Brownian Motion near a Soft Surface

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MC24 - Simulations des colloïdes

Brownian motion

- ▶ 1827, Robert Brown: random motion of pollen particles;
- 1901, Louis Bachelier: theory of speculation;
- ▶ 1905, Albert Einstein: diffusive model; $D_{\text{bulk}} = \frac{k_{\text{B}}T}{6\pi nr}$
- 1908, Paul Langevin: equations of motions;
- ▶ 1909, Jean Perrin: experiments to measure N_A;





Brownian motion of pollen J. Perrin, in *Atoms*, London: Constable **1914**, pp. 115.

Brownian motion of stock price

Confined Brownian motion





L. Faucheux, A. Libchaber. Phys. Rev. E. 1994, 49(6), 5158.



M. Lavaud, et al. Phys. Rev. Res. 2021, 3(3), L032011.



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 \circ ElastoHydroDynamic lift force



J. Skotheim, L. Mahadevan. Phys. Rev. Lett. 2004, 92, 245509.



Z. Zhang, et al. Phys. Rev. Lett. 2020, 124(5), 054502.

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 \odot Situation of the problem

Brownian motion

Confined

ElastoHydroDynamics

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\odot Situation of the problem



\odot Elastohydrodynamic interactions



$$\begin{aligned} x &= X_{\rm G} \cdot r\sqrt{2\varepsilon} \\ \delta &= \Delta \cdot r\varepsilon \\ \theta &= \Theta \cdot \sqrt{2\varepsilon} \\ t &= T \cdot r\sqrt{2\varepsilon} \end{aligned}$$

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\odot Elastohydrodynamic interactions



$$\begin{split} \ddot{X}_{\rm G} &+ \frac{2\varepsilon\xi}{3}\frac{\dot{X}_{\rm G}}{\sqrt{\Delta}} + \frac{\kappa\varepsilon\xi}{6}\left[\frac{19}{4}\frac{\dot{\Delta}\dot{X}_{\rm G}}{\Delta^{7/2}} - \frac{\dot{\Delta}\dot{\Theta}}{\Delta^{7/2}} + \frac{1}{2}\frac{\ddot{\Theta} - \ddot{X}_{\rm G}}{\Delta^{5/2}}\right] = 0\\ \ddot{\Delta} &+ \xi\frac{\dot{\Delta}}{\Delta^{3/2}} + \frac{\kappa\xi}{4}\left[21\frac{\dot{\Delta}^2}{\Delta^{9/2}} - \frac{(\dot{\Theta} - \dot{X}_{\rm G})^2}{\Delta^{7/2}} - \frac{15}{2}\frac{\ddot{\Delta}}{\Delta^{7/2}}\right] = 0\\ \ddot{\Theta} &+ \frac{4\varepsilon\xi}{3}\frac{\dot{\Theta}}{\sqrt{\Delta}} + \frac{\kappa\varepsilon\xi}{3}\left[\frac{19}{4}\frac{\dot{\Delta}\dot{\Theta}}{\Delta^{7/2}} - \frac{\dot{\Delta}\dot{X}_{\rm G}}{\Delta^{7/2}} + \frac{1}{2}\frac{\ddot{X}_{\rm G} - \ddot{\Theta}}{\Delta^{5/2}}\right] = 0 \end{split}$$

T. Salez, and L. Mahadevan, J. Fluid Mech. 2015, 779, 181-196

\odot Langevin equation

$$\dot{v} = -\gamma v + \delta F/m$$

P. Langevin, Compt. Rendus 1908, 146, 530-533.

Langevin equation
$$\rightarrow v(t) \rightarrow \langle v^2(t) \rangle \rightarrow$$
 noise amplitudes
 $\langle v(0)v(t) \rangle \rightarrow$ mean square displacement (MSD)

diffusion coefficients

\odot Modified fluctuation-dissipation relation

 $\begin{array}{c} \dot{v}_i \text{ coefficients} \longrightarrow \text{mass matrix } M_{\alpha\beta}(\kappa, \Delta) \\ & & \text{real mass } m_i \longrightarrow \text{effective friction } \gamma_{\text{eff}}(\kappa, \Delta) \\ \hline v_i \text{ coefficients} \longrightarrow \text{friction matrix } \gamma_{\alpha\beta}(\kappa, \Delta) \end{array}$

$$\gamma_{\mathrm{eff}} = M_{lphaeta}^{-1} \cdot m_{lpha} \cdot \gamma_{lphaeta}$$

