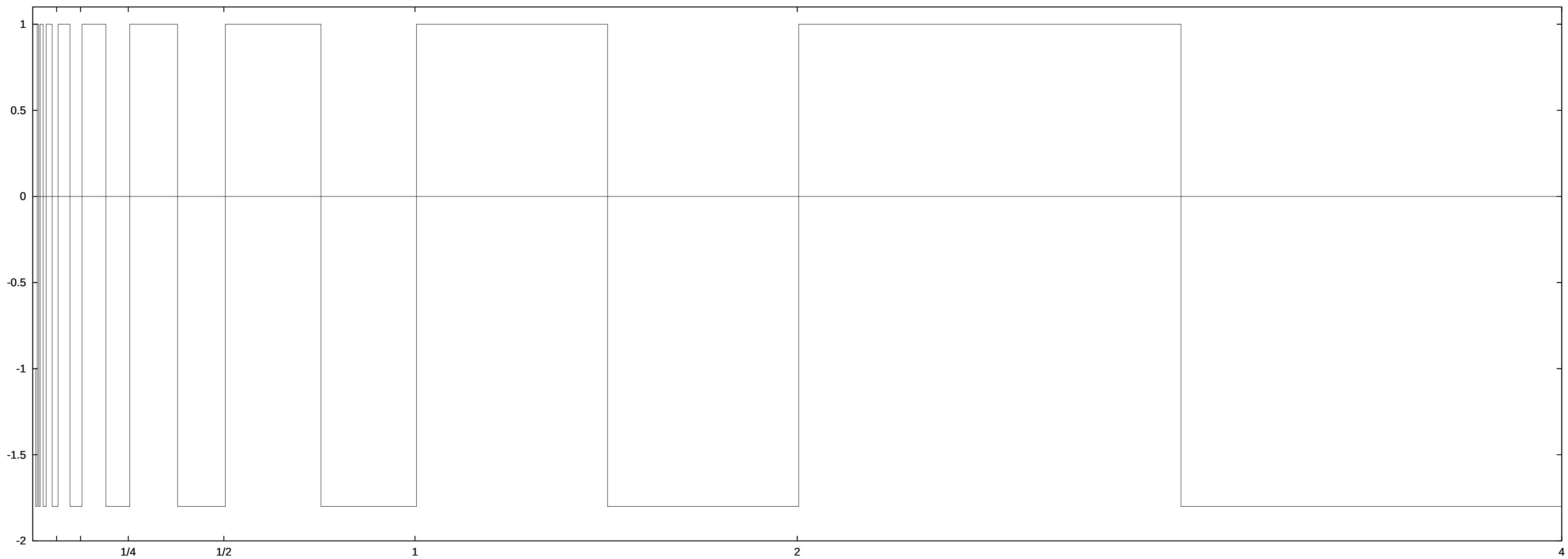
(counter example in the spirit of Schatzman [22], Ballard [1])

$$
\begin{array}{rcl}
u(0) & = & 0, \\
q(t) & = & \displaystyle\int_0^t u(s)\ \mathrm{ds} \quad \forall t \in I, \\
\dot{u}(t) & = & f(t) + \lambda, \\
\mathrm{supp}(\lambda) & \subset & \{t\ ,\ \ q(t) = 0\}, \\
u^+ & = & u^- - P_{\mathcal{N}_q} u^- \quad \forall t \in I,
\end{array}
$$

where $\mathcal{N}_q$ is $\{0\}$ whenever $q > 0$, and $\mathbb{R}^-$ as soon as $q = 0$.

Force field

$$
f(t) = \left| \begin{array}{lll} 1 & \text{for} & t \in \left(\dfrac{1}{2^{k+1}}, \dfrac{1}{2^{k+1}} + \dfrac{1}{2^{k+2}} \right) \\ & & \\ -\alpha & \text{for} & t \in \left(\dfrac{1}{2^{k+1}} + \dfrac{1}{2^{k+2}}, \dfrac{1}{2^{k}} \right) \end{array} \right\} k \in \mathbb{Z}\ ,\quad k \geq -4.
$$



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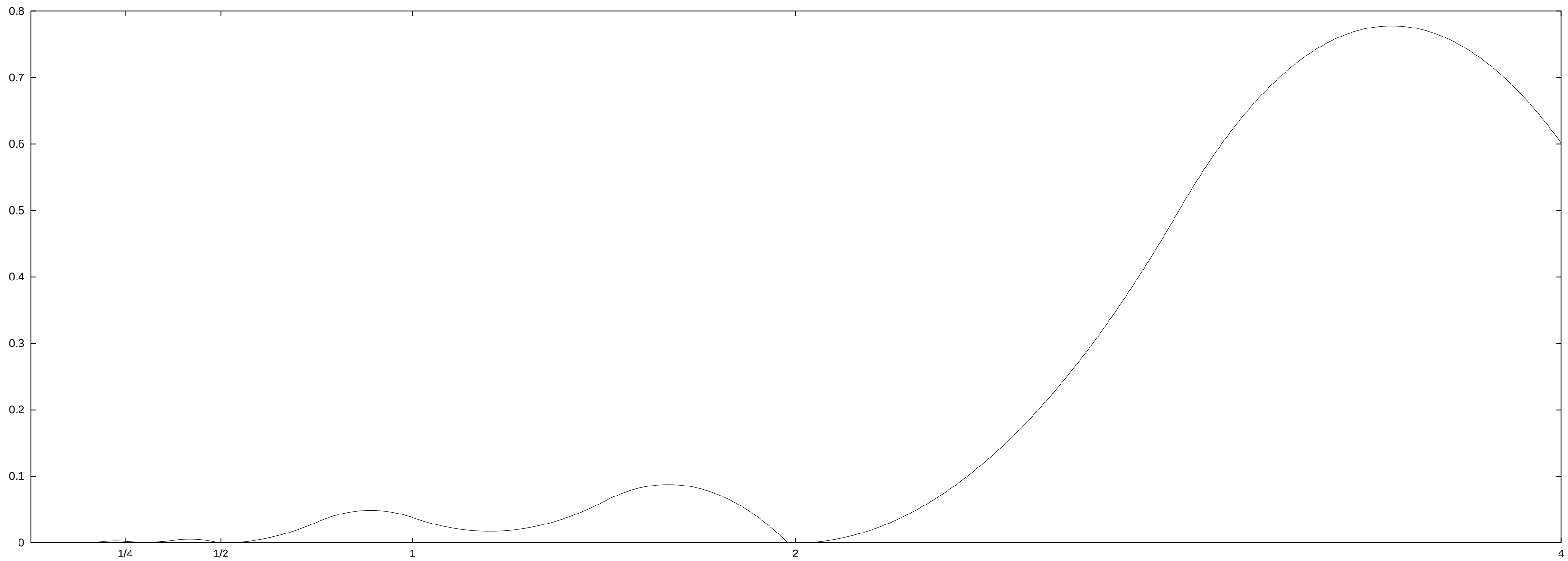
1
2
4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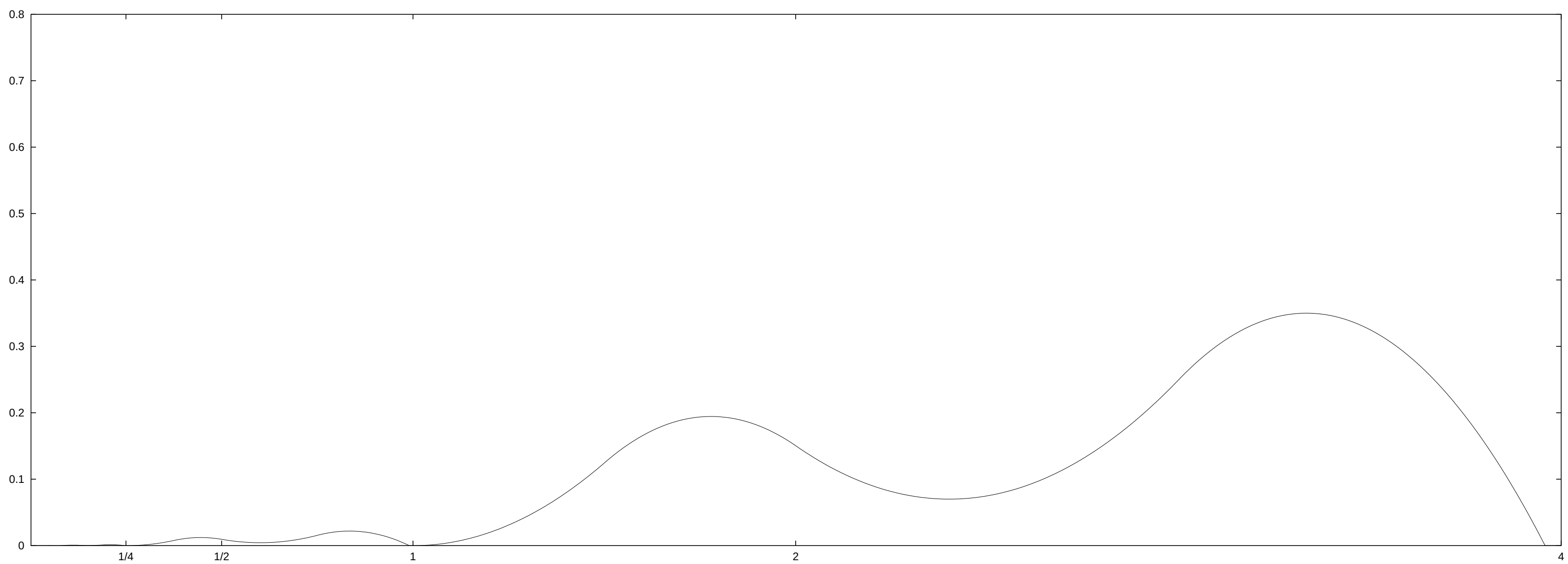
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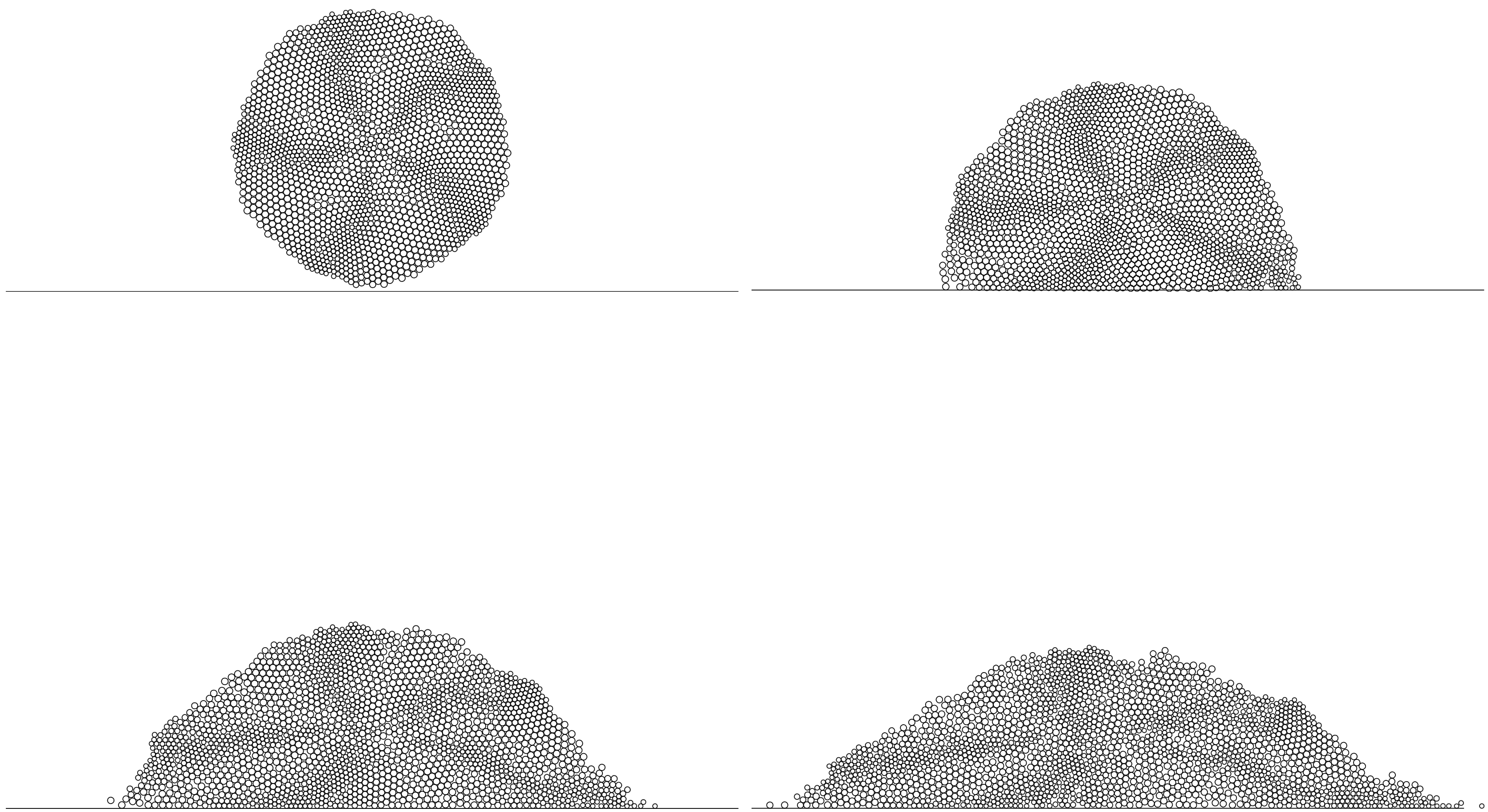
Large time steps in a many-body situation (every 3 time steps shots)



Stochastic forcing

$$\mathbf{q}(t) = \mathbf{q}_0 + \int_0^t \mathbf{u}(s)\,\mathrm{ds} \ \in Q_0 \quad \forall\, t \ \in I$$

$$d\mathbf{u} = \mathbf{f}(\mathbf{q}, t)\,dt + \sum_{i<j} d\lambda_{ij}\mathbf{G}_{ij}(\mathbf{q}(t)) + \sigma d\mathbf{w}$$

$$\mathrm{supp}(d\lambda_{ij}) \subset \{t, D_{ij}(\mathbf{q}(t)) = 0\},$$

$$\mathbf{u}^+(t) = P_{C_\mathbf{q}}\mathbf{u}^-(t) \quad \forall t \in I,$$

Numerically:

$$\mathbf{u}_h^{n+1} = \arg \min_{\mathbf{u}\in \mathrm{C}_h(\mathbf{q}_h^n)} \frac{1}{2}\left|\mathbf{u} - \mathbf{u}_h^n - h\mathbf{f}_h^{n+1}(\mathbf{q}_h^n) - \sqrt{h}\,\sigma\mathbf{w}^{n+1}\right|$$

1D problem

Unconstrained problem : primitive of the Brownian motion
$q = \int_0^t w(s)\, ds$.

