ESR 12: LBM-DEM simulations of suspensions

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1 Introduction and aim

Suspensions of solid particles dispersed in fluid are ubiquitous in nature and industry. High-fidelity simulations fully resolving the fluid motion are required to study the influence of fluid inertia. Therefore, a coupling between the lattice Boltzmann method (LBM) and the discrete element method (DEM) is applied to study dense suspension flow.

2 Methodology

DEM to track particles (LIGGGHTS):

$$m\ddot{x}=F=F_{contact}+F_{hydrodynamic}+F_{lub,correction}$$

$$F_{contact}=k_n\delta n_{ij}+k_t\delta t_{ij} \quad \text{and} \quad F_t\leqslant x_\mu F_n \quad \text{where} \quad x_\mu=0 \quad \text{(frictionless)}$$

LBM for the fluid phase (Palabos):

$$\frac{f_i(\vec{x}+\vec{c}_i,t+\Delta t)-f_i(\vec{x},t)}{\Delta t}=\frac{(1-B_i)}{\tau}\left(f_i^{eq}(\vec{u}_f,\vec{x},t)-f_i(\vec{x},t)\right)+B_i\Omega_i^s$$

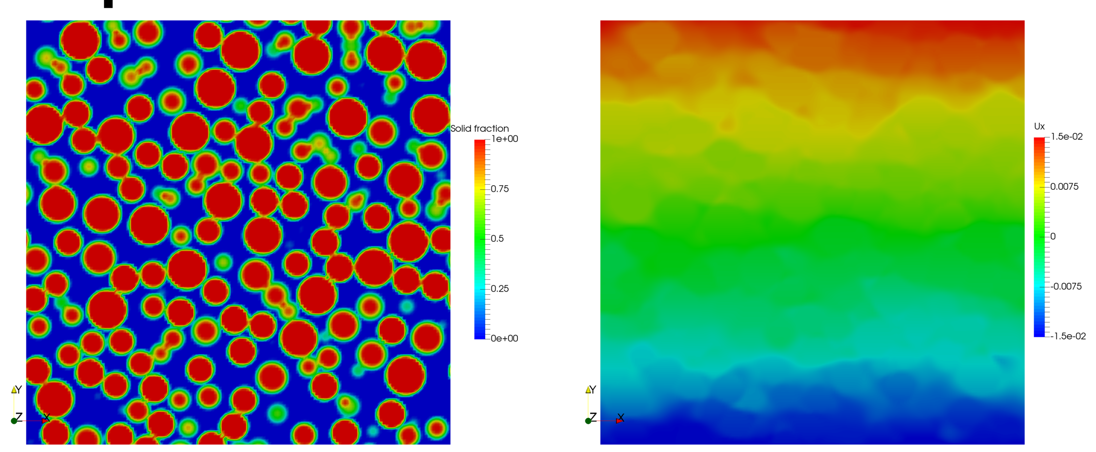
Coupling based on [1] by considering the particle presence by a solid fraction weighted ($B_i=\varepsilon_i^s=[0,1]$) bounce back term $\Omega_i^s=f_{-i}-f_i+f_i^{eq}(\vec{u}_s,\vec{x},t)-f_{-i}^{eq}(\vec{u}_f,\vec{x},t)$:

$$F_{hydrodynamic}=\frac{h^3}{\Delta t}\sum_s B^s\sum_i \Omega_i^s e_i$$

For inertialess flow, we can combine in DEM $F_{hydrodynamic}$ and $F_{lub,correction}$ to the grand-resistance matrix with an external force imposed on the particles to obtain a sheared state without making use of a coupling to LBM.

3 Simulation set-up

- 3D simulations of bidisperse (1:1.4) suspensions (>2000 particles)
- Apply simple shear using Lees-Edwards boundary conditions for particles [2] and fluid phase [3]
- Solid fraction ranges from 0.3 – 0.5
- Low shear rate, i.e. Re < 1
- Stress computation:

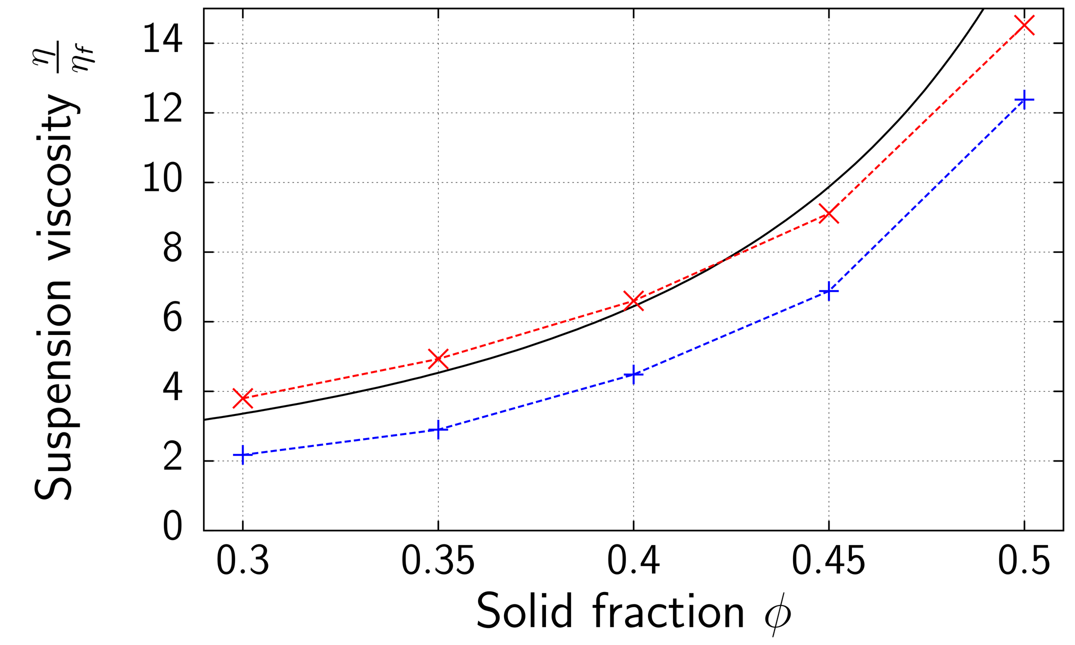


Particle packing (left) and fluid velocity in shearing direction (right) for a suspension of $\phi=0.5$

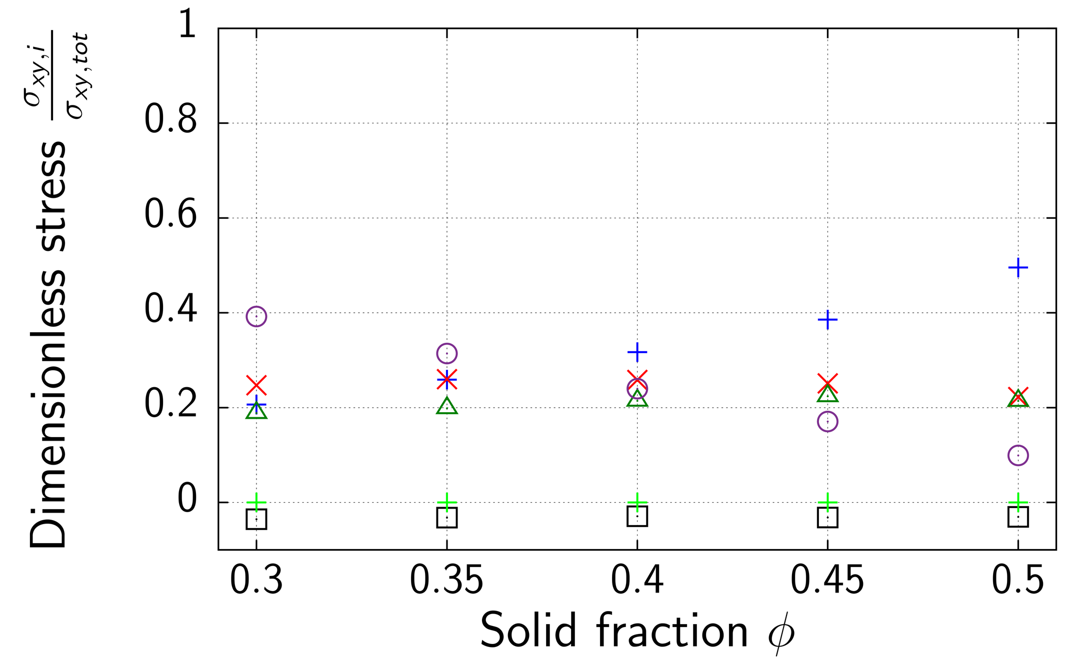
$$\sigma_{Contact/Lubrication}=\frac{1}{V}\sum_i\sum_{j\neq i} r_{ij}F_{ij}^{C/L} \qquad \sigma_{kin.energy}=\frac{1}{V}\sum_i m_i v_i' v_i' \qquad \sigma_{Stresslet,lk}=\frac{1}{2V}\int_{S_p}(\sigma_{ln}x_k+\sigma_{kn}x_l)n_n\,dS$$

