DNS of polydisperse suspensions of spherical and cylindrical particles:

Application to rheology of complex fluids.

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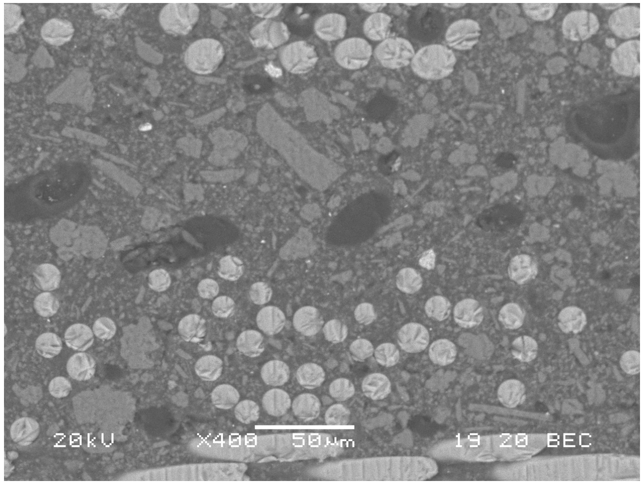
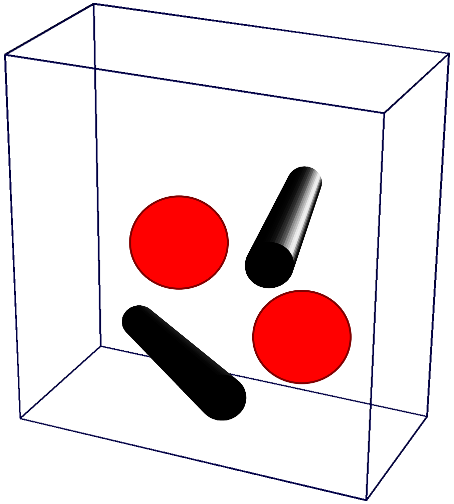
Determination of macroscopic parameters of complex fluids by numerical homogenization

- **Industrial application:** injection of BMC





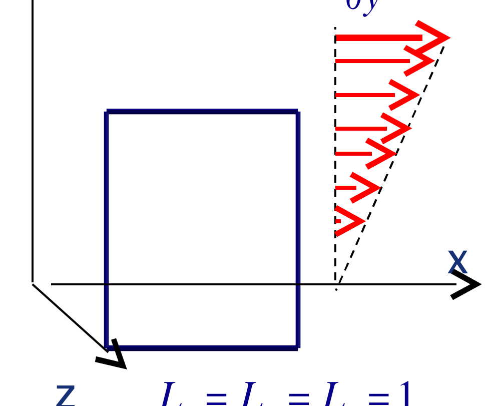
- Fluid chosen: newtonian fluid charged with solid particles (fibers + spheres)

Numerical homogenization in a REV :

Mesoscopic scale
particle level

- **shear** fixed
- numerical simulations of fluid-particles flows

$$\frac{\partial v_x}{\partial y} = \langle \dot{\gamma} \rangle = cte$$



$$L_x = L_y = L_z = 1$$

→

Macroscopic scale
mold size

- "volumic" average of various values
- **Macroscopic parameters**

  average viscosity
  average orientation

Mumerical Method:

- **Multi-domain approach:** (Fictitious domain method **[Glowinski *et al.* 1999]**)

Fluid domain: → **characteristic function** I_{Ω_f}

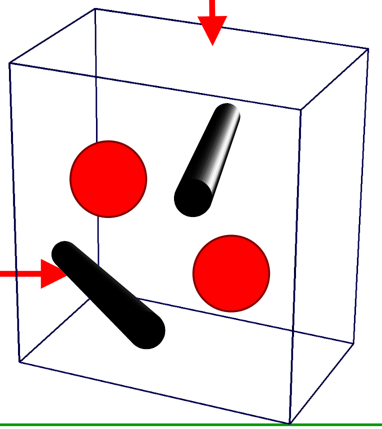
$$\nabla . \underline{\underline{\sigma}} = 0$$ **(Navier) Stokes for injection process**

$$\underline{\underline{\sigma}} = -p \underline{\underline{I_d}} + 2\eta_f \underline{\underline{\dot{\varepsilon}}}(u)$$ **Newtonian behavior**

$$\nabla . u = 0$$ **incompressibility**

Solid domain: **particules 1,…N** → I_{Ω_s}

$\underline{\underline{\dot{\varepsilon}}}(u) = 0$ **and** $\nabla . u = 0$



•New Formulation in Solid Domain

$$\rho_s \left[\frac{\partial \vec{u}}{\partial t} + \vec{u} \, . \, \nabla \vec{u} \right] = \rho_s \, \vec{g} + \nabla \, . \, \underline{\underline{\sigma}}$$

$$\nabla \, . \, \vec{u} = 0$$

$$\underline{\underline{\dot{\epsilon}}}(\vec{u}) = 0$$

Rigid motion

$$[[\vec{u}]]_{\partial \Omega_s} = 0$$

$$[[\underline{\underline{\sigma}}.\vec{n}]]_{\partial \Omega_s} = 0$$

Boundary conditions

Stress tensor

$$\underline{\underline{\sigma}} = \eta_s \underline{\underline{\dot{\epsilon}}}(\vec{u}) - p\mathbb{I} + \underline{\underline{\lambda}}$$

Penalization factor

Lagrangian multiplier

Numerical procedure :

- Computation of velocity field

  finite element method for the Stokes with P1+/P1 element and multi-domain approach

  (no inertia, no gravity)

