ERROR ANALYSIS OF A STOCHASTIC IMMERSED BOUNDARY METHOD INCORPORATING THERMAL FLUCTUATIONS

PAUL J. ATZBERGER * AND PETER R. KRAMER †

Abstract. A stochastic numerical scheme for an extended immersed boundary method which incorporates thermal fluctuations for the simulation of microscopic biological systems consisting of fluid and immersed elastica was introduced in (1). The numerical scheme uses techniques from stochastic calculus to overcome stability and accuracy issues associated with standard finite difference methods. The numerical scheme handles a range of time steps in a unified manner, including time steps which are greater than the smallest time scales of the system. The time step regimes we shall investigate can be classified as small, intermediate, or large relative to the time scales of the fluid dynamics of the system. Small time steps resolve in a computationally explicit manner the dynamics of all the degrees of freedom of the system. Large time steps resolve in a computationally explicit manner only the degrees of freedom of the immersed elastica, with the contributions of the dynamics of the fluid degrees of freedom accounted for in only a statistical manner over a time step. Intermediate time steps resolve in a computationally explicit manner only some degrees of freedom of the fluid with the remaining degrees of freedom accounted for statistically over a time step. In this paper, uniform bounds are established for the strong error of the stochastic numerical method for each of the time step regimes. The scaling of the numerical error with respect to the parameters of the method is also given.

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

1. Introduction. With experimental advances in optical tweezers, fluorescent probes, and protein assays, there has been a steady increase in the amount of biochemical, structural, and even mechanical information available for cellular and intracellular processes (4; 26; 37). Integrating this information to formulate models of biological processes within the cell is challenging given the wide range of active length and time scales. While molecular dynamics yields insight into the role of individual molecules and small assemblies (35), understanding complex processes involved in cell division and motility (3; 14; 34; 39) or in the functioning of organelles such as the golgi apparatus and endoplasmic reticulum (2) requires modeling on a more coarse-grained level (8). Which spatial and temporal scales are modeled depends on the mechanisms being studied. The mechanics of many biological systems to a first approximation can be thought of in terms of immersed elastic structures which interact with a fluid (3; 23). The immersed boundary method of (29) has been used to model the mechanics of many macroscopic biological systems such as blood flow in the heart (30), wave propagation in the cochlea (12), and lift generation in insect flight (25). However, for cellular and intracellular processes thermal fluctuations also play an important role (13; 16; 28; 33). An extended immersed boundary method which incorporates thermal fluctuations for modeling of the elastic mechanics and fluid dynamics of microscopic biological systems was recently introduced in (1; 18).

The extended immersed boundary method incorporates thermal fluctuations through appropriate stochastic forcing terms in the fluid equations consistent with the principles of statistical mechanics. Integrating these equations numerically poses a number of difficulties arising from fast time scales introduced by the stochastic forcing terms. This leads to stiffness in the fluid equations, which severely restricts admissible time steps for standard finite difference methods, such as explicit or implicit Runge-Kutta

*Rensselaer Polytechnic Institute, Department of Mathematics , Troy, NY 12180
†Rensselaer Polytechnic Institute, Department of Mathematics , Troy, NY 12180

methods (17). To overcome these restrictions, a numerical scheme was devised in (1) using results from stochastic calculus to avoid a full discretization in time of the fluid equations, thereby allowing large time steps to be taken.

We shall be concerned here with the accuracy of the proposed stochastic numerical method. Given the analytic manner in which the dynamics of the fluid is partially integrated using stochastic calculus, a high level of accuracy can be attained even for relatively large time steps, provided certain asymptotic conditions are met by the time step relative to the parameters of the method. This requires that a somewhat different approach be taken to understand the accuracy of the method than in standard numerical analysis in which one typically analyzes the limit as the time step is made small relative to all time scales of the problem (36).

Instead, we shall perform analysis of the numerical method by rigorously establishing, under a few natural assumptions, general error bounds which hold uniformly over all time steps. The terms in these bounds will then be further estimated in asymptotic regimes in which the time step is of a size which is small, intermediate, or large relative to the time scales associated with the dynamics of the fluid degrees of freedom. This approach allows for the accuracy of the scheme to be understood in a variety of different parameter regimes depending on the desired mode of operation of the method and the specific physical system being simulated.

The paper is organized as follows. In Section 2, the extended framework of the immersed boundary method incorporating thermal fluctuations is introduced along with a summary of the numerical scheme formulated in (1). Some notational conventions that will be used throughout the paper are then discussed in Section 3. In Section 4, general error estimates are proved for the numerical method. To investigate how the errors scale for small, intermediate, and large time steps, further refinements of the general error estimates are made in Sections 5–7. Finally, in Section 8, the scaling of the numerical error with respect to the parameters of the method is given.

2. The Immersed Boundary Method with Thermal Fluctuations. In microscopic biological systems, the Reynolds number is very small and to a good approximation the fluid dynamics is governed by the Stokes' equations (22):

$$\rho\frac{\partial \mathbf{u}(\mathbf{x},t)}{\partial t} = \mu\Delta\mathbf{u}(\mathbf{x},t) - \nabla p + \mathbf{f}(\mathbf{x},t) \tag{2.1}$$

$$\nabla\cdot\mathbf{u} = 0 \tag{2.2}$$

where p is the pressure arising from the incompressibility constraint, ρ is the fluid density, μ is the dynamic viscosity, and $\mathbf{f}$ is a force density acting on the fluid. In the immersed boundary method with thermal fluctuations, the force density has two components:

$$\mathbf{f}(\mathbf{x},t) = \mathbf{f}_{\mathrm{prt}}(\mathbf{x},t) + \mathbf{f}_{\mathrm{thm}}(\mathbf{x},t). \tag{2.3}$$

The component $\mathbf{f}_{\mathrm{thm}}$ represents a forcing of the fluid equations which represents thermal fluctuations of the system. The detailed form of this force will be discuss at greater length below.

The force density $\mathbf{f}_{\mathrm{prt}}(\mathbf{x},t)$ arises from forces acting on structures immersed in the fluid, such as particles, polymers, and membranes. These structures can be represented in the immersed boundary method through discretization into a finite set of moving control points which we shall refer to as "elementary particles". The force density has the form:

$$\mathbf{f}_{\text{prt}}(\mathbf{x},t) = \sum_{j=1}^{M} \mathbf{F}^{[j]}(\{\mathbf{X}(t)\})\ \delta_a(\mathbf{x} - \mathbf{X}^{[j]}(t)) \tag{2.4}$$

where $\mathbf{X}^{[j]}$ and $\mathbf{F}^{[j]}$ denote respectively the position and force acting on the of the j^{th} elementary particle. If the forces were, for example, governed by a general potential function V, then we would have $\mathbf{F}^{[j]} = -\nabla_{\mathbf{X}^{[j]}} V(\{\mathbf{X}\})$. The notation $\{\mathbf{X}(t)\}$ denotes the composite vector of all particle positions. The factor δ_a is a weight function which integrates to one and represents the spatial region occupied by a particle. The parameter a designates the approximate size of a particle which corresponds to the region on which δ_a is non-zero (9; 24).

To update the position of an elementary particle, an interpolation of the fluid velocity is performed in the vicinity of the particle:

$$\frac{d\mathbf{X}^{[j]}(t)}{dt} = \int_{\Lambda} \delta_a(\mathbf{x} - \mathbf{X}^{[j]}(t))\mathbf{u}(\mathbf{x},t)d\mathbf{x} \tag{2.5}$$

with the integral taken over the entire spatial domain Λ of the fluid.

The equations 2.1 – 2.5 constitute what we refer to as the immersed boundary method with thermal fluctuations (1). We shall now discuss a spatial discretization of these equations and the thermal forcing term which, for a given discretization, is chosen in such a manner as to be consistent with laws of statistical mechanics.

The discretization used for equations 2.1 and 2.2 in space is:

$$\begin{aligned} \rho\frac{d\mathbf{u}_{\mathbf{m}}}{dt} &= \mu\sum_{\ell=1}^{3} \frac{\mathbf{u}_{\mathbf{m}-\mathbf{e}_\ell}(t) - 2\mathbf{u}_{\mathbf{m}}(t) + \mathbf{u}_{\mathbf{m}+\mathbf{e}_\ell}(t)}{\Delta x^2} \\ &\quad - \sum_{\ell=1}^{3} \frac{p_{\mathbf{m}+\mathbf{e}_\ell} - p_{\mathbf{m}-\mathbf{e}_\ell}}{2\Delta x}\mathbf{e}_\ell + \mathbf{f}_{\text{total}}(\mathbf{x}_{\mathbf{m}},t) \end{aligned} \tag{2.6}$$

$$\sum_{\ell=1}^{3} \frac{\mathbf{u}^{(\ell)}_{\mathbf{m}+\mathbf{e}_\ell}(t) - \mathbf{u}^{(\ell)}_{\mathbf{m}-\mathbf{e}_\ell}(t)}{2\Delta x} = 0 \tag{2.7}$$

where $\mathbf{e}_\ell$ denotes the standard basis vector with all zero entries except for a one in the ℓ^{th} position. The parenthesized superscripts denote the vector component. The subscripts denote the indices of the lattice points used in the discretization.

The fluid-structure coupling equations 2.4 and 2.5 are discretized by:

$$\mathbf{f}_{\text{prt}}(\mathbf{x}_{\mathbf{m}},t) = \sum_{j=1}^{M} \mathbf{F}^{[j]}(\{\mathbf{X}(t)\})\ \delta_a(\mathbf{x}_{\mathbf{m}} - \mathbf{X}^{[j]}(t)) \tag{2.8}$$

$$\frac{d\mathbf{X}^{[j]}(t)}{dt} = \mathbf{U}(\mathbf{X}^{[j]}(t),t) \tag{2.9}$$

$$\mathbf{U}(\mathbf{x},t) = \sum_{\mathbf{m}} \delta_a(\mathbf{x}_{\mathbf{m}} - \mathbf{x})\mathbf{u}(\mathbf{x}_{\mathbf{m}},t)\Delta x^3. \tag{2.10}$$

All quantities with subscript $\mathbf{m} = (m_1, m_2, m_3)$ are specified on a cubic lattice with N points in each direction. We define L as the edge length of the cubic computational domain, so the spacing between grid points is $\Delta x = L/N$. The position of the grid point with index $\mathbf{m}$ is denoted by $\mathbf{x_m}$. In addition, periodic boundary conditions are imposed.

To handle the equations numerically, the following Discrete Fourier Transform (DFT) will be used (5; 31):

$$\hat{\mathbf{u}}_{\mathbf{k}} = \frac{1}{N^3}\sum_{\mathbf{m}} \mathbf{u}_{\mathbf{m}} \exp\left(-i2\pi \mathbf{k}\cdot\mathbf{m}/N\right) \tag{2.11}$$

$$\mathbf{u}_{\mathbf{m}} = \sum_{\mathbf{k}} \hat{\mathbf{u}}_{\mathbf{k}} \exp\left(i2\pi \mathbf{k}\cdot\mathbf{m}/N\right) \tag{2.12}$$

where each of the sums in the above equations runs over any translate of the N^3 lattice points defined by $0 \leq \mathbf{k}^{(\ell)} \leq N-1$ and $0 \leq \mathbf{m}^{(\ell)} \leq N-1$ where $\ell = 1,2,3$.

Under the discrete Fourier Transform (DFT), the Stokes equation can be expressed in differential notation as:

$$d\hat{\mathbf{u}}_{\mathbf{k}} = -\alpha_{\mathbf{k}}\wp_{\mathbf{k}}^{\perp}\hat{\mathbf{u}}_{\mathbf{k}}dt + \rho^{-1}\wp_{\mathbf{k}}^{\perp}\hat{\mathbf{f}}_{\mathrm{prt},\mathbf{k}}dt + \rho^{-1}\wp_{\mathbf{k}}^{\perp}\hat{\mathbf{f}}_{\mathrm{thm},\mathbf{k}}dt \tag{2.13}$$

where

$$\alpha_{\mathbf{k}} = \frac{2\mu}{\rho\Delta x^2}\sum_{j=1}^{3}(1-\cos(2\pi\mathbf{k}^{(j)}/N))). \tag{2.14}$$

The incompressibility constraint becomes:

$$\hat{\mathbf{g}}_{\mathbf{k}}\cdot\hat{\mathbf{u}}_{\mathbf{k}} = 0 \tag{2.15}$$

with

$$\hat{\mathbf{g}}_{k}^{(j)} = \sin(2\pi\mathbf{k}^{(j)}/N)/\Delta x. \tag{2.16}$$

In 2.13, this constraint is handled by the projection method (6) where the projection operator in the direction orthogonal to $\hat{\mathbf{g}}_{\mathbf{k}}$ is denoted by:

$$\wp_{\mathbf{k}}^{\perp} = \left(\mathcal{I} - \frac{\hat{\mathbf{g}}_{\mathbf{k}}\hat{\mathbf{g}}_{\mathbf{k}}^{T}}{|\hat{\mathbf{g}}_{\mathbf{k}}|^2}\right). \tag{2.17}$$

For those modes for which $\hat{\mathbf{g}}_{\mathbf{k}} = \mathbf{0}$, the projections is defined as $\wp_{\mathbf{k}}^{\perp} = \mathcal{I}$. The set of indices on which $\hat{\mathbf{g}}_{\mathbf{k}} = \mathbf{0}$ is given by:

$$\mathcal{K} = \left\{(\mathbf{k}^{(1)},\mathbf{k}^{(2)},\mathbf{k}^{(3)}) \mid \mathbf{k}^{(j)} = 0 \ \vee\ \mathbf{k}^{(j)} = N/2,\ j = 1,2,3\right\}. \tag{2.18}$$

For the above discretization, the thermal forcing was derived in (1) and is given by:

$$\hat{\mathbf{f}}_{\mathrm{thm},\mathbf{k}}(t)dt = \sqrt{2D_{\mathbf{k}}}\wp_{\mathbf{k}}^{\perp}d\tilde{\mathbf{B}}_{\mathbf{k}}(t) \tag{2.19}$$

where

$$D_{\mathbf{k}} = \begin{cases} \frac{k_BT}{\rho L^3}\alpha_{\mathbf{k}} & ,\ \mathbf{k}\in\mathcal{K} \\ \frac{k_BT}{2\rho L^3}\alpha_{\mathbf{k}} & ,\ \mathbf{k}\notin\mathcal{K} \end{cases} \tag{2.20}$$

and $\tilde{\mathbf{B}}_{\mathbf{k}}(t)$ denotes a three dimensional complex-valued stochastic process which in each real and imaginary component is a standard Brownian motion. In 2.13 and 2.19, the use of differential notation is made as is common when working with stochastic processes to avoid taking derivatives of Brownian motion, which do not exist as a consequence of the order $\sqrt{\Delta t}$ scaling of increments of $\tilde{\mathbf{B}}(t+\Delta t)-\tilde{\mathbf{B}}(t)$. All stochastic differential expressions are to be interpreted in the sense of Itô (11; 27).

The requirement that the velocity field of the fluid be real-valued gives the following condition which must be satisfied by solutions of equation 2.13:

$$\overline{\hat{\mathbf{u}}_{\mathbf{N}-\mathbf{k}}} = \hat{\mathbf{u}}_{\mathbf{k}}, \tag{2.21}$$

where $\mathbf{N}$ is shorthand for $(N,N,N)^T$ and the overbar denotes complex conjugation. Provided the force is real-valued, it can be shown that if this constraint holds for the initial conditions, then it will be satisfied for all time.

2.1. Summary of the Numerical Method. Each time step the following operations are performed to advance the velocity field of the fluid and the configuration of the immersed structures, as represented by the positions of the elementary particles:

1. The forces acting on the elementary particles are computed and the force density field which is applied to the fluid is obtained from

$$\mathbf{f}^n(\mathbf{x}) = \sum_{j=1}^{N} \mathbf{F}^{[j]}(\{\mathbf{X}^n\})\ \delta_a(\mathbf{x}-\mathbf{X}^{n,[j]}) \tag{2.22}$$

The Fourier coefficients $\hat{\mathbf{f}}_{\mathbf{k}}^n$ are computed using a discrete Fast Fourier Transform (FFT).

