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A NOTE ON THE CORRESPONDENCE OF AN IMMERSSED BOUNDARY METHOD INCORPORATING THERMAL FLUCTUATIONS WITH STOKESIAN-BROWNIAN DYNAMICS

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Abstract. In this paper a direct correspondence is made between the effective stochastic dynamics of elastic structures of an Immersed Boundary Method incorporating thermal fluctuations and Stokesian-Brownian Dynamics. The correspondence is made in the limit of small Reynolds number, in which the fluid relaxes rapidly on the time scale of the motion of the immersed structures, by performing an averaging procedure directly on the stochastic equations of the Immersed Boundary Method. It is found that there is agreement with Stokesian-Brownian Dynamics for the far-field hydrodynamic interactions and that a fluctuation-dissipation relation is satisfied for the stochastic fluctuations of the effective equations.

Key words. Stochastic Processes, Fluid Dynamics, Brownian Dynamics, Statistical Mechanics, Immersed Boundary Method.

1. Introduction. In Stokesian-Brownian Dynamics (3; 6) elastic structures immersed in a fluid are modeled by discretization into a set of interacting particles which evolve according to effective stochastic equations. The effective equations are obtained by eliminating the fluid degrees of freedom by making a steady-state approximation in which it is assumed that the fluid relaxes rapidly given the forces impinging on the fluid for the instantaneous configuration of the particles (3; 6).

In the Immersed Boundary Method (17) both the particle and fluid degrees of freedom are dynamically modeled. A feature of the Immersed Boundary Method distinguishing it from other hydrodynamic models is the simple manner in which fluid-particle coupling is handled. The hydrodynamic equations in the Immersed Boundary Method can be viewed as conservation equations for the momentum of both the fluid body and particles in a Eulerian reference frame. In the Immersed Boundary Method a weight function δ_a , which integrates to one, is used to assign momentum to an immersed structure and to transmit forces acting on a structure to the fluid. Given this difference with hydrodynamic models in which stresses at the structures' interface are used to couple the fluid and structures, an important question for the Immersed Boundary Method incorporating thermal fluctuations (1; 14) is whether or not in the limit of small Reynolds number and fast relaxation of the fluid the effective stochastic equations for the immersed structure degrees of freedom are consistent with the hydrodynamic effects captured by other methods such as Stokesian-Brownian Dynamics.

In previous work (13), a correspondence was established using a rigorous, but somewhat abstract, stochastic mode reduction procedure (10) on the Kolomogorov-Backward equations (16) associated with an Immersed Boundary Method incorporating thermal fluctuations. It was remarked in this work that the effective stochastic equations are not obvious from the primitive equations due to the nature of the simultaneous fluid and structure dynamics. In this work we show how a more direct, but

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less rigorous, approach can be taken working directly with the primitive stochastic equations.

In Section 2, we discuss an Immersed Boundary Method which incorporates thermal fluctuations (1; 14). A correspondence between the Immersed Boundary Method and Stokesian-Brownian Dynamics is made in Section 3. The effective stochastic equations for multiple particles is then derived in Section 3.1. We then discuss in Section 3.1 the hydrodynamic coupling matrix derived for particles represented in the Immersed Boundary Method and show that a fluctuation-dissipation relation holds for the correlations of the effective thermal fluctuations and the hydrodynamic coupling. In Section 3.2 we discuss the effective stochastic equations for a single particle and show that the fluctuation-dissipation relation reduces to the classical Einstein relation (5), provided the friction coefficient of a particle is defined appropriately. The Smoluchowsky dynamics (20) of a single Brownian particle is also shown to be recovered.

2. The Immersed Boundary Method Incorporating Thermal Fluctuations. For microscopic systems on the order of tens of microns or smaller where the structures undergoing Brownian motion are immersed in water at room temperature, the Reynolds number is very small. This allows in the Navier-Stokes equations for the nonlinear advection term to be neglected, but not the derivative in time, which can not be dropped as a consequence of the fast time scales associated with the thermal fluctuations of the fluid. In this regime the hydrodynamics can be modeled by the stochastically forced Stokes equations (2; 7; 8):

$$(2.1) \quad \rho \frac{\partial \mathbf{u}(\mathbf{x}, t)}{\partial t} = \mu \Delta \mathbf{u}(\mathbf{x}, t) - \nabla p + \mathbf{f}_{\text{prt}}(\mathbf{x}, t) + \mathbf{f}_{\text{thm}}(\mathbf{x}, t)$$

$$(2.2) \quad \nabla \cdot \mathbf{u} = 0,$$

where p is the pressure arising from the incompressibility constraint, ρ is the fluid density, μ is the dynamic viscosity, and $\mathbf{f}_{\text{prt}}, \mathbf{f}_{\text{thm}}$ are force densities which model the particle forces and thermal fluctuations of the fluid, respectively. The details of the particle force \mathbf{f}_{prt} and thermal force \mathbf{f}_{thm} will be discussed below. We shall consider the fluid equations in three dimensions on a cubic domain Λ having sides L with periodic boundary conditions.

