Lattice Boltzmann simulations of droplet dynamics in time-dependent flows

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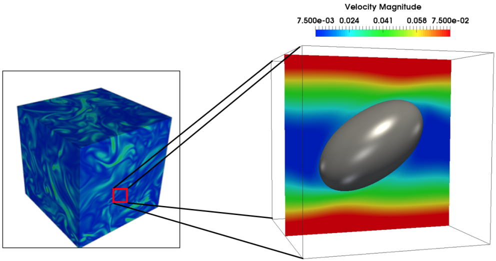
Droplets in turbulence

- analysis of the deformation of a confined droplet in an oscillatory shear flow
- the deformation of the fully resolved droplet (Lattice Boltzmann) is in good agreement with a point like phenomenological approximation(MM-model)
- Lattice Boltzmann Method (LBM) confirms droplet transparency effect for high frequency oscillatory flows

The scale separation between turbulence and microfluidics



Scale separation: turbulent flow ↔ droplet size

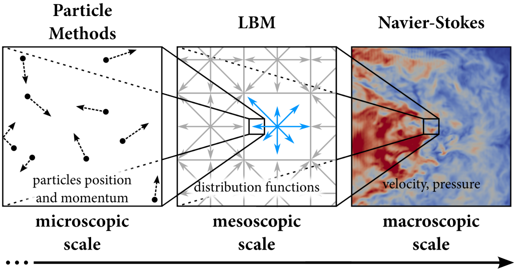
- impossible to resolve both length scales simultaneously
- solution: simulate a single fully resolved droplet under the influence of turbulent fluctuations

The meso-scale

Navier-Stokes equations (incompressible flows)

$$\nabla \cdot \mathbf{v} = 0$$

$$\partial_t \mathbf{v} + \mathbf{v} \cdot \nabla \mathbf{v} = -\frac{1}{\rho} \nabla p + \nu \nabla^2 \mathbf{v}$$



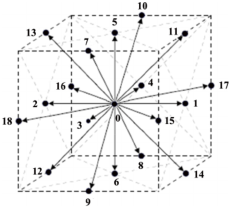
The Lattice Boltzmann Method

Boltzmann equation and Lattice Boltzmann Equation (LBE)

$$\partial_t g(\mathbf{x}, t) + \mathbf{v} \cdot \nabla g(\mathbf{x}, t) = \Omega(g(\mathbf{x}, t))$$

$$\underbrace{g_i(\mathbf{x} + \mathbf{c}_i \Delta t, t + \Delta t) - g_i(\mathbf{x}, t)}_{\textbf{Streaming}} = \underbrace{\Delta t\, \Omega(\{g_i(\mathbf{x}, t)\})}_{\textbf{Collision}}$$

- $\rho(\mathbf{x}, t) = \sum_i g_i$
- $\mathbf{v}(\mathbf{x}, t) = \frac{1}{\rho(\mathbf{x}, t)} \sum_i g_i \mathbf{c}_i$

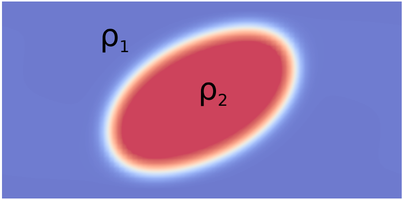


Shan-Chen Multicomponent model (SCMC)

Shan-Chen Multicomponent Coupling

Pseudo potential : $\psi_\sigma = \rho_\sigma$

SCMC Force : $\mathbf{F}_\sigma(\mathbf{x}) = -\psi_\sigma(\mathbf{x}) \sum_{\substack{i \\ \sigma \neq \sigma'}} G_{\sigma,\sigma'}\, w_i\, \psi_{\sigma'}(\mathbf{x} + \mathbf{c}_i)\mathbf{c}_i$

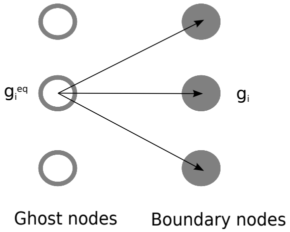


Two component system with ρ_1 and ρ_2

Boundary method

Ghost node storage of boundary values ρ_b and $\mathbf{u}$

$$g_i^{\text{ghost}} = g_i^{\text{eq}}(\rho_b, \mathbf{u}) = w_i \rho_b \left[1 + 3(\mathbf{c}_i \cdot \mathbf{u}) + \frac{9}{2}(\mathbf{c}_i \cdot \mathbf{u})^2 - \frac{3}{2}\mathbf{u}^2\right]$$



Streaming step of the ghost nodes to the boundary layer.