4 Preliminary results

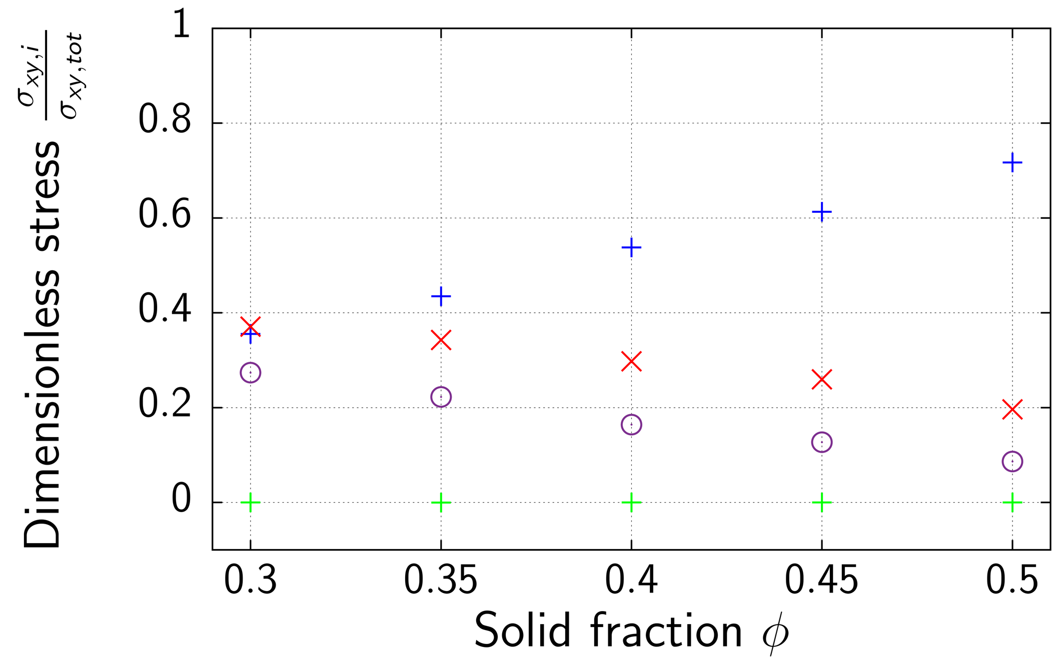
- Difference in viscosity between DEM and LBDEM for low-Re flows
- Difference is probably caused by stresslet computation and missing shearing lubrication force correction in LBDEM
- Normal and shearing lubrication force have similar magnitudes



(a)



(b)



(c)

(a): Comparison of DEM (x) and LBDEM (+) to Krieger-Dougherty correlation (black solid line)
(b)/(c): Stress contributions for (b) DEM and (c) LBDEM. Legend:
+: Contact stress, x: Normal lubrication (correction) contribution, △: Shearing lubrication contribution, □: Rotational lubrication contribution, O: Stresslet, +: Kinetic energy contribution

5 Challenges & future work

Main challenges:

- Improve (stresslet) accuracy for LBM-DEM simulations

Future simulations of sheared dense suspensions to investigate:

- Influence of different stress contributions on suspension viscosity
- Hydrodynamic stress and microstructure evolution during unsteady shear flow

References

[1] Noble and Torczynski, Int. J. Mod. Phys. C, 1998, 9(8):1189-1201
[2] Lees and Edwards, J. Phys. C:, 1972, 5:1921-1929
[3] Wagner and Pagonabarraga, J. Stat. Phys, 2002, 107(112):521-537

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