Lattice-Boltzmann Simulations of Particle Suspensions in Sheared Flow

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Outline

• Lattice-Boltzmann Method (LBM)
• Suspension Modeling with LBM
• Lees-Edwards Boundary Conditions (LEBC) for LBM Suspensions
• Rheology of Suspensions (Validation of LEBC)
• Some Cluster Properties
Lattice-Boltzmann Method (LBM)
LBM’s Predecessor: Lattice-Gas Automaton

- identical particles on a lattice (space, time AND velocities discrete)
- propagation
- collision: particles reshuffled, mass and momentum conserved

- Frisch, Hasslacher, Pommeau (1986): LGA on hexagonal lattice → Navier-Stokes
Lattice-Boltzmann method

- particles replaced by their ensemble average (reduction of noise): distribution function $f_i(r, t)$, giving the probability of finding a particle at site $r$ at time $t$ flying with velocity $c_i$
- evolution follows the Boltzmann-equation for a dilute gas,

$$\partial_t f_i(x, v, t) + v \nabla_x f_i(x, v, t) + \frac{F}{m} f_i(x, v, t) = \text{coll}(f(x, v, t)),$$

in its discretized form (here, the simplest LBGK scheme, single-relaxation time)

$$f_i(r + e_i, t + 1) - f_i(r, t) + F_i = \frac{1}{\tau} (f^\text{eq}_i(r, t) - f_i(r, t))$$

where: $e_i$ velocity, pointing to adjacent node
$\tau$ relaxation time.
- kinematic viscosity $\nu = (2\tau - 1)/6$
Lattice-Boltzmann method

• moments of $f_i$: density, momentum, momentum flux density

$$\rho(r, t) = \sum_{i} Q f_i(r, t)$$

$$\rho(r, t) \cdot u(r, t) = \sum_{i} e_i f_i(r, t)$$

$$\Pi = \sum_{i} e_i e_i f_i(r, t)$$

• equilibrium function (for a weakly compressible fluid) for $\text{Ma} \ll 1$

$$f_i^{eq}(r, t) = \rho(r, t) \left(A_i + B_i (e_i \cdot u) + C_i (e_i \cdot u)^2 + D_i u^2\right)$$

agrees with Maxwell-Boltzmann distribution up to $O(u^2)$

• direction dependent coefficients determined by conservation of mass, momentum and kinetic energy (total energy $\rho\theta + \rho uu$ for thermal LBM)
D2Q9 LBM

- isotropy requires at least 9 velocities in 2 dimensions

\[
\begin{align*}
e_0 &= (0, 0), \\
e_1 &= (1, 0), \quad e_2 = (0, 1), \\
e_3 &= (-1, 0), \quad e_4 = (0, -1), \\
e_5 &= (1, 1), \quad e_6 = (-1, 1), \\
e_7 &= (-1, -1), \quad e_8 = (1, -1)
\end{align*}
\]

- coefficients in \( f_i^{eq} \)

<table>
<thead>
<tr>
<th>( i )</th>
<th>( A_i )</th>
<th>( B_i )</th>
<th>( C_i )</th>
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<td>1/12</td>
<td>1/8</td>
<td>-1/24</td>
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</table>
Modelling of Suspensions with LBM
The ALD method for suspended particles

(Aidun, Lu, Ding, 2003)

• particles mapped to lattice → broken links
• virtual fluid inside shell
• arbitrary surfaces possible

• solid-fluid interaction: (bounce-back at the links with moving wall)

\[
f_i(x, t + 1) = \begin{cases} 
  f_{-i}(x, t^+) + 2\rho B_i u_b \cdot e_i & \text{if BL} \\
  f_i(x + e_{-i}, t^+) & \text{else}
\end{cases}
\]

• momentum exchange, force, torque:

\[
\delta p_i = 2e_i[f_i(x, t + 1) - \rho B_i u_b \cdot e_i]
\]

\[
F_i(x, t_0 + 1/2) = \delta p_i / \Delta t, \quad T_i(x, t_0 + 1/2) = (x - X(t_0) \times F_i(x, t_0 + 1/2))
\]
Lees-Edwards Boundary Conditions for LBM Suspensions
Lees-Edwards Boundaries for Suspensions

**Procedure for boundary-crossing densities:**
- Mapping to off-grid copy (distribute $f$ over destination nodes according to sub-grid shift ratio):

$$f_5(x, 1) = (1 - \text{mod}_1[ut]) \cdot f_5(x + \text{int}[x - ut], y_{\text{max}}) + \text{mod}_1[ut] \cdot f_5(x + \text{int}[x - ut - 1], y_{\text{max}})$$
Lees-Edwards Boundaries for Suspensions

