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

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Yukawa Insitute for Theoretical Physics
Kyoto University

Rheology of disordered particle part 1, YITP, June 22nd 2018

Outline

YUKAWA INSTITUTE FOR THEORETICAL PHYSICS

Suspensions

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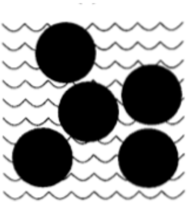

Solid particles suspended in solvent fluid

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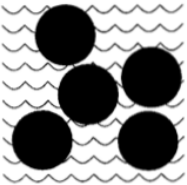

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$$\nabla p = \eta \nabla^2 \mathbf{u}$$

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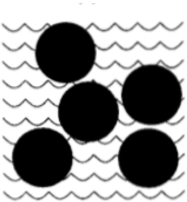

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Suspensions rheology have unique behavior!

Discontinuous shear thickening

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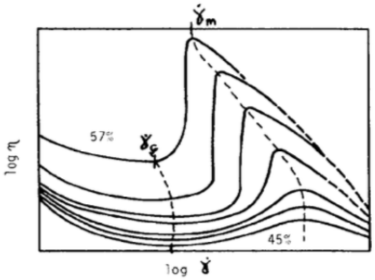

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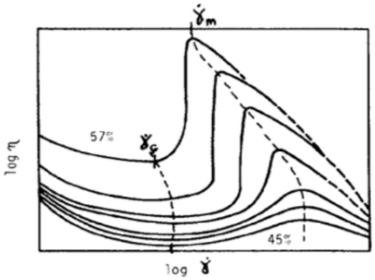

- R. G. Egres and N. J. Wagner J. Rheol. 49 3 , 719-746(2015)

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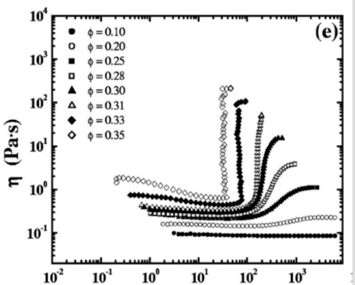

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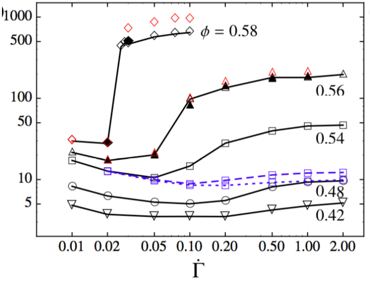

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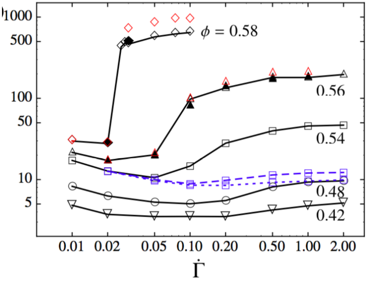

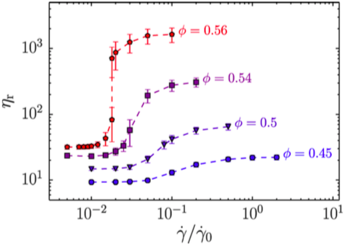

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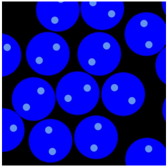
Motivations:

- Recover DST using LBM
- Decompose all contributions to the shear stress
  - Helpful for the theoretical construction

Lattice Boltzmann vs Stokesian Dynamics

Lattice Boltzmann

Stokesian Dynamics



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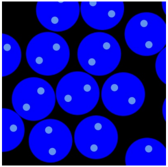

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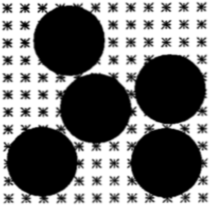
Lattice Boltzmann (susp3d)



- Hydrodynamic fields are calculated *locally* at each lattice point.
- *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:

$$m \cdot \frac{d}{dt}\begin{pmatrix}\mathbf{U}\\ \mathbf{\Omega}\end{pmatrix} = \sum_{\alpha}\begin{pmatrix}\mathbf{F}_{\alpha}\\ \mathbf{T}_{\alpha}\end{pmatrix}$$

$$\sum_{\alpha}\mathbf{F}_{\alpha} = \mathbf{F}^{h} + \mathbf{F}^{c} + \mathbf{F}^{R}$$

