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The Lagrangian approach for fiber suspension flows

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Outline

1. Motivation
2. Basics
3. One-way coupling
4. Fiber interactions
5. Two-way coupling

Motivation

Voith papermaking production line

Fluid phase :

$$\frac{\partial u}{\partial t}+u\cdot\nabla u=-\nabla p+\nabla\cdot(2\nu D)$$

$$\nabla\cdot u=0$$

Fiber suspension :

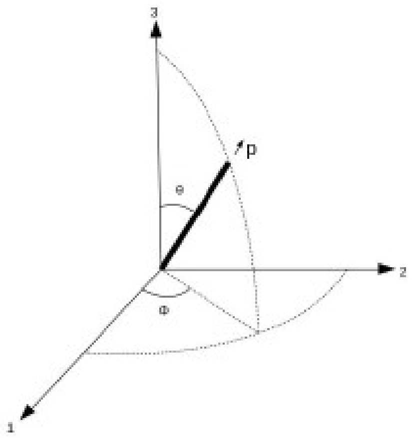
Lagrangian Approach :

- **Accurate (specially near solid boundaries)**
- **Costly, each fiber must be tracked individually**

Eulerian Approach :

- **Cannot describe the detailed motion of individual fibers**
- **Computationally more efficient**

The Lagrangian Approach



$$p_1 = sin(\theta)cos(\phi),$$

$$p_2 = sin(\theta)sin(\phi),$$

$$p_3 = cos(\theta).$$

ODE for the center of mass Xi, of the i-th fiber :

$$\frac{dX_i}{dt} = u(X_i), \qquad X_i(0) = X_i^0$$

Jeffery equation for the fiber orientation :

$$\frac{dp_i}{dt} = W \cdot p_i + \lambda [D \cdot p_i - D : (p_i \otimes p_i) \cdot p_i], \qquad p_i(0) = p_i^0$$

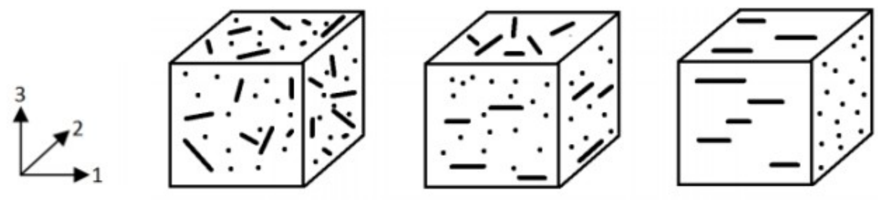
p = Orientation vector, W = Spin tensor, D = Strain rate tensor, λ= Shape parameter

Orientation Tensors

The 2nd and 4th order orientation tensors :

$$A(x,t)=\langle nn\rangle=\int_S (p\otimes p)\psi(p,x,t)dp$$

$$\mathbb{A}(x,t)=\langle nnnn\rangle=\int_S (p\otimes p\otimes p\otimes p)\psi(p,x,t)dp$$



$$a_{ij}=\begin{pmatrix}\frac{1}{3} & 0 & 0\\ 0 & \frac{1}{3} & 0\\ 0 & 0 & \frac{1}{3}\end{pmatrix}\qquad a_{ij}=\begin{pmatrix}\frac{1}{2} & 0 & 0\\ 0 & \frac{1}{2} & 0\\ 0 & 0 & 0\end{pmatrix}\qquad a_{ij}=\begin{pmatrix}1 & 0 & 0\\ 0 & 0 & 0\\ 0 & 0 & 0\end{pmatrix}$$

a) 3D random b) Planar random c) Aligned

Example of different orientation states and corresponding orientation tensors [1]

Where ψ(p,x,t) denote the probability of finding a fiber parallel to the orientation vector *p*.

Fokker-Planck equation :

$$\frac{\partial\psi}{dt}+u\cdot\nabla_x\psi+\frac{1}{2}\nabla_p\cdot(\dot{p}\psi)=\Delta_p(D_r\psi),$$

[1] Lukáš LIKAVČAN et al. 2014

Orientation Tensors

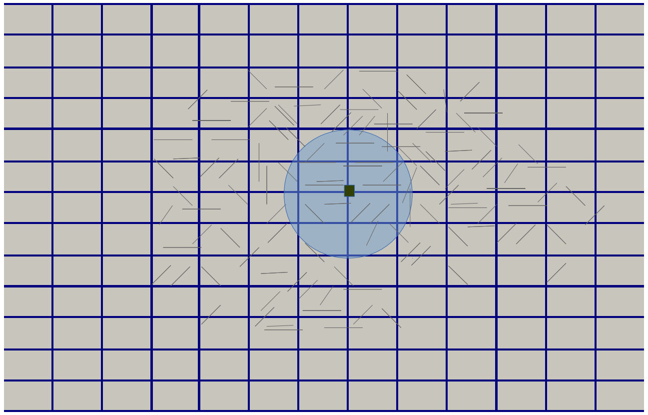
In an Eulerian framework :

$$\frac{\partial A}{dt}+u\cdot\nabla A=(A\cdot W-W\cdot A)+\lambda(A\cdot D+D\cdot\mathbb{A}-2A:D)$$

