# Collision Strategy for Direct Simulation of Moving Fibers

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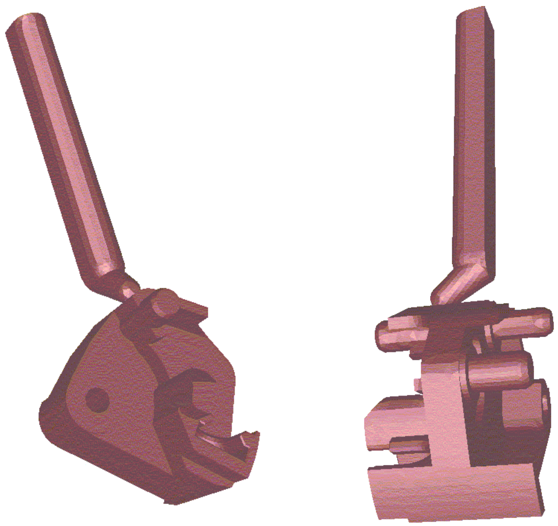
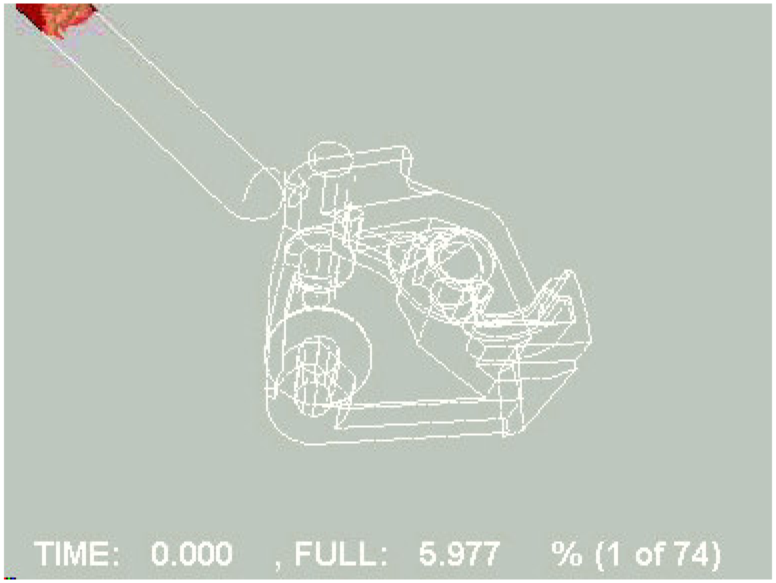
# Introduction (1)

- **Injection of thermoplastic**

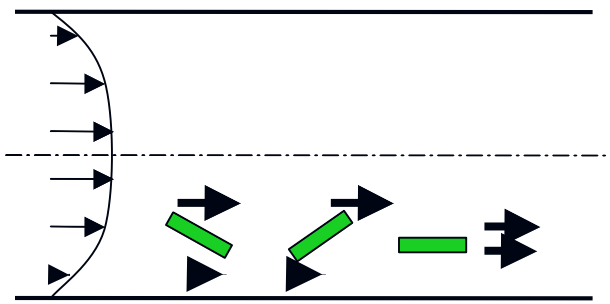




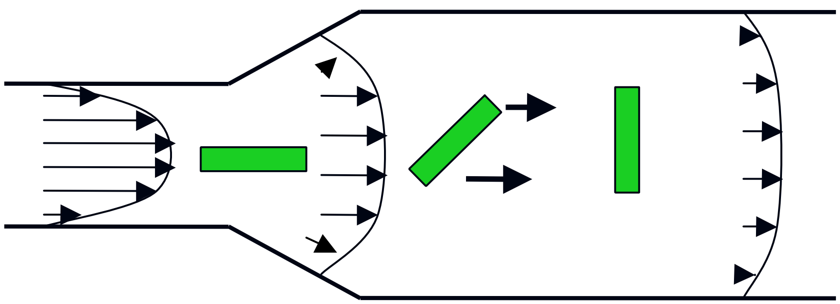

- **Injection of fiber-reinforced polymer**
  - use the same process as classical thermoplastic
  - complex composite products with improved mechanical properties
  - mechanical properties depend on fiber orientation

# Introduction (2)

- **Fiber orientation in flow motion**

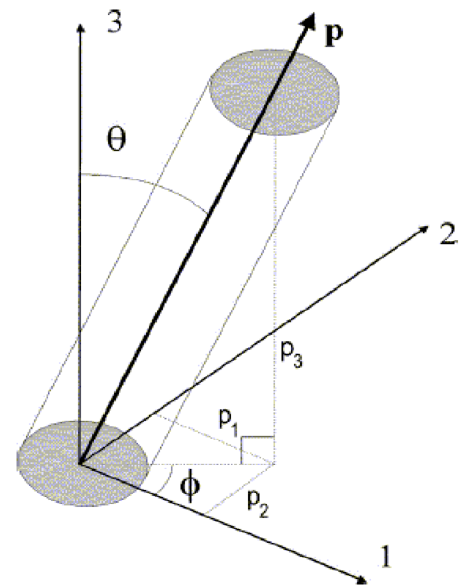


**Shear flow**



**Elongational flow**

# Background & Motivations




**p** orientation vector

- **Macroscopic modelling**
  - Dilute suspension → Jeffery's equation [Jeffery 1922]

    Newtonian fluid –slender body theory

$$\frac{dp}{dt} = \Omega p + \lambda\left(\dot{\varepsilon}\, p - \left(\dot{\varepsilon} : [p \otimes p]\right) p\right)$$

f( β = aspect ratio)

  - Semi-concentrated suspension → Folgar and Tucker's equation [Folgar 1984]

**Population of fiber :** $a_2 = \int_p \psi(p)\, p \otimes p\, dp = \frac{1}{N}\sum_{k=1}^{N} p_k \otimes p_k$

$$\frac{D\underline{\underline{a}}_2}{Dt} = \underline{\underline{\Omega}}\,\underline{\underline{a}}_2 - \underline{\underline{a}}_2\underline{\underline{\Omega}} + \lambda\left(\underline{\underline{\dot{\varepsilon}}}\,\underline{\underline{a}}_2 + \underline{\underline{a}}_2\underline{\underline{\dot{\varepsilon}}} - 2\underline{\underline{\dot{\varepsilon}}} : \underline{\underline{a}}_4\right) + 2C_I \dot{\bar{\varepsilon}}\left(\underline{\underline{I}}_d - 3\underline{\underline{a}}_2\right)$$

