

Simulation model for concentrated suspension *lubrication and contact force*

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1 Targets

Contact forces Friction, rolling friction, cohesion, these contact forces might have some influence of suspension rheology. We may expect that such contact forces tend to glow up force correlation (force chains).

Criteria of particle contact It becomes a question that how particles can get in contact when lubrication forces act between particles in sheared suspensions.

$$\mathbf{F}_{\text{lub}} = -\frac{1}{4h}(\mathbf{v}_i - \mathbf{v}_j) \cdot \mathbf{n}\mathbf{n} \quad (1)$$

This factor $1/h$ is drastic. However, it is not Coulomb type repulsive force. The divergence factor $1/h$ is in the resistance coefficient. Even if the distance is nearly zero $h \ll 1$, the lubrication force can be small if the normal element of the relative velocity is small.

In sheared suspensions, gaps between particles can become very small. If they are perfect spheres, these gaps are finite positive mathematically. In real system, particles can be get into contact due to various factors of reality. We need to introduce some persuasive manner to allow the direct contact in simulation model. We may introduce a parameter to control this nature systematically.

The replacement of $1/h$ by $1/h'$ is a possible way, where $h' \equiv r - 2a'$ with $a' < a$. This $1/h'$ does not diverge at $h = 2a$. But, this modification systematically affects overall hydrodynamic interaction. This is why this is not the best way.

We can introduce a cutoff gap h^* .

$$\alpha(h) = \begin{cases} \frac{1}{4h}, & h > h^* \\ \frac{1}{4h^*}, & h \leq h^* \end{cases} \quad (2)$$

Force chains If volume fraction of suspension is the same, the increase of viscosity can be realized by efficient configuration of particles. Many particles seem to cooperate for the resistance of flowing. Force chains are the evidence of the cooperation. Chain-like 1D structures in 3D suspension indicate the efficiency of particles' collaboration. So, understanding the law of shear-induced force chains is key task to explain shear thickening.

Avoiding ordering Shear induces layering or latticed chains [Catherall et al., 2000]. The shear induced order seems to be a simple tendency.

In packing problem, monodisperse smooth spheres tend to order. Poly- or bidispersity can prevent this.

For the case of the shear induced ordering, we may expect the mixture of different sizes can avoid in some extent. We plan to check this by introducing bi-disperse simulation.

2 Simulation method

To solve the problems, we start to work with particle scale simulation. In order to capture some large scale structure and to keep aggressive investigation, we plan to introduce a simplified model than Stokesian dynamics. We plan to follow Ball & Melrose strategy (1995-2004). They introduced lubrication dynamics to simulate concentrated suspensions. They took only the leading order terms of the two-body lubrication forces, which diverges at zero gap $h \rightarrow 0$. The force balance equations ($\mathbf{F}_H + \mathbf{F}_B + \mathbf{F}_C = \mathbf{0}$) are solved. The benefits of the lubrication dynamics is the drastic reduction of the calculation cost from Stokesian dynamics: (1) we can build the resistance matrix without matrix inversion, (2) we can solve equation by using sparse matrix algorithm. The limitation is it should be valid for only concentrated suspensions.

The main extension from Ball & Melrose model (or Stokesian dynamics) is the introduction of the direct contact forces between particles. We are preparing to combine contact models to the lubrication dynamics. We can also introduce bidisperse simulation to control shear induced ordering, though we don't know how much we can avoid it.

3 Previous works

Ball and Merlose model

Ball-1995

Ball and Melrose [1995] "Lubrication breakdown in hydrodynamic simulations of concentrated colloids" reported the difficulty of the simulation including lubrication force. Their model is FT-level ($6N$ -vectors).

$$\mathbf{F}_H = -\mathbf{R}\mathbf{V} \quad (3)$$

is used for the over damped motion.

$$\mathbf{F}_H = \mathbf{F}_C = 0. \quad (4)$$

The leading order of the pair-wise squeeze hydrodynamic force was used.

$$\mathbf{f}_i = - \sum_j \frac{3\pi\mu}{8h_{ij}} \{(\mathbf{v}_i - \mathbf{v}_j) \cdot \mathbf{n}_{ij}\} \mathbf{n}_{ij} \quad (5)$$

They reported the singular results obtained by this model. The minimum gap and viscosity depend on simulation detail, such as time step. They concluded “The ideal problem of smooth hard spheres in a Newtonian fluid under simple shear appears to be singular in nature”.

We are dubious about their modeling. Their lubrication model (5) is not the same as the leading order of Jeffrey [1992].

Melrose-1995

The article by Melrose and Ball [1995] titled “*The Pathological Behaviour of Sheared Hard Spheres with Hydrodynamic Interactions*” also discussed the difficulty with the same level.

The divergent squeeze terms in principle prevent overlap of particles, but computations with fured time steps lead to overlap.

Melrose-1996

In Melrose et al. [1996] titled “*Continuous shear thickening and colloid surfaces*”, they moved on the problem of rheology by using the model.

Ball-1997

Simulation method was reviewed by Ball and Melrose [1997], titled “*A simulation technique for many spheres in quasi-static motion under frame-invariant pair drag and Brownian forces*”.

The equation (12) in the paper is

$$-\mathbf{R}(\mathbf{V} - \mathbf{V}_0) + \mathbf{F}^C + \mathbf{F}^B - \mathbf{R}\mathbf{V}_0 = 0 \quad (6)$$

The final term in Eq. (12) is often termed the shear tensor. Here it is evaluated at the frame-invariant pair level of the basic approximation. (If the shear tensor and the matrix R are formulated separately, as, for example, in moment expansions, it may be that frame invariance is broken and this should be checked for in practice.)