A phenomenological model for droplet deformation

Maffettone-Minale model (MM)

$$\frac{dM_{ij}}{dt} = \underbrace{[f_2(Ca)(S_{ik}M_{kj} + M_{ik}S_{kj}) + \Omega_{ik}M_{kj} - M_{ik}\Omega_{kj}]}_{\textbf{droplet stretching}}$$

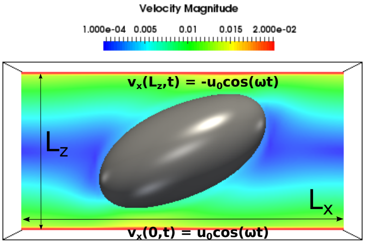
$$- \underbrace{f_1(Ca)\left(M_{ij} - \frac{1}{3}g(M_{ij})\delta_{ij}\right)}_{\textbf{droplet relaxation}}$$

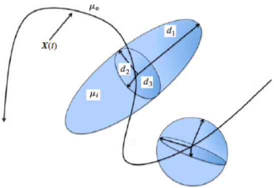
M_{ij}: Droplet deformation tensor S_{ij}, Ω_{ij}: Shear tensor parts

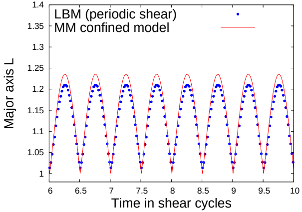
$Ca = \frac{\mu_o RG}{\sigma}$: Capillary number

Maffettone, Minale, J. Non-Newtonian Fluid Mech., 78 (1998) 227–241

Droplet deformation via an oscillatory shear flow







Time dependent deformation of the major axis L

First order solution for the time-dependent MM-model

First order Ca expansion of the morphology tensor

$$M_{ij}(t) = \delta_{ij} + Ca(t)\, M_{ij}^{(1)}(t) + \mathcal{O}(Ca^2)$$

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Time-dependent first order solution

$$L^2 = 1 + Ca_{\max} f_2 \frac{\omega t_d \cos(\omega t_d t) - f_1 \sin(\omega t_d t)}{f_1^2 + \omega^2 t_d^2} + \mathcal{O}(Ca^2)$$

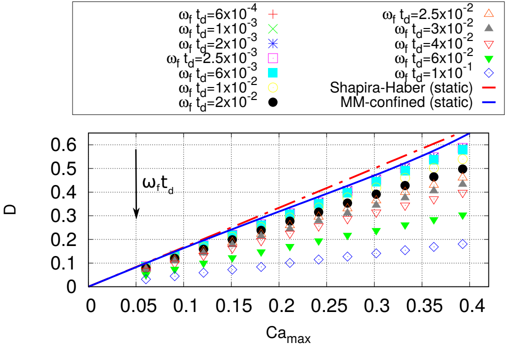
$$W^2 = 1 - Ca_{\max} f_2 \frac{\omega t_d \cos(\omega t_d t) - f_1 \sin(\omega t_d t)}{f_1^2 + \omega^2 t_d^2} + \mathcal{O}(Ca^2)$$

$$B^2 = 1 + \mathcal{O}(Ca^2)$$

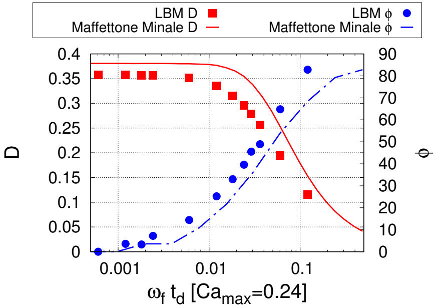
$$\phi = \arctan\left(\frac{\omega t_d}{f_1}\right) + \mathcal{O}(Ca^2)\, (t_d : \text{Droplet relaxation time})$$

Phase space

G: shear amplitude & $\omega_f t_d$: normalised shear frequency



Deformation D for shear frequencies $\omega_f t_d$



Deformation D and phase shift ϕ against the shear frequency $\omega_f t_d$

- out of phase response of the droplet to the oscillatory shear flow $\Rightarrow$ rapid decrease in deformation parameter D
- the point like phenomenological MM-model and the fully resolved LBM scheme match well

F.Milan, M.Sbragaglia, L.Biferale, F.Toschi: arXiv:1711.05498

Time-dependent droplet break up

- successful benchmark of LBM & MM-model
- move to a regime where the MM-model is not correct $\rightarrow$ droplet break up
- scan of the phase space: critical capillary number Ca_{cr} vs shear frequency $\omega_f t_d$

Time-dependent droplet dynamics in generic flows

Planar hyperbolic flow

$$\text{Stress tensor : } S_{ij} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \Omega_{ij} = 0$$

Conclusion

- phenomenological MM-model and fully resolved LBM simulations are in good agreement
- droplet transparency effect in respect to high normalised shear frequency $\omega_f t_d$
- use fully resolved LBM scheme for quantitative study of droplet break up in generic oscillatory flows

Future:

- introducing turbulent fluctuations to the LBM boundary scheme
- multi-scale analysis of droplet morphology in a turbulent flow

Acknowledgements

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