- Update particle position

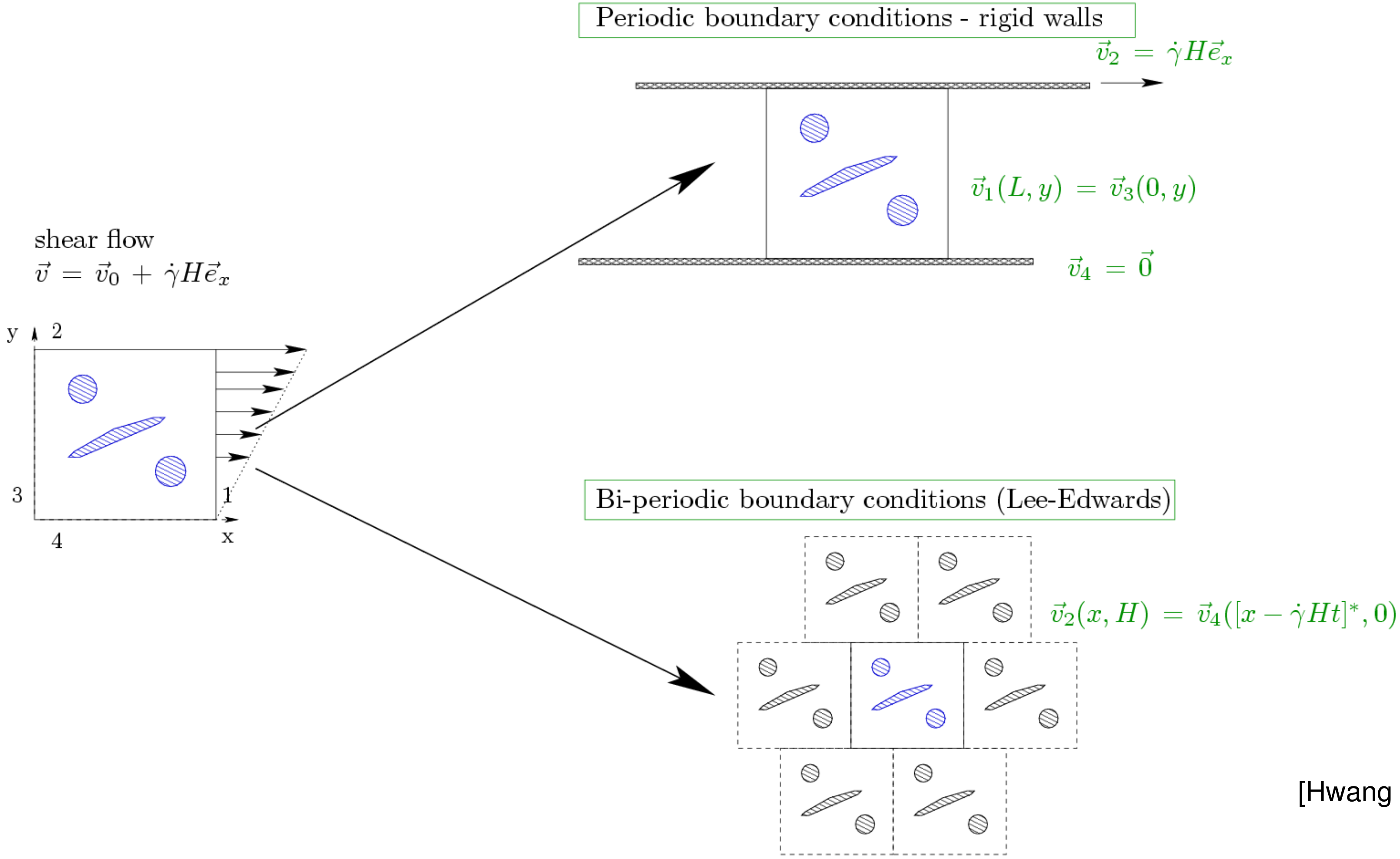
  Particle method

- Computation of characteristic functions I_{Ω_s}

  level set method

Simulations are made with $\gamma = 1$ and $\eta_f = 1$

How to impose periodic boundary conditions and mean shear rate ?