*fiber-fiber interaction term*

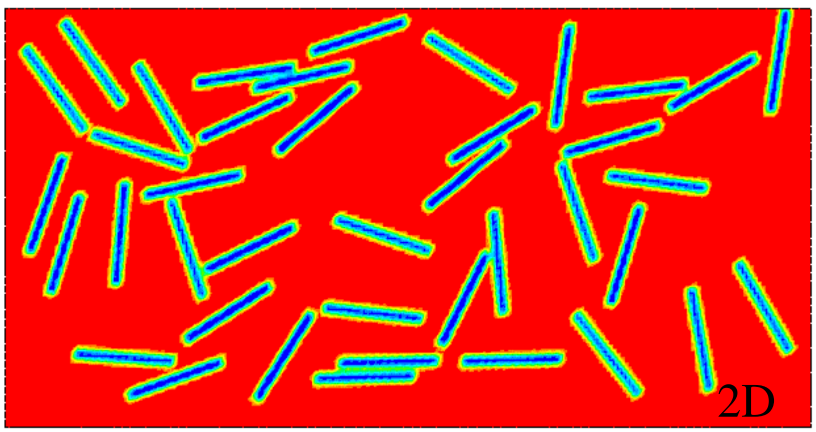
→ **Closure approximation, Ci ?**

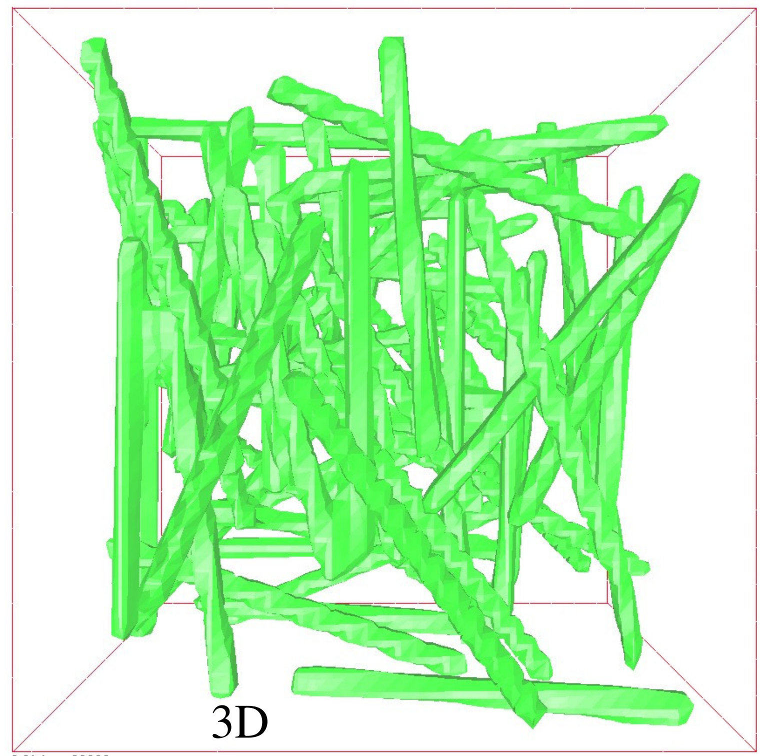
# Objectives : Micromechanic modelling approach

## Micromechanic approach → Direct simulation

**Simulate directly the motion of a dense population of fiber in a REV**

**Particle interactions are given by a fluid-structure coupling**




**Gives macroscopic informations on tensor $a_2$ and rheological properties**

# Numerical Procedure

t

1. Computation of velocity field

   *finite element method for the Stokes equation with multi-domain approach*

   *(no inertia, no gravity)*

2. Update particle position

   *particle method*

3. Computation of characteristic functions associated to each domain

   *voxelisation method*

$t + \Delta t$

- **Numerical approach similar to Glowinski & Joseph's modelling [Glowinski 1999]**

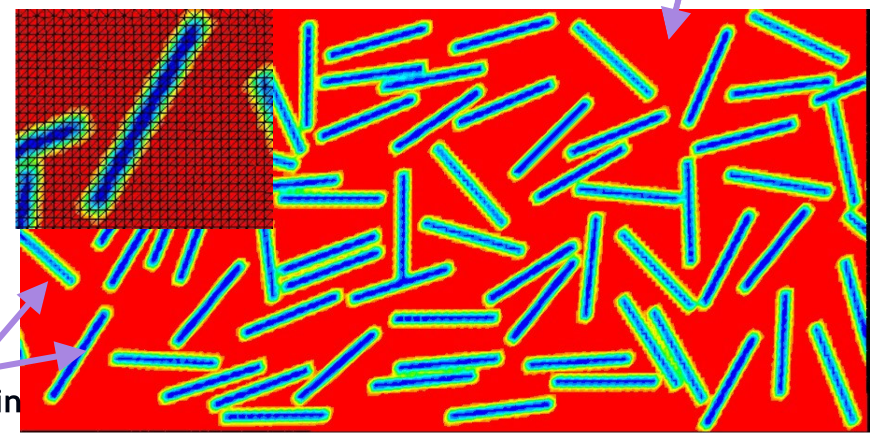
  **(Fictitious domain method for particulate flows)**

# Computation of Velocity field (1)

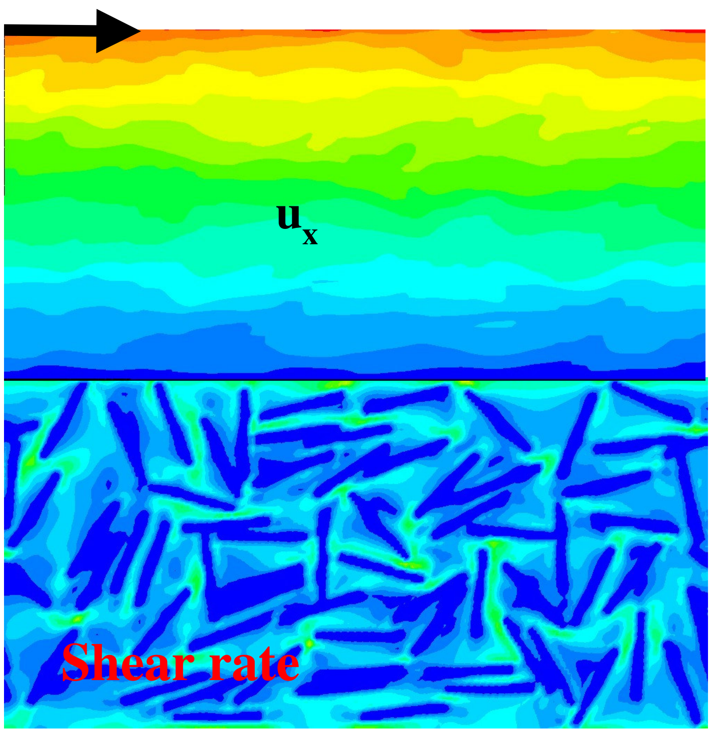
### 1) Characteristic function

$$1_{\Omega_j}(x,t) = \begin{cases} 1 & x \in \Omega_j \\ 0 & x \notin \Omega_j \end{cases}$$

j = fluid or solid (fibers)




$$\Omega_s = \bigcup_i^n \Omega_{si}$$




### 2) Velocity field

$$\nabla . \sigma = 0$$

$$\int_\Omega 1_{\Omega_f} 2\eta \varepsilon(u) : \varepsilon(v)\, d\Omega + \int_\Omega 1_{\Omega_s} \mathbf{r}\, \varepsilon(u) : \varepsilon(v)\, d\Omega$$