2. The velocity field of the fluid is updated by the stochastic recurrence

$$\hat{\mathbf{u}}_{\mathbf{k}}^{n+1} = e^{-\alpha_{\mathbf{k}}\Delta t}\hat{\mathbf{u}}_{\mathbf{k}}^n + \frac{1}{\rho\alpha_{\mathbf{k}}}\left(1-e^{-\alpha_{\mathbf{k}}\Delta t}\right)\wp_{\mathbf{k}}^{\perp}\hat{\mathbf{f}}_{\mathbf{k}}^n + \wp_{\mathbf{k}}^{\perp}\hat{\boldsymbol{\Xi}}_{\mathbf{k}}^n \tag{2.23}$$

where $\wp_{\mathbf{k}}^{\perp}$ denotes the projection orthogonal to $\hat{\mathbf{g}}_{\mathbf{k}}$ defined in 2.16 and is used to enforce the incompressibility constraint 2.15. The factor $\hat{\boldsymbol{\Xi}}_{\mathbf{k}}^n = \sigma_{\mathbf{k}}\boldsymbol{\eta}_{\mathbf{k}}$ accounts for potentially rapid fluctuations over the time step. In the notation $\boldsymbol{\eta}_{\mathbf{k}}$ denotes a complex vector-valued random variable independent in $\mathbf{k}$ having independent real and imaginary components, each of which are Gaussian random variables with mean zero and variance one. The variance of $\hat{\boldsymbol{\Xi}}_{\mathbf{k}}^n$ is determined in (1) and is given by

$$\sigma_{\mathbf{k}}^2 = \frac{D_{\mathbf{k}}}{\alpha_{\mathbf{k}}}\left(1-\exp\left(-2\alpha_{\mathbf{k}}\Delta t\right)\right) \tag{2.24}$$

where $\alpha_{\mathbf{k}}$ is defined in 2.14 and $D_{\mathbf{k}}$ is defined in 2.20.

3. The particle positions are updated by

$$\mathbf{X}^{n+1,[j]} - \mathbf{X}^{n,[j]} = \sum_{\mathbf{m}} \delta_a(\mathbf{x}_{\mathbf{m}}-\mathbf{X}^{n,[j]})\boldsymbol{\Gamma}_{\mathbf{m}}^n\Delta x^3 \tag{2.25}$$

where $\boldsymbol{\Gamma}_{\mathbf{m}}^n$ is the time integrated velocity field of the fluid. It is obtained by a discrete Inverse Fast Fourier Transform (IFFT) of appropriately generated random variables $\hat{\boldsymbol{\Gamma}}_{\mathbf{k}}^n$ in Fourier space:

$$\boldsymbol{\Gamma}_{\mathbf{m}}^n = \int_{t_n}^{t_{n+1}} \mathbf{u}_{\mathbf{m}}(s)ds = \sum_{\mathbf{k}} \hat{\boldsymbol{\Gamma}}_{\mathbf{k}}^n \cdot \exp\left(i2\pi\mathbf{k}\cdot\mathbf{m}/N\right). \tag{2.26}$$

The $\hat{\boldsymbol{\Gamma}}_{\mathbf{k}}^n$ are computed from

$$\hat{\boldsymbol{\Gamma}}_{\mathbf{k}}^n = \hat{\mathbf{Z}}_{\mathbf{k}} + c_{1,\mathbf{k}}\wp_{\mathbf{k}}^{\perp}\hat{\boldsymbol{\Xi}}_{\mathbf{k}}^n + c_{2,\mathbf{k}}\wp_{\mathbf{k}}^{\perp}\hat{\mathbf{G}}_{\mathbf{k}} \tag{2.27}$$

where $\hat{\boldsymbol{\Xi}}_{\mathbf{k}}^n$ is obtained from step 2 and $\hat{\mathbf{Z}}_{\mathbf{k}}$ is computed from step 1 and 2 by

$$\hat{\mathbf{Z}}_{\mathbf{k}} = \frac{1-\exp\left(-\alpha_{\mathbf{k}}\Delta t\right)}{\alpha_{\mathbf{k}}}\hat{\mathbf{u}}_{\mathbf{k}}^n + \left(\frac{\Delta t}{\alpha_{\mathbf{k}}} + \left(\frac{1}{\alpha_{\mathbf{k}}}\right)^2\left(\exp\left(-\alpha_{\mathbf{k}}\Delta t\right)-1\right)\right)\rho^{-1}\wp_{\mathbf{k}}^{\perp}\hat{\mathbf{f}}_{\mathbf{k}}^n. \tag{2.28}$$

The random variable $\hat{\mathbf{G}}_{\mathbf{k}}$ is computed from scratch for each mode $\mathbf{k}$ by generating a complex vector-valued random variable having independent real and imaginary components, each of which are Gaussian random variables with mean zero and variance one. The constants in 2.27 are given by

$$c_{1,\mathbf{k}} = \frac{1}{\alpha_{\mathbf{k}}}\tanh\left(\frac{\alpha_{\mathbf{k}}\Delta t}{2}\right) \tag{2.29}$$

and

$$c_{2,\mathbf{k}} = \sqrt{\left(\frac{2D_{\mathbf{k}}}{\alpha_{\mathbf{k}}^3}\right)\left(\alpha_{\mathbf{k}}\Delta t - 2\tanh\left(\frac{\alpha_{\mathbf{k}}\Delta t}{2}\right)\right)} \tag{2.30}$$

In this manner the time integrated velocity field is generated consistently with the correct correlations with $\{\mathbf{u}_{\mathbf{k}}^n\}$ and $\{\mathbf{u}_{\mathbf{k}}^{n+1}\}$ from steps 1 and 2. This procedure is discussed in greater detail in (1).

The computational complexity of the method, when excluding the application specific forces acting on the elementary particles, is dominated by the FFT and IFFT which for a three dimensional lattice requires $O(N^3\ln(N^3))$ arithmetic steps.

3. Error Estimates of the Numerical Method. To quantify the accuracy of the method, the strong error will be considered, following (17). The strong error for the $\mathbf{k}^{th}$ mode of the fluid is defined as:

$$\hat{e}_{\text{fld},\mathbf{k}}(\Delta t) := E\left(\left|\hat{\mathbf{u}}_{\mathbf{k}}(\Delta t) - \hat{\tilde{\mathbf{u}}}_{\mathbf{k}}(\Delta t)\right|\right). \tag{3.1}$$

For the velocity field expressed in physical space, the associated strong error is defined by:

$$e_{\text{fld}}(\Delta t) := E\left(\frac{1}{L^3}\sum_{\mathbf{m}}\left|\mathbf{u}_{\mathbf{m}}(\Delta t) - \tilde{\mathbf{u}}_{\mathbf{m}}(\Delta t)\right|\Delta x^3\right). \tag{3.2}$$

The strong error of an elementary particle constituting the immersed structures is defined by:

$$e_{\text{prt}}(\Delta t) := E\left(\left|\mathbf{X}(\Delta t) - \tilde{\mathbf{X}}(\Delta t)\right|\right). \tag{3.3}$$

In the notation, $\mathbf{X}(t)$ denotes the exact solution of equation 2.9 for the elementary particles and $\hat{\mathbf{u}}_{\mathbf{k}}(t)$ denotes the exact solution to equation 2.6 for the Fourier modes of the velocity field of the fluid. The numerically computed trajectories of the elementary particles are denoted by $\tilde{\mathbf{X}}(t)$ and the numerically computed fluid modes are denoted by $\tilde{\mathbf{u}}_{\mathbf{k}}(t)$. Since we are interested in analyzing the error incurred only over a time step we shall assume that the numerically computed particle positions and fluid modes are the same as the exact solution at the beginning of each time step, which for convenience will be taken as time 0. The superscript j is dropped throughout the discussion since we shall be interested in the generic error associated with a typical elementary particle.

Error estimates will be established rigorously for the strong error of the numerical method for both the fluid and structural degrees of freedom as defined in 3.1, 3.2, and 3.3 under a few specified assumptions. An important feature of the numerical method is that depending on the time scales of the problem simulated and the choice of time step, the dynamics of the fluid can be either resolved in detail or under-resolved with the contributions of such degrees of freedom handled statistically over a time step (1).

We will always assume here that the structural degrees of freedom are resolved, so our analysis is most relevant for the situation in which the dynamics of some of the fluid modes is fast compared to the dynamical time scale of the immersed structures. This is a rather general situation in microbiology, where the Kubo and Reynolds numbers are small (19; 20). Unlike standard numerical methods which are typically analyzed when the time step is taken smaller than all time scales of the problem, for the stochastic immersed boundary method we shall be interested in analyzing the error even when the time step is taken larger than some of the time scales of the problem.

To obtain estimates of the error in the different regimes of the time step, we first establish general error bounds which hold uniformly for all time steps which resolve the structural degrees of freedom. This is done in Propositions 4.1 and 4.2. To obtain more insight into how the error behaves in each of the time step regimes, more specialized error expressions are derived from the general estimates. The analysis reveals that there are four natural regimes to consider.

The first regime, which we shall refer to as the small time step regime, occurs when all time scales of the fluid and immersed structures are explicitly resolved by the numerical method. The second and third regime, to which we shall refer collectively as the intermediate time step regimes, occur when some of the fluid modes are under-resolved while other fluid modes and all structural modes are explicitly resolved. There are two regimes as a consequence of the fluid-structure coupling 2.8. One regime occurs when the time step is taken sufficiently small to resolve all of the relevant fluid modes which contribute to the dynamics of the structures while still under-resolving some of the fastest modes of the fluid dynamics with high wavenumbers. The other regime occurs when some, but not all, of the fluid modes which contribute non-negligibly to the structural dynamics are under-resolved. The fourth time step regime occurs when all of the fluid modes are under-resolved, and this is referred to as the large time step regime.

We first derive in Sections 5–7 several bounds for the numerical errors, each of which are uniformly valid for time steps which resolve the structural degrees of freedom (but not necessarily the fluid degrees of freedom). In each of the time regimes described above, one of the rigorous bounds is in fact fairly sharp, and the estimates are correspondingly organized into sections according to the regime for which they are best suited. To better elucidate the error incurred by the method in each of the time step regimes, the scaling of the error estimates with respect to the parameters of the numerical method are given in Section 8.

3.1. Notation Used in the Error Analysis. Throughout the analysis it will be useful to decompose the positions of the elementary particles and the modes of the fluid into two contributions. The first consists of a component that arises primarily from the forces acting on the particles and is associated with the local systematic drift in the fluid velocity. The second arises primarily from the thermal fluctuations of the system and is drift-free. We shall make this decomposition more precise by introducing a number of notational conventions and definitions.

The notation $\sqcup$ will be used to demarcate contributions to the dynamics that arise primarily from the structural forces. For the terms associated with the thermal fluctuations of the system, the symbol $\sqcap$ will be used. With this convention the Fourier modes of the fluid are decomposed into the contributions:

$$\hat{\mathbf{u}}_{\mathbf{k}}(t) = \overset{\sqcup}{\hat{\mathbf{u}}}_{\mathbf{k}}(t) + \overset{\sqcap}{\hat{\mathbf{u}}}_{\mathbf{k}}(t) \tag{3.4}$$

where we define:

$$\overset{\sqcup}{\hat{\mathbf{u}}}_{\mathbf{k}}(t) := \rho^{-1}\int_0^t e^{-\alpha_{\mathbf{k}}(t-s)}\wp_{\mathbf{k}}^{\perp}\hat{\mathbf{f}}_{\mathbf{k}}(s)ds + e^{-\alpha_{\mathbf{k}}t}\,\overset{\sqcup}{\hat{\mathbf{u}}}_{\mathbf{k}}(0) \tag{3.5}$$

and

$$\overset{\sqcap}{\hat{\mathbf{u}}}_{\mathbf{k}}(t) := \sqrt{2D_{\mathbf{k}}}\int_0^t e^{-\alpha_{\mathbf{k}}(t-s)}\wp_{\mathbf{k}}^{\perp}d\tilde{\mathbf{B}}_{\mathbf{k}}(s) + e^{-\alpha_{\mathbf{k}}t}\,\overset{\sqcap}{\hat{\mathbf{u}}}_{\mathbf{k}}(0) \tag{3.6}$$

where $\hat{\mathbf{f}}_{\mathbf{k}}(s)$ is the Discrete Fourier Transform of the force density of the fluid at time s.

In the analysis we shall assume that the fluid velocity components at the beginning of the time step at time 0 are random variables with probability distributions defined by:

$$\overset{\sqcup}{\hat{\mathbf{u}}}_{\mathbf{k}}(0) := \rho^{-1}\int_{-\infty}^0 e^{\alpha_{\mathbf{k}}s}\wp_{\mathbf{k}}^{\perp}\hat{\mathbf{f}}_{\mathbf{k}}(s)ds \tag{3.7}$$

and

$$\overset{\sqcap}{\hat{\mathbf{u}}}_{\mathbf{k}}(0) := \sqrt{2D_{\mathbf{k}}}\int_{-\infty}^0 e^{\alpha_{\mathbf{k}}s}\wp_{\mathbf{k}}^{\perp}d\tilde{\mathbf{B}}_{\mathbf{k}}(s). \tag{3.8}$$

These expressions should be regarded as weak definitions in the sense that only the probability distributions of the random variables have been specified. The analysis will only use features of the distributions, making the results independent of which specific strong definition of the random variables is used.

In 3.7, the probability is defined for a given distribution of the forces acting on the fluid for $s \leq 0$, features of which will be discussed further in the analysis. From the definition of the Itô integral, we can more directly define the fluid velocity at the beginning of the time step (3.8) as a vector-valued random variable having in each component an independent Gaussian distribution with mean 0 and variance $\frac{D_{\mathbf{k}}}{\alpha_{\mathbf{k}}}$ which is then projected by $\wp_{\mathbf{k}}^{\perp}$ to ensure incompressibility. We remark that for this random variable

$$E\left(\left|\overset{\sqcap}{\hat{\mathbf{u}}}_{\mathbf{k}}(0)\right|^2\right) = \Upsilon_{\mathbf{k}}\frac{k_BT}{\rho L^3}$$

where $\Upsilon_{\mathbf{k}}$ is defined in A.4.

The above definitions lead naturally to the definitions:

$$\overset{\sqcup}{\mathbf{u}}_{\mathbf{m}}(t) := \sum_{\mathbf{k}} \overset{\sqcup}{\hat{\mathbf{u}}}_{\mathbf{k}}(t) \exp\left(i2\pi\mathbf{k}\cdot\mathbf{m}/N\right) \tag{3.9}$$

and

$$\overset{\sqcup}{\mathbf{U}}(\mathbf{x},t) := \sum_{\mathbf{m}} \delta_a(\mathbf{x}_{\mathbf{m}} - \mathbf{x}) \overset{\sqcup}{\mathbf{u}}_{\mathbf{m}}(t)\Delta x^3 \tag{3.10}$$

with $\overset{\sqcap}{\mathbf{u}}_{\mathbf{m}}$ and $\overset{\sqcap}{\mathbf{U}}(\mathbf{x},t)$ defined similarly.

For the particle trajectory $\mathbf{X}(t)$, we make a similar decomposition by defining:

$$\overset{\sqcup}{\mathbf{X}}(t) = \overset{\sqcup}{\mathbf{X}}(0) + \int_0^t \overset{\sqcup}{\mathbf{U}}(\mathbf{X}(s),s)ds \tag{3.11}$$

$$\overset{\sqcap}{\mathbf{X}}(t) = \overset{\sqcap}{\mathbf{X}}(0) + \int_0^t \overset{\sqcap}{\mathbf{U}}(\mathbf{X}(s),s)ds \tag{3.12}$$

so that:

$$\mathbf{X}(t) = \overset{\sqcup}{\mathbf{X}}(t) + \overset{\sqcap}{\mathbf{X}}(t). \tag{3.13}$$

The subsequent analysis does not depend on the precise definition of the quantities $\overset{\sqcup}{\mathbf{X}}(0)$ and $\overset{\sqcap}{\mathbf{X}}(0)$, provided that $\mathbf{X}(0) = \overset{\sqcup}{\mathbf{X}}(0) + \overset{\sqcap}{\mathbf{X}}(0)$. For concreteness, we shall make the explicit definition $\overset{\sqcup}{\mathbf{X}}(0) = \mathbf{X}(0)$ and $\overset{\sqcap}{\mathbf{X}}(0) = \mathbf{0}$.