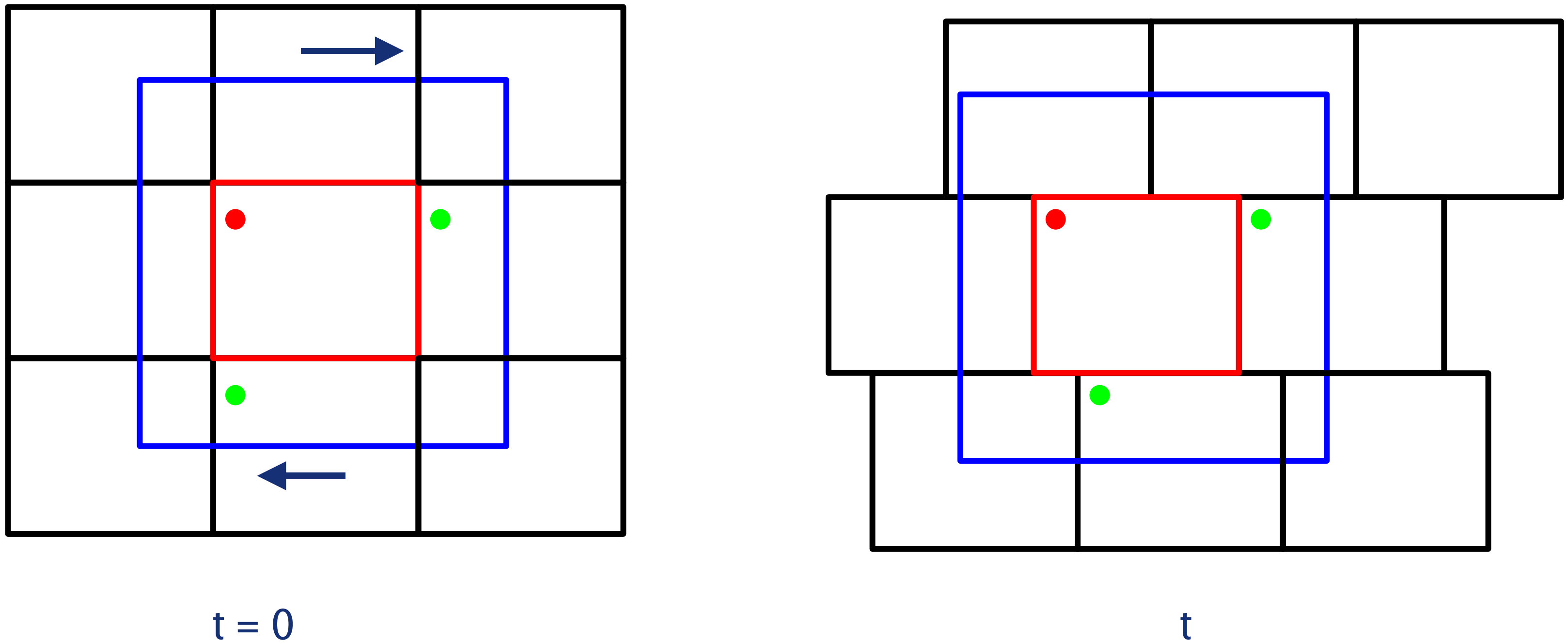


[Hwang 2004]

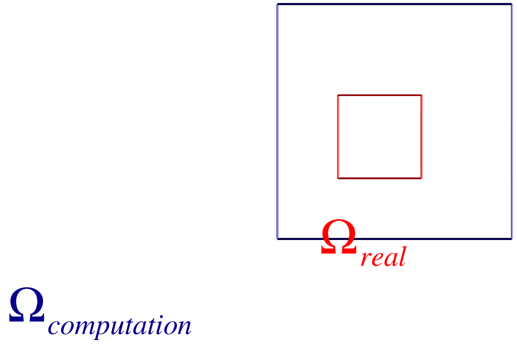
- Bi-periodic boundary conditions:

- Lagrangian multiplier [Hwang *et al.* 2004]
  (in 3D -> large linear system and difficulties with the parallelization)

- Pseudo-periodicity: velocity imposed on horizontal boundaries of Ω computation

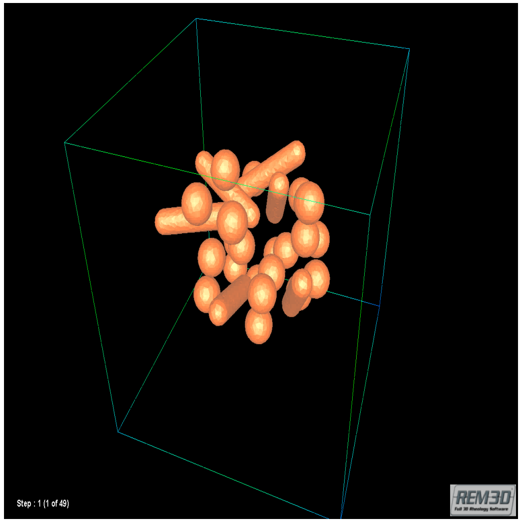


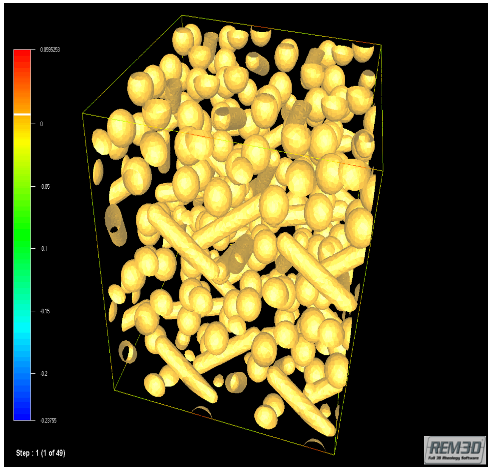
Example of pseudo –periodicity:



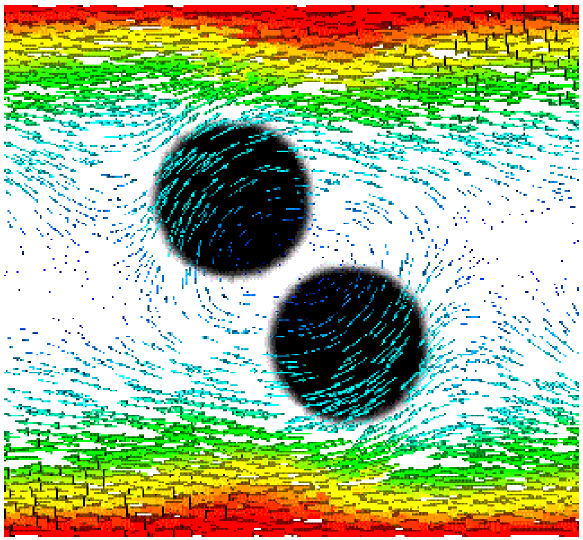
Studied suspension

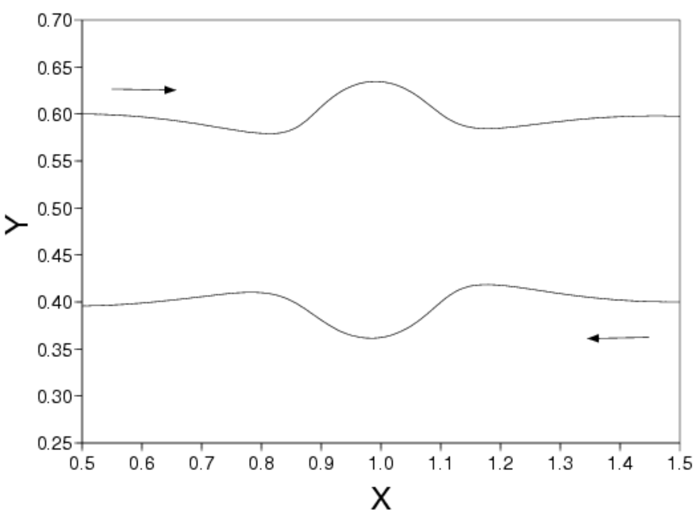
Added particles



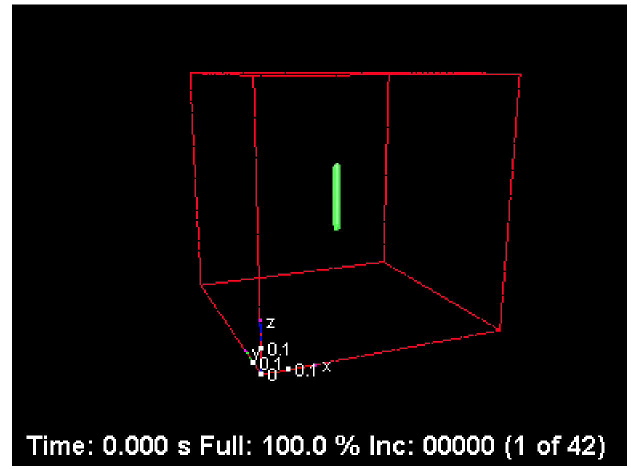


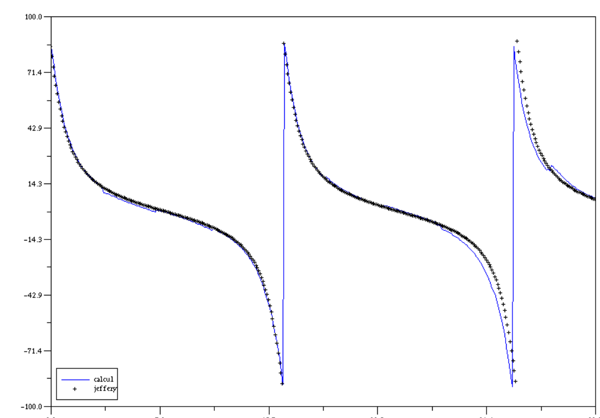
Simple computations: elementary square/cube domains





Rotation period for one fiber:





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

Effective viscosity

- **Homogenization :** $\langle \underline{\underline{\sigma}} \rangle_\Omega = \langle \underline{\underline{\sigma_f}} \rangle_\Omega + \langle \underline{\underline{\sigma_s}} \rangle_\Omega$

- **Stress tensor :**

$$\langle \underline{\underline{\sigma^s}} \rangle_\Omega = -\langle p \rangle_{\Omega_s} \underline{\underline{I}} + \langle \lambda \rangle_{\Omega_s}$$

$$\langle \underline{\underline{\sigma}}_{xy} \rangle_\Omega = 2\eta_f \langle \underline{\underline{\dot{\epsilon}}}(\vec{u})_{xy} \rangle_{\Omega_f} + \langle \lambda \; xy \rangle_{\Omega_s}$$

- **Effective viscosity (γ fixed)**

$$\eta_{eff} = \frac{\langle \underline{\underline{\sigma}}_{xy} \rangle_\Omega}{\dot{\gamma}}$$

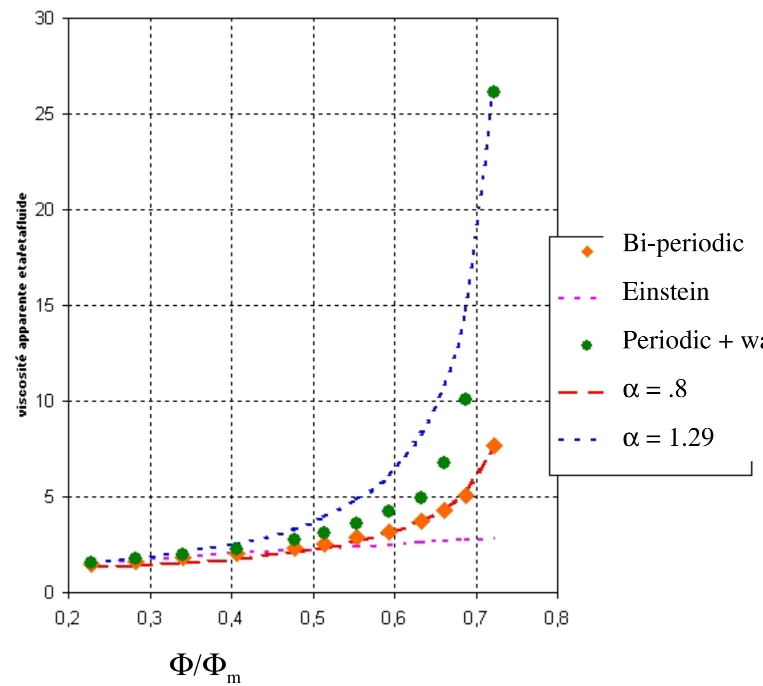
- **Theoretical model**

$$\eta_{eff}(\varphi) = \eta_f \left(1 - \frac{\varphi}{\varphi_m}\right)^{-\alpha}$$