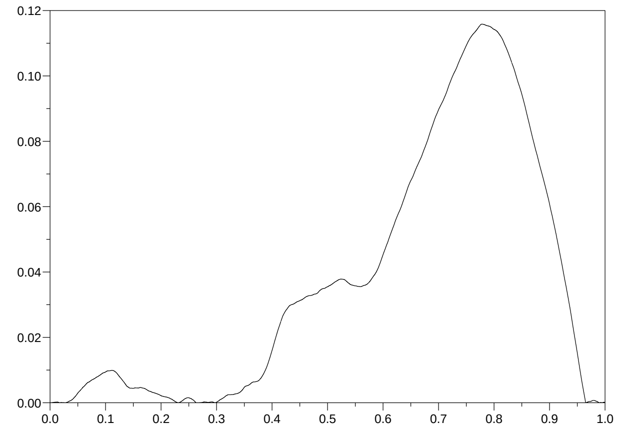
$\{t\ ,\ \ q(t) = 0\}$ has a.s. a single cluster point at 0,

Constrained problem :

$$\begin{aligned} du &= \sigma dw + d\lambda \\ dq &= u\, dt \\ u^+ &= P_{\mathcal{C}_q} u^- \end{aligned}$$

Almost surely: points of $Z = \{t\ ,\ \ q(t) = 0\}$ are left-hand cluster points of Z itself, but for a countable infinity (take off instants).
N.B. : u is no longer in BV.

Analysis : see Bertoin [3]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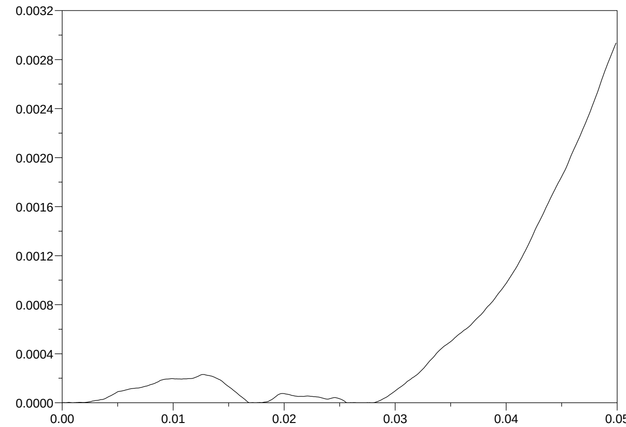
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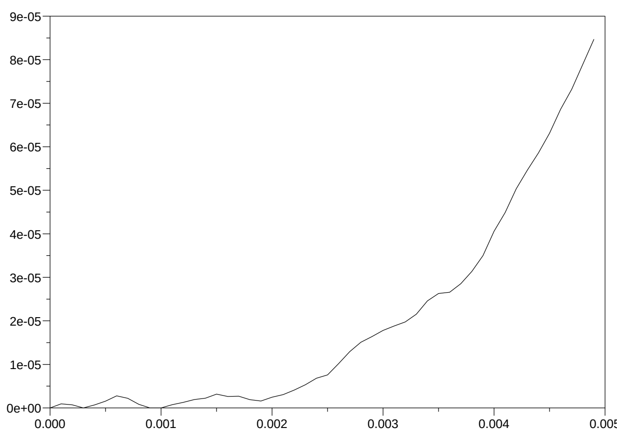
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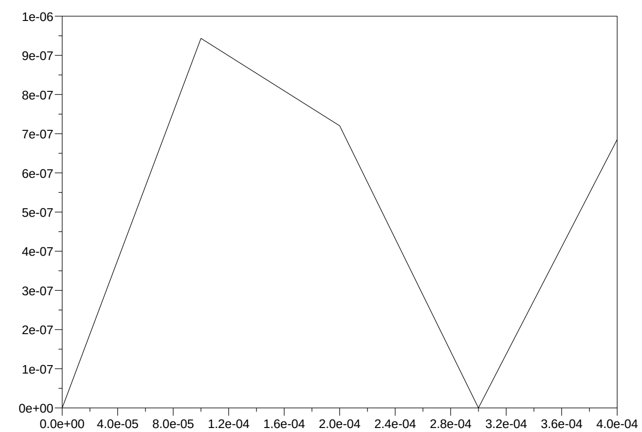
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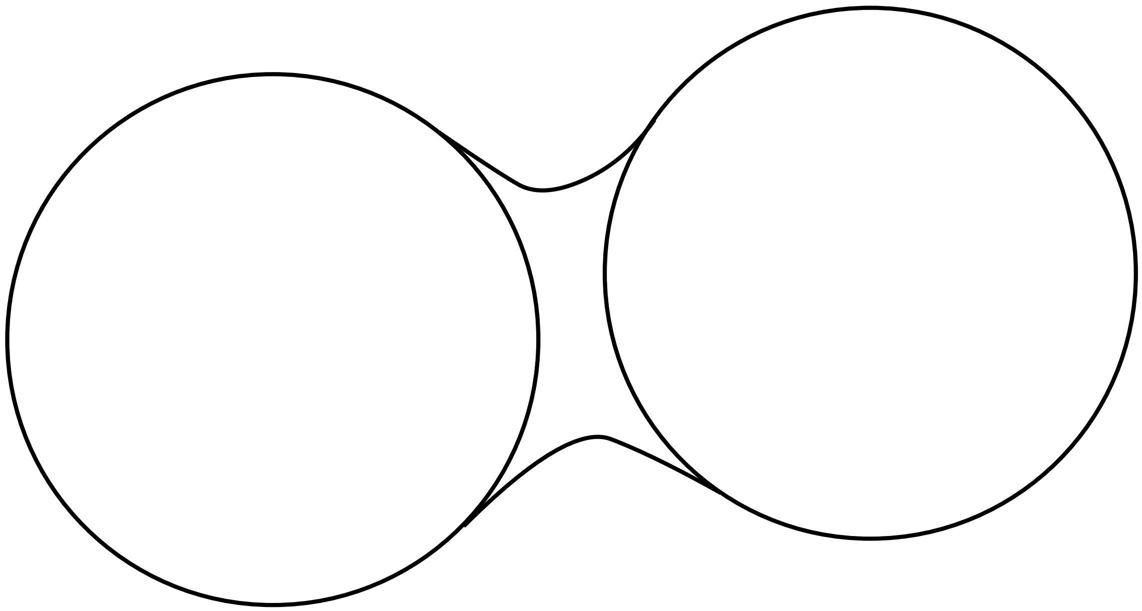
Capillary forces (with common radius r):



$$F_{ji} = -F_{ij} = \pi\gamma r \left(\exp\left(-AD_{ij} + B\right) + C\right) \mathbf{e}_{ij} \text{ if } D_{ij} < D_{\text{rupt}}.$$

→41-42

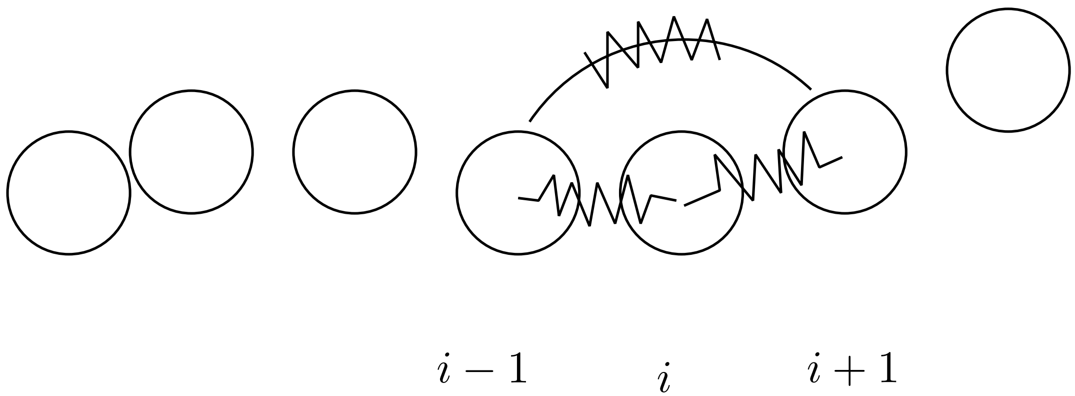
Further experiments

Many-body simulations →50-52-54

Macroscopic bodies

$$\text{Additional force}: \mathbf{F} = -\nabla_{\mathbf{q}} V ,$$

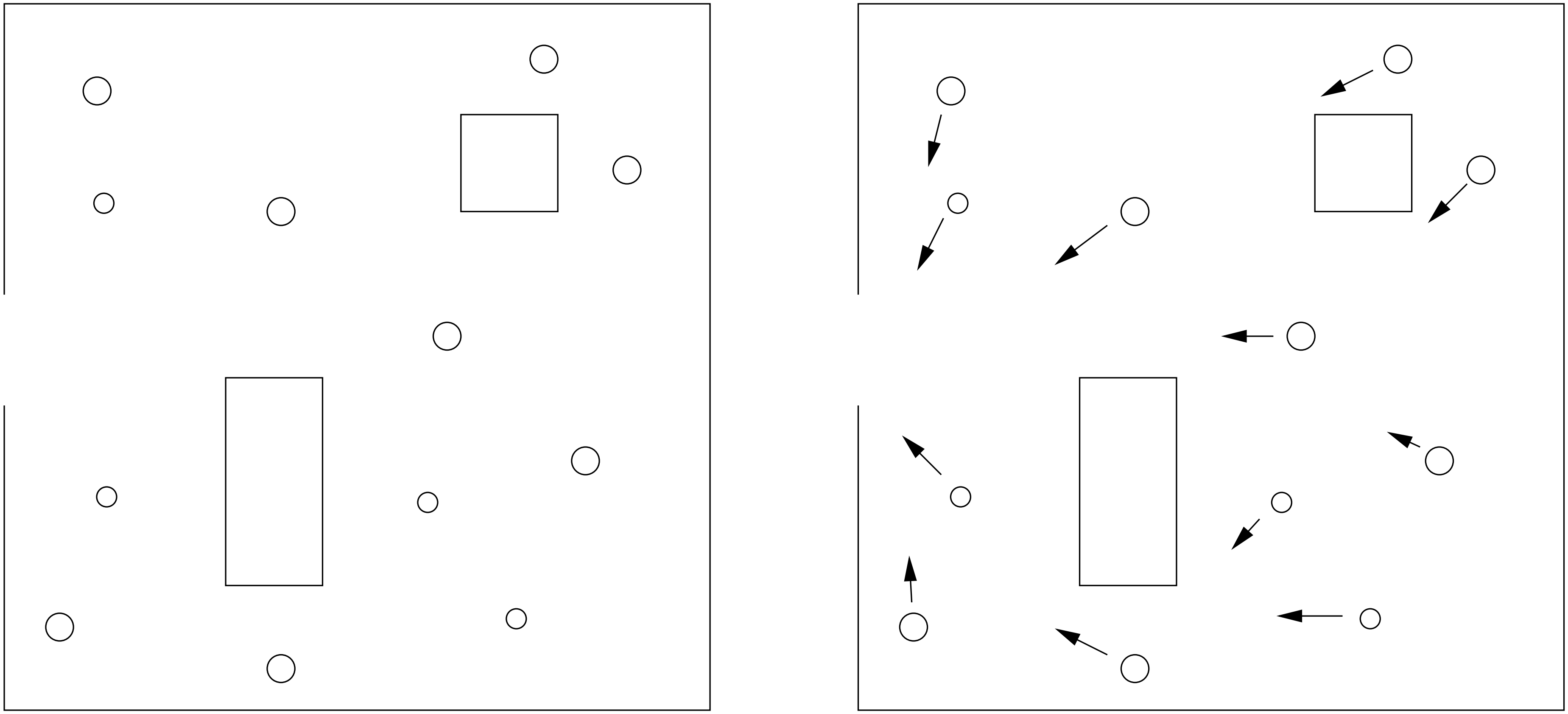
$$V = \frac{k}{2}\sum \left(|\mathbf{q}_{i+1} - \mathbf{q}_i| - \ell\right)^2 + \frac{k_a}{2}\sum \frac{\mathbf{q}_{i+1} - \mathbf{q}_i}{|\mathbf{q}_{i+1} - \mathbf{q}_i|} \cdot \frac{\mathbf{q}_{i-1} - \mathbf{q}_i}{|\mathbf{q}_{i-1} - \mathbf{q}_i|}.$$



