Particle pair interactions

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with illustrations by Sylvie Pic

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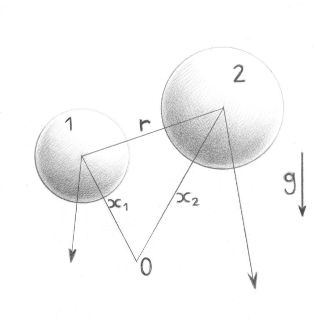
Cambridge Texts in Applied Mathematics

1. Sedimenting pair
   - Method of reflections
2. A pair in a shear
3. Pair lubrication interactions
   - Two spheres in squeeze flow
4. Stokesian dynamics

Sedimenting pair



$$\mathbf{F_1^e} = \frac{4}{3}\pi a_1^3(\rho_p - \rho)\mathbf{g}$$

$$\mathbf{F_2^e} = \frac{4}{3}\pi a_2^3(\rho_p - \rho)\mathbf{g}$$

- Balance of force

$$\mathbf{F_1^h} + \mathbf{F_1^e} = 0 \quad \text{and} \quad \mathbf{F_2^h} + \mathbf{F_2^e} = 0$$

- Mobility formulation

$$\begin{pmatrix} \mathbf{U_1} \\ \mathbf{U_2} \end{pmatrix} = \begin{pmatrix} \mathbf{M_{11}} & \mathbf{M_{12}} \\ \mathbf{M_{21}} & \mathbf{M_{22}} \end{pmatrix} \cdot \begin{pmatrix} \mathbf{F_1^e} \\ \mathbf{F_2^e} \end{pmatrix}$$

- When $r \to \infty$

$$\mathbf{M_{12}} = \mathbf{M_{21}} = 0 \quad \mathbf{M_{11}} = \frac{\mathbf{I}}{6\pi\mu a_1} \quad \mathbf{M_{22}} = \frac{\mathbf{I}}{6\pi\mu a_2}$$

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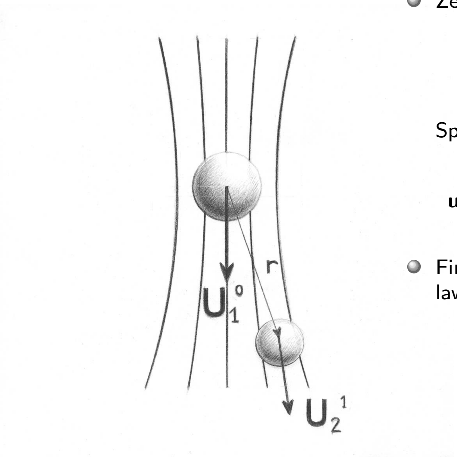
Method of reflections



- Zeroth reflection

$$\mathbf{U_1^0} = \frac{\mathbf{F_1^e}}{6\pi\mu a_1} \quad \text{and} \quad \mathbf{U_2^0} = \frac{\mathbf{F_2^e}}{6\pi\mu a_2}$$

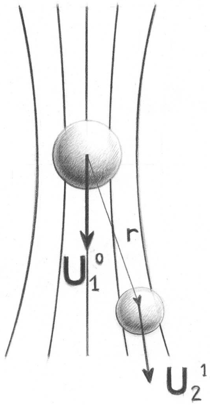
Sphere 1 causes a fluid velocity disturbance

$$\mathbf{u_1^0} = (\frac{\mathbf{I}}{r} + \frac{\mathbf{xx}}{r^3}) \cdot \frac{\mathbf{F_1^e}}{8\pi\mu} + (\frac{\mathbf{I}}{3r^3} - \frac{\mathbf{xx}}{r^5}) \cdot \frac{a^2\mathbf{F_1^e}}{8\pi\mu}$$

- First reflection on sphere 2 given by Faxen law

$$\begin{aligned} \mathbf{U_2^1} &= \mathbf{u_1^0}(\mathbf{r}) + \frac{a_2^2}{6}\nabla^2\mathbf{u}_1^0(\mathbf{r}) \\ &= \frac{1}{8\pi\mu}(\frac{\mathbf{I}}{r} + \frac{\mathbf{rr}}{r^3}) \cdot \mathbf{F_1^e} + O(r^{-3}) \end{aligned}$$

