A Fully-Resolved Immersed Boundary Numerical Method to Simulate Particle-Laden Viscoelastic Flows

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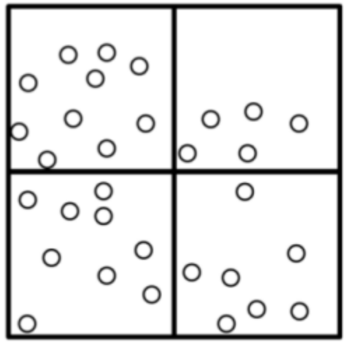
Motivation

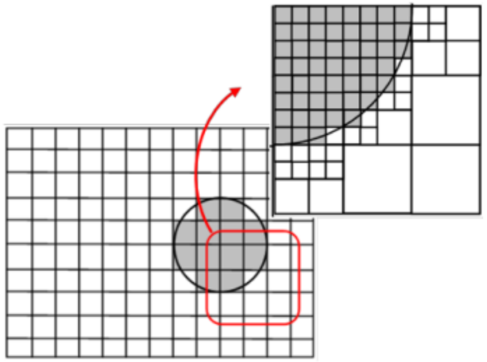
Hydraulic Fracturing + Polymer Composites

Fluid-particle interaction

CFDEM coupling **Computational Fluid Dynamics (CFD)** + **Discrete Element Method (DEM)** LIGGGHTS



- **unresolved CFD-DEM**
- **resolved CFD-DEM**



- CFD-DEM
- coarse grained CFD-DEM
- MP-PIC

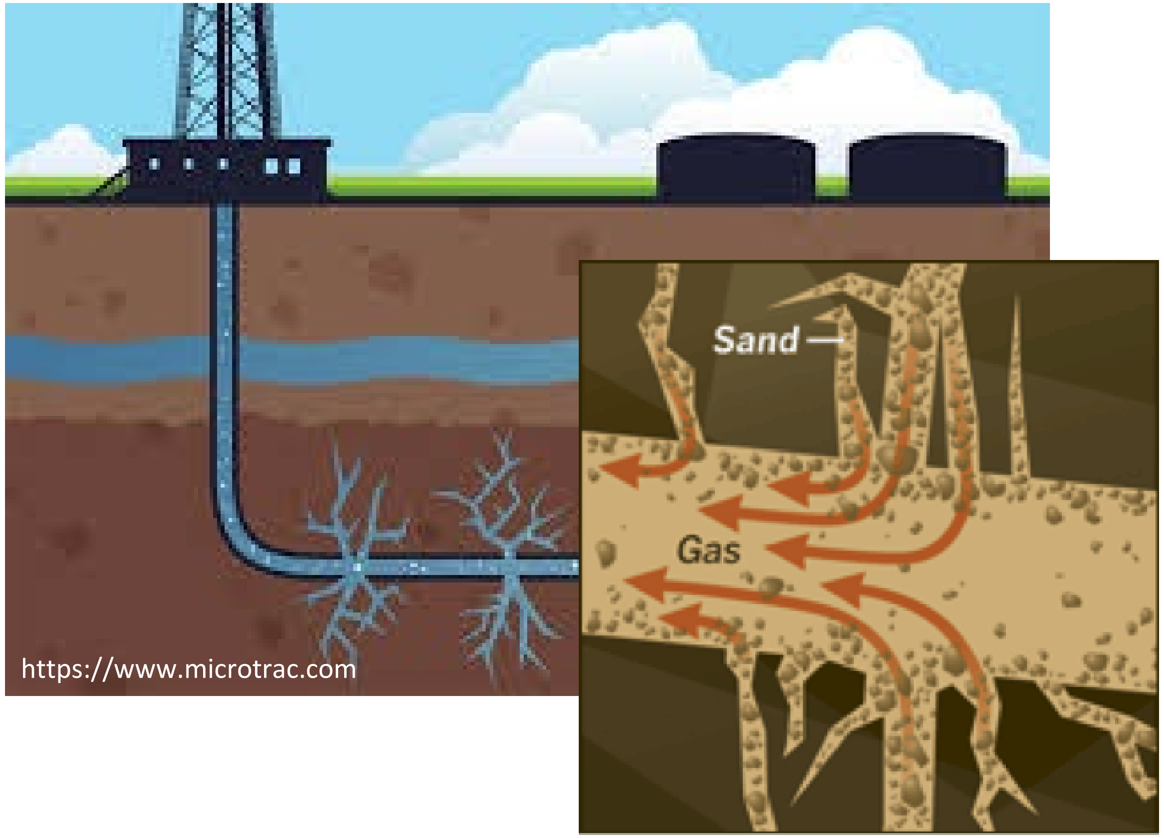
- Immersed Boundary Method
- Fictitious Domain Method

*Christoph Kloss, Christoph Goniva and Stefan Pirker (2013), LIGGGHTS and CFDEM coupling – Modelling of macroscopic particle processes based on LAMMPS technology, DEM6 Conference