→62-64

First-order evolution equation :

a crowd motion model (with Juliette Venel [16])



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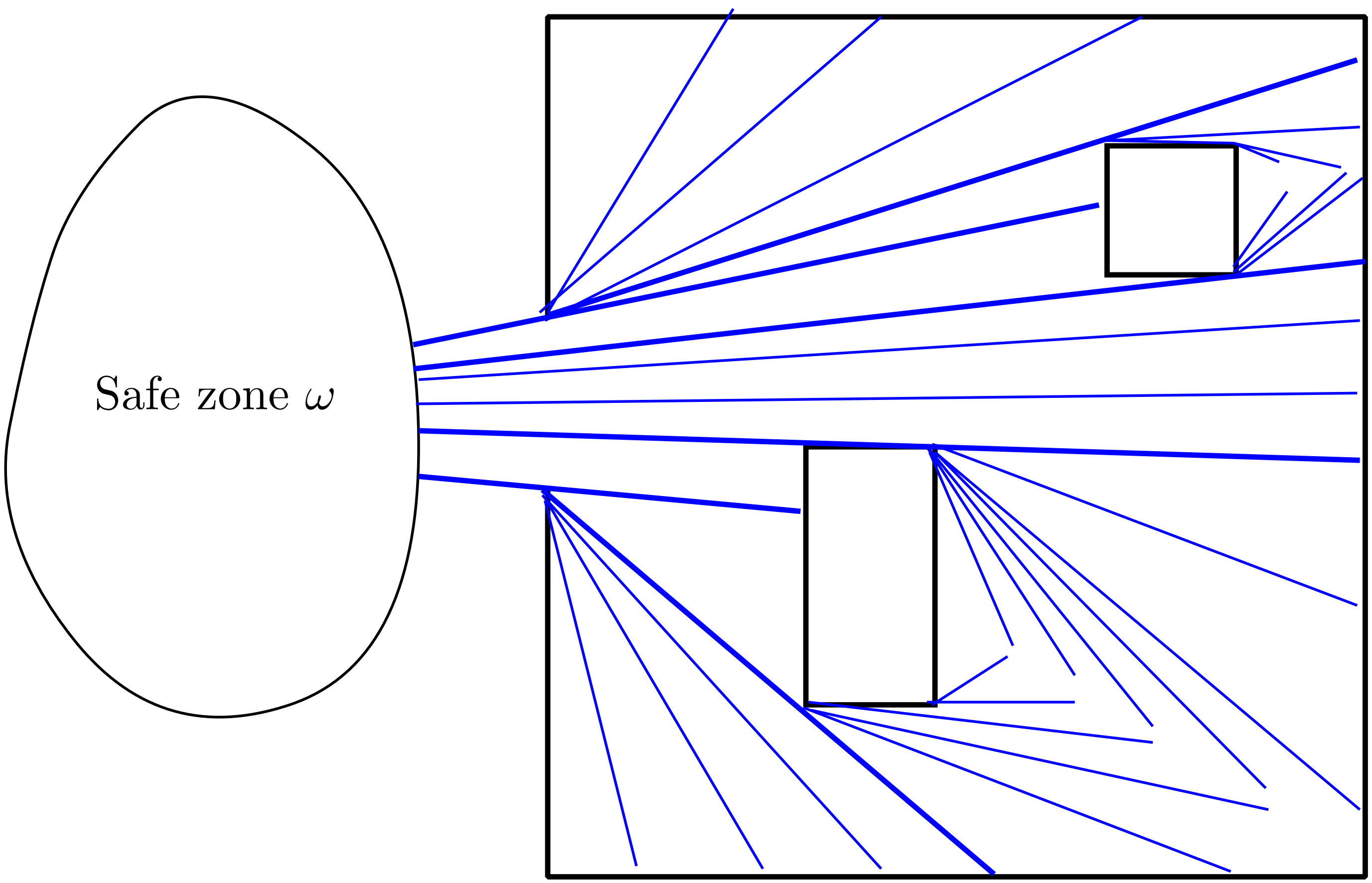


Evolution equation : $\dfrac{d\mathbf{q}}{dt} = P_{\mathcal{C}_{\mathbf{q}}}\mathbf{U}(\mathbf{q}) \quad \text{or} \quad \dfrac{d\mathbf{q}}{dt} + \mathcal{N}_{\mathbf{q}} \ni \mathbf{U}.$

$\rightarrow$70-72-73

Convergence of the scheme

Functional framework ($I =]0, T[$, N spheres in $\mathbb{R}^d$)

$\mathbf{q} \in W^{1,1}$: set of dN vector-valued functions, abs. continuous over I.

$\mathbf{u} \in \mathrm{BV}$: set of dN vector-valued functions with bounded variation over I:

$$\sup_{S \in \Lambda} \sum_{n=1}^{N_S} |\mathbf{u}(t_n) - \mathbf{u}(t_{n-1})| < \infty,$$

where $S = (t_0, t_1, \ldots, t_{N_S})$ runs over the set of subdivisions of I.

$\boldsymbol{\mu} \in \mathcal{M}^1 =$ set of $N(N-1)/2$ vector-valued bounded measures on I :
$\boldsymbol{\mu} = (\mu_{ij})_{1 \le i < j \le N}$ with μ_{ij} a continuous linear functional over $C_0(I)$

Component-wise positive measures:

$$\mathcal{M}^1_+ = \left\{ \boldsymbol{\mu} = (\mu_{ij})_{1 \le i < j \le N} \in \mathcal{M}^1, \, \langle \mu_{ij}, \varphi \rangle \ge 0 \quad \forall \varphi \in C_0(I), \, \varphi \ge 0 \right\}.$$

Condition on $\mathbf{f}$: Carathéodory type (see Coddington [6])

$$\exists F \in L^1(I) \text{ s.t. } |\mathbf{f}(\mathbf{q},t)| \leq F(t) \quad \forall (\mathbf{q},t) \in Q_0 \times I,$$

and $\mathbf{f}$ is uniformly Lipschitz with respect to $\mathbf{q}$

$$\exists k \ , \ \ |\mathbf{f}(\mathbf{q}',t) - \mathbf{f}(\mathbf{q},t)| \leq k\,|\mathbf{q}' - \mathbf{q}| \quad a.e. \text{ in } I \quad \forall \mathbf{q},\, \mathbf{q}' \in Q_0.$$

Rk: forces like $\mathbf{f} = -K\nabla V(|q_2 - q_1|)$ with $V(d) = K/d$, are OK.

Discrete functions

$$X_h = \left\{ \mathbf{q}_h = (\mathbf{q}_i) : I \to Q \ , \ \ \mathbf{q}_i \in (\mathrm{P}^1_h)^d \ , \ \ 1 \leq i \leq N \right\},$$

$$V_h = \left\{ \mathbf{u}_h = (\mathbf{u}_i) : I \to \ \mathrm{T}_Q \ , \ \ \mathbf{u}_i \in (\mathrm{P}^0_h)^d \ , \ \ 1 \leq i \leq N \right\},$$

$$R_h = \left\{ \boldsymbol{\mu}_h = (\mu_{ij}) : I \to \ \mathbb{R}^r \ , \ \ \mu_{ij} \in \mathrm{P}^0_h \ , \ \ 1 \leq i < j \leq N \right\},$$

where $r = N(N-1)/2$ is the number of constraints.

For any $\mathbf{u}_h \in V_h$ (resp. $\boldsymbol{\mu}_h \in R_h$) $\mathbf{u}_h^n$ (resp. $\boldsymbol{\mu}_h^n$) denotes the constant value in the subinterval $\big[(n-1)h, nh\big)$.

Similarly, $\mathbf{q}_h^n$ denotes $\mathbf{q}_h(nh)$, for any $\mathbf{q}_h \in X_h$.

Theorem (for a single contact)s

Let $(\mathbf{q}_h, \mathbf{u}_h, \mu_h)_h$ be a sequence of approximate solutions, with $h \to 0$. There exists a subsequence of time steps (still denoted by h), and

$$(\mathbf{q}, \mathbf{u}, \lambda) \in W^{1,1} \times \mathrm{BV} \times \mathcal{M}^1_+$$

such that

$$\mathbf{q}_h \longrightarrow \mathbf{q} \quad \text{in } W^{1,1},$$

$$\lambda_h \overset{\star}{\rightharpoonup} \lambda \quad \text{in } \mathcal{M}^1,$$

and $(\mathbf{q}, \mathbf{u}, \lambda)$ is *a* solution to the initial problem.

PROOF

1) The scheme produces feasible configurations only: $\mathbf{q}_h(t) \in Q_0$.

2) The family $(\mathbf{u}_h)$ is uniformly bounded, *i.e.*,

$$\exists C_\infty \ , \quad |\mathbf{u}_h(t)| \leq C_\infty \quad \forall t \in [0,T] \ , \quad \forall h > 0.$$

3) The fields $\mathbf{u}_h$ have uniform bounded variation, *i.e.*,

$$\exists C_{\mathrm{var}} \ , \quad \mathrm{var}(\mathbf{u}_h) = \sum_{n=1}^{N} |\mathbf{u}_h^n - \mathbf{u}_h^{n-1}| \leq C_{\mathrm{var}} \quad \forall h.$$

4) The familly $(\mathbf{u}_h)$ is relatively compact in $L^1(I)$. One can extract a subsequence (still denoted $\mathbf{q}_h$) such that $\mathbf{q}_h \longrightarrow \mathbf{q}$ in $W^{1,1}$. The limit velocity $\mathbf{u} = \dot{\mathbf{q}} = \lim \dot{\mathbf{q}}_h$ is in BV, and the limit motion $\mathbf{q}$ is feasible.

5) The sequence $(\lambda_h)_h$ is bounded in L^1: up to a subsequence, it converges weak-$\star$ to a vector-valued bounded measure $\lambda \in \mathcal{M}^1_+$.

6) The pair $(\mathbf{u}, \lambda)$ verifies the momentum equation.

7) Complementarity slackness condition (unformally $\lambda D = 0$):

$$\mathrm{supp}(\lambda) \subset \{t \;, \;\; D(q(t)) = 0\}.$$

8) The initial condition is verified.

9) The jump equation $\mathbf{u}^{+} = P_{\mathcal{C}_{\mathbf{q}}} \mathbf{u}^{-}$ is verified.

1) Feasibility ($\mathbf{q}_h(t) \in Q_0 \quad \forall h > 0, \forall t$).

Convexity of $\mathbf{q} \mapsto D_{ij}(\mathbf{q})$ implies

$$
\begin{aligned}
D_{ij}(\mathbf{q}_h^{n+1}) &= D_{ij}(\mathbf{q}_h^n + h\mathbf{u}_h^{n+1}) \\
&\geq D_{ij}(\mathbf{q}_h^n) + h\mathbf{G}_{ij}(\mathbf{q}_h^n) \cdot \mathbf{u}_h^{n+1} \quad \text{(since } D_{ij} \text{ is convex)} \\
&\geq 0.
\end{aligned}
$$

2) Uniform boundedness of the velocity: due to the implicit character of the scheme.

$$
\frac{\mathbf{u}_h^{n+1} - \mathbf{u}_h^n}{h} + \partial I_{\mathrm{C}_h(\mathbf{q}_h^n)}\left(\mathbf{u}_h^{n+1}\right) \ni \mathbf{f}_h^{n+1}(\mathbf{q}_h^n)
$$

$\mathrm{C}_h(\mathbf{q}_h^n)$ closed and convex $\implies$ Operator $I + \partial I_{\mathrm{C}_h(\mathbf{q}_h^n)}$ is a contraction.

3) Uniformly bounded variation of the velocity. Not trivial, as the number of collisions (i.e. number of instants at which the velocity is likely to be discontinuous) is not bounded, even for regular data.

Core of the proof: compactness argument (Brezis 1973).

THEOREM

$$\frac{du}{dt} + Au \ni f(t),$$

with $A : H \to H$ maximal monotone operator , $f \in L^1(I, H)$. If the domain of A has a nonempty interior, then the solution u is BV.