In a Lagrangian framework :

$$A_{ij}=\frac{1}{N_f}\sum_{i=1}^{N_f}p_i p_j$$

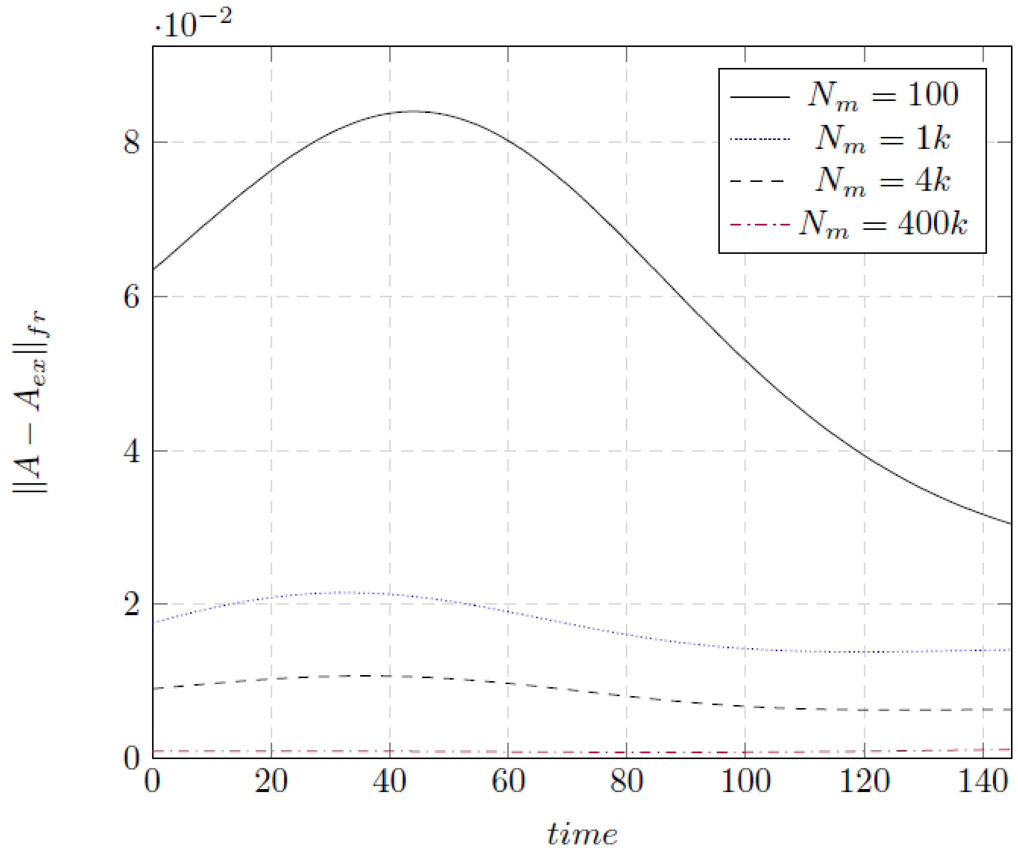
$$\mathbb{A}_{ijkl}=\frac{1}{N_f}\sum_{i=1}^{N_f}p_i p_j p_k p_l$$



Influence of the number of fibers

The velocity gradient for the planar elongation is defined by :

