Systematic Reductions in the Stochastic Eulerian-Lagrangian Method for Fluid-Structure Interactions with Thermal Fluctuations

Author: Gil Tabak. *Advisor:* Paul Atzberger

May 31, 2013

Acknowledgements

I deeply thank my advisor, Paul J. Atzberger, for his help, support, and active collaboration. I could not have completed this project otherwise.

I also thank Aleksandar Donev for thoughtful comments and remarks.

Contents

1 Table of Constants

Value	Description
Υ_0	Fluid-structure momentum coupling constant.
ρ	Density of the fluid.
ℓ	Characteristic structure length-scale.
m	Excess mass of a structure.
$m_0 = \rho\ell^3$	Mass of fluid in the volume ℓ^3.
$k_B T$	Boltzmann's constant $\times$ temperature.
$\tau_v = \Upsilon_0/m$	Relaxation time-scale of the structure velocity.
$\tau_k = \sqrt{m_0\ell^2/k_B T}$	Characteristic diffusion time-scale.
$\kappa = \rho\ell^3/m = m_0/m$	Fluid-structure density ratio.
$\epsilon = \tau_v/\tau_k$	Inertial vs diffusive time-scale ratio.
$\alpha = \Phi_0/k_B T$	Scale of potential energy w.r.t. thermal energy.

2 Abstract

We are interested in the dynamics of structures immersed within a fluid, including thermal fluctuations. We present a systematic analysis in several limiting regimes of interest, including (i) the coupling between the fluid and the structure is strong or infinite (ii) the excess mass of the structures is small in comparison to that of the displaced fluid, and (iii) the hydrodynamic relaxation to a quasi-steady state occurs rapidly in comparison to the structure motion. Our derivation is based on a singular perturbation analysis of the Backward Kolmogorov equations of the stochastic process describing the dynamical system. Our description of the system is based on the Stochastic Eulerian Lagrangian Method (SELM), which describes both the fluid and structure dynamics. In order to perform the reduction, we use a dimensional analysis of the SELM equations to identify key non-dimensional groups and to characterize precisely each of the limiting physical regimes. The reduced equations offer insights to the effective behavior of the SELM equations, while avoiding rapid time-scales in the dynamics. This allows for the development of more efficient computational methods for systems of interest.

3 Background

3.1 Introduction

The focus of this work is fluid-structure interactions. This subject has many different applications. These include diverse applications like aerodynamic oscillations that occur to study airplane wings [18, 23, 16], animal locomotion such as swimming or flying [42, 34, 49], climate modeling [39, 40], and biological phenomena including the flow of blood through heart vavles [26, 47, 9] as well as the inner workings of cells [56, 48, 3]. In some examples, like living cells, the length scales are sufficiently small that thermal fluctuations have a significant contribution to the behavior of the system. This leads to phenomena like stochastic reasonance that can only occur in noisy systems [41, 24]. In such a situation, the fluctuations due to noise allows the system's configuration to alternate between multiple stable states. Such phenomena demonstrate that it may be necessary to include stochastic terms in the equations of motion to fully capture the features of the system in a predictive model.

There are many situations in which the fluid dynamics play an important role. Some specific situations are nanofluidics and microfluidics, as well as the dynamical behavior of microbiological systems [54, 33]. In addition, there are situations in which the coupling of the fluid and the structure might be the key to understanding the system. For instance, the intricate geometries and behavior of the structure may affect the fluid flow. The dynamics that lead to momentum transfer between the fluid and structure could not be captured with a model that only uses the structural degrees of freedom. One well-known example where complicated fluid dynamics result from somewhat simple interaction with a structure is the Kármán vortex street, where an alternating pattern of vortices forms in the flow around a cylindrical object [55].

Another recent example of the importance of the fluid-structure coupling was an elegent study of the locomotion of water striders [28]. It demonstrated that the insects propel themselves mostly by generating tiny vertices in the fluid, as opposed to relying on surface waves for momentum transfer. A related current area of interest is flying birds and insects, and the bio-inspired design and control of micro air vehicles (MAVs) [21, 35]. These bio-inspired projects include non-rigid (membrane) wings. The flapping motion of these wings seems to be crucial below a certain length scale, presumably because of the complicated fluid motion interacting with the structure. Such structures are difficult to study directly due to their size, so accurate and

efficient simulations are crucial.

A central difficulty arises in modeling systems with fluid-structure interactions and thermal fluctuations, which may lead to descriptions for which computational cost becomes an issue. It is therefore important to find approximate methods that capture the essential features while allowing for tractable numerical calculations.

Many computational methods have been developed to understand fluid-structure interactions. These methods include the Stochastic Immersed Boundary Method [30, 38, 4, 1, 5], Fluctuating Immersed Material Dynamics [12], Computational Fluctuating Fluid Dynamics [8], Arbitrary Lagrangian Method [53, 17, 27], Lattice Boltzmann methods [19, 20], and Accelerated Stokesian Dynamics [7, 10]. In particular, some recent work focused on including thermal fluctuations into such methods. In our approach, we will use the Stochastic Eulerian Lagrangian Method (SELM) as a framework, which generalizes Immersed Boundary Methods. This will allow to incorporate thermal fluctuations in our system that preserve detailed balance and agree with the Bolzmann statistics in quasi-steady equilibrium. Such features are important in accurately preserving the underlying physics of the dynamical system.

One central issue this work will address is the coupling between the fluid and the structure. In many cases of interest, a traditional treatment would require solving for the boundary conditions of the fluid and the structure. This assumption is often made due to agreement with experimental results in many situations, although there are systems where other conditions may be more appropriate [33, 22]. Imposing a condition like no-slip may be difficult in general because these boundary conditions may be complex for structures of interest.

Frameworks like SELM may not explicitly impose boundary conditions, but instead impose drag on both using a coupling operator. Unfortunately, imposing a no-slip or weak-slip condition would require strong coupling, which introduces stiffness to the dynamical equations. Our approach is to use the timescale separation that results from the "fast" coupling (the relaxation timescale of fluid-structure momentum transfer) and the other timescales in the system for an asymptotic analysis. The result is a reduced system that approximates