α = 1.29

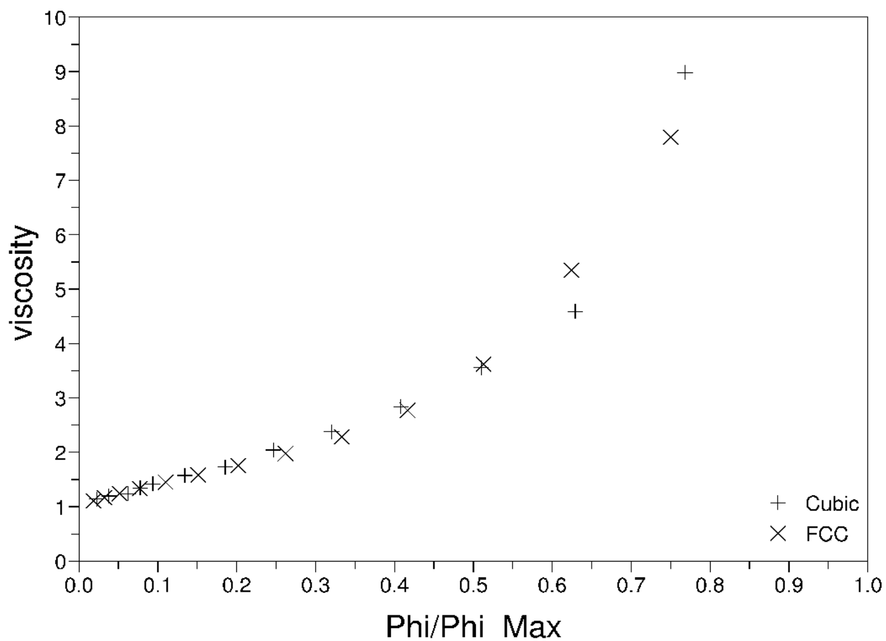
ϕ_m = maximal volume fraction

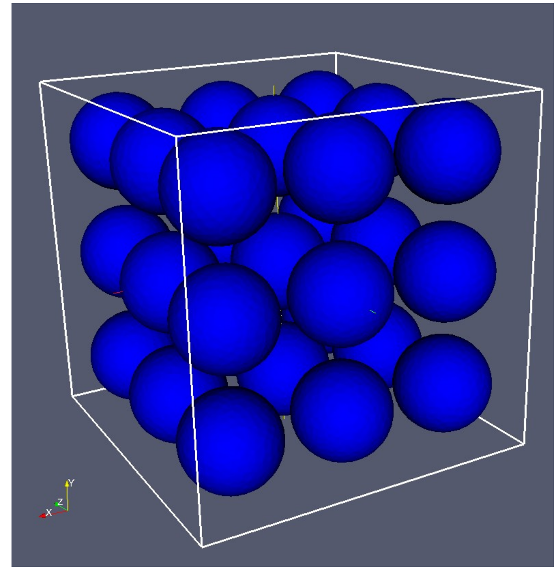
$\eta_{eff}\,(\Phi)$



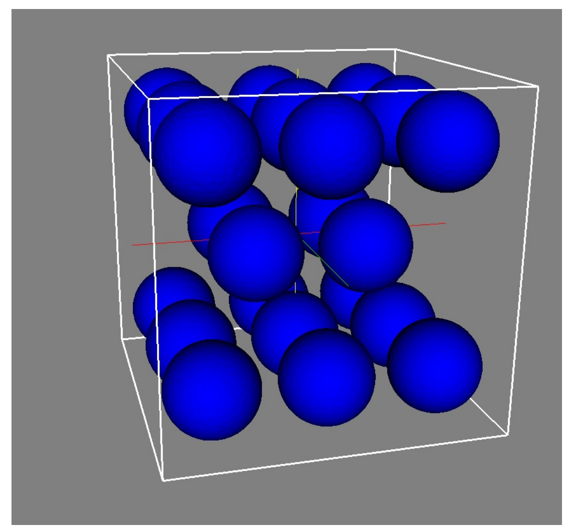
Wall influence

Effective viscosity (3D Spheres):





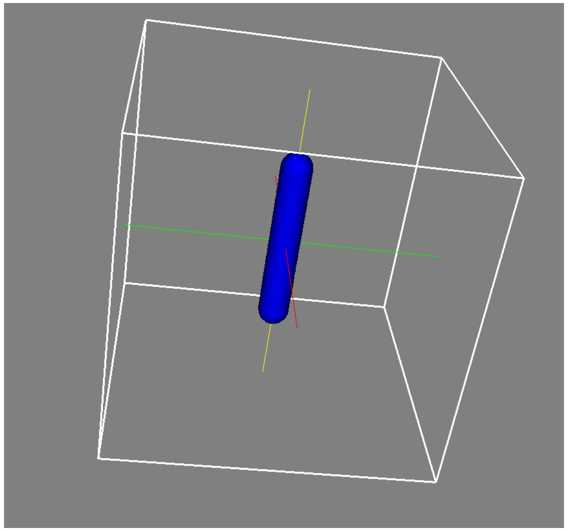
cubic lattice
27 spheres

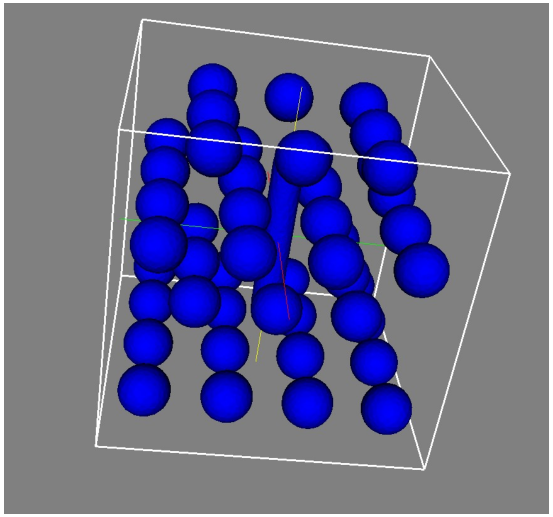


Face-centered
cubic lattice
(22 spheres)

Slight dependence with particle positions
for small concentration.