To bound the strong error of the particle position in terms of the two contributions 3.11 and 3.12 defined above, we introduce:

$$\overset{\sqcup}{e}_{\mathrm{prt}}(\Delta t) := E\left(\left|\overset{\sqcup}{\mathbf{X}}(\Delta t) - \overset{\sqcup}{\tilde{\mathbf{X}}}(\Delta t)\right|\right) \tag{3.14}$$

and

$$\overset{\sqcap}{e}_{\mathrm{prt}}(\Delta t) := E\left(\left|\overset{\sqcap}{\mathbf{X}}(\Delta t) - \overset{\sqcap}{\tilde{\mathbf{X}}}(\Delta t)\right|\right). \tag{3.15}$$

The strong error of the particle position is then bounded by:

$$e_{\mathrm{prt}}(\Delta t) \leq \overset{\sqcup}{e}_{\mathrm{prt}}(\Delta t) + \overset{\sqcap}{e}_{\mathrm{prt}}(\Delta t). \tag{3.16}$$

Two statistics appear frequently in the estimates and will be denoted by the following correlation functions:

$$\psi(s,r) := \sup_{1\leq\beta\leq 3,\ \mathbf{X}(0)\in\Omega} E\left(\left(\overset{\sqcap}{\mathbf{X}}^{(\beta)}(s) - \overset{\sqcap}{\mathbf{X}}^{(\beta)}(0)\right)\cdot\left(\overset{\sqcap}{\mathbf{X}}^{(\beta)}(r) - \overset{\sqcap}{\mathbf{X}}^{(\beta)}(0)\right)\right) \tag{3.17}$$

(3.18)
$$\phi(s,r) := \sup_{1\leq\alpha,\beta\leq 3,\ \mathbf{X}(0)\in\Omega} E\left(\nabla \overset{\sqcap}{\mathbf{U}}^{(\alpha,\beta)}(\mathbf{X}(0),s)\cdot\nabla \overset{\sqcap}{\mathbf{U}}^{(\alpha,\beta)}(\mathbf{X}(0),r)\right).$$

The single superscripts denote the index of a vector component. The double superscripts denote the indices of a matrix entry. We remark that the fluid-particle equations are discretized on a finite lattice. The expectations appearing in 3.17 and 3.18 do not depend on the external forces acting on the elementary particles and are nearly translation invariant except for a dependence on the shift of $\mathbf{X}(0)$ relative to the lattice points. This gives a periodic dependence of the expectations with period Δx in each direction.

A further notation that will be used in the analysis is the following. For any function $f : \mathbb{R}^N \to \mathbb{R}$ we define the class of functions $O(f(\mathbf{y}))$ by the condition that $g(\mathbf{y}) \in O(f(\mathbf{y}))$ if and only if there exists a constant C independent of $\mathbf{y}$ such that:

$$|g(\mathbf{y})| \leq Cf(\mathbf{y}) \tag{3.19}$$

for all $\mathbf{y}$. A common abuse of notation that we shall use is that expressions of the form:

$$h(\mathbf{y}) = O(f(\mathbf{y})) \text{ or } h(\mathbf{y}) \leq O(f(\mathbf{y})) \tag{3.20}$$

should be interpreted as $h(\mathbf{y}) \in O(f(\mathbf{y}))$. These notations are in the same spirit as those typically used in asymptotics (15).

4. The General Error Estimates. A general error estimate for the numerical method 2.22 – 2.30 is now established. The method is designed to allow underresolution of some or all of the fluid modes, but is intended to be used only with time steps that resolve the structural degrees of freedom. We formalize the latter restriction by the following standing assumption on the time step:

- *Assumption T1:* The time step satisfies $0 < \Delta t \leq \tau_{\text{mov}}(a)$, where

  $$\tau_{\text{mov}}(a) = E\left(\inf\{t > 0 : |\mathbf{X}(t) - \mathbf{X}(0)| = a\}\right) \tag{4.1}$$

  represents the time scale on which a particle moves a distance comparable to its size, and can be thought of as the fastest time scale for the motion of the immersed structures.

Our subsequent study of various regimes of underresolution or resolution of the fluid modes is meaningful under Assumption (T1) because typically at least some of the fluid degrees of freedom are faster than those of the immersed structures. This is due to the generally low Kubo and Reynolds number in microbiology (19). This assumption will be used in our calculations in a more precise manner through the technical assumption (A1) described below.

In the immersed boundary method, the elementary particle dynamics are governed by local averages of the velocity field of the fluid. This poses a number of difficulties in the analysis of the system, as is common in stochastic transport problems (7; 10; 38). To make the analysis tractable we shall make a few technical assumptions about the coupling of the dynamics of the elementary particles and fluid. More specifically these are:

- *Assumption A1:* There exists a positive constant C_{A1} uniform with respect to all parameters such that for time steps satisfying condition (T1), the following inequality holds:

$$E\left(\left|\int_0^{\Delta t} \mathbf{U}(\mathbf{X}(s),s) - \mathbf{U}(\mathbf{X}(0),s)ds\right|\right)$$
$$\leq C_{A1} E\left(\left|\int_0^{\Delta t} \nabla\mathbf{U}(\mathbf{X}(0),s)\cdot(\mathbf{X}(s)-\mathbf{X}(0))\,ds\right|\right).$$

We remark that the assumption A1 is made to avoid technicalities that arise when using the Mean-Value Theorem and Taylor Expansion in the context of stochastic processes (11; 17). Indeed, the statement with $C_{A1} = 1$ corresponds to a first order Taylor approximation, which is expected to be accurate provided $|\mathbf{X}(s) - \mathbf{X}(0)| \ll a$, the length scale on which $\mathbf{U}$ varies. The time step restriction T1 reflects this criterion.

- *Assumption A2:* There exists a positive constant C_{A2} uniform with respect to all parameters so that:

$$E\left(\nabla\mathbf{W}^{(\alpha,\beta)}(\mathbf{X}(0),s)\mathbf{Y}^{(\beta)}(s)\nabla\mathbf{W}^{(\alpha,\beta)}(\mathbf{X}(0),r)\mathbf{Y}^{(\beta)}(r)\right)$$
$$\leq C_{A2}\left|E\left(\nabla\mathbf{W}^{(\alpha,\beta)}(\mathbf{X}(0),s)\nabla\mathbf{W}^{(\alpha,\beta)}(\mathbf{X}(0),r)\right)E\left(\mathbf{Y}^{(\beta)}(s)\mathbf{Y}^{(\beta)}(r)\right)\right|$$

where $\mathbf{W}=\overset{\sqcup}{\mathbf{U}}$ or $\mathbf{W}=\overset{\sqcap}{\mathbf{U}}$ and $\mathbf{Y}\,(t)=\overset{\sqcup}{\mathbf{X}}\,(t)-\overset{\sqcup}{\mathbf{X}}\,(0)$ or $\mathbf{Y}\,(t)=\overset{\sqcap}{\mathbf{X}}\,(t)-\overset{\sqcap}{\mathbf{X}}\,(0)$.

One motivation for such an inequality is the Corrsin conjecture (7; 10; 38), which amounts to the unproven but plausible approximation that the position and instantaneous velocity of a particle in a random flow become nearly independent on time scales which are large compared to the correlation time τ_{fld} of the flow. Using the Corrsin Conjecture would imply equality in the above expression for $\max(s,r) \gg \tau_{\text{fld}}$ with $C_{A2} = 1$.

For small time values, $s, r \ll \tau_{\text{fld}}$, the particle velocity $\mathbf{U}$ is highly correlated with its initial value, and to leading order we can approximate each of $\mathbf{U}(\mathbf{X}(0),s)$ and $\mathbf{U}(\mathbf{X}(0),r)$ by the constant random variable $\mathbf{U}(\mathbf{X}(0),0)$. (We use here also the notion that for general microbiological applications, the Kubo number is small (1; 18): $\tau_{\text{fld}} \ll \tau_{\text{mov}}(a)$.) Then our assumption reduces to a statement concerning the control of a fourth-order correlation of the random variables $\mathbf{U}(\mathbf{X}(0),0)$ and $\nabla\mathbf{U}(\mathbf{X}(0),0)$ in terms of their variances. Such an inequality holds for jointly Gaussian random variables. It would only be violated were weight to concentrate in the tails of the joint probability distributions of these random variables under certain admissible parameter choices – we see no reason for this to happen. Having argued for the plausibility of the inequality for very short times and very long times, a case for the plausibility of the bound for all times can be made by an interpolation argument.

- *Assumption A3:* We shall assume throughout that both the particle force $\mathbf{F}^{[j]}(\{\mathbf{X}\})$ and the particle representation function $\delta_a(\mathbf{x})$ are Lipschitz continuous, that $|\mathbf{F}^{[j]}| \leq F^*$ uniformly in j, and that $\delta_a(\mathbf{x}) \geq 0$. For the force, we assume that the Lipschitz constant L_F is uniform in j and $\{\mathbf{X}\}$ so that:

$$|\mathbf{F}^{[j]}(\{\mathbf{Y}\}) - \mathbf{F}^{[j]}(\{\mathbf{X}\})| \leq L_F|\{\mathbf{Y}\} - \{\mathbf{X}\}| \tag{4.2}$$

where $\{\mathbf{X}\}$ and $\{\mathbf{Y}\}$ denotes the composite vector consisting of the configurations of all of the elementary particles.

In our derivations, we shall for simplicity assume that the particle representation function $\delta_a(\mathbf{x})$ is also continuously differentiable. Our arguments can be readily extended to the slightly more general situation of functions with bounded and piecewise continuous derivatives through standard approximation arguments, the details of which we omit. With this in mind, our estimates can be shown to hold without modification for one particle representation function widely used in practice (29), which is only piecewise smooth. To make transparent how our bounds generalize, we shall express estimates in terms of Lipschitz constants rather than gradient norms.

A further technical assumption we shall make concerning δ_a is that the elementary particle size is an integer multiple of the fluid resolution length scale, and so in particular $a \geq \Delta x$.

These assumptions will be used in the derivation of the error estimates in this section, which will in turn be developed into more specialized error estimates for various time step regimes in subsequent sections. Therefore, the above assumptions (T1), (A1), (A2), and (A3) should be understood as standing assumptions underlying all results.

PROPOSITION 4.1. *For the numerical method 2.22 – 2.30, the following estimate holds for the strong error of the fluid dynamics:*

(4.3)

$$e_{fld,\mathbf{k}}(\Delta t) \leq \left[E\left(|\hat{\mathbf{u}}_{\mathbf{k}}(\Delta t) - \hat{\tilde{\mathbf{u}}}_{\mathbf{k}}(\Delta t)|^2\right)\right]^{1/2} \leq \left(\rho^{-1}M^2 L_F \hat{\delta}^*_{a,\mathbf{k}} + \rho^{-1}MF^* L_{\delta,\mathbf{k}}\right) \cdot \\ \cdot \left[B_0\left(\frac{1}{\alpha_{\mathbf{k}}}\right)^2\left(\alpha_{\mathbf{k}}\Delta t - 1 + e^{-\alpha_{\mathbf{k}}\Delta t}\right) \right. \\ \left. + \sqrt{3}\int_0^{\Delta t} e^{-\alpha_{\mathbf{k}}(\Delta t - s)}\left(\psi(s,s)\right)^{\frac{1}{2}}\, ds\right]$$

where the function $\psi(r,s)$ is defined in 3.17 and the constants are defined in Table C.3.

Proof.

Before we give the analysis of the fluid error, we first establish a few basic estimates which will be used in this and later derivations. Using equation 3.9 we can bound the magnitude of the contributions associated with the systematic drift of the fluid by:

$$\text{(4.4)} \qquad |\overset{\sqcup}{\mathbf{u}}_{\mathbf{m}}(t)| = |\sum_{\mathbf{k}} \overset{\sqcup}{\hat{\mathbf{u}}}_{\mathbf{k}}(t)\exp\left(i2\pi\mathbf{k}\cdot\mathbf{m}/N\right)| \\ \leq \sum_{\mathbf{k}}\int_{-\infty}^{t}\rho^{-1}e^{-\alpha_{\mathbf{k}}(t-s)}|\hat{\mathbf{f}}_{\mathbf{k}}(s)|ds.$$

The Fourier coefficients of the force density arising from the particle forces acting on the fluid are bounded by:

$$\text{(4.5)} \qquad |\hat{\mathbf{f}}_{\mathbf{k}}(s)| = |\sum_j \mathbf{F}^{[j]}\hat{\delta}_{a,\mathbf{k}}(\mathbf{X}^{[j]}(s))| \\ \leq MF^*\hat{\delta}^*_{a,\mathbf{k}}$$

where M denotes the number of elementary particles, F^* denotes the maximum force applied to a particle, and $\hat{\delta}^*_{a,\mathbf{k}}$ denotes the maximum of the Fourier coefficient of the δ_a representation function over all shifts (see Appendix B). We remark that in the force density, the reference "prt" has been dropped in the notation since all forces associated with the thermal fluctuations of the system will be written out explicitly.

From this we obtain the following bound which holds uniformly in $\mathbf{m}$ and t:

$$|\overset{\sqcup}{\mathbf{u}}_{\mathbf{m}}(t)| \leq B_0 \tag{4.6}$$

where

$$B_0 := \frac{MF^*}{\rho}\sum_{\mathbf{k}}\frac{\hat{\delta}^*_{a,\mathbf{k}}}{\alpha_{\mathbf{k}}}. \tag{4.7}$$

The constant B_0 is the largest magnitude the drift of the fluid can attain from the forces acting on the particles.

From the definitions 3.10, 3.11, and the pointwise bound 4.6, we have the following bound for the component of the particle displacement associated with the structural forces over the time interval $[0,t]$:

$$|\overset{\sqcup}{\mathbf{X}}(t) - \overset{\sqcup}{\mathbf{X}}(0)| \leq B_0 t. \tag{4.8}$$

The contributions to the error of the particle displacement associated with the thermal fluctuations can be estimated using the Cauchy-Schwartz inequality:

$$\begin{aligned} E\left(|\overset{\sqcap}{\mathbf{X}}(t) - \overset{\sqcap}{\mathbf{X}}(0)|\right) &\leq \left[E\left(|\overset{\sqcap}{\mathbf{X}}(t) - \overset{\sqcap}{\mathbf{X}}(0)|^2\right)\right]^{\frac{1}{2}} \\ &= \sqrt{3}\left(\psi(t,t)\right)^{\frac{1}{2}} \end{aligned} \tag{4.9}$$

where ψ is defined in 3.17.

From 4.8, 4.9 and the triangle inequality, this gives the following bound:

$$E\left(|\mathbf{X}(t) - \mathbf{X}(0)|\right) \leq \left[E\left(|\mathbf{X}(t) - \mathbf{X}(0)|^2\right)\right]^{1/2} \leq B_0 t + \sqrt{3}\left(\psi(t,t)\right)^{\frac{1}{2}}. \tag{4.10}$$

Now using the above estimates, we shall establish expressions for the error incurred for the $\mathbf{k}^{th}$ Fourier mode of the fluid. In the numerical scheme the force is approximated as constant over the time step. From the definition of the strong error in 3.1 and 2.23 this gives:

(4.11)

$$\begin{aligned} e_{\mathrm{fld},\mathbf{k}}(\Delta t) &\leq \left[E\left(|\hat{\mathbf{u}}_{\mathbf{k}}(\Delta t) - \hat{\tilde{\mathbf{u}}}_{\mathbf{k}}(\Delta t)|^2\right)\right]^{1/2} \\ &\leq \left[E\left(\left|\rho^{-1}\int_0^{\Delta t} e^{-\alpha_{\mathbf{k}}(\Delta t - s)}|\hat{\mathbf{f}}_{\mathbf{k}}(s) - \hat{\mathbf{f}}_{\mathbf{k}}(0)|ds\right|^2\right)\right]^{1/2}. \end{aligned}$$

We remark that in the analysis, the range in the integrand is from 0 to Δt and refers to a time step in which both the exact solution and numerical solutions start from the same value at time 0.

