

Supplement Document:

Janus microdimer swimming in oscillating magnetic field

Jinyou Yang

NUMERICAL METHOD

Boundary element method

In this section, we explain a numerical method for Janus particles swimming in fluid. Due to the small size of Janus particle, we neglect inertial effects in the flow field and assume Stokes flow. We assume that Janus particles are immersed in incompressible Newtonian fluid with viscosity η and density ρ_{liquid} . We also assume the Janus particles located on an infinite plane wall of $x_3 = 0$ when investigated the surface walk of Janus particles. In the Stokes flow regime, the velocity field around the Janus microdimer in integral form is given by

$$\mathbf{u}_i(\mathbf{x}) - \mathbf{u}_i^\infty(\mathbf{x}) = -\frac{1}{8\pi\eta} \int_{particle} G_{ij}(\mathbf{x} - \mathbf{y}) t_j(\mathbf{y}) dA_c, \quad (1)$$

where $\mathbf{u}(\mathbf{x})$ is the velocity at position \mathbf{x} , $\mathbf{u}^\infty(\mathbf{x})$ is the background velocity, A_c is the surface of the Janus microdimer, and \mathbf{t} is the traction force. \mathbf{G} is referred to as free-space Green's function or simply the Stokeslet, in the form of

$$G_{ij}(\mathbf{x} - \mathbf{y}) = \left(\frac{\delta_{ij}}{r} + \frac{r_i r_j}{r^3} \right), \quad (2)$$

Where $\mathbf{y} = (y_1, y_2, y_3)$, $r = [(x_1 - y_1)^2 + (x_2 - y_2)^2 + (x_3 - y_3)^2]^{1/2}$,

Consider a wall in the x_1, x_2 plane at $x_3 = 0$, \mathbf{G}^w for the half space bounded by a no-slip wall, given by:

$$G_{ij}^w(\mathbf{x} - \mathbf{y}) = \left(\frac{\delta_{ij}}{r} + \frac{r_i r_j}{r^3} \right) - \left(\frac{\delta_{ij}}{R} + \frac{R_i R_j}{R^3} \right) + 2h(\delta_{j\alpha} \delta_{\alpha k} - \delta_{j3} \delta_{3k}) \frac{\partial}{\partial R_k} \left\{ \frac{h R_i}{R^3} - \left(\frac{\delta_{i3}}{R} + \frac{R_i R_3}{R^3} \right) \right\}, \quad (3)$$

where $\mathbf{y} = (y_1, y_2, h)$, $r = [(x_1 - y_1)^2 + (x_2 - y_2)^2 + (x_3 - h)^2]^{1/2}$, $R = [(x_1 - y_1)^2 + (x_2 - y_2)^2 + (x_3 + h)^2]^{1/2}$ and $\alpha = 1, 2$.

The surface A of particle is determined by two curvilinear coordinate system (ξ^1, ξ^2) , which express the coordinate \mathbf{x} as $\mathbf{x}(\xi, \gamma)$. The normal vector of the surface is given by

$$\mathbf{n} = \frac{1}{J} \frac{\partial \mathbf{x}}{\partial \xi^1} \times \frac{\partial \mathbf{x}}{\partial \xi^2}, \quad \text{with } J = \left| \frac{\partial \mathbf{x}}{\partial \xi^1} \times \frac{\partial \mathbf{x}}{\partial \xi^2} \right|, \quad (4)$$

The Jacobian of the transformation. An infinitely small surface element has area

$$dA_c = J d\xi^1 d\xi^2, \quad (5)$$

To calculate the integral equation, we use a Gaussian numerical integration scheme with a linear interpolation function. This method approximates the integral of function as a weighted sum of function values at specified points within the domain of the element. In this study flat triangles have been used to form the boundary surface. In a given element, the coordinates (ξ^1, ξ^2) are replaced by the intrinsic coordinates in an isoparametric triangular element (γ^1, γ^2) with the interval of $[0,1]$. The integral is then discretized by:

$$\begin{aligned} \int t(\mathbf{x}) dA_c &= \int t(\xi^1, \xi^2) J d\xi^1 d\xi^2 \approx \sum_{element} \int_0^1 \int_0^{1-\gamma^2} t(\gamma^1, \gamma^2) J d\gamma^1 d\gamma^2 = \\ &\frac{1}{2} \sum_{element} \sum_{k=1}^{28} J t(k) w_k, \end{aligned} \quad (6)$$

Note that Eq.(6) includes a singularity. When an observation point \mathbf{x} is located near a source point \mathbf{y} , a special operation is needed to avoid numerical errors arising from the singularity. For the singular elements, we use a coordinate transformation from (γ^1, γ^2) to polar coordinates (ζ, θ) as

$$\int_0^1 \int_0^{1-\gamma^2} t(\gamma^1, \gamma^2) J d\gamma^1 d\gamma^2 = \int_0^{\frac{\pi}{2}} \int_0^{R(\theta)} t(\zeta, \theta) J \zeta d\zeta d\theta, \quad (7)$$

Where $R(\theta)$ is the distance from \mathbf{x} to the opposite edge of the triangle at angle θ .