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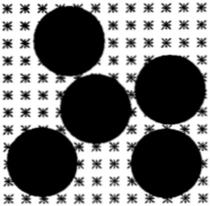

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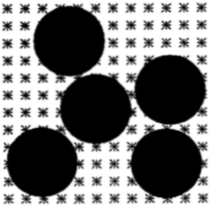
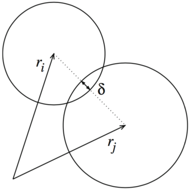


Contact between particles



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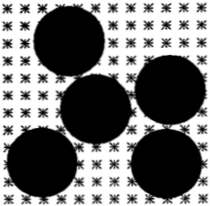

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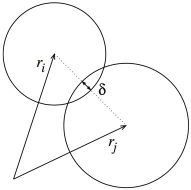
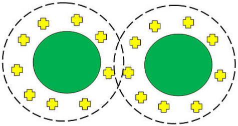


Electrostatic repulsive forces



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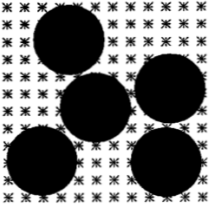

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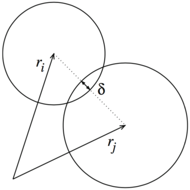

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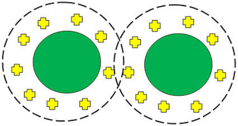

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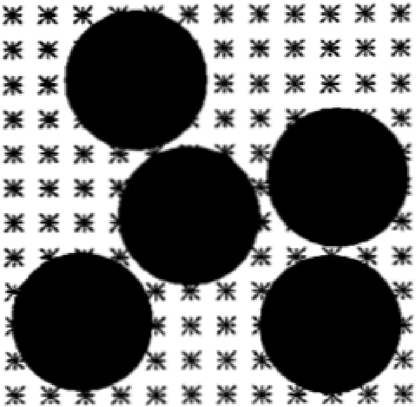

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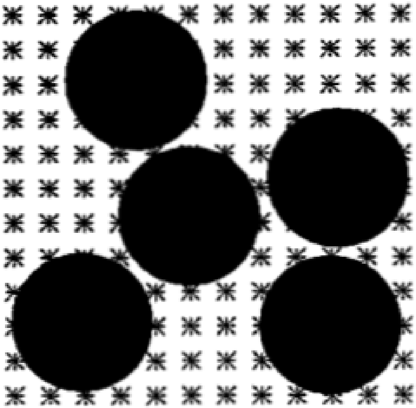

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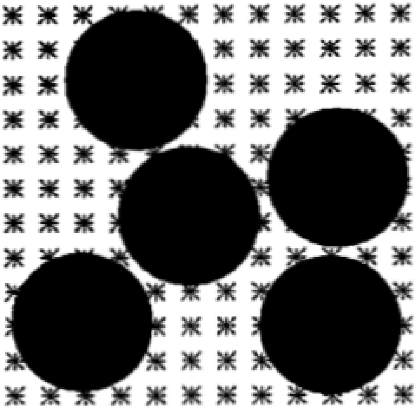

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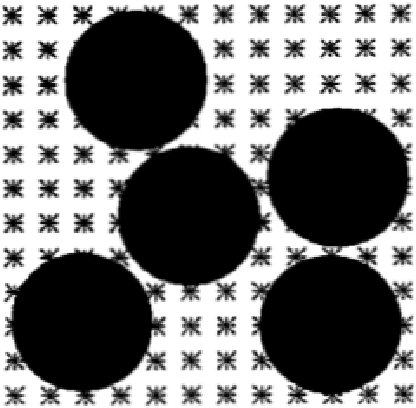

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All quantities below are written in lattice units!

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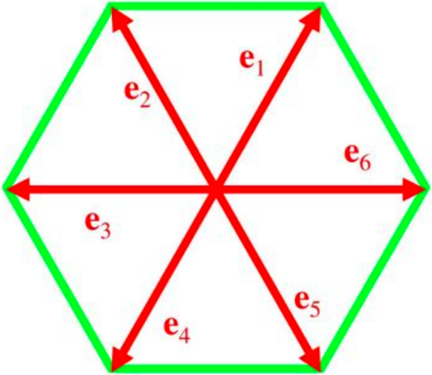

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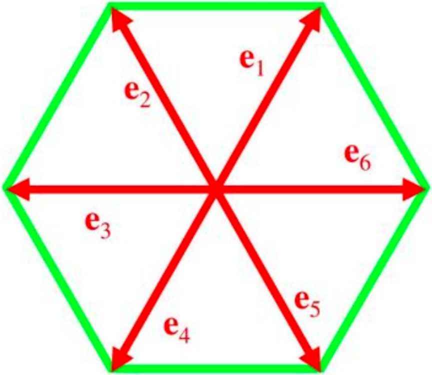

- Now, LBM is widely used for various computational fluid dynamics simulation.