$$\nabla u = \begin{pmatrix} g & 0 \\ 0 & -g \end{pmatrix}$$



Comparison between the frameworks

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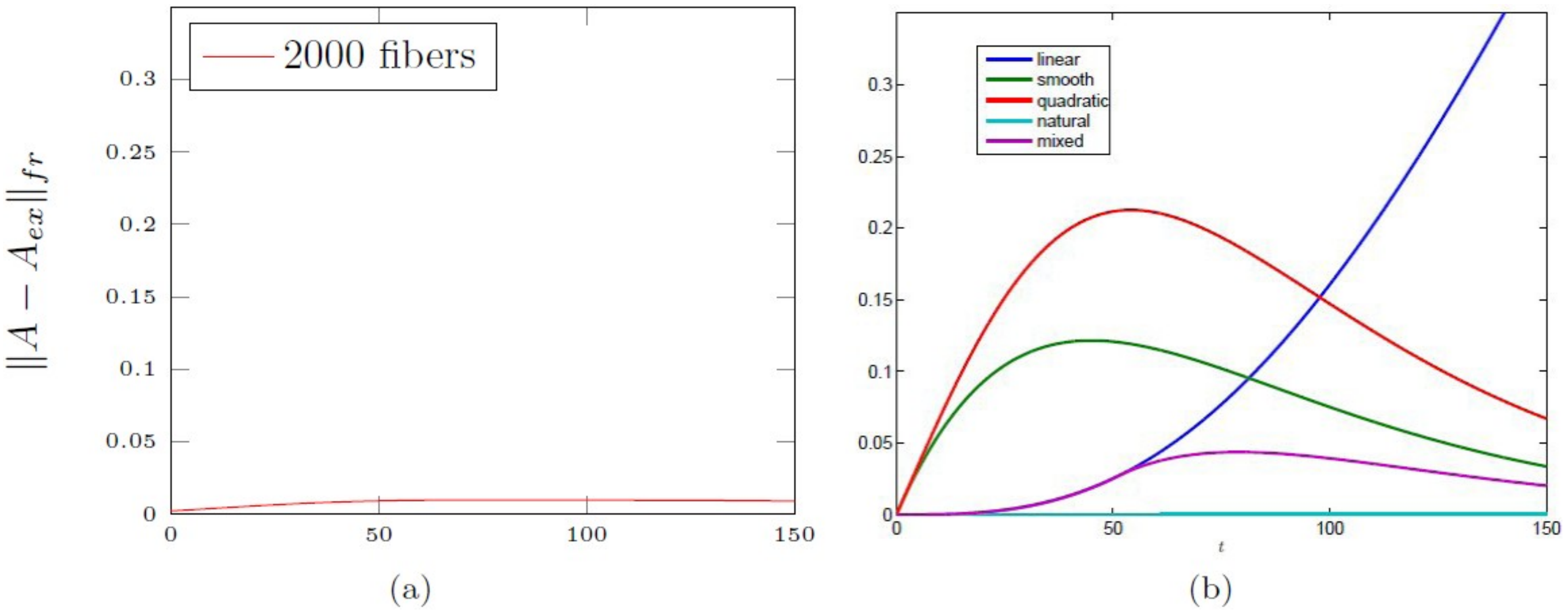
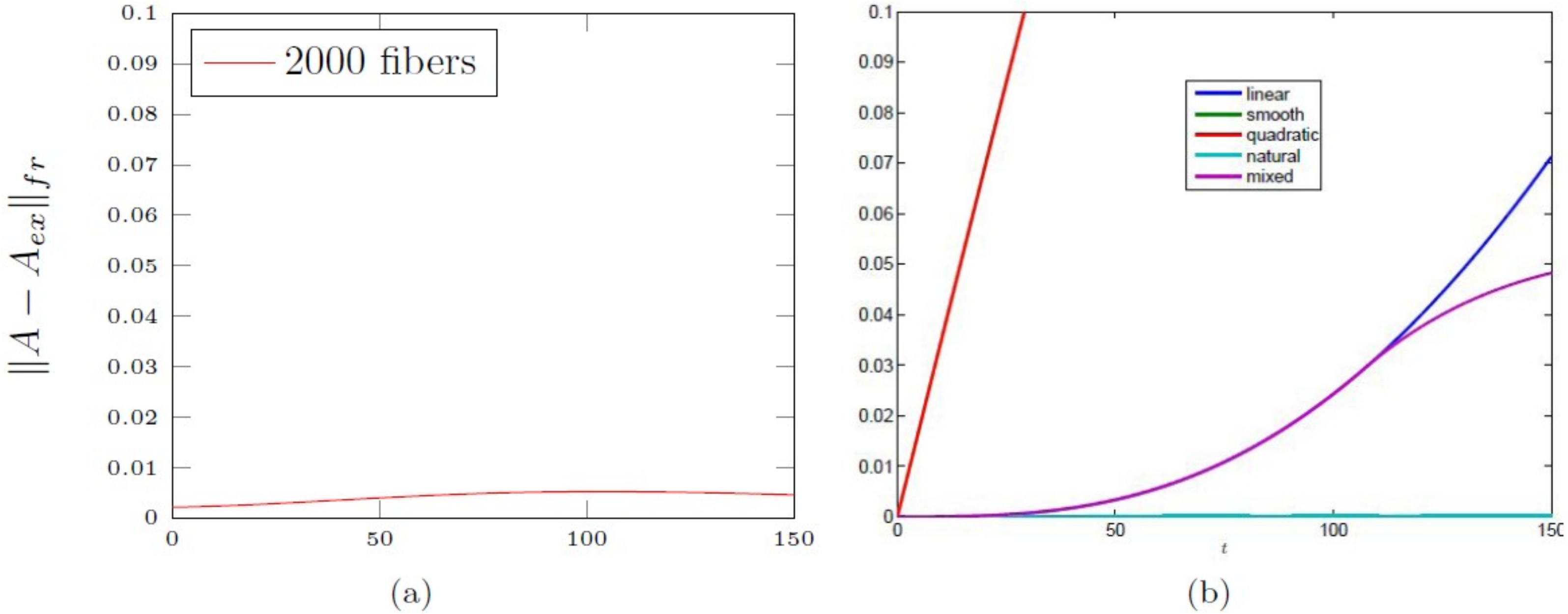


Comparison between a) Lagrangian simulation and (b) Eulerian approaches *[1]*

Comparison between the frameworks

The velocity gradient for the shear flow is defined by :