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$$\gamma_{\mathrm{eff}} = M_{\alpha\beta}^{-1} \cdot m_{lpha} \cdot \gamma_{lphaeta}$$

$$v_{i} = v_{i0} + \kappa \cdot v_{i1} \longrightarrow \langle v_{i0} v_{i1} \rangle (t, \kappa) \longrightarrow$$

$$\gamma_{i} = \gamma_{i0}(\Delta) + \kappa \cdot \gamma_{i1}(\Delta) \longrightarrow$$
noise correlator amplitude
$$\delta F_{i} = \delta F_{i0} + \kappa \cdot \delta F_{i1} \longrightarrow \langle \delta F_{i0} \delta F_{i1} \rangle (\kappa)$$

$$\langle \delta F_i(\tau_1) \delta F_i(\tau_2) \rangle \propto 2k_{\rm B}T \ m_i \ \gamma_{i0} \ \delta(\tau_1 - \tau_2) \cdot \left[1 - \kappa \cdot \frac{\gamma_{i1}(\Delta)}{\gamma_{i0}(\Delta)} \right]$$

 • Simulation with **fixed** height (Δ) - Effect of a rigid wall ($\kappa = 0$)



$$\epsilon = 0.1$$
 $\xi = 1.0$ $\Delta \equiv \Delta(0)$
 $X_{\rm G}(0) = \dot{X}_{\rm G}(0) = \Theta(0) = \dot{\Theta}(0) = 0$
At long time:

$$\left\langle \Delta X_{\rm G}^2 \right\rangle \propto 2D(\kappa, \Delta)\Delta T$$

$$\log \left\langle \Delta X_{\rm G}^2 \right\rangle = \log \Delta T + \log D(0, \Delta) + C$$

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• Simulation with **fixed** height (Δ) - Effect of a rigid wall ($\kappa = 0$)



• Simulation with **fixed** height (Δ) - Effect of compliance ($\kappa \neq 0$)

$$\begin{aligned} \epsilon &= 0.1 \quad \xi = 1.0 \quad \Delta \equiv \Delta(0) \\ X(0) &= \dot{X}(0) = \Theta = \dot{\Theta} = 0 \\ \log \left\langle \Delta X_{\rm G}^2 \right\rangle &= \log \Delta T + \log D(\kappa, \Delta) + C \\ &+ \log \left[1 - \kappa \cdot \frac{\gamma_{i1}(\Delta)}{\gamma_{i0}(\Delta)} \right] + C \end{aligned}$$



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$$\begin{aligned} \epsilon &= 0.1 \quad \xi = 1.0 \quad \Delta \equiv \Delta(0) \\ X(0) &= \dot{X}(0) = \Theta = \dot{\Theta} = 0 \\ \log \left\langle \Delta X_{\rm G}^2 \right\rangle &= \log \Delta T + \log D(\kappa, \Delta) + C \\ &+ \log \left[1 - \kappa \cdot \frac{\gamma_{i1}(\Delta)}{\gamma_{i0}(\Delta)} \right] + C \end{aligned}$$

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• Simulation with **unfixed** Δ - Electrostatic repel of rigid wall ($\kappa = 0$)



• Simulation with **unfixed** Δ - Effect of compliance ($\kappa \neq 0$)

$$\epsilon = 0.1$$
 $\xi = 1.0$ $X(0) = \dot{X}(0) = 0$ $\overline{D}(\kappa) = \int_{z_{\min}}^{z_{\max}} P(\Delta) D(\kappa, \Delta) d\Delta$

$$D(\kappa, \Delta) = D(0, \Delta) \left[1 - \kappa \cdot \frac{\gamma_{i1}(\Delta)}{\gamma_{i0}(\Delta)} \right]$$

$$\log \left\langle \Delta X_{\rm G}^2 \right\rangle = \log \Delta T + \log \overline{D}(\kappa) + C$$



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Summary

Noise-correlator amplitude affected by soft surface:

$$\langle \delta F_i(\tau_1) \delta F_i(\tau_2) \rangle \propto 2k_{\rm B}T \ m_i \ \delta(\tau_1 - \tau_2) \cdot (\gamma_{i0} - \kappa \cdot \gamma_{i1})$$

Less time consumed to enter the diffusive region;

Diffusion coefficients affected by softer surface;

$$D(\kappa, \Delta) = D(0, \Delta) \left[1 - \kappa \cdot rac{\gamma_{i1}(\Delta)}{\gamma_{i0}(\Delta)}
ight]$$



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Perspective





V. Bertin, et al. J. Fluid Mech. 2022, 933, A23.



- 2D toy model toward the 3D case;
 - Experimental verifications;
 - "Target finding" diffusion near soft walls;

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