In the Immersed Boundary Method the immersed structures are represented by a discretization into a finite number of interacting “elementary particles”. A particle of size a immersed in the fluid is modeled by a Lagrangian coordinate $\mathbf{X}(t)$ with the fluid-particle coupling handled by treating the particle as part of the fluid body. In particular, the Stokes equation are viewed as conservation equations for the total momentum of both the fluid and particles. The momentum associated with a particle is obtained by averaging the fluid momentum in the vicinity of the particle position $\mathbf{X}(t)$. The following equation of motion is used to model the particle dynamics (17):

$$(2.3) \quad \frac{d\mathbf{X}(t)}{dt} = \mathbf{U}(\mathbf{X}(t), t)$$

with \mathbf{U} defined by:

$$(2.4) \quad \mathbf{U}(\mathbf{x}, t) := \int_{\Lambda} \delta_a(\mathbf{y} - \mathbf{x}) \mathbf{u}(\mathbf{y}, t) d\mathbf{y}$$

where δ_a is a weight function which integrates to one (17) and Λ denotes the periodic.

To account for the forces that act on the particles the following force density is used:

$$(2.5) \quad \mathbf{f}_{\text{prt}}(\mathbf{x}, t) = \sum_j \mathbf{F}^{[j]}(t) \delta_a(\mathbf{x} - \mathbf{X}^{[j]}(t)).$$

The fluid-particle coupling equations 2.3 - 2.5 has been demonstrated to be an effective approach in modeling many biological systems, see (11; 12; 17).

The Fourier transform of the Stokes equations 2.1 and 2.2 give:

$$(2.6) \quad \frac{d\hat{\mathbf{u}}_{\mathbf{k}}}{dt} = -\alpha_{\mathbf{k}} \hat{\mathbf{u}}_{\mathbf{k}} + \rho^{-1} \wp_{\mathbf{k}}^{\perp} \hat{\mathbf{f}}_{\text{prt}, \mathbf{k}} + \rho^{-1} \wp_{\mathbf{k}}^{\perp} \hat{\mathbf{f}}_{\text{thm}, \mathbf{k}}$$

$$(2.7) \quad \hat{\mathbf{g}}_{\mathbf{k}} \cdot \hat{\mathbf{u}}_{\mathbf{k}} = 0,$$

where

$$(2.8) \quad \alpha_{\mathbf{k}} := \frac{4\pi^2 \mu}{\rho L^2} |\mathbf{k}|^2$$

$$(2.9) \quad \hat{\mathbf{g}}_{\mathbf{k}} := \frac{2\pi \mathbf{k}}{L}.$$

The projection operator which enforces incompressibility (4) is defined by:

$$(2.10) \quad \wp_{\mathbf{k}}^{\perp} := \left(\mathcal{I} - \frac{\hat{\mathbf{g}}_{\mathbf{k}} \hat{\mathbf{g}}_{\mathbf{k}}^T}{|\hat{\mathbf{g}}_{\mathbf{k}}|^2} \right).$$

In the case that $\hat{\mathbf{g}}_{\mathbf{k}} = 0$ the incompressibility constraint becomes trivial and we define $\wp_{\mathbf{k}}^{\perp} = \mathcal{I}$.

The requirement that the Fourier coefficients represent a real-valued velocity field gives the extra constraint:

$$(2.11) \quad \overline{\hat{\mathbf{u}}_{-\mathbf{k}}} = \hat{\mathbf{u}}_{\mathbf{k}}.$$

To model thermal fluctuations of the system the thermal force is given by Fourier modes proportional formally to “white noise” (16):

$$(2.12) \quad \hat{\mathbf{f}}_{\text{thm}, \mathbf{k}}(t) = \sqrt{2D_{\mathbf{k}}} \frac{d\tilde{\mathbf{B}}_{\mathbf{k}}(t)}{dt}$$

where the factors $\tilde{\mathbf{B}}_{\mathbf{k}}$ are independent complex-valued Brownian motions (16). To ensure the thermal forcing is real-valued the following constraint is imposed:

$$(2.13) \quad \overline{d\tilde{\mathbf{B}}_{-\mathbf{k}}} = d\tilde{\mathbf{B}}_{\mathbf{k}}.$$

The coefficients $D_{\mathbf{k}}$ were derived in (1) and satisfy the following fluctuation-dissipation relation (15; 19):

$$(2.14) \quad D_{\mathbf{k}} = \frac{k_B T}{2\rho L^3} \alpha_{\mathbf{k}}.$$

This gives the following formal representation of the thermal force density:

$$(2.15) \quad \mathbf{f}_{\text{thm}}(\mathbf{x}, t) = \sum_{\mathbf{k}} \sqrt{2D_{\mathbf{k}}} \frac{d\tilde{\mathbf{B}}_{\mathbf{k}}(t)}{dt} \exp(i2\pi \mathbf{k} \cdot \mathbf{x}).$$