$$\nabla u = \begin{pmatrix} 0 & g \\ 0 & 0 \end{pmatrix}$$



Comparison between a) Lagrangian simulation and (b) Eulerian approaches *[1]*

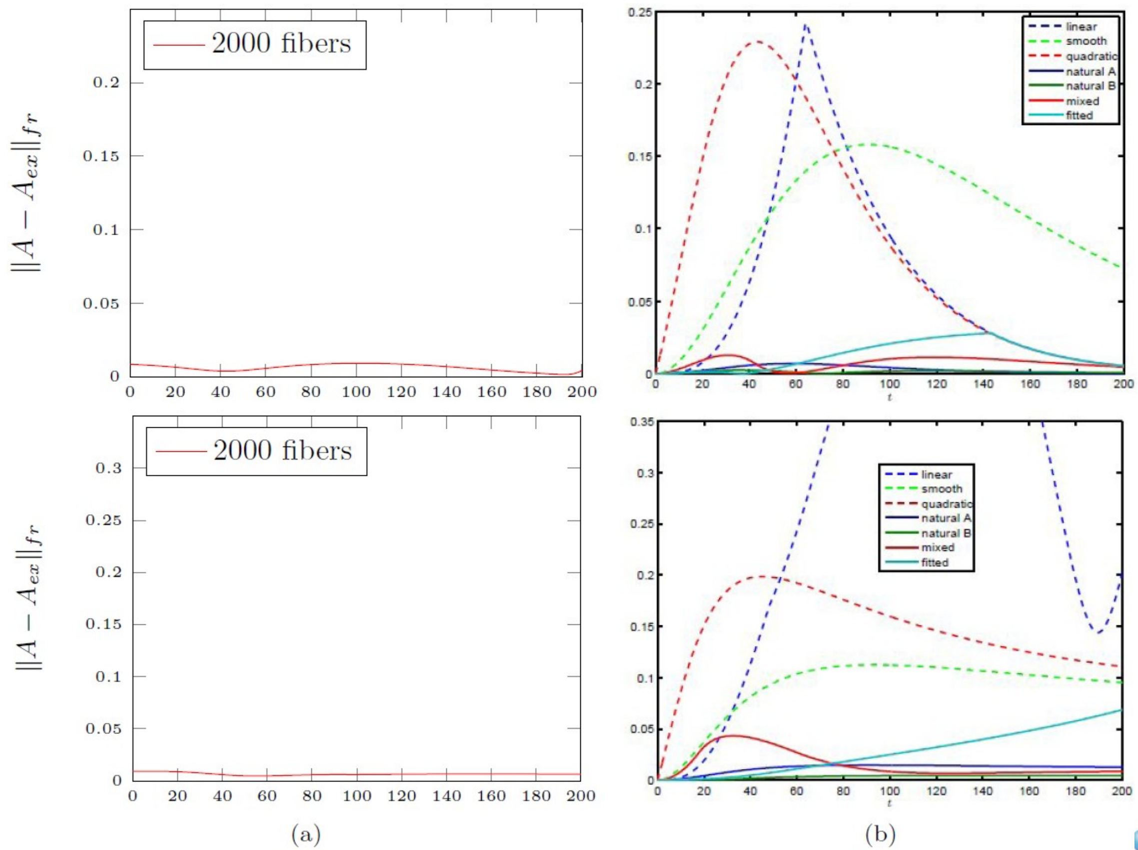
Comparison between the frameworks

3D uniaxial elongation flow :

$$\nabla u = \begin{pmatrix} 0.02 & 0.0 & 0.0 \\ 0.0 & -0.01 & 0.0 \\ 0.0 & 0.0 & -0.01 \end{pmatrix}$$

3D shear flow :

$$\nabla u = \begin{pmatrix} 0.0 & 0.05 & 0.0 \\ 0.0 & 0.00 & 0.0 \\ 0.0 & 0.0 & 0.0 \end{pmatrix}$$



Comparison between a) Lagrangian simulation and (b) Eulerian approaches *[1]*

Fiber-fiber interactions

Fokker-Planck equation :

$$\frac{\mathrm{d}\psi}{\mathrm{d}t} + \nabla_{\mathrm{p}} \cdot (\dot{\mathbf{p}}\psi) = D_r \Delta_{\mathrm{p}} \psi$$

An additional diffusion-like term to take the fiber-fiber interactions into account :

$$q = D_r \frac{1}{\psi} \nabla_p \psi,$$

where *Dr* is a rotary diffusion coefficient.

After solving the Jeffery equation :

$$p_i^n = p_i^n + D_r \frac{1}{\psi} \nabla_p \psi$$

Fiber-fiber interactions

Wiener process (random walk) - Cartesian Approach

$$p_i^n = p_i^n + d_i\sqrt{\Delta t}\zeta,$$

d = diffusion coefficient, ζ = a random number uniformely distributed between [-a,a]

Analytical solution of the diffusion equation :

$$A(x,t) = \prod_{i=1,2,3} \frac{1}{2\sqrt{Dt\pi}} e^{\frac{-x_i^2}{4Dt}}$$

The variance (strength, width or mean square displacement) of this function :

$$\sigma^2 = 2Dt$$

Fiber-fiber interactions

Central limit theorem : The sum of infinitely many random numbers tends toward a normal Gaussian distribution.

The variance of the random walk using the Central Limit Theorem :

$$\sigma^2 = \frac{td^2}{12}$$

The random number is uniformly distributed between [-0.5,0.5]

```
% a = 1d array
% n = a large number of fibers
% rand = a random number uniformly distributed in [0,1]
for i=1 : n
  a(i) = (rand-0.5)
end
mean(a) % mean of the perturbations ≃ 0
var(a) % variance of the perturbations ≃ 1/12
```

The diffusion coefficient : $d = \sqrt{24D},$

Random walk : $p_i^n = p_i^n + \sqrt{12}\sqrt{2D\Delta t}\zeta,$

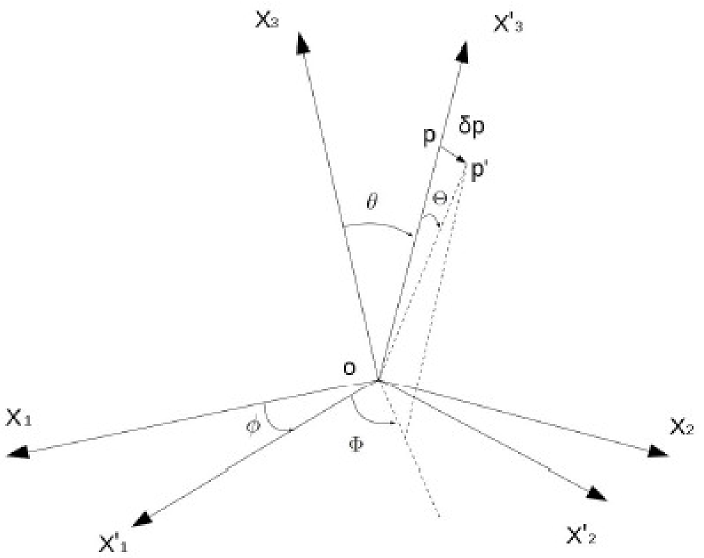
Fiber-fiber interactions

Laplacian equation in the spherical coordinates :

$$\Delta = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial f}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial f}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2 f}{\partial\phi^2}$$