$$- \int_\Omega p \nabla.v \; d\Omega = 0$$

**Penalization ~ $10^3\, \eta$**

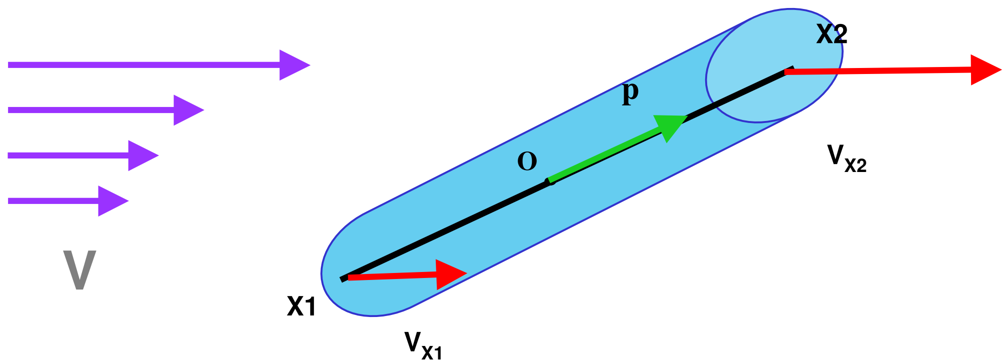
$$\varepsilon(u) = 0$$

$$\nabla . u = 0 \qquad - \int_\Omega q \nabla.u \; d\Omega = 0$$

# Update fiber position and orientation (2)

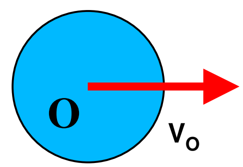
**Particle method**

**Langrangian updating of the position**




$$X_i(t+\Delta t) = X_i + V_{X_i}\Delta t$$

**Rigid motion**




$$O\,(t+\Delta t) = O + V_O\,\Delta t$$

$$\vec{p} = \frac{\overrightarrow{X_2X_1}}{\left\|\overrightarrow{X_2X_1}\right\|}$$

**Vector orientation**

$$O = \frac{X_1 + X_2}{2}$$

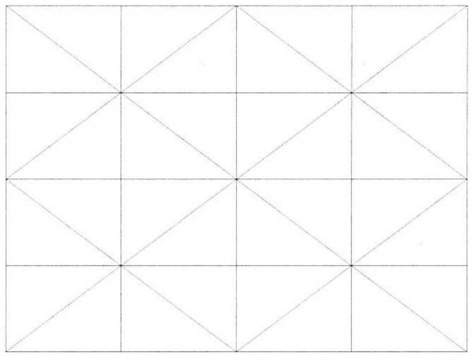
**Fiber center**

## Advantages

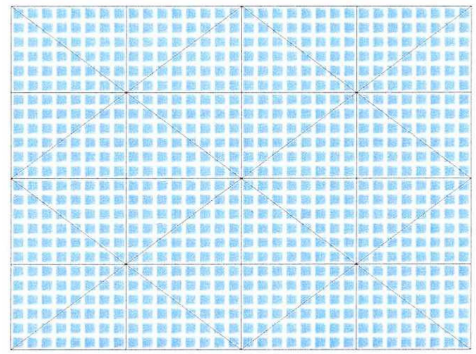
- **Perfect rigid motion of each fiber**
- **Conservation of the length**
- **No mumerical diffusion**