Mobility formulation



- Total velocity of sphere 2 using principle of superposition

$$\mathbf{U}_2^0+\mathbf{U}_2^1=\frac{\mathbf{I}}{6\pi\mu a_2}\cdot\mathbf{F}_2^e+\frac{1}{8\pi\mu}(\frac{\mathbf{I}}{r}+\frac{\mathbf{rr}}{r^3})\cdot\mathbf{F}_1^e+O(r^{-3})$$

- Mobility relation

$$\begin{pmatrix}\mathbf{U_1}\\ \mathbf{U_2}\end{pmatrix} = \boldsymbol{\mathcal{M}}\cdot\begin{pmatrix}\mathbf{F_1^e}\\ \mathbf{F_2^e}\end{pmatrix}$$

$$\boldsymbol{\mathcal{M}}=\begin{pmatrix}\frac{\mathbf{I}}{6\pi\mu a_1} & \frac{1}{8\pi\mu}(\frac{\mathbf{I}}{r}+\frac{\mathbf{rr}}{r^3})\\ \frac{1}{8\pi\mu}(\frac{\mathbf{I}}{r}+\frac{\mathbf{rr}}{r^3}) & \frac{\mathbf{I}}{6\pi\mu a_2}\end{pmatrix}$$

with an error of $O(r^{-3})$

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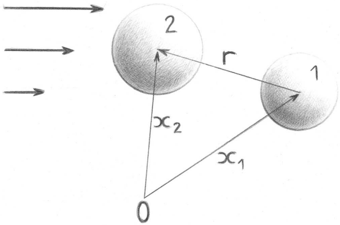
Pair of freely suspended spheres in a simple shear flow



pair approach one another as the result of the ambient motion

- Ambient shear flow

$$\mathbf{u}^\infty = \mathbf{G}^\infty\cdot\mathbf{x} = (\mathbf{E}^\infty + \boldsymbol{\Omega}^\infty)\cdot\mathbf{x}$$

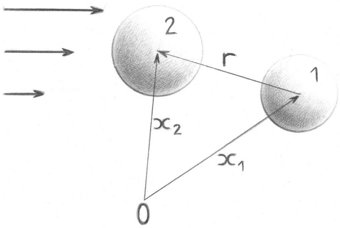
- Isolated particle motions ($r \to \infty$)

$$\begin{aligned}\mathbf{U}_1^\infty &= \mathbf{u}^\infty(\mathbf{x}_1) \quad \text{and} \quad \boldsymbol{\omega}_1^\infty = \boldsymbol{\omega}^\infty(\mathbf{x}_1),\\ \mathbf{U}_2^\infty &= \mathbf{u}^\infty(\mathbf{x}_2) \quad \text{and} \quad \boldsymbol{\omega}_2^\infty = \boldsymbol{\omega}^\infty(\mathbf{x}_2)\end{aligned}$$

- Relative motion of a pair at large separation

$$\mathbf{U}_{\mathrm{rel}} = \mathbf{U}_2^\infty - \mathbf{U}_1^\infty = \mathbf{G}^\infty\cdot(\mathbf{x}_2 - \mathbf{x}_1) = \mathbf{G}^\infty\cdot\mathbf{r}$$

Particle velocity disturbances



- Spheres deviate from the isolated-particle motions in order to satisfy the requirement of remaining force- and torque-free
- Sphere 2 causes a fluid velocity disturbance at the position of sphere 1

$$\mathbf{u}(\mathbf{x_1}) - \mathbf{u}^\infty \sim r^{-2} \quad \text{due to stresslet-induced flow}$$