In Appendix A, more explicit calculations are give. \mathbf{f}_i and \mathbf{g}_i are force and torque acting on particle $i = 1, 2$.

$$\begin{aligned} \mathbf{f}_1 &= -\mathbf{f}_2 \\ &= -a_{sq}\mathbf{N}(\mathbf{v}_1 - \mathbf{v}_2) - a_{sh}\left(\frac{2}{r}\right)^2 \mathbf{P}(\mathbf{v}_1 - \mathbf{v}_2) + \left(\frac{2}{r}\right) a_{sh}\mathbf{n} \times \mathbf{P}(\mathbf{w}_1 + \mathbf{w}_2) \\ \mathbf{g}_1 &= -\left(\frac{2}{r}\right) a_{sh}\mathbf{n} \times \mathbf{P}(\mathbf{v}_1 - \mathbf{v}_2) - a_{sh}\mathbf{P}(\mathbf{w}_1 + \mathbf{w}_2) - a_{pu}\mathbf{P}(\mathbf{w}_1 - \mathbf{w}_2) - a_{tw}\mathbf{N}(\mathbf{w}_1 - \mathbf{w}_2) \\ \mathbf{g}_2 &= -\left(\frac{2}{r}\right) a_{sh}\mathbf{n} \times \mathbf{P}(\mathbf{v}_1 - \mathbf{v}_2) - a_{sh}\mathbf{P}(\mathbf{w}_1 + \mathbf{w}_2) + a_{pu}\mathbf{P}(\mathbf{w}_1 - \mathbf{w}_2) + a_{tw}\mathbf{N}(\mathbf{w}_1 - \mathbf{w}_2) \end{aligned}$$

where $\mathbf{N} = \mathbf{n}\mathbf{n}$, $\mathbf{P} = 1 - \mathbf{n}\mathbf{n}$, and $r = d + h$.

$$\begin{aligned}
a_{\text{sq}} &= \frac{3\pi\mu d}{2} \left(\frac{d}{4h} + \frac{18}{40} \ln\left(\frac{d}{2h}\right) + \frac{9}{84} \frac{h}{d} \ln\left(\frac{d}{2h}\right) \right) \\
a_{\text{sh}} &= \frac{\pi\mu d}{2} \ln\left(\frac{d}{2h}\right) \frac{(d+h)^2}{4} \\
a_{\text{pu}} &= \frac{\pi\mu d^3}{8} \left\{ \frac{3}{20} \ln\left(\frac{d}{2h}\right) + \frac{63}{250} \frac{h}{d} \ln\left(\frac{d}{2h}\right) \right\} \\
&= 8\pi\mu a^3 \left\{ \frac{3}{160} \ln\left(\frac{a}{h}\right) + \frac{63}{4000} \frac{h}{a} \ln\left(\frac{a}{h}\right) \right\} \\
&\quad (\uparrow 3/160 \text{ should be } 3/40 \text{ according to Kumar's thesis}) \\
a_{\text{tw}} &= \frac{\pi\mu d^3 h}{4 d} \ln\left(\frac{2}{2h}\right) \quad (\Leftarrow 2d/2h?)
\end{aligned}$$

Farr-1997

Farr et al. [1997] “*Kinetic theory of jamming in hard-sphere startup flows*” discussed the physics.

Silbert-1997

Silbert et al. [1997] “Colloidal microdynamics: Pair-drag simulations of model-concentrated aggregated systems”

Silbert-1999-1

Silbert et al. [1999a] “*A structural analysis of concentrated, aggregated colloids under flow*” added an attractive force to cause aggregation and analyzed the structure.

Silbert-1999-2

Silbert et al. [1999b] “Stress distributions in flowing aggregated colloidal suspensions” also include the attractive force. They studied force correlations.

Catherall-2000

Catherall et al. [2000] “Shear thickening and order-disorder effects in concentrated colloids at high shear rates” discussed the order formation and the stability.

Melrose-2004-1

Melrose and Ball [2004a] “Continuous shear thickening transitions in model concentrated colloids –The role of interparticle forces”

They still used (5).

Melrose-2004-2

Melrose and Ball [2004b] “*Contact networks* in continuously shear thickening colloids”

Kumer

Kumar and Higdon [2010]: Origins of the anomalous stress behavior in charged colloidal suspensions under shear

He followed the same approach with Melrose and Ball. The detail description is in his thesis (Kumar [2010])

Marchioro

Marchioro and Acrivos [2001]: Shear-induced particle diffusivities from numerical simulations

Jamali

Jamali et al. [2013]: Bridging the gap between microstructure and macroscopic behavior of monodisperse and bimodal colloidal suspensions

Stokesian dynamics

- Bossis and Brady [1984]: Dynamic simulation of sheared suspensions. I. General method
- Brady and Bossis [1985]: The rheology of concentrated suspensions of spheres in simple shear flow by numerical simulation
- Brady and Bossis [1988]: Stokesian dynamics
- Bossis et al. [1988]: Shear-induced structure in colloidal suspensions I. numerical simulation
- Phung and Brady [1996]: Stokesian dynamics simulation of Brownian suspensions
- Brady and Morris [1997]: Microstructure of strongly sheared suspensions and its impact on rheology and diffusion
- Foss and Brady [2000]: Structure, diffusion and rheology of Brownian suspensions by Stokesian dynamics simulation
- Sierou and Brady [2002]: Rheology and microstructure in concentrated noncolloidal suspensions
- Morris and Katyal [2002]: Microstructure from simulated Brownian suspension flows at large shear rate
- Sierou and Brady [2004]: Shearinduced selfdiffusion in noncolloidal suspensions
- Wagner and Brady [2009]: Shear thickening in colloidal dispersions

- [Morris \[2009\]](#): A review of microstructure in concentrated suspensions and its implications for rheology and bulk flow
- [Nazockdast \[2012\]](#) Smoluchowski theory for concentrated colloidal dispersions far from equilibrium

Experiments

- [Bender and Wagner \[1996\]](#): Reversible shear thickening in monodisperse and bidisperse colloidal dispersions
- [Melrose et al. \[1996\]](#): Continuous shear thickening and colloid surfaces
- [Maranzano and Wagner \[2001a\]](#): The effects of particle size on reversible shear thickening of concentrated colloidal dispersions
- [Maranzano and Wagner \[2001b\]](#): The effects of interparticle interactions and particle size on reversible shear thickening: Hard-sphere colloidal dispersions
- [Maranzano and Wagner \[2002\]](#) Flow-small angle neutron scattering measurements of colloidal dispersion microstructure evolution through the shear thickening
- [Lee and Wagner \[2003\]](#) Dynamic properties of shear thickening colloidal suspensions

4 Questions on lubrication forces

Leading order or higher order? For near touching particles, the leading terms including the $1/h$ factor dominate to determine the particle velocities. However, there seems to be some significant differences between the leading order lubrication force and full order lubrication force.