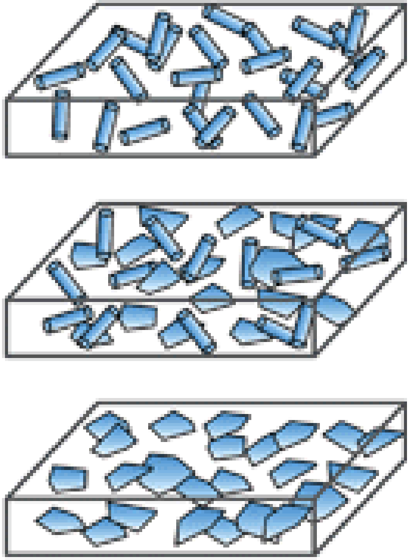
Motivation

Hydraulic Fracturing + Polymer Composites

Hydraulic Fracturing



Polymer Composites

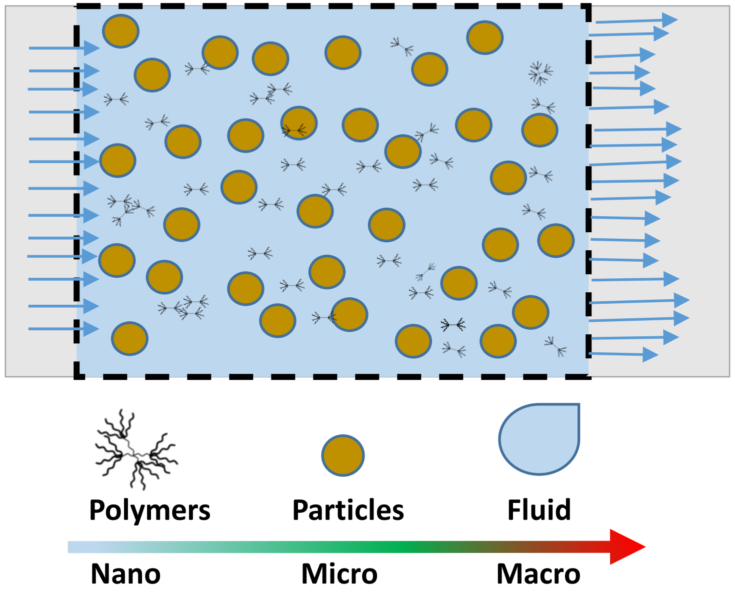


DOI: 10.1039/C4TC01998A

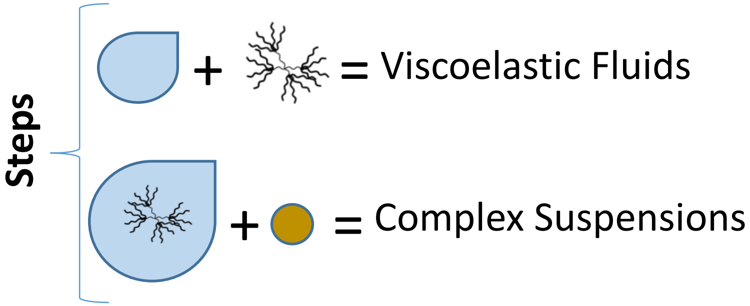
*Barbati, Alexander C., et al. (2016). *Annual review of chemical and biomolecular engineering*, 7:415–453

Numerical Approach

Eulerian-Lagrangian & Particle-based Model



Structural length scales

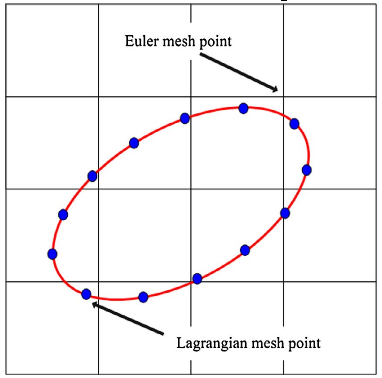


$$\rho\frac{D\boldsymbol{u}}{Dt} = \boldsymbol{\nabla}.\boldsymbol{\sigma} + \rho\boldsymbol{g} \quad \rightarrow \boldsymbol{\sigma} = -p\boldsymbol{I} + \boldsymbol{\sigma_s} + \boldsymbol{\sigma_p}$$

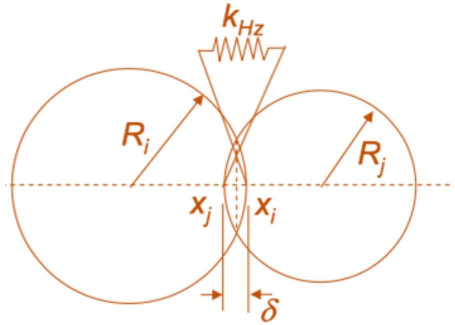
Solvent stress: $\boldsymbol{\sigma_s} = \mu_s\left(\boldsymbol{\nabla}\mathbf{u} + (\boldsymbol{\nabla}\mathbf{u})^T\right)$

Polymeric stress: $\boldsymbol{\sigma_p} + \lambda_1\overset{\triangledown}{\boldsymbol{\sigma}}_{\boldsymbol{p}} = \mu_p\left(\boldsymbol{\nabla}\mathbf{u} + (\boldsymbol{\nabla}\mathbf{u})^T\right)$ (e.g. Oldroyd-B)

$$\delta x < d_p$$



Immersed Boundary Method



Discrete Element Method

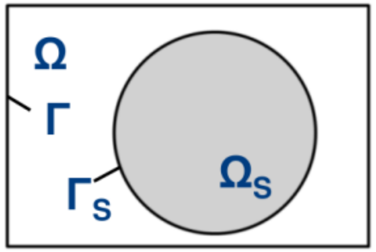
$$\begin{cases} m_i\dfrac{\mathrm{d}\mathbf{U}_i^p}{\mathrm{d}t} = \displaystyle\sum_{j=1}^{n_i^c}\mathbf{F}_{ij}^c + \mathbf{F}_i^f + \mathbf{F}_i^g \\ I_i\dfrac{\mathrm{d}\boldsymbol{\omega}_i}{\mathrm{d}t} = \displaystyle\sum_{j=1}^{n_i^c}\mathbf{M}_{ij} \end{cases}$$

*Hager A, Kloss C, Pirker S, Goniva C (2014). *J Comp Mult Flows*, 6:13–27
*https://www.cfdem.com/media/DEM/docu/gran_model_hertz.html

Numerical Implementation

Eulerian-Lagrangian & Particle-based Model

Integration of the **interface condition**:



$$\int_{\Gamma_S} \boldsymbol{\sigma} \cdot \hat{\mathbf{n}} \, d\Gamma_S = \int_{\Gamma_S} \mathbf{t}_{\Gamma_S} d\Gamma_S$$

