Discontinuous shear thickening on dense non-Brownian suspensions via lattice Boltzmann method

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Outline

Introduction
  Outline of our model
Hydrodynamics: lattice Boltzmann method
Particle contacts
Electrostatic repulsive forces
Sheared suspensions simulations
Results
Discussions
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Suspensions

Solid particles suspended in solvent fluid

Fluids are described by Stokes equation ($\text{Re} \rightarrow 0$):

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

$$\nabla \mathbf{p} = \eta \nabla^2 \mathbf{u}$$

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- Lubrication (Brady’s group)
- Granular systems (Otsuki and Hayakawa, 2011)
- Boundary effect (Brown and Jaeger, 2012) and (Allen, et al, 2017) (Brown’s group)

Motivations:
- Recover DST using LBM
- Decompose all contributions to the shear stress
- Helpful for the theoretical construction
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- Hydrodynamic fields are calculated by solving the resistance matrix.
- Separate lubrication calculation.
Lattice Boltzmann vs Stokesian Dynamics

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Lattice Boltzmann (susp3d)

- Hydrodynamic fields are calculated \textit{locally} at each lattice point.
- \textit{mesoscopic}, possible to have simple local rules between fluid and solid.
- Particle motion obey the Newton equations.
- Separate lubrication calculation.
Outline of our model

Equation of motions:

\[ m \cdot \frac{d}{dt} \begin{pmatrix} U \\ \Omega \end{pmatrix} = \sum_{\alpha} \begin{pmatrix} F_{\alpha} \\ T_{\alpha} \end{pmatrix} \]

\[ \sum_{\alpha} F_{\alpha} = F^h + F^c + F^R \]

\[ \sum_{\alpha} T_{\alpha} = T^h + T^c + T^R \]

\[ U(t + \Delta t) = U(t) + \frac{\Delta t}{m} F(t) \]

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By using LBM, we need to discretize the unit length \( a \) (particle radius) to lattice unit \( \Delta x \)!

Our simulation used \( \Delta x = 0.1 \).

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History of LBM

- Initially devised as an extension of the Lattice Gas Automata by McNamara and Zanetti (McNamara, Zanetti, 1988)
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- Now, LBM is widely used for various computational fluid dynamics simulation.
The discrete distribution function (He and Luo, 1997)

$n \rightarrow$ particle velocity ($v$) distribution function on space time point ($r, t$)
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\( n \rightarrow \) particle velocity (\( \mathbf{v} \)) distribution function on space time point (\( \mathbf{r}, t \))

time evolution of \( n \) in continuous space:

\[
\partial_t n + \mathbf{v} \cdot \nabla n = \left( \frac{dn}{dt} \right)_{\text{coll}}
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we can project to the Hermite bases:

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which is linear combination of the moments of \( n \)

The first few of the Hermite polynomials (\( H^{(l)}(v) \)):

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H^{(0)}(v) = 1 \\
H^{(1)}(v) = v_\alpha \\
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the Gaussian weight function:

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\omega(v) = \frac{1}{(2\pi)^{D/2}} \exp \left( -\frac{v^2}{2} \right)
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From Boltzmann equation to LBE

**Truncate:** (to several orders of $K$)

$$n(r, v, t) = \omega(v) \sum_{l=0}^{K} \frac{1}{l!} A^{(l)} H^{(l)}(v)$$
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**only finite sets of velocities are needed!** we can compute the integral for $A$ with Gauss-Hermite quadrature.

$(\rho(v) \rightarrow \text{arbitrary polynomial of } v, c_i \rightarrow \text{discrete lattice velocity}, w_i \rightarrow \text{quadrature weight} )$

$$\int d\mathbf{v} \omega(v) \rho(v) = \sum_{i=1}^{b} w_i \rho(c_i)$$
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$$= \sum_{i=1}^{b} w_i \frac{n(r, v, t)}{\omega(\mathbf{v})} c_i \cdots c_i$$

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discrete distribution function $\rightarrow n_i(r, c_i, t) = w_i n(r, v, t) / \omega(v)$
the lattice Boltzmann method

Evolving equation:

\[ n_i(r + c_i, t + 1) = n_i(r, t) + \Delta_i(r, t) \]
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Hydrodynamic fields:

Mass density  \[ \rho = \sum_i n_i \]

Momentum density  \[ j = \sum_i n_i \mathbf{c}_i \]

Momentum flux  \[ \Pi = \sum_i n_i \mathbf{c}_i \mathbf{c}_i \]
LBM: Collision operator

Linearized collision operator

\[ \Delta_i(n) = \Delta_i(n_i^{eq}) + \sum_j L_{ij} n_j^{neq} \]
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\[ n_{eq}^i = \rho \left( \frac{m}{2\pi k_b T} \right)^{\frac{3}{2}} \exp \left( \frac{-m(v - u) \cdot (v - u)}{2k_b T} \right) \]