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From Boltzmann equation to LBE

Truncate: (to several orders of K)

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($p(\mathbf{v}) \rightarrow$ arbitrary polynomial of $\mathbf{v}$, $\mathbf{c}_i \rightarrow$ discrete lattice velocity, $w_i \rightarrow$ quadrature weight)

$$\int d\mathbf{v}\omega(\mathbf{v})p(\mathbf{v}) = \sum_{i=1}^{b} w_i p(\mathbf{c}_i)$$

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$$\begin{aligned}
\int d\mathbf{v} n(\mathbf{r}, \mathbf{v}, t) \mathbf{v} \cdots \mathbf{v} &= \int d\mathbf{v} \frac{\omega(\mathbf{v})}{\omega(\mathbf{v})} n(\mathbf{r}, \mathbf{v}, t) \mathbf{v} \cdots \mathbf{v} \\
&= \sum_{i=1}^{b} w_i \frac{n(\mathbf{r}, \mathbf{v}, t)}{\omega(\mathbf{v})} \mathbf{c}_i \cdots \mathbf{c}_i \\
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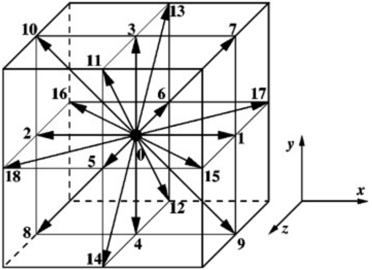
discrete distribution function $\rightarrow n_i(\mathbf{r}, \mathbf{c}_i, t) = w_i n(\mathbf{r}, \mathbf{v}, t)/\omega(\mathbf{v})$

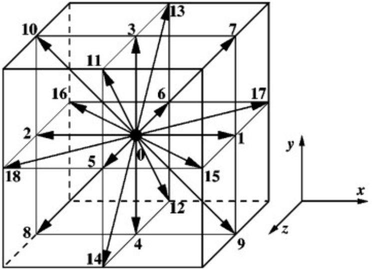
the lattice Boltzmann method



Evolving equation:

$$n_i(\mathbf{r} + \mathbf{c}_i, t + 1) = n_i(\mathbf{r}, t) + \Delta_i(\mathbf{r}, t)$$

the lattice Boltzmann method



Evolving equation:

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streaming

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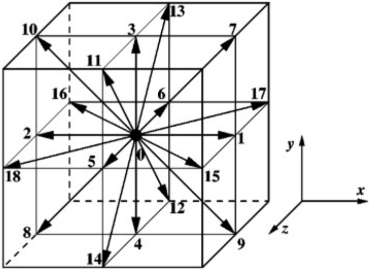

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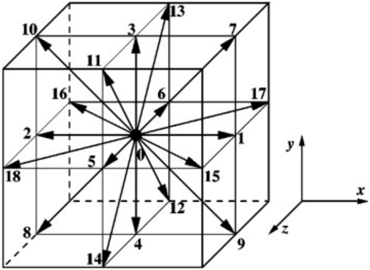

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streaming collision

Hydrodynamic fields:

mass density $\rho = \sum_i n_i$

momentum density $\mathbf{j} = \sum_i n_i \mathbf{c}_i$

momentum flux $\mathbf{\Pi} = \sum_i n_i \mathbf{c}_i \mathbf{c}_i$

LBM: Collision operator

Linearized collision operator

$$\Delta_i(n) = \Delta_i(n_i^{eq}) + \sum_j \mathcal{L}_{ij} n_j^{neq}$$

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$$n^{eq} = \rho \left(\frac{m}{2\pi k_b T} \right)^{\frac{3}{2}} \exp\left(\frac{-m(\mathbf{v} - \mathbf{u}) \cdot (\mathbf{v} - \mathbf{u})}{2 k_b T} \right)$$