Here: second order equation, but the time discretization scheme reads

$$\frac{\mathbf{u}_h^{n+1} - \mathbf{u}_h^n}{h} + \partial I_{\mathrm{C}_h(\mathbf{q}_h^n)}\left(\mathbf{u}_h^{n+1}\right) \ni \mathbf{f}_h^{n+1}(\mathbf{q}_h^n)$$

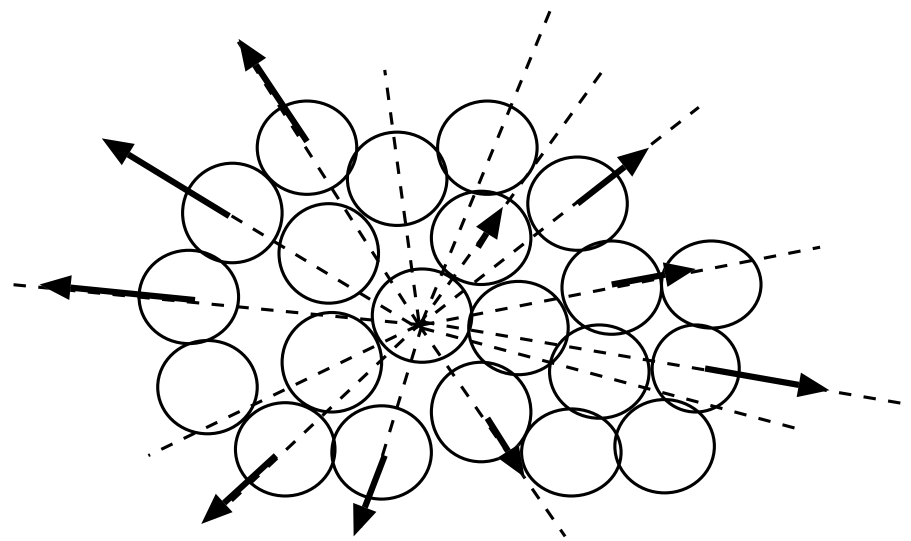
which is basically

$$\frac{d\mathbf{u}}{dt} + \partial I_{C(\mathbf{q}(t))}\mathbf{u} \ni \mathbf{f}(\mathbf{q}(t), t)$$

Key-point in the proof of Brezis theorem: fix an interior point in $D(A)$.

$\longrightarrow$ does there exist $\mathbf{u}_0 \in \overset{o}{\mathrm{C}}_h(\mathbf{q}_h(t))$?

$$\mathrm{C}_h(\mathbf{q}_h^n) = \{\mathbf{u} \in \mathrm{T}_Q, D_{ij}(\mathbf{q}_h^n) + h\mathbf{G}_{ij}(\mathbf{q}_h^n) \cdot \mathbf{u} \geq 0\}.$$



Steps 4, 5, 6, 7, and 8 straightforward.

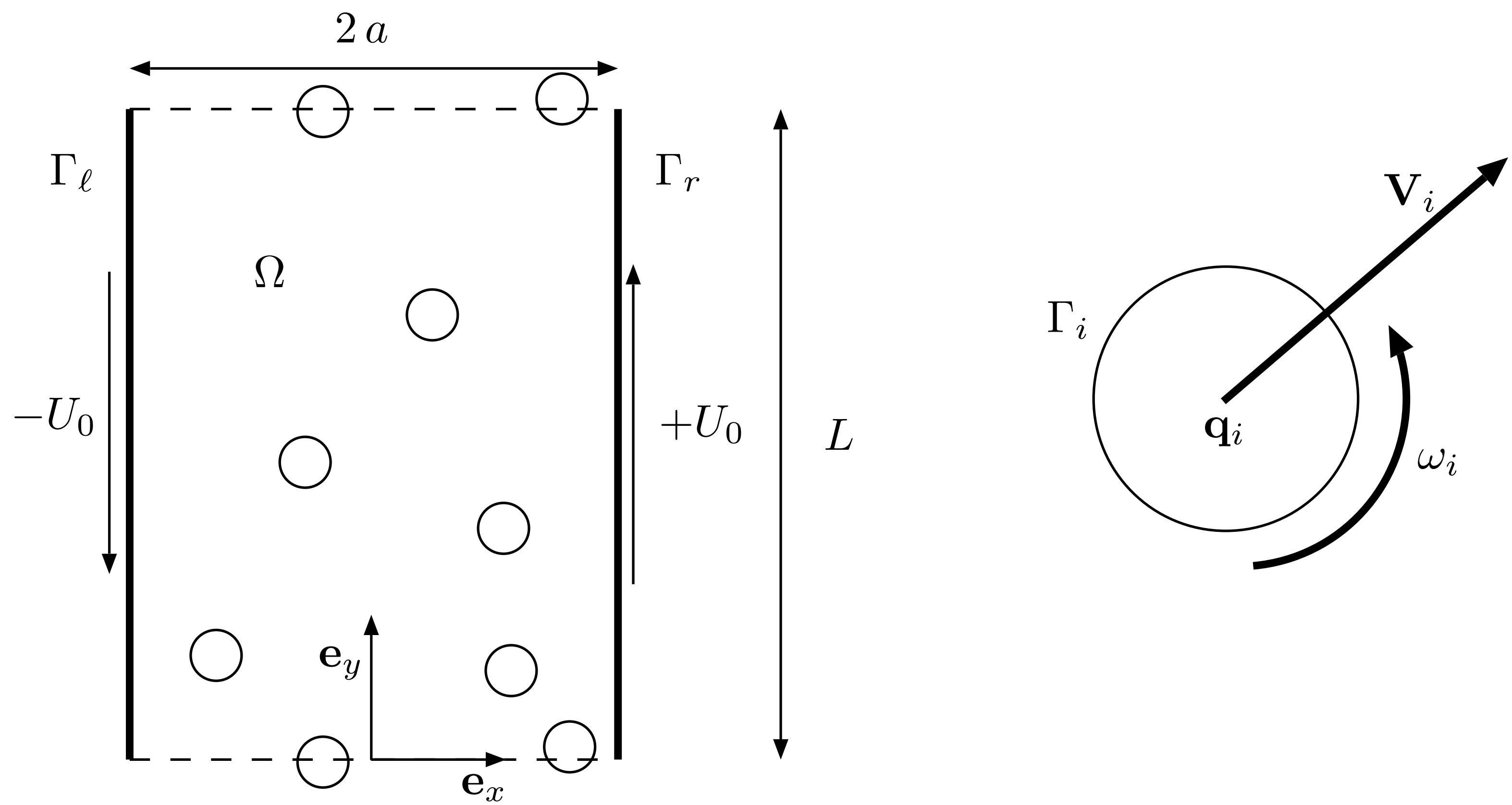
Step 9 : $\mathbf{u}^+ = P_{\mathcal{C}_\mathbf{q}} \mathbf{u}^-$, given $\mathbf{u}_h \longrightarrow \mathbf{u}$ in L^1 (see [17]).

LUBRICATED CONTACT

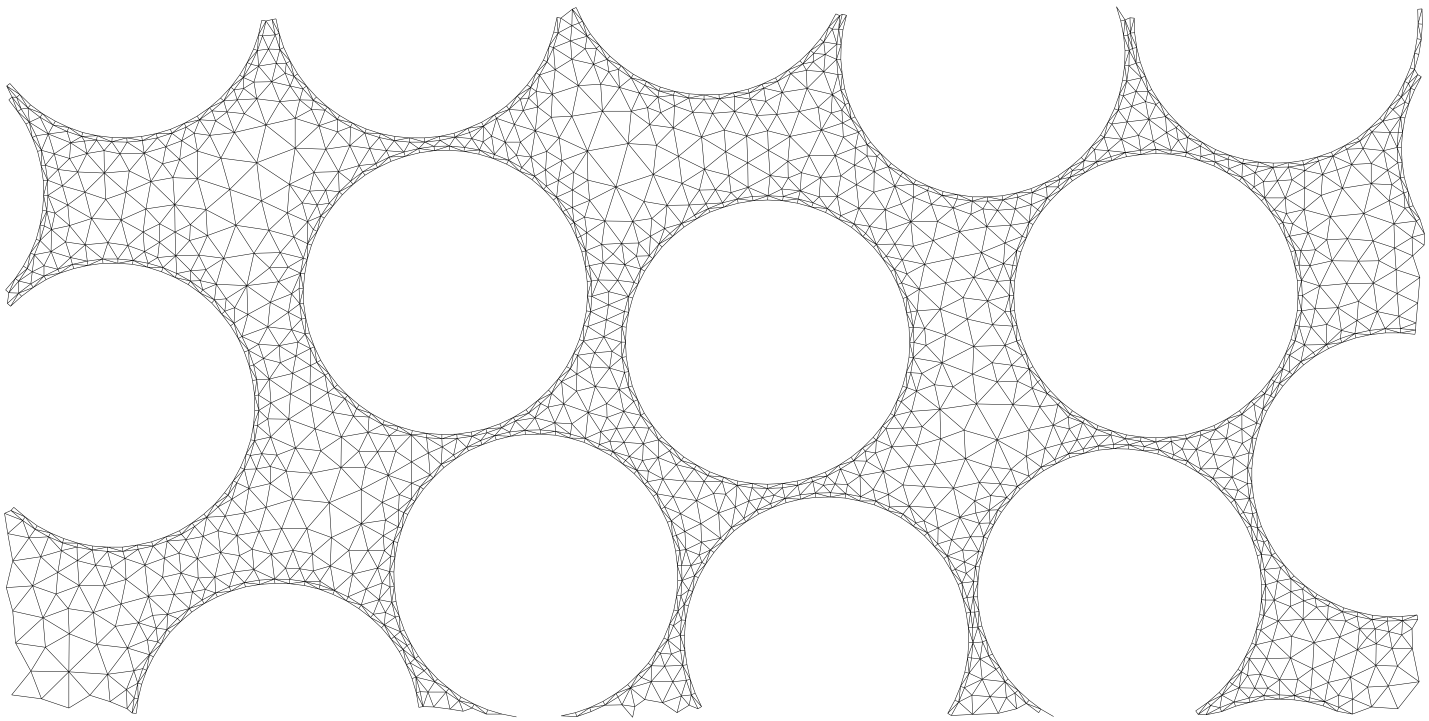
Motivation

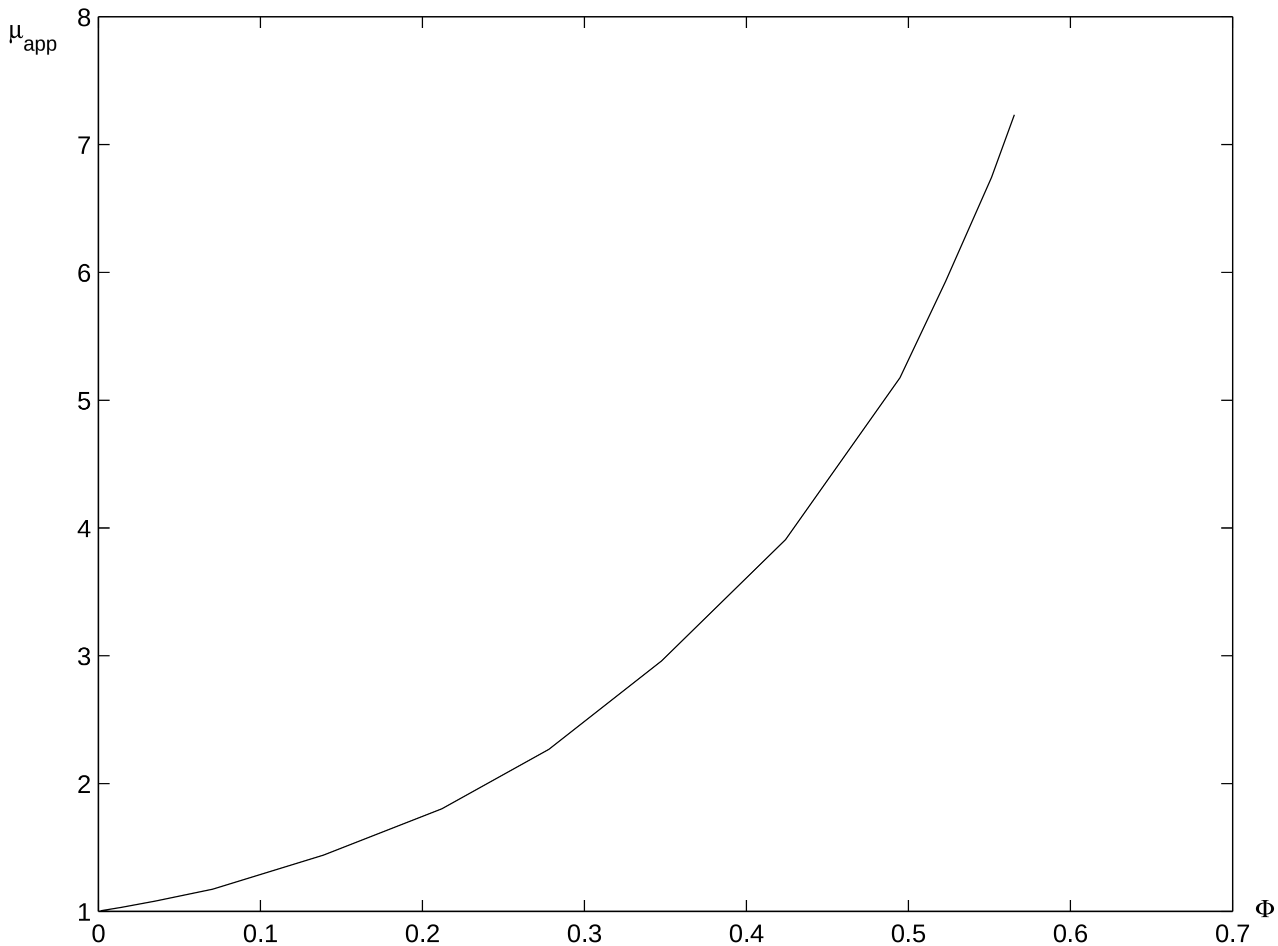
Body-body lubrication model : scheme I (see [14]).