- The simplified lubrication model includes only the squeezed mode lubrication force.
- In the full lubrication model, the tangential force and torque diverge as $\log h^{-1}$
- In the full lubrication model, the lubrication forces are depend on the orientation of two particles.

According to [Kumar \[2010\]](#), δ -log δ FLD gives good agreement with SD. (But, it is not clear how good SD is in concentrated suspension.)

Ball&Melrose model The lubrication force used in [Ball and Melrose \[1997\]](#) is the leading order terms of the full expression given by [Jeffrey \[1992\]](#). In order to simulate polydisperse system, we need to derive the leading terms from [Jeffrey \[1992\]](#).

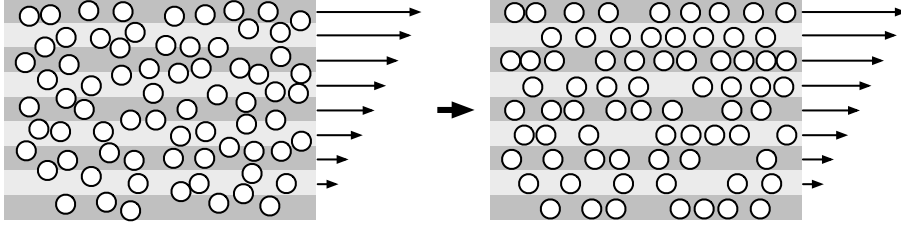
What is singularity at $Pe \rightarrow \infty$? [Ball and Melrose \[1995\]](#) and [Melrose and Ball \[1995\]](#) reported singularity of pure hydrodynamic limit. What is the reason for that? This affects the physics?

Frame invariant pair drag model

[Ball and Melrose \[1997\]](#) claims that simulation model should satisfy frame invariant. It points out that the addition of diagonal terms corresponding to Stokes drag forces relative to an assumed background shear flow breaks this invariant property. I don't understand why this approximation is so bad.

Such models are physically peculiar because they correspond to a set of particles each of which moves relative to the frame of its own independently sheared fluid.

Our first model includes the diagonal terms corresponding to Stokes drag forces. As [Ball and Melrose \[1997\]](#) pointed out, we can expect that the profile of undisturbed background flow appears in particle configuration after some shearing. Stokesian dynamics has less this tendency since the background flow can be disturbed.



$$\mathbf{R} = \mathbf{R}_{\text{onebody}} + \mathbf{R}_{\text{pair}} \quad (7)$$

$$\mathbf{R}_{\text{onebody}} = \mathbf{I}.$$

$$\begin{aligned} \mathbf{F}_H &= -\mathbf{R}(\mathbf{U} - \mathbf{U}^\infty) + \mathbf{G}\mathbf{E}^\infty \\ &= -(\mathbf{R}_{\text{onebody}} + \mathbf{R}_{\text{pair}})(\mathbf{U} - \mathbf{U}^\infty) + \mathbf{G}\mathbf{E}^\infty \end{aligned}$$

The background flow and the drag forces acting on particles are modeled by $\mathbf{U}^\infty(\mathbf{r})$ and the diagonal matrix $\mathbf{R}_{\text{onebody}}$. We may introduce a parameter s : $0 < s < 1$ for the diagonal matrix $\mathbf{R}_{\text{onebody}}$.

$$\mathbf{R}_{\text{onebody}} = s\mathbf{I} \quad (8)$$

In the dilute limit, s should converge to 1. So, a possible way is

$$s \approx \frac{(\phi_{\text{max}} - \phi)}{\phi_{\text{max}}} \quad (9)$$

$$\begin{aligned} \mathbf{F}_H &= 0 \\ \rightarrow (\mathbf{R}_{\text{onebody}} + \mathbf{R}_{\text{pair}})(\mathbf{U} - \mathbf{U}^\infty) &= \mathbf{G}\mathbf{E}^\infty \end{aligned}$$

We can find some implementation Kumar's thesis Chapter 6 (Fast lubrication dynamics algorithm) [Kumar \[2010\]](#). He extract the optimal values by comparing with Stokesian dynamics.

$$\mathbf{R}_0 = \begin{pmatrix} R_{\text{FU}}^0 & 0 & 0 \\ 0 & R_{\text{T}\Omega}^0 & 0 \\ 0 & 0 & R_{\text{SE}}^0 \end{pmatrix} \quad (10)$$

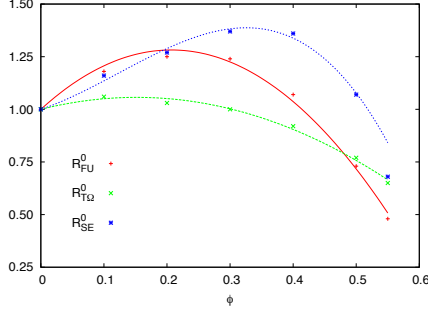


Figure 6.5: Optimal isotropic constants. Best fits in the plots are given by $R_{FU}^0 = 1 + 2.725\phi - 6.583\phi^2$, $R_{T\Omega}^0 = 1 + 0.749\phi - 2.469\phi^2$, $R_{SE}^0 = 1 + 0.9972\phi + 4.8409\phi^2 - 13.0510\phi^3$. Lubrication cutoff of $2.5a$ was used in this calculation.

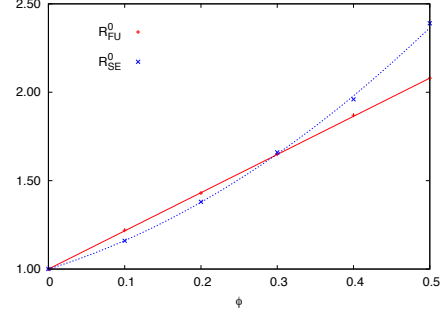


Figure 6.6: Optimal isotropic constants. Best fits in the plots are given by $R_{FU}^0 = 1 + 2.16\phi$, and $R_{SE}^0 = 1 + 1.33\phi + 2.80\phi^2$. Lubrication cutoff of $2.5a$ was used in this calculation.