3. Correspondence with Stokesian-Brownian Dynamics. In Stokesian-Brownian Dynamics (3; 6), the fluid is eliminated by a steady-state approximation and the elastic structures are modeled by discretization into a set of interacting particles with stochastic dynamics of the form:

$$(3.1) \quad d\mathbf{X}(t) = \tilde{H}\mathbf{F}(\mathbf{X}(t))dt + \tilde{C}d\mathbf{B}(t)$$

where for M particles $\mathbf{X}, \mathbf{F}, \mathbf{B} \in \mathbb{R}^{3M}$ and $\tilde{H}, \tilde{C} \in \mathbb{R}^{3M \times 3M}$. The term $\mathbf{X}(t)$ denotes the composite vector of particle positions, \mathbf{F} denotes the composite vector of forces acting on the particles, and $\mathbf{B}(t)$ denotes the vector-valued stochastic process which in each component is an independent real-valued Brownian motion (16). The term \tilde{H} is a positive definite matrix and models the hydrodynamic coupling of the particles (3; 6). The term \tilde{C} corresponds to the correlations of the effective thermal forces acting on the particles and for a given temperature T is defined as $\tilde{C} = \sqrt{2k_B T} \cdot \tilde{H}$, where k_B is Boltzmann's constant (7; 19).

3.1. The Effective Stochastic Dynamics of Multiple Particles. We shall now consider the effective stochastic equations for the immersed structures as represented by the elementary particles and force interactions in the Immersed Boundary Method with thermal fluctuations. We shall obtain the effective equations in the small Reynolds number limit in which the hydrodynamic dynamics relax rapidly on the time scales associated with the motion of the structures. The hydrodynamic equations 2.6 and 2.7 can be rewritten in terms of the following integral equation:

$$(3.2) \quad \hat{\mathbf{u}}_{\mathbf{k}}(t) = \rho^{-1} \int_{-\infty}^t e^{-\alpha_{\mathbf{k}}(t-s)} \wp_{\mathbf{k}}^{\perp} \hat{\mathbf{F}}_{\mathbf{k}}(\{\mathbf{X}^{[j]}(s)\}, s) ds \\ + \sqrt{2D_{\mathbf{k}}} \int_{-\infty}^t e^{-\alpha_{\mathbf{k}}(t-s)} \wp_{\mathbf{k}}^{\perp} d\tilde{\mathbf{B}}_{\mathbf{k}}(s).$$

This expression is obtained by an analogue of the method of integrating factors in Ito Calculus (16). The last term is obtained from the representation of the thermal forcing $\hat{\mathbf{f}}_{\text{thm}, \mathbf{k}}$ in 2.12 with integration to be interpreted in the sense of an Ito Integral (16). In the notation, the j^{th} elementary particle is denoted by $\mathbf{X}^{[j]}$ with $\{\mathbf{X}^{[j]}\}$ denoting the collection of all particle positions and $\hat{\mathbf{F}}_{\mathbf{k}}$ is used as short-hand for the Fourier transform of the particle force $\hat{\mathbf{f}}_{\text{prt}, \mathbf{k}}$.

This leads to a natural decomposition of $\hat{\mathbf{u}}_{\mathbf{k}}$ into a part containing the drift of the dynamics and a part which is drift-free. We make the following definition for the drift term:

$$(3.3) \quad \hat{\mathbf{v}}_{\mathbf{k}}(t) = \rho^{-1} \int_{-\infty}^t e^{-\alpha_{\mathbf{k}}(t-s)} \wp_{\mathbf{k}}^{\perp} \hat{\mathbf{F}}_{\mathbf{k}}(\{\mathbf{X}^{[j]}(s)\}, s) ds$$

and the following definition for the drift-free term:

$$(3.4) \quad \hat{\mathbf{w}}_{\mathbf{k}}(t) = \sqrt{2D_{\mathbf{k}}} \int_{-\infty}^t e^{-\alpha_{\mathbf{k}}(t-s)} \wp_{\mathbf{k}}^{\perp} d\tilde{\mathbf{B}}_{\mathbf{k}}(s).$$

In addition, we make the definitions:

$$(3.5) \quad \mathbf{v}(\mathbf{x}, t) = \sum_{\mathbf{k}} \hat{\mathbf{v}}_{\mathbf{k}}(t) \exp(i2\pi\mathbf{k} \cdot \mathbf{x})$$

and

$$(3.6) \quad \mathbf{w}(\mathbf{x}, t) = \sum_{\mathbf{k}} \hat{\mathbf{w}}_{\mathbf{k}}(t) \exp(i2\pi\mathbf{k} \cdot \mathbf{x}).$$