Weight coefficients:

\[ a_0 = 12 \]
\[ a_1 = 2 \]
\[ a_\sqrt{2} = 1 \]
\[ c_s = \sqrt{k_b T} \rightarrow \text{lattice sound speed} \]
\[ A : B = \text{Tr}(AB) \]
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Expanding with Hermite polynomials up to 2nd order, with coefficients:

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\[ \sum_i L_{ij} = 0 \quad \sum_i c_i L_{ij} = 0 \quad \sum_i c_i c_i L_{ij} = \lambda c_j c_j \quad \sum_i c_i^2 L_{ij} = \lambda \nu c_j^2 \]

\( c_j c_j \rightarrow \) traceless
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Only the second moment of \( n_i^{eq} \) that is affected by collision
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Only the second moment of \( n_i^{eq} \) that is affected by collision

Post collision distribution function:

\[ n_i^* = a^c_i \left( \rho + \frac{j \cdot c_i}{c_s^2} + \frac{(\rho uu + \Pi^{neq,*}) : (c_i c_i - c_s^2 1)}{2c_s^4} \right) \]
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$c_j c_j \to$ traceless

discrete equilibrium distribution function:

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Only the second moment of $n_{i\,eq}^c$ that is affected by collision

Post collision distribution function:

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$\longrightarrow$ Calculate $\Pi_{neq,\,*}^{\text{eq}}$
LBM: Collision operator $\Pi^{neq,*}$

\[
\Pi^{neq} = \Pi - \Pi^{eq} \quad \Pi = \sum_i n_i c_i c_i
\]
LBM: Collision operator $\Pi^{neq,*}$

$$\Pi^{neq} = \Pi - \Pi^{eq} \quad \Pi = \sum_i n_i c_i c_i$$
	nonequilibrium second moments obtained from the eigen equation of $L_{ij}$:

$$\sum_i L_{ij} = 0 \quad \sum_i c_i L_{ij} = 0 \quad \sum_i c_i c_i L_{ij} = \lambda c_j c_j \quad \sum_i c_i^2 L_{ij} = \lambda_\nu c_j^2$$

What will happen on the solid boundary conditions (surface of the particles)?
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$$\Pi^{neq,*} = (1 + \lambda)\tilde{\Pi}^{neq} + \frac{1}{3}(1 + \lambda_\nu)(\Pi^{neq} : 1)$$

$\lambda$ and $\lambda_\nu$ are related to shear $\eta$ and bulk $\eta_\nu$ viscosities from the multiscale analysis:

$$\eta = -\rho c_s^2 \Delta t \left( \frac{1}{\lambda} + \frac{1}{2} \right) \quad \eta_\nu = -\rho c_s^2 \Delta t \left( \frac{2}{3\lambda_\nu} + \frac{1}{3} \right)$$
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What will happen on the solid boundary conditions (surface of the particles)?
Solid-fluid boundary condition

Anthony Ladd’s bounce-back rule:

(a)

\[ n_b'(r, t + \Delta t) = n_b^*(r, t) - \frac{2a_c \rho_0 u_b \cdot c_b}{c_s^2} \]

Velocity of the boundary nodes:

\[ u_b = U + \Omega \times (r_b - R) \]

R is the center of mass of the particle.
Solid-fluid boundary condition

Forces exerted at the boundary nodes:

\[ f(r_b, t + \frac{1}{2} \Delta t) = \frac{\Delta x^3}{\Delta t} \left[ 2n_b^*(r, t) - \frac{2a_c \rho_0 u_b \cdot c_b}{c_s^2} \right] c_b \]
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Sum over all boundary nodes within a particle:
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Sum over all boundary nodes within a particle:

\[ F^h = \sum_b f(r_b) \]
\[ T^h = \sum_b r_b \times f(r_b) \]
\[ \sigma^h = \sum_b r_b f(r_b) \]
Shared nodes

need separated lubrication forces calculation!
Shared nodes

need separated lubrication forces calculation!
Lubrications

If gap between particle is less than 1 lattice unit ..
Lubrications

If gap between particle is less than 1 lattice unit..
Grand-resistance formulation (Nguyen and Ladd, 2002)
Lubrications

If gap between particle is less than 1 lattice unit...