Figure 1: Figure from Kumar's thesis. R_{FU}^0 can be larger than 1. The left one is with δ -log δ level, and the right one with δ level,

5 Lubrication forces

Jeffrey (1992)

Interaction between particles 1 and 2 can be written in a linear form:

$$\begin{pmatrix} \mathbf{F} \\ \mathbf{T} \\ \mathbf{S} \end{pmatrix} = -\mu \begin{pmatrix} \mathbf{A} & \tilde{\mathbf{B}} & \tilde{\mathbf{G}} \\ \mathbf{B} & \mathbf{C} & \tilde{\mathbf{H}} \\ \mathbf{G} & \mathbf{H} & \mathbf{M} \end{pmatrix} \begin{pmatrix} \mathbf{U} - \mathbf{U}_\infty \\ \boldsymbol{\Omega} - \boldsymbol{\Omega}_\infty \\ -\mathbf{E}_\infty \end{pmatrix} \quad (11)$$

Two particles are included in the expression:

$$\mathbf{F} = \begin{pmatrix} \mathbf{F}_1 \\ \mathbf{F}_2 \end{pmatrix}, \quad \mathbf{T} = \begin{pmatrix} \mathbf{T}_1 \\ \mathbf{T}_2 \end{pmatrix}, \quad \mathbf{S} = \begin{pmatrix} \mathbf{S}_1 \\ \mathbf{S}_2 \end{pmatrix}, \quad \mathbf{U} = \begin{pmatrix} \mathbf{U}_1 \\ \mathbf{U}_2 \end{pmatrix}, \quad \boldsymbol{\Omega} = \begin{pmatrix} \boldsymbol{\Omega}_1 \\ \boldsymbol{\Omega}_2 \end{pmatrix}, \quad \mathbf{E}^\infty = \begin{pmatrix} \mathbf{E}^\infty \\ \mathbf{E}^\infty \end{pmatrix} \quad (12)$$

The matrices also consist of submatrices, e.g. \mathbf{A} is written as

$$\mathbf{A} = \begin{pmatrix} \mathbf{A}_{11} & \mathbf{A}_{12} \\ \mathbf{A}_{21} & \mathbf{A}_{22} \end{pmatrix}. \quad (13)$$

Variables:

$$\mathbf{r} \equiv \mathbf{r}_2 - \mathbf{r}_1, \quad \mathbf{n} \equiv \frac{\mathbf{r}}{r} \quad (14)$$

$$s \equiv \frac{2r}{a_1 + a_2}, \quad \lambda \equiv \frac{a_2}{a_1}, \quad \xi \equiv s - 2 \quad (15)$$

Symmetries: 2-indices:

$$A_{ij}^{\alpha\beta} = A_{ji}^{\beta\alpha} \quad (16)$$

3-indices:

$$G_{ijk}^{\alpha\beta} = G_{jik}^{\alpha\beta}, \quad G_{iik}^{\alpha\beta} = H_{iik}^{\alpha\beta} = 0, \quad \tilde{G}_{ijk}^{\alpha\beta} = G_{jki}^{\beta\alpha} \quad (17)$$

4-indices:

$$M_{iikl}^{\alpha\beta} = 0, \quad M_{iikl}^{\alpha\beta} = M_{lkij}^{\beta\alpha} \quad (18)$$

Adimensional tensors: The following adimensional transformation is given in [Jeffrey and Onishi \[1984\]](#)

$$\hat{\mathbf{A}}_{\alpha\beta} = \frac{\mathbf{A}_{\alpha\beta}}{3\pi(a_\alpha + a_\beta)}, \quad \hat{\mathbf{B}}_{\alpha\beta} = \frac{\mathbf{B}_{\alpha\beta}}{\pi(a_\alpha + a_\beta)^2}, \quad \hat{\mathbf{C}}_{\alpha\beta} = \frac{\mathbf{C}_{\alpha\beta}}{\pi(a_\alpha + a_\beta)^3} \quad (19)$$

The following adimensional transformation is given in [Jeffrey \[1992\]](#)

$$\hat{\mathbf{G}}_{\alpha\beta} = \frac{\mathbf{G}_{\alpha\beta}}{\pi(a_\alpha + a_\beta)^2}, \quad \hat{\mathbf{H}}_{\alpha\beta} = \frac{\mathbf{H}_{\alpha\beta}}{\pi(a_\alpha + a_\beta)^3}, \quad \hat{\mathbf{M}}_{\alpha\beta} = \frac{\mathbf{M}_{\alpha\beta}}{(5/6)\pi(a_\alpha + a_\beta)^3} \quad (20)$$

Scalar functions From [Jeffrey and Onishi \[1984\]](#):

$$\hat{A}_{ij}^{(\alpha\beta)} = X_{\alpha\beta}^A n_i n_j + Y_{\alpha\beta}^A (\delta_{ij} - n_i n_j) \quad (21)$$

$$\hat{B}_{ij}^{(\alpha\beta)} = \hat{B}_{ji}^{(\beta\alpha)} = Y_{\alpha\beta}^B \varepsilon_{ijk} n_k \quad (22)$$

$$\hat{C}_{ij}^{\alpha\beta} = X_{\alpha\beta}^C n_i n_j + Y_{\alpha\beta}^C (\delta_{ij} - n_i n_j) \approx X_{\alpha\beta}^C n_i n_j \quad (23)$$