Vanishing viscosity limit: scheme II (see [15, 12]).

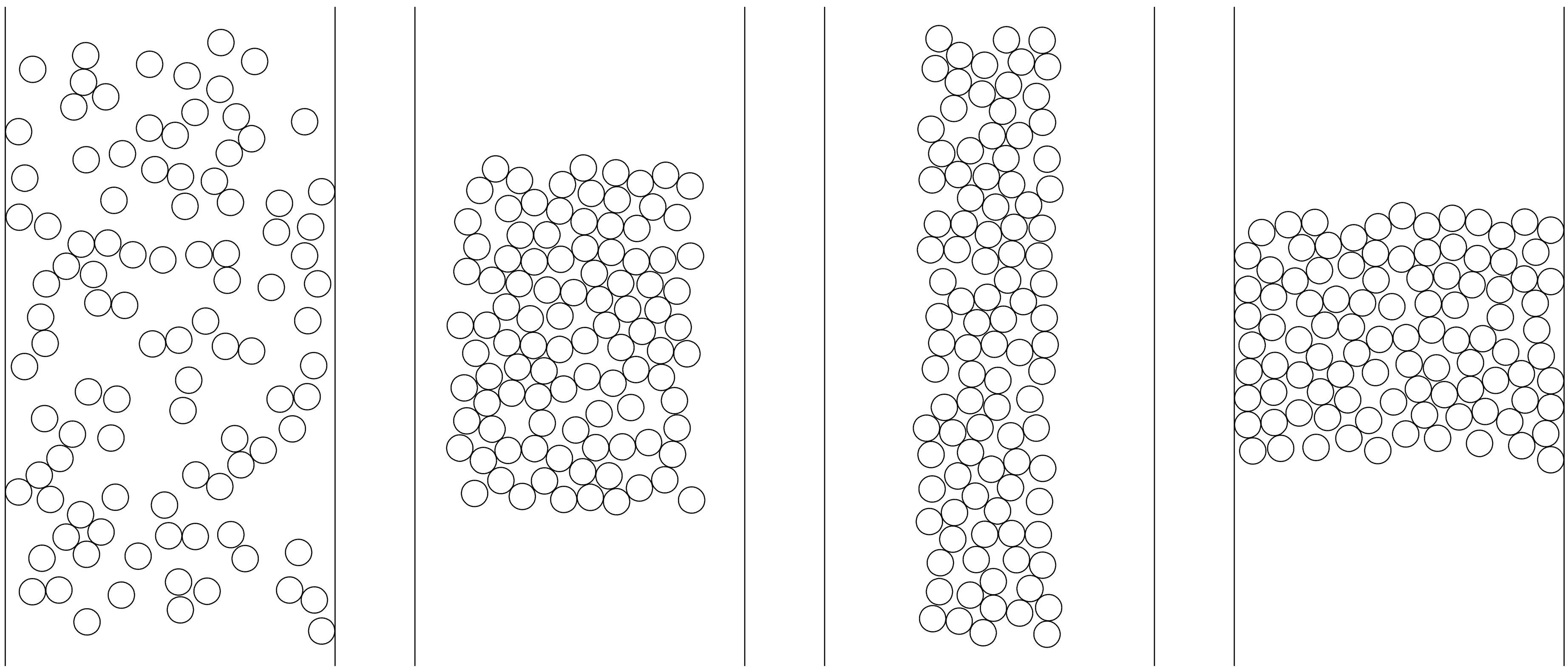


$2\,a$
Γ_ℓ
Γ_r
Ω
$-U_0$
$+U_0$
L
$\mathbf{e}_y$
$\mathbf{e}_x$
$\mathbf{V}_i$
Γ_i
$\mathbf{q}_i$
ω_i

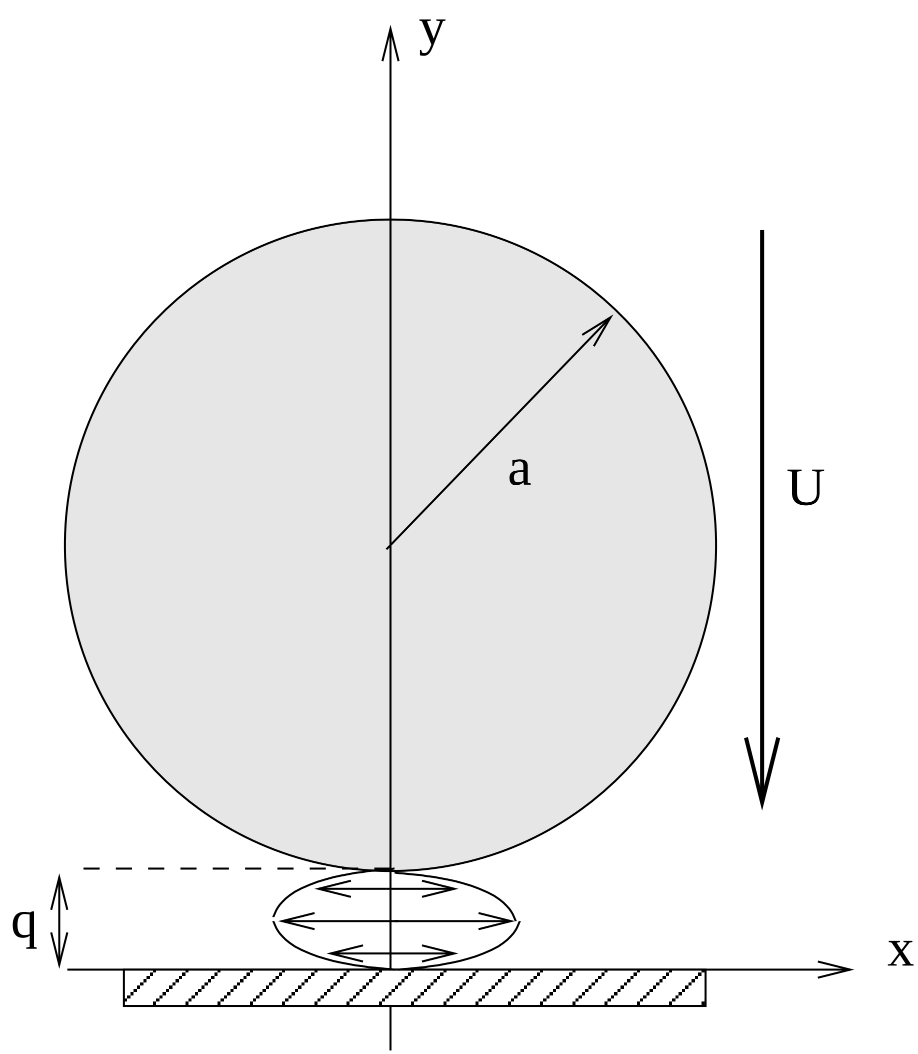




μ_{app}
8
7
6
5
4
3
2
1
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
Φ

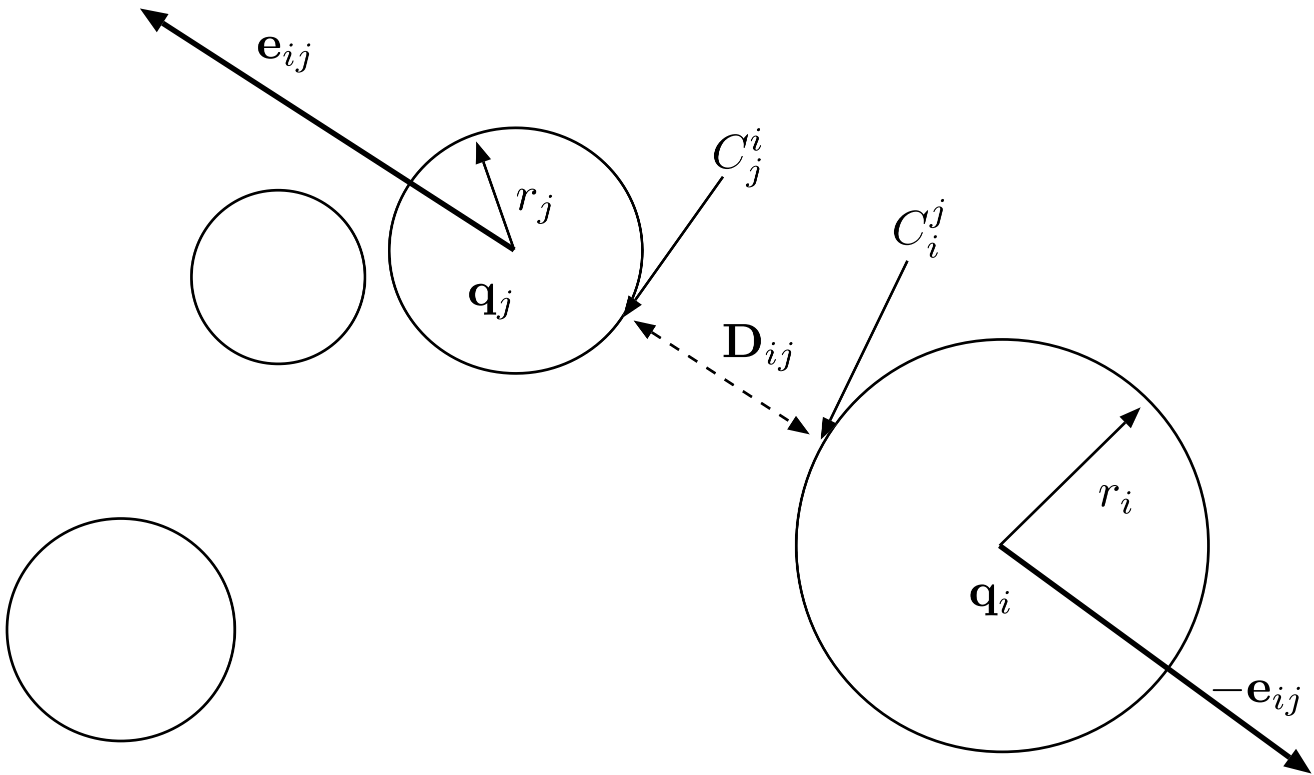


Apparent viscosities 2.0, 2.45, 1.62, and 6.54



$F_{lub} \sim -6\pi\mu a^2 \frac{U}{q} \mathbf{e}_y$ (See Brenner [7] or Kim [9])

Notations



$\mathbf{e}_{ij}$
C_j^i
r_j
C_i^j
$\mathbf{q}_j$
$\mathbf{D}_{ij}$
r_i
$\mathbf{q}_i$
$-\mathbf{e}_{ij}$

$$\mathbf{F}_i^j = -\mathbf{F}_j^i = -\kappa\,(\mathrm{D}_{ij})\,\left[(\dot{\mathbf{C}}_i^j - \dot{\mathbf{C}}_j^i)\cdot\mathbf{e}_{ij}\right]\;\mathbf{e}_{ij}\;,$$

which can be written

$$\mathbf{F}_i^j = \left[-\kappa\,(\mathrm{D}_{ij})\,\mathbf{e}_{ij}\otimes\mathbf{e}_{ij}\right]\cdot(\dot{\mathbf{C}}_i^j - \dot{\mathbf{C}}_j^i)\;,\quad \kappa\,(d) = \mu\;\,1/d.$$

$$m_i\,\ddot{\mathbf{q}}_i = \mathbf{\Phi}_i + \sum_{j\neq i}\;\mathbf{F}_i^j(\dot{\mathbf{C}}_i^j,\dot{\mathbf{C}}_j^i).$$

$$M\,\ddot{\mathbf{q}} = \Phi - \sum_{i<j}\left[\kappa\,(\mathrm{D}_{ij})\,\mathbf{G}_{ij}\otimes\mathbf{G}_{ij}\right]\cdot\dot{\mathbf{q}}$$

The velocity $\mathbf{u} = \dot{\mathbf{q}}$ verifies the associated energy balance

$$\frac{d}{dt}\,\left(\frac{1}{2}\,M\mathbf{u}\cdot\mathbf{u}\right) - \Phi\cdot\mathbf{u} + \Psi(\mathbf{u},\mathbf{u}) = 0\;,$$

with Φ symmetric, nonnegative bilinear form.