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Expanding with Hermite polynomials
up to 2nd order, with coefficients:

$$A_{eq}^0 = \rho$$
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function:

$$n_i^{eq} = a^{c_i} \left(\rho + \frac{\mathbf{j}\cdot\mathbf{c}_i}{c_s^2} + \frac{(\rho\mathbf{u}\mathbf{u}) : (\mathbf{c}_i\mathbf{c}_i - c_s^2 1)}{2c_s^4} \right)$$

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$$A_{eq}^0 = \rho$$
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Weight coefficients:

$$a^0 = 12 \qquad a^1 = 2$$
$$a^{\sqrt{2}} = 1$$

discrete equilibrium distribution
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$$n_i^{eq} = a^{c_i}\left(\rho + \frac{\mathbf{j}\cdot\mathbf{c}_i}{c_s^2} + \frac{(\rho\mathbf{u}\mathbf{u}) : (\mathbf{c}_i\mathbf{c}_i - c_s^2 1)}{2c_s^4}\right)$$

$c_s = \sqrt{k_b T} \rightarrow$ lattice sound speed
$\mathbf{A} : \mathbf{B} = Tr(\mathbf{AB})$

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Post collision distribution function:

$$n_i^{*} = a^{c_i} \left(\rho + \frac{\mathbf{j} \cdot \mathbf{c}_i}{c_s^2} + \frac{(\rho \mathbf{u}\mathbf{u} + \mathbf{\Pi}^{neq,*}) : (\mathbf{c}_i \mathbf{c}_i - c_s^2 1)}{2 c_s^4} \right)$$

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$\longrightarrow$ Calculate $\mathbf{\Pi}^{neq,*}$

LBM: Collision operator $\mathbf{\Pi}^{neq,*}$

$\mathbf{\Pi}^{neq} = \mathbf{\Pi} - \mathbf{\Pi}^{eq} \qquad \mathbf{\Pi} = \sum_i n_i \mathbf{c}_i \mathbf{c}_i$

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nonequilibrium second moments obtained from the eigen equation of $\mathcal{L}_{ij}$:

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$$\mathbf{\Pi}^{neq,*} = (1+\lambda)\bar{\mathbf{\Pi}}^{neq} + \frac{1}{3}(1+\lambda_\nu)(\mathbf{\Pi}^{neq} : 1)1$$

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λ and λ_ν are related to shear η and bulk η_ν viscosities from the multiscale analysis:

$$\eta = -\rho c_s^2 \Delta t \left(\frac{1}{\lambda} + \frac{1}{2} \right) \qquad \eta_\nu = -\rho c_s^2 \Delta t \left(\frac{2}{3\lambda_\nu} + \frac{1}{3} \right)$$

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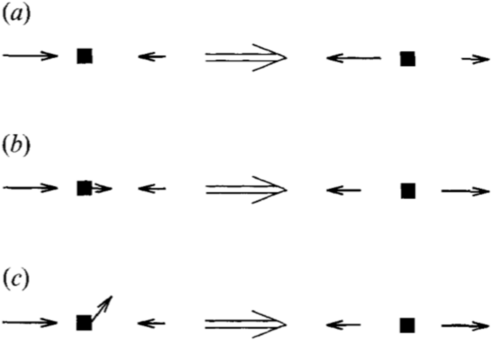
What will happen on the solid boundary conditions (surface of the particles) ?

Solid-fluid boundary condition

Anthony Ladd's bounce-back rule:



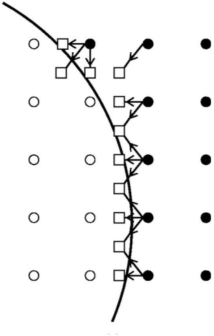
$$n_{b'}(\mathbf{r}, t + \Delta t) = n_b^*(\mathbf{r}, t) - \frac{2a^{c_b}\rho_0 \mathbf{u}_b \cdot \mathbf{c}_b}{c_s^2}$$

Velocity of the boundary nodes:

$$\mathbf{u}_b = \mathbf{U} + \mathbf{\Omega} \times (\mathbf{r}_b - \mathbf{R})$$

R is the center of mass of the particle

Solid-fluid boundary condition



Forces exerted at the boundary nodes:

$$\mathbf{f}(\mathbf{r}_b, t+\frac{1}{2}\Delta t) = \frac{\Delta x^3}{\Delta t}\left[2n_b^*(\mathbf{r}, t) - \frac{2a^{c_b}\rho_0\mathbf{u}_b\cdot\mathbf{c}_b}{c_s^2}\right]\mathbf{c}_b$$