To decompose over the time interval $[0, t]$ the contributions of the drift and drift-free parts to the elementary particle displacement we make the following definitions:

$$(3.7) \quad \bar{\mathbf{X}}^{[\ell]}(t) - \mathbf{X}^{[\ell]}(0) = \int_0^t \int_{\Omega} \delta_a(\mathbf{y} - \mathbf{X}^{[\ell]}(s)) \mathbf{v}(\mathbf{y}, s) d\mathbf{y} ds$$

and

$$(3.8) \quad \hat{\mathbf{X}}^{[\ell]}(t) - \mathbf{X}^{[\ell]}(0) = \int_0^t \int_{\Omega} \delta_a(\mathbf{y} - \mathbf{X}^{[\ell]}(s)) \mathbf{w}(\mathbf{y}, s) d\mathbf{y} ds$$

where on the right hand side and at time 0 the full particle displacement is used.

To derive the effective stochastic equations for the structures we shall eliminate the fluid degrees of freedom by taking the limit in which the fluid rapidly relaxes to a statistical steady-state for the current forces acting on the fluid induced by the instantaneous configuration of the particles. For a physical system in which the fluid is undergoing Stokes flow it follows from 3.2 that the time scale on which the fluid relaxes to statistical steady-state for the \mathbf{k}^{th} mode is $\tau_{\mathbf{k}} = 1/\alpha_{\mathbf{k}}$ provided that $\mathbf{k} \neq 0$. We shall denote the longest relaxation time scale by $\tau_{\text{fld}} = \max\{\tau_{\mathbf{k}}\}$. For the system with periodic boundary conditions this time scale is given by $\tau_{\text{fld}} = \rho L^2 / 4\pi^2 \mu$.

For an individual physical particle in a fluid with Stokes flow the time scale on which a particle moves a displacement comparable to its size a is $\tau_{\text{prt}} = \min\{a^2/D, a\gamma/F\}$, where $\gamma \approx 6\pi\mu a$ denotes the friction coefficient of the particle, $D \approx \frac{K_B T}{\gamma}$ denotes the diffusion coefficient of the particle, and F denotes the force acting directly on the particle. Considering the low Reynolds number limit in which $\mu \rightarrow \infty$, holding all other non-derived physical parameters fixed, we have $\alpha_{\mathbf{k}} \rightarrow \infty$ uniformly for all modes $\mathbf{k} \neq 0$, $\gamma \rightarrow \infty$, and $D \rightarrow 0$. Consequently, $\tau_{\text{fld}} \rightarrow 0$ while $\tau_{\text{prt}} \rightarrow \infty$ and there is a separation of time scales indicated for the physical system between the motion of the structures and the relaxation of the fluid.

To determine the drift of the effective stochastic equation for a given configuration of the elementary particles $\mathbf{X}(0)$ we shall take the following limit and define $H : \mathbb{R}^{3M} \rightarrow \mathbb{R}^{3M}$ by its action on arbitrary \mathbf{F} :

$$(3.9) \quad H\mathbf{F} := \lim_{\substack{\Delta t \rightarrow 0, \mu \rightarrow \infty \\ \mu\Delta t \rightarrow \infty}} \frac{\langle \bar{\mathbf{X}}(\Delta t) - \bar{\mathbf{X}}(0) \rangle}{\Delta t}.$$

In the notation, $\bar{\mathbf{X}}$ denotes the composite vector of all displacements of the elementary particles as defined in 3.7.

To determine the strength of the thermal fluctuations in the effective equations for a given configuration of the elementary particles $\mathbf{X}(0)$ we shall take the following limit and define $\Gamma : \mathbb{R}^{3M} \rightarrow \mathbb{R}^{3M}$ by:

$$(3.10) \quad \Gamma := \lim_{\substack{\Delta t \rightarrow 0, \mu \rightarrow \infty \\ \mu\Delta t \rightarrow \infty}} \frac{\langle (\hat{\mathbf{X}}(\Delta t) - \hat{\mathbf{X}}(0)) (\hat{\mathbf{X}}(\Delta t) - \hat{\mathbf{X}}(0))^T \rangle}{\Delta t}.$$

In the notation, $\hat{\mathbf{X}}$ denotes the composite vector of all displacements of the elementary particles as defined in 3.8.

We now compute each of these terms directly from the primitive stochastic equations of the immersed boundary method. In the limit $\alpha_{\mathbf{k}} \rightarrow \infty$ the drift term can be computed using the following quasi-steady-state approximation which follows directly from 2.6 and 3.3:

$$(3.11) \quad \hat{\mathbf{v}}_{\mathbf{k}}(s) \approx \frac{\rho^{-1} \wp_{\mathbf{k}}^{\perp} \hat{\mathbf{F}}_{\mathbf{k}}(\{\mathbf{X}^{[j]}\}, s)}{\alpha_{\mathbf{k}}}.$$

The factors $\hat{\mathbf{F}}_{\mathbf{k}}$ are the Fourier coefficients of the elementary particle force density acting on the fluid given by:

$$(3.12) \quad \hat{\mathbf{F}}_{\mathbf{k}} = \sum_j \mathbf{F}^{[j]} \hat{\delta}_{a,\mathbf{k}}(\mathbf{X}^{[j]}).$$

The short-hand notation $\hat{\delta}_{a,\mathbf{k}}(\mathbf{X}^{[j]})$ denotes the Fourier coefficient in \mathbf{x} of the function $\delta_a(\mathbf{x} - \mathbf{X}^{[j]})$ and includes the phase factor arising from the shift of δ_a from the origin.