(in its kernel: rigid motion of clusters)

Numerical strategy: decoupling of $\mathbf{q}$ and the distances.

$$\dot{\mathrm{D}}_{pq} = \mathbf{G}_{pq} \cdot \dot{\mathbf{q}}\,, \quad \ddot{\mathrm{D}}_{pq} = \mathbf{G}_{pq} \cdot \ddot{\mathbf{q}} + \dot{\mathbf{G}}_{pq} \cdot \dot{\mathbf{q}}\,,$$

$$\begin{aligned} \Longrightarrow \ddot{\mathrm{D}}_{pq} \quad &= \quad \mathbf{G}_{pq} \cdot \mathrm{M}^{-1}\boldsymbol{\Phi} - \mu\, \frac{\dot{\mathrm{D}}_{pq}}{\mathrm{D}_{pq}}\, \mathbf{G}_{pq} \cdot \mathrm{M}^{-1}\mathbf{G}_{pq} \\ &\quad -\frac{1}{2}\sum_{i \neq j}\, \kappa\,(\mathrm{D}_{ij})(\mathbf{G}_{ij} \cdot \mathbf{u})\,(\mathbf{G}_{pq} \cdot \mathrm{M}^{-1}\mathbf{G}_{ij}) \end{aligned}$$

One keeps D_{pq} implicit, the other distances explicit

$\longrightarrow \ddot{D} = -\mu\dot{D}/D + f$

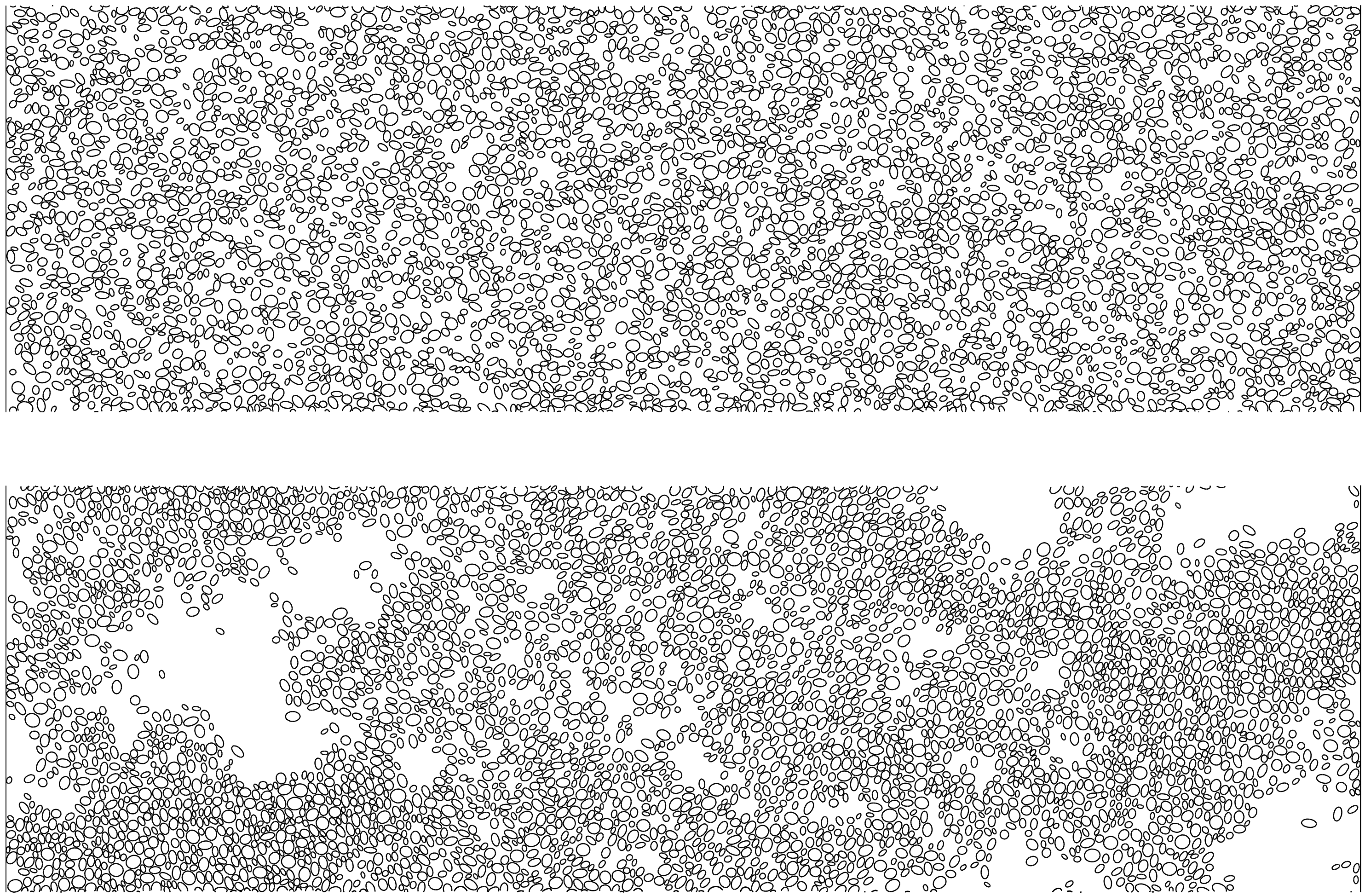
1) Compute the distances (ODE).

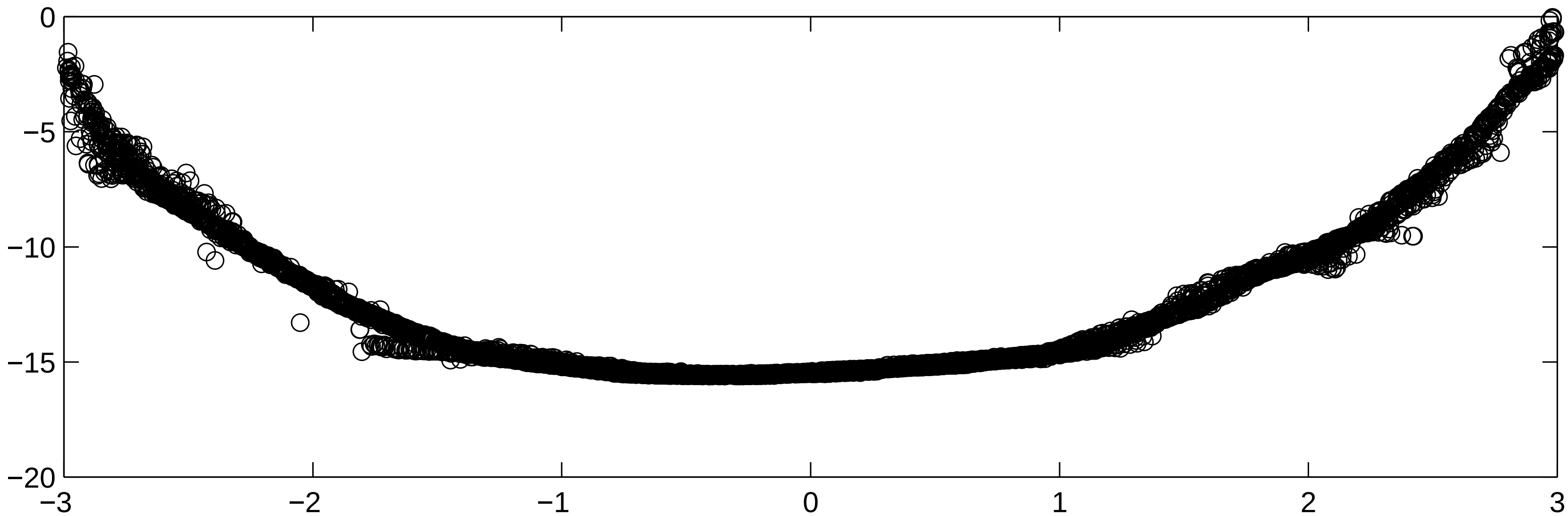
2) Compute the matrix

$$A = \sum_{i<j} \left[\kappa \left(\mathrm{D}_{ij} \right) \mathbf{G}_{ij} \otimes \mathbf{G}_{ij} \right]$$

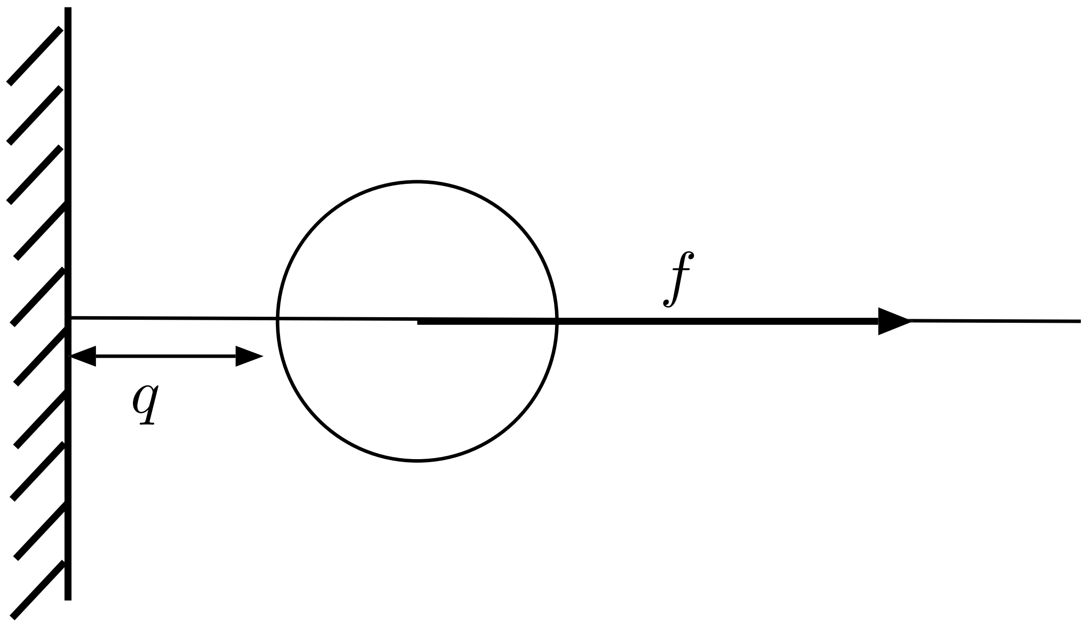
3) Compute velocities and positions

$$M \frac{\mathbf{u}^{n+1} - \mathbf{u}^{n}}{h} + A\mathbf{u}^{n+1} = \Phi$$





0
−5
−10
−15
−20
−3
−2
−1
0
1
2
3



$$\left|\begin{array}{l} \ddot{q}_\varepsilon = -\varepsilon \dfrac{\dot{q}_\varepsilon}{q_\varepsilon} + f(t), \\ \\ q_\varepsilon(0) = q^0 > 0 \ , \ \ \dot{q}_\varepsilon(0) = u^0, \end{array}\right.$$

Theorem Let $\varepsilon > 0$ and $f \in L^1_{\text{loc}}(\mathbb{R}^+)$ be given. Then the problem admits a unique global solution $q_\varepsilon \in W^{1,\infty}_{\text{loc}}(\mathbb{R}^+)$.

Proof. There exists a maximal solution defined on $[0, \tau[$.

$$\frac{1}{2}|\dot{q}_\varepsilon|^2 \leq \frac{1}{2}|\dot{q}_\varepsilon|^2 + \varepsilon \int_0^t \frac{|\dot{q}_\varepsilon|^2}{q_\varepsilon} \leq \frac{1}{2}|u^0|^2 + \int_0^t |f||\dot{q}_\varepsilon| \Longrightarrow |\dot{q}_\varepsilon| \leq |u^0| + \int_0^t |f|.$$

$\dot{q}_\varepsilon$ cannot blow up within a finite time

if $\tau < \infty$, then necessarily q_ε goes to 0 as t goes to τ^-. But

$$\dot{q}_\varepsilon(t) = u^0 - \varepsilon \ln\left(\frac{q_\varepsilon(t)}{q^0}\right) + \int_0^t f(s)\, ds,$$

so that $q_\varepsilon \to 0$ implies $\dot{q}_\varepsilon(t) \longrightarrow +\infty$, hence a contradiction.

Asymptotic behaviour

$$\left|\begin{array}{l}
\text{Find } q \in W^{1,\infty}(I) \text{ with } \dot{q} \in BV(I)\,,\;\; \gamma \in BV(I)\,,\;\; \mu \in \mathcal{M}(I)\,, \quad \text{such that} \\[2ex]
\ddot{q} = f + \lambda \text{ in } \mathcal{M}(I)\,, \\[2ex]
\mathrm{supp}(\lambda) \in \{t,\, q(t) = 0\}\,, \\[2ex]
\dot{q}^+ = P_{C_q}\dot{q}^-\,, \\[2ex]
\dot{\gamma} = -\lambda\,,\;\; \gamma \le 0\,,\;\; q \ge 0\,,\;\; q\gamma = 0 \quad \text{a.e. in } I\,, \\[2ex]
q(0) = q^0 > 0\,,\;\; \dot{q}(0) = u^0,
\end{array}\right.$$