From assumption (A3), expressions 4.2 and B.1, and using the definition of the force field 2.8, we have:

(4.12)

$$
\begin{aligned}
|\hat{\mathbf{f}}_{\mathbf{k}}(s) - \hat{\mathbf{f}}_{\mathbf{k}}(0)| = \Bigg| & \sum_j \left[\mathbf{F}^{[j]}(\{\mathbf{X}(s)\}) - \mathbf{F}^{[j]}(\{\mathbf{X}(0)\})\right] \hat{\delta}_{a,\mathbf{k}}(\mathbf{X}^{[j]}(s)) \\
& + \sum_j \mathbf{F}^{[j]}(\{\mathbf{X}(0)\}) \left[\hat{\delta}_{a,\mathbf{k}}(\mathbf{X}^{[j]}(s)) - \hat{\delta}_{a,\mathbf{k}}(\mathbf{X}^{[j]}(0))\right] \Bigg| \\
& \leq \sum_j L_F \sum_{j'} |\mathbf{X}^{[j']}(s) - \mathbf{X}^{[j']}(0)| \hat{\delta}^*_{a,\mathbf{k}} + \sum_j F^* L_{\delta,k} |\mathbf{X}^{[j]}(s) - \mathbf{X}^{[j]}(0)| \\
& \leq \left(M L_F \hat{\delta}^*_{a,\mathbf{k}} + F^* L_{\delta,k}\right) \sum_j |\mathbf{X}^{[j]}(s) - \mathbf{X}^{[j]}(0)| \\
& \leq \left(M L_F \hat{\delta}^*_{a,\mathbf{k}} + F^* L_{\delta,\mathbf{k}}\right) \left(M B_0 s + \sum_j |\overset{\sqcap}{\mathbf{X}}^{[j]}(s) - \overset{\sqcap}{\mathbf{X}}^{[j]}(0)| \right).
\end{aligned}
$$

Plugging 4.12 into 4.11 and using the triangle inequality of the L^2 norm we have:

(4.13)

$$
\begin{aligned}
\left[E\left(|\hat{\mathbf{u}}_{\mathbf{k}}(\Delta t) - \tilde{\hat{\mathbf{u}}}_{\mathbf{k}}(\Delta t)|^2\right)\right]^{1/2} \leq & \left(M L_F \hat{\delta}^*_{a,\mathbf{k}} + F^* L_{\delta,\mathbf{k}}\right) \cdot \\
& \cdot \left(\left[E\left(\left|\rho^{-1}\int_0^{\Delta t} e^{-\alpha_{\mathbf{k}}(\Delta t - s)} M B_0 s ds\right|^2\right)\right]^{1/2} \right. \\
& \left. + \sum_j \left[E\left(\left|\rho^{-1}\int_0^{\Delta t} e^{-\alpha_{\mathbf{k}}(\Delta t - s)} |\overset{\sqcap}{\mathbf{X}}^{[j]}(s) - \overset{\sqcap}{\mathbf{X}}^{[j]}(0)| ds\right|^2\right)\right]^{1/2} \right) \\
\leq & \left(M L_F \hat{\delta}^*_{a,\mathbf{k}} + F^* L_{\delta,\mathbf{k}}\right) \cdot \\
& \cdot \left(\rho^{-1}\int_0^{\Delta t} e^{-\alpha_{\mathbf{k}}(\Delta t - s)} M B_0 s ds \right. \\
& \left. + \sum_j \rho^{-1}\int_0^{\Delta t} e^{-\alpha_{\mathbf{k}}(\Delta t - s)} \left[E\left(\left|\overset{\sqcap}{\mathbf{X}}^{[j]}(s) - \overset{\sqcap}{\mathbf{X}}^{[j]}(0)\right|^2\right)\right]^{1/2} ds \right)
\end{aligned}
$$

Performing the integration and using equation 4.9 establishes the general error estimate for the fluid 4.3.

□

Proposition 4.2. *For the numerical method 2.22 – 2.30 , the following estimate for the error of the elementary particle dynamics can be established:*

(4.14)

$$
e_{prt}(\Delta t) \leq 9 C_{A1} L_{\delta,a} A_a B_0 \left[B_0 \frac{\Delta t^2}{2} + \sqrt{C_{A2}} \left(\int_0^{\Delta t} \int_0^{\Delta t} \psi(s,r) dr ds \right)^{\frac{1}{2}} \right]
$$

$$
\begin{aligned}
&+ \sum_{\mathbf{k}} \left(\rho^{-1} M^2 L_F \hat{\delta}^*_{a,\mathbf{k}} + \rho^{-1} M F^* L_{\delta,\mathbf{k}}\right) \cdot \\
&\cdot \left[B_0 \left(\frac{1}{\alpha_{\mathbf{k}}}\right)^2 \left(\alpha_{\mathbf{k}} \frac{\Delta t^2}{2} - \Delta t + \left(\frac{1}{\alpha_{\mathbf{k}}}\right)\left(1 - e^{-\alpha_{\mathbf{k}}\Delta t}\right)\right) \right. \\
&\quad \left. + \sqrt{3} \int_0^{\Delta t} \int_0^s e^{-\alpha_{\mathbf{k}}(s-r)} \left(\psi(r,r)\right)^{\frac{1}{2}} drds \right] \\
&+ 9 B_0 C_{A1} \sqrt{C_{A2}} \left(\int_0^{\Delta t} \int_0^{\Delta t} \phi(s,r) srdrds \right)^{\frac{1}{2}} \\
&+ 9 C_{A1} \sqrt{C_{A2}} \left(\int_0^{\Delta t} \int_0^{\Delta t} \phi(s,r)\psi(s,r) drds \right)^{\frac{1}{2}}.
\end{aligned}
$$

where the constants are defined in Table C.3.

Proof.

Using the definitions 3.3, 3.11, and 3.12 as well as the triangle inequality, the strong error over the time step can be bounded by:

(4.15)
$$
e_{\text{prt}}(\Delta t) \leq \overset{\sqcup}{e}_{\text{prt}}(\Delta t) + \overset{\sqcap}{e}_{\text{prt}}(\Delta t)
$$

where $\overset{\sqcup}{e}_{\text{prt}}(\Delta t)$ and $\overset{\sqcap}{e}_{\text{prt}}(\Delta t)$ denote the natural decomposition of the strong error of the particle using the drift and drift-free contributions to the particle positions defined in 3.11 and 3.12.

From 2.25 and 3.11, we have for the contributions associated with the systematic drift of the particle:

$$
\overset{\sqcup}{e}_{\text{prt}}(\Delta t) = E\left(\left| \overset{\sqcup}{\mathbf{X}}(\Delta t) - \overset{\sqcup}{\tilde{\mathbf{X}}}(\Delta t) \right| \right) \leq \overset{\sqcup}{A}_1 + \overset{\sqcup}{A}_2
$$

where

$$
\begin{aligned}
\overset{\sqcup}{A}_1 &:= E\left(\left| \int_0^{\Delta t} \overset{\sqcup}{\mathbf{U}}(\mathbf{X}(s),s) - \overset{\sqcup}{\mathbf{U}}(\mathbf{X}(0),s) ds \right| \right) \\
\overset{\sqcup}{A}_2 &:= E\left(\left| \int_0^{\Delta t} \overset{\sqcup}{\mathbf{U}}(\mathbf{X}(0),s) - \overset{\sqcup}{\tilde{\mathbf{U}}}(\mathbf{X}(0),s) ds \right| \right).
\end{aligned}
$$

From assumption (A1) we have:

(4.16)
$$
E\left(\left| \int_0^{\Delta t} \overset{\sqcup}{\mathbf{U}}(\mathbf{X}(s),s) - \overset{\sqcup}{\mathbf{U}}(\mathbf{X}(0),s) ds \right| \right) \leq C_{A1} E\left(\left| \int_0^{\Delta t} \nabla \overset{\sqcup}{\mathbf{U}}(\mathbf{X}(0),s) \cdot (\mathbf{X}(s) - \mathbf{X}(0))\, ds \right| \right).
$$

The estimate can be further broken down into:

(4.17)
$$
\overset{\sqcup}{A}_1 \leq \overset{\sqcup}{A}_{1,1} + \overset{\sqcup}{A}_{1,2}
$$

with

(4.18)

$$\overset{\sqcup}{A}_{1,1} := C_{A1} E\left(\left|\int_0^{\Delta t} \nabla \overset{\sqcup}{\mathbf{U}} (\mathbf{X}(0), s)\cdot\left(\overset{\sqcup}{\mathbf{X}} (s) - \overset{\sqcup}{\mathbf{X}} (0)\right) ds\right|\right)$$

$$\overset{\sqcup}{A}_{1,2} := C_{A1} E\left(\left|\int_0^{\Delta t} \nabla \overset{\sqcup}{\mathbf{U}} (\mathbf{X}(0), s)\cdot\left(\overset{\sqcap}{\mathbf{X}} (s) - \overset{\sqcap}{\mathbf{X}} (0)\right) ds\right|\right),$$

where 3.13 has been used.

From 3.10, 4.6 and 4.8, the following estimate can be obtained:

(4.19)

$$\begin{aligned}\overset{\sqcup}{A}_{1,1} &\leq C_{A1} E\left(\sum_{\alpha,\beta=1}^{3}\left|\int_0^{\Delta t} \nabla \overset{\sqcup}{\mathbf{U}}^{(\alpha,\beta)} (\mathbf{X}(0), s)\cdot\left(\overset{\sqcup}{\mathbf{X}}^{(\beta)} (s) - \overset{\sqcup}{\mathbf{X}}^{(\beta)} (0)\right) ds\right|\right) \\ &\leq C_{A1}\sum_{\alpha,\beta}\sum_{\mathbf{m}} |\nabla\delta_a(\mathbf{x}_{\mathbf{m}} - \mathbf{X}(0))| B_0 \Delta x^3 \cdot \int_0^{\Delta t} B_0 s ds \\ &= 9 C_{A1} L_{\delta,a} A_a B_0^2 \frac{\Delta t^2}{2}\end{aligned}$$

where $L_{\delta,a}$ is the Lipschitz constant of $\delta_a(\mathbf{x})$, and $A_a = n\Delta x^3$ with n the number of lattice points on which δ_a is non-zero.

The second term can be estimated using the Cauchy-Schwartz inequality and assumption (A2) to obtain:

(4.20)

$$\begin{aligned}\overset{\sqcup}{A}_{1,2} &\leq C_{A1}\sum_{\alpha,\beta=1}^{3} E\left(\left|\int_0^{\Delta t} \nabla \overset{\sqcup}{\mathbf{U}}^{(\alpha,\beta)} (\mathbf{X}(0), s)\cdot\left(\overset{\sqcap}{\mathbf{X}}^{(\beta)} (s) - \overset{\sqcap}{\mathbf{X}}^{(\beta)} (0)\right) ds\right|^2\right)^{\frac{1}{2}} \\ &\leq 9 C_{A1}\sqrt{C_{A2}}\left(\int_0^{\Delta t}\int_0^{\Delta t} E\left(\nabla \overset{\sqcup}{\mathbf{U}}^{(\alpha,\beta)} (\mathbf{X}(0), s)\cdot \nabla \overset{\sqcup}{\mathbf{U}}^{(\alpha,\beta)} (\mathbf{X}(0), r)\right)\right. \\ &\qquad\qquad \left. E\left(\left(\overset{\sqcap}{\mathbf{X}}^{(\beta)} (s) - \overset{\sqcap}{\mathbf{X}}^{(\beta)} (0)\right)\left(\overset{\sqcap}{\mathbf{X}}^{(\beta)} (r) - \overset{\sqcap}{\mathbf{X}}^{(\beta)} (0)\right)\right) dr ds\right)^{\frac{1}{2}} \\ &\leq 9 C_{A1}\sqrt{C_{A2}} L_{\delta,a} A_a B_0 \left(\int_0^{\Delta t}\int_0^{\Delta t} \psi(s,r) dr ds\right)^{\frac{1}{2}}\end{aligned}$$

where $\psi(s,r)$ is defined in 3.17, and $L_{\delta,a}$ and A_a are defined as in 4.19.

Combining the estimates 4.19 and 4.20 gives:

$$\overset{\sqcup}{A}_{1} \leq 9 C_{A1} L_{\delta,a} A_a B_0 \left(B_0 \frac{\Delta t^2}{2} + \sqrt{C_{A2}}\left(\int_0^{\Delta t}\int_0^{\Delta t} \psi(s,r) dr ds\right)^{\frac{1}{2}}\right). \tag{4.21}$$

To estimate $\overset{\sqcup}{A}_2$ we shall use:

$$\left|\overset{\sqcup}{\mathbf{u}}_{\mathbf{m}} (s) - \overset{\sqcup}{\tilde{\mathbf{u}}}_{\mathbf{m}} (s)\right| \leq \sum_{\mathbf{k}} e_{\text{fld},\mathbf{k}}(s). \tag{4.22}$$

From the estimate established for $e_{\text{fld},\mathbf{k}}(s)$ in 4.3 and using that $\sum_{\mathbf{m}} \delta_a(\mathbf{x}_{\mathbf{m}} - \mathbf{X}(0))\Delta x^3 = 1$, we have:

$$\overset{\sqcup}{A}_2 \leq E\left(\int_0^{\Delta t} \sum_{\mathbf{m}} \delta_a(\mathbf{x}_{\mathbf{m}} - \mathbf{X}(0)) \left| \overset{\sqcup}{\mathbf{u}}_{\mathbf{m}}(s) - \overset{\sqcup}{\tilde{\mathbf{u}}}_{\mathbf{m}}(s) \right| \Delta x^3 ds\right) \tag{4.23}$$
$$\leq \sum_{\mathbf{k}} \left(\rho^{-1} M^2 L_F \hat{\delta}^*_{a,\mathbf{k}} + \rho^{-1} M F^* L_{\delta,\mathbf{k}}\right) \cdot$$
$$\cdot \left[B_0 \left(\frac{1}{\alpha_{\mathbf{k}}}\right)^2 \left(\alpha_{\mathbf{k}} \frac{\Delta t^2}{2} - \Delta t + \left(\frac{1}{\alpha_{\mathbf{k}}}\right)\left(1 - e^{-\alpha_{\mathbf{k}} \Delta t}\right)\right) \right.$$
$$\left. + \sqrt{3} \int_0^{\Delta t} \int_0^s e^{-\alpha_{\mathbf{k}}(s-r)} \left(\psi(r,r)\right)^{\frac{1}{2}} dr ds \right].$$

By combining 4.21 and 4.23, an estimate is obtained for $\overset{\sqcup}{e}_{\text{prt}}(\Delta t)$.

An estimate for the error of the particle displacement in the component associated with the thermal fluctuations is now established. Since 2.23 of the numerical method resolves the contributions of the thermal fluctuations of the fluid dynamics exactly over a time step, we have:

$$\overset{\sqcap}{\tilde{\mathbf{U}}}(\mathbf{X}(0), s) = \overset{\sqcap}{\mathbf{U}}(\mathbf{X}(0), s). \tag{4.24}$$

From assumption (A1) and the triangle inequality we obtain:

(4.25)

$$\overset{\sqcap}{e}_{\text{prt}}(\Delta t) = E\left(\left| \int_0^{\Delta t} \overset{\sqcap}{\mathbf{U}}(\mathbf{X}(s), s) - \overset{\sqcap}{\tilde{\mathbf{U}}}(\mathbf{X}(0), s) ds \right|\right)$$
$$\leq \overset{\sqcap}{A}_1 + \overset{\sqcap}{A}_2$$

where

$$\overset{\sqcap}{A}_1 := C_{A1} E\left(\left| \int_0^{\Delta t} \nabla \overset{\sqcap}{\mathbf{U}}(\mathbf{X}(0), s) \cdot \left(\overset{\sqcup}{\mathbf{X}}(s) - \overset{\sqcup}{\mathbf{X}}(0)\right) ds \right|\right) \tag{4.26}$$

$$\overset{\sqcap}{A}_2 := C_{A1} E\left(\left| \int_0^{\Delta t} \nabla \overset{\sqcap}{\mathbf{U}}(\mathbf{X}(0), s) \cdot \left(\overset{\sqcap}{\mathbf{X}}(s) - \overset{\sqcap}{\mathbf{X}}(0)\right) ds \right|\right). \tag{4.27}$$

To estimate $\overset{\sqcap}{A}_1$ and $\overset{\sqcap}{A}_2$ we shall use Cauchy-Schwartz inequality and assumption (A2), which gives:

(4.28)

$$\overset{\sqcap}{A}_1 \leq C_{A1}\sqrt{C_{A2}} \sum_{\alpha,\beta=1}^{3} \left(\int_0^{\Delta t} \int_0^{\Delta t} E\left(\nabla \overset{\sqcap}{\mathbf{U}}^{(\alpha,\beta)}(\mathbf{X}(0), s) \cdot \nabla \overset{\sqcap}{\mathbf{U}}^{(\alpha,\beta)}(\mathbf{X}(0), r)\right) \right.$$
$$\left. E\left(\left(\overset{\sqcup}{\mathbf{X}}^{(\beta)}(s) - \overset{\sqcup}{\mathbf{X}}^{(\beta)}(0)\right)\left(\overset{\sqcup}{\mathbf{X}}^{(\beta)}(r) - \overset{\sqcup}{\mathbf{X}}^{(\beta)}(0)\right)\right) ds dr \right)^{\frac{1}{2}}$$
$$\leq 9 C_{A1}\sqrt{C_{A2}} B_0 \left(\int_0^{\Delta t} \int_0^{\Delta t} \phi(s,r) s r dr ds \right)^{\frac{1}{2}}$$

and

(4.29)

$$\overset{\sqcap}{A}_2 \leq C_{A1}\sqrt{C_{A2}} \sum_{\alpha,\beta=1}^{3} \left(\int_0^{\Delta t} \int_0^{\Delta t} E\left(\nabla \overset{\sqcap}{\mathbf{U}}^{(\alpha,\beta)} (\mathbf{X}(0),s) \cdot \nabla \overset{\sqcap}{\mathbf{U}}^{(\alpha,\beta)} (\mathbf{X}(0),r) \right) E\left(\left(\overset{\sqcap}{\mathbf{X}}^{(\beta)} (s) - \overset{\sqcap}{\mathbf{X}}^{(\beta)} (0) \right) \left(\overset{\sqcap}{\mathbf{X}}^{(\beta)} (r) - \overset{\sqcap}{\mathbf{X}}^{(\beta)} (0) \right) \right) dsdr \right)^{\frac{1}{2}}$$

$$\leq 9C_{A1}\sqrt{C_{A2}} \left(\int_0^{\Delta t} \int_0^{\Delta t} \phi(s,r)\psi(s,r)drds \right)^{\frac{1}{2}}.$$

The function $\phi(s,r)$ is defined in 3.18 and $\psi(s,r)$ is defined in 3.17. From 4.28 and 4.29 we obtain the estimate for $\overset{\sqcup}{e}_{\text{prt}}(\Delta t)$.

