Numerical Simulation of Red Blood Cells: a “Stokesian Dynamics” Approach

S. Faure, S. Martin, B. Maury & T. Takahashi

Groupe de Travail “Méthodes numériques”
Laboratoire Jacques Louis-Lions

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**Aim:** Individual and collective behaviour of Red Blood Cells: aggregates, lateral migration...
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Numerical tool: C++ program for granular flows (accurate handling of contacts between rigid spheres)
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**Numerical tool:** C++ program for granular flows (accurate handling of contacts between rigid spheres)

**Modeling:** Fluid-RBC interactions, from dilute to dense suspensions...
Fictitious domain methods:

Wang, Pan & Glowinski: (2008)
References

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**Lattice Boltzmann methods:**

Binder et al.: *J. Colloid Interface Sci.* (2006)
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Other methods:
1. A brief description of SCoPI

2. How to simulate one single Red Blood Cell?

3. Fluid / Red Blood Cells interactions in *dilute* suspensions

4. Fluid / Red Blood Cells interactions in *dense* suspensions
A brief description of SCoPI

- **SCoPI** (*simulation of collections of particles in interaction*):
  - ✔ written by Aline Lefebvre
  - ✔ accurate handling of contacts between rigid spheres

\[
M \cdot \frac{dU}{dt} = F_{\text{ext}}, \quad \text{in } \mathbb{R}^3
\]

Algorithm:
\[
M \cdot U_{n+1} = M \cdot U_n + h F_n_{\text{ext}},
\]
\[
q_{n+1} = q_n + h U_{n+1}
\]

handling of contacts by Uzawa technique

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  - Euler scheme

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A brief description of SCoPI

- **Idea** (Maury, 2006): projection onto the set of admissible velocities:

\[
K(q^n) = \left\{ \mathbf{V} \in \mathbb{R}^{3N}, \; D_{ij}(q^n) + h \mathbf{G}_{ij}(q^n) \cdot \mathbf{V} \geq 0, \; \forall i < j \right\}
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- **Constrained minimization problem**: splitting scheme:

\[
\begin{align*}
U^{n+1/2} &= U^n + h M^{-1} \cdot F_{\text{ext}} \\
U^{n+1} &= \min_{V \in K(q^n)} \frac{1}{2} \left| V - U^{n+1/2} \right|^2
\end{align*}
\]
A brief description of SCoPI

- **Saddle-point problem:** the minimization problem reads as

\[
\begin{aligned}
\text{Find } (U^{n+1}, \mu^{n+1}) \in W \text{ such that }
\mathcal{L}(U^{n+1}, \lambda) &\leq \mathcal{L}(U^{n+1}, \mu^{n+1}) \leq \mathcal{L}(V, \mu^{n+1}), \\
&\forall (V, \lambda) \in W,
\end{aligned}
\]

with \( W = \mathbb{R}^{3N} \times \mathbb{R}_+^{N(N-1)/2} \) and

\[
\mathcal{L}(V, \lambda) = \mathcal{F}(V) - \sum_{1 \leq i < j \leq N} \lambda_{ij} (D_{ij}(q^n) + h G_{ij}(q^n) \cdot V)
\]

where \( \mathcal{F} \) denotes the unconstrained functional...

- **Numerical computations** by Uzawa algorithm.
Numerical modeling of a Red Blood Cell:

- Macro-body made of 11 rigid spheres
- Shape of the RBC: two- / three-body interactions between the spheres
- “Fake” overlapping of the annular spheres
How to simulate one single Red Blood Cell?

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- **Film 1** — formation of 1 RBC (with VTK)
- **Film 2** — formation of 1 RBC (with post-processing: POVRAY)
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- **Film 2** — formation of 1 RBC (with post-processing: POVRAY)
- **Film 3** — formation of 30 RBC (with post-processing)
- **Film 4** — formation of 500 RBC (with post-processing)
How to simulate one single Red Blood Cell?

Formation of 1 RBC (initialization)

Formation of 1 RBC (at fixed time)
How to simulate one single Red Blood Cell?