From [Jeffrey \[1992\]](#)

$$\hat{G}_{ijk}^{\alpha\beta} = X_{\alpha\beta}^G \left(n_i n_j - \frac{1}{3} \delta_{ij} \right) n_k + Y_{\alpha\beta}^G (n_i \delta_{jk} + n_j \delta_{ik} - 2n_i n_j n_k) \quad (24)$$

$$\hat{H}_{ij}^{\alpha\beta} = Y_{\alpha\beta}^H (n_i \varepsilon_{jkm} n_m + n_j \varepsilon_{ikm} n_m) \quad (25)$$

$$\hat{M}_{ijkl}^{\alpha\beta} = \frac{3}{2} X_{\alpha\beta}^M \left(n_i n_j - \frac{1}{3} \delta_{ij} \right) \left(n_k n_l - \frac{1}{3} \delta_{kl} \right) \quad (26)$$

$$+ \frac{1}{2} Y_{\alpha\beta}^M (n_i \delta_{jl} n_k + n_j \delta_{il} n_k + n_i \delta_{jk} n_l + n_j \delta_{ik} n_l - 4n_i n_j n_k n_l) \quad (27)$$

$$+ \frac{1}{2} Z_{\alpha\beta}^M (\delta_{ik} \delta_{jl} + \delta_{jk} \delta_{il} - \delta_{ij} \delta_{kl} + n_i n_j \delta_{kl} + \delta_{ij} n_k n_l + n_i n_j n_k n_l) \quad (28)$$

$$- n_i \delta_{jl} n_k - n_j \delta_{il} n_k - n_i \delta_{jk} n_l - n_j \delta_{ik} n_l) \quad (29)$$

$$X_{\alpha\beta}^G(s, \lambda) = -X_{(3-\alpha)(3-\beta)}^G(s, \lambda^{-1}), \quad (30)$$

$$Y_{\alpha\beta}^G(s, \lambda) = -Y_{(3-\alpha)(3-\beta)}^G(s, \lambda^{-1}), \quad (31)$$

$$Y_{\alpha\beta}^H(s, \lambda) = Y_{(3-\alpha)(3-\beta)}^G(s, \lambda^{-1}), \quad (32)$$

$$X_{\alpha\beta}^M(s, \lambda) = X_{\beta\alpha}^M(s, \lambda) = X_{(3-\alpha)(3-\beta)}^M(s, \lambda^{-1}), \quad (33)$$

$$Y_{\alpha\beta}^M(s, \lambda) = Y_{\beta\alpha}^M(s, \lambda) = Y_{(3-\alpha)(3-\beta)}^M(s, \lambda^{-1}), \quad (34)$$

$$Z_{\alpha\beta}^M(s, \lambda) = Z_{\beta\alpha}^M(s, \lambda) = Z_{(3-\alpha)(3-\beta)}^M(s, \lambda^{-1}), \quad (35)$$

$$(36)$$

The leading terms include the factor ξ^{-1} . The leading order of scalar functions are given as follows:

$$g_1(\lambda) \approx \frac{2\lambda^2}{(1+\lambda)^3}, \quad g_1(1) \approx \frac{1}{4}$$

$$X_{11}^A \approx g_1(\lambda)\xi^{-1}, \quad X_{11}^A \approx \frac{1}{4\xi} \quad (37)$$

$$X_{12}^A \approx -\frac{2}{1+\lambda}g_1(\lambda)\xi^{-1}, \quad X_{12}^A \approx -\frac{1}{\xi} \quad (38)$$

$$X_{11}^C \approx \mathcal{O}(1) + \mathcal{O}(\xi \ln \xi^{-1}) \quad (39)$$

$$X_{12}^C \approx \mathcal{O}(1) + \mathcal{O}(\xi \ln \xi^{-1}) \quad (40)$$

$$X_{11}^G \approx \frac{3}{2}g_1(\lambda)\xi^{-1}, \quad X_{11}^G \approx \frac{3}{8}\xi^{-1} \quad (41)$$

$$X_{12}^G \approx \frac{-6}{(1+\lambda)^2}g_1(\lambda)\xi^{-1}, \quad X_{12}^G \approx -\frac{3}{8}\xi^{-1}, \quad (42)$$

$$X_{11}^M \approx \frac{3}{5}g_1(\lambda)\xi^{-1}, \quad X_{11}^M \approx \frac{3}{20}\xi^{-1} \quad (43)$$

$$X_{12}^M \approx \frac{8\lambda}{(1+\lambda)^3}g_1(\lambda)\xi^{-1}, \quad X_{12}^M \approx \frac{1}{4}\xi^{-1} \quad (44)$$

Leading order If we consider only the leading terms for the nearly contacting particles ($\xi \rightarrow 0$), only \mathbf{A} and \mathbf{G} give the leading contribution to the forces.

$$\begin{pmatrix} \mathbf{F}_1 \\ \mathbf{F}_2 \end{pmatrix} \approx -\mu \begin{pmatrix} \mathbf{A}_{11} & \mathbf{A}_{12} \\ \mathbf{A}_{21} & \mathbf{A}_{22} \end{pmatrix} \begin{pmatrix} \mathbf{U}_1 - \mathbf{U}_1^\infty \\ \mathbf{U}_2 - \mathbf{U}_2^\infty \end{pmatrix} + \mu \begin{pmatrix} \tilde{\mathbf{G}}_{11} & \tilde{\mathbf{G}}_{12} \\ \tilde{\mathbf{G}}_{21} & \tilde{\mathbf{G}}_{22} \end{pmatrix} \begin{pmatrix} \mathbf{E}_\infty \\ \mathbf{E}_\infty \end{pmatrix} \quad (45)$$

$$\begin{pmatrix} \mathbf{S}_1 \\ \mathbf{S}_2 \end{pmatrix} \approx -\mu \begin{pmatrix} \mathbf{G}_{11} & \mathbf{G}_{12} \\ \mathbf{G}_{21} & \mathbf{G}_{22} \end{pmatrix} \begin{pmatrix} \mathbf{U}_1 - \mathbf{U}_1^\infty \\ \mathbf{U}_2 - \mathbf{U}_2^\infty \end{pmatrix} + \mu \begin{pmatrix} \tilde{\mathbf{M}}_{11} & \tilde{\mathbf{M}}_{12} \\ \tilde{\mathbf{M}}_{21} & \tilde{\mathbf{M}}_{22} \end{pmatrix} \begin{pmatrix} \mathbf{E}_\infty \\ \mathbf{E}_\infty \end{pmatrix} \quad (46)$$