- First reflection approximation of the velocity of sphere 1

$$\mathbf{U}_1' = \mathbf{U_1} - \mathbf{u}^\infty(\mathbf{x_1}) \sim r^{-2}$$

- For equal-sized particles

$$\mathbf{U}_2' = -\mathbf{U}_1'$$

Resistance formulation

- Resistance relation in condensed notation

$$\begin{pmatrix} \hat{\mathbf{F}}^{\mathbf{h}} \\ \mathbf{S}^{\mathbf{h}} \end{pmatrix} = \begin{pmatrix} \mathbf{0} \\ \mathbf{S}^{\mathbf{h}} \end{pmatrix} = - \begin{pmatrix} \hat{\mathbf{R}}^{\mathbf{FU}} & \hat{\mathbf{R}}^{\mathbf{FE}} \\ \hat{\mathbf{R}}^{\mathbf{SU}} & \mathbf{R}^{\mathbf{SE}} \end{pmatrix} \cdot \begin{pmatrix} \hat{\mathbf{U}}' \\ -\mathbf{E}^{\infty} \end{pmatrix}$$

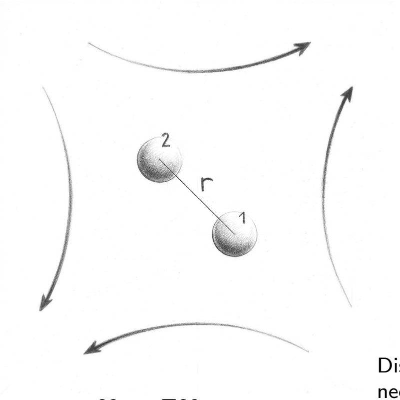
with $\hat{\mathbf{F}}^{\mathbf{h}} = (\mathbf{F}^{\mathbf{h}}, \mathbf{T}^{\mathbf{h}})$ and $\hat{\mathbf{U}}' = (\mathbf{U} - \mathbf{U}^{\infty}, \boldsymbol{\omega} - \boldsymbol{\omega}^{\infty})$

- Pair motions

$$\begin{aligned} \hat{\mathbf{U}}' = \hat{\mathbf{U}} - \hat{\mathbf{U}}^{\infty} &= (\hat{\mathbf{R}}^{\mathbf{FU}})^{-1} \cdot \hat{\mathbf{R}}^{\mathbf{FE}} : \mathbf{E}^{\infty} \\ &= \hat{\mathbf{M}} \cdot \mathbf{F}^{\mathbf{E}} \end{aligned}$$

with
  - $\hat{\mathbf{M}} = (\hat{\mathbf{R}}^{\mathbf{FU}})^{-1}$ translational-rotational mobility
  - $\mathbf{F}^{\mathbf{E}} = \hat{\mathbf{R}}^{\mathbf{FE}} : \mathbf{E}^{\infty}$ forces (and torques) due to the interaction of the pair in a shear flow

Origin of the hydrodynamic force associated with the pair motion in a straining flow



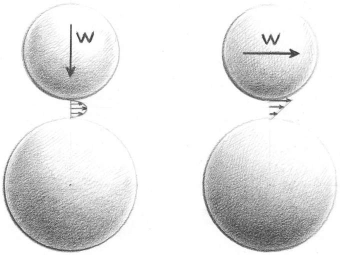
$$\mathbf{u}^{\infty} = \mathbf{E}^{\infty} \cdot \mathbf{x}$$

- As the particle surfaces approach
  - each particle encounters the flow generated by the other as each pushes fluid in front of it
  - an elevated pressure is formed between the pair of particles
  - the particles experience a hydrodynamic force which resists the relative motion, equal to $\hat{\mathbf{R}}^{\mathbf{FE}}:\mathbf{E}^{\infty}$
- In order that the hydrodynamic force and torque be zero, the particles must move with a velocity differing from the bulk motion such that

$$-\hat{\mathbf{R}}^{\mathbf{FU}}\cdot(\mathbf{U} - \mathbf{U}^{\infty}) + \hat{\mathbf{R}}^{\mathbf{FE}}:\mathbf{E}^{\infty} = 0$$

Disturbance translational velocities $\equiv$ magnitude necessary to obtain a zero hydrodynamic force