… applying **Divergence Theorem** and assuming a **Viscoelastic** fluid:

$$\int_{\Omega_S} \left[-\nabla p + \nabla \cdot \left(\mu_S \left(\nabla \mathbf{u} + (\nabla \mathbf{u})^T \right) \right) + \nabla \cdot \boldsymbol{\sigma}_P \right] d\Omega_S = \int_{\Gamma_S} \mathbf{t}_{\Gamma_S} d\Gamma_S$$

$$\xRightarrow[]{\substack{\nabla \cdot (\nabla \mathbf{u}) = \nabla^2 \mathbf{u} + \nabla (\nabla \cdot \mathbf{u}) \\ \nabla \cdot (\nabla \mathbf{u})^T = 0}} \int_{\Omega_S} \left[-\nabla p + \mu_S \nabla^2 \mathbf{u} + \nabla \cdot \boldsymbol{\sigma}_P \right] d\Omega_S = \int_{\Gamma_S} \mathbf{t}_{\Gamma_S} d\Gamma_S$$

Numerical integration yields

$$F_{drag} = \sum_{c \in \overline{T}_h} (-\nabla p + \mu_S \nabla^2 \mathbf{u} + \nabla \cdot \boldsymbol{\sigma}_P)(c) \cdot V(c)$$

$$F_{torques} = \sum_{c \in \overline{T}_h} \left[\mathbf{r}(c) \times \left(-\nabla p + \mu_S \nabla^2 \mathbf{u} + \nabla \cdot \boldsymbol{\sigma}_P \right)(c) \right] \cdot V(c)$$

$\hat{\mathbf{n}} \equiv$ outward normal unit vector to Γ_S

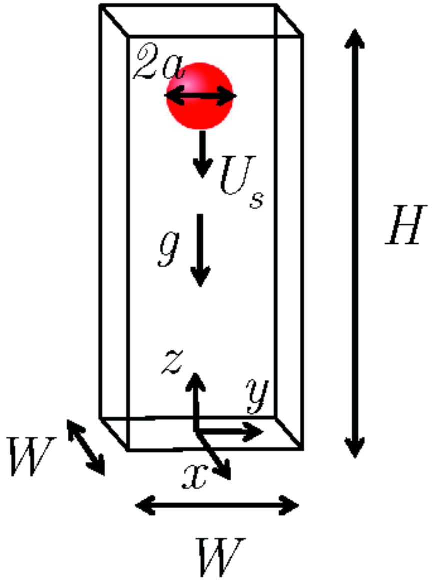
$\mathbf{t}_{\Gamma_S} \equiv$ stress vector acting from the fluid on the solid body interface

$\overline{T}_h \equiv$ set of all solid-covered cells

$V(c) \equiv$ volume of cell c

FV-IB-DEM Solver Validation

1. Sedimentation of a sphere in a Newtonian fluid

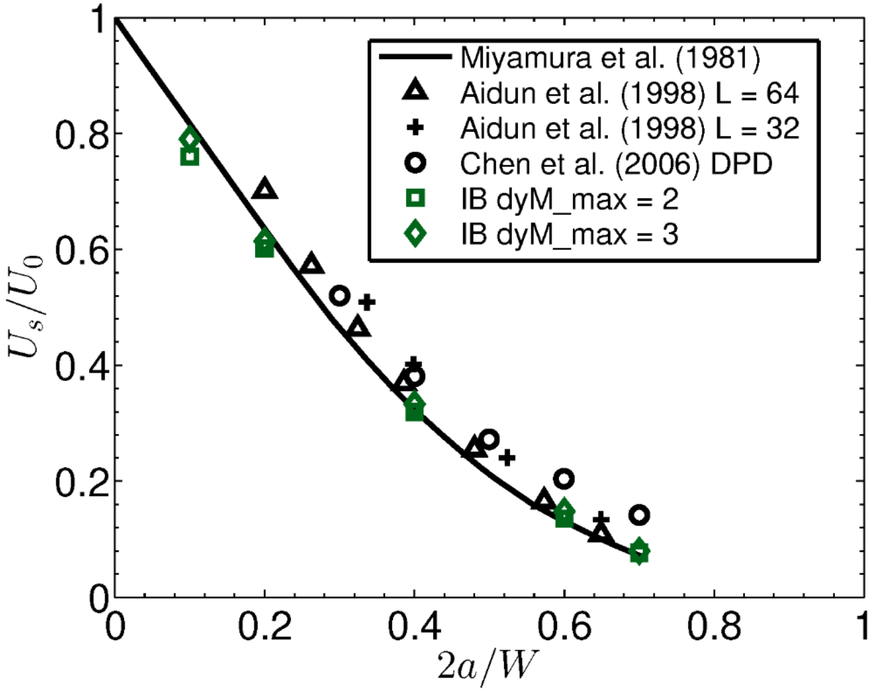


$$H/W = 4$$

$$\rho_s/\rho_f = 2.5$$

$$Re \equiv 2\rho_f U_0 a/\mu = 0.36$$

$$U_0 = \frac{(4/3)\pi a^3(\rho_s - \rho_f)g}{6\pi\mu a} = \frac{2a^2(\rho_s - \rho_f)g}{9\mu}$$



*Miyamura A, Iwasaki S, Ishii T (1981). *Int J of Mult Flow,* 7:41–46
*Aidun C K, Lu Y, Ding E –J (1998). *J Fluid Mech*, 373:287–311
*Chen S, Phan-Thien N, Khoo B C, Fan X J (2006). *Physics of Fluids*, 18:1–14