Considering a second coordinate system : $\{X_1', X_2', X_3'\}$

$$\Delta_p = \frac{1}{\sin\Theta}\frac{\partial}{\partial\Theta}\left(\sin\Theta\frac{\partial f}{\partial\Theta}\right) + \frac{1}{\sin^2\Theta}\frac{\partial^2 f}{\partial\Phi^2}.$$



Corresponding diffusion equation :

$$\frac{\partial f}{\partial t} = \frac{D_r}{\sin\Theta}\frac{\partial}{\partial\Theta}\left(\sin\Theta\frac{\partial f}{\partial\Theta}\right)$$

Fiber-fiber interactions

Quadratic angular displacement (variance) :

$$< \theta^2 >= \sigma^2 = 4D\Delta t, \text{ for } D\Delta t \ll 1$$

The small angular movement :

$$\Theta = \sqrt{12}\sqrt{4D\Delta t}\zeta.$$

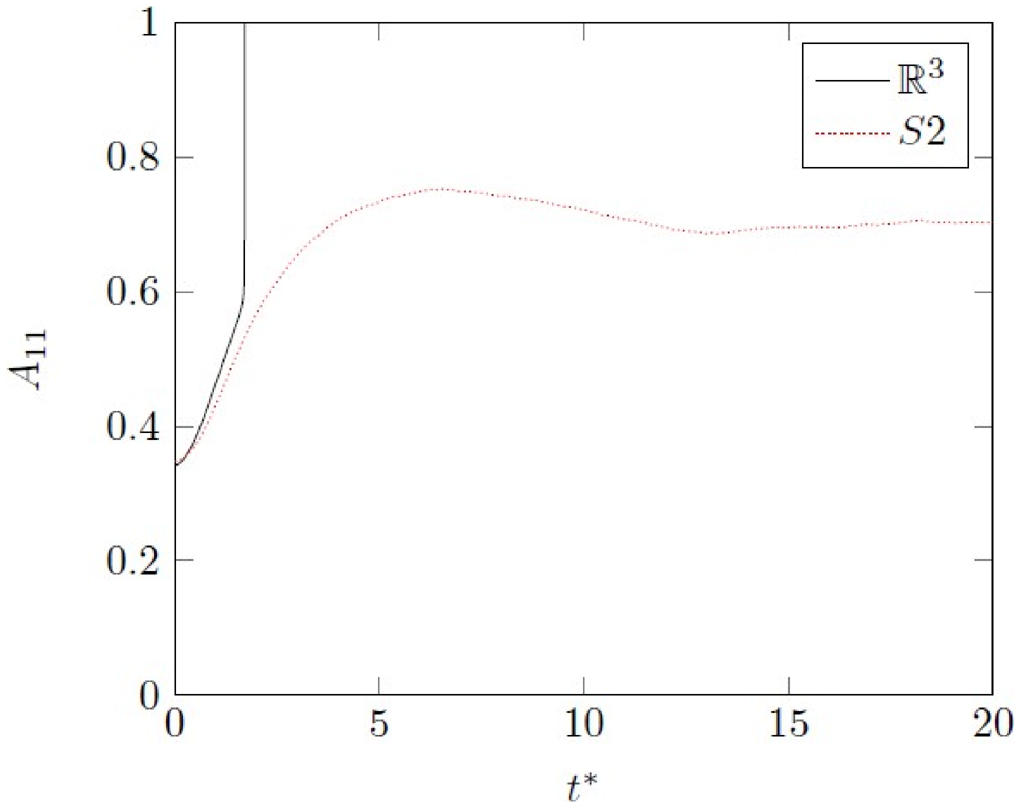
Since the perturbation can happen in any azimuth angle :

$$\Phi = 2\pi(\zeta + 0.5),$$

The coordinate transformation for finding the perturbations to be added to Jeffery equation :