$$\begin{aligned} F_i^{(1)} &\approx -\mu A_{ij}^{(11)}(U_j^{(1)} - U_j^{(1)\infty}) - \mu A_{ij}^{(12)}(U_j^{(2)} - U_j^{(2)\infty}) + \mu \tilde{G}_{ijk}^{(11)} E_{jk}^\infty + \mu \tilde{G}_{ijk}^{(12)} E_{jk}^\infty \\ &= -6\pi\mu a_1 \hat{A}_{ij}^{(11)}(U_j^{(1)} - U_j^{(1)\infty}) - 3\pi\mu(a_1 + a_2) \hat{A}_{ij}^{(12)}(U_j^{(2)} - U_j^{(2)\infty}) \\ &\quad + 4\pi\mu a_1^2 \hat{\tilde{G}}_{ijk}^{(11)} E_{jk}^\infty + \pi\mu(a_1 + a_2)^2 \hat{\tilde{G}}_{ijk}^{(12)} E_{jk}^\infty \\ &= -6\pi\mu a_1 \hat{A}_{ij}^{(11)}(U_j^{(1)} - U_j^{(1)\infty}) - 3\pi\mu(a_1 + a_2) \hat{A}_{ij}^{(12)}(U_j^{(2)} - U_j^{(2)\infty}) \\ &\quad + 4\pi\mu a_1^2 \hat{\tilde{G}}_{jki}^{(11)} E_{jk}^\infty + \pi\mu(a_1 + a_2)^2 \hat{\tilde{G}}_{jki}^{(21)} E_{jk}^\infty \\ &= -6\pi\mu a_1 X_{11}^A(s, \lambda) n_i n_j (U_j^{(1)} - U_j^{(1)\infty}) - 3\pi\mu(a_1 + a_2) X_{12}^A(s, \lambda) n_i n_j (U_j - U_j^{(2)\infty}) \\ &\quad + 4\pi\mu a_1^2 X_{11}^G(s, \lambda) n_i \left(n_j n_k - \frac{\delta_{jk}}{3} \right) E_{jk}^\infty + \pi\mu(a_1 + a_2)^2 X_{21}^G(s, \lambda) n_i \left(n_j n_k - \frac{\delta_{jk}}{3} \right) E_{jk}^\infty \\ &= -6\pi\mu a_1 X_{11}^A(s, \lambda) n_i n_j (U_j^{(1)} - U_j^{(1)\infty}) - 3\pi\mu(a_1 + a_2) X_{12}^A(s, \lambda) n_i n_j (U_j - U_j^{(2)\infty}) \\ &\quad + 4\pi\mu a_1^2 X_{11}^G(s, \lambda) n_i \left(n_j n_k - \frac{\delta_{jk}}{3} \right) E_{jk}^\infty - \pi\mu(a_1 + a_2)^2 X_{12}^G(s, \lambda^{-1}) n_i \left(n_j n_k - \frac{\delta_{jk}}{3} \right) E_{jk}^\infty \\ &= 6\pi\mu \left(-a_1 \frac{g_1(\lambda)}{\xi} n_i n_j (U_j^{(1)} - U_j^{(1)\infty}) + \frac{a_1 + a_2}{1 + \lambda} \frac{g_1(\lambda)}{\xi} n_i n_j (U_j^{(2)} - U_j^{(2)\infty}) \right. \\ &\quad \left. + a_1^2 \frac{g_1(\lambda)}{\xi} n_i \left(n_j n_k - \frac{\delta_{jk}}{3} \right) E_{jk}^\infty + \frac{\lambda^2}{(1 + \lambda)^2} (a_1 + a_2)^2 \frac{g_1(1/\lambda)}{\xi} n_i \left(n_j n_k - \frac{\delta_{jk}}{3} \right) E_{jk}^\infty \right) \end{aligned}$$

- $\tilde{G}_{ijk}^{(11)} = G_{jki}^{(11)}$, $\tilde{G}_{ijk}^{(12)} = G_{jki}^{(21)}$, $\tilde{G}_{ijk}^{(21)} = G_{jki}^{(12)}$, $\tilde{G}_{ijk}^{(22)} = G_{jki}^{(22)}$.
- $X_{11}^G(s, \lambda) = -X_{22}^G(s, \lambda^{-1})$ and $X_{21}^G(s, \lambda) = -X_{12}^G(s, \lambda^{-1})$
- $X_{11}^A(s, \lambda) \approx g_1(\lambda) \frac{1}{\xi}$, $X_{12}^A(s, \lambda) \approx -\frac{2}{1+\lambda} g_1(\lambda) \frac{1}{\xi}$
 $X_{11}^G(s, \lambda) \approx \frac{3}{2} g_1(\lambda) \frac{1}{\xi}$, $X_{12}^G(s, \lambda) \approx -\frac{6}{(1+\lambda)^2} g_1(\lambda) \frac{1}{\xi}$

Monodisperse $a_\alpha = a_\beta = a$, $g_1(1) = 1/4$.

$$\begin{aligned} F_i^{(1)} &= \frac{6\pi\mu a}{4\xi} \left(-n_i n_j (U_j^{(1)} - U_j^{(1)\infty}) + n_i n_j (U_j^{(2)} - U_j^{(2)\infty}) + 2a n_i \left\{ n_j n_k - \frac{\delta_{jk}}{3} \right\} E_{jk}^\infty \right) \\ &= -\frac{3\pi\mu a}{2\xi} \left(n_i n_j (U_j^{(1)} - U_j^{(1)\infty}) - n_i n_j (U_j^{(2)} - U_j^{(2)\infty}) - 2a n_i n_j E_{jk}^\infty n_k + 2a n_i (E_{xx}^\infty + E_{yy}^\infty + E_{zz}^\infty) \right) \end{aligned} \quad (47)$$

cf. Ball&Melrose expression:

$$F_i^{(1)} = -\frac{3\pi\mu a^2}{2h_{ij}} \left(n_i n_j (U_j^{(1)} - U_j^{(1)\infty}) - n_i n_j (U_j^{(2)} - U_j^{(2)\infty}) - (2 + h/a) n_i n_j E_{jk} n_k \right) \quad (48)$$