# Computation of Characteristic Function (3)

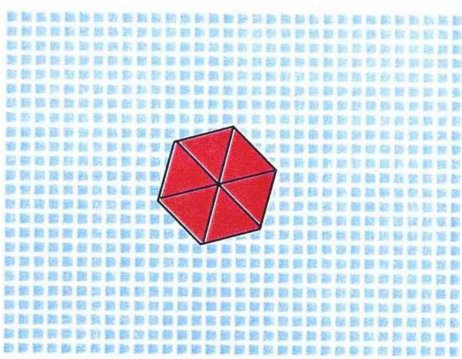
## Voxelisation method



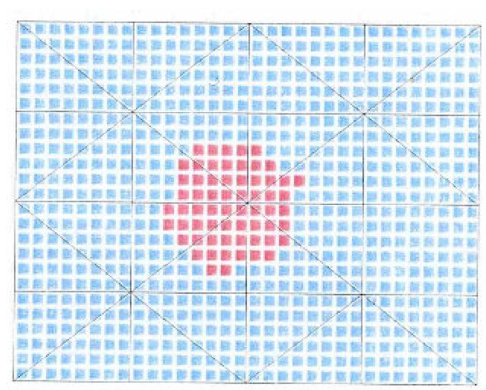
Cavity mesh



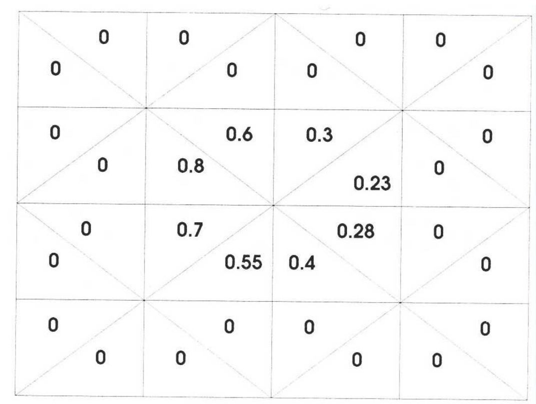
Voxelisation



Add fiber mesh

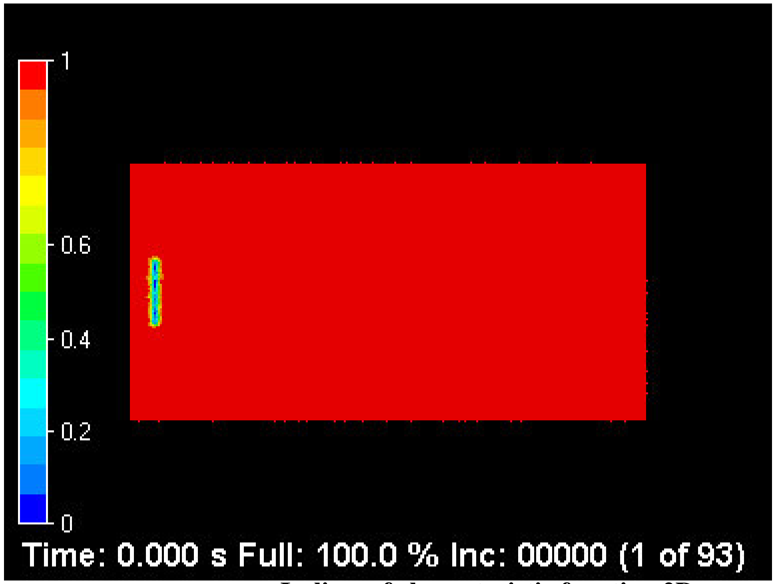


switch on pixels

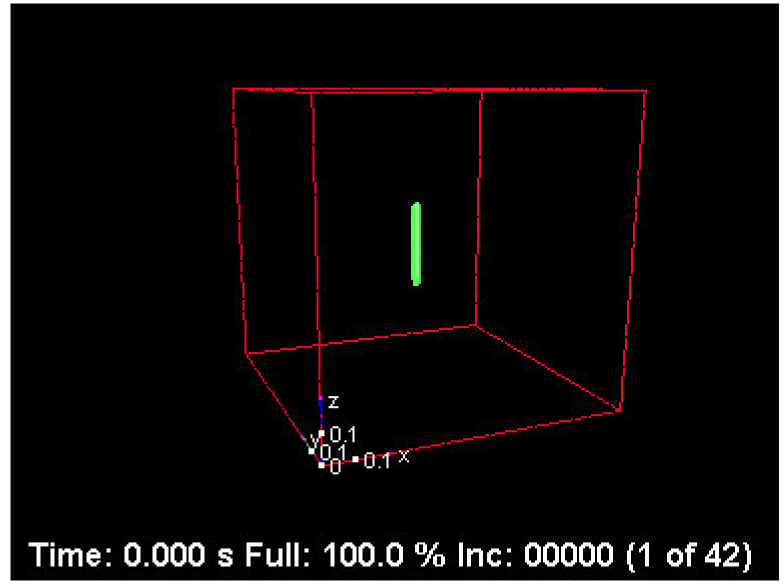



Get values

# Single Fiber Motion in shear flow



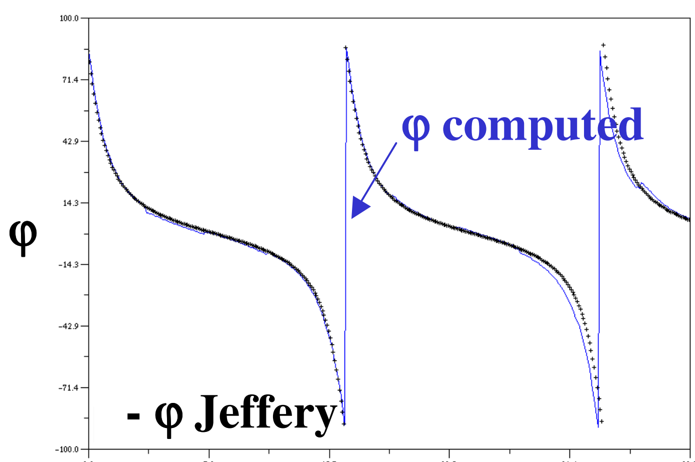

Isoline of characteristic function 2D




Isoline of characteristic function 3D

**Shear flow, Periodic Cell**

**Equivalent aspect ratio $\beta_{ref}$**




**Evolution of φ vs time**

**Find Jeffery's orbit for a shear flow**

→ **Periodic motion**

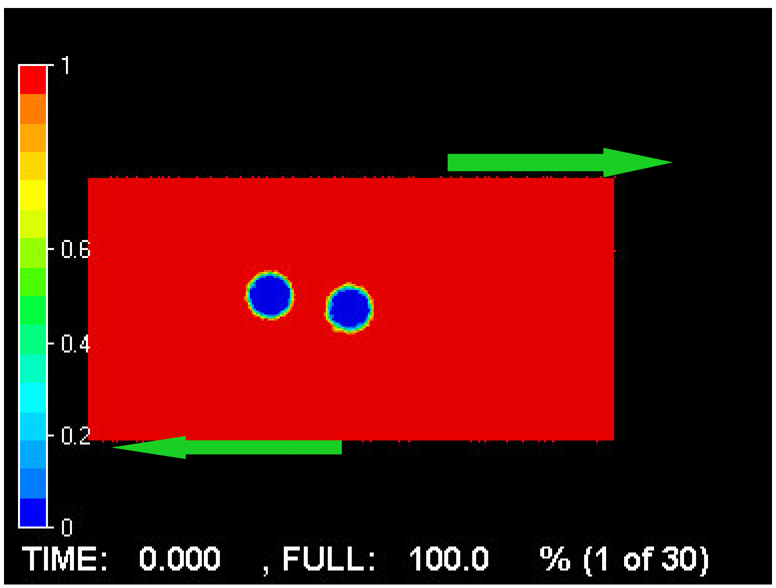
$$T = \frac{2\pi}{\dot{\gamma}} \left( \beta_{ref} + \frac{1}{\beta_{ref}} \right)$$

# Hydrodynamical Interactions

**It is not necessary to have an explicit form** **(as in [Yamane 1994] , [Fan 1998])**

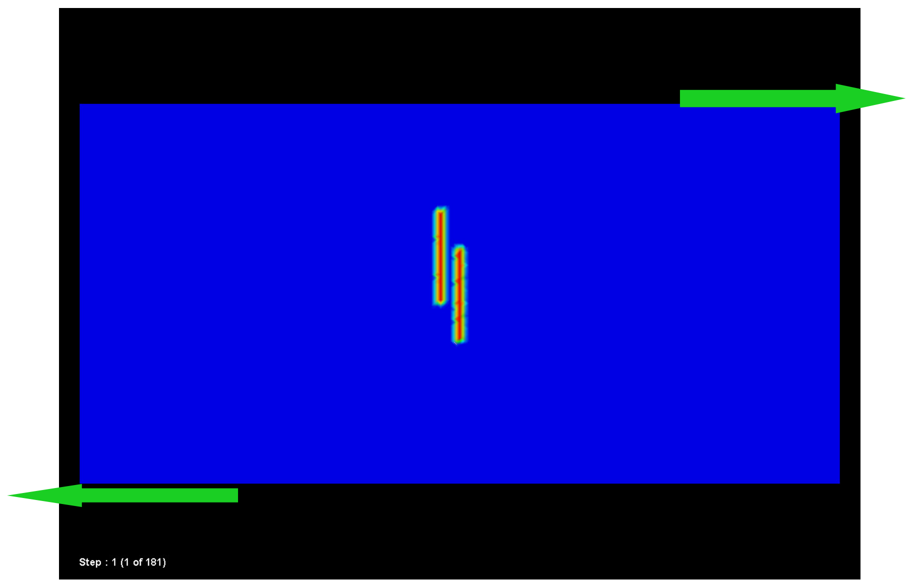
- **drag forces**
- **lubrification forces (short range interactions)**