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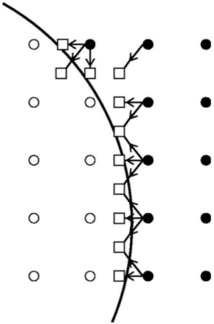

Sum over all boundary nodes within a particle:

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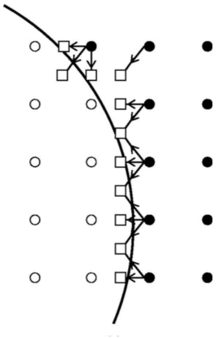

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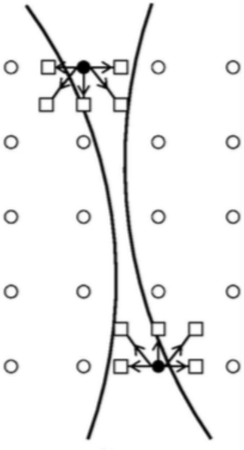
Sum over all boundary nodes within a particle:

$$\mathbf{F}^h = \sum_b \mathbf{f}(\mathbf{r}_b)$$

$$\mathbf{T}^h = \sum_b \mathbf{r}_b \times \mathbf{f}(\mathbf{r}_b)$$

$$\sigma^h = \sum_b \mathbf{r}_b\mathbf{f}(\mathbf{r}_b)$$

Shared nodes



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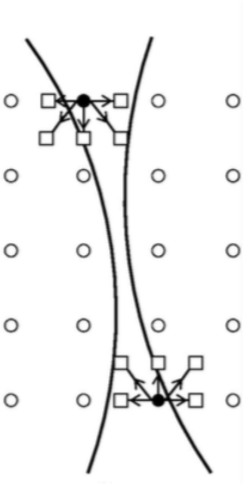

need separated lubrication forces calculation!

Lubrications

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

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Grand-resistance formulation (Nguyen and Ladd, 2002)

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$$\begin{pmatrix} \mathbf{F}_1 \\ \mathbf{T}_1 \\ \mathbf{T}_2 \\ \mathbf{S}_1 \\ \mathbf{S}_2 \end{pmatrix} = - \begin{pmatrix} \mathbf{A}_{11} & -\mathbf{B}_{11} & \mathbf{B}_{22} \\ \mathbf{B}_{11} & \mathbf{C}_{11} & \mathbf{C}_{12} \\ -\mathbf{B}_{22} & \mathbf{C}_{12} & \mathbf{C}_{22} \\ \mathbf{G}_{11} & \mathbf{H}_{11} & \mathbf{H}_{12} \\ \mathbf{G}_{22} & -\mathbf{H}_{21} & \mathbf{H}_{22} \end{pmatrix} \begin{pmatrix} \mathbf{U}_{12} \\ \mathbf{\Omega}_1 \\ \mathbf{\Omega}_2 \end{pmatrix}$$

(Kim and Karilla, 1991)

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

$\mathbf{d} \rightarrow$ displacement unit vector along axis. $\epsilon \rightarrow$ Levi-Civita symbol

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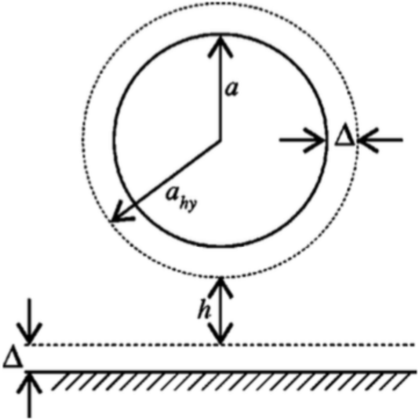
Each scalar function is a function of gap h and $\beta = \frac{a_i}{a_j}$ i.e

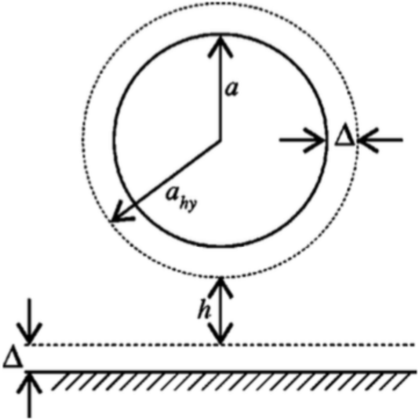
$$Y_{12}^H = 8 \log\left(\frac{1}{h}\right) \pi \eta a_i \frac{2\beta^2(1+7\beta)}{5(1+\beta)^5}$$