Expression in LFDEM

$$\begin{pmatrix} \mathbf{F}_1 \\ \mathbf{F}_2 \end{pmatrix} \approx -\mu \begin{pmatrix} \mathbf{A}_{11} & \mathbf{A}_{12} \\ \mathbf{A}_{21} & \mathbf{A}_{22} \end{pmatrix} \begin{pmatrix} \mathbf{U}_1 - \mathbf{U}_1^\infty \\ \mathbf{U}_2 - \mathbf{U}_2^\infty \end{pmatrix} + \mu \begin{pmatrix} \tilde{\mathbf{G}}_{11} & \tilde{\mathbf{G}}_{12} \\ \tilde{\mathbf{G}}_{21} & \tilde{\mathbf{G}}_{22} \end{pmatrix} \begin{pmatrix} \mathbf{E}_\infty \\ \mathbf{E}_\infty \end{pmatrix} \quad (49)$$

$$\begin{pmatrix} \mathbf{S}_1 \\ \mathbf{S}_2 \end{pmatrix} \approx -\mu \begin{pmatrix} \mathbf{G}_{11} & \mathbf{G}_{12} \\ \mathbf{G}_{21} & \mathbf{G}_{22} \end{pmatrix} \begin{pmatrix} \mathbf{U}_1 - \mathbf{U}_1^\infty \\ \mathbf{U}_2 - \mathbf{U}_2^\infty \end{pmatrix} + \mu \begin{pmatrix} \tilde{\mathbf{M}}_{11} & \tilde{\mathbf{M}}_{12} \\ \tilde{\mathbf{M}}_{21} & \tilde{\mathbf{M}}_{22} \end{pmatrix} \begin{pmatrix} \mathbf{E}_\infty \\ \mathbf{E}_\infty \end{pmatrix} \quad (50)$$

6 Ball&Melrose model

One-body limit:

$$\mathbf{F}_i^{\text{self}} = -6\pi\mu a(\mathbf{v}_i - \mathbf{U}^\infty(\mathbf{r}_i)) \quad (51)$$

$$\mathbf{T}_i^{\text{self}} = -8\pi\mu a^3(\boldsymbol{\omega}_i - \boldsymbol{\Omega}^\infty) \quad (52)$$

Melrose and Ball [2004a] used the leading squeeze mode of lubrication force:

$$\mathbf{F}_{ij}^{\text{pair}} = -\alpha_n(h_{ij})\{(\mathbf{v}_i - \mathbf{v}_j) \cdot \mathbf{n}_{ij}\}\mathbf{n}_{ij} \quad (53)$$

$$\mathbf{T}_{ij}^{\text{pair}} = \mathbf{0}, \quad (54)$$

where

$$\alpha_n(h_{ij}) = \frac{3\pi\mu a^2}{2h_{ij}}. \quad (55)$$

Hydrodynamic interaction acting on particle i is given by

$$\mathbf{F}_i^{\text{H}} = \mathbf{F}_i^{\text{self}} + \sum_j \mathbf{F}_{ij}^{\text{pair}} \quad (56)$$

$$\mathbf{T}_i^{\text{H}} = \mathbf{T}_i^{\text{self}} \quad (57)$$

Dimensionless equations

The unit of length, velocity and force are given: $L_0 = a$, $v_0 = a\dot{\gamma}$, and $F_0 \equiv 6\pi\mu a v_0$.

The dimensionless variables are introduced: $\tilde{h}_{ij} = h_{ij}/L_0$, $\tilde{\mathbf{v}}_i = \mathbf{v}_i/U_0$, and $\tilde{\mathbf{F}}_{ij}^{\text{pair}} = \mathbf{F}_{ij}^{\text{pair}}/F_0$.

The relations are written as follows:

$$\tilde{\mathbf{F}}_i^{\text{self}} = -(\tilde{\mathbf{v}}_i - \tilde{\mathbf{U}}^\infty(\tilde{\mathbf{r}}_i)) \quad (58)$$

$$\tilde{\mathbf{F}}_{ij}^{\text{pair}} = -\frac{1}{4\tilde{h}_{ij}}\{(\tilde{\mathbf{v}}_i - \tilde{\mathbf{v}}_j) \cdot \mathbf{n}_{ij}\}\mathbf{n}_{ij} \quad (59)$$

$$\mathbf{U}^\infty(\mathbf{r}) = \dot{\gamma}z\mathbf{e}_x \quad (60)$$

$$\Rightarrow \tilde{\mathbf{U}}^\infty(\tilde{\mathbf{r}}) = \dot{\gamma}z\mathbf{e}_x/U_0 = \dot{\gamma}z\mathbf{e}_x/(\dot{\gamma}a) = \tilde{z}\mathbf{e}_x \quad (61)$$

Matrix form

$$\begin{aligned} \mathbf{F}_{\alpha\beta}^{\text{pair}} &= -\frac{1}{4h_{\alpha\beta}}\{(\mathbf{v}_\alpha - \mathbf{v}_\beta) \cdot \mathbf{n}_{\alpha\beta}\}\mathbf{n}_{\alpha\beta} \\ &= -\frac{1}{4h_{\alpha\beta}}\left[\{(\mathbf{v}_\alpha - \mathbf{U}_\alpha^\infty) - (\mathbf{v}_\beta - \mathbf{U}_\beta^\infty) + \mathbf{U}_\alpha^\infty - \mathbf{U}_\beta^\infty\} \cdot \mathbf{n}_{\alpha\beta}\right]\mathbf{n}_{\alpha\beta} \end{aligned}$$