Grand-resistance formulation (Nguyen and Ladd, 2002)

\[
\begin{pmatrix}
F_1 \\
T_1 \\
T_2 \\
S_1 \\
S_2
\end{pmatrix} = -
\begin{pmatrix}
A_{11} & -B_{11} & B_{22} \\
B_{11} & C_{11} & C_{12} \\
-B_{22} & C_{12} & C_{22} \\
G_{11} & H_{11} & H_{12} \\
G_{22} & -H_{21} & H_{22}
\end{pmatrix}
\begin{pmatrix}
U_{12} \\
\Omega_1 \\
\Omega_2
\end{pmatrix}
\]

(Kim and Karilla, 1991)
Lubrications

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(Kim and Karilla, 1991)

$$U_{12} = U_1 - U_2$$ relative velocity
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Each coefficients can be expressed in terms of scalar function i.e
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Each coefficients can be expressed in terms of scalar function i.e

\(H_{12} = Y_{12}^H (\epsilon_{\alpha\gamma\delta} d_\delta d_\beta + \epsilon_{\beta\gamma\delta} d_\delta d_\alpha)\)

\(d \rightarrow\) displacement unit vector along axis. \(\epsilon \rightarrow\) Levi-Civita symbol
Lubrications

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\[d \rightarrow \text{displacement unit vector along axis. } \epsilon \rightarrow \text{Levi-Civita symbol}\]

Each scalar function is a function of gap \(h\) and \(\beta = \frac{a_i}{a_j}\) i.e

\[Y_{12}^H = 8 \log \left(\frac{1}{h}\right) \pi \eta a_i \frac{2\beta^2(1 + 7\beta)}{5(1 + \beta)^5}\]
Lubrications

Cutoff length \( \delta = \frac{a_{\text{contact}} - a_{\text{hydro}}}{a_{\text{contact}}} \) to allow contact
Lubrications

Cutoff length $\delta = \frac{a_{contact} - a_{hydro}}{a_{contact}}$ to allow contact

We used $\delta = 0.01$
Particle contacts
Contact model

Linear spring dashpot model (Luding, 2008)
Contact model

Linear spring dashpot model (Luding, 2008) \( \mathbf{F}_{ij}^c = \mathbf{F}_{ij}^{nor} + \mathbf{F}_{ij}^{tan} \)

(Fleischmann, 2015)
Contact model

Coulomb friction rules:

\[ |\mathbf{F}_{ij}^{\tan}| \geq \mu(|\mathbf{F}_{ij}^{\text{nor}}|) \rightarrow \]
Contact model

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Stress contribution from contact:
Normal:
\[ \sigma_{\alpha\beta}^{\text{nor}} = -\frac{1}{2V} \sum_i \sum_{j \neq i} (r_{ij,\alpha} \mathbf{F}_{ij,\beta}^{\text{nor}} + r_{ij,\beta} \mathbf{F}_{ij,\alpha}^{\text{nor}}) \]
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Contact model

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Electrostatic repulsive forces (Israelachvili, 2001)

\[ F_{ij} = \frac{1}{\lambda} \left( a_i a_j + a_j a_i \right) F^* \exp(-h/\lambda) \hat{n}_{ij} \lambda \rightarrow \text{Debye length} \]

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Electrostatic repulsive forces (Israelachvili, 2001)

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we used \( \lambda = 0.2a \)
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\]
Sheared suspensions

Wall moves with velocity $u_{\text{wall}}$ to $x$ and $-x$ directions.

All simulation uses $N=512$ particles.
Sheared suspensions

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Rheology

Shear stress:

$$\sigma_{\alpha\beta} = \sigma^h_{\alpha\beta} + \sigma^{tan}_{\alpha\beta} + \sigma^{nor}_{\alpha\beta} + \sigma^r_{\alpha\beta}$$
Rheology

Shear stress:

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Apparent viscosity:

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Rheology

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Sheared Suspensions: $\frac{\eta}{\eta_0}$ vs $\dot{\gamma}^*$, compared with results from (Mari, et al, 2014)
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Contributions to shear viscosity for $\phi = 0.57$
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Contributions to shear viscosity for $\phi = 0.54$ and 0.48
Contributions to shear viscosity for $\phi = 0.54$ and $0.48$
Time evolution of shear viscosity $\phi = 0.57$ and $\phi = 0.48$
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Time evolution of contact number for $\phi = 0.57$
Time evolution of contact number for $\phi = 0.57$
Evolution of the contact network ($\phi = 0.57$)

- high shear rate
- low shear rate
Discussions

- Slight deviation from Seto’s
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  - Need to allow separate ”switching” length between boundary nodes and lubrication calculation for normal, tangential, and rotation modes
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  - Our simulation used $\Delta x = 0.1a$, to let $Re < 1$, one need typical particle speed $U < 0.016 \frac{\Delta x}{\Delta t}$. 

To travel a distance of its radius, one particles needs $>6200$ time steps.
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Future prospects

- Good starting point for the theoretical works
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- Use more realistic boundary conditions
References