Finally, by substituting 4.21 4.23, 4.28, and 4.29 into 4.15 we obtain the general estimate 4.14 for the strong error $e_{\text{prt}}(\Delta t)$ incurred in computing the trajectory of an elementary particle each time step. □

5. Uniform Bounds Suited for Small Time Steps. In this section, we develop uniform bounds on the numerical error which are designed to give tight scaling estimates for small time steps $\Delta t \ll \min 1/\alpha_{\mathbf{k}}$ in which the dynamics of the fluid is explicitly resolved by the numerical method. In particular, the inequalities defining the bounds for the small time step regime considered in this section will follow essentially from asymptotic expansions of the terms in the general bound. The bounds will in fact, with some apparent fortune, also serve as uniform bounds over the broader range of time steps restricted by Assumption (T1), which requires the time step be sufficiently small to resolve the dynamics of the immersed structures. The form of the bounds which we present in this section follows from rigorous mathematical analysis, under the assumptions discussed in Section 4. The results are presented in a somewhat technical form in terms of various mathematical quantities related to the smoothness and bounds of various functions entering the numerical method. For ease in interpretation, we present in Section 8 more transparent versions of the error estimates presented here, which exhibit the scaling of the errors with respect to fundamental physical and numerical parameters. We follow a similar approach for the other two time step regimes in subsequent sections.

We now establish uniform error estimates which are essentially sharp for small time steps $\Delta t \ll \min 1/\alpha_{\mathbf{k}}$:

Proposition 5.1. *The error incurred by the numerical method 2.22 – 2.30 for the dynamics of the fluid is bounded by:*

(5.1)

$$e_{fld,\mathbf{k}}(\Delta t) \leq E\left(|\hat{\mathbf{u}}_{\mathbf{k}}(\Delta t) - \hat{\tilde{\mathbf{u}}}_{\mathbf{k}}(\Delta t)|^2 \right)^{1/2}$$

(5.2)

$$\leq \left(\rho^{-1} M^2 L_F \hat{\delta}^*_{a,\mathbf{k}} + \rho^{-1} M F^* L_{\delta,\mathbf{k}} \right) \cdot \cdot \left[B_0 + \sqrt{3} \left(\frac{k_B T}{\rho} \sum_{\mathbf{m}} \delta_a^2(\mathbf{x}_{\mathbf{m}}) \Delta x^3 \right)^{1/2} \right] \frac{\Delta t^2}{2} \cdot \cdot \left(1 + O\left(1/N^3\right) + O\left(\Delta x/a\right) \right).$$

Proof. The velocity autocorrelation function is bounded by (see Appendix A):

(5.3)
$$E\left(\overset{\sqcap}{\mathbf{u}}_{\mathbf{m}}(s)\cdot\overset{\sqcap}{\mathbf{u}}_{\mathbf{n}}(r)\right)\leq\frac{k_BT}{\rho L^3}\sum_{\mathbf{k}}\Upsilon_{\mathbf{k}}\exp\left(i2\pi\mathbf{k}\cdot(\mathbf{m}-\mathbf{n})/N\right)$$
$$\leq 3\frac{k_BT}{\rho}\frac{\chi_{\mathbf{m},\mathbf{n}}}{\Delta x^3}\left(1+O\left(1/N^3\right)\right)$$

where $\chi_{\mathbf{m},\mathbf{n}}$ is the Kronecker delta function which is one if $\mathbf{m}=\mathbf{n}$ and zero otherwise. The error contribution $O\left(1/N^3\right)$ arises when approximating the sum by the discrete Fourier transform of the Kronecker delta function because of the 8 modes which have $\Upsilon_{\mathbf{k}}=2$.

From 5.3 and the smoothness of δ_a we have the following bound:

(5.4)
$$\psi(s,r)=\frac{1}{3}\int_0^s\int_0^r\sum_{\mathbf{m},\mathbf{n}}\delta_a(\mathbf{x_m})\delta_a(\mathbf{x_n})E\left(\overset{\sqcap}{\mathbf{u}}_{\mathbf{m}}(s)\cdot\overset{\sqcap}{\mathbf{u}}_{\mathbf{n}}(r)\right)\Delta x^6 drds\cdot$$
$$\cdot\ (1+O(\Delta x/a))$$
$$\leq\frac{k_BT}{\rho}\left(\sum_{\mathbf{m}}\delta_a^2(\mathbf{x_m})\Delta x^3\right)sr\left(1+O\left(1/N^3\right)+O(\Delta x/a)\right).$$

The error contribution $O(\Delta x/a)$ arises from shifting the arguments of the particle representation functions δ_a in the lattice sums so that the arguments fall on the lattice, and is estimated quantitatively by noting that the shifts are bounded by Δx in each coordinate direction and that the global Lipschitz constant for δ_a is bounded uniformly by a multiple of $1/a$ (Appendix B).

Substituting 5.4 into the general error estimate 4.3 and taking the Taylor expansion of the exponential terms, the fluid error 5.1 is obtained. We remark that this in fact turns out to furnish a uniform inequality by the negativity of the neglected terms in the expansion. ∎

PROPOSITION 5.2. *The numerical method 2.22 – 2.30 incurs an error for the particle error which can be bounded by:*

(5.5)
$$e_{prt}(\Delta t)\leq\Bigg\{\Bigg[9C_{A1}L_{\delta,a}A_aB_0\left(B_0+\sqrt{C_{A2}}\left(\frac{k_BT}{\rho}\sum_{\mathbf{m}}\delta_a^2(\mathbf{x_m})\Delta x^3\right)^{\frac{1}{2}}\right)$$
$$+\ 9B_0C_{A1}\sqrt{C_{A2}}\left(\frac{k_BT}{\rho}L_{\delta,a}^2A_a\right)^{\frac{1}{2}}$$
$$+\ 9C_{A1}\sqrt{C_{A2}}\left(\left(\frac{k_BT}{\rho}\right)^2L_{\delta,a}^2A_a\sum_{\mathbf{m}}\delta_a^2(\mathbf{x_m})\Delta x^3\right)^{\frac{1}{2}}\Bigg]\frac{\Delta t^2}{2}$$
$$+\sum_{\mathbf{k}}\rho^{-1}\left(M^2L_F\hat{\delta}^*_{a,\mathbf{k}}+MF^*L_{\delta,\mathbf{k}}\right)$$
$$\left(B_0+\sqrt{3}\left(\frac{k_BT}{\rho}\sum_{\mathbf{m}}\delta_a^2(\mathbf{x_m})\Delta x^3\right)^{\frac{1}{2}}\right)\frac{\Delta t^3}{6}\Bigg\}\cdot$$
$$\cdot\ \left(1+O\left(1/N^3\right)+O\left(\Delta x/a\right)\right).$$

Proof. To obtain the bound, we shall estimate for small time steps the function ϕ, ψ and the integrals that appear in the general error expression 4.14. Using the definition of ϕ given in 3.17 and approximating the velocity autocorrelation function using 5.3, we obtain:

(5.6)
$$\phi(s,r) \leq \frac{1}{3}\sum_{\mathbf{m},\mathbf{n}} \nabla\delta_a^{(\beta)}(\mathbf{x_m})\nabla\delta_a^{(\beta)}(\mathbf{x_n})E\left(\overset{\sqcap}{\mathbf{u}}_{\mathbf{m}}(s)\cdot \overset{\sqcap}{\mathbf{u}}_{\mathbf{n}}(r)\right)\Delta x^6\left(1+O(\Delta x/a)\right)$$
$$\leq \frac{k_BT}{\rho}\left(\sum_{\mathbf{m}}\left(\nabla\delta_a(\mathbf{x_m})\right)^2\Delta x^3\right)\left(1+O\left(1/N^3\right)+O\left(\Delta x/a\right)\right)$$
$$\leq \frac{k_BT}{\rho}\left(L_{\delta,a}^2 A_a\right)\left(1+O\left(1/N^3\right)+O\left(\Delta x/a\right)\right).$$

The last expression was obtained using an argument similar to that in 4.19.

Together with 5.4, this yields the following approximations for the integrals appearing in the general particle error estimate 4.14:

(5.7)
$$\int_0^{\Delta t}\int_0^{\Delta t}\psi(s,r)drds$$
$$\leq \frac{k_BT}{\rho}\left(\sum_{\mathbf{m}}\delta_a^2(\mathbf{x_m})\Delta x^3\right)\frac{\Delta t^4}{4}\cdot\left(1+O\left(1/N^3\right)+O\left(\Delta x/a\right)\right).$$

(5.8)
$$\int_0^{\Delta t}\int_0^{\Delta t}\phi(s,r)srdrds$$
$$\leq \frac{k_BT}{\rho}\left(\sum_{\mathbf{m}}\left(\nabla\delta_a(\mathbf{x_m})\right)^2\Delta x^3\right)\frac{\Delta t^4}{4}\left(1+O\left(1/N^3\right)+O\left(\Delta x/a\right)\right)$$
$$\leq \frac{k_BT}{\rho}\left(L_{\delta,a}^2 A_a\right)\frac{\Delta t^4}{4}\left(1+O\left(1/N^3\right)+O\left(\Delta x/a\right)\right).$$

(5.9)
$$\int_0^{\Delta t}\int_0^{\Delta t}\phi(s,r)\psi(s,r)drds$$
$$\leq \left(\frac{k_BT}{\rho}\right)^2\left(\sum_{\mathbf{m}}\left(\nabla\delta_a(\mathbf{x_m})\right)^2\Delta x^3\right)\left(\sum_{\mathbf{m}}\delta_a^2(\mathbf{x_m})\Delta x^3\right)\frac{\Delta t^4}{4}\cdot$$
$$\cdot\left(1+O\left(1/N^3\right)+O\left(\Delta x/a\right)\right)$$
$$\leq \left(\frac{k_BT}{\rho}\right)^2\left(L_{\delta,a}^2 A_a\right)\left(\sum_{\mathbf{m}}\delta_a^2(\mathbf{x_m})\Delta x^3\right)\frac{\Delta t^4}{4}\cdot$$
$$\cdot\left(1+O\left(1/N^3\right)+O\left(\Delta x/a\right)\right).$$

(5.10)
$$\int_0^{\Delta t}e^{-\alpha_{\mathbf{k}}(s-r)}\left(\psi(r,r)\right)^{\frac{1}{2}}drds$$

$$\leq \left(\frac{k_BT}{\rho}\sum_{\mathbf{m}}\delta_a^2(\mathbf{x_m})\Delta x^3\right)^{\frac{1}{2}}\frac{\Delta t^2}{2}\cdot$$
$$\cdot\left(1+O\left(1/N^3\right)+O\left(\Delta x/a\right)\right).$$

Using the estimates 5.7 – 5.10 in the general particle error bound 4.14, the expression 5.5 for the small time step regime is obtained.
□

6. Uniform Bounds Suited for Large Time Steps. Error estimates designed for the regime $\max 1/\alpha_{\mathbf{k}} \ll \Delta t$ in which the dynamics of the fluid are under-resolved by the numerical method are now discussed. As always, an upper limit $\Delta t \leq \tau_{\mathrm{mov}}(a)$ is imposed on the size of the time step (Assumption (T1)) so that the structural degrees of freedom are resolved and assumption (A1) is reasonable. We remark that the error estimates hold uniformly for all time steps consistent with (T1), but are tight in the large time step regime $\max 1/\alpha_{\mathbf{k}} \ll \Delta t \ll \tau_{\mathrm{mov}}(a)$.

PROPOSITION 6.1. *The numerical method 2.22 – 2.30 incurs an error for the fluid dynamics bounded by:*

(6.1)
$$e_{\mathit{fld},\mathbf{k}}(\Delta t) \leq \left[E\left(|\hat{\mathbf{u}}_{\mathbf{k}}(\Delta t)-\hat{\tilde{\mathbf{u}}}_{\mathbf{k}}(\Delta t)|^2\right)\right]^{1/2}$$
(6.2)
$$\leq \rho^{-1}\left(M^2L_F\hat{\delta}^*_{a,\mathbf{k}}+MF^*L_{\delta,\mathbf{k}}\right)\left(B_0\frac{\Delta t}{\alpha_{\mathbf{k}}}+\sqrt{6D}\frac{\Delta t^{\frac{1}{2}}}{\alpha_{\mathbf{k}}}\right)\cdot$$
$$\cdot\ (1+O(\Delta x/a))$$

where the constants are defined in Table C.3.

Proof.

In this regime we shall use the velocity autocorrelation function derived in Appendix A:

$$E\left(\overset{\sqcap}{\mathbf{u}}_{\mathbf{m}}(s)\cdot\overset{\sqcap}{\mathbf{u}}_{\mathbf{n}}(r)\right)=\frac{k_BT}{\rho L^3}\sum_{\mathbf{k}}\Upsilon_{\mathbf{k}}e^{-a_{\mathbf{k}}|s-r|}\exp\left(i2\pi(\mathbf{n}-\mathbf{m})\cdot\mathbf{k}/N\right). \tag{6.3}$$

To estimate ψ and ϕ we shall use the fact that the correlation statistics appearing in 3.17 and 3.18 only depend with period Δx on $\mathbf{X}(0)$ with respect to the shift relative to the lattice points, and can therefore relate the lattice sums to the case where $\mathbf{X}(0)$ is lattice node with $O(\Delta x/a)$ error, as in the proof of Proposition 5.1.

From 3.17, 3.18 and the smoothness of δ_a, we have:

(6.4)
$$\psi(s,r)\leq\frac{1}{3}\sum_{\mathbf{m},\mathbf{n}}\delta_a(\mathbf{x_m})\delta_a(\mathbf{x_n})\int_0^s\int_0^r E\left(\overset{\sqcap}{\mathbf{u}}_{\mathbf{m}}(p)\cdot\overset{\sqcap}{\mathbf{u}}_{\mathbf{n}}(q)\right)dpdq\Delta x^6\left(1+O(\Delta x/a)\right)$$
$$\leq\left[2D\min(s,r)-\frac{k_BTL^3}{3\rho}\sum_{\mathbf{k}}\frac{|\hat{\delta}_{a,\mathbf{k}}|^2\Upsilon_{\mathbf{k}}}{\alpha_{\mathbf{k}}^2}\left(1+e^{-\alpha_{\mathbf{k}}|s-r|}-e^{-\alpha_{\mathbf{k}}s}-e^{-\alpha_{\mathbf{k}}r}\right)\right]\cdot$$
$$\cdot\ (1+O(\Delta x/a))$$

where D is defined by:

$$D:=\frac{k_BTL^3}{3\rho}\sum_{\mathbf{k}}\frac{|\hat{\delta}_{a,\mathbf{k}}|^2\Upsilon_{\mathbf{k}}}{\alpha_{\mathbf{k}}} \tag{6.5}$$

and $\Upsilon_{\mathbf{k}}$ is defined in A.4; see (1). The factor D can be interpreted as the diffusion coefficient of a particle (1; 18). From 6.4 we have for all s, r:

$$\psi(s,r) \leq 2D\min(s,r)\left(1 + O(\Delta x/a)\right). \tag{6.6}$$

From 6.6 we have the bound:

$$\int_0^{\Delta t} e^{-\alpha_{\mathbf{k}}(\Delta t - s)}\left(\psi(s,s)\right)^{\frac{1}{2}} ds \leq \sqrt{2D}\frac{(\Delta t)^{\frac{1}{2}}}{\alpha_{\mathbf{k}}}\left(1 + O(\Delta x/a)\right). \tag{6.7}$$

To obtain expression 6.1 for the error associated with the modes of the fluid, the estimate 6.7 is substituted into 4.3 and the explicit terms are bounded by their large Δt asymptotics.
□

PROPOSITION 6.2. *The numerical scheme 2.22 – 2.30 incurs an error for the particle dynamics which can be bounded by:*