Formation of 1 RBC (initialization)

Formation of 1 RBC (at fixed time)
**Faxen laws** (Faxen, 1922):

- rigid sphere (radius $a$, velocity $U$),
- Stokes flow (viscosity $\mu$, velocity field $v^\infty$).

\[ F = -6\pi \mu a \left( U - v^\infty_{|x=0} \right) + \pi \mu a^3 \nabla^2 v^\infty_{|x=0} \]
Fluid / Red Blood Cells interactions (dilute suspensions)

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- **Couette flow** (**Film 5**):

Tank-treading motion (t) and tumbling motion (b)
**Langevin formulation:**

\[ M \cdot \frac{dU}{dt} = F_H + F_P, \quad \text{in } \mathbb{R}^{3N} \]

- **F}_H : hydrodynamic forces
- **F}_P : non hydrodynamic forces
Langevin formulation:

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SCoPI algorithm:

- Definition of the so-called “grand resistance” matrix:
  \[ \mathbf{F}_H = -\mathbf{R} \cdot \mathbf{U} + \mathbf{F} \]

- Implicit procedure:
  \[
  (M + h \mathbf{R}^n) \cdot \mathbf{U}^{n+1} = h (\mathbf{F}^n + \mathbf{F}_P^n), \\
  q^{n+1} = q^n + h \mathbf{U}^{n+1}
  \]
Stokesian Dynamics (Brady & Bossis, 1988):
- suspension of rigid, non-Brownian particles
- bulk macroscopic shear flow
- the Reynolds particle number is small
Fluid / Red Blood Cells interactions (dense suspensions)

- **Stokesian Dynamics** (Brady & Bossis, 1988):
  - ✓ suspension of rigid, non-Brownian particles
  - ✓ bulk macroscopic shear flow
  - ✓ the Reynolds particle number is small

- Relationship between hydrodynamic forces and velocities (Happel & Brenner, 1965; Brenner & O’Neill, 1972):
  - ✓ resistance formulation: $F_H = -\mathcal{R} \cdot (\mathbf{U} - \mathbf{v}^\infty) + \Phi : \mathcal{E}(\mathbf{v}^\infty)$
  - ✓ mobility formulation: $\mathcal{M} = \mathcal{R}^{-1}$
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- **Assumption:** *pairwise additivity of the interactions*
For two spheres, all elements of the resistance / mobility matrix for all separation are known exactly (Jeffrey & Onishi, 1984).

✓ At large separations, far-field expressions (method of reflections,...)
✓ At small separations, analytical results from lubrication theory
✓ At intermediate separations, tabulated results
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Resistance matrix...

- Resistance / mobility matrix defined for two spheres in interaction.
- The grand resistance matrix is obtained by pairwise additivity...

\[ R = (\mathcal{M}^\infty)^{-1} + R_{2B} - R_{2B}^\infty \]
**Far-field forces** (Smoluchowski, 1911; Luke, 1989; Guazzelli, 2003)

\[-U_2 = \frac{1}{6\pi\mu a} F_2 + \frac{1}{8\pi\mu} \left( \frac{I}{r} + \frac{r \cdot r}{r^3} \right) \cdot F_1 + \frac{a^2}{4\pi\mu} \left( \frac{I}{3r^3} - \frac{r \cdot r}{r^5} \right) \cdot F_1 + \ldots \]
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- **Lubrication forces** (Jeffrey & Onishi, 1984; Dance & Maxey, 2003)

\[
F_{j \to i} \cdot \mathbf{n}_{i \to j} = -\frac{3\pi \mu a^2}{2} \frac{(\mathbf{U}_i - \mathbf{U}_j) \cdot \mathbf{n}_{i \to j}}{r} + O(\ln r)
\]
Fluid / Red Blood Cells interactions (dense suspensions)

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- **Intermediate-field forces** (Kim & Karrila, 1991)
Fluid / Red Blood Cells interactions (dense suspensions)

Film 6 — without lubrication forces

Film 7 — with lubrication forces
Conclusion and perspectives

- **To be improved:**
  - Far-field forces:
    - method of reflections
    - cut-off distance (Satoh, 2001)
  - Lubrication:
    - method of boxes (complexity in $N \log N$ instead of $N^2$)
    - tangential contributions
    - wall-particle lubrication
**Conclusion and perspectives**

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  - ✓ Periodic boundary conditions
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To be discussed:

✓ Lateral migration
✓ Aggregates (Film 8)
Red blood cell aggregates in a shear flow
Spheres in a Poiseuille flow
Conclusion and perspectives

Polymer chains in a Poiseuille flow