Direct Simulation of the motion of rigid fibers in viscous fluid

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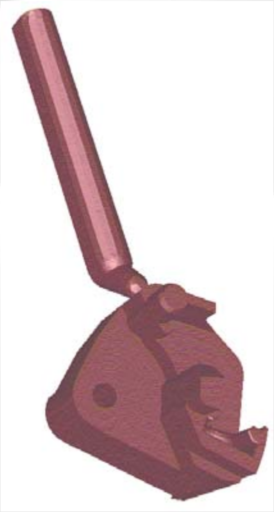
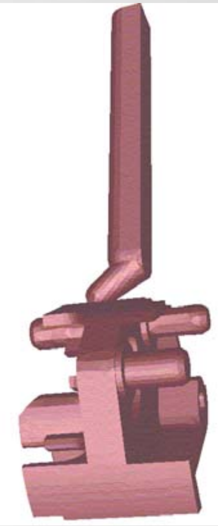
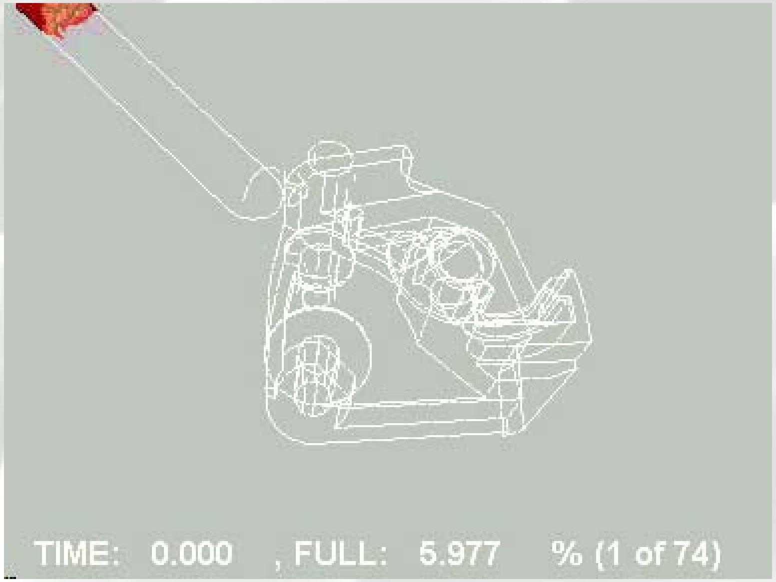
Introduction (1)

- **Injection of thermoplastic**



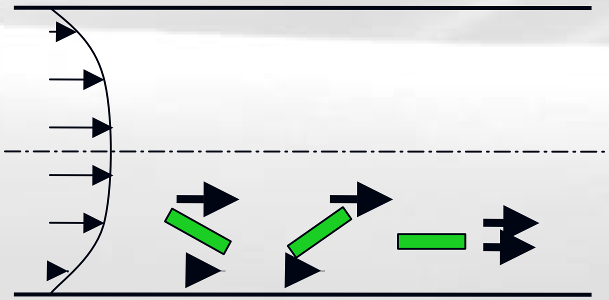




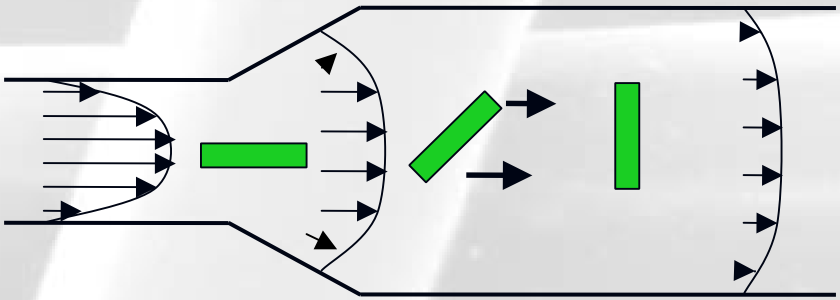
- **Injection of fiber-reinforced polymer**
  - use the same process as classical thermoplastic
  - complex composite products with improved mechanical properties
  - mechanical properties depend on fiber orientation

Introduction (2)

- **Fiber orientation in flow motion**



Shear flow



Elongational flow

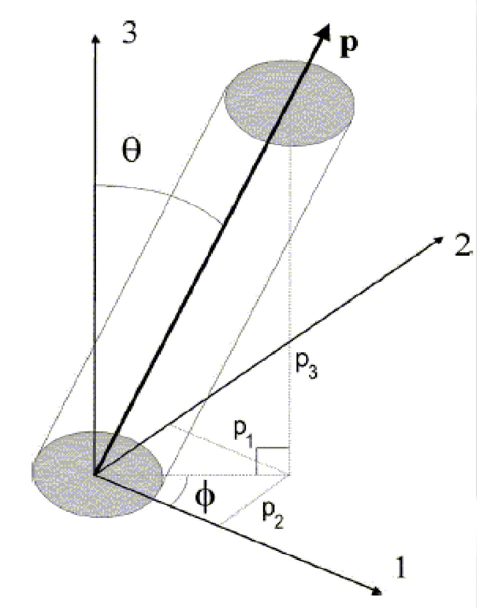
Background & Motivations

- **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)