(6.8)
$$\begin{aligned}
e_{prt}(\Delta t) \leq \Bigg\{ & 9C_{A1}L_{\delta,a}A_a B_0\left(B_0\frac{\Delta t^2}{2} + \left(\frac{2C_{A2}}{3}D\right)^{1/2}\Delta t^{3/2}\right) \\
& + \sum_{\mathbf{k}}\left(\rho^{-1}M^2 L_F \hat{\delta}^*_{a,\mathbf{k}} + \rho^{-1}MF^* L_{\delta,\mathbf{k}}\right)\left(\frac{B_0}{2\alpha_{\mathbf{k}}}\Delta t^2 + 2\sqrt{\frac{2D}{3}}\frac{\Delta t^{3/2}}{\alpha_{\mathbf{k}}}\right) \\
& + 9B_0C_{A1}\sqrt{C_{A2}}\left(\frac{2}{9}\frac{k_BTL^3}{\rho}\sum_{\mathbf{k}}\frac{L^2_{\delta,\mathbf{k}}\Upsilon_{\mathbf{k}}}{\alpha_{\mathbf{k}}}\right)^{1/2}\Delta t^{3/2} \\
& + 9C_{A1}\sqrt{C_{A2}}\left(\frac{2D}{3}\frac{k_BTL^3}{\rho}\sum_{\mathbf{k}}\frac{L^2_{\delta,\mathbf{k}}\Upsilon_{\mathbf{k}}}{\alpha_{\mathbf{k}}}\right)^{1/2}\Delta t\Bigg\}\left(1 + O(\Delta x/a)\right).
\end{aligned}$$

Proof.
To obtain the bound 6.8 we shall use estimates of the functions ϕ, ψ and the integrals appearing in 4.14.
To estimate ϕ we use 6.3 to obtain:

$$\begin{aligned}
\phi(s,r) &\leq \frac{1}{3}\sum_{\mathbf{m},\mathbf{n}}\nabla\delta_a^{(\beta)}(\mathbf{x_m})\nabla\delta_a^{(\beta)}(\mathbf{x_n})E\left(\overset{\sqcap}{\mathbf{u}}_{\mathbf{m}}(s)\cdot\overset{\sqcap}{\mathbf{u}}_{\mathbf{n}}(r)\right)\Delta x^6\,\cdot \\
&\quad\cdot\left(1 + O(\Delta x/a)\right) \\
&\leq \frac{1}{3}\frac{k_BTL^3}{\rho}\sum_{\mathbf{k}}|\widehat{\nabla\delta}^{(\beta)}_{a,\mathbf{k}}|^2\Upsilon_{\mathbf{k}}e^{-\alpha_{\mathbf{k}}|s-r|} \\
&\quad\cdot\left(1 + O(\Delta x/a)\right) \\
&\leq \frac{1}{3}\frac{k_BTL^3}{\rho}\sum_{\mathbf{k}}L^2_{\delta,\mathbf{k}}\Upsilon_{\mathbf{k}}e^{-\alpha_{\mathbf{k}}|s-r|} \\
&\quad\cdot\left(1 + O(\Delta x/a)\right)
\end{aligned} \tag{6.9}$$

where the notation $\widehat{\nabla\delta}^{(\beta)}_{a,\mathbf{k}}$ refers to the β vector component of the Fourier transform of $\nabla\delta_a(\mathbf{x})$.

To estimate the integrals, the following estimates will be useful:

$$\int_0^{\Delta t}\int_0^{s} e^{-\alpha_{\mathbf{k}}(s-r)} r dr ds \le \frac{\Delta t^2}{2\alpha_{\mathbf{k}}} \tag{6.10}$$

and

$$\int_0^{\Delta t}\int_0^{\Delta t} e^{-\alpha_{\mathbf{k}}|s-r|} s r dr ds \le \frac{2}{3}\frac{\Delta t^3}{\alpha_{\mathbf{k}}}. \tag{6.11}$$

From 6.6 we have:

$$\begin{aligned}\int_0^{\Delta t}\int_0^{\Delta t} \psi(s,r) dr ds &\le \int_0^{\Delta t}\int_0^{\Delta t} 2D\min(s,r) dr ds \left(1+O(\Delta x/a)\right)\\ &= \frac{2}{3} D\Delta t^3 \left(1+O(\Delta x/a)\right).\end{aligned} \tag{6.12}$$

It follows from 6.7 that:

$$\begin{aligned}\int_0^{\Delta t}\int_0^{s} e^{-\alpha_{\mathbf{k}}(s-r)} \left(\psi(s,r)\right)^{\frac{1}{2}} dr ds &\le \sqrt{2D}\int_0^{\Delta t} \frac{s^{\frac{1}{2}}}{\alpha_{\mathbf{k}}} ds \left(1+O(\Delta x/a)\right)\\ &\le \frac{2}{3}\frac{\sqrt{2D}}{\alpha_{\mathbf{k}}}\Delta t^{3/2} \left(1+O(\Delta x/a)\right).\end{aligned} \tag{6.13}$$

Using 6.6, 6.9, and 6.10, we obtain:

$$\begin{aligned}\int_0^{\Delta t}\int_0^{\Delta t} \phi(s,r)\psi(s,r) dr ds \le \frac{2D}{3}\left(\frac{k_B T L^3}{\rho}\sum_{\mathbf{k}}\frac{L_{\delta,\mathbf{k}}^2 \Upsilon_{\mathbf{k}}}{\alpha_{\mathbf{k}}}\right)\Delta t^2 \cdot\\ \cdot\ \left(1+O(\Delta x/a)\right).\end{aligned} \tag{6.14}$$

From 6.9 and 6.11 we have:

$$\begin{aligned}\int_0^{\Delta t}\int_0^{\Delta t} \phi(s,r) s r dr ds &\le \sum_{\mathbf{m},\mathbf{n}} \nabla\delta_a^{(\beta)}(\mathbf{x}_{\mathbf{m}})\nabla\delta_a^{(\beta)}(\mathbf{x}_{\mathbf{n}}) \cdot\\ &\cdot\ \frac{k_B T}{\rho L^3}\sum_{\mathbf{k}}\int_0^{\Delta t}\int_0^{\Delta t} \Upsilon_{\mathbf{k}} e^{-\alpha_{\mathbf{k}}|s-r|} s r dr ds \exp\left(i2\pi(\mathbf{m}-\mathbf{n})\cdot\mathbf{k}/N\right)\Delta x^6 \cdot\\ &\cdot\ \left(1+O(\Delta x/a)\right)\\ &\le \frac{2}{9}\frac{k_B T L^3}{\rho}\sum_{\mathbf{k}}\frac{L_{\delta,\mathbf{k}}^2 \Upsilon_{\mathbf{k}}}{\alpha_{\mathbf{k}}}\Delta t^3 \left(1+O(\Delta x/a)\right).\end{aligned} \tag{6.15}$$

By substituting 6.12, 6.13, 6.14, 6.15 into 4.14 we obtain 6.8.

□

7. Uniform Bounds Suited for Intermediate Time Steps. We shall now discuss the error when the time step is in the intermediate range:

$$\min \frac{1}{\alpha_{\mathbf{k}}} \lesssim \Delta t \lesssim \max \frac{1}{\alpha_{\mathbf{k}}}. \tag{7.1}$$

In this regime at least some of the modes of the fluid are under-resolved by the numerical method. An important feature of the immersed boundary method which is relevant in this regime is that the particle dynamics depend on the fluid velocity though a convolution with the function $\delta_a(\mathbf{x})$. As a consequence of the rapid decay of $\hat{\delta}_{a,\mathbf{k}}$ for $|\mathbf{k}| >> (L/a)$, only a subset of the fluid modes contribute non-negligibly to the particle dynamics. This requires that two intermediate time step regimes be considered. The first regime occurs when a significant number of the modes which contribute to the particle dynamics are under-resolved:

$$\frac{\rho a^2}{\mu} \ll \Delta t \lesssim \max \frac{1}{\alpha_{\mathbf{k}}}. \tag{7.2}$$

In this regime the thermal component of the displacement of a particle over a time step $\overset{\sqcap}{\mathbf{X}}(\Delta t) - \overset{\sqcap}{\mathbf{X}}(0)$ is expected to have diffusive-like $\Delta t^{1/2}$ scaling. The second intermediate time step regime occurs when all of the fluid modes which contribute non-negligibly to the particle dynamics are resolved:

$$\min \frac{1}{\alpha_{\mathbf{k}}} \lesssim \Delta t \ll \frac{\rho a^2}{\mu}. \tag{7.3}$$

The scaling of the thermal component of the particle displacement $\overset{\sqcap}{\mathbf{X}}(\Delta t) - \overset{\sqcap}{\mathbf{X}}(0)$ over a time step in this regime is expected to have ballistic Δt scaling. Much of the analysis proceeds in the same manner as in the case of the small and large time step regimes with only a few changes made to the error estimates which take into account the features mentioned above concerning the dependence of the particle dynamics on the fluid modes.

We shall first establish a proposition concerning estimates of ψ which is used to bound the thermal component of the particle displacement over a time step. We then establish estimates for the fluid and particle dynamics in each of the intermediate time step regimes. For convenience we shall consider only the case when $s \geq r$, with the other case when $s \leq r$ following similarly by symmetry of the function ψ in the parameters s and r.

Two uniform estimates will be established for ψ. Which estimate is better depends on the specific regime of the time step. The first estimate will be used in the regime $s, r \leq \rho a^2/\mu$. The second estimate will be used in the regime $s > \rho a^2/\mu$.

LEMMA 7.1. *The following two bounds for $\psi(s,r)$ hold uniformly for $0 < r \leq s$:*

$$\psi(s,r) \leq \frac{k_B T L^3}{3\rho} \sum_{\mathbf{k}} \Upsilon_{\mathbf{k}} \delta_{a,\mathbf{k}}^2 s r \tag{7.4}$$

$$\psi(s,r) \leq \frac{2 k_B T L^3}{3\rho} \sum_{\mathbf{k}} \Upsilon_{\mathbf{k}} \frac{\delta_{a,\mathbf{k}}^2}{\alpha_{\mathbf{k}}} r. \tag{7.5}$$

Proof.
From 3.17 we have:

$$\psi(s,r) = \frac{k_B T L^3}{3\rho} \sum_{\mathbf{k}} \Upsilon_{\mathbf{k}} \delta_{a,\mathbf{k}}^2 Q_{\mathbf{k}}(s,r) \tag{7.6}$$

where

(7.7)

$$\begin{aligned} Q_{\mathbf{k}}(s,r) &= \int_0^s \int_0^r e^{-\alpha_{\mathbf{k}}|s'-r'|} dr' ds' \\ &= 2\left(\frac{1}{\alpha_{\mathbf{k}}}\right)^2 \left(\alpha_{\mathbf{k}} r - \left(1 - e^{-\alpha_{\mathbf{k}} r}\right)\right) - \left(\frac{1}{\alpha_{\mathbf{k}}}\right)^2 \left(e^{-\alpha_{\mathbf{k}}(s-r)} - 1 - e^{-\alpha_{\mathbf{k}} s} + e^{-\alpha_{\mathbf{k}} r}\right) \end{aligned}$$

when $r \leq s$. The estimates for ψ are a direct consequence of bounding the terms in the sum 7.6 using the following two inequalities for $Q_{\mathbf{k}}(s,r)$, which hold uniformly for $0 < r \leq s$:

$$Q_{\mathbf{k}}(s,r) \leq sr \tag{7.8}$$

$$Q_{\mathbf{k}}(s,r) \leq \frac{2r}{\alpha_{\mathbf{k}}}. \tag{7.9}$$

□

The corresponding regimes in which the estimates are optimal can be established by using the scaling of $\alpha_{\mathbf{k}}$ given in Table C.1.

We shall now consider the fluid and particle errors for the regime in which

$$\frac{\rho a^2}{\mu} \ll \Delta t \lesssim \max \frac{1}{\alpha_{\mathbf{k}}}. \tag{7.10}$$

When the time step under-resolves the $\mathbf{k}^{th}$ mode of the fluid, the error estimate for $e_{\text{fld},\mathbf{k}}(\Delta t)$ in Proposition 6.1 suffices. When the time step is sufficiently small to resolve the $\mathbf{k}^{th}$ mode of the fluid, the error estimate for $e_{\text{fld},\mathbf{k}}(\Delta t)$ can be improved relative to the estimate for the resolved case established in proposition 5.1. This occurs since the thermal component of the particle displacement is now expected to scale in a diffusive-like $\Delta t^{1/2}$ fashion as a consequence of the under-resolved modes.

More precisely, the error of the $\mathbf{k}^{th}$ fluid mode is bounded best by proposition 6.1 when $\alpha_{\mathbf{k}}\Delta t \gg 1$ and by the following estimate when $\alpha_{\mathbf{k}}\Delta t \ll 1$:

Proposition 7.2.

(7.11)

$$\begin{aligned} e_{\mathit{fld},\mathbf{k}}(\Delta t) &\leq \left[E\left(|\hat{\mathbf{u}}_{\mathbf{k}} - \hat{\tilde{\mathbf{u}}}_{\mathbf{k}}|^2\right)\right]^{1/2} \\ &\leq \rho^{-1}\left(M^2 L_F \hat{\delta}_{a,\mathbf{k}}^* + M F^* L_{\delta,\mathbf{k}}\right)\left(B_0 \Delta t^2 + \frac{2}{3}\sqrt{6D}\Delta t^{3/2}\right) \cdot \\ &\quad \cdot \left(1 + O(\Delta x / a)\right) \end{aligned}$$

where D is defined in 6.5.

Proof.

From the second estimate in Lemma 7.1 and the definition of the diffusion coefficient given in 6.5, we have:

$$\psi(s,r) \leq 2D\min(s,r)\left(1 + O(\Delta x/a)\right). \tag{7.12}$$

From 7.12, we have the bound:

$$\int_0^{\Delta t} e^{-\alpha_{\mathbf{k}}(\Delta t - s)}\left(\psi(s,s)\right)^{1/2} ds \leq \frac{2}{3}\sqrt{2D}\Delta t^{3/2}\left(1 + O(\Delta x/a)\right). \tag{7.13}$$

To obtain expression 7.11 for the error associated with the modes of the fluid over intermediate time steps, the estimate 7.13 is substituted into 4.3 and the exponential terms are bounded by their second order Taylor expansion in Δt. □

For the time step regime

$$\frac{\rho a^2}{\mu} \ll \Delta t \lesssim \max\frac{1}{\alpha_{\mathbf{k}}} \tag{7.14}$$

the estimate for the particle error in Proposition 6.2 suffices.

The second intermediate regime occurs for the time step:

$$\min\frac{1}{\alpha_{\mathbf{k}}} \lesssim \Delta t \ll \frac{\rho a^2}{\mu}. \tag{7.15}$$

In this regime all of the fluid modes which contribute non-negligibly to the particle dynamics are resolved over the time step. This follows since for time steps in this regime the smallest wavenumber $\mathbf{k}$ for which the fluid dynamics is under-resolved satisfies $|\mathbf{k}| \gg L/a$. As a consequence, the particle error $e_{\mathrm{prt}}(\Delta t)$ in this regime is also tightly bounded by the estimate of Proposition 5.2. The only error estimate which can be substantially improved from the previous analysis is the fluid error for under-resolved modes. More precisely the error of the $\mathbf{k}^{th}$ fluid mode when $\alpha_{\mathbf{k}}\Delta t \ll 1$ is given by proposition 5.1 and when $\alpha_{\mathbf{k}}\Delta t \gg 1$ is bounded tightly by:

PROPOSITION 7.3.

(7.16)

$$\begin{aligned} e_{\mathit{fld},\mathbf{k}}(\Delta t) &\leq \left[E\left(|\hat{\mathbf{u}}_{\mathbf{k}} - \hat{\tilde{\mathbf{u}}}_{\mathbf{k}}|^2\right)\right]^{1/2} \\ &\leq \rho^{-1}\left(M^2 L_F \hat{\delta}^*_{a,\mathbf{k}} + MF^* L_{\delta,\mathbf{k}}\right)\left(B_0\frac{\Delta t}{\alpha_{\mathbf{k}}} + \sqrt{3}\left(\frac{k_B T}{\rho}\sum_{\mathbf{m}}\delta_a^2(\mathbf{x}_{\mathbf{m}})\Delta x^3\right)^{1/2}\frac{\Delta t^2}{2}\right)\cdot \\ &\quad \cdot \left(1 + O(\Delta x/a)\right). \end{aligned}$$

Proof. The integral involving ψ in the general error expression 4.3 can be handled in this regime using the uniform estimate 7.4. The integrals are then handled in otherwise the same manner as in estimate 5.4 in Proposition 5.1. □

8. Scaling of the Error Estimates in the Parameters of the Method. To better elucidate the numerical error, we shall use the uniform estimates in Sections 5–7 to bound the error using the best approximation among the bounds in each of the asymptotic scaling regimes of the time step. To make the estimates as transparent as possible, the scaling of the expressions with respect to the parameters used in the numerical method 2.22 – 2.30 will be derived. The scaling of key terms that appear in the estimates are summarized in Table C.1. To estimate the fluid error in physical space, as defined in 3.2, we use the fact that L^1 averages are bounded by L^2 averages. Along with Plancherel's Theorem, we can then obtain the spatial fluid error in terms of our L^2 estimates for the error of the fluid Fourier modes:

$$e_{\text{fld}}(\Delta t) \leq \left(\sum_{\mathbf{k}} E\left(|\hat{\mathbf{u}}_{\mathbf{k}}(\Delta t) - \hat{\tilde{\mathbf{u}}}_{\mathbf{k}}(\Delta t)|^2 \right) \right)^{1/2}. \tag{8.1}$$

To simplify the discussion, it will be assumed throughout that the particle size is no larger than the length scale of variation of the force fields: $a \lesssim \ell_F$.