Lubrications



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

Lubrications



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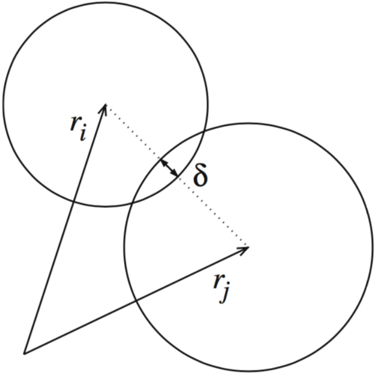
We used $\delta = 0.01$

Particle contacts



Contact model

Linear spring dashpot model (Luding, 2008)

Contact model

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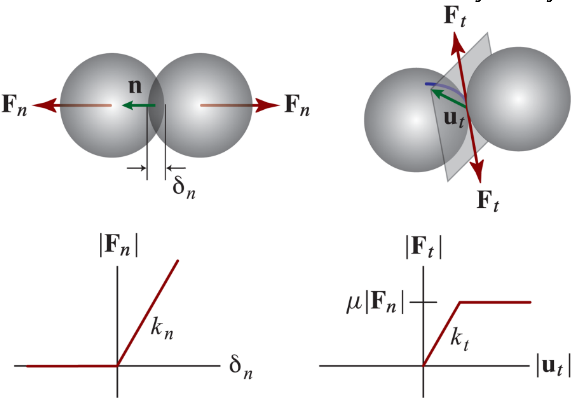

(Fleischmann, 2015)

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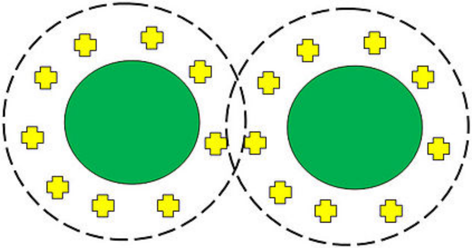
Electrostatic repulsive forces (Israelachvili, 2001)



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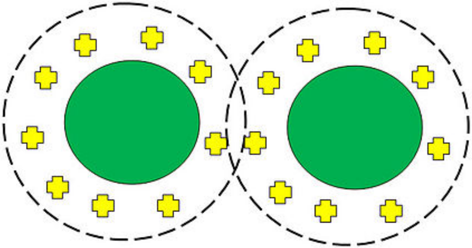

$$\mathbf{F}_{ij}^R = \frac{1}{\lambda}\left(\frac{a_i a_j}{a_i + a_j}\right) F^* \exp(-h/\lambda)\hat{\mathbf{n}}_{ij} \qquad \lambda \to \text{Debye length}$$

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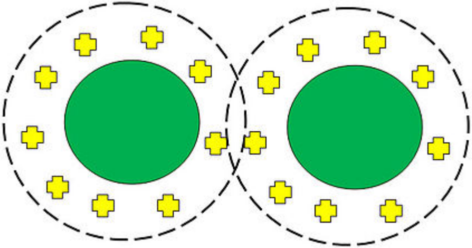

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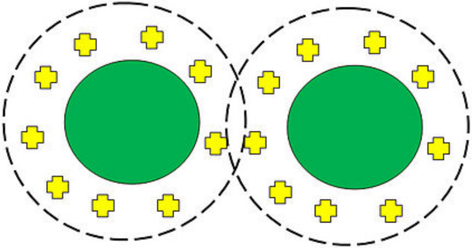

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Sheared suspensions

Sheared suspensions

- wall moves with velocity u_{wall} to x and $-x$ directions
- All simulation use N=512 particles.

