Methods for Simulating Fluid-Structure Interactions with Thermal Fluctuations

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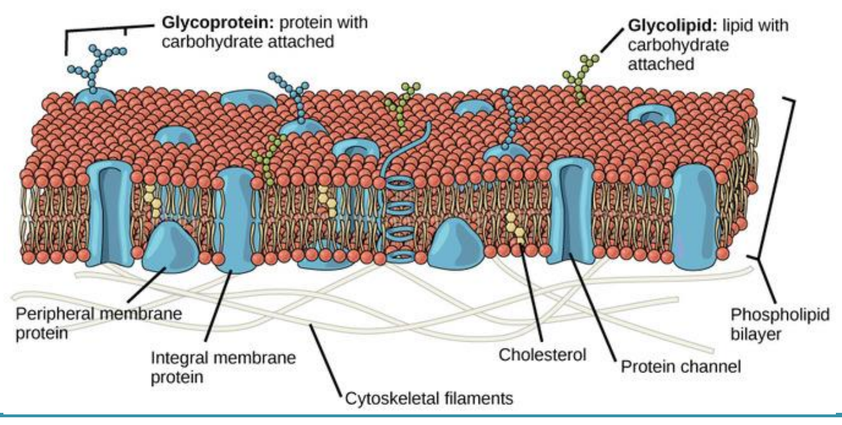
1. Introduction

Motivated by problems in biophysics in which elastic structures interact in a fluid-like medium, we introduce approaches for modeling such systems. At these length scales, because the interaction energy of the immersed structures is on the order of $k_B T$, thermal fluctuations of the fluid medium will contribute significantly to the dynamics of the system and must be taken into account.

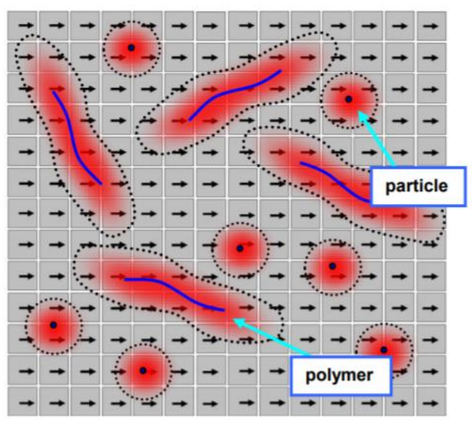


2. Model

Because actual liquids contain far too many molecules than would be computationally tractable, we use a continuum description for the fluid, using the following equations (a statement of Newton's 2nd law) to model the fluid dynamics. We account for the dissipative stresses (like friction) and pressure (molecules pushing in on each other) in the fluid, the forces from the immersed structures that affect the fluid flow, and the thermal fluctuations.

$$\rho \frac{d\mathbf{u}}{dt} = \mu \nabla^2 \mathbf{u} - \nabla p + \mathbf{f}_{total}$$

$$\mathbf{f}_{total} = \mathbf{f}_{prt} + \mathbf{f}_{thm}$$



3. Fluid-Structure Coupling

A number of approaches could be taken to couple the dynamics of the fluid and microstructures. Because even the simplest biological systems can consist of thousands of molecules/structures, we take an approach in our model that balances accuracy and efficiency. To determine the microstructures' velocities, we average the velocity of the local fluid environment, and to determine the particle forces acting on a point in the fluid, we average the forces that neighboring microstructures experience from each other.

$$\mathbf{f}_{prt}(\mathbf{x}) = \sum_{j=1}^{M} -\nabla_{\mathbf{X}^{(j)}} V(\mathbf{X}^{(j)}(t)) \delta_a(\mathbf{x} - \mathbf{X}^{(j)}(t))$$

$$\frac{d\mathbf{X}^{(j)}}{dt} = \int_{\Omega} \mathbf{u}(\mathbf{x}, t) \delta_a(\mathbf{x} - \mathbf{X}^{(j)}(t)) d\mathbf{x}$$