Squeezing and shearing problems

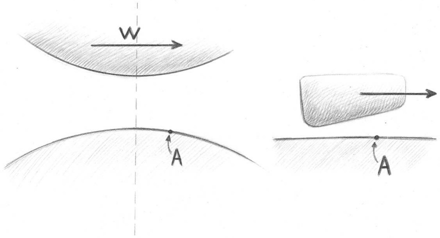


$F_{sq} \sim \mu a W \epsilon^{-1}$ $F_{sh} \sim \mu a W \ln \epsilon$

- Surface separation $r - 2a = h_0 = \epsilon a$ with $\epsilon \ll 1$
- Large pressure in the gap $p \sim (\mu W/a)\epsilon^{-2}$
- Divergence of force in the squeezing motion

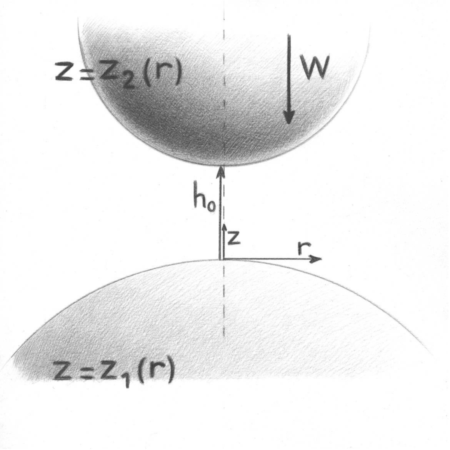
$$\begin{aligned} F_{sq} &\sim p \times S \\ &\sim (\mu W/a)\epsilon^{-2} \times \epsilon a^2 \\ &\sim \mu a W \epsilon^{-1} \end{aligned}$$

Shearing and sliding block problems



- Positive pressure at point A in either case
- Negative pressure at the mirror image point of A for the spheres: positive and negative pressures cancel in the vertical direction, normal to the motion
- Divergence of force in the shearing motion: logarithmic singularity

Geometry approximation



$a = \frac{a_1 a_2}{a_1 + a_2}$

- For $r \ll a_2$

$$\begin{aligned} z_2 &= a_2 + h_0 - (a_2^2 - r^2)^{\frac{1}{2}} \\ &\approx h_0 + \frac{r^2}{2a_2} \end{aligned}$$

- For $r \ll a_1$

$$z_1 = -a_1 + (a_1^2 - r^2)^{\frac{1}{2}} \approx -\frac{r^2}{2a_1}$$

- Distance between spheres

$$\begin{aligned} h(r) &= z_2 - z_1 \approx h_0 + \frac{r^2}{2}(\frac{1}{a_2} + \frac{1}{a_1}) \\ &\approx h_0 + \frac{r^2}{2a} = h_0(1 + \frac{r^2}{2ah_0}) \end{aligned}$$

Length and velocity scales

Continuity equation

$$\frac{1}{r}\frac{\partial(ru)}{\partial r} + \frac{\partial w}{\partial z} = 0$$

$$O\left(\frac{U}{\sqrt{ah_0}}\right) \qquad O\left(\frac{W}{h_0}\right)$$

- axial z-length scale: $h_0 = \epsilon a$ with $\epsilon \ll 1$
- radial r-length scale: $\sqrt{ah_0} = \epsilon^{1/2} a$
- axial z-velocity scale: W
- radial r-velocity scale: $U = W\sqrt{a/h_0} = \epsilon^{-1/2} W \gg W$

Flow approximately unidirectional

Lubrication approximation

- r-component of momentum equation for $\epsilon \ll 1$

$$
\begin{array}{cccc}
 & -\dfrac{\partial p}{\partial r} & + & \mu\dfrac{\partial}{\partial r}[\dfrac{1}{r}\dfrac{\partial(ru)}{\partial r}] + \mu\dfrac{\partial^2 u}{\partial z^2} = 0 \\
 & O(\dfrac{P}{\sqrt{ah_0}}) & & O(\dfrac{\mu W\sqrt{\frac{a}{h_0}}}{ah_0}) \ll O(\dfrac{\mu W\sqrt{\frac{a}{h_0}}}{h_0^2}) \\
\therefore & -\dfrac{\partial p}{\partial r} & + & \mu\dfrac{\partial^2 u}{\partial z^2} = 0
\end{array}
$$