FV-IB-DEM Solver Validation

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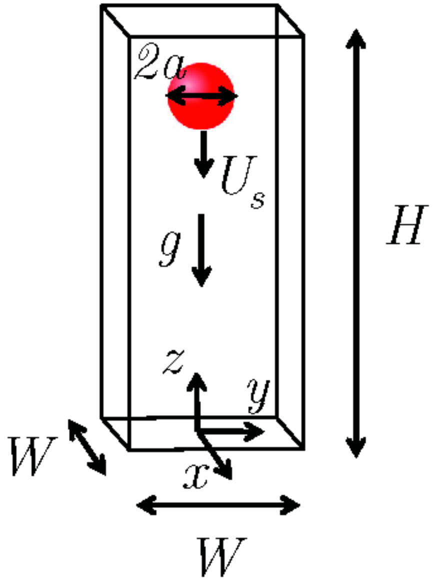

$H/W = 4$

$\rho_s/\rho_f = 2.5$

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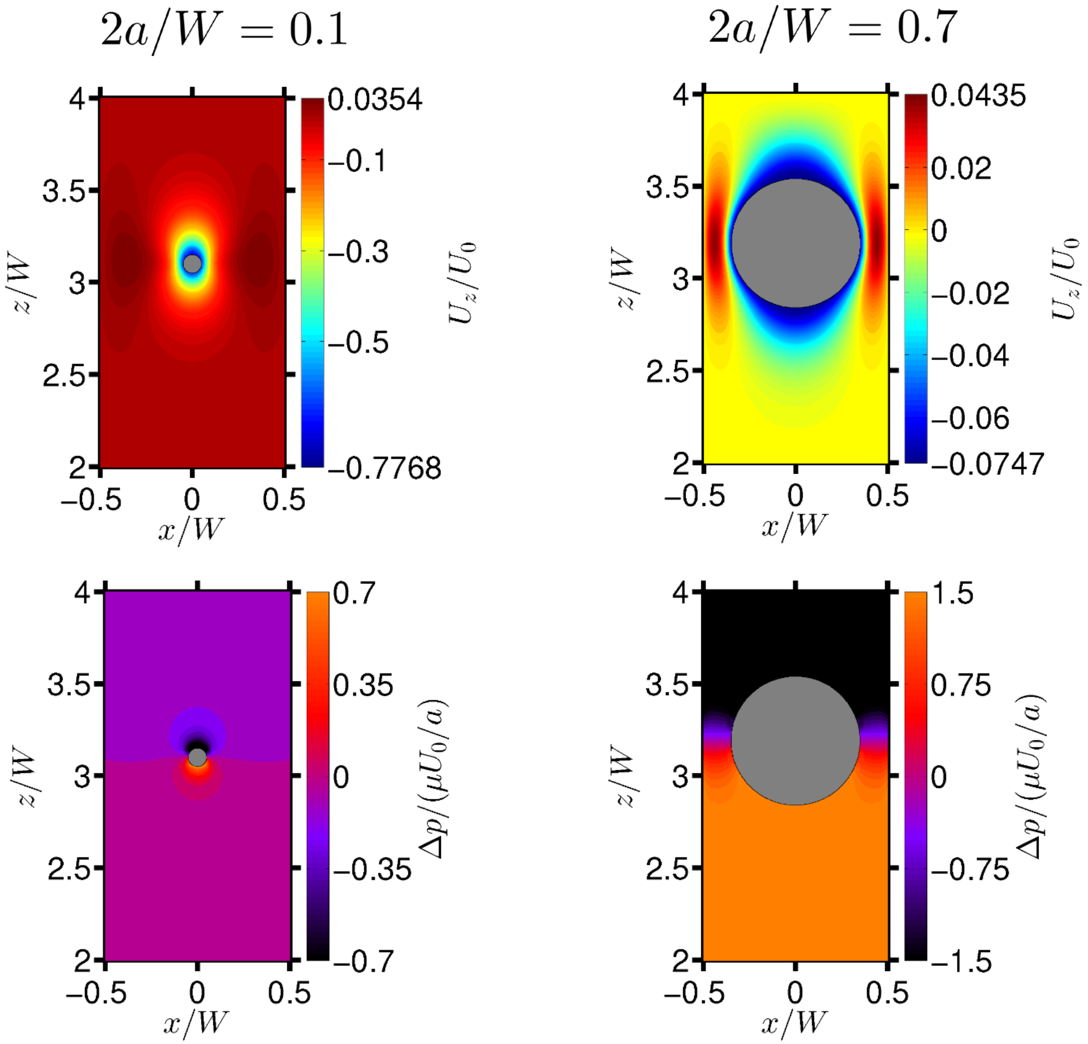


FV-IB-DEM Solver Validation

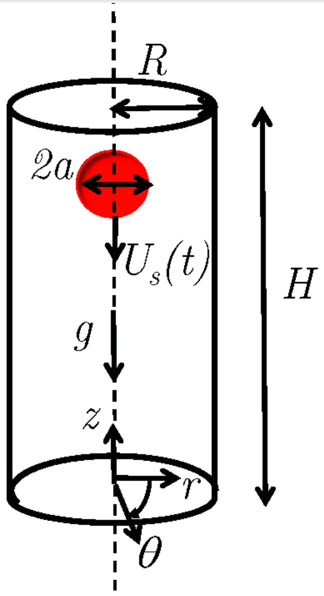
2. Sedimentation of a sphere in viscoelastic fluids