**The central particle moves due to hydrodynamical interactions**

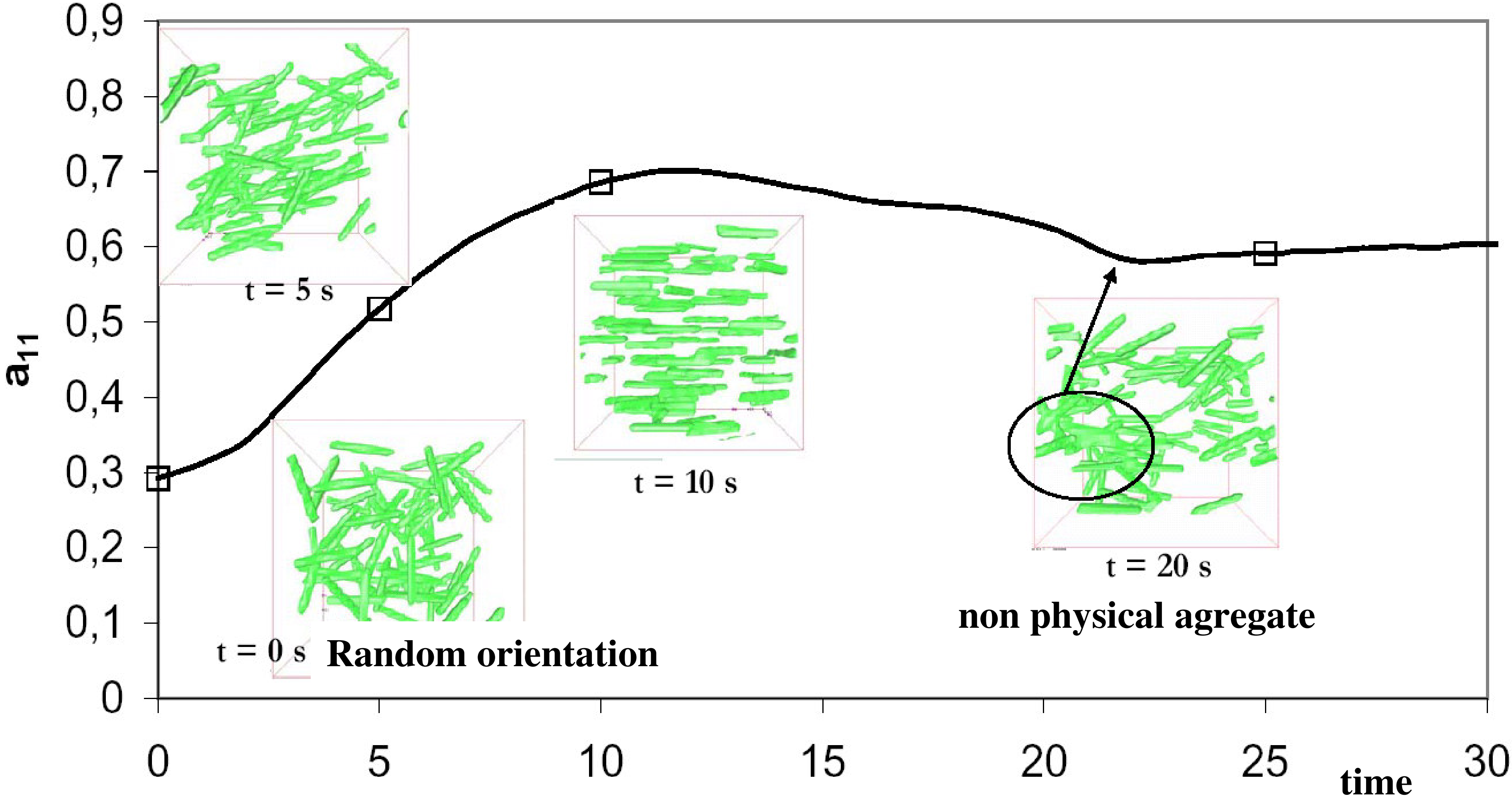



**Sphericals particles in Couette Flow**

**The period of rotation changes**

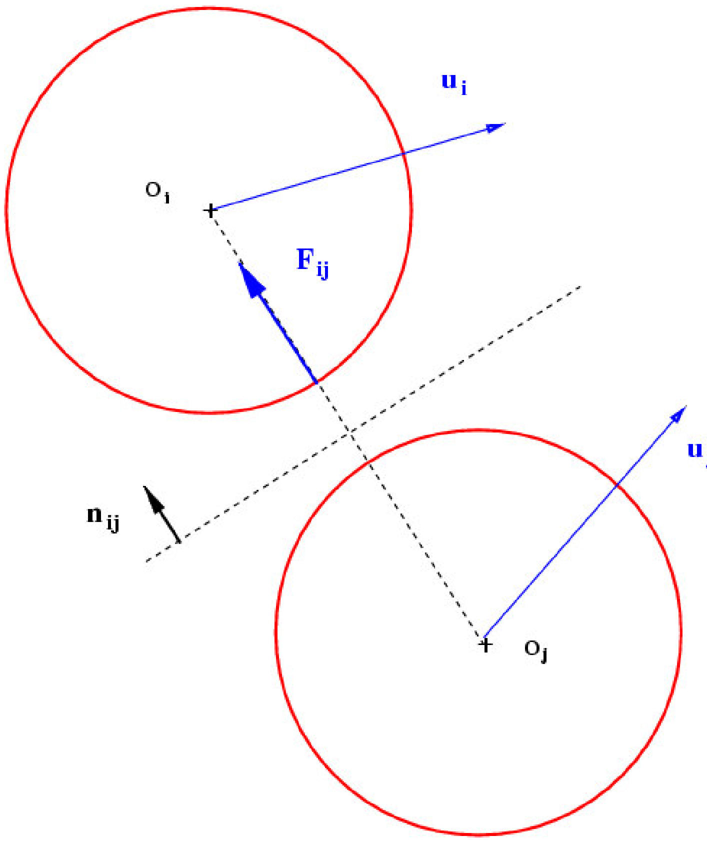


# Many Fibers – Collision Strategy



# Spheres – short-range hydr. forces (moderate concentration)

**Lubrification theory :**
**repulsion force exerted by *j* on *i* //** $\mathbf{n}_{ij} = \dfrac{\overrightarrow{O_j O_i}}{||\overrightarrow{O_j O_i}||}$




$$F_{ij} = -\frac{3}{2}\,\pi\,R^2\,\eta\,\frac{(\mathbf{u}_i - \mathbf{u}_j)\,.\,\mathbf{n}_{ij}}{||\overrightarrow{O_j O_i}|| - 2\,R}\,\mathbf{n}_{ij}$$

$F_{ij}$ ↗ as $O_i \longrightarrow O_j$

➡

- **Modifies $u_i$ and moves $O_i$ in the $n_{ij}$ direction**
- **Accurate computation needs a small region between two spheres**

$$||\overrightarrow{O_j O_i}|| > 2\,R + \underline{\alpha}$$

**depends on mesh**

# Spheres - Collisions (concentrated suspension)

## Assumptions :

**<u>no fluid between spheres</u>**
**same mass**
**elastic choc, no friction**

**If P collision point :**

$$\left(\mathbf{u}_i^+(P) - \mathbf{u}_j^+(P)\right) \, . \, \mathbf{n}_{ij} \; = \; -\left(\mathbf{u}_i^-(P) - \mathbf{u}_j^-(P)\right) \, . \, \mathbf{n}_{ij}$$

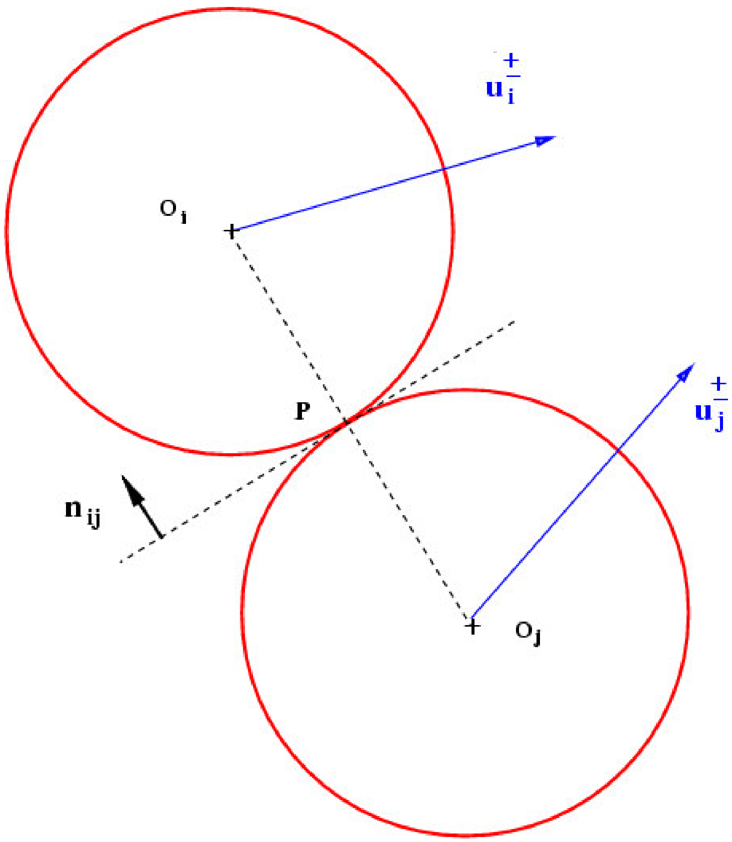
**Modifies center velocities**

$$\mathbf{u}_i^+ \;=\; \mathbf{u}_i^- - \delta_u \; \mathbf{n}_{ij}$$

**with**

$$\mathbf{u}_j^+ \;=\; \mathbf{u}_j^- + \delta_u \; \mathbf{n}_{ij}$$

$$\delta_u = \left[ (\mathbf{u}_i^- - \mathbf{u}_j^-) \; . \; \mathbf{n}_{ij} \right] \qquad < \quad 0$$