Effective viscosity (Spheres + fiber):





48 spheres + 1 fiber

$\Phi \sim \Phi_{spheres} = 12\ \%$

η_{eff} (spheres) = 1.80

η_{eff} (fiber) = 1.04

η_{eff} (spheres+fiber) = 2.17

Macroscopic relation ?
Replace η_f by η_{eff}(spheres) ?

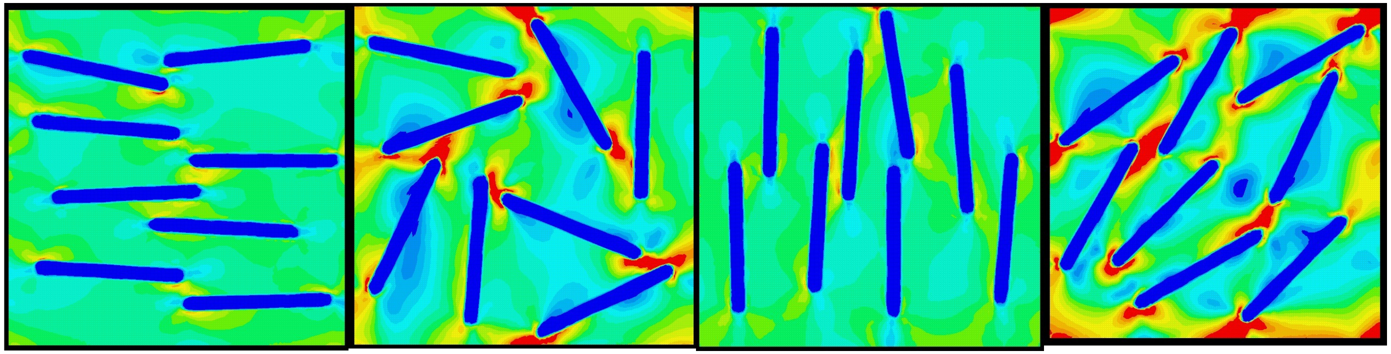
Fibers suspension (2D):

- Direct computation of fiber orientations:

$$\underline{\underline{a_2}} = \sum_{i \in V} p_i \otimes p_i$$

$$\underline{\underline{\underline{a_4}}} = \sum_{i \in V} p_i \otimes p_i \otimes p_i \otimes p_i$$

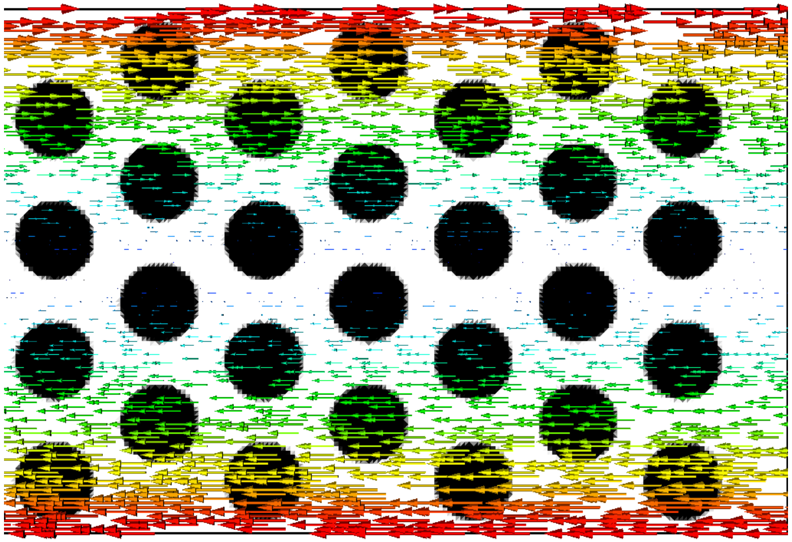
- Computations made for various orientations:



$$\langle \underline{\underline{\sigma}}_p \rangle = N_s \left[\langle \underline{\underline{\dot{\varepsilon}}} \rangle . \underline{\underline{a_2}} + \underline{\underline{a_2}} . \langle \underline{\underline{\dot{\varepsilon}}} \rangle \right] + N_p \left[\underline{\underline{\underline{a_4}}} : \langle \underline{\underline{\dot{\varepsilon}}} \rangle \right]$$

Ns = .4 ; Np = 5.0

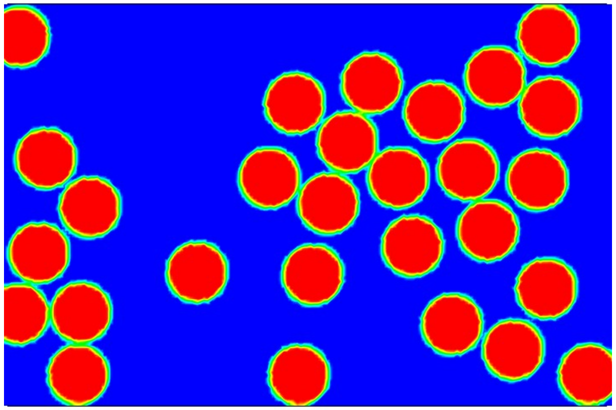
Dynamic viscosity with rigid horizontal wall