Using 3.11 the contribution of the drift term to the particle displacement, as defined in 3.7, can be expressed as:

$$(3.13) \quad \begin{aligned} \bar{\mathbf{X}}^{[\ell]}(\Delta t) - \mathbf{X}^{[\ell]}(0) &= \int_0^{\Delta t} \int_{\Omega} \delta_a(\mathbf{y} - \mathbf{X}^{[\ell]}(s)) \sum_{\mathbf{k}} \sum_j \frac{\rho^{-1} \wp_{\mathbf{k}}^{\perp} \mathbf{F}^{[j]} \hat{\delta}_{a,\mathbf{k}}(\mathbf{X}^{[j]}) L^3}{\alpha_{\mathbf{k}} L^3} \exp(i2\pi \mathbf{k} \cdot \mathbf{y}) \, d\mathbf{y} ds \\ &= \sum_j \int_{\Omega} \int_{\Omega} \int_0^{\Delta t} \delta_a(\mathbf{y} - \mathbf{X}^{[\ell]}(s)) \delta_a(\mathbf{y} - \mathbf{X}^{[j]}(s)) \mathbf{Q}^{[j]}(\mathbf{y} - \mathbf{y}', s) \, ds d\mathbf{y} d\mathbf{y}' \end{aligned}$$

where

$$(3.14) \quad \mathbf{Q}^{[j]}(\mathbf{z}, s) := \sum_{\mathbf{k}} \frac{\rho^{-1} \wp_{\mathbf{k}}^{\perp} \mathbf{F}^{[j]}(s)}{\alpha_{\mathbf{k}} L^3} \exp(i2\pi \mathbf{k} \cdot \mathbf{z}).$$

The second equality in 3.13 follows from the Fourier Convolution Theorem.

From 3.13 the limit in 3.9 is computed as:

$$(3.15) \quad (\mathbf{H}\mathbf{F}(t))^{[\ell]} = \sum_j \int_{\Omega} \int_{\Omega} \delta_a(\mathbf{y} - \mathbf{X}^{[\ell]}(t)) \delta_a(\mathbf{y} - \mathbf{X}^{[j]}(t)) \mathbf{Q}^{[j]}(\mathbf{y} - \mathbf{y}', t) \, d\mathbf{y} d\mathbf{y}'.$$

From 3.14 it follows that the drift is a linear function of the elementary particle forces. The entries of the matrix H can be computed by substituting $\mathbf{F} = \mathbf{e}_{q'}^{[\ell']}$ for the force. The notation $\mathbf{e}_{q'}^{[\ell']}$ denotes a composite vector in \mathbb{R}^{3M} where all components are zero except for the entry corresponding to q^{th} vector component of the ℓ^{th} elementary particle force. In other words, the non-zero entry has index $3\ell' + q'$ in the composite vector $\mathbf{e}_{q'}^{[\ell']}$.

Making this substitution the entries of H are given by:

$$(3.16) \quad H_{q,q'}^{[\ell,\ell']}(s) = \int_{\Omega} \int_{\Omega} \delta_a(\mathbf{y} - \mathbf{X}^{[\ell]}(s)) \delta_a(\mathbf{y}' - \mathbf{X}^{[\ell']}(s)) \sum_{\mathbf{k}} \frac{\rho^{-1} (\wp_{\mathbf{k}}^{\perp})_{q,q'}}{\alpha_{\mathbf{k}} L^3} \exp(i2\pi \mathbf{k} \cdot (\mathbf{y} - \mathbf{y}')) \, d\mathbf{y} d\mathbf{y}'$$

where $(\wp_{\mathbf{k}}^\perp)_{q,q'}$ denotes the entry corresponding to the q^{th} row and q'^{th} column of the matrix. The notation $H_{q,q'}^{[\ell,\ell']}(s)$ denotes the entry corresponding with the $3\ell + q$ row and $3\ell' + q'$ column of the matrix.