Rheology

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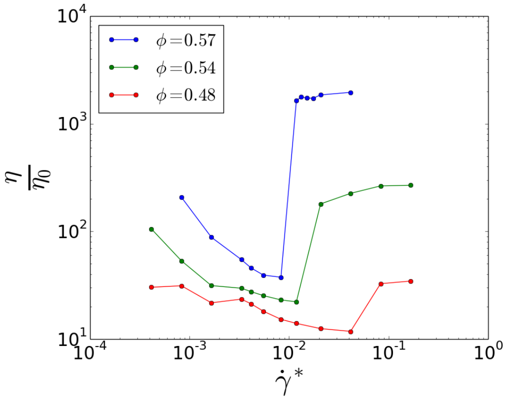
Sheared Suspensions: $\frac{\eta}{\eta_0}$ vs $\dot{\gamma}^*$, compared with results from (Mari, et al, 2014)



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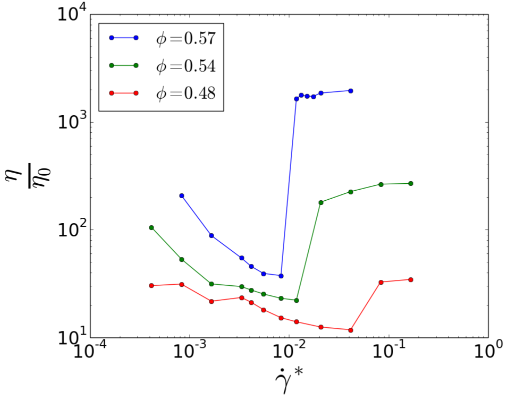

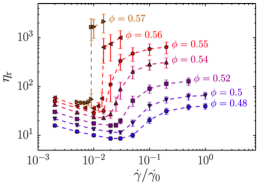

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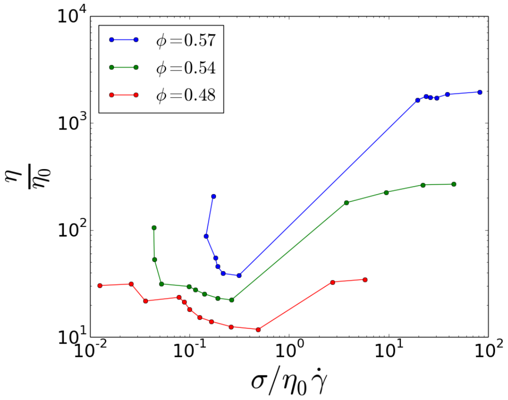

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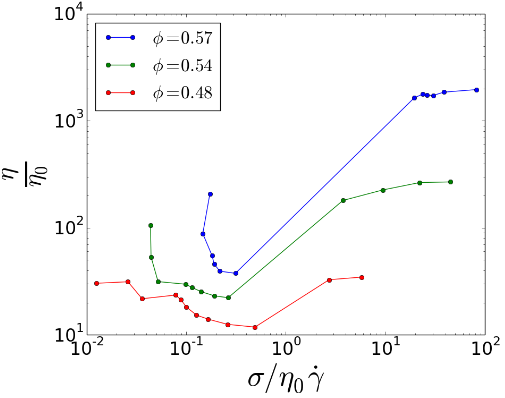
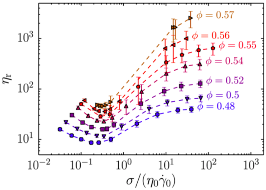
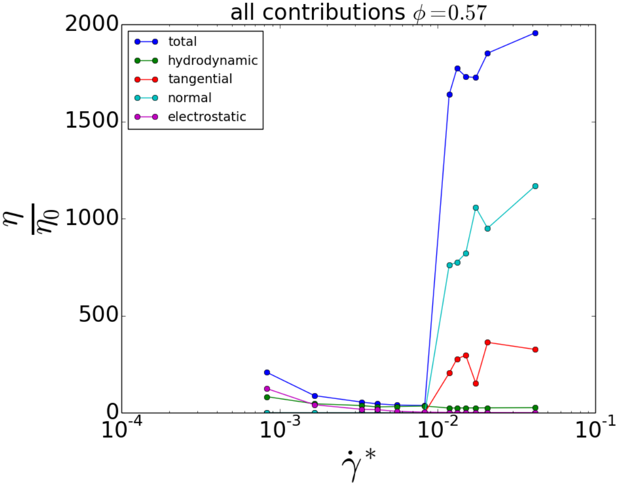