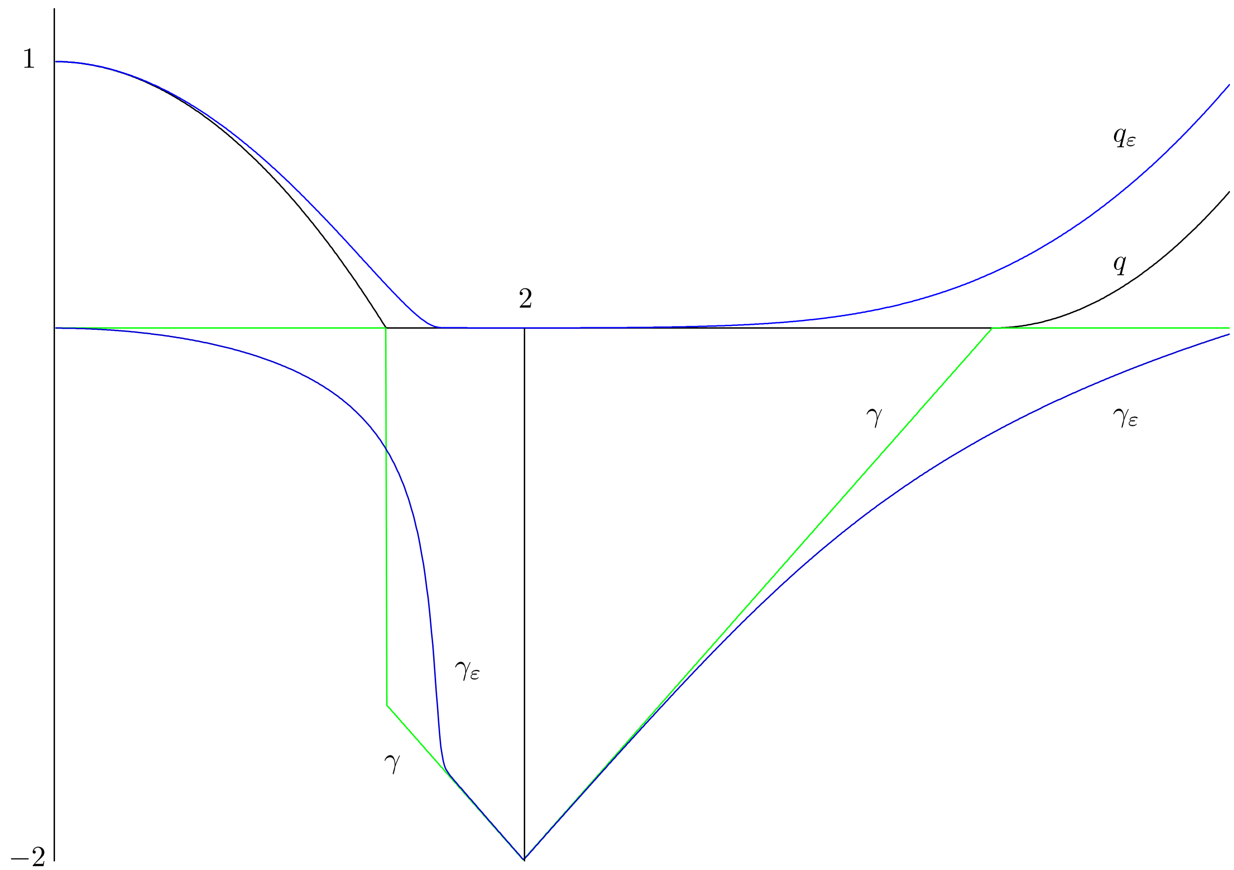
$$\text{with } C_q = \left|\begin{array}{lll}
\mathbb{R} & \text{if} & q > 0\,, \\
\mathbb{R}^+ & \text{if} & q = 0 \text{ and } \gamma^- = 0\,, \\
\{0\} & \text{if} & q = 0 \text{ and } \gamma^- < 0.
\end{array}\right.$$

Alternative formulation (equivalent for a finite number of contacts)

$$\left|\begin{array}{l} \text{Find } q \in W^{1,\infty}(I)\ ,\quad \gamma \in L^{\infty}(I),\ \text{such that} \\[2ex] \dot{q} + \gamma = \tilde{u} = u^0 + \displaystyle\int_0^t f(s)\,ds \quad \text{a.e. in } I\ , \\[2ex] \gamma \leq 0\ ,\quad q \geq 0\ ,\quad q\gamma = 0 \quad \text{a.e. in } I\ , \\[2ex] q(0) = q^0 > 0\ ,\quad \dot{q}(0) = u^0. \end{array}\right.$$

Numerical scheme

$$
q^n > 0 \left\{
\begin{array}{l}
u^{n+1} = u^n + hf(t^{n+1}) \ , \\[2ex]
\tilde{q}^{n+1} = q^n + hu^{n+1} \ , \\[2ex]
\text{if } \tilde{q}^{n+1} < 0 \left| \begin{array}{l} q^{n+1} = 0 \ , \\ \gamma^{n+1} = u^{n+1} \ , \end{array} \right. \\[4ex]
\text{if } \tilde{q}^{n+1} \geq 0 \left| \begin{array}{l} q^{n+1} = \tilde{q}^{n+1} \ , \\ \gamma^{n+1} = 0 \ , \end{array} \right.
\end{array}
\right.
\qquad
q^n = 0 \left\{
\begin{array}{l}
\gamma^{n+1} = \gamma^n + hf(t^{n+1}) \ , \\[2ex]
\text{if } \gamma^{n+1} \leq 0 \left| \begin{array}{l} q^{n+1} = 0 \ , \\ u^{n+1} = 0 \ , \end{array} \right. \\[4ex]
\text{if } \gamma^{n+1} > 0 \left| \begin{array}{l} u^{n+1} = \gamma^{n+1} \ , \\ q^{n+1} = q^n + hu^{n+1} \end{array} \right.
\end{array}
\right.
$$



1
-2
2
q_ε
q
γ
γ_ε
γ_ε
γ

THEOREM Let $q^0 > 0$, $u^0 \in \mathbb{R}$, a time interval $I =]0, T[$ and $f \in L^1(I)$ be given. We denote by $q_\varepsilon \in W^{1,\infty}(I)$ the unique solution in $\overline{I}$, and we set $\gamma_\varepsilon = \varepsilon \ln q_\varepsilon$. When ε goes to 0, there exists a subsequence, still denoted by (q_ε), $q \in W^{1,\infty}(I)$, $\gamma \in L^\infty(I)$, such that

$$\begin{array}{cccl} q_\varepsilon & \longrightarrow & q & \text{uniformly ,} \\ \gamma_\varepsilon & \overset{\star}{\rightharpoonup} & \gamma & \text{in } L^\infty \text{ weak} - \star, \end{array}$$

and the couple (q, γ) is a solution to the limit problem.

Energy balance: (q_ε) in $W^{1,\infty}(I)$

One extracts a subsequence (still denoted by q_ε) such that q_ε converges uniformly to some $q \in W^{1,\infty}$, and $\dot{q}_\varepsilon$ converges to $u = \dot{q}$ in the weak-$\star$ sense.

Let γ_ε be defined as $\varepsilon \ln q_\varepsilon$. One has

$$\dot{q}_\varepsilon + \gamma_\varepsilon = u^0 + \gamma_\varepsilon^0 + \int_0^t f,$$

where $\gamma_\varepsilon^0 = \gamma_\varepsilon(0) = \varepsilon \ln q^0$ goes to 0 with ε.

As a consequence, γ_ε converges weak-$\star$ in L^∞ towards $\gamma \in L^\infty$ such that

$$\dot{q} + \gamma = u^0 + \int_0^t f = \tilde{u}(t).$$

Next step: $\dot{q} = \tilde{u}$ in $I_0 = \{t, q(t) > 0\}$.

We introduce, for any $\eta > 0$, the set $I_\eta(q) = \{t \in]0, T[\ ,\ \ q(t) > \eta\}$. As q_ε converges uniformly to q, $I_\eta(q) \subset I_{\eta/2}(q_\varepsilon)$ for ε sufficiently small.

As a consequence, $\gamma_\varepsilon = \varepsilon \ln q_\varepsilon$ goes uniformly to 0 on $I_\eta(q)$, thus $\dot{q}_\varepsilon$ cv uniformly towards the unconstrained velocity $\tilde{u}$ in $I_\eta(q)$, for all $\eta > 0$.

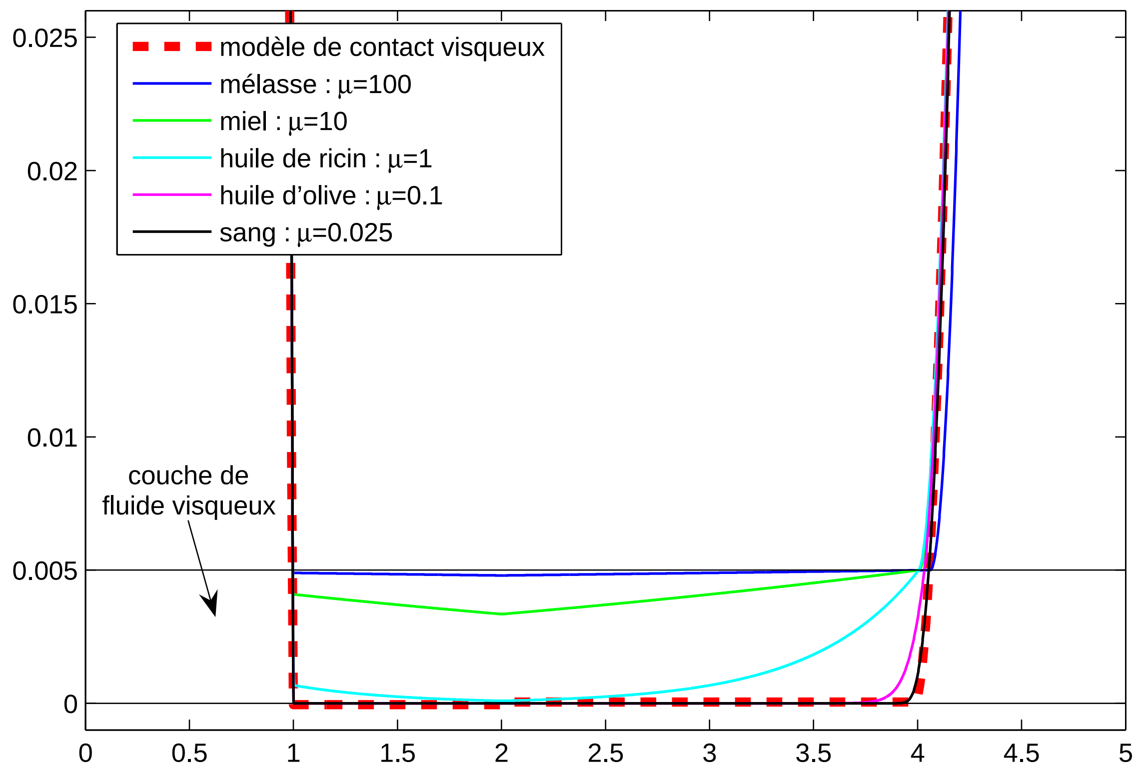
The limit q is therefore C^1 on I_0, with $\dot{q} = \tilde{u}$, and γ is identically 0 on I_0.

On $I_0^c(q) = \{t,\, q(t) = 0\}$, q is constant, so that $\dot{q} = 0$ almost everywhere, thus $\gamma = \tilde{u}$ a.e.

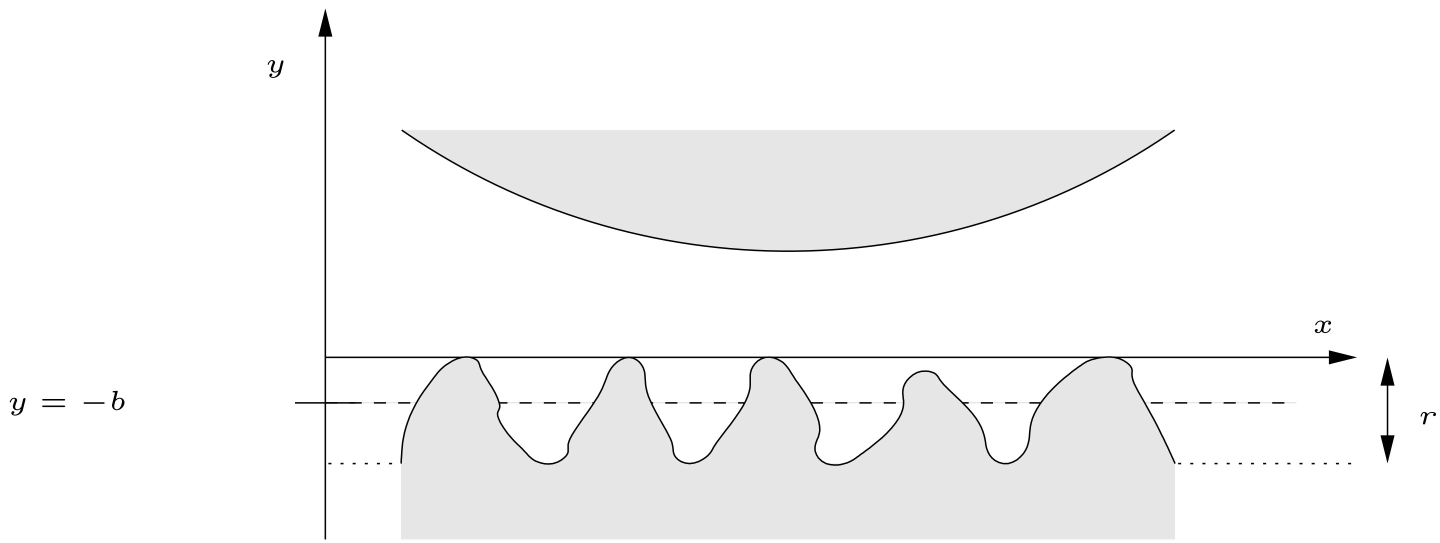
Besides, as γ_ε is negative as soon as $q_\varepsilon < 1$, one has $\gamma \leq 0$ on I_0^c.

Modelling issues

Paradox: modeling of contacts with a highly viscous interstitial fluid obtained as a vanishing viscosity limit.