We now compute the effective thermal fluctuations of the structures when the fluid degrees of freedom are eliminated:

$$(3.17) \quad \left\langle \left(\hat{\mathbf{X}}_q^{[\ell]}(\Delta t) - \mathbf{X}_q^{[\ell]}(0) \right) \left(\hat{\mathbf{X}}_{q'}^{[\ell']}(\Delta t) - \mathbf{X}_{q'}^{[\ell']}(0) \right) \right\rangle \\ = \left\langle \int_{\Omega} \int_0^{\Delta t} \delta_a(\mathbf{y} - \mathbf{X}^{[\ell]}(s)) \mathbf{w}_q(\mathbf{y}, s) ds dy \cdot \int_{\Omega} \int_0^{\Delta t} \delta_a(\mathbf{y}' - \mathbf{X}^{[\ell']}(s')) \mathbf{w}_{q'}(\mathbf{y}', s') ds' dy' \right\rangle.$$

The notation \mathbf{w}_q denotes the q^{th} vector component of \mathbf{w} . We denote by $\hat{\mathbf{X}}_q^{[\ell]}$ the $3\ell + q$ vector component of $\hat{\mathbf{X}}$ with the other terms to be interpreted similarly.

To avoid computing the full expectation above we shall assume a separation of time scales between the time scale of the elementary particle motion and the fluid dynamics so that $\tau_{\text{fld}} \ll \Delta t \ll \tau_{\text{prt}}$. For such Δt the elementary particles move a negligible distance relative to their size over the time increment $[0, \Delta t]$. Approximating the particle position as constant gives:

$$(3.18) \quad \left\langle \left(\hat{\mathbf{X}}_q^{[\ell]}(\Delta t) - \mathbf{X}_q^{[\ell]}(0) \right) \left(\hat{\mathbf{X}}_{q'}^{[\ell']}(\Delta t) - \mathbf{X}_{q'}^{[\ell']}(0) \right) \right\rangle \\ \approx \int_{\Omega} \int_{\Omega} \delta_a(\mathbf{y} - \mathbf{X}^{[\ell]}(0)) \delta_a(\mathbf{y}' - \mathbf{X}^{[\ell']}(0)) \cdot \int_0^{\Delta t} \int_0^{\Delta t} \langle \mathbf{w}_q(\mathbf{y}, s) \mathbf{w}_{q'}(\mathbf{y}', s') \rangle ds' ds dy' dy.$$

From 3.4 we can express the expectation by:

$$(3.19) \quad \langle \mathbf{w}_q(\mathbf{y}, s) \mathbf{w}_{q'}(\mathbf{y}', s') \rangle \\ = \sum_{\mathbf{k}, \mathbf{k}'} 2D_{\mathbf{k}} \int_{-\infty}^s \int_{-\infty}^{s'} e^{-\alpha_{\mathbf{k}}(s+s'-r-r')} \left\langle \wp_{\mathbf{k}}^\perp d\tilde{\mathbf{B}}_{\mathbf{k}}(r) \overline{\left(\wp_{\mathbf{k}}^\perp d\tilde{\mathbf{B}}_{\mathbf{k}'}(r') \right)^T} \right\rangle_{q,q'} ds' ds$$

where $\langle \cdot \rangle_{q,q'}$ denotes the (q, q') entry of the expectation of the matrix.

From the properties of the complex-valued Brownian motion driving the system with constraint 2.13 we have:

$$(3.20) \quad \left\langle \wp_{\mathbf{k}}^\perp d\tilde{\mathbf{B}}_{\mathbf{k}}(r) \overline{\left(\wp_{\mathbf{k}}^\perp d\tilde{\mathbf{B}}_{\mathbf{k}'}(r') \right)^T} \right\rangle = \wp_{\mathbf{k}}^\perp \left\langle d\tilde{\mathbf{B}}_{\mathbf{k}}(r) \overline{d\tilde{\mathbf{B}}_{\mathbf{k}'}^T(r')} \right\rangle (\wp_{\mathbf{k}}^\perp)^T \\ = \wp_{\mathbf{k}}^\perp 2\mathcal{I} \delta(r - r') \delta_{\mathbf{k}, \mathbf{k}'} (\wp_{\mathbf{k}}^\perp)^T \\ = 2\wp_{\mathbf{k}}^\perp \delta(r - r') \delta_{\mathbf{k}, \mathbf{k}'}$$

where $\delta(r - r')$ denotes the Dirac δ -function and $\delta_{\mathbf{k}, \mathbf{k}'}$ denotes the Kronecker δ -function. To obtain the last expression we also use that $(\wp_{\mathbf{k}}^\perp)^T = \wp_{\mathbf{k}}^\perp$ and $(\wp_{\mathbf{k}}^\perp)^2 = \wp_{\mathbf{k}}^\perp$ which follow from 2.10.