p orientation vector

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

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

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

fiber-fiber interaction term

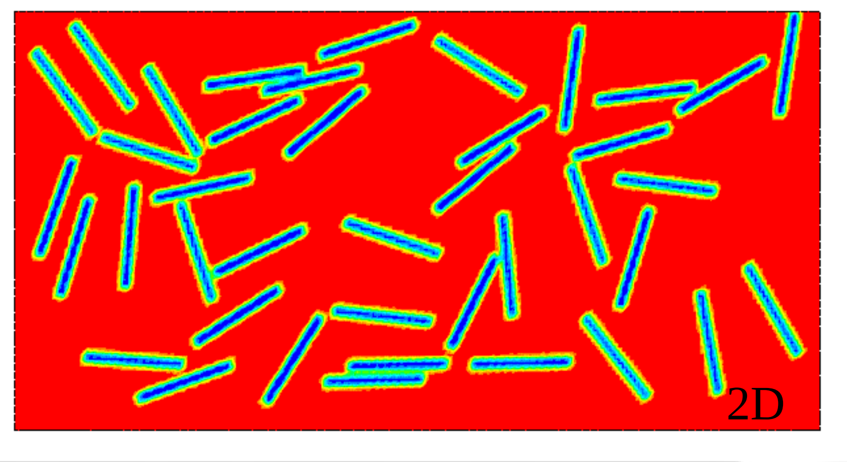
Closure approximation, Ci ?

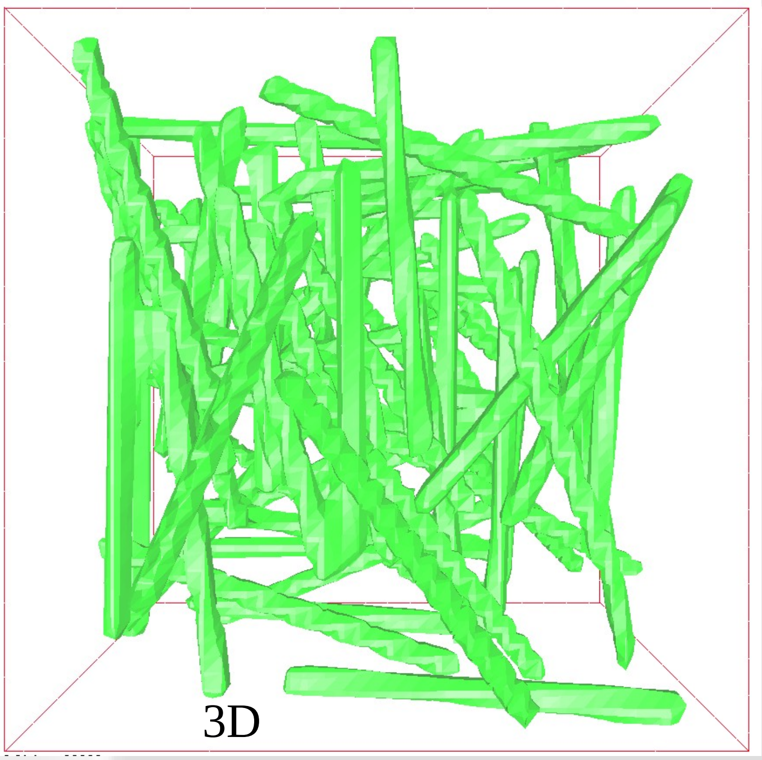
Objectives : Micromechanic modelling approach

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 with **Rem3D**
   finite element method for the Stokes equation with multi-domain approach
   (no inertia, no gravity)

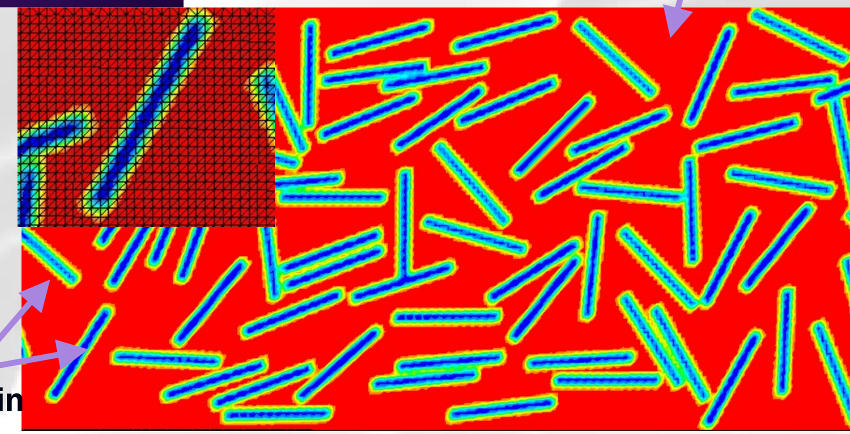
2. Update particle position
   particle method

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)

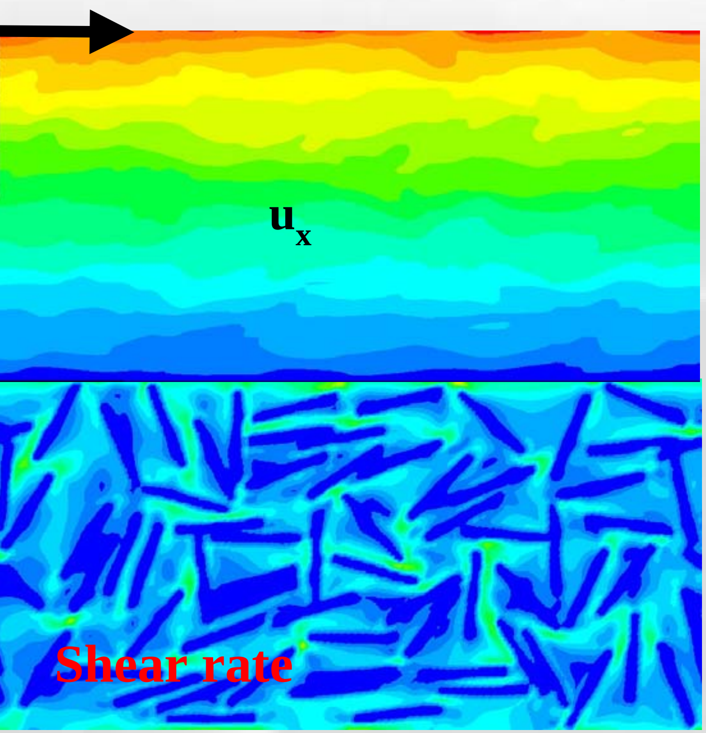


1) Characteristic function

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

j = fluid or solid (fibers)