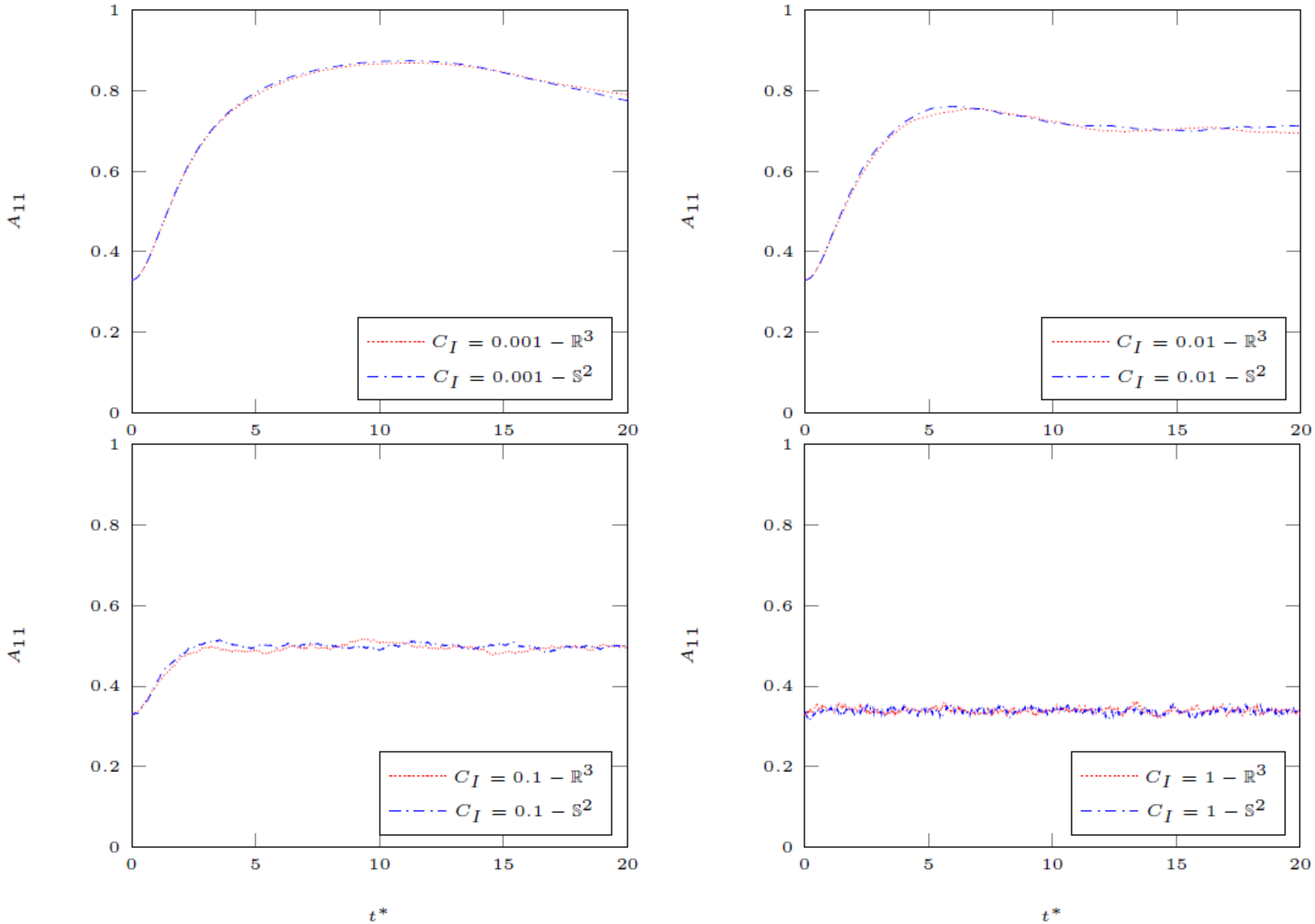
$$\begin{bmatrix} \delta p_1 \\ \delta p_2 \\ \delta p_3 \end{bmatrix} = \begin{bmatrix} \sin\phi & \cos\theta\cos\phi & \sin\theta\cos\phi \\ -\cos\phi & \cos\theta\sin\phi & \sin\theta\sin\phi \\ 0 & -\sin\theta & \cos\theta \end{bmatrix} \times \begin{bmatrix} \sin\Theta\cos\Phi \\ \sin\Theta\sin\Phi \\ \cos\Theta \end{bmatrix} - \begin{bmatrix} \sin\theta\cos\phi \\ \sin\theta\sin\phi \\ \cos\theta \end{bmatrix}.$$

Fiber-fiber interactions



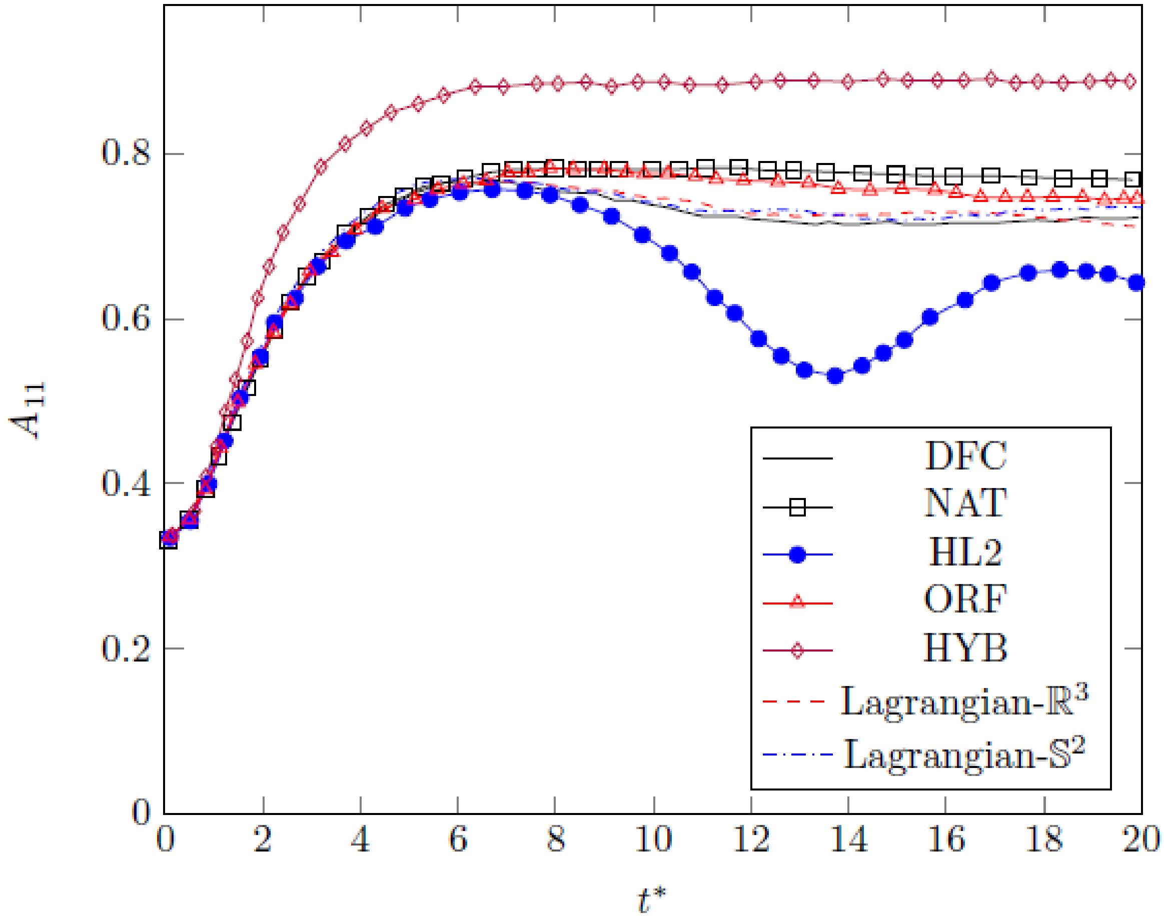
Comparison between the two stochastic approaches without normalization(C_I = 0.01).