In the notation, factors C will be superscripted with primes and are non-dimensional constants approximately independent of the physical parameters. These factors can be thought of as order unity constants. To avoid cumbersome notation and unduly emphasizing the role of these factors, the notation is reused in each equation, with the understanding that C denotes distinct factors for each estimate.

We remark that in the following sections we are discussing our rigorous mathematical results in a more physically intuitive manner. Given the less formal approach of these sections, we shall discuss the the error estimates as approximate equalities rather than inequalities. This is meant to convey the intended content of the inequalities derived in the previous sections, which could be shown to be approximate equalities in the corresponding asymptotic regimes.

8.1. Scaling for Small Time Steps which Fully Resolve the Fluid Dynamics. The scaling is now discussed for the error estimates 5.1 and 5.5 in the regime $\Delta t \ll \min \frac{1}{\alpha_{\mathbf{k}}}$, where the time step is taken sufficiently small so that the dynamics of all modes of the fluid are resolved by the stochastic immersed boundary method.

From the estimates 4.3 and 4.14 with the scalings of key terms given in Table C.1, we obtain for the numerical errors:

$$\hat{e}_{\text{fld},\mathbf{k}}(\Delta t) \approx \frac{MF^*}{\rho}\hat{\delta}^*_{a,\mathbf{k}} \left(\frac{M}{\ell_F} + C\frac{1}{a} \right) \left(C' v_{\text{frc}} + C'' v_{\text{thm}} \right) \Delta t^2 \tag{8.2}$$

$$e_{\text{fld}}(\Delta t) \approx \frac{MF^*}{\rho a^{3/2} L^{3/2}} \left(\frac{M}{\ell_F} + C\frac{1}{a} \right) \left(C' v_{\text{frc}} + C'' v_{\text{thm}} \right) \Delta t^2 \tag{8.3}$$

$$\begin{aligned} e_{\text{prt}}(\Delta t) \approx & \left(C v_{\text{thm}}^2 + C' v_{\text{frc}} v_{\text{thm}} + C'' v_{\text{frc}}^2 \right) \frac{\Delta t^2}{a} \\ & + \frac{MF^*}{\rho a^3} \left(\frac{M}{\ell_F} + C''' \frac{1}{a} \right) \left(C'''' v_{\text{frc}} + C''''' v_{\text{thm}} \right) \Delta t^3, \end{aligned} \tag{8.4}$$

where the parameters are defined in Table C.2 and C.3. To simplify the notation and aid in interpretation of the estimates, two factors were introduced. The first $v_{\text{thm}} = \sqrt{k_B T / \rho a^3}$ is the typical thermal velocity associated with a particle under the equipartition theorem of statistical mechanics (21; 32). The second $v_{\text{frc}} = MF^*/\mu a$ is the velocity scale of a particle in a viscous fluid subject to a force of magnitude MF^*.

These error estimates indicate that the stochastic immersed boundary method behaves like a strong first order accurate method when the time step is taken sufficiently small. For more details, see the discussion in reference (1).

8.2. Scaling for Large Time Steps which Under-resolve All Fluid Modes. We now present estimates for how the numerical error scales in the physical parameters when the time step is taken large enough to under-resolve all modes of the fluid, but always small enough to resolve the elementary particle dynamics:

$$\max \frac{1}{\alpha_{\mathbf{k}}} \ll \Delta t \ll \tau_{\mathrm{mov}}(a). \tag{8.5}$$

The notation $\tau_{\mathrm{mov}}(a)$ denotes the typical time required for an elementary particle to move a displacement equal to its size a, either by advection or diffusion. It can be estimated to scale with respect to physical parameters as follows:

$$\tau_{\mathrm{mov}}(a) \approx \min(Ca/v_{\mathrm{frc}}, C'a^2/D).$$

In the regime 8.5, the numerical error scales as:

$$\hat{e}_{\mathrm{fld},\mathbf{k}}(\Delta t) \approx \frac{MF^*L^2}{\mu|\mathbf{k}|^2}\hat{\delta}^*_{a,\mathbf{k}}\left(\frac{M}{\ell_F} + C\frac{1}{a}\right)\left(C'v_{\mathrm{frc}}\Delta t + C''\sqrt{D}\Delta t^{1/2}\right) \tag{8.6}$$

$$e_{\mathrm{fld}}(\Delta t) \approx \sqrt{\frac{a}{L}}\frac{MF^*}{\mu L}\left(\frac{M}{\ell_F} + C\frac{1}{a}\right)\left(C'v_{\mathrm{frc}}\Delta t + C''\sqrt{D}\Delta t^{1/2}\right) \tag{8.7}$$

$$\begin{aligned} e_{\mathrm{prt}}(\Delta t) \approx {} & C\frac{D}{a}\Delta t \\ & + \left(C'\frac{M}{\ell_F} + C''\frac{1}{a}\right)\left(\sqrt{D}v_{\mathrm{frc}}\Delta t^{3/2} + v_{\mathrm{frc}}^2\Delta t^2\right) \end{aligned} \tag{8.8}$$

where D denotes the diffusion coefficient of an elementary particle defined in 6.5, which scales with respect to the parameters as:

$$D \approx C\frac{k_B T}{\mu a}. \tag{8.9}$$

The factors C denote order unity nondimensional constants. For the definitions of the parameters of the method, see Tables C.2 and C.3.

The smaller powers of Δt appearing in the error estimates may suggest that the accuracy is deteriorating more rapidly with respect to the time step in the under-resolved regime under discussion, but in fact the opposite is true. The error estimates reported above are in fact considerably smaller than the error estimates in Subsection 8.1, for the range of time steps defining the under-resolved regime. Indeed, the ratio of terms appearing in the above estimates to corresponding terms in the equations in Subsection 8.1 involve ratios such as $\rho L^2/(\mu|\mathbf{k}|^2\Delta t)$, $D^{1/2}/(v_{\mathrm{thm}}\Delta t^{1/2})$, and $L^{1/2}a^{3/2}\rho/\mu\Delta t$, all of which are much smaller than one in the asymptotic regime defined by 8.5.

A more important point is that the numerical errors remain small relative to the changes in the system variables throughout this range of time steps, so that the numerical method maintains accuracy for all $\Delta t \lesssim \tau_{\text{mov}}(a)$. We emphasize that unlike traditional numerical analysis, the presence of terms proportional to Δt in the error estimate 8.8 does not imply that the method is inconsistent. It must be remembered that these error estimates are good approximations not in the $\Delta t \downarrow 0$ limit, but rather in the asymptotic regime 8.5. See (1) for a more detailed discussion.

8.3. Scaling for Intermediate Time Steps which Under-resolve Only Some Fluid Modes. An important feature of the stochastic numerical scheme is that time steps can be chosen which only partially resolve the dynamics of the fluid. This corresponds to the time step Δt falling into the range:

$$\min \frac{1}{\alpha_{\mathbf{k}}} \lesssim \Delta t \lesssim \max \frac{1}{\alpha_{\mathbf{k}}}. \tag{8.10}$$

In this case, there are in fact two asymptotic regimes of the time step for the scaling of the numerical error:

$$\frac{\rho a^2}{\mu} \ll \Delta t \lesssim \max \frac{1}{\alpha_{\mathbf{k}}} \tag{8.11}$$

and

$$\min \frac{1}{\alpha_{\mathbf{k}}} \lesssim \Delta t \ll \frac{\rho a^2}{\mu}. \tag{8.12}$$

The first regime corresponds to the situation in which a significant number of the fluid modes which influence the dynamics of the immersed structures is under-resolved over a time step. The second corresponds to the case when all of the fluid modes which contribute non-negligibly to the dynamics of the immersed structures are resolved over a time step.

Most scaling estimates can be derived in a similar fashion to those in the other time step regimes. Only the spatial fluid error (8.1) requires special attention because it involves a sum over the errors of the fluid Fourier modes, which switch between two forms depending on the magnitude of the wavenumber $\mathbf{k}$. The critical wavenumber for the transition between the regimes $\alpha_{\mathbf{k}}\Delta t \ll 1$ and $\alpha_{\mathbf{k}}\Delta t \gg 1$ is given by:

$$k_c = \left(\frac{\rho L^2}{\mu \Delta t}\right)^{1/2}. \tag{8.13}$$

We then split the sum over wavenumbers in 8.1 into two parts consisting of wavenumbers for which the fluid dynamics are resolved and under-resolved. We shall obtain the scalings using the following integral approximations for each part of the sum:

$$\sum_{|\mathbf{k}| \le k_c} \hat{\delta}^*_{a,\mathbf{k}} \approx C \int_1^{\min\{k_c, L/a\}} \frac{1}{L^3} r^2 dr \tag{8.14}$$

and

$$\sum_{|\mathbf{k}| > k_c} \frac{\hat{\delta}_{a,\mathbf{k}}}{|\mathbf{k}|^2} \approx C \int_{k_c}^{L/a} \frac{1}{L^3} dr. \tag{8.15}$$

In the first regime:

$$\frac{\rho a^2}{\mu} \ll \Delta t \lesssim \max \frac{1}{\alpha_{\mathbf{k}}}, \tag{8.16}$$

we have:

$$\sum_{|\mathbf{k}| \leq k_c} \hat{\delta}^*_{a,\mathbf{k}} \ll \frac{C}{L^3} \left(\frac{\rho L^2}{\mu \Delta t} \right)^{3/2} \tag{8.17}$$

and

$$\sum_{|\mathbf{k}| > k_c} \frac{\hat{\delta}^*_{a,\mathbf{k}}}{|\mathbf{k}|^2} \approx \frac{C}{aL^2}. \tag{8.18}$$

From the scaling of the summation terms above, Table C.1, and using the best approximation among the established bounds for the fluid and particle error for this regime, the following estimates are obtained. For those fluid modes which are well resolved in this regime ($\alpha_{\mathbf{k}} \Delta t \ll 1$), we have from Proposition 7.2 that:

$$\hat{e}_{\text{fld},\mathbf{k}}(\Delta t) \approx \frac{MF^*}{\rho} \hat{\delta}^*_{a,\mathbf{k}} \left(\frac{M}{\ell_F} + C\frac{1}{a} \right) \left(C' v_{\text{frc}} \Delta t^2 + C'' \sqrt{D} \Delta t^{3/2} \right). \tag{8.19}$$

For the under-resolved modes (with $\alpha_{\mathbf{k}} \Delta t \gg 1$), we have the same error estimate 8.8 as in the fully under-resolved case.

The errors incurred in the physical space variables describing the velocity and elementary particle positions can be estimated in this asymptotic regime as:

$$e_{\text{fld}}(\Delta t) \approx \frac{MF^*}{\rho \nu^{3/4} L^{3/2}} \left(\frac{M}{\ell_F} + C\frac{1}{a} \right) \left(C' v_{\text{frc}} \Delta t^{5/4} + C'' \sqrt{D} \Delta t^{3/4} \right) \tag{8.20}$$

and

$$\begin{aligned} e_{\text{prt}}(\Delta t) \approx{}& C\frac{D}{a}\Delta t \\ &+ \left(\frac{M}{\ell_F} + C'\frac{1}{a} \right) \left[\sqrt{D} v_{\text{frc}} \Delta t^{3/2} + v_{\text{frc}}^2 \Delta t^2 \right] \end{aligned} \tag{8.21}$$

where $\nu = \mu/\rho$.

In the second regime:

$$\min \frac{1}{\alpha_{\mathbf{k}}} \lesssim \Delta t \ll \frac{\rho a^2}{\mu}, \tag{8.22}$$

we have:

$$\sum_{|\mathbf{k}| \leq k_c} \hat{\delta}^*_{a,\mathbf{k}} \approx \frac{C}{a^3} \tag{8.23}$$

and the contribution from large wavenumbers is comparatively negligible. For these time steps, all error estimates presented in Subsection 8.1 for the fully resolved regime remain good approximations for the particle error, spatial fluid error, and resolved fluid Fourier mode errors. The estimate for the individual under-resolved fluid modes can be improved in this intermediate regime using Proposition 7.3 to obtain:

$$\hat{e}_{\mathrm{fld},\mathbf{k}}(\Delta t) \approx \frac{MF^{*}L^{2}}{\mu|\mathbf{k}|^{2}}\left(\frac{M}{\ell_F} + C\frac{1}{a}\right)\hat{\delta}^{*}_{a,\mathbf{k}}\left(C' v_{\mathrm{frc}} + C'' v_{\mathrm{thm}}\right)\Delta t. \tag{8.24}$$

As with the other regimes, the estimates can be used to show that the errors are small relative to the magnitude of the changes of the actual system variables over a time step. For a further discussion see (1).

9. Conclusions. By using stochastic calculus to integrate analytically some of the degrees of freedom in the immersed boundary method with thermal fluctuations, a stable and accurate numerical method was obtained, even in regimes when the time step is larger than some time scales of the system. In this paper it was shown how numerical analysis can be carried out for the method, including the regimes where some dynamical features of the system are under-resolved.

The basic approach was to decompose the error contributions of the fluid and particle degrees of freedom in such a manner that general bounds holding uniformly for all time steps could be obtained in terms of the correlation functions ψ, ϕ of the system, as defined in 3.17 and 3.18. The terms of the general bound were then further developed by obtaining more specific estimates of the correlation functions for each time step regime. The scaling of the estimates with respect to the parameters of the method were then developed. The scaling of the estimates yields information about how the error behaves in each regime, giving insight into how to determine an appropriate time step or into numerical issues that can arise for specific parameter regimes when using the method in practice. The numerical analysis shown in this paper for the stochastic immersed boundary method may also be applicable in a similar fashion to other "multiscale" explicit integrators which under-resolve dynamics on small time scales arising from stochastic forcing terms.

References.

[1] P. J. Atzberger, P. R. Kramer, and C. S. Peskin, *A Stochastic Immersed Boundary Method for Biological Fluid Dynamics at Microscopic Length Scales*, (submitted J. Comp. Phys.)

[2] B. Alberts, A. Johnson, J. Lewis, M. Raff, K. Roberts, and P. Walker, *Molecular Biology of the Cell*, Garland Publishing, 2002.

[3] D. Boal, *Mechanics of the Cell*, Cambridge University Press, Cambridge, U.K., 2002.

[4] L. C. de Hoog and M. Mann, *Proteomics*, Annu. Rev. Genomics Hum. Genet. 2004. 5:267–293.

[5] D. C. Champeney, *A handbook of Fourier theorems*, Cambridge University Press, Cambridge, 1987. ISBN 0-521-26503-7.

[6] A. J. Chorin, *Numerical Solution of the Navier-Stokes Equations*, Math. Comp., vol. 22, (1968), pp. 745.

[7] S. Corrsin, *Atmospheric Diffusion and Air Pollution, edited by F. N. Frenkiel and P.A. Shappard*, vol. 6, 1960.

[8] C. P. Fall, E. S. Marland, J. M. Wagner, and J. J. Tyson, eds., *Computational cell biology*, vol. 20 of Interdisciplinary Applied Mathematics, Springer-Verlag, New York, 2002.

[9] L. J. Fauci and A. L. Fogelson, *Truncated Newton Method and the Modeling of Complex Immersed Elastic Structures*, Communication on Pure and Applied Mathematics, XLVI (1993), pp. 787–818.

[10] L. Fradkin, *Comparison of Lagrangian and Eulerian approaches to turbulent diffusion*, Plasma Physics and Controlled Fusion, 33 (1991), pp. 685–701.

[11] C. W. Gardiner, *Handbook of stochastic methods*, Springer Series in Synergetics, 1985

[12] E. Givelberg and J. Bunn, *Detailed simulation of the cochlea: Recent progress using large shared memory parallel computers*, CACR Technical Report CACR-190, (2001).

[13] N. Gov and S. A. Safran, *Red-blood cell membrane fluctuations and shape controlled by ATP-induced cytoskeletal defects*, Biophysical Journal BioFAST, (2004).

[14] H. P. Grimm, A. B. Verkhovsky, A. Mogilner, and J. J. Meister, *Analysis of actin dynamics at the leading edge of crawling cells: implications for the shape of keratocyte lamellipodia*, European Biophysical Journal, 32 (2003), pp. 563 – 577.

[15] M. Holmes, *Introduction to Perturbation Methods*, Springer.