$$H/R \approx 17.2$$

$$\mathcal{K} = a/R \approx 0.243$$

$$\rho_s/\rho_f = 4.29$$

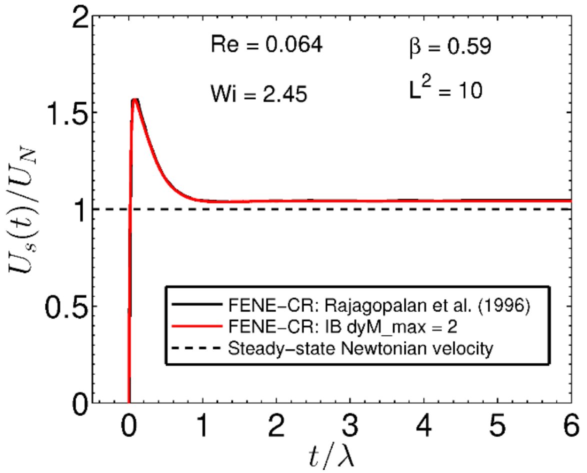
$$\beta = \eta_S/\eta_0 \approx 0.59$$

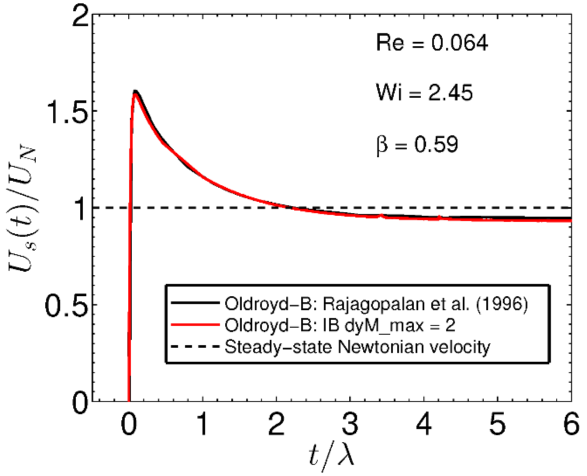


$$U_N = \frac{(4/3)\pi a^3(\rho_s - \rho_f)g}{6\pi\eta_0 a K_N(\mathcal{K})} = \frac{2a^2(\rho_s - \rho_f)g}{9\eta_0 K_N(\mathcal{K})}$$

$$Re \equiv 2a\rho_f U_N/\eta_0 \approx 0.064$$

$$Wi \equiv \lambda U_N/a \approx 2.45$$





*Rajagopalan D, Arigo M T, McKinley G H (1996). *Journal of Non-Newtonian Fluid Mechanics*, 65:17–46
*Happel J, Brenner H (1983). Low Reynolds Number Hydrodynamics, Dordrecht

FV-IB-DEM Solver Validation

2. Sedimentation of a sphere in viscoelastic fluids

FV-IB-DEM Solver Validation

2. Sedimentation of a sphere in viscoelastic fluids

Simulation Challenge: resolving stress overshoot

We extended our numerical approach to work with the log-conformation tensor providing the possibility to perform stable simulations at very large values of the Weissenberg (*Wi*) number.

$$\boldsymbol{\sigma}_P = \frac{\eta_p}{\lambda}(\mathbf{A} - \mathbf{I})$$

Extra stress tensor

Conformation tensor

Symmetric Positive Definite

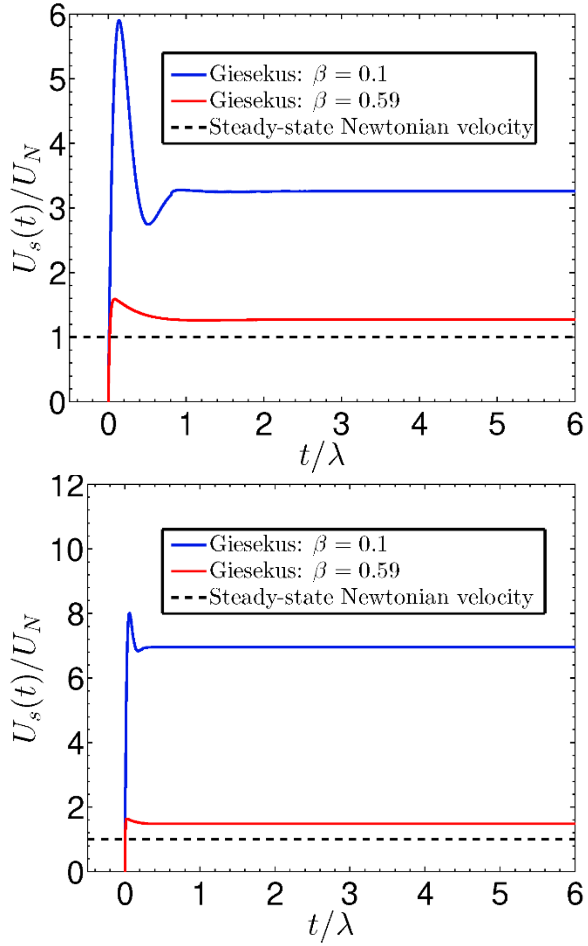
$$\boldsymbol{\Theta} = \log \mathbf{A}$$

Log-Conformation tensor

$\alpha = 0.2$

$Wi = 2.45$

$Wi = 10$



*Fattal R, Kupferman R (2005). *Journal of Non-Newtonian Fluid Mechanics*,126:23-37

*Pimenta F, Alves MA (2017). *Journal of Non-Newtonian Fluid Mechanics*, 239:85-104

FV-IB-DEM Solver Validation

2. Sedimentation of a sphere in viscoelastic fluids

$$Wi = 2.45$$

$\beta = 0.1$

$\beta = 0.59$

FV-IB-DEM Solver Validation

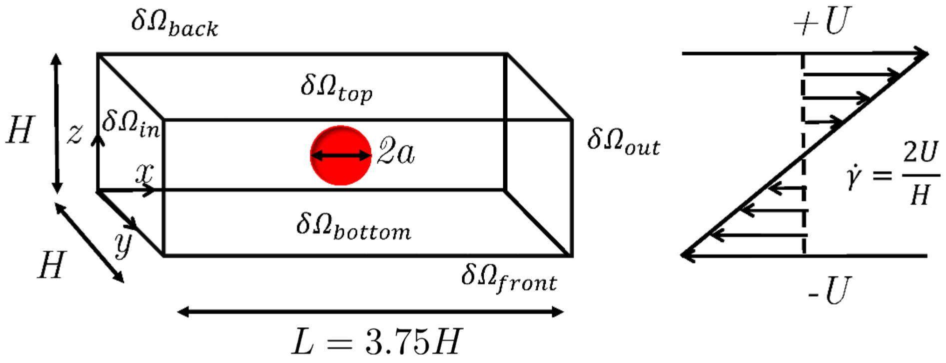
2. Sedimentation of a sphere in viscoelastic fluids