$$\Delta \mathbf{v} \equiv (\mathbf{v} - \mathbf{U}^\infty)$$

$$\begin{aligned} \Delta \mathbf{v} \cdot \mathbf{n} \mathbf{n} &= (\Delta v_x n_x + \Delta v_y n_y + \Delta v_z n_z) n_x \mathbf{i} \\ &\quad + (\Delta v_x n_x + \Delta v_y n_y + \Delta v_z n_z) n_y \mathbf{j} \\ &\quad + (\Delta v_x n_x + \Delta v_y n_y + \Delta v_z n_z) n_z \mathbf{k} \\ &= \begin{pmatrix} n_x n_x & n_y n_x & n_z n_x \\ n_x n_y & n_y n_y & n_z n_y \\ n_x n_z & n_y n_z & n_z n_z \end{pmatrix} \begin{pmatrix} \Delta v_x \\ \Delta v_y \\ \Delta v_z \end{pmatrix} \\ (\Delta \mathbf{v} \cdot \mathbf{n} \mathbf{n})_i &= n_i n_j \Delta v_j \end{aligned}$$

$$\begin{aligned} \mathbf{F}_\alpha &= -\Delta \mathbf{v}_\alpha - \sum_\beta \frac{1}{4h_{\alpha\beta}} (\mathbf{n}_{\alpha\beta}(\mathbf{n}_{\alpha\beta} \cdot \Delta \mathbf{v}_\alpha) - \mathbf{n}_{\alpha\beta}(\mathbf{n}_{\alpha\beta} \cdot \Delta \mathbf{v}_\beta) + \mathbf{n}_{\alpha\beta} \{ \mathbf{n}_{\alpha\beta} \cdot (\mathbf{U}_\alpha^\infty - \mathbf{U}_\beta^\infty) \}) \\ &= -\Delta \mathbf{v}_\alpha - \sum_\beta \frac{1}{4h_{\alpha\beta}} (\mathbf{n}_{\alpha\beta}(\mathbf{n}_{\alpha\beta} \cdot \Delta \mathbf{v}_\alpha) - \mathbf{n}_{\alpha\beta}(\mathbf{n}_{\alpha\beta} \cdot \Delta \mathbf{v}_\beta) + \mathbf{n}_{\alpha\beta} \{ \dots \}) \\ &= -\Delta \mathbf{v}_\alpha - \sum_\beta \frac{1}{4h_{\alpha\beta}} (\mathbf{n}_{\alpha\beta}(\mathbf{n}_{\alpha\beta} \cdot \Delta \mathbf{v}_\alpha) - \mathbf{n}_{\alpha\beta}(\mathbf{n}_{\alpha\beta} \cdot \Delta \mathbf{v}_\beta) - r_{\alpha\beta} \mathbf{n}_{\alpha\beta} \{ \mathbf{n}_{\alpha\beta} \cdot (\mathbf{E}^\infty \mathbf{n}_{\alpha\beta}) \}) \end{aligned}$$

$$\mathbf{n}_{\alpha\beta} = \mathbf{r}^\beta - \mathbf{r}^\alpha$$

$$\begin{aligned} \mathbf{n}_{\alpha\beta} \{ \dots \} &= \mathbf{n}_{\alpha\beta} \{ \mathbf{n}_{\alpha\beta} \cdot (\Omega^\infty \times (\mathbf{r}^\alpha - \mathbf{r}^\beta) + \mathbf{E}^\infty(\mathbf{r}^\alpha - \mathbf{r}^\beta)) \} \\ &= r_{\alpha\beta} \mathbf{n}_{\alpha\beta} \{ (\mathbf{n}_{\alpha\beta} \cdot \Omega^\infty \times \mathbf{n}_{\alpha\beta} - \mathbf{n}_{\alpha\beta} \cdot (\mathbf{E}^\infty \mathbf{n}_{\alpha\beta})) \} \\ &= -r_{\alpha\beta} \mathbf{n}_{\alpha\beta} \{ \mathbf{n}_{\alpha\beta} \cdot (\mathbf{E}^\infty \mathbf{n}_{\alpha\beta}) \} \end{aligned}$$

$$\begin{aligned} F_i^\alpha &= -\Delta v_i^\alpha - \frac{1}{4h} \left(n_i n_j \Delta v_j^\alpha - n_i n_j \Delta v_j^\beta - r n_i n_j n_k E_{jk} \right) \\ &= -\Delta v_i^\alpha - \frac{1}{4h} \left(n_i n_j \Delta v_j^\alpha - n_i n_j \Delta v_j^\beta - r n_i n_j n_k E_{jk} \right) \end{aligned}$$

$$\begin{pmatrix} \vdots \\ \mathbf{F}_i \\ \vdots \\ \mathbf{F}_j \\ \vdots \end{pmatrix} = \begin{pmatrix} \vdots \\ \mathbf{F}_i^{\text{self}} + \mathbf{F}_{ij}^{\text{pair}} \\ \vdots \\ \mathbf{F}_j^{\text{self}} + \mathbf{F}_{ji}^{\text{pair}} \\ \vdots \end{pmatrix} \quad (62)$$

$$= - \begin{pmatrix} \dots & \dots & \dots & \dots & \dots \\ \dots & 1 + \frac{1}{4h_{ij}} \mathbf{n}_{ij} \otimes \mathbf{n}_{ij} & \dots & -\frac{1}{4h_{ij}} \mathbf{n}_{ij} \otimes \mathbf{n}_{ij} & \dots \\ \dots & \dots & \dots & \dots & \dots \\ \dots & -\frac{1}{4h_{ji}} \mathbf{n}_{ji} \otimes \mathbf{n}_{ji} & \dots & 1 + \frac{1}{4h_{ji}} \mathbf{n}_{ji} \otimes \mathbf{n}_{ji} & \dots \\ \dots & \dots & \dots & \dots & \dots \end{pmatrix} \begin{pmatrix} \vdots \\ \Delta \mathbf{v}_i \\ \vdots \\ \Delta \mathbf{v}_j \\ \vdots \end{pmatrix} \quad (63)$$

$$+ \begin{pmatrix} \vdots \\ -\frac{1}{4h_{ij}} \frac{(z_i - z_j)(x_i - x_j)}{r_{ij}} \mathbf{n}_{ij} \\ \vdots \\ -\frac{1}{4h_{ji}} \frac{(z_j - z_i)(x_j - x_i)}{r_{ji}} \mathbf{n}_{ji} \\ \vdots \end{pmatrix} \quad (64)$$

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