[16] J. Howard, *Mechanics of Motor Proteins and the Cytoskeleton*, Sinauer Associates, Sunderland, CN, 2001.

[17] P. E. Kloeden and E. Platen, *Numerical solution of stochastic differential equations*, Springer-Verlag, 1992.

[18] P. R. Kramer and C. S. Peskin , *Incorporating thermal fluctuations into the immersed boundary method*, Proceedings of the Second MIT Conference on Computational Fluid and Solid Mechanics, K. K. Bathe, ed. Elsevier, 2 (2003), pp. 1755–1758.

[19] P. R. Kramer and A. J. Majda, *Stochastic mode reduction for the immersed boundary method*, SIAM J. Appl. Math., 64 (2003/04), pp. 369–400 (electronic).

[20] R. Kubo, M. Toda, and N. Hashitsume, *Statistical physics. II*, Springer-Verlag, Berlin, second ed., 1991, section 4. Nonequilibrium statistical mechanics.

[21] L. D. Landau and E. M. Lifshitz, *Course of theoretical physics. Vol. 9: Statistical physics*, Pergamon Press, Oxford, 1980, ch. IX.

[22] L. D. Landau and E. M. Lifshitz, *Course of theoretical physics. Vol. 6: Fluid Mechanics*, Butterworth-Heinemann, Oxford, 1987, ch. II.

[23] R. Lipowsky, *Statistical Mechanics of Biocomplexity*, Springer, 1999.

[24] X. Meng, *A computational model of flow through porous media at the microscale*, Ph.D. thesis, Department of Mathematics, Tulane University, New Orleans, Louisiana 70118. July 1998.

[25] L. Miller and C. Peskin, *When vortices stick: an aerodynamic transition in tiny insect flight*, J Exp Biol., 207 (2004), pp. 3073–3088.

[26] K. C. Neuman and S. M. Block, *Optical trapping*, Review of Scientific Instruments, volume 75, number 9, (2004).

[27] B. Oksendal, *Stochastic Differential Equations: An Introduction with Applications.* Springer, 2000

[28] G. Oster and A. Mogilner, *Force generation by cellular polymers. Supramolecular Polymers*, A. Ciferri (ed.), New York:Dekker (in press), 2005.

[29] C. S. Peskin, *The immersed boundary method*, Acta Numerica, 11 (2002), pp. 1–39.

[30] C. Peskin and D. McQueen, *Shared-memory parallel vector implementation*

of the immersed boundary method for the computation of blood flow in the beating mammalian heart., Journal of Supercomputing, 11 (1997), pp. 213–236.
[31] W. H. Press and Saul A. Teukolsky and W. T. Vetterling and B. P. Flannery, *Numerical Recipes*, Cambridge University Press, 2002
[32] L. E. Reichl, *A modern course in statistical physics*, John Wiley & Sons Inc., New York, second ed., 1998
[33] P. Reimann, *Introduction to the physics of Brownian motors*, Appl. Phys A, 75 (2002), pp. 169–178.
[34] D. N. Robinson and J. A. Spudich, *Mechanics and regulation of cytokinesis*, Current Opinion in Cell Biology, 16 (2004), pp. 182–188.
[35] T. Schlick, *Molecular Modeling and Simulation: An Interdisciplinary Guide*, vol. 21 of Interdisciplinary Applied Mathematics, Springer-Verlag, Berlin, 2002.
[36] J. C. Strikwerda, *Finite difference schemes and partial differential equations*, Chapman & Hall, New York.
[37] Tanke HJ, Dirks RW, and Raap T, *FISH and immunocytochemistry: towards visualising single target molecules in living cells*, Curr Opin Biotechnol 16, 49-54.
[38] J. Weinstock, *Lagrangian Eulerian relation and the independence approximation*, Physics of Fluids, 19 (1976), pp. 1702–1711.
[39] T. Wittman, A. Hyman, and A. Desai, *The spindle: a dynamic assembly of microtubules and motors*, Nature Cell Biology, 3 (2001), pp. E28 – E34.

Appendix A. The Autocorrelation Function of the Velocity Field of the Fluid. In this section the autocorrelation function is computed for the component of the velocity field $\overset{\sqcap}{\mathbf{u}}_{\mathbf{m}}$ which is driven by the thermal force, as defined below 3.9. This is done by representing the velocity field in Fourier space and computing the autocorrelation function for each mode $\mathbf{k}$. From equation 3.6 and 3.8 and standard stochastic calculus, the steady-state autocorrelation function of the $\mathbf{k}^{th}$ mode when $s > r$ is

$$E\left(\overline{\overset{\sqcap}{\hat{\mathbf{u}}}_{\mathbf{k}}(s)}\cdot \overset{\sqcap}{\hat{\mathbf{u}}}_{\mathbf{k}}(r)\right) \tag{A.1}$$

$$= 2D_{\mathbf{k}}E\left(\overline{\int_{-\infty}^{s} e^{-\alpha_{\mathbf{k}}(s-w)}\wp_{\mathbf{k}}^{\perp}d\tilde{\mathbf{B}}_{\mathbf{k}}(w)}\cdot\int_{-\infty}^{r} e^{-\alpha_{\mathbf{k}}(r-q)}\wp_{\mathbf{k}}^{\perp}d\tilde{\mathbf{B}}_{\mathbf{k}}(q)\right), \tag{A.2}$$

where the notation $\wp_{\mathbf{k}}^{\perp}$ denotes projection orthogonal to $\hat{\mathbf{g}}_{\mathbf{k}}$ as defined in 2.16.

By applying Ito's Isometry to A.2, and observing the symmetry under the interchange $s \leftrightarrow r$, the autocorrelation function is given by

$$E\left(\overline{\overset{\sqcap}{\hat{\mathbf{u}}}_{\mathbf{k}}(s)}\cdot \overset{\sqcap}{\hat{\mathbf{u}}}_{\mathbf{k}}(r)\right) = \begin{cases} 3\frac{D_{\mathbf{k}}}{\alpha_{\mathbf{k}}}e^{-\alpha_{\mathbf{k}}|s-r|} & \text{if } \mathbf{k}\in\mathcal{K} \\ 4\frac{D_{\mathbf{k}}}{\alpha_{\mathbf{k}}}e^{-\alpha_{\mathbf{k}}|s-r|} & \text{if } \mathbf{k}\notin\mathcal{K} \end{cases} \tag{A.3}$$

$$= \Upsilon_{\mathbf{k}}\frac{k_BT}{\rho L^3}e^{-\alpha_{\mathbf{k}}|s-r|},$$

where

$$\Upsilon_{\mathbf{k}} = \begin{cases} 3, & \mathbf{k}\in\mathcal{K} \\ 2, & \mathbf{k}\notin\mathcal{K}, \end{cases} \tag{A.4}$$

and the index set $\mathcal{K}$ is defined in 2.18. The factor $\Upsilon_{\mathbf{k}}$ arises from the incompressibility constraint 2.15, the real-valuedness constraint 2.21, and the dimensionality of the space orthogonal to $\hat{\mathbf{g}}_{\mathbf{k}}$.

The spatio-temporal correlation function of the thermal velocity field $\overset{\sqcap}{\mathbf{u}}$ is then given by:

$$\begin{aligned} E\left(\overset{\sqcap}{\mathbf{u}}_{\mathbf{m}}(s)\cdot\overset{\sqcap}{\mathbf{u}}_{\mathbf{n}}(r)\right) &= \sum_{\mathbf{k}}\sum_{\mathbf{k}'} E\left(\overline{\overset{\sqcap}{\hat{\mathbf{u}}}_{\mathbf{k}}(s)}\cdot\overset{\sqcap}{\mathbf{u}}_{\mathbf{k}'}(r)\right)\exp\left(i2\pi(\mathbf{n}\cdot\mathbf{k}'-\mathbf{m}\cdot\mathbf{k})/N\right) \\ &= \sum_{\mathbf{k}} E\left(\overline{\overset{\sqcap}{\hat{\mathbf{u}}}_{\mathbf{k}}(s)}\cdot\overset{\sqcap}{\hat{\mathbf{u}}}_{\mathbf{k}}(r)\right)\exp\left(i2\pi(\mathbf{n}-\mathbf{m})\cdot\mathbf{k}/N\right) \qquad \text{(A.5)} \\ &= \frac{k_B T}{\rho L^3}\sum_{\mathbf{k}}\Upsilon_{\mathbf{k}} e^{-a_{\mathbf{k}}|s-r|}\exp\left(i2\pi(\mathbf{n}-\mathbf{m})\cdot\mathbf{k}/N\right). \end{aligned}$$

To obtain the second equality, we used the statistical independence of the Fourier modes of the velocity field when the indices $\mathbf{k}$ and $\mathbf{k}'$ are distinct and do not correspond to conjugate modes (see 2.21). When the indices $\mathbf{k}$ and $\mathbf{k}'$ do refer to conjugate, but distinct, modes then the average vanishes because a mean zero random variable Z with independent and identically distributed real and imaginary components satisfies $\langle Z^2\rangle = 0$. The last equality follows by substitution from equation A.3.

Appendix B. Technical Properties of the Particle Representation Function δ_a.

Throughout the paper it will be useful to consider the Fourier coefficients of the function $\delta_a(\mathbf{x}-\mathbf{X})$ used to represent an elementary particle situated at position $\mathbf{X}$. While the function is defined for all $\mathbf{x}\in\Lambda$, it is often useful to consider the restriction of the function to the discrete lattice points $\{\mathbf{x}_{\mathbf{m}} = \mathbf{m}\Delta x | \mathbf{m}\in\mathbb{Z}_N^3\}$.

We will use the following notation to denote the discrete Fourier transform of the particle representation function restricted to the lattice:

$$\hat{\delta}_{a,\mathbf{k}}(\mathbf{X}) = \frac{1}{N^3}\sum_{\mathbf{m}}\delta_a(\mathbf{x}_{\mathbf{m}}-\mathbf{X})\exp\left(-i2\pi\mathbf{k}\cdot\mathbf{m}/N\right).$$

The dependence of the Fourier coefficients on the particle position $\mathbf{X}$ (relative to the lattice) is explicitly noted. When the dependence on $\mathbf{X}$ is not explicitly noted, then we will be referring implicitly to the discrete Fourier transform of the delta function when centered on a lattice point: $\hat{\delta}_{a,\mathbf{k}} := \hat{\delta}_{a,\mathbf{k}}(\mathbf{0})$.

Continuous differentiability of δ_a (part of Assumption A3) implies the existence of a global Lipshitz constant $L_{\delta,\mathbf{k}}$ for the shift dependent Fourier coefficients of δ_a so that:

$$|\hat{\delta}_{a,\mathbf{k}}(\mathbf{y}) - \hat{\delta}_{a,\mathbf{k}}(\mathbf{x})| \leq L_{\delta,\mathbf{k}}|\mathbf{y}-\mathbf{x}|. \qquad \text{(B.1)}$$

In implementations, the δ_a depends only on the parameter a as a length scale parameter:

$$\delta_a(\mathbf{x}) = \frac{1}{a^3}\phi\left(\frac{\mathbf{x}^{(1)}}{a}\right)\phi\left(\frac{\mathbf{x}^{(2)}}{a}\right)\phi\left(\frac{\mathbf{x}^{(3)}}{a}\right), \qquad \text{(B.2)}$$

where $\phi(r)$ is a non-dimensional "shape" function for an elementary particle. Moreover, this shape function has the property that the sum of ϕ over any translate of the integer lattice is equal to one (29). From these properties of the particle representation function, we can readily derive the following asymptotics for the Fourier coefficients:

$$\hat{\delta}^*_{a,\mathbf{k}} \approx \left\{\begin{array}{ll} 1/L^3 & |\mathbf{k}| \ll L/a \\ 0 & |\mathbf{k}| \gg L/a \end{array}\right. . \qquad \text{(B.3)}$$

and also establish the existence of a constant C independent of all parameters such that:

$$|L_{\delta,\mathbf{k}}| \leq C/a.$$

Appendix C.

Table C.1
Scaling of Key Terms

$\alpha_{\mathbf{k}} \propto \mu\lvert\mathbf{k}\rvert^2/\rho L^2$	$\sum_{\mathbf{m}} \delta_a^2(\mathbf{x}_{\mathbf{m}})\Delta x^3 \propto 1/a^3$	$\sum_{\mathbf{m}} \left(\nabla\delta_a(\mathbf{x}_{\mathbf{m}})\right)^2 \Delta x^3 \propto 1/a^5$
$A_a \propto a^3$	$\sum_{\mathbf{k}} \hat{\delta}_{a,\mathbf{k}} \propto 1/a^3$	$\sum_{\mathbf{k}} \widehat{\nabla\delta}_{a,\mathbf{k}} \propto 1/a^4$
$B_0 \propto MF^*/\mu a$	$\sum_{\mathbf{k}} \hat{\delta}_{a,\mathbf{k}}/\lvert\mathbf{k}\rvert^2 \propto 1/aL^2$	$\sum_{\mathbf{k}} \widehat{\nabla\delta}_{a,\mathbf{k}}/\lvert\mathbf{k}\rvert^2 \propto 1/a^2L^2$
$L_F \propto MF^*/\ell_F$	$\sum_{\mathbf{k}} \hat{\delta}^2_{a,\mathbf{k}}/\lvert\mathbf{k}\rvert^2 \propto 1/aL^5$	$\sum_{\mathbf{k}} \left(\widehat{\nabla\delta}_{a,\mathbf{k}}\right)^2/\lvert\mathbf{k}\rvert^2 \propto 1/a^3L^5$
$\lvert\delta_a^*\rvert \propto 1/a^3$	$\sum_{\mathbf{k}} \hat{\delta}^2_{a,\mathbf{k}}/\lvert\mathbf{k}\rvert^4 \propto (1/L^6)$	
$L_{\delta,a} \propto 1/a^4$		

Table C.2
Parameters of the Numerical Method

Parameter	Description
k_B	Boltzmann's constant
T	Temperature
L	Period Length of Fluid Domain
μ	Fluid Dynamic Viscosity
ρ	Fluid Density
a	Effective Elementary Particle Size (approximate radius)
N	Number of Grid Points in each Dimension
M	The Number of Elementary Particles
Δt	Time Step
Δx	Space Between Grid Points L/N

Table C.3
Notational Conventions

Notation	Description
δ_a	Representation function of an immersed elementary particle of size a.
$\delta_{a,\mathbf{k}}$	The $\mathbf{k}^{th}$ Fourier coefficient of the particle representation function, as defined in Appendix B.
$\hat{\delta}^*_{a,\mathbf{k}}$	The maximum value of the $\mathbf{k}^{th}$ Fourier coefficient defined in Appendix B.
$L_{\delta,\mathbf{k}}$	The Lipschitz constant defined in B.1 of the Fourier coefficient $\delta_{a,\mathbf{k}}$ defined in Appendix B.
$L_{\delta,a}$	The Lipschitz constant of the function $\delta_a(\mathbf{x})$
$\alpha_{\mathbf{k}}$	Damping time scale of the $\mathbf{k}^{th}$ Fourier mode, defined in 2.14.
$D_{\mathbf{k}}$	Strength of the thermal forcing of the $\mathbf{k}^{th}$ Fourier mode, defined in 2.20.
$\wp^{\perp}_{\mathbf{k}}$	Incompressibility projection operator, defined in 2.17.
$\mathbf{u}_m$	Fluid velocity at the $\mathbf{m}^{th}$ grid point.
$\hat{\mathbf{u}}_k$	The $\mathbf{k}^{th}$ Fourier mode of the fluid velocity field.
$\mathbf{U}$	Smoothed fluid velocity field for elementary particles, defined in 2.10.
$\mathbf{x}_m$	Position vector of the $\mathbf{m}^{th}$ Eulerian grid point.
$\mathbf{X}^{[j]}$	Position vector of the j^{th} elementary particle.
D	The particle diffusion coefficient, defined in 6.5.
A_a	The volume of the region over which δ_a is non-zero.
$\Upsilon_{\mathbf{k}}$	Mode dependent factor in the velocity autocorrelation function, defined in A.4.
$\mathbf{f}_{\text{prt}}$	Force density arising from the immersed structures.
$\mathbf{f}_{\text{thm}}$	Force density arising from the thermal forcing.
$\hat{\mathbf{f}}_k$	The $\mathbf{k}^{th}$ Fourier mode of the force field.
F^*	The largest force acting on an individual elementary particle.
B_0	The maximum fluid velocity induced by the structural forces, defined in 4.7.
L_F	The Lipschitz constant of the structural force field, defined in 4.2.
ℓ_F	Length scale associated with the structure force: $L_F = F^*/\ell_F$.
v_{frc}	Typical particle velocity arising from the forces, $MF^*/\mu a$.
v_{thm}	Typical particle velocity arising from thermal fluctuations, $k_B T/\rho a^3$.