$$Wi = 10$$

$\beta = 0.1$ | $\beta = 0.59$

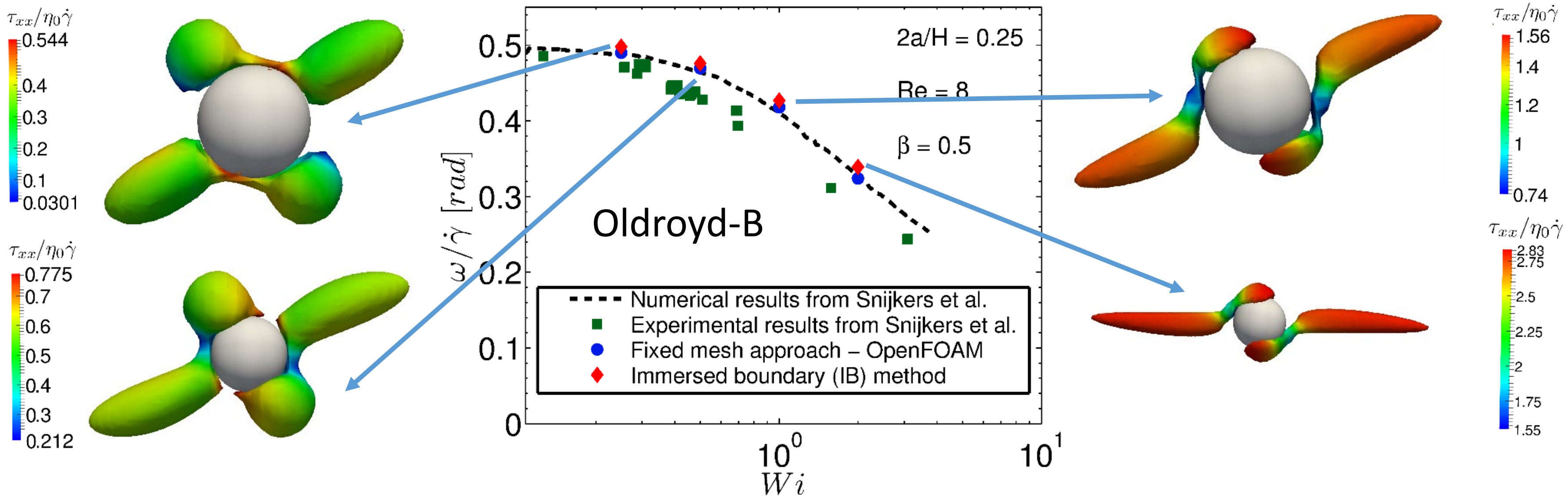
FV-IB-DEM Solver Validation

3. Rotation of a sphere in a fluid subjected to steady shear flow



$$\omega = \frac{\dot{\gamma}}{2}$$

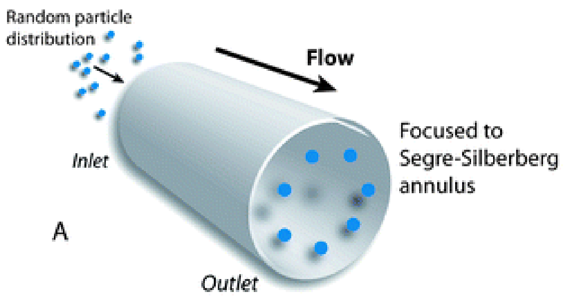
For Newtonian (*Wi* = 0)

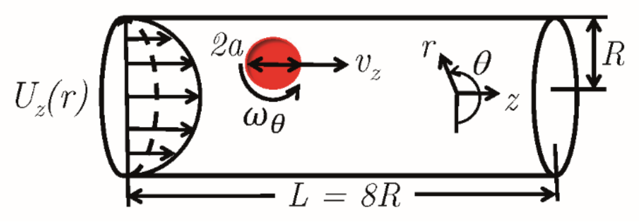


*Snijkers F, D’Avino G, Maffettone P L, Greco F, Hulsen M A, Vermant J (2011). *Journal of Non-Newtonian Fluid Mechanics*, *166*:363–372

FV-IB-DEM Solver Validation

4. Cross-stream migration of a neutrally buoyant sphere in Poiseuille flow

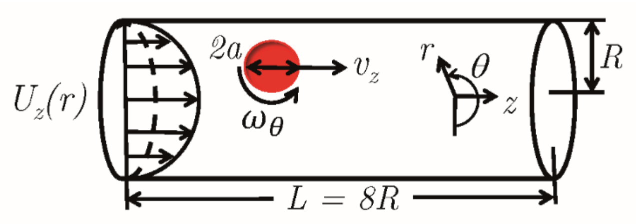




*Di Carlo D (2009). *Lab on a Chip,* 9:3038–3046
*Segré G, Silberberg A (1961). *Nature,* 189:209–210