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



2) Velocity field

$$\nabla . \sigma = 0$$

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

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

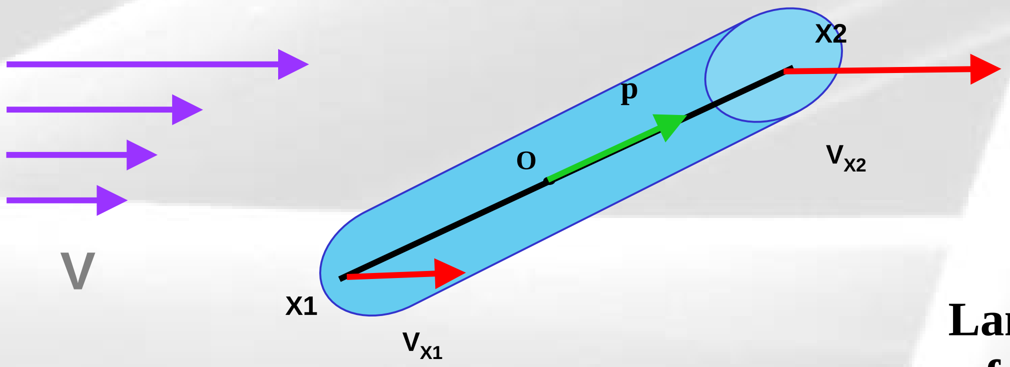
Penalization ~ $10^3\,\eta$

$$\varepsilon(u) = 0$$

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

Update fiber position and orientation (2)

Particle method



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

Langrangian updating of the position of the two extremities of each fiber

Rigid motion

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

Vector orientation

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

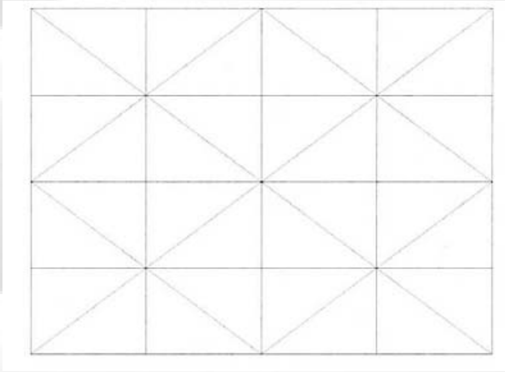
Fiber center

Advantages

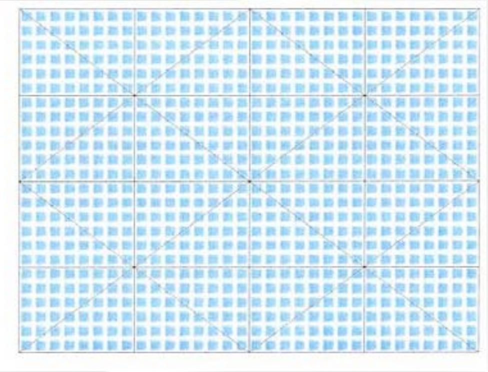
- **Perfect rigid motion of each fiber**
- **Conservation of the length**
- **No mumerical diffusion**

Computation of Characteristic Function (3)

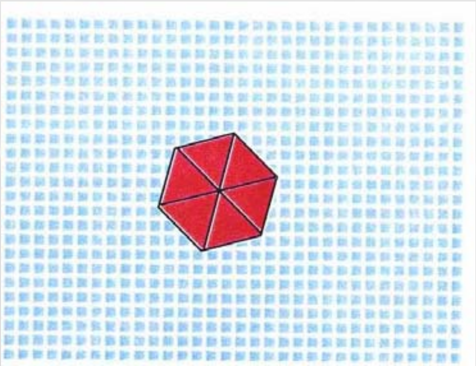
Voxelisation method



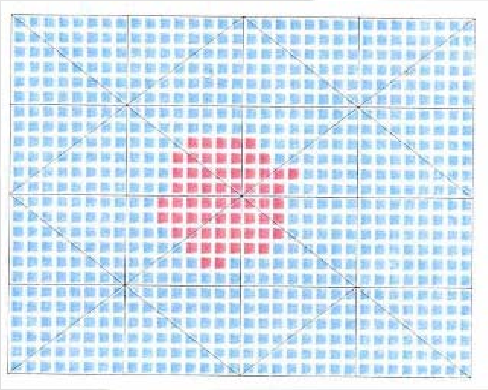
Cavity mesh



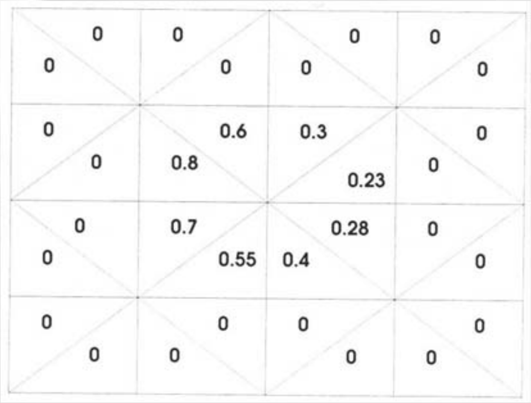
Voxelisation



Add fiber mesh

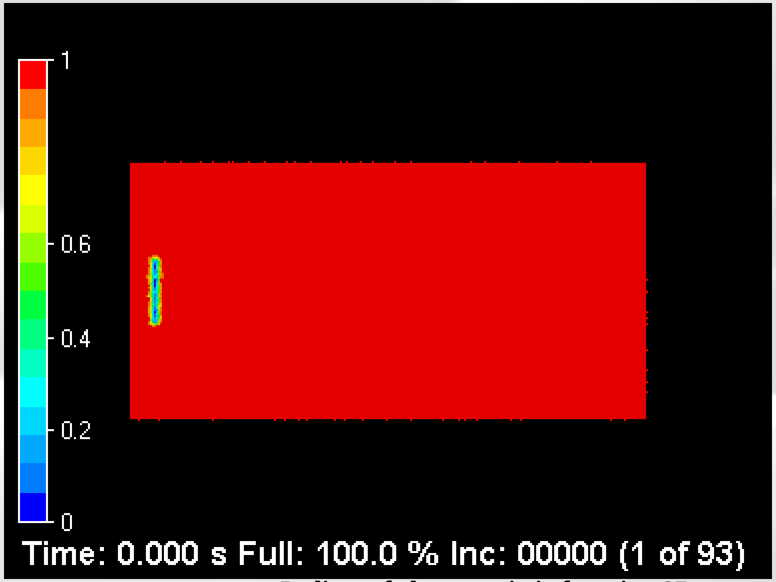


switch on pixels

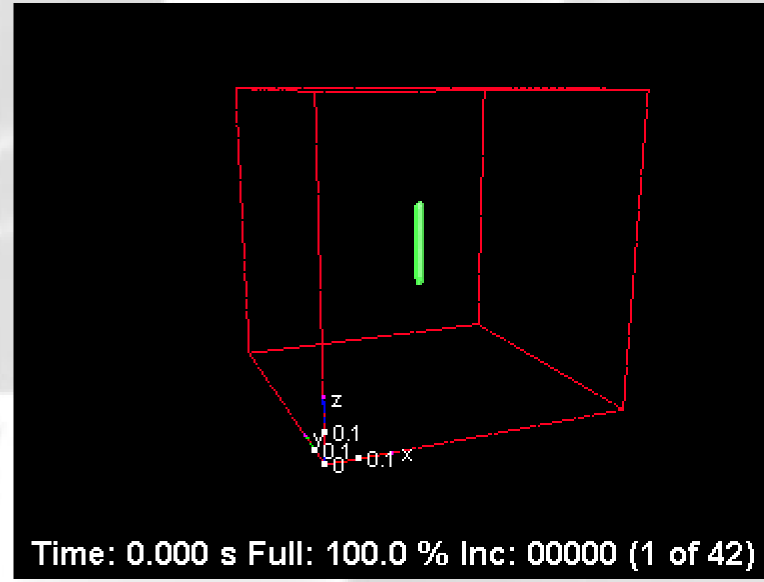


Get values

Single Fiber Motion in shear flow

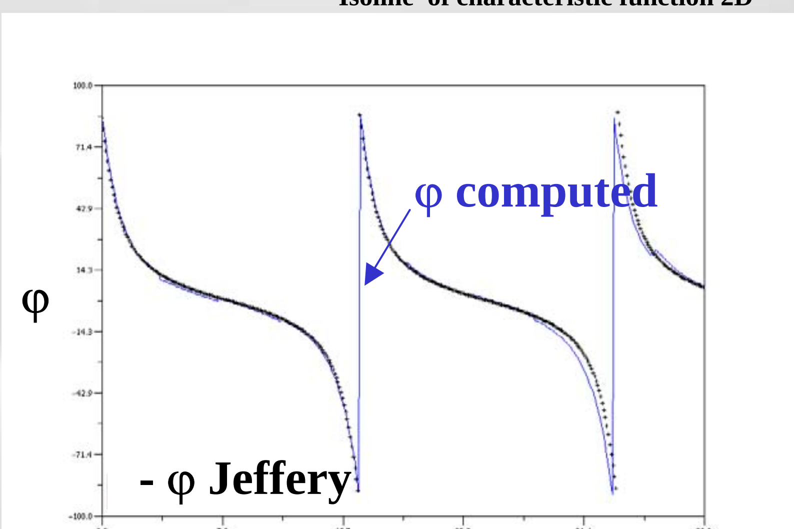


Isoline of characteristic function 2D



Isoline of characteristic function 3D

Shear flow, Periodic Cell
aspect ratio β=10



Evolution of φ vs time

Find Jeffery's orbit for a shear flow

→ **Periodic motion**

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

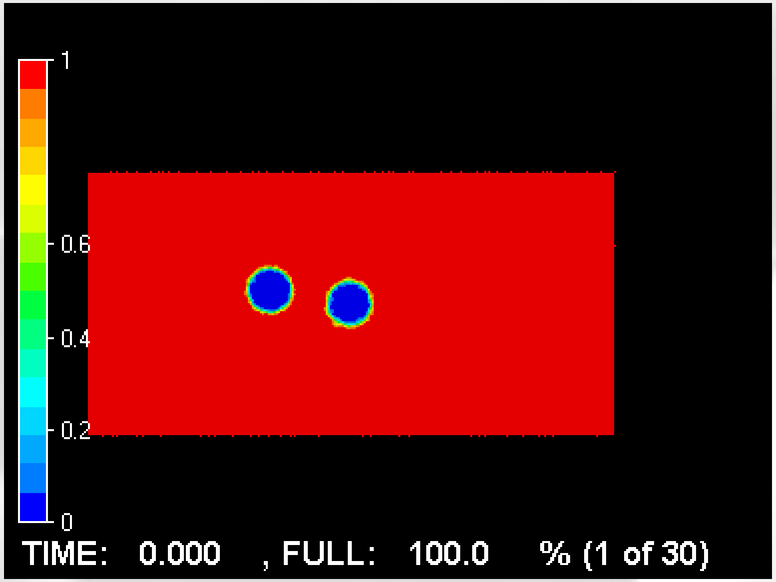
Hydrodynamical Interactions

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

- drag forces

- lubrification forces (short range interactions)

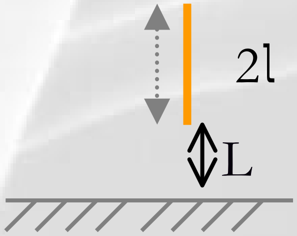
→ An example of hydrodynamical interactions



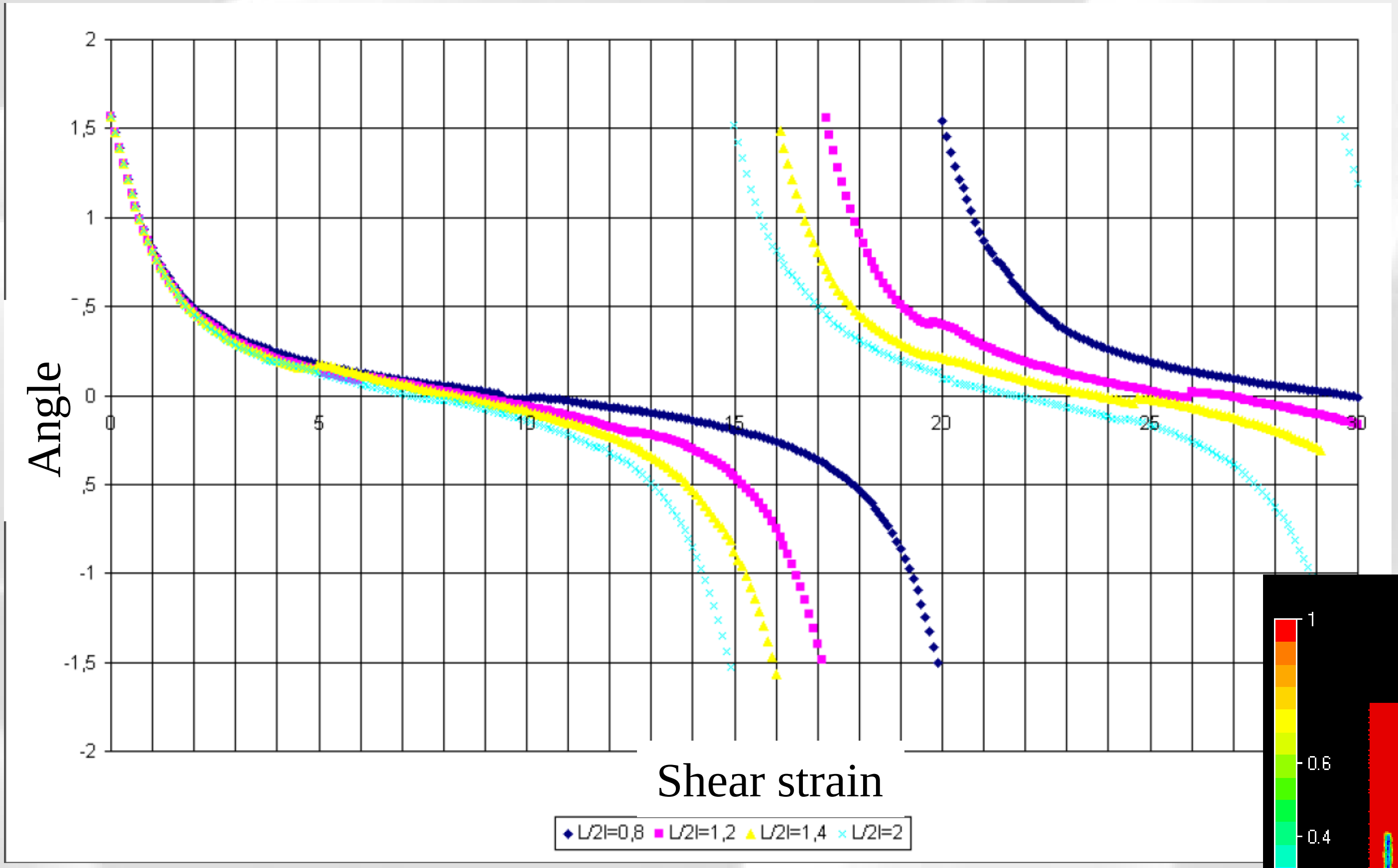
Sphericals particles in Couette Flow

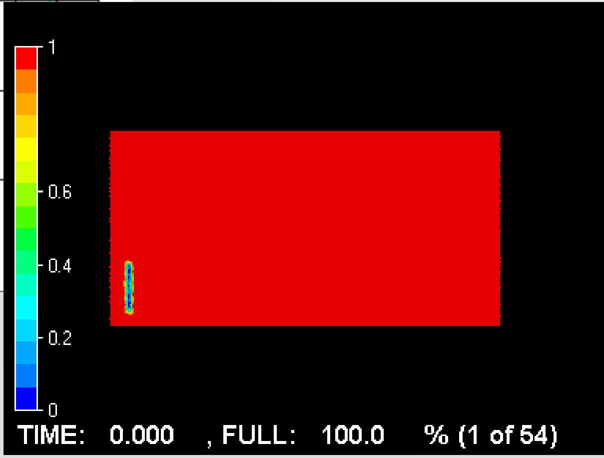
The central particle moves due to hydrodynamical interactions

Fiber – Wall interaction (1)



- Fiber initially perpendicular to the wall

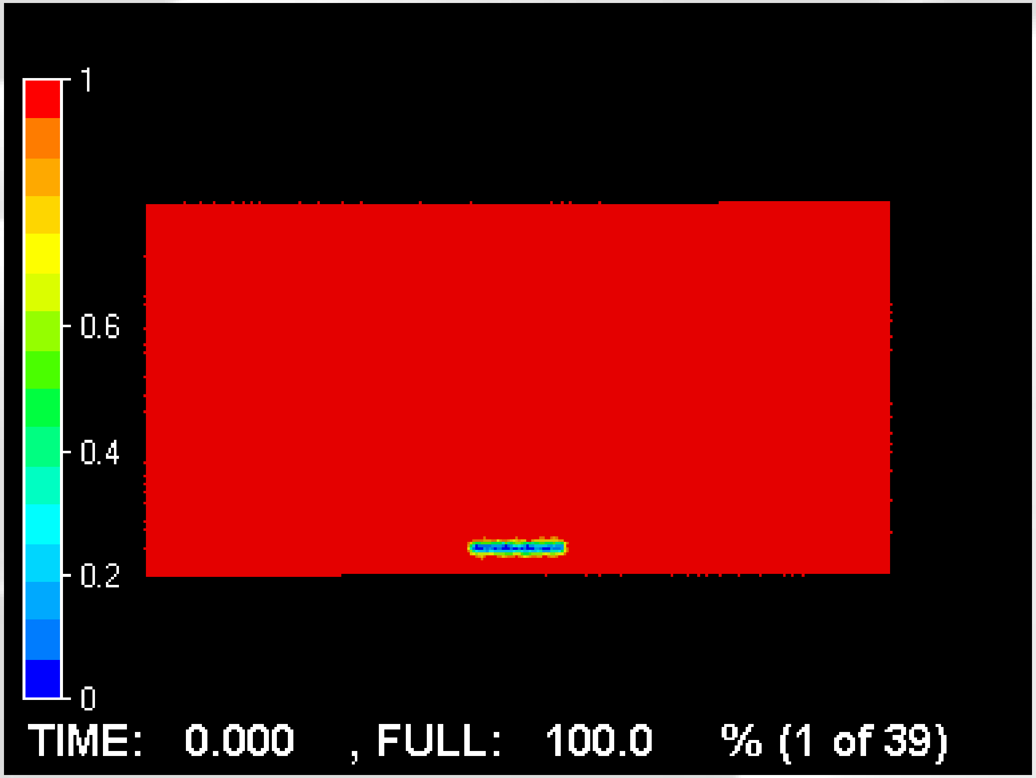


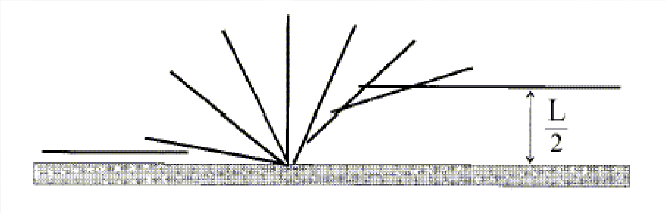


⇒ T ↗ as L ↘

Fiber – Wall interaction (2)

- **Fiber initially parallel to the wall**

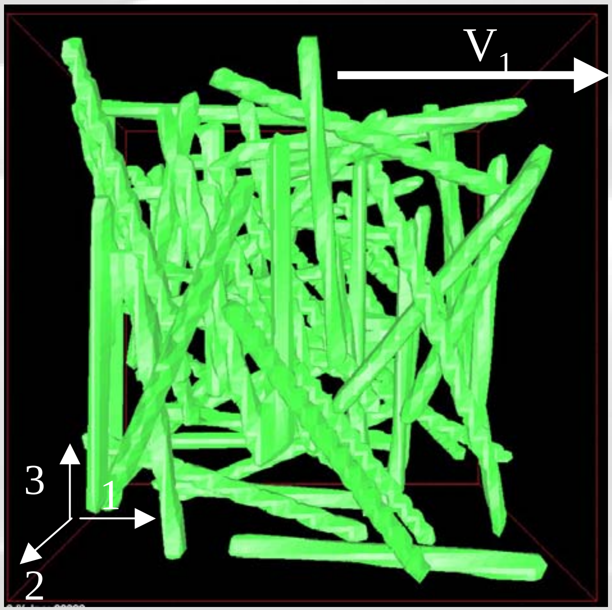




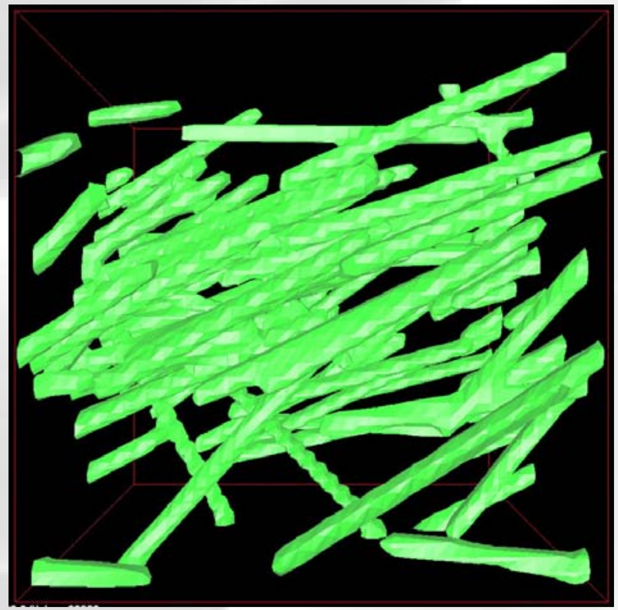
Fiber migration and alignment near the wall

Statistical studies - 3D example -

- **Aspect ratio β = 12, concentrated suspension**
- **Shear flow**



Initial time



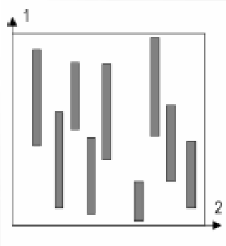
Shear strain 5

Shear strain 10

Get a_2 and a_4 on time

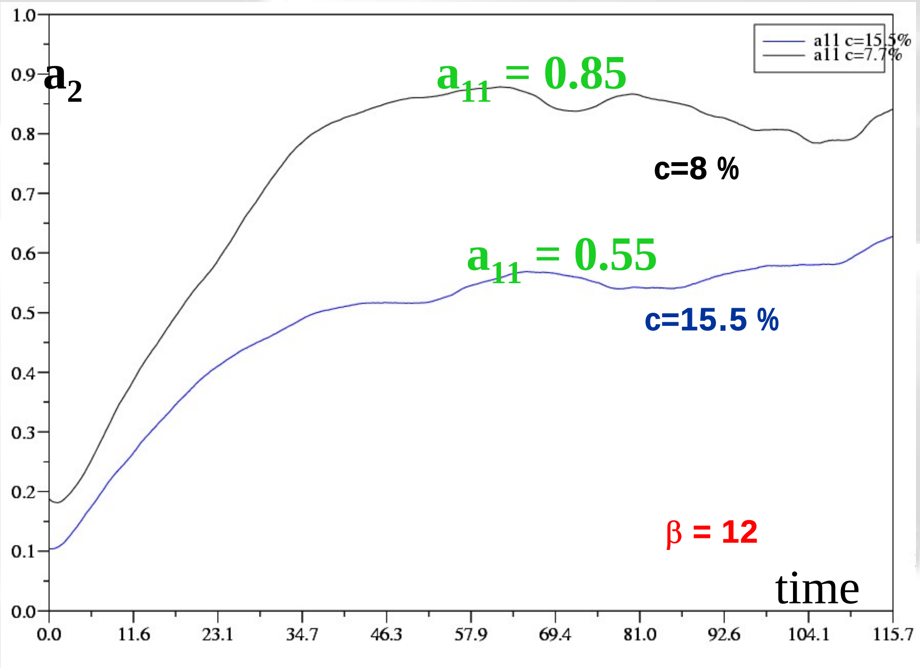
$$a_2 = \frac{1}{60}\sum_{k=1}^{60} p_k \otimes p_k$$

Statistical studies (1) -Evolution of a_2 -

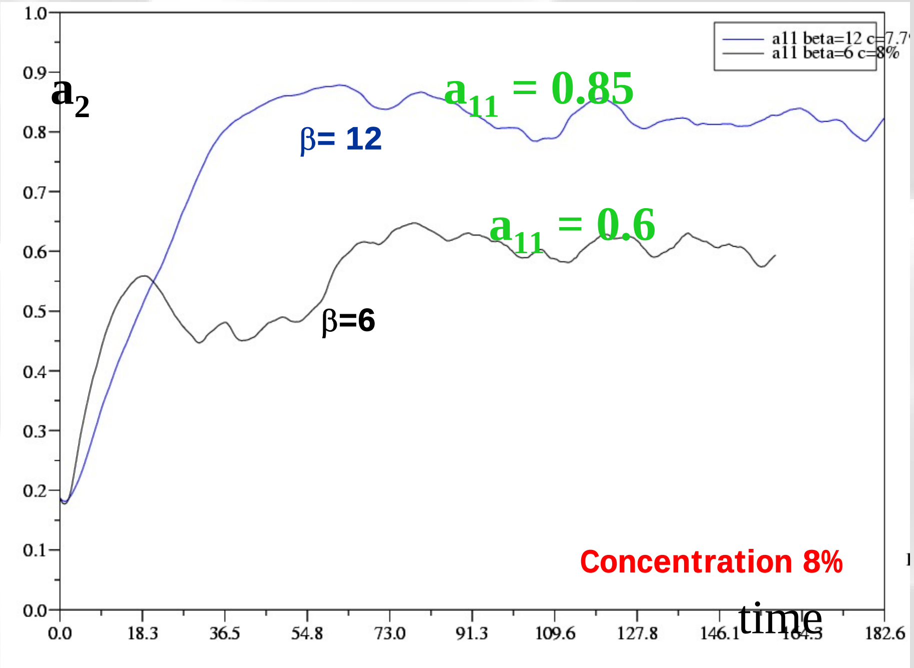


$$a_2 = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$$

- Effect of the concentration



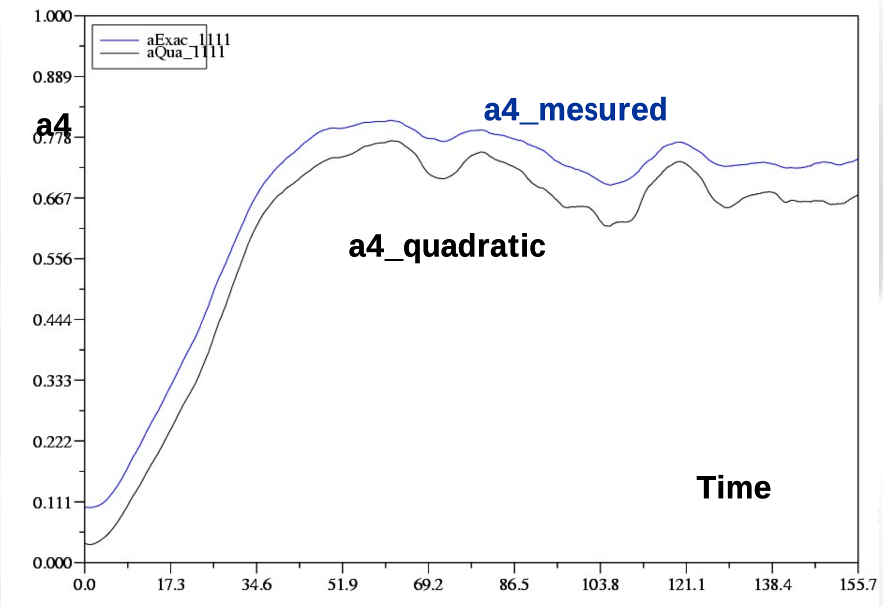
- Effect of the aspect ratio

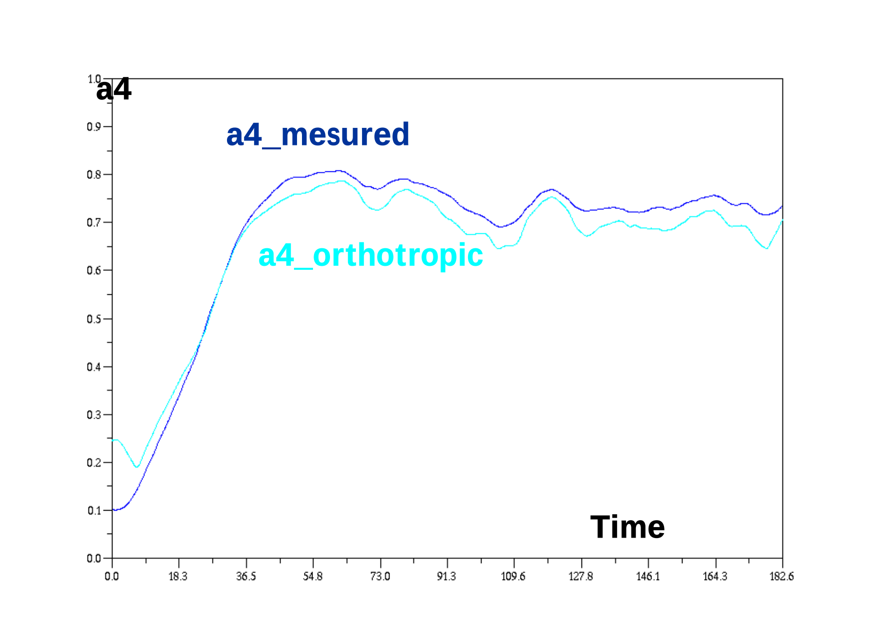


- Sensibility of simulations to the concentration and the aspect ratio
  - Interaction
  - Closure approximation

Statistical studies (2) - Closure approximation -

- Test of Closure approximation
  - a_{4_model} = function ($a_{2\_mesured}$)
  - Comparison $a_{4\_mesured}$ & a_{4_model}
- 60 fibers in shear flow, β = 12





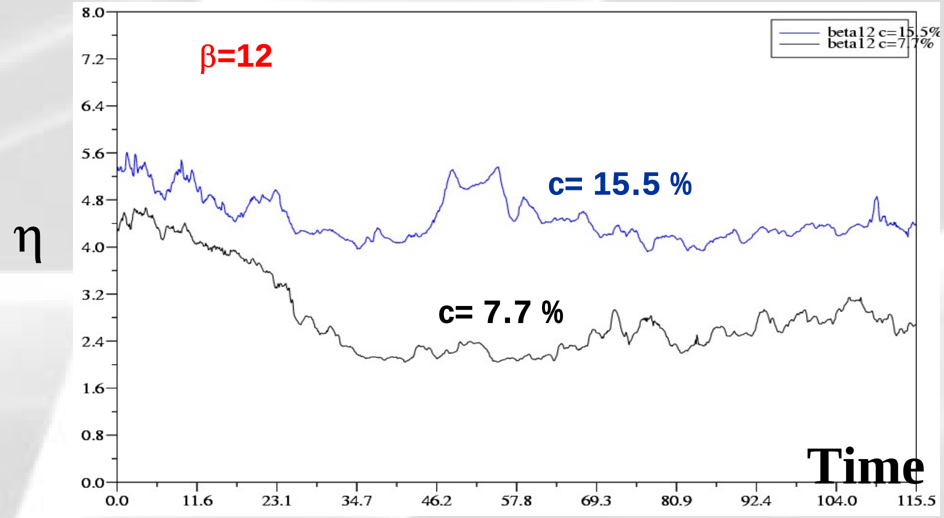
Quadractic closure : correct evolution in shear flow

Orthotropic closure : more accurate

Statistical studies in progress (3)   - Rheology-

- Evolution of the viscosity in shear flow

$$\eta_{apparent} = \frac{\sigma_{imposed}}{\dot{\gamma}_{apparent\ REV}}$$



- Evolution of the Cauchy stress tensor

$$\sigma = \sigma_{fluid} + \sigma_{fibers}$$

Study of rheological parameters

Newtonian fluids $$\sigma_{fibers} = 2\eta_f \, N_p \, \varepsilon(u) : a_4$$

Conclusions

- **We have developed a micromechanical modelling approach**
  - **Simulate directly the motion of a dense population of fibers**
  - **Model the exact particle interaction by using a multi-domain approach**
- **Very encouraging results for the**
  - **Study of macroscopic parameters as :**
    - **interaction between particles**
    - **closure approximations**
  - **Study of the suspension's rheology : η and stress tensor**
- **Next Step**
  - **Multiple populations of fibers**
  - **Flexibility**
  - **Viscoelasticity**