4. Thermal Fluctuations

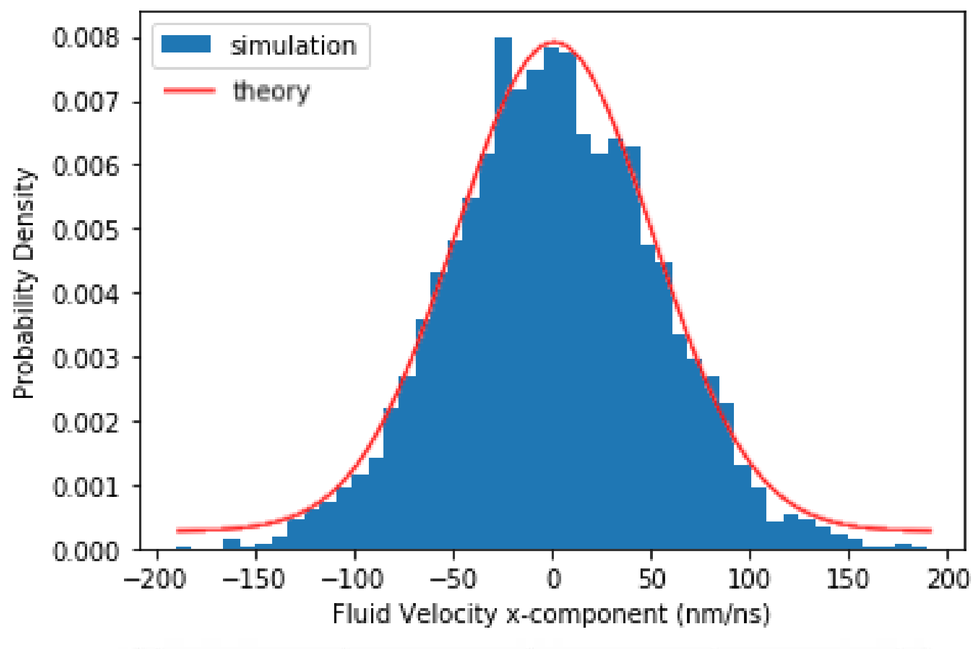
The theory of statistical mechanics tells us that the equilibrium fluctuations of the fluid velocity should follow the Gibbs-Boltzmann distribution. Imposing this condition on our system, we can determine what the thermal forcing on the fluid should be in order to properly account for these fluctuations.

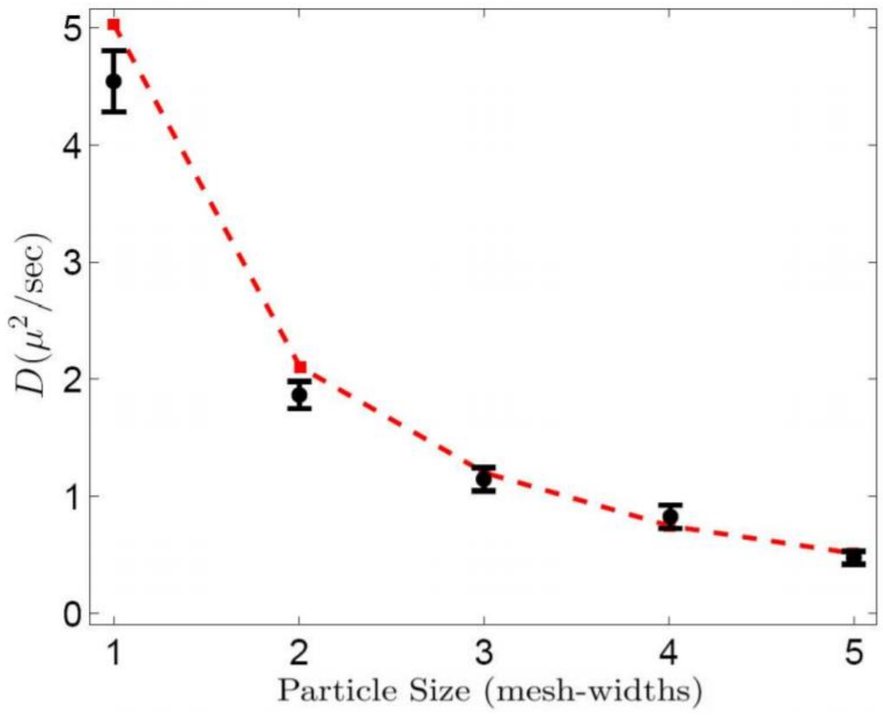
$$\mathbf{f}_{thm} = Q \frac{d\mathbf{B}_t}{dt}$$

$$QQ^T = -(LC_{eq} + C_{eq}L^T)$$

5. Validation of Methodology

In order to test the validity of our model, we perform some basic checks to see whether essential features of the physics are retained. Plotted below is the equilibrium distribution of the fluid velocity and diffusivity of the microstructures estimated from numerical simulations, which closely match the theoretical predictions. This suggests the methodology holds promise for more sophisticated simulation of biophysical systems.





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