From this it follows that:

$$(3.21) \quad \langle \mathbf{w}_q(\mathbf{y}, s) \mathbf{w}_{q'}(\mathbf{y}', s') \rangle = \sum_{\mathbf{k}} \frac{2D_{\mathbf{k}}}{\alpha_{\mathbf{k}}} (\wp_{\mathbf{k}}^{\perp})_{q,q'} e^{-\alpha_{\mathbf{k}}|s-s'|} \exp(i2\pi\mathbf{k} \cdot (\mathbf{y} - \mathbf{y}'))$$

and

$$(3.22) \quad \int_0^{\Delta t} \int_0^{\Delta t} \langle \mathbf{w}_q(\mathbf{y}, s) \mathbf{w}_{q'}(\mathbf{y}', s') \rangle ds' ds = \sum_{\mathbf{k}} \frac{4D_{\mathbf{k}}}{\alpha_{\mathbf{k}}} (\wp_{\mathbf{k}}^{\perp})_{q,q'} \frac{1}{\alpha_{\mathbf{k}}} \left(\Delta t - \frac{1}{\alpha_{\mathbf{k}}} (1 - e^{-\alpha_{\mathbf{k}}\Delta t}) \right).$$

Substituting this into equation 3.18 and taking the limit in 3.10 we obtain:

$$(3.23) \quad \Gamma_{q,q'}^{[\ell,\ell']} = 2k_B T \int_{\Omega} \int_{\Omega} \delta_a(\mathbf{y} - \mathbf{X}^{[\ell]}(0)) \delta_a(\mathbf{y}' - \mathbf{X}^{[\ell']}(0)) \cdot \sum_{\mathbf{k}} \frac{\rho^{-1} (\wp_{\mathbf{k}}^{\perp})_{q,q'}}{\alpha_{\mathbf{k}} L^3} \exp(i2\pi\mathbf{k} \cdot (\mathbf{y} - \mathbf{y}')) d\mathbf{y} d\mathbf{y}'.$$

From 3.16 and 3.23 it follows that a fluctuation-dissipation relation holds for the effective equations (15; 19):

$$(3.24) \quad \Gamma_{q,q'}^{[\ell,\ell']} = 2k_B T \cdot H_{q,q'}^{[\ell,\ell']}.$$

We now discuss the correspondence between the Immersed Boundary Method and Stokesian-Brownian Dynamics. The equation 3.16 for the hydrodynamic coupling matrix H can be expressed by computing the Inverse Fourier Transform:

$$(3.25) \quad H_{q,q'}^{[\ell,\ell']}(s) = \int_{\Omega} \delta_a(\mathbf{y} - \mathbf{X}^{[\ell]}(s)) \int_{\Omega} \mathcal{T}_{q,q'}(\mathbf{y}' - \mathbf{y}) \delta_a(\mathbf{y}' - \mathbf{X}^{[\ell']}(s)) d\mathbf{y}' d\mathbf{y}$$

where

$$(3.26) \quad \mathcal{T}(\mathbf{r}) = \frac{\rho}{8\pi\mu|\mathbf{r}|} \left(\mathcal{I} + \frac{\mathbf{r}\mathbf{r}^T}{|\mathbf{r}|^2} \right).$$

From 3.25 the matrix H is symmetric and positive definite so that a matrix C can be found from 3.24 with:

$$(3.27) \quad \Gamma = CC^T.$$

The matrix C can be expressed from 3.24 as:

$$(3.28) \quad C = \sqrt{2k_B T \cdot H}.$$

In practice, C can be found by numerically performing a Cholesky factorization of H (18).

The effective stochastic dynamics of the structures in the Immersed Boundary Method can then be expressed as:

$$(3.29) \quad d\mathbf{X}(t) = H\mathbf{F}(\mathbf{X}(t), t)dt + \sqrt{2k_B T \cdot H} d\mathbf{B}(t).$$

From 3.25 we find that the hydrodynamic coupling in the effective elementary particle dynamics recovers the Oseen tensor \mathcal{T} used in Stokesian-Brownian Dynamics (3; 6) (also referred to as the Green's function of Stokes equation or the Stokeslet tensor). A notable difference in how this tensor arises in the Immersed Boundary Method is that the force is spread out over a region determined by the function δ_a . In Stokesian-Brownian Dynamics in which a particle is represented on small scales with a sharply delineated boundary with the fluid, the forces act on the fluid through stresses integrated over the surface of the particles (3; 6).

In numerical practice carrying out this integration would be expensive so the integral is often handled only approximately. A simple approximation often used is to treat the force acting on the fluid only at a single point at the center of a particle (3; 6). For small particles which are far apart relative to their size the differences between the Stokesian-Brownian Dynamics approach and that associated with the effective dynamics of particles in the Immersed Boundary Method in 3.25 is small.

To deal with particles when they become close in Stokesian-Brownian Dynamics an additional hydrodynamic lubrication term is often included to capture the effects of the small scale flow in which the fluid is "squeezed out" from between the rigid boundaries of the particles as they approach one another (3; 6). In the Immersed Boundary Method no such near-field lubrication term is explicitly included.

For microscopic biological systems the boundaries of the structures when approaching molecular length scales are less rigid or sharply delineated with the fluid than in systems encountered in the engineering applications which originally motivated the Stokesian-Brownian Dynamics approach (3; 6). In some circumstances even the no-slip boundary condition of a particle may be called into question (9). Thus determining appropriate hydrodynamic lubrication terms in the biological context poses a number of interesting challenges and is possibly application specific.