Fiber-fiber interactions



Comparison between the two stochastic approaches with different interaction coefficients

Fiber-fiber interactions



Comparison between the Eulerian approaches and the Lagrangian simulations with 2000 fibers. DFC is the reference solution *[1]*

[1] Cintra & Tucker : Orthotropic closure approximations for flow induced fiber orientation , 1995

Two-way coupling

The momentum equation for the flow of a non-Newtonian fluid :

$$\rho \frac{\mathrm{D}\mathbf{U}}{\mathrm{D}t} = -\nabla p + \nabla \cdot \left(\tau^{\mathrm{N}} + \tau^{\mathrm{NN}} \right)$$

A simple model to compute the non-Newtonian stress (<nnnn> is the 4th order orientation tensor) :

$$\tau^{\mathrm{NN}} = 2\mu N_P \mathbf{D} : \langle \mathbf{nnnn} \rangle_{\Psi},$$

Brenner's theory :

$$\begin{aligned}\tau^{\mathrm{NN}} = {} & 2\mu_0 \mathbf{D} + \mu_1 \mathbf{1}(\mathbf{D} : \langle \mathbf{nn} \rangle_{\Psi}) + \mu_2 \mathbf{D} : \langle \mathbf{nnnn} \rangle_{\Psi} \\ & + 2\mu_3(\langle \mathbf{nn} \rangle_{\Psi} \cdot \mathbf{D} + \mathbf{D} \cdot \langle \mathbf{nn} \rangle_{\Psi}) \\ & + 2\mu_4 D_r (3\langle \mathbf{nn} \rangle_{\Psi} - \mathbf{1}),\end{aligned}$$

Two-way coupling

Brenner's theory :

$$\tau^{\mathrm{NN}} = 2\mu_0\mathbf{D} + \mu_1\mathbf{1}\left(\mathbf{D} : \langle\mathbf{nn}\rangle_\Psi\right) + \mu_2\mathbf{D} : \langle\mathbf{nnnn}\rangle_\Psi$$
$$+ 2\mu_3\left(\langle\mathbf{nn}\rangle_\Psi \cdot \mathbf{D} + \mathbf{D}\cdot \langle\mathbf{nn}\rangle_\Psi\right) + 2\mu_4 D_r\left(3\langle\mathbf{nn}\rangle_\Psi - \mathbf{1}\right),$$

Having isotropic orientation tensor :

$$\langle\mathbf{nn}\rangle_\Psi = \frac{1}{3}\mathbf{1} = \begin{pmatrix} \frac{1}{3} & 0 & 0 \\ 0 & \frac{1}{3} & 0 \\ 0 & 0 & \frac{1}{3} \end{pmatrix}$$

Analytical solution for the non-Newtonian stress :

$$\begin{aligned} \tau &= \tau^{\mathrm{N}} + \tau^{\mathrm{NN}}_{\mathrm{isotropic}} \\ &= 2\left(\mu + \mu_0 + \frac{1}{15}\mu_2 + \frac{2}{3}\mu_3 + \frac{1}{5}\mu_4\right)\mathbf{D} \\ &= 2\mu_{\mathrm{eff}}\mathbf{D}. \end{aligned}$$

By setting r=150, and volume fraction of 1 % :