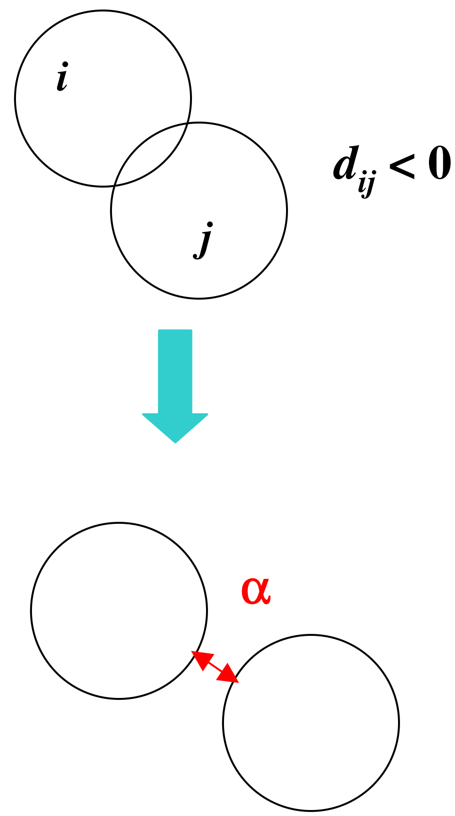
# Spheres - algorithm

**If $u_i \sim u_j$ → the action of hydrodynamic forces and analogy with collision process by imposing at time $t + \Delta t$**

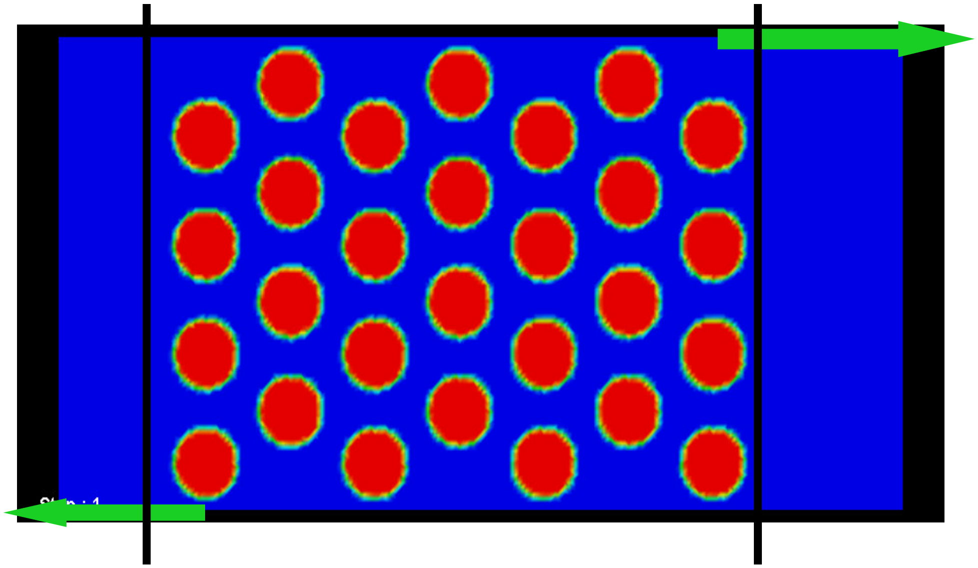
$$\min_{i,j} (d_{ij}) \geq 0 \quad \text{with} \quad d_{ij} = ||\overrightarrow{O_j O_i}|| - 2\ R - \alpha$$

**Converge in few iterations**

```
while ( min(d_ij)  < 0 )
    loop on spheres  i
      loop on spheres j <> i

         compute the smallest D_i =  min_j(d_ij)

          if ( D_i < 0)
            delta_u = |D_i|/Delta_t/2
            u_i = u_i + delta_u  n_ij
            u_j = u_j - delta_u  n_ij
          endif

      end loop j
      compute D = min_i(D_i)
    end loop i
    D = min_ij (d_ij)
end while
```

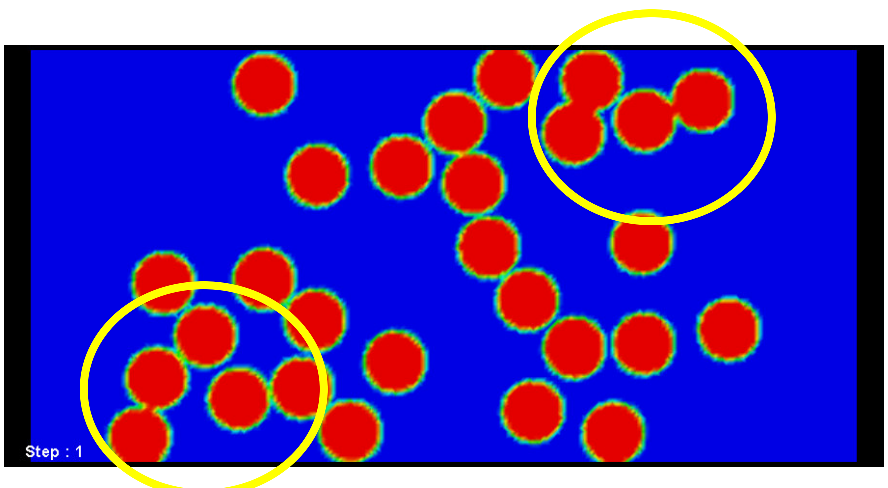


# Examples with Spheres (1)

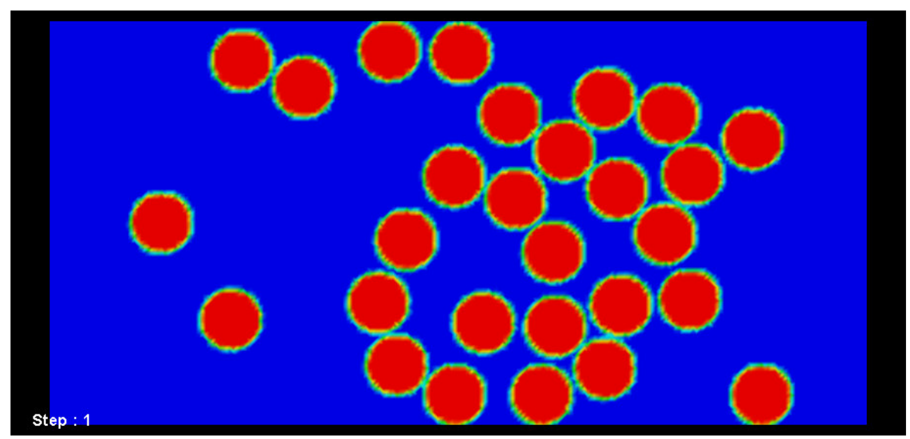


NE = 58 000 , $\Delta t = .05$ , $\gamma = 1$
Size = 1.5 x 1, R = .075, $\phi = 50\ \%$ ,