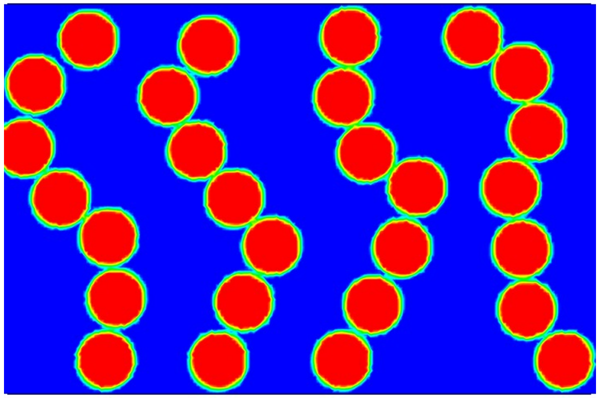


Shear induced diffusion

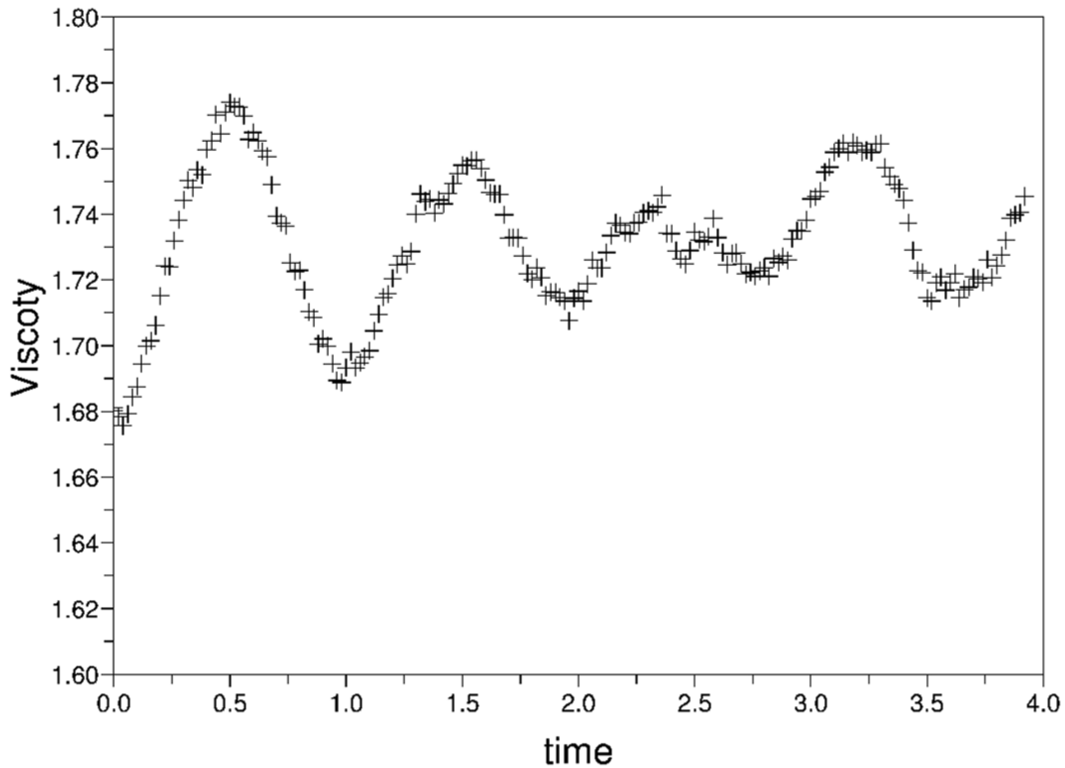
Formation of cluster and hole

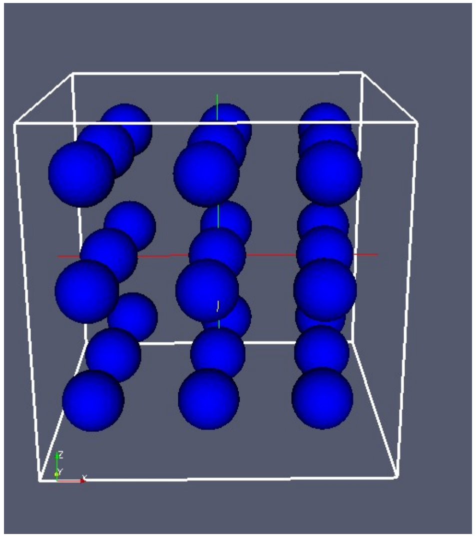
Blocking structure



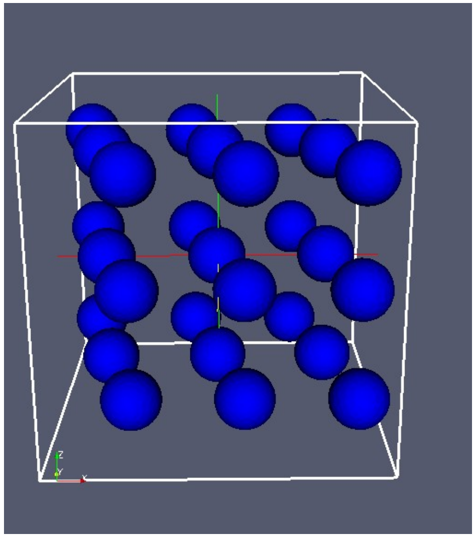


Pseudo bi-periodic conditions





Min

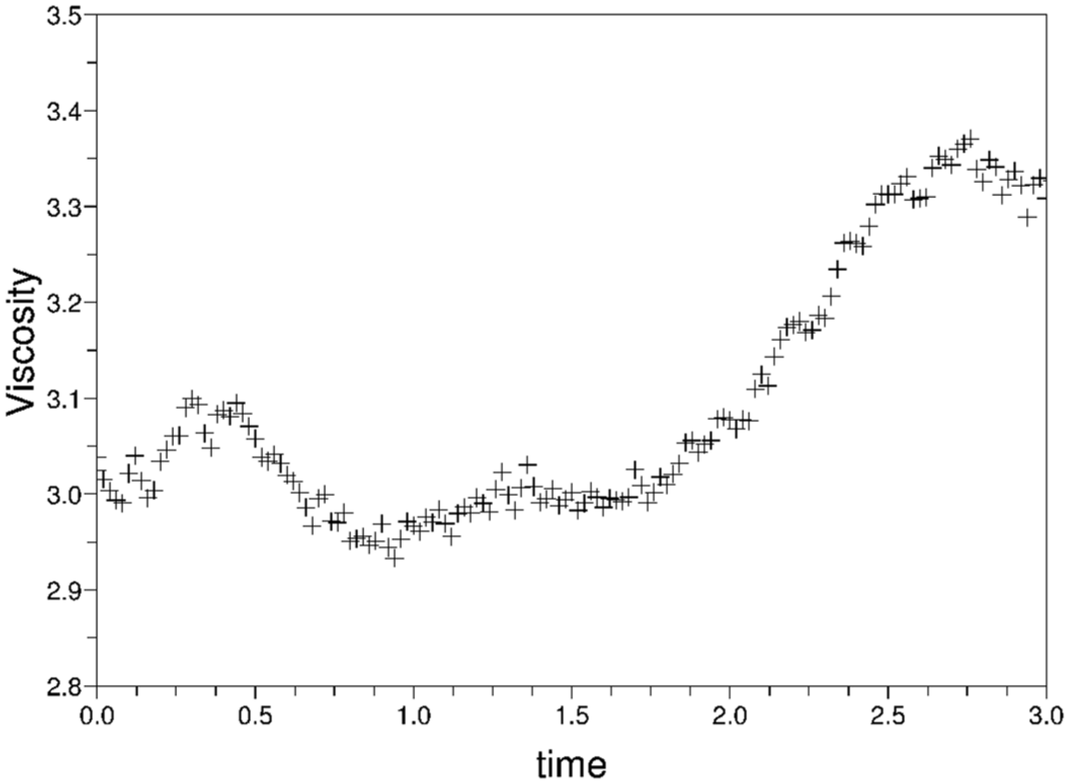


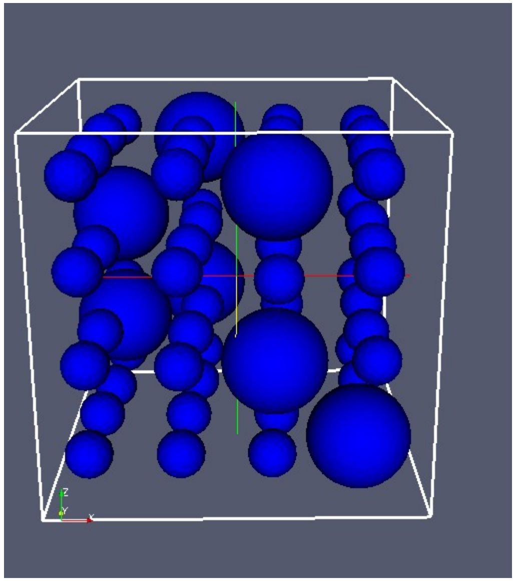
Max

Concentration = 11 %

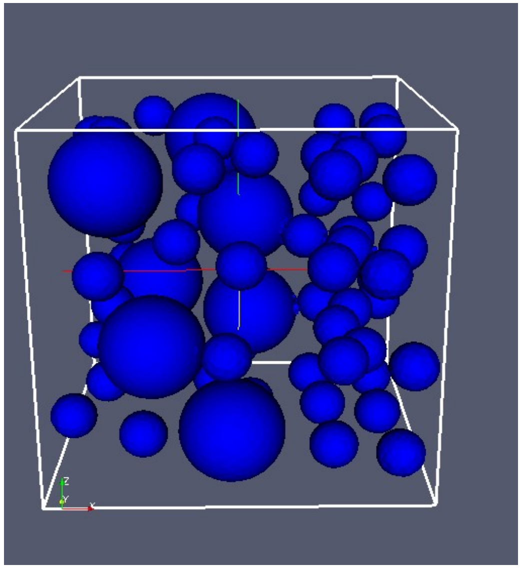
Relative error ~ 5% if $\eta_{eff} = < \eta_{eff} >_t$

Bi-disperse suspension





t = 0



t = 2.6

$\Phi = 20\ \%$; η_{eff} (nonodisperse)~ 2.3

$R_1/R_2 = 2$

Conclusions

- **We have developed an efficient numerical tools**
  - **Compute directly the motion of a dense population of polydisperse particles**
  - **Model the exact particle interactions by using a multi-domain approach**
- **Very encouraging results :**
  - **Study of the suspension's rheology : η_{eff}**
  - **Coupling effect between rheology and fiber orientation**
- **Next Step**
  - **Add h-adaptation for mesh to study higher concentration.**
  - **Introduce an equation which describes the evolution of $\Phi(x,t)$ (shear-induced diffusion process)**

■ Conclusion :

-Développement d’une méthode de simulation numérique à l’échelle microscopique – évolution d’un fluide chargé sphères/fibres

-Validation de la méthode sur des cas tests élémentaires (interaction hydrodynamique entre 2 sphères, viscosité effective)

■ Perspectives :

- efficacité numérique (parrallélisation, robustesse) pour des simulations longues en 3D

- Mélanges plus complexes (fibres/sphères), et migration de particules