A Stochastic Immersed Boundary Method Incorporating Thermal Fluctuations: Coarse-Grained Micromechanics

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Introduction

Motivated by recent advances in experimental biology, we consider mechanics at small-length scales in which elastic structures interact with a fluid in the presence of thermal fluctuations. Potential application areas include: cell motility, molecular motor proteins, and membrane dynamics. In this poster a framework is presented which extends the Immersed Boundary Method (IB) formalism by incorporation of appropriate stochastic forcing terms in the fluid equations. However, the formalism yields a stiff system of equations. A stochastic numerical method is presented allowing for the system dynamics to be efficiently integrated. Application to a coarse-grained lipid bilayer membrane model and molecular motor protein model are discussed.

Immersed Boundary Method

Stokes Fluid Equations (R << 1):

\[ \rho \frac{d^2 u(x,t)}{dt^2} = -\nabla p + F_{ext}(x,t) \]

\[ \nabla \cdot \mathbf{u}(x,t) = 0 \]

Fluid-Particle Coupling (IB Method):

\[ \frac{dX_k(t)}{dt} = \frac{1}{\Delta x^2} \sum_{j=1}^{N} \delta(x-X^j(t)) \mathbf{u}(x) \text{dx} \]

\[ F_{ext}(x,t) = F_{ext}(x) + F_{inter}(x,t) \]

Fluid-Particle Coupling:

\[ \frac{dX_k(t)}{dt} = \frac{1}{\Delta x^2} \sum_{j=1}^{N} \delta(x-X^j(t)) \mathbf{u}(x) \text{dx} \]

Semi-discretized Equations

Stokesian Fluid Equations (N\^2 Lattice):

\[ \frac{d u_{nm}(t)}{dt} = -\nabla p + F_{ext}(x,t) \]

\[ \frac{d u_{nm}(t)}{dt} = \frac{1}{\Delta x^2} \sum_{j=1}^{N} \delta(x-X^j(t)) \mathbf{u}(x) \text{dx} \]

Fluid-Particle Coupling:

\[ \frac{d X_k(t)}{dt} = \frac{1}{\Delta x^2} \sum_{j=1}^{N} \delta(x-X^j(t)) \mathbf{u}(x) \text{dx} \]

Fourier Representation

Fluid Equations:

\[ \frac{d \hat{u}_k(t)}{dt} = -\frac{1}{\Delta x} \hat{X}_k(t) \cdot \hat{u}_k(t) + \sum_{j=1}^{N} \delta(x-X^j(t)) \mathbf{u}(x) \text{dx} \]

\[ \hat{u}_k(t) = 0 \]

\[ \hat{u}_k(t) = \delta_{kn} \hat{X}_n(t) \text{ (incompressibility)} \]

\[ \hat{u}_k(t) = \frac{1}{\Delta x} \hat{X}_k(t) \hat{u}_k(t) \text{ (real-valued)} \]

where,

\[ \alpha_k = -\frac{2\nu}{\rho \Delta x^2} \frac{1}{j=1} (1 - \cos(2\pi k/j)) \]

\[ \hat{X}_k(t) = \frac{1}{\Delta x} \hat{X}_k(t) \]

\[ \mathbf{v}_p = \mathbf{v}_p(t) \]

Thermal Forcing

Stationary probability distribution

\[ w(\mathbf{u}_k) = \frac{1}{2\pi} e^{-\frac{\alpha_k u_k^2}{2}} \]

Energy of Fourier Modes by Parseval’s Lemma

\[ \mathcal{E}[\mathbf{u}_k] = \frac{2\pi}{2N} \sum_{m=1}^{N} u_{k,m}^2 \Delta x^2 = \frac{\rho L^2}{2} \sum_{k} |u_k|^2 = \mathcal{E}[\mathbf{u}_k] \]

Boltzmann’s distribution

\[ w(\mathbf{u}_k) = \frac{1}{2\pi} e^{-\frac{\alpha_k u_k^2}{2}} \]

Thermal forcing strength

\[ D_k = \left\{ \begin{array}{ll} \frac{\beta u_k^2}{2}, & k \in K \\ \frac{\beta u_k^2}{2} \alpha_k, & k \notin K \end{array} \right. \]

(Time Scale: typical)

Length-scale: \( L = 1 \mu m \)

Number modes resolved: \( N = 32 \)

Relaxation time scales for modes \( k \) (water):

\[ \tau_k = \frac{1}{\alpha_k} \]

min \( \frac{1}{\alpha_k} \approx 10ns \)

\[ \tau_{diff}(1mm) \approx 10ns \]

max \( \frac{1}{\alpha_k} \approx 10^{-6} \)

\[ \tau_{diff}(10mm) \approx 10^{-6} \]

Numerical Method

Fluid:

\[ \frac{d \mathbf{v}_p(t)}{dt} = -\nabla p + F_{ext}(x,t) \]

\[ \mathbf{v}_p(t) \text{ (generated consistently with } \mathcal{E}) \]

Immersed Elementary Particles:

\[ \frac{d X_k(t)}{dt} = \frac{1}{\Delta x^2} \sum_{j=1}^{N} \delta(x-X^j(t)) \mathbf{u}(x) \text{dx} \]

\[ \mathcal{E} = \sigma_k (0,1) \text{ (complex-valued Gaussian)} \]

\[ \sigma_k^2 = \frac{D_k}{\alpha_k} (1 - e^{-2\alpha_k \Delta t}) \]

Polynomial Mode Variances

\[ \langle \mathbf{v}_p(t) \mathbf{v}_p(t) \rangle = \sigma_k^2 (0,1) \text{ (complex-valued Gaussian)} \]

\[ \mathcal{E} = \langle \mathbf{v}_p(t) \mathbf{v}_p(t) \rangle \]

\[ \langle \mathbf{v}_p(t) \mathbf{v}_p(t) \rangle = \sigma_k^2 (0,1) \text{ (complex-valued Gaussian)} \]

\[ \mathcal{E} = \langle \mathbf{v}_p(t) \mathbf{v}_p(t) \rangle \]

Applications

Molecular Motor Proteins:

Mean Velocity vs. Load

Polynomial Mode Variances

Physical Fidelity

• Correct scaling of the diffusion coefficient in the physical parameters.

• Well known hydrodynamic memory effect of Brownian motion captured where the velocity autocorrelation function has long time algebraic decay.

• Stationary statistics appear Boltzmann for the fluctuations of the immersed particles and fluid.

Conclusion

A stochastic IB method has been presented which allows for long time steps to be taken while carefully taking into account the statistical contributions of the fastest dynamics of the system. The method captures many well known microscopic physical phenomena suggesting the promise of the method to correctly simulate biological mechanical processes at small length scales.