$\alpha = .005$




t = 27

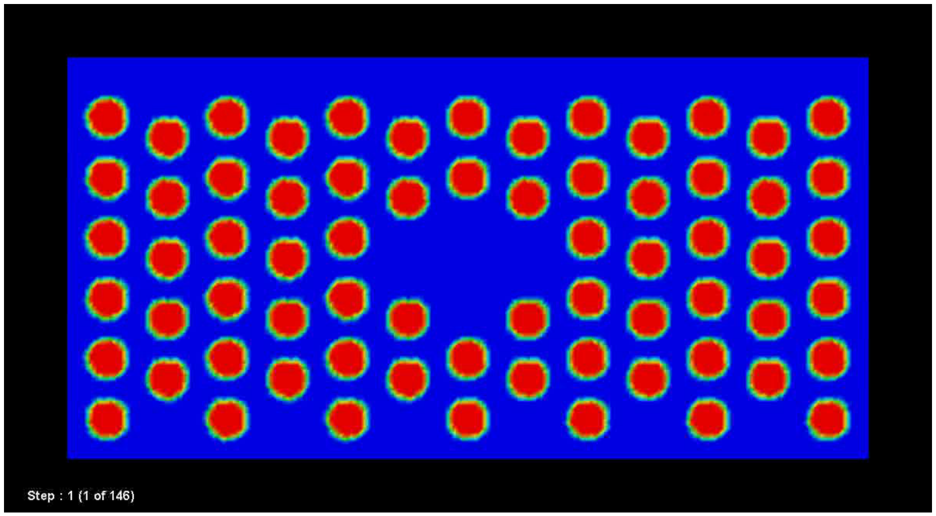


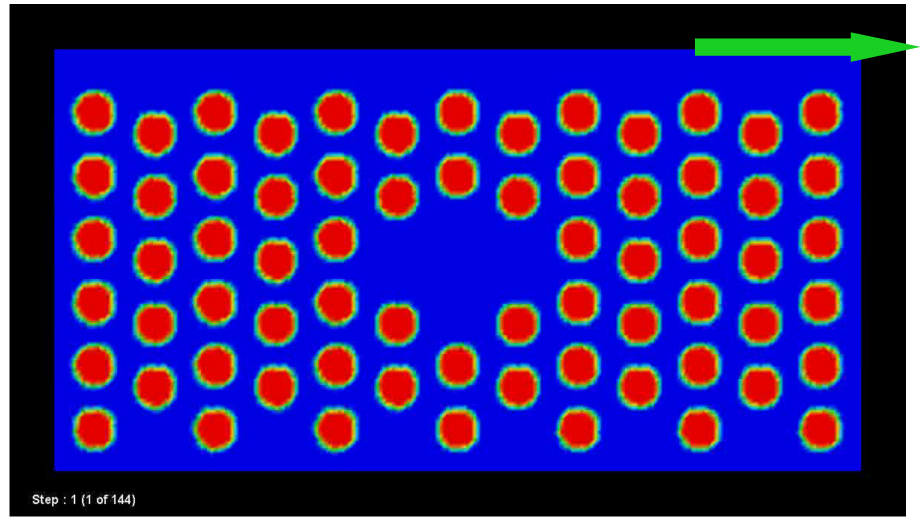

t = 30

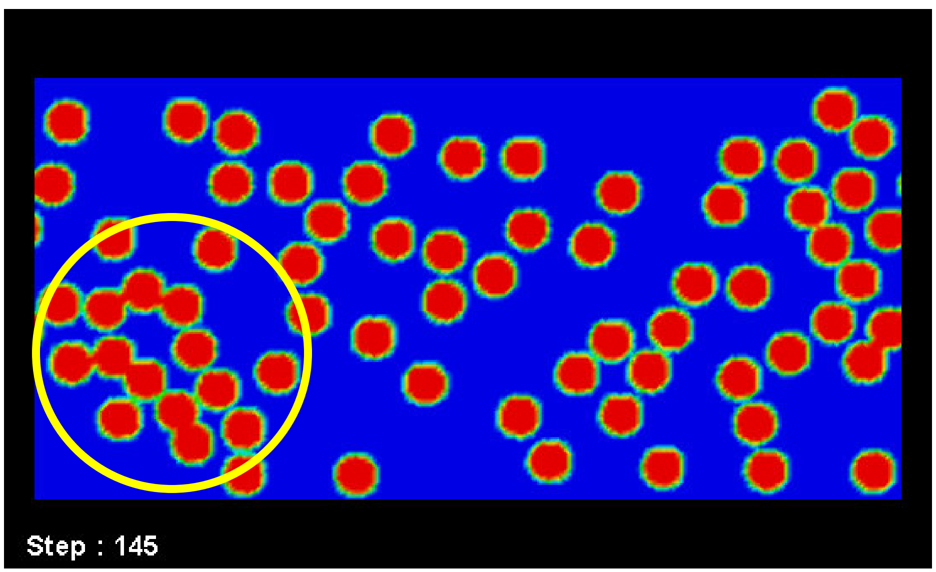
# Examples with Spheres (3)