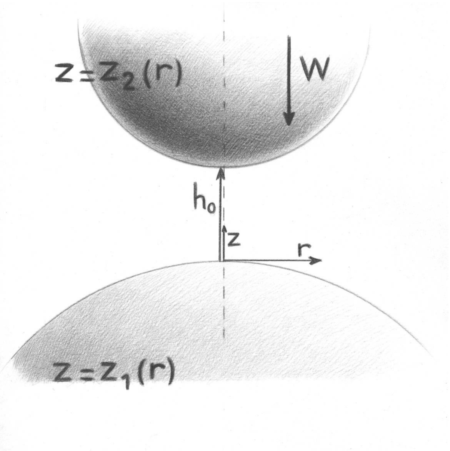
scale for the pressure: $P = \dfrac{\mu a W}{h_0^2} = \dfrac{\mu W}{a}\epsilon^{-2}$

- z-component of momentum equation for $\epsilon \ll 1$

$$
\begin{array}{ccccccc}
 & -\dfrac{\partial p}{\partial z} & + & \mu\dfrac{1}{r}\dfrac{\partial}{\partial r}(r\dfrac{\partial w}{\partial r}) + \mu\dfrac{\partial^2 w}{\partial z^2} = 0 & & & \\
 & O(\dfrac{P}{h_0}) & \gg & O(\dfrac{\mu W}{ah_0}) & \ll & O(\dfrac{\mu W}{h_0^2}) & \\
\therefore & \dfrac{\partial p}{\partial z} & = & 0 & & &
\end{array}
$$

pressure constant across the gap: $p = p(r)$

Velocity field



- Lubrication equation

$$-\frac{dp(r)}{dr} + \mu \frac{\partial^2 u(r,z)}{\partial z^2} = 0$$

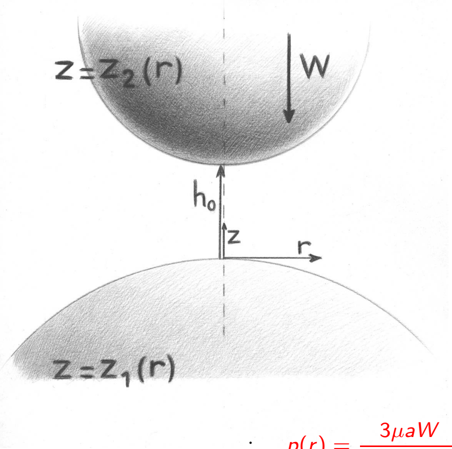
- Boundary conditions

$$u(r, z_1) = u(r, z_2) = 0$$

- Parabolic velocity profile

$$u(r,z) = \frac{1}{2\mu}\frac{dp}{dr}[z - z_1(r)][z - z_2(r)]$$

Pressure field



- Mass conservation equation

$$\begin{aligned}\pi r^2 W &= 2\pi r \int_{z_1}^{z_2} u(r,z)dz \\ &= -2\pi r \frac{h^3}{12\mu}\frac{dp}{dr}\end{aligned}$$

- Pressure

$$\begin{aligned}\int_r^{r\to\infty} -dp &= 6\mu W \int_r^{\infty} \frac{r}{h^3} dr \\ &= 6\mu a W \int_h^{\infty} \frac{dh}{h^3}\end{aligned}$$

$$\therefore \quad p(r) = \frac{3\mu a W}{(h_0 + \frac{r^2}{2a})^2} = \frac{3\mu W/a}{\epsilon^2(1+\frac{r^2}{2a^2\epsilon})^2}$$

Lubrication force

- Pressure $O(\frac{\mu a W}{h_0^2})$ dominates viscous stresses $O(\frac{\mu W \sqrt{\frac{a}{h_0}}}{h_0})$
- Magnitude of lubrication force