Galilei-Transformation of boundary-crossing densities to new reference frame

- difference in $f_i$ to get momentum transfer right (all macroscopic variables and their derivatives will stay the same, image is moving as block at const velocity)

$$\Delta f_5 = f_5(u + u_w) - f_5(u)$$

$$\approx f_5^{eq}(u + u_w) - f_5^{eq}(u)$$

$$-\tau (\partial_t[f_5^{eq}(u + u_w) - f_5^{eq}(u)] + u_5 \partial_r[f_5^{eq}(u + u_w) - f_5^{eq}(u)])$$

$$\approx f_5^{eq}(u + u_w) - f_5^{eq}(u)$$

- last step: only $u$-dependence kept, skip $O(\partial)$ terms because their 0th and 1st moments neglectible (Wagner, Pagonabarraga, 2006)
Sub-grid Boundary Reflection (according to sub-grid shift ratio):

- modification of distribution step to allow fluid-solid interaction

\[
f_i(x, t+1) = (1 - \text{mod}_1[u_w t]) \cdot \left\{ \begin{array}{ll}
f_i(x - \text{int}[x - u_w t] + e_i, t^+) & \text{if } \text{BL} \\
f_{-i}(x, t^+) - \rho B_i u_b \cdot e_i & \text{if } \text{BL}
\end{array} \right.
+ \text{mod}_1[u_w t] \cdot \left\{ \begin{array}{ll}
f_i(x - \text{int}[x - u_w t + 1] + e_i, t^+) & \text{if } \text{BL} \\
f_{-i}(x, t^+) - \rho B_i u_b \cdot e_i & \text{if } \text{BL}
\end{array} \right.
\]
Rheology of Suspensions
Apparent Viscosity, Dependence on Concentration $\phi$

- for a dilute dispersed suspension (Einstein, 1906): $\nu_{\text{app}} = \nu_f (1 + 2.5\phi)$
  - assumptions: no hydrodynamical interaction ($\sim \phi^2$), Brownian motion insignificant
- semi-empirical Krieger-Dougherty relation:

$$\nu_{\text{app}} = \nu_f \left(1 - \frac{\phi}{\phi_{\text{max}}}\right)^{[\eta]\phi_{\text{max}}} \tag{1}$$

- simulation results for $R = 8$, $Re = 0.001$
App. Viscosity $\nu_{\text{app}}$ as a Function of Shear Rate $\dot{\gamma}$

- generic behaviour

- I - Newtonian plateau: Brownian motion dominates
- II - shear-thinning: increasing shear decreases disorder of particle structure
- III - Newtonian plateau: particles strongly orientated
- IV - shear-thickening: local structures, broken by shear, momentum transfer via particles dominates
- V - unknown: some experimental results show repeated shear-thinning
Shear-Thickening

- $R_p = 8, L_{x,y} = 259 \approx 16 \cdot 2R_p, \phi = 0.40, \nu_f = 0.0125, u_w < 0.0864$

Lees-Edwards vs. planar Couette scheme

- clear: Couette scheme suffers from wall effects at higher shear rates $\dot{\gamma}$
  - wall induces different particle structures $\rightarrow$ depletion zone $\rightarrow$ wall slip $\rightarrow$ lower apparent viscosity
Particle Clusters
Emerging Particle Clusters

Snapshot of a sheared suspension

$R_{part} = 3.75$, $Re_{shear,part} \approx 0.1$, $\phi = 0.431$, red~high pressure
Cluster Properties

- **Definition:** Cluster = agglomeration of particles, connected via links \( d < d_{\text{crit}} = 2.2 R_p \) (Max in PDF)
- Angle distribution of linked particles shows strong anisotropy
  → mostly aligned to a direction diagonal to shear
- Rod-like clusters in diagonal direction are perfect tools to transport momentum through the system → possible explanation for shear thickening behaviour

- **KCM model** (Raiskinmäki, 2004)
  - tube rotates in shear: particles initially uncorrelated, density of centres of mass Poisson distributed
  - tube deforms, particles collide

\[
 n(m) \sim m^{-1.5} \exp(-m/m_0)
\]

\[
 m_0 = 1/(\lambda - \log(\lambda) - 1), \lambda = \phi/\phi_c(\dot{\gamma})
\]

- cutoff cluster size \( m_0 \) diverges when \( \phi \rightarrow \phi_c(\dot{\gamma}) \)
Outlook

- integration into the COAST multi-scale environment

Further objective: blood flow

- implementation of (deformable) RBC-like particles
- implementation of walls, LCs and their sticking behaviour (LC rolling)

Thank you!