The Immersed Boundary Method as a consequence can only be expected to reliably capture hydrodynamic effects at large separation distances between the particles. These differences show that when particles become close in the Immersed Boundary Method care must be taken in how the particle dynamics are handled and additional correction terms may be warranted. To summarize, we find that the effective stochastic dynamics of particles in the Immersed Boundary Method agrees well with Stokesian-Brownian Dynamics when considering only the far-field hydrodynamic coupling interactions.

3.2. The Effective Stochastic Dynamics of a Single Particle. The effective dynamics of a single particle can readily be obtained by reduction of the multiple particle expressions. For the hydrodynamic drift term we have:

$$(3.30) \quad H(s) = \int_{\Omega} \int_{\Omega} \delta_a(\mathbf{y} - \mathbf{X}(s)) \delta_a(\mathbf{y}' - \mathbf{X}(s)) \sum_{\mathbf{k}} \frac{\rho^{-1} \varrho_{\mathbf{k}}^{\perp}}{\alpha_{\mathbf{k}} L^3} \exp(i2\pi\mathbf{k} \cdot (\mathbf{y} - \mathbf{y}')) d\mathbf{y} d\mathbf{y}'$$

and for the correlations of the thermal fluctuations we have:

$$(3.31) \quad CC^T = 2k_B T \int_{\Omega} \int_{\Omega} \delta_a(\mathbf{y} - \mathbf{X}(0)) \delta_a(\mathbf{y}' - \mathbf{X}(0)) \cdot$$

$$\sum_{\mathbf{k}} \frac{\rho^{-1} \wp_{\mathbf{k}}^{\perp}}{\alpha_{\mathbf{k}} L^3} \exp(i2\pi \mathbf{k} \cdot (\mathbf{y} - \mathbf{y}')) dy dy'.$$

Using the definition 2.10 and assuming rotational symmetry for $\delta_a(\mathbf{z})$ about the origin it can be shown that the off-diagonal terms of the matrix H are zero. Moreover, the diagonal entries can be shown to be equal. This allows for an effective friction coefficient γ to be defined for the particle:

(3.32)

$$\gamma := \left(\int_{\Omega} \int_{\Omega} \delta_a(\mathbf{y} - \mathbf{X}(s)) \delta_a(\mathbf{y}' - \mathbf{X}(s)) \sum_{\mathbf{k}} \frac{\rho^{-1} (\wp_{\mathbf{k}}^{\perp})_{q,q}}{\alpha_{\mathbf{k}} L^3} \exp(i2\pi \mathbf{k} \cdot (\mathbf{y} - \mathbf{y}')) dy dy' \right)^{-1}.$$

We remark that this definition is independent of both the index (q, q) used for the diagonal entry and the particle location $\mathbf{X}(s)$.

From 3.28 and 3.32 we have that:

$$(3.33) \quad \begin{aligned} C &= \sqrt{2k_B T \cdot H} \\ &= \sqrt{\frac{2k_B T}{\gamma} \mathcal{I}}. \end{aligned}$$

In the absence of a particle force the effective stochastic equation 3.29 can be solved exactly and the diffusion coefficient of the particle is given by:

$$(3.34) \quad \begin{aligned} D &= \frac{1}{6} \text{trace}(C^2) \\ &= \frac{k_B T}{\gamma}. \end{aligned}$$

This shows that the classical Einstein's relation (5) for a Brownian particle holds for a particle modeled by the effective stochastic equations of the Immersed Boundary Method when the effective friction coefficient is defined by 3.32.

When a force \mathbf{F} acts on the particle the drift term can be expressed from 3.30 and 3.32 as:

$$(3.35) \quad H\mathbf{F} = \frac{1}{\gamma} \mathbf{F}.$$

For a single particle the effective stochastic equations, when defining the particle friction coefficient by 3.32, reduces to classical Smoluchowsky dynamics (20):

$$(3.36) \quad d\mathbf{X}(t) = \frac{1}{\gamma} \mathbf{F} dt + \sqrt{2D} d\mathbf{B}(t).$$

4. Conclusion. In this work, a correspondence of an Immersed Boundary Method incorporating thermal fluctuations was made with Stokesian-Brownian Dynamics by working directly with the stochastic equations. It was found in the small Reynolds number limit that the effective stochastic dynamics of structures of the Immersed Boundary Method are in agreement with Stokesian-Brownian Dynamics with respect to the far-field hydrodynamic interactions. Further, it was found that the effective stochastic dynamics obey a fluctuation-dissipation relation which reduces in the case of a single particle to Einstein's relation, provided the particle friction coefficient is defined appropriately. These results indicate that the Immersed Boundary Method incorporating thermal fluctuations captures in a physically accurate manner phenomena associated with the fluctuations of immersed structures in microscopic hydrodynamic systems.

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