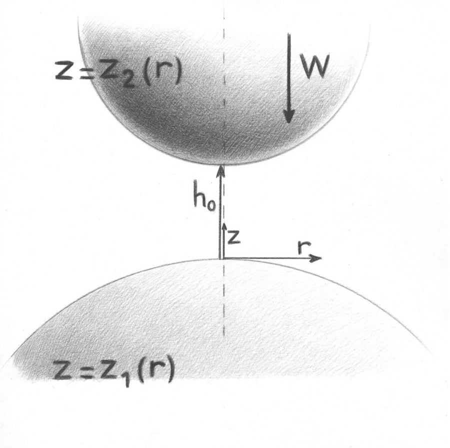
$$
\begin{aligned}
F^l &= \int_{r=0}^{r\to\infty} p(r) 2\pi r dr = \int_{h=h_0}^{h\to\infty} p(h) 2\pi a dh \\
&= 6\pi\mu a^2 W \int_{h_0}^{\infty} \frac{dh}{h^2} = 6\pi\mu a^2 W / h_0 = 6\pi\mu a W \epsilon^{-1}
\end{aligned}
$$

- Distance between sphere for constant imposed force $F^l = 6\pi\mu a^2 \frac{dh_0}{dt} / h_0$

$$
h_0(t) = h_0(t_0) \exp[-\frac{F_l}{6\pi\mu a^2}(t - t_0)]
$$

infinite time before touching but in reality contact in a finite time because of roughness and/or van der Waals force!

Resistance formulation



Resistance matrix
for the squeeze flow problem:

$$\begin{pmatrix} \mathbf{F}_1^l \\ \mathbf{F}_2^l \end{pmatrix} = -\mathcal{R}^l \cdot \begin{pmatrix} \mathbf{U}_1 \\ \mathbf{U}_2 \end{pmatrix}$$

$$\mathcal{R}^l = \frac{6\pi\mu a^2}{h_0} \begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix}$$

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Stokesian dynamics [Brady and Bossis, 1988]

Molecular-dynamics-like approach for dynamically simulating the behavior of many particles suspended or dispersed in a fluid medium

$$\text{Langevin equation: } m\frac{d\mathbf{U}}{dt} = \mathbf{F}^{\mathbf{h}} + \mathbf{F}^{\mathbf{e}} + \mathbf{F}^{\mathbf{b}}$$

- $\mathbf{F}^{\mathbf{h}}$ hydrodynamic force
- $\mathbf{F}^{\mathbf{e}}$ interparticle and external forces typically derivable from a potential
- $\mathbf{F}^{\mathbf{b}}$ random Brownian force representing the effect of a continuous series of collisions with the molecules of the underlying fluid

SD for non-Brownian particles in Stokes-flow conditions

- Balance of force (no inertia): $\mathbf{F^h} + \mathbf{F^e} = 0$
- Resistance formulation

$$\begin{pmatrix} \hat{\mathbf{F}} \\ \mathbf{S} \end{pmatrix} = -\mathcal{R}\cdot \begin{pmatrix} \hat{\mathbf{U}} - \hat{\mathbf{U}}^\infty \\ -\mathbf{E}^\infty \end{pmatrix} \text{ with } \hat{\mathbf{F}}^\mathbf{h} = (\mathbf{F^h}, \mathbf{T^h}) \text{ and } \hat{\mathbf{U}} = (\mathbf{U}, \boldsymbol{\omega})$$

- Grand resistance matrix

$$\mathcal{R} = \begin{pmatrix} \hat{\mathbf{R}}^\mathbf{FU} & \hat{\mathbf{R}}^\mathbf{FE} \\ \hat{\mathbf{R}}^\mathbf{SU} & \mathbf{R}^\mathbf{SE} \end{pmatrix} \quad \text{constructed as } \mathcal{R} = (\mathcal{M}^\infty)^{-1} + \mathcal{R}^l - \mathcal{R}^{l,\infty}$$

- Equation for particle motions

$$\hat{\mathbf{U}} - \hat{\mathbf{U}}^\infty = (\hat{\mathbf{R}}^\mathbf{FU})^{-1} \cdot (\hat{\mathbf{F}}^\mathbf{e} + \hat{\mathbf{R}}^\mathbf{FE} : \mathbf{E}^\infty)$$

General reference on Stokesian dynamics

Brady, J. F., and Bossis, G. 1988. Stokesian Dynamics. *Annu. Rev. Fluid Mech.*, **20**, 111–157.