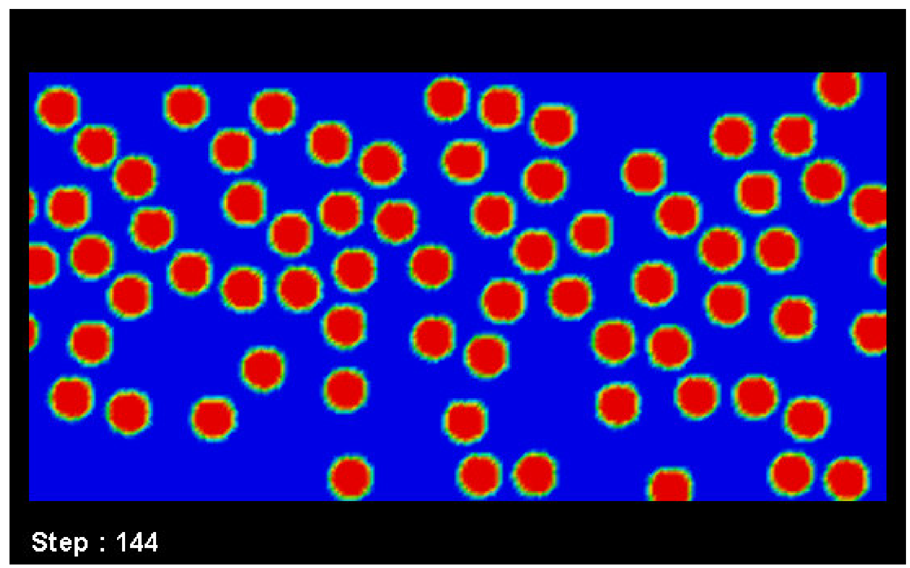
**No collision strategy**

$\alpha = .02$



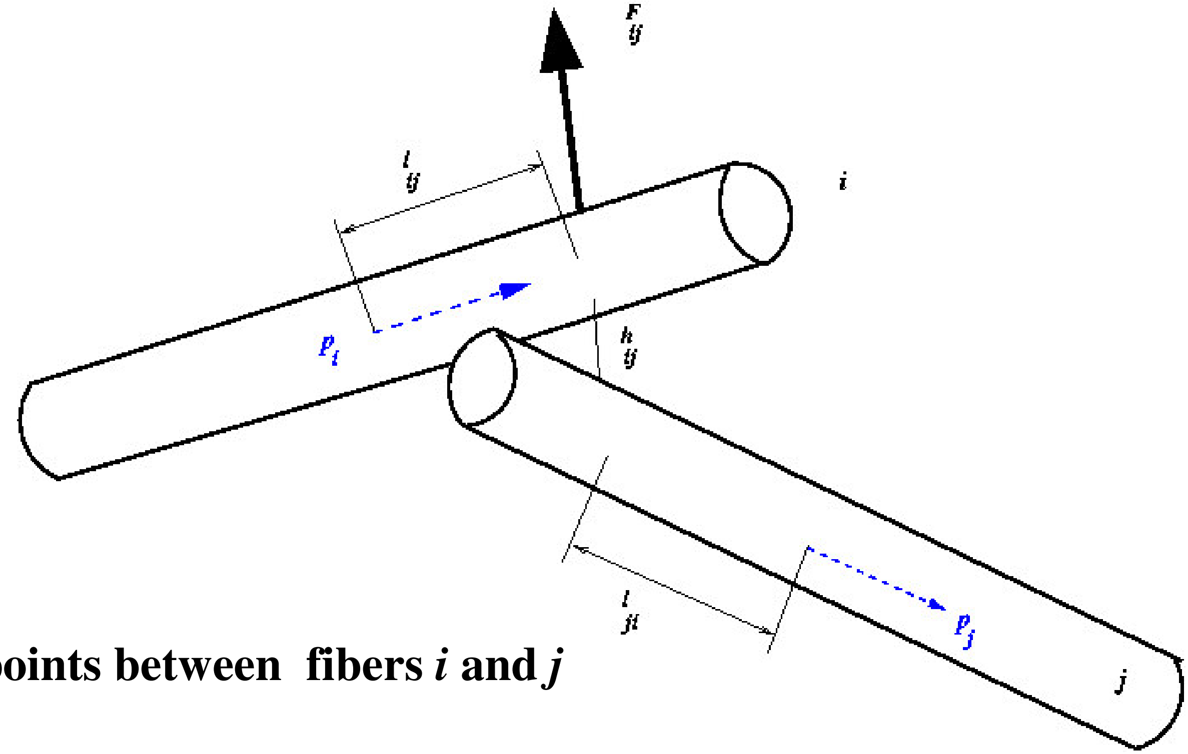



# Cylindrical Fibers ?

**3D case :**

**Repelling force // $p_i \wedge p_j$**



**Determination of the closest points between fibers *i* and *j***

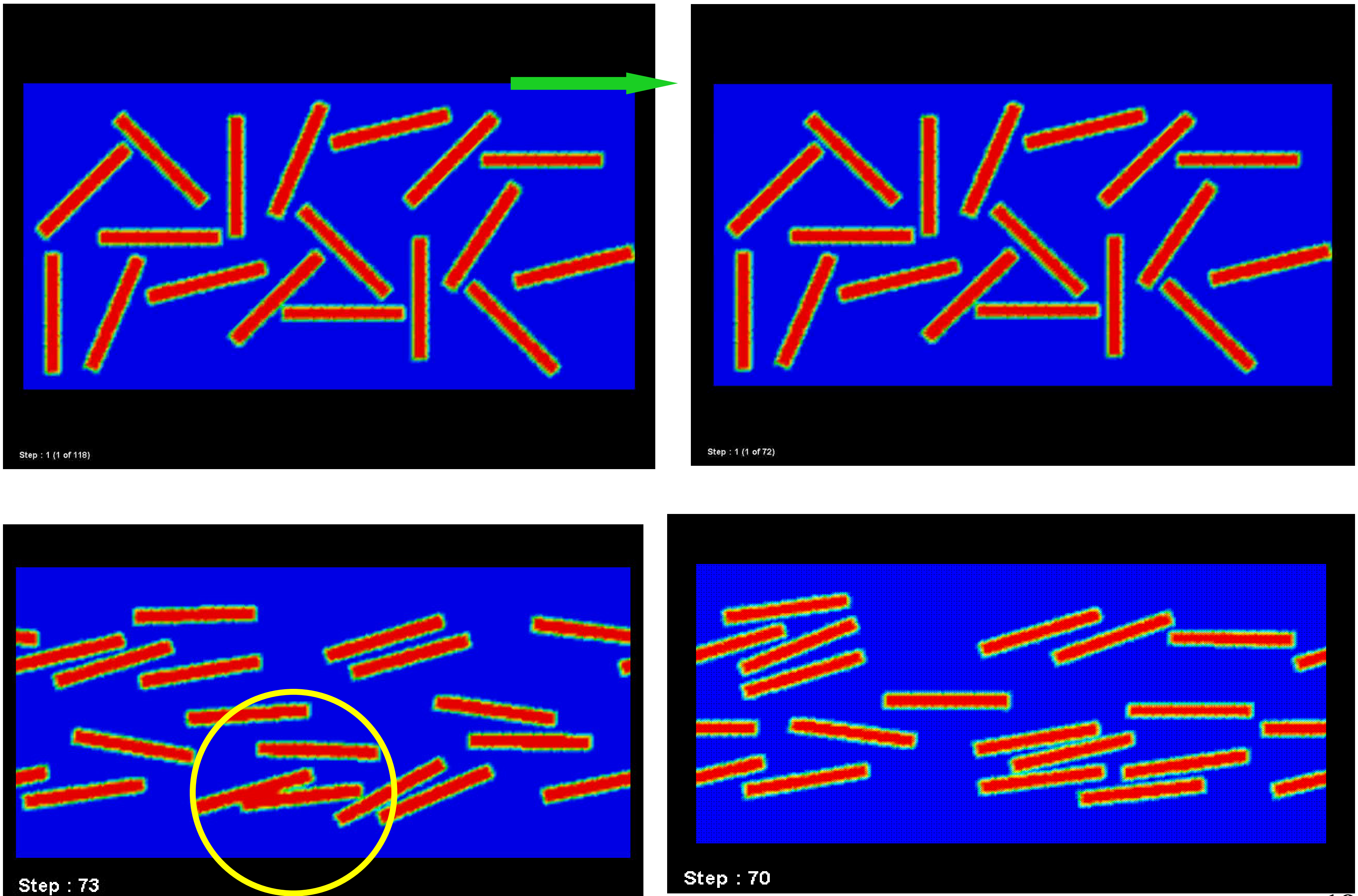
$$l_{ij} = \frac{\overrightarrow{O_iO_j} \, . \, \mathbf{p}_i - (\mathbf{p}_i \, . \, \mathbf{p}_j) \, (\overrightarrow{O_iO_j} \, . \, \mathbf{p}_j)}{1 - (\mathbf{p}_i \, . \, \mathbf{p}_j)^2}$$

$$h_{ij} = \frac{|\overrightarrow{O_iO_j}.(\mathbf{p}_i \wedge \mathbf{p}_j)|}{|\mathbf{p}_i \wedge \mathbf{p}_j|}$$

**Conditions : $h_{ij} > 2R + \alpha$ if $l_{ij}, l_{ji} < L_f / 2$**

# Examples with fibers

No collision strategy



# Conclusions

- **We have developed a micromechanical modelling approach**

  - **compute directly the motion of a dense population of fibers**

  - **Model the exact particle interaction by using a multi-domain approach and collision strategy.**

- **In Progress studies of macroscopic properties :**

  - **Influence of security zone $\alpha$**
  - **Computation of coefficient interaction ($C_i$)**
  - **Check closure approximations**
  - **Rheology of suspension ( $\eta$ and stress tensor )**