In real life: ruguous walls. Contact actually occurs at distance $\delta > 0$. If the distance below which the models produces significant forces is $\delta_\varepsilon < \delta$, the model does not make sense.



Numerically: cut-off applied to γ below some threshlod value.

Many-body situation

$$\left\{\begin{array}{rcl}\dfrac{d\mathbf{u}}{dt} & = & \mathbf{f}+\displaystyle\sum_{i<j}\lambda_{ij}\mathbf{G}_{ij}\\[2ex] \mu_{ij}\in\mathcal{M}(I)\ ,\ \ \mathrm{supp}(\mu_{ij}) & \subset & \{t\ ,\ \ D_{ij}(\mathbf{q}(t))=0\},\\[2ex] \mathbf{u}^{+} & = & P_{\mathcal{C}_{\mathbf{q}}}\mathbf{u}^{-},\\[2ex] \dot{\gamma}_{ij} & = & -\lambda_{ij}.\end{array}\right.$$

$$\mathcal{C}_{\mathbf{q}}=\{\mathbf{v}\in \mathrm{T}_Q\ ,\ \ D_{ij}(\mathbf{q})=0\Rightarrow \mathbf{G}_{ij}\cdot\mathbf{v}\geq 0\ ,\ \ \gamma_{ij}<0\Rightarrow \mathbf{G}_{ij}\cdot\mathbf{v}=0\}\,,$$

Remark: tangential forces can be included.

→80-81-82-84-85-86-87-88

Links with macroscopic models

Instantaneous saddle point problem:

$$\begin{cases} \mathbf{u} + B^\star \lambda & = & \mathbf{U} \\ B\mathbf{u} & \leq & 0. \end{cases}$$

$\mathbf{U}$ velocity before the collision, $\mathbf{u}$ after the collision.

Rows of B: gradients $-\mathbf{G}_{ij}$.

B expresses a unilateral incompressibility (divergence)

(saturated zones cannot be further compressed)

$B^\star$ is a gradient like operator:

$$-B^\star \lambda = \sum \lambda_{ij} \mathbf{G}_{ij}.$$

Analogy with a unilateral Darcy-like problem

$$\left\{\begin{array}{lcl} \mathbf{u} + B^\star \lambda & = & \mathbf{U} \\ \\ B\mathbf{u} & \leq & 0. \end{array}\right. \qquad \left\{\begin{array}{lcl} \mathbf{u} + \nabla p & = & \mathbf{F} \\ \\ -\nabla \cdot \mathbf{u} & \leq & 0. \end{array}\right.$$

Continuous problem on Ω with free outlet ($p = 0$ on $\partial\Omega$):

$$B \,:\, L^2(\Omega)^2 \mapsto H^{-1},$$

$$\langle B\mathbf{v}, q\rangle = \int_\Omega \mathbf{v} \cdot \nabla q.$$

One has $||B^\star q|| = ||\nabla q||_{L^2} \geq ||q||_{H^1(\Omega)}$ (Poincaré inequality), so that B is surjective

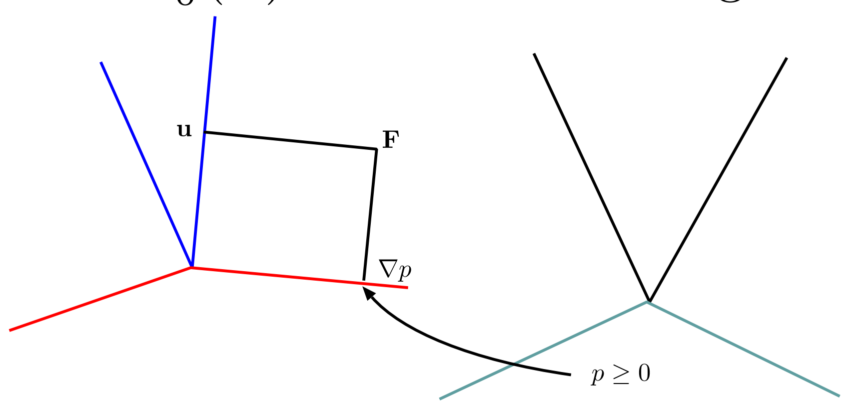
$\Longrightarrow$ the problem is well-posed ($\exists!$ $(\mathbf{u}, p)$ s.t. $\ldots$).

Analogy (continued)

The Lagrange multiplier field minimizes

$$J(q) = \frac{1}{2}\left|\nabla p - \mathbf{F}\right|^2$$

over all those fields in $H_0^1(\Omega)$ which are non negative a.e.



Turns out to be an obstacle problem, whose saddle point formulation is

$$\left\{\begin{array}{rcl} -\triangle \mathrm{p} - \mu & = & -\nabla \cdot \mathbf{F} \\ \\ -\mathrm{p} & \leq & 0. \end{array}\right.$$

The underlying operator is a Laplacian.

Back to the granular situation:

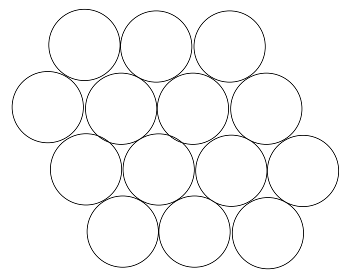
$$\left\{\begin{array}{rcl} \mathbf{u} + B^{\star}\lambda & = & \mathbf{U} \\ \\ B\mathbf{u} & \leq & 0. \end{array}\right.$$

First remark: λ is not unique in general.

Indeed (2D situation):

number of equations ($\approx 2N$) $>$ number of unknowns ($\approx 3N$)

Minimal set: 14 discs (28 primal DOFs), 29 contacts



In open (expandable) situations, uniqueness holds for the homogeneous problem

$$B^\star \lambda = 0\ ,\quad \lambda \geq 0 \Longrightarrow \lambda = 0$$

which simply means that $\ker B^\star \cap (\mathbb{R}_+)^r = \{0\}$.

But in general $B^\star \lambda = F$ admits infinitely many solutions.

It suffices that there exists a solution $\lambda \in]0, +\infty[^r$.

For the dry contact case: no consequence

For the lubricated case: huge consequences

$$\dot{\gamma}_{ij} = -\lambda_{ij},$$

and γ_{ij} conditions the take-off instant.

$\longrightarrow$ beside the non-uniqueness in time for non analytical data, the evolution problem admits a continuum of solutions, as soon as degeneracy occurs sometimes.

Degeneracy: many particles have more than 4 neighbours, in 2D, more than 6 in 3D: generic situation for monodisperse packed suspensions.

→90

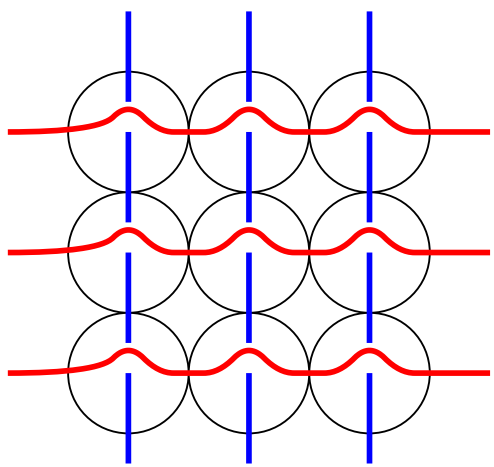
Analogy (continued).

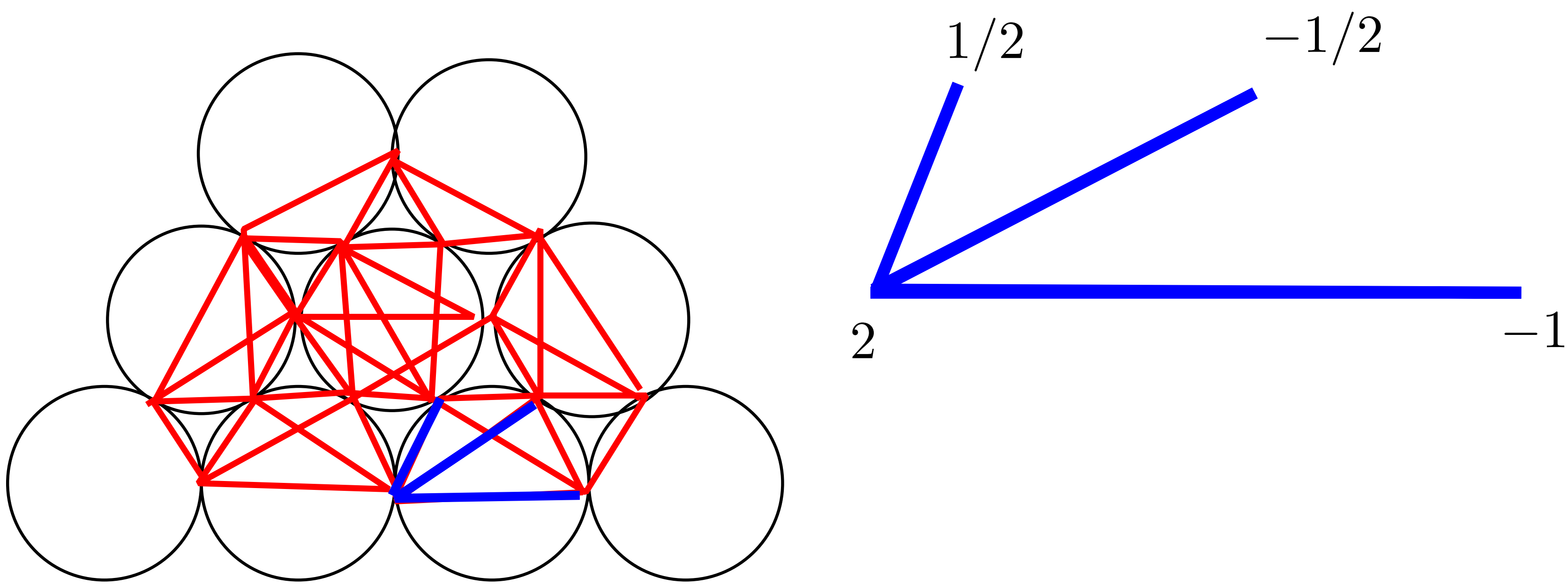
B plays the role of the divergence.

$\longrightarrow$ nature of $BB^\star$? (N.B. it conditions the computational cost)

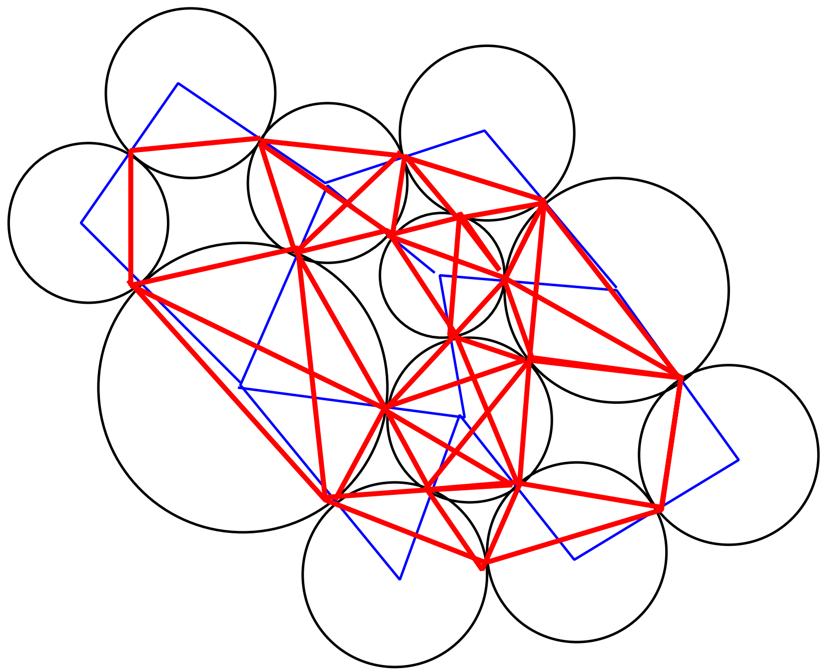
For 1D problems : $BB^\star$ is exactly the discrete Laplacian.

In higher dimensions: depends on the structure




1/2
−1/2
2
−1

General situation



Macroscopic models

Macroscopic pressureless gas model

$$
\begin{aligned}
\partial_t \rho + \nabla \cdot (\rho \mathbf{u}) &= 0, \\
\partial_t (\rho \mathbf{u}) + \nabla \cdot (\rho \mathbf{u} \otimes \mathbf{u}) + \nabla \mathrm{p} &= 0 \\
\rho &\leq 1 \\
(1 - \rho)\mathrm{p} &= 0 \\
\mathbf{u}^+ &= P_{\mathcal{C}_\rho} \mathbf{u}^-
\end{aligned}
$$

Well-posedness issues ?

Possibilities to integrate some structural parameter.

Macroscopic lubricated model

Asymptotic limit (?)

$$
\left|\begin{array}{rcr}
\partial_t \rho + \partial_x(\rho u) & = & 0 \\[2ex]
\partial_t(\rho u) + \partial_x(\rho u^2) + \partial_x p & = & f \\[2ex]
\partial_t \gamma + \partial_x(\gamma u) & = & -\mathrm{p} \\[2ex]
\gamma \le 0\ ,\quad \rho \le 1\ ,\quad \gamma(1-\rho) & = & 0
\end{array}\right.
$$

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