FV-IB-DEM Solver Validation

4. Cross-stream migration of a neutrally buoyant sphere in Poiseuille flow

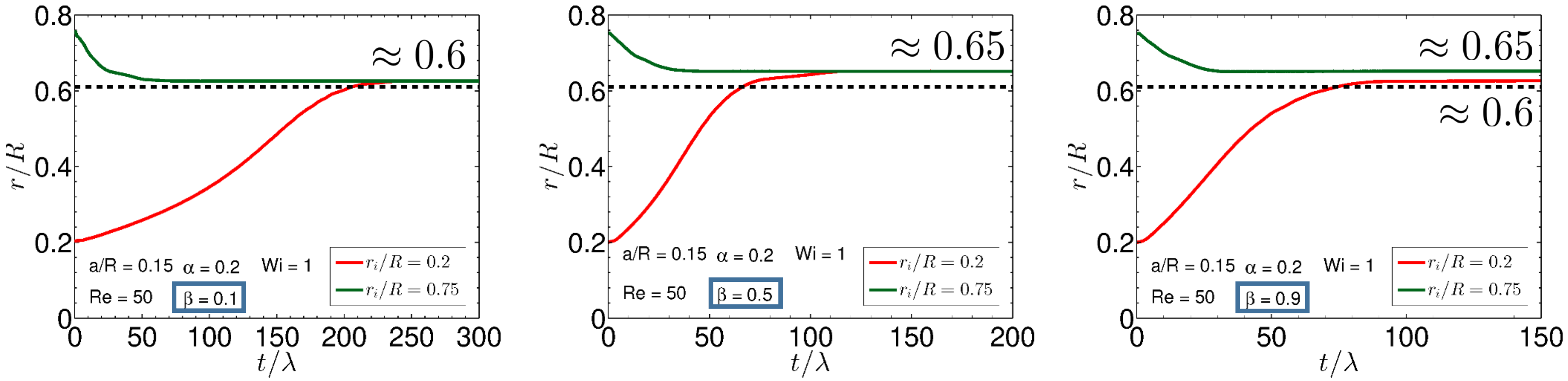


Giesekus

$\alpha = 0.2$

$Wi = 1$

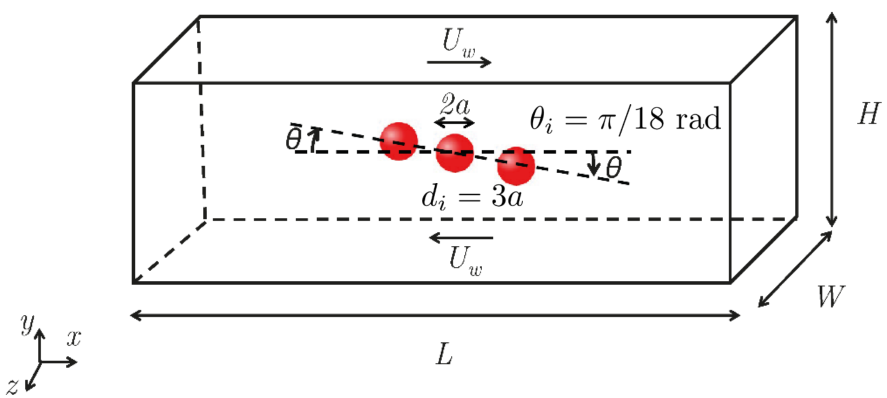
Study the effect of the retardation ratio $\beta = \frac{\eta_S}{\eta_S + \eta_P}$



The effects of the fluid elasticity has a complex transiente effect on the equilibrium position of the sphere, which requires further investigation that will be considered in future works.

Particle Alignment

Mesh convergence study



$$Re \equiv 2\rho_f U_w/\eta_0 = 0.1$$

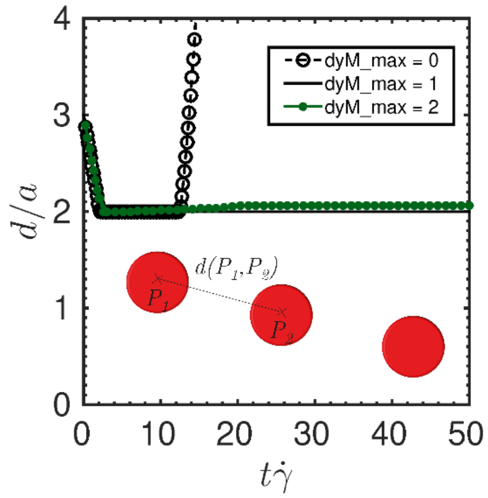
$$Wi \equiv \lambda\dot{\gamma} = 3$$

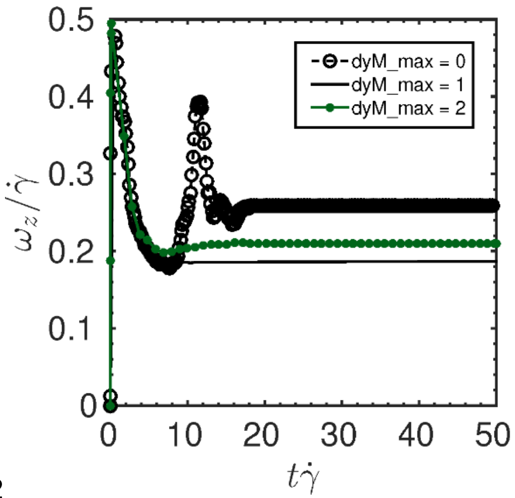
$$\beta = 0.1$$

$$\alpha = 0.1$$

Domain $L \times W \times H$	Total number of mesh cells	Estimated number of cells covered by the particles (solid fraction)	DOF
$40a \times 10a \times 16a$	51 200	2144	524 864
$20a \times 10a \times 8a$	12 800	2144	140 864

Mesh	dyM_max	Total number of mesh cells	d_f/a	Relative error (%)	$(\omega_z)_f/\dot{\gamma}$	Relative error (%)
M1	0	12800	–	–	0.259	18.8
M2	1	$\sim$ 20 000	2.001	3.9	0.186	14.7
M3	2	$\sim$ 45 000	2.062	1.0	0.210	3.7
Extrapolated	∞	–	2.082	–	0.218	–