Contributions to shear viscosity for $\phi = 0.57$



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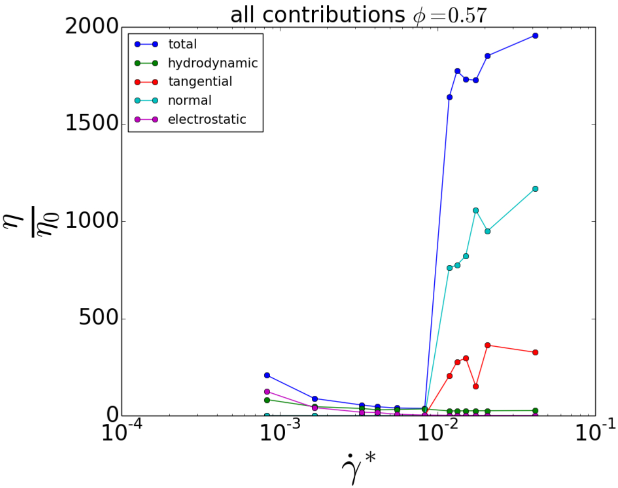

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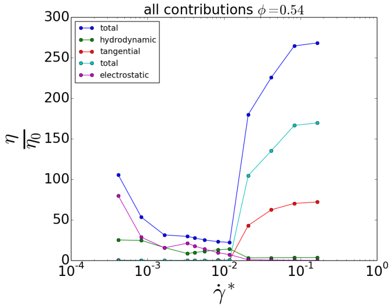

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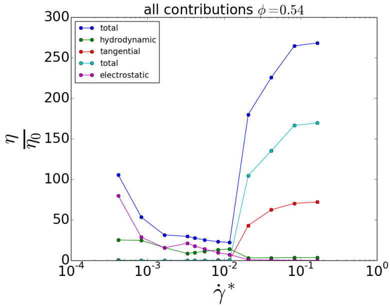

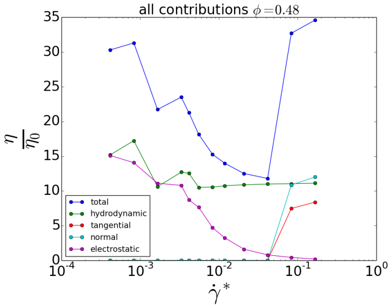

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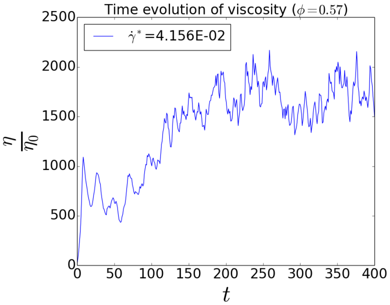

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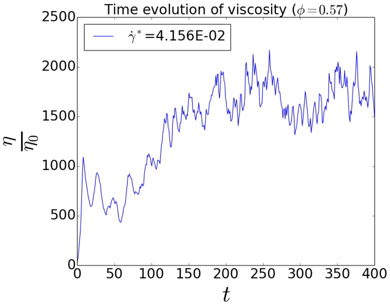

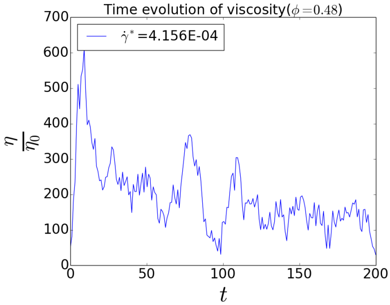

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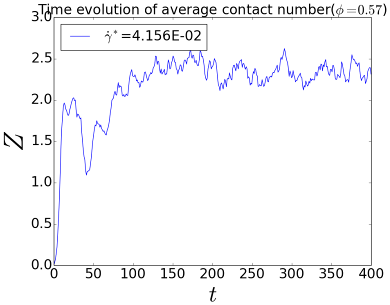

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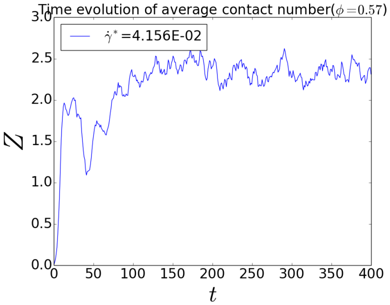

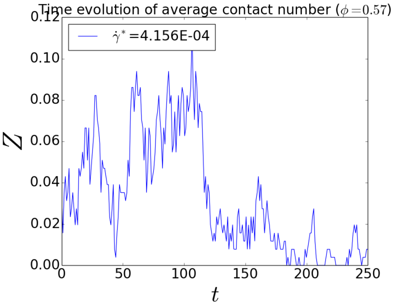

Evolution of the contact network ($\phi = 0.57$)

high shear rate

low shear rate

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References

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