Exploring Brownian Motion using Hydrodynamic Memory Kernels

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Introduction

- At **low particle to fluid density ratios** ($\rho_p/\rho_f \approx 1$) observed in many microfluidic systems, Brownian motion needs to account for **Drag, Added Mass and History Effects**
- **Novel multiscale method** presented capable of modelling Brownian motion while incorporating these effects

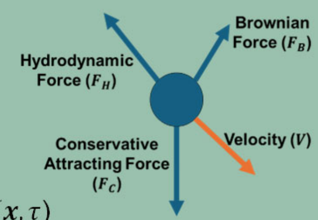
Generalised Langevin Equation (GLE)

$$m_p \frac{dV}{dt} = \boldsymbol{F_H} + \boldsymbol{F_B} + \boldsymbol{F_C}$$

$$\boldsymbol{F_H} = -\int_0^t \boldsymbol{K}(\boldsymbol{x}, t-\tau).\boldsymbol{V}(\tau)d\tau$$

Drag, Added Mass & History Effects included

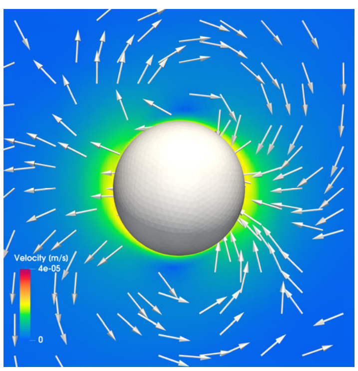
$$\langle F_{B,i}(t-\tau) \cdot F_{B,j}(t) \rangle = k_B T K_{ij}(\boldsymbol{x}, \tau)$$



Hydrodynamic Force $\boldsymbol{F_H}$ ⟵ Memory kernel $(\boldsymbol{K}(t,\tau))$ ⟶ Random Brownian Force $\boldsymbol{F_B}$

Multiscale Simulation Method using GLE

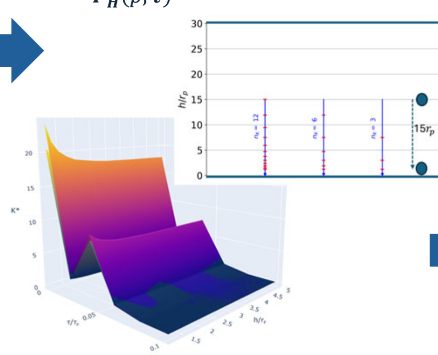
Short Direct Numerical Simulations to determine Hydrodynamic Force $(F_H(p,\tau))$



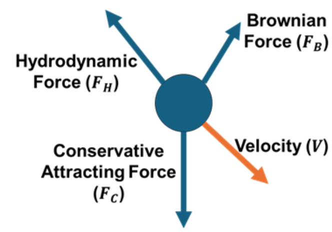
$$\int_S (-p\delta_{ij} + \tau_{ij})n_j dS = \boldsymbol{F_H}(p, \boldsymbol{\tau})$$

Generate memory kernel library by running short DNS at different locations in the domain

$$\frac{\boldsymbol{F_H}(\boldsymbol{K},\boldsymbol{V}) - \boldsymbol{F_H}(p,\boldsymbol{\tau})}{\boldsymbol{F_H}(p,\boldsymbol{\tau})} = C(\boldsymbol{K}) \Rightarrow \boldsymbol{K}(\boldsymbol{x})$$



Lagrangian Particle Tracking (LPT) evolves particle trajectory: Generate Hydrodynamic and Brownian forces from Kernels

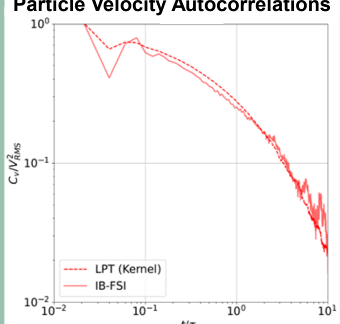


$\boldsymbol{K}(\boldsymbol{x})$ ⟶ $\boldsymbol{F_H}(\boldsymbol{K},\boldsymbol{V})$ No analytical models
$\boldsymbol{K}(\boldsymbol{x})$ ⟶ $\boldsymbol{F_B}(\boldsymbol{K})$

$$m_p \frac{dV}{dt} = \boldsymbol{F_H}(\boldsymbol{K},\boldsymbol{V}) + \boldsymbol{F_B}(\boldsymbol{K}) + \boldsymbol{F_C}$$

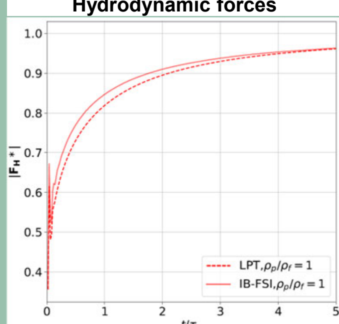
Validation

Particle Velocity Autocorrelations



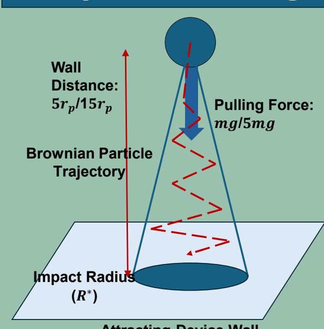
Brownian motion modelled incorporating added mass and history effects

Hydrodynamic forces



Hydrodynamic force is accurately captured without analytical models

Study of a Settling Brownian Particle

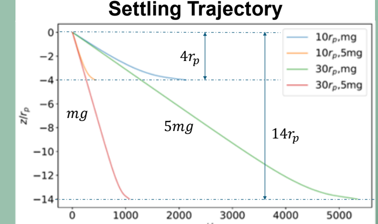


Simulation of Brownian particle pulled towards a wall using a constant force

Alternative Pure DNS method

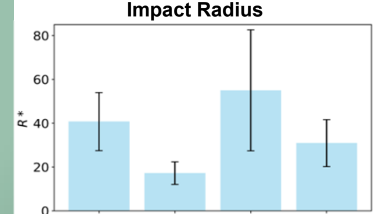
Highlights

Settling Trajectory



Hydrodynamic hindrance increases close to the wall slowing the particles down

Impact Radius



Impact radius increases with domain size and decreases with pulling force strength

Conclusion

A novel multiscale method based on memory kernels is used to accurately model Brownian motion of a particle incorporating memory effects. Wall bounded settling simulations using the method captured increased hindrance from wall and changes in impact region.

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