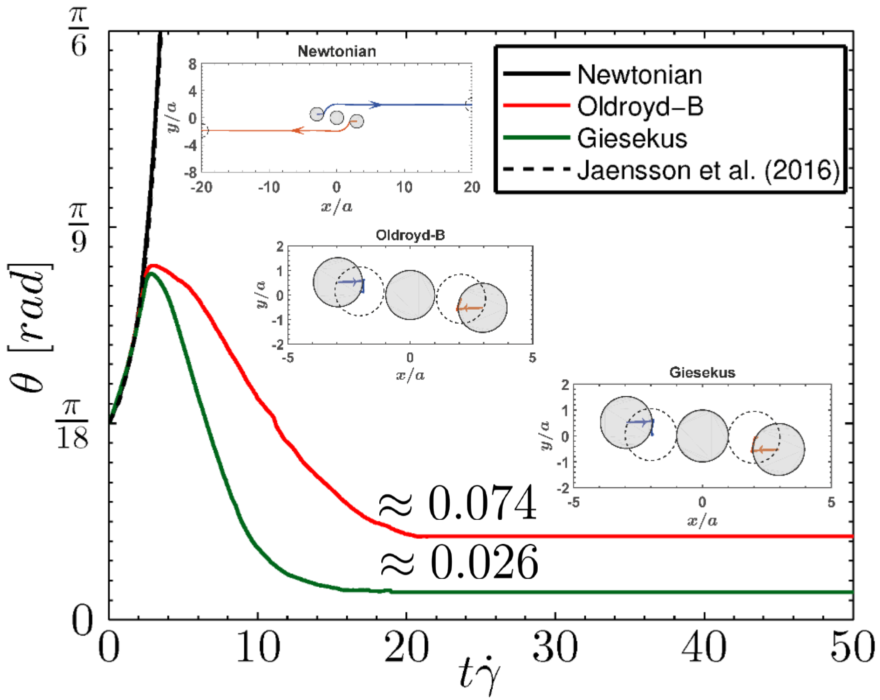


*Jaensson N O, Hulsen M A, Anderson P D (2016). *Journal of Non-Newtonian Fluid Mechanics*, 235:125–142

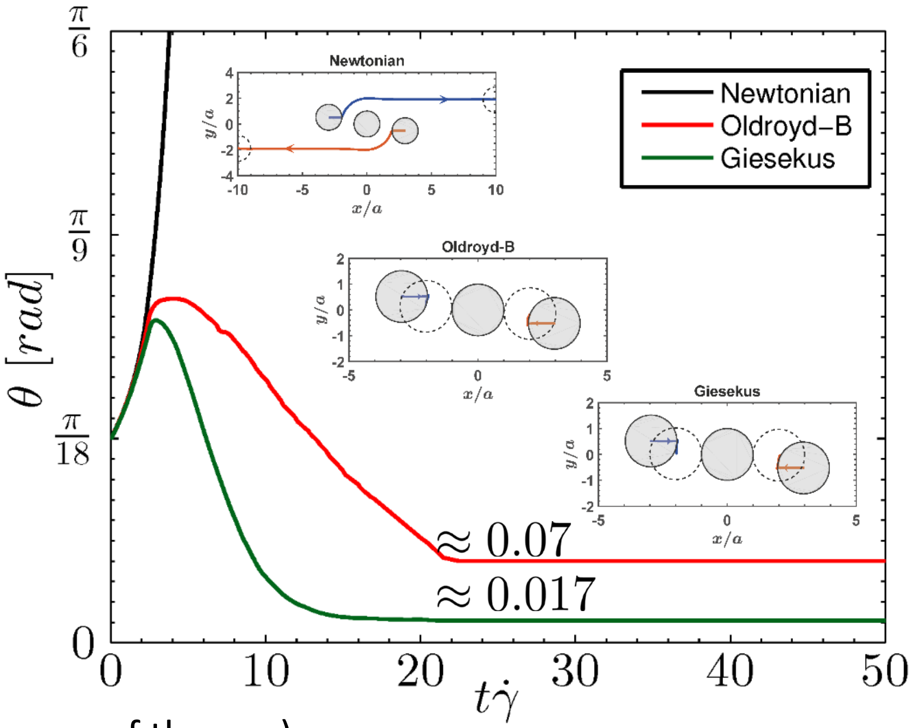
Particle Alignment

Effect of rheology and blockage ratio

$2a/H = 1/8$



$2a/H = 1/4$



With the increase of the blockage ratio (i.e. decrease of the gap), the particle aligment gets:

- 5.4 % of reduction for the Oldroyd-B fluid
- 34.6 % of reduction for the Giesekus fluid

Shear-thinning enhances particle aligment

*Jaensson N O, Hulsen M A, Anderson P D (2016). *Journal of Non-Newtonian Fluid Mechanics*, 235:125–142

Conclusions

- ✓ **The validation of a fully-resolved numerical algorithm for the simulation of solid particles in viscoelastic fluids was presented, including:**
  - Sedimentation of a sphere;
  - Rotation of a sphere in a fluid subjected to steady shear flow;
  - Cross-stream migration of a sphere in Poiseuille flow.
- ✓ **The capabilities of the developed code were tested in a challenging physical problem, the shear-induced particle alignment in wall-bounded Newtonian and viscoelastic fluids.**
  - Particle alignment occurs only in viscoelastic fluids, when normal stress differences are present, and the phenomena is enhanced by shear-thinning;
  - Particle alignment rate increases as the gap is reduced and the blockage ratio increases.

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University of Minho

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For further details please see:

C. Fernandes, S.A. Faroughi, O.S. Carneiro, J. Miguel Nóbrega, G.H. McKinley (2019). Fully-resolved simulations of particle-laden viscoelastic fluids using an immersed boundary method. *Journal of Non-Newtonian Fluid Mechanics*, *266*:80–94
doi: https://doi.org/10.1016/j.jnnfm.2019.02.007