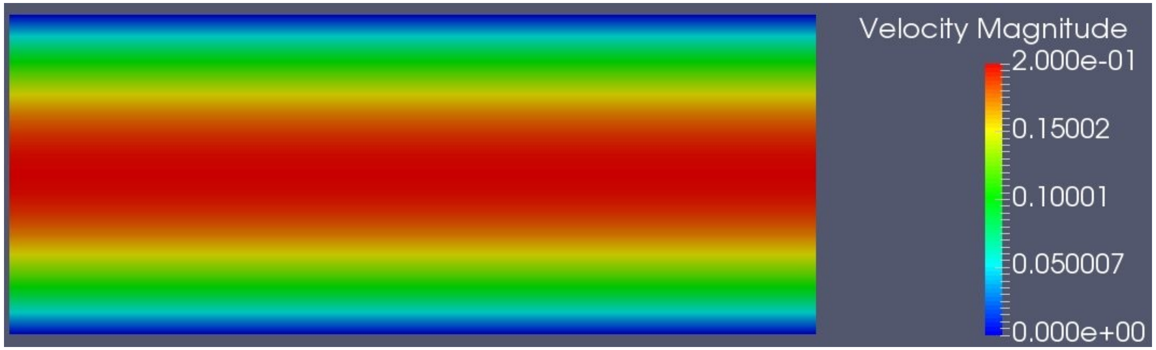
$$\mu_{\mathrm{eff}}/\mu = 4.584$$

Two-way coupling – Channel flow

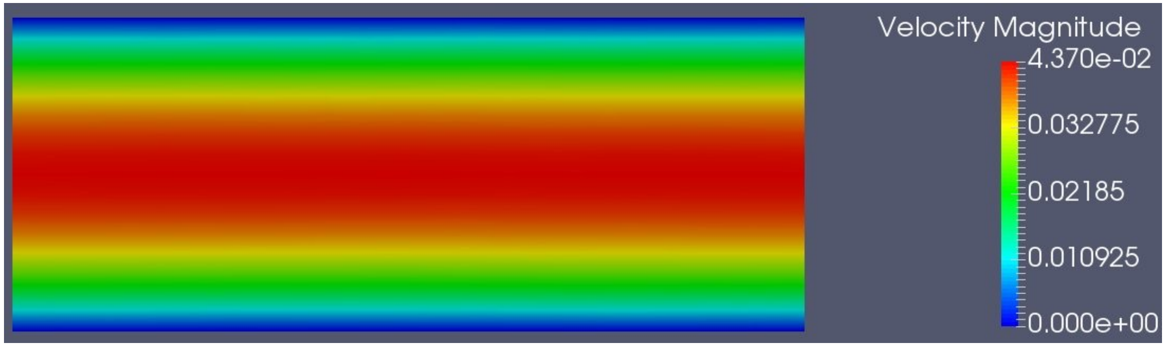
Analytical solution for channel flow :

$$\langle U\rangle(z) = -\frac{1}{\mu_{\text{eff}}}\frac{\mathrm{d}\langle p\rangle}{\mathrm{d}x}hz\left(1-\frac{z}{2h}\right).$$

$$U_c = \langle U\rangle(z=h) = -\frac{1}{2\mu_{\text{eff}}}\frac{\mathrm{d}\langle p\rangle}{\mathrm{d}x}h^2.$$



Without Fiber

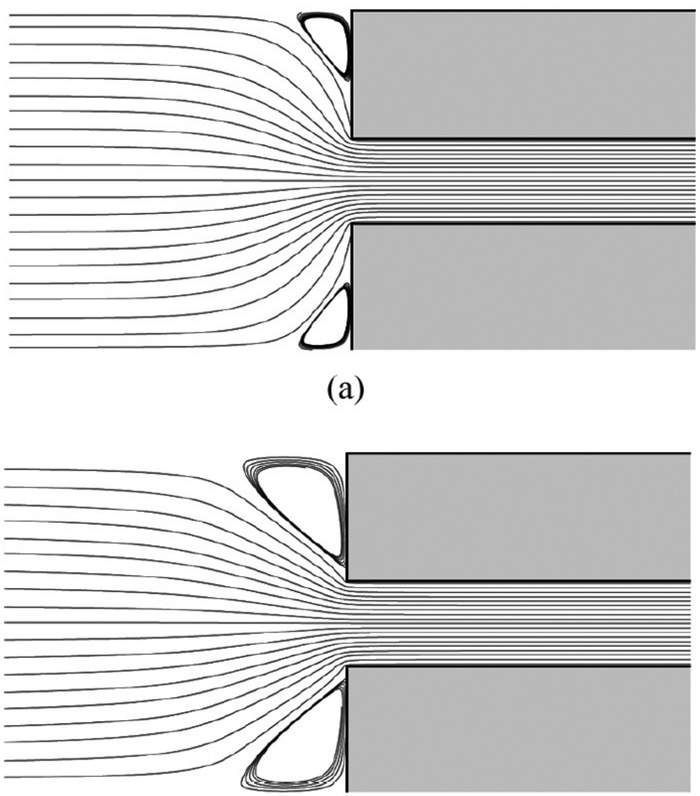


With Fiber

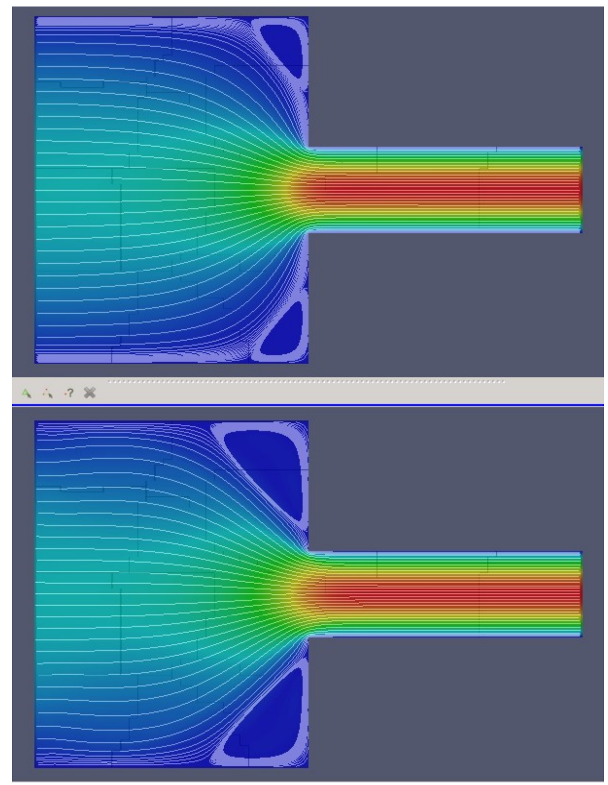
Relative error : 0.15 %

Two-way coupling – 4:1 contraction

Stress model for fibers : $\tau^{\mathrm{NN}} = 2\mu N_P \mathbf{D} : \langle \mathbf{nnnn} \rangle_{\Psi},$



Results of Manhart [1]



Without Fiber

With Fiber-1%

next steps

- **Validation of 3D Axisymmetric contraction with experimental data.**
- **Combining the Eulerian and the Lagrangian approach ?!**
- **More complex geometries, polymer flows, etc.**

THANKS FOR YOUR ATTENTION