Numerical simulation of suspensions: lubrication correction including fluid correction

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joint work with Flore Nabet

CMAP – Ecole polytechnique

Workshop "Collective behavior of particles in fluids"

December 14-17, 2020

ANR
RheoSuNN

Mud from wastewater treatment

Industrial process

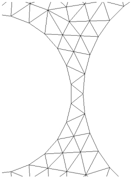
Micro-swimmers

- Suspensions of rigid particles in Stokes flow
- Macroscopic properties
- Dense suspensions

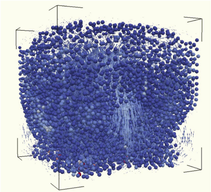
Need for numerical simulations

Direct numerical simulations

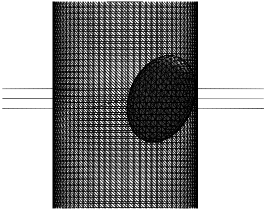
- Solving the fluid particle PDEs
- Underlying mesh
- Approximation of the velocity and pressure fields
- Converging results



FreeFem++

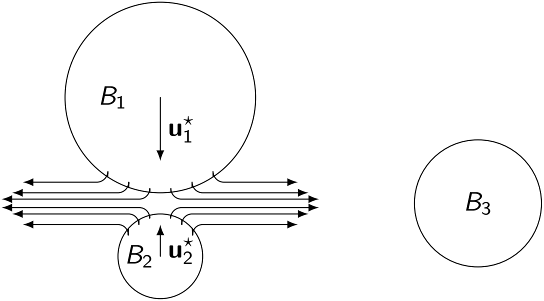


CAFES (LMO - CMAP)



MyBEM/Gypsilab (CMAP)

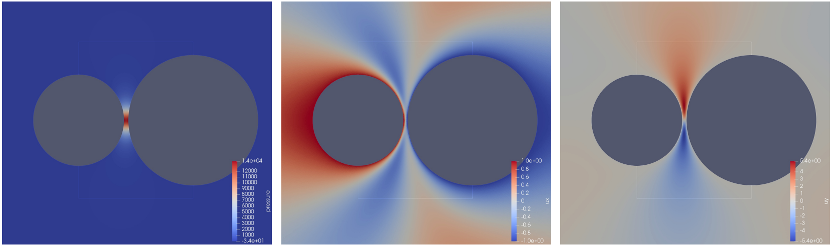
Lubrication in dense suspensions



- Multi-particule effects
- Macroscopic effects

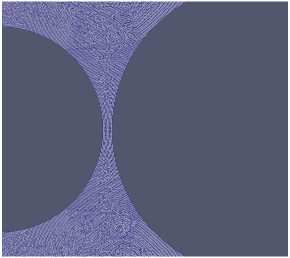
Behaviour for small distances

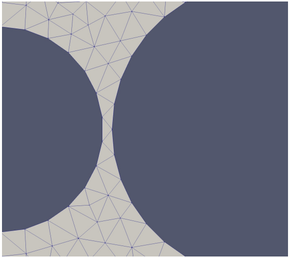
- $r_1 = 0.07,\ r_2 = 1,\ d = r_2/10,\ \mathbf{u}_1^\star = \mathbf{e}_x,\ \mathbf{u}_2^\star = -\mathbf{e}_x,$



- Pressure field not bounded
- Pressure field localized in space
- Velocity field exhibiting high variations

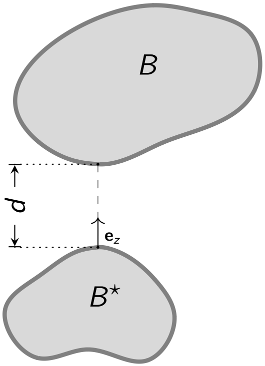
Numerical consequences





- Need to develop strategies to take lubrication into account in direct numerical simulations.

Forces: asymptotic behaviour for 2 particles [Cox, 1974]

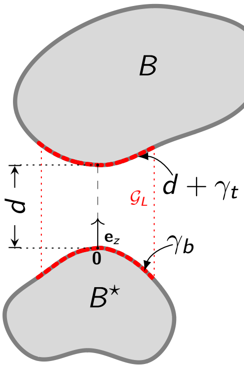


A Dirichlet to Neumann problem:

$$
\begin{aligned}
-\Delta \mathbf{u} + \nabla p = 0 \quad & \text{in } \mathcal{F};\\
\operatorname{div} \mathbf{u} = 0 \quad & \text{in } \mathcal{F};\\
\mathbf{u} = u_z^\star \mathbf{e}_z \quad & \text{on } \partial B^\star;\\
\mathbf{u} = 0 \quad & \text{on } \partial B.
\end{aligned}
$$

Remark: can be extended to more general configurations.

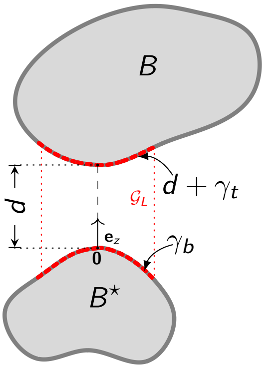
Notations



A Dirichlet to Neumann problem:

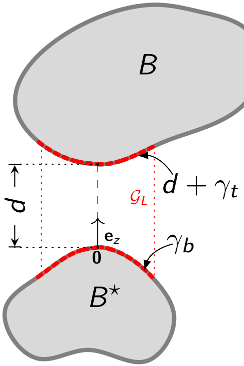
$$\begin{aligned} -\Delta \mathbf{u} + \nabla p = 0 &\quad \text{in } \mathcal{F}; \\ \operatorname{div} \mathbf{u} = 0 &\quad \text{in } \mathcal{F}; \\ \mathbf{u} = u_z^\star \mathbf{e}_z &\quad \text{on } \partial B^\star; \\ \mathbf{u} = 0 &\quad \text{on } \partial B. \end{aligned}$$

First order approximation in $\mathcal{G}_L$



$$
\begin{aligned}
u_x(x,y,z) &= \frac{1}{\sqrt{d}}\tilde{u}_x\left(\frac{x}{\sqrt{d}},\frac{y}{\sqrt{d}},\frac{z}{d}\right)\\
u_y(x,y,z) &= \frac{1}{\sqrt{d}}\tilde{u}_y\left(\frac{x}{\sqrt{d}},\frac{y}{\sqrt{d}},\frac{z}{d}\right)\\
u_z(x,y,z) &= \tilde{u}_z\left(\frac{x}{\sqrt{d}},\frac{y}{\sqrt{d}},\frac{z}{d}\right)\\
p(x,y,z) &= \frac{1}{d^2}\tilde{p}\left(\frac{x}{\sqrt{d}},\frac{y}{\sqrt{d}},\frac{z}{d}\right)
\end{aligned}
$$

First order approximation in $\mathcal{G}_L$



$$-\partial_{zz} v_x + \partial_x \mathrm{q}_{in} = 0 \qquad (1)$$

$$-\partial_{zz} v_y + \partial_y \mathrm{q}_{in} = 0 \qquad (2)$$

$$\partial_z \mathrm{q}_{in} = 0 \qquad (3)$$

$$\partial_x v_x + \partial_y v_y + \partial_z v_z = 0 \qquad (4)$$

$$v_x = v_y = v_z = 0 \text{ on } z = d + \gamma_t(x, y) \qquad (5)$$

$$v_x = v_y = 0 \text{ on } z = \gamma_b(x, y) \qquad (6)$$

$$v_z = v_z^\star \text{ on } z = \gamma_b(x, y) \qquad (7)$$

First order approximation in $\mathcal{G}_L$

$$-\partial_{zz} v_x + \partial_x \mathrm{q}_{in} = 0 \qquad (1)$$

$$-\partial_{zz} v_y + \partial_y \mathrm{q}_{in} = 0 \qquad (2)$$

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$$\partial_x v_x + \partial_y v_y + \partial_z v_z = 0 \qquad (4)$$

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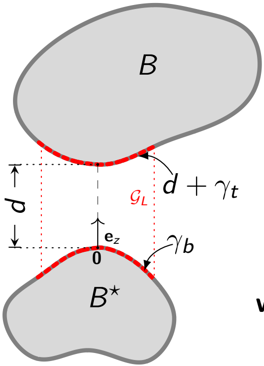
First order approximation in $\mathcal{G}_L$



- $\mathrm{q}_{in} = \mathrm{q}_{in}(x, y)$ defined in $B(0, L)$:

$$\left\{ \begin{array}{rcl} -\dfrac{1}{12}\,\mathrm{div}(\gamma^3 \nabla \mathrm{q}_{in}) & = & u_z^\star \\ \mathrm{q}_{in} & = & 0. \end{array} \right.$$

- $v = \mathbf{w}[\mathrm{q}_{in}]$ in $\mathcal{G}_L$

$$\mathbf{w}[\mathrm{q}]_{x,y}(\cdot, z) = \frac{1}{2}(z - (d + \gamma_t))(z - \gamma_b)\nabla \mathrm{q}$$

$$w[\mathrm{q}]_z(\cdot, z) = \mathrm{div}_{x,y}\left[\int_z^{d+\gamma_t} \mathbf{w}[\mathrm{q}]_{x,y}(\cdot, s)\, ds\right]$$

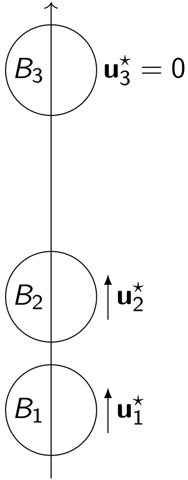
Lubrication forces: asymptotic expansion

- Estimate $F_z^{sing} = \int_{\partial B} \sigma(\mathbf{u})\mathbf{n} \cdot \mathbf{e}_z$
- 2 spheres:

$$F_z^{sing} \sim -6\pi\mu \frac{r_1^2 r_2^2}{(r_1 + r_2)^2} \frac{u_z^\star}{d} \mathbf{e}_z$$

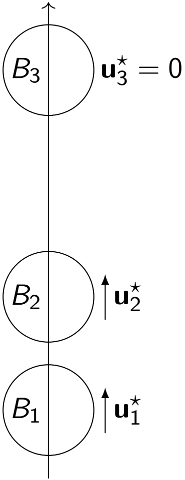
- Can be generalized to
  - any rigid movement
  - any (convex) form of particle

Application to numerical simulations: the Stokesian Dynamics [Brady, Bossis, 1984]



Application to numerical simulations: the Stokesian Dynamics [Brady, Bossis, 1984]

$$
\begin{aligned}
\mathbf{F}^L_{SD} &= \mathbf{F}^L + \left(\mathbf{F}^{sing}_{2B}(d) - \mathbf{F}^{sing,L}_{2B}(d) \right) \\
&= \begin{pmatrix} f_1^L \\ f_2^L \\ f_3^L \end{pmatrix} + \begin{pmatrix} c_1 \\ c_2 \\ 0 \end{pmatrix}
\end{aligned}
$$



- Correction of the forces exerted on the particles
- The flow $(\mathbf{u}, \mathrm{p})$ is not corrected
- Restricted to monodisperse suspensions

Numerical challenge

- Design of numerical methods taking the lubrication forces into account in the whole flow with a reasonable computational cost
- Handle non-spherical and polydisperse particles

Stokesian Dynamics: decomposition of the force

$$\begin{aligned} \mathbf{F}_{SD}^{L} &= \left(\mathbf{F}^{L} - \mathbf{F}_{2B}^{sing,L}(d)\right) + \mathbf{F}_{2B}^{sing}(d) \\ &= \mathbf{F}_{L}^{reg} + \mathbf{F}^{sing} \end{aligned}$$

New method: decomposition of the flow

$$\begin{aligned} \mathbf{u} &= \mathbf{u}^{reg} + \mathbf{u}^{\mathrm{sing}} \\ \mathrm{p} &= \mathrm{p}^{reg} + \mathrm{p}^{\mathrm{sing}} \end{aligned}$$

- In [L, Merlet, Nguyen, 2015] : tabulation of the singular flow
- In this work: use an explicit asymptotic development

$$\mathbf{u} = \mathbf{u}^{\mathrm{reg}} + \mathbf{u}^{\mathrm{sing}} \quad \text{and} \quad \mathrm{p} = \mathrm{p}^{\mathrm{reg}} + \mathrm{p}^{\mathrm{sing}}.$$

Suppose $(\mathbf{u}^{\mathrm{sing}}, \mathrm{p}^{\mathrm{sing}})$ is known and solve

$$\begin{aligned} -\Delta \mathbf{u}^{\mathrm{reg}} + \nabla \mathrm{p}^{\mathrm{reg}} &= \Delta \mathbf{u}^{\mathrm{sing}} - \nabla \mathrm{p}^{\mathrm{sing}} && \text{in } \mathcal{F}; \\ \operatorname{div} \mathbf{u}^{\mathrm{reg}} &= -\operatorname{div} \mathbf{u}^{\mathrm{sing}} && \text{in } \mathcal{F}; \\ \mathbf{u}^{\mathrm{reg}} &= \mathbf{u}_i^{\star} - \mathbf{u}^{\mathrm{sing}} && \text{on } \partial B_i. \end{aligned}$$

Find a suitable field $(\mathbf{u}^{\mathrm{sing}}, \mathrm{p}^{\mathrm{sing}})$ s.t. the field $(\mathbf{u}^{\mathrm{reg}}, \mathrm{p}^{\mathrm{reg}})$ is "regular" i.e.

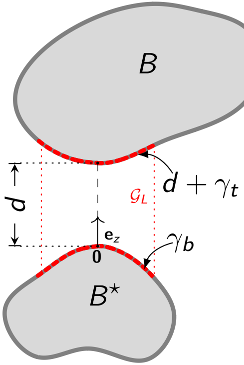
$$\|\mathbf{u}^{\mathrm{reg}}\| + \|\mathrm{p}^{\mathrm{reg}}\| \leq C,$$

with C independent of d.

$\Longrightarrow$ [M. Hillairet, T. Kelai, 2015]

$\Longrightarrow$ H^{-1} bound for $\Delta \mathbf{u}^{\mathrm{sing}} - \nabla \mathrm{p}^{\mathrm{sing}}$ and $\operatorname{div} \mathbf{u}^{\mathrm{sing}}$

Choice for the singular pressure field in $\mathcal{F}$



- $\mathrm{q}_{in} = \mathrm{q}_{in}(x, y)$ in $B(0, L)$:

$$\begin{cases} -\dfrac{1}{12}\,\mathrm{div}(\gamma^3 \nabla \mathrm{q}_{in}) & = & u_z^\star \\ \mathrm{q}_{in} & = & 0. \end{cases}$$

Truncated pressure field

$$\begin{aligned} \mathrm{p}^{\mathrm{sing}}(x, y, z) &= \mathrm{p}^{\mathrm{sing}}(x, y) \\ &= \mathrm{q}_{in}(x, y)\chi_L(x, y). \end{aligned}$$

Choice for the inner singular velocity field in $\mathcal{G}_L$

Find $\mathbf{u}_{in}$ in $\mathcal{G}_L$ such that $\Delta \mathbf{u}_{in} - \nabla \mathsf{p}^{\mathrm{sing}}$ bounded

$$\Delta w[\mathsf{q}]_z - \nabla_z \mathsf{p}^{\mathrm{sing}} = \Delta w[\mathsf{q}]_z$$

$$\begin{aligned}\Delta \mathbf{w}[\mathsf{q}]_{x,y} - \nabla_{x,y} \mathsf{p}^{\mathrm{sing}} &= \Delta_{x,y} \mathbf{w}[\mathsf{q}]_{x,y} + \partial^2_{zz} \mathbf{w}[\mathsf{q}]_{x,y} - \nabla_{x,y} \mathsf{p}^{\mathrm{sing}}, \\ &= \Delta_{x,y} \mathbf{w}[\mathsf{q}]_{x,y} + \nabla_{x,y} \mathsf{q} - \nabla_{x,y} \mathsf{p}^{\mathrm{sing}}\end{aligned}$$

Velocity field in $\mathcal{G}_L$

$$\mathbf{u}_{in} = \mathbf{w}[\mathsf{p}^{\mathrm{sing}}] = \mathbf{w}[\mathsf{q}_{in}\chi_L] \text{ in } \mathcal{G}_L$$

Extension of the inner singular velocity field to $\mathcal{F}$

Find $\mathbf{u}_{ext}$ such that $\mathbf{u}^{\text{sing}} = \mathbf{u}_{in} + \mathbf{u}_{ext}$ satisfies the BC

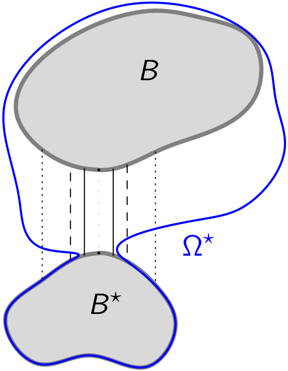
Outer velocity field

$\mathbf{u}_{ext}$ is solution to a Stokes problem in an outer domain $\Omega^\star$ with

$$\mathbf{u}_{ext} = \mathbf{u}^\star - \mathbf{u}_{in} \text{ on } \partial\Omega^\star$$

Choice for $\Omega^\star$??

- $\mathbf{u}^{\text{sing}}$ satisfies the boundary conditions
  $\Rightarrow \{\mathbf{u} \neq \mathbf{u}_{in}\} \subset \partial\Omega^\star$
- RHS bounded independently of d
  $\Rightarrow \Omega^\star$ independent of d
  $\Rightarrow B \subset (\Omega^\star)^c$ for all d



Asymptotic result [M. Hillairet, T. Kelai, 2015]

$(\mathbf{u}^{\mathrm{sing}}, p^{\mathrm{sing}})$ are such that

$$|\mathbf{u}^{\mathrm{reg}}|_{H^1} + |\mathrm{p}^{\mathrm{reg}}|_{L^2} \leq C$$

with $C > 0$ not depending on the distance.

Modification of the singular field for numerical purpose

$$\Delta \mathbf{w}[\mathsf{q}]_{x,y} - \nabla_{x,y}\mathsf{p}^{\text{sing}} = \Delta_{x,y}\mathbf{w}[\mathsf{q}]_{x,y} + \partial^2_{zz}\mathbf{w}[\mathsf{q}]_{x,y} - \nabla_{x,y}\mathsf{p}^{\text{sing}},$$

$$= \Delta_{x,y}\mathbf{w}[\mathsf{q}]_{x,y} + \nabla_{x,y}\mathsf{q} - \nabla_{x,y}\mathsf{p}^{\text{sing}}$$

$$\Delta w[\mathsf{q}]_z - \nabla_z\mathsf{p}^{\text{sing}} = \Delta w[\mathsf{q}]_z$$

New singular velocity field

$$\bar{\mathbf{u}}^{\text{sing}}_{x,y} = \mathbf{w}[\mathsf{p}^{\text{sing}}]_{x,y} \quad \text{and} \quad \bar{\mathbf{u}}^{\text{sing}}_z = \chi_L\,\mathbf{w}[\mathsf{q}_{in}]_z$$

- vanishes outside $\mathcal{G}_L$
- less derivatives of χ_L to be computed

$$\mathbf{u} = \bar{\mathbf{u}}^{\mathrm{reg}} + \bar{\mathbf{u}}^{\mathrm{sing}} \quad \text{and} \quad \mathrm{p} = \mathrm{p}^{\mathrm{reg}} + \mathrm{p}^{\mathrm{sing}}.$$

Asymptotic result [L, Nabet, 2020]

$(\bar{\mathbf{u}}^{\mathrm{sing}}, p^{\mathrm{sing}})$ are such that

$$|\bar{\mathbf{u}}^{\mathrm{reg}}|_{H^1} + |\mathrm{p}^{\mathrm{reg}}|_{L^2} \leq C$$

with $C > 0$ not depending on the distance.

- use the estimation of $\mathbf{u}_{ext}$
- estimate $\mathbf{u}_{in} - \bar{\mathbf{u}}^{\mathrm{sing}}$

And what about numerical implementation ?

Find $(\mathbf{u}_h^{\mathrm{reg}}, p_h^{\mathrm{reg}}) \in V_h \times M_h$:

$$\left\{ \begin{array}{rcll} -\triangle \mathbf{u}_h^{\mathrm{reg}} + \nabla p_h^{\mathrm{reg}} & = & \triangle \mathbf{u}^{\mathrm{sing}} - \nabla p^{\mathrm{sing}} & \text{in } \Omega \setminus \cup B_i \\ \nabla \cdot \mathbf{u}_h^{\mathrm{reg}} & = & -\nabla \cdot \mathbf{u}^{\mathrm{sing}} & \text{in } \Omega \setminus \cup B_i \\ \mathbf{u}_h^{\mathrm{reg}} & = & \mathbf{u}_i - \mathbf{u}^{\mathrm{sing}} & \text{on } \partial B_i \end{array} \right.$$

- Estimations of convergence independent of the distance
- Classical Stokes problem: fast numerical methods
- "Exact" computations for the integrals in the right-hand side
- Numerical difficulty: discrete compatibility condition...

And what about numerical implementation ?

Find $(\mathbf{u}_h^{\text{reg}}, p_h^{\text{reg}}) \in V_h \times M_h$:

$$\begin{cases} -\triangle \mathbf{u}_h^{\text{reg}} + \nabla p_h^{\text{reg}} &= \triangle \mathbf{u}^{\text{sing}} - \nabla p^{\text{sing}} \quad \text{in } \Omega \setminus \cup B_i \\ \varepsilon p_h^{\text{reg}} + \nabla \cdot \mathbf{u}_h^{\text{reg}} &= -\nabla \cdot \mathbf{u}^{\text{sing}} \quad \text{in } \Omega \setminus \cup B_i \\ \mathbf{u}_h^{\text{reg}} &= \mathbf{u}_i - \mathbf{u}^{\text{sing}} \quad \text{on } \partial B_i \end{cases}$$

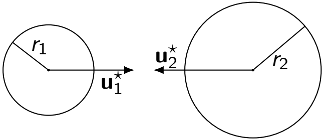
- Estimations of convergence independent of the distance
- Classical Stokes problem: fast numerical methods
- "Exact" computations for the integrals in the right-hand side
- Numerical difficulty: discrete compatibility condition...

Numerical results

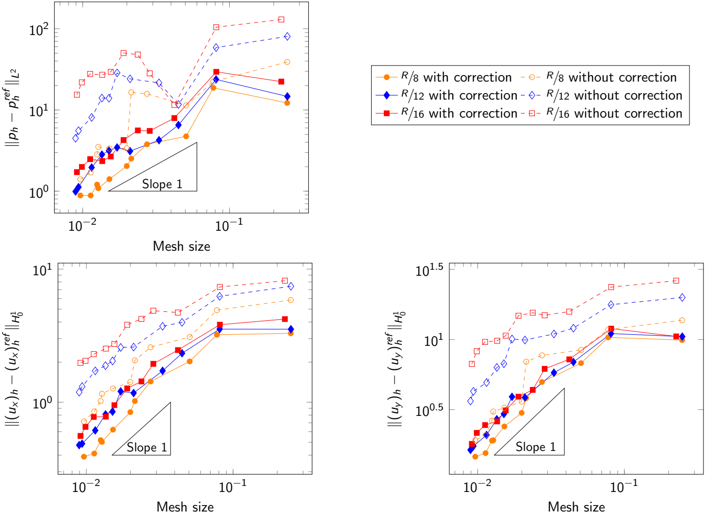
- FreeFem++, direct solver
- P1isoP2 / P1
- Reference: very fine mesh, direct solver
- Singularity taken into account: normal translation.

Two spherical particles moving along the line of their centers.

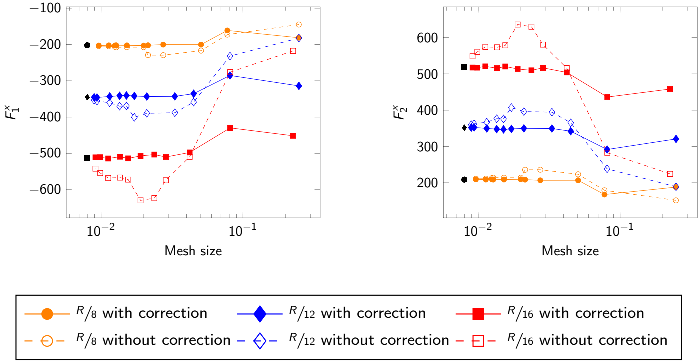
- $r_1 = 0.07$, $r_2 = 0.1$, $d = r_2/\alpha$;
- $\mathbf{u}_1^\star = \mathbf{e}_x$, $\mathbf{u}_2^\star = -\mathbf{e}_x$;



Error on the flow

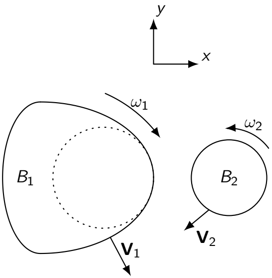


Estimation of the forces

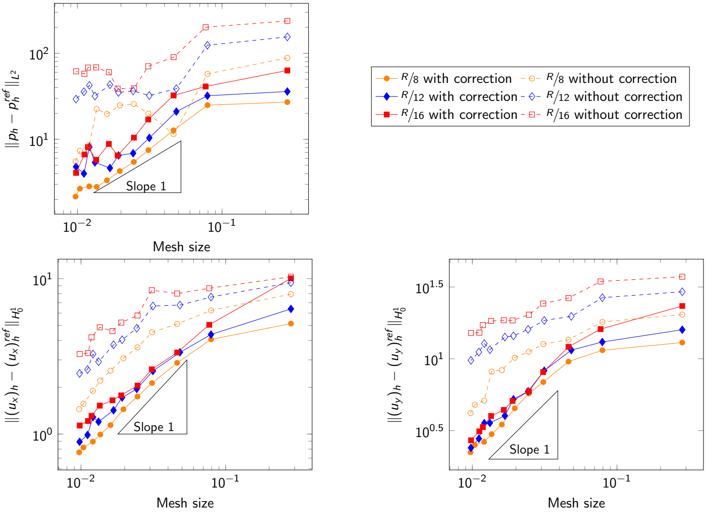


Non-spherical particles with general rigid motions

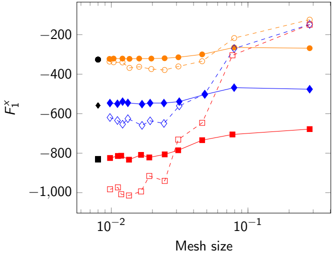
- $\mathbf{u}_i^\star = \mathbf{V}_i + \omega_i(\mathbf{x} - \mathbf{x}_i)^\perp$
- $\mathbf{v}_1 = (1, 1)$, $\mathbf{v}_2 = (-1, -2)$
- $\omega_1 = 3$ and $\omega_2 = 5$
- Singularity taken into account: normal relative velocity
- Approximation of the geometry: osculating circles

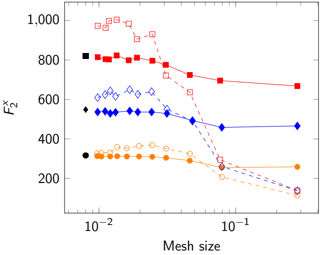


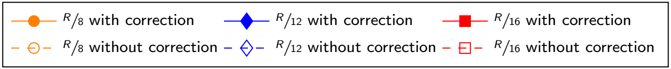
Error on the flow



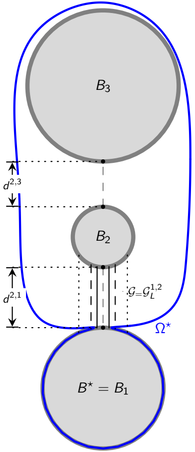
Estimation of the forces

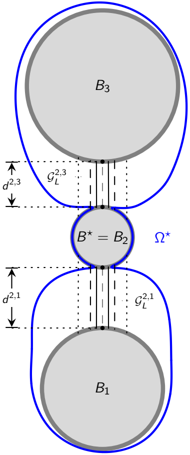




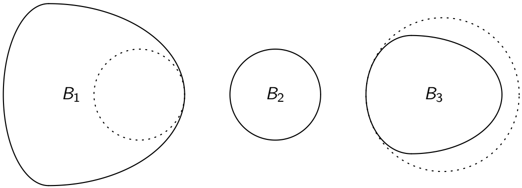


Three particles case: an example



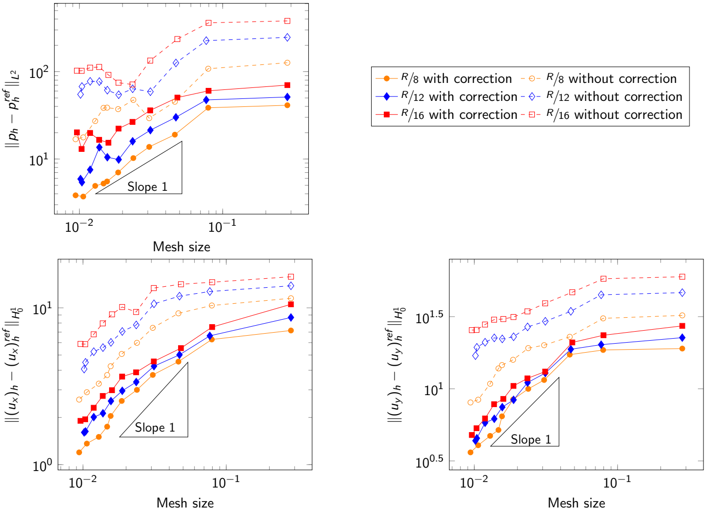


Numerical test

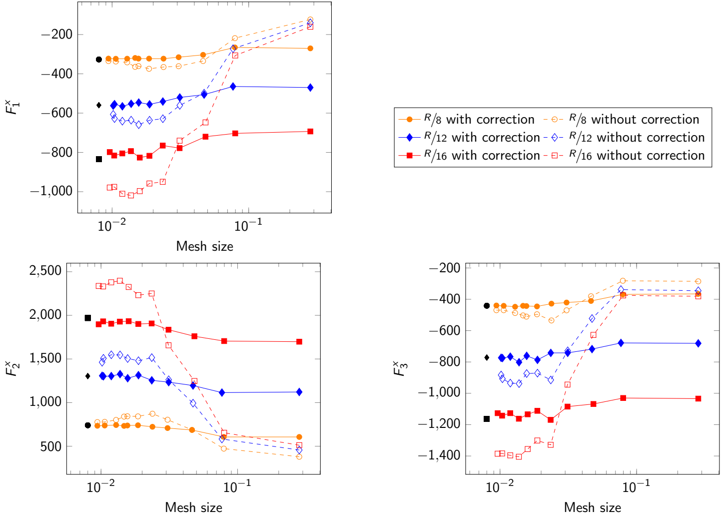


- $\mathbf{u}_i^\star = \mathbf{V}_i + \omega_i(\mathbf{x} - \mathbf{x}_i)^\perp$
- $\mathbf{v}_1 = (1, 1)$, $\mathbf{v}_2 = (-1, -2)$, $\mathbf{v}_3 = (1.5, -2)$
- $\omega_1 = 3$, $\omega_2 = 5$, $\omega_3 = 5$
- Singularities taken into account: normal relative velocities
- Approximation of the geometry: osculating circles

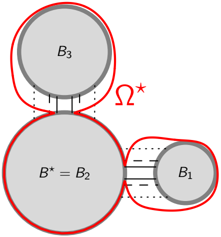
Error on the flow

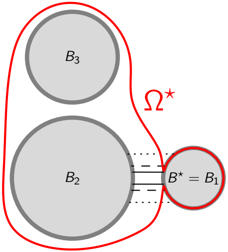


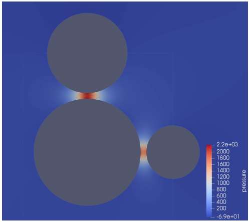
Estimation of the forces



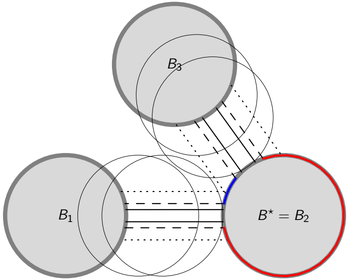
L-shape configuration

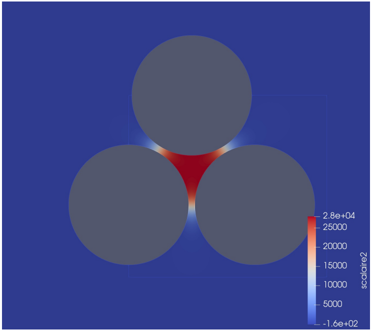






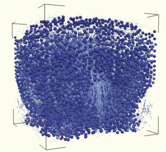
A limitation in 2 dimensions





- new numerical method taking lubrication into account
- direct simulation: do not introduce new model
- velocity and pressure fields corrected
- can handle polydisperse suspensions
- can handle non-spherical of particles

On-going work:



- multiparticle effects?
- 3D-Multi-particle suspensions
  - Implementation into solver CAFES [L. Gouarin, B. Fabrèges]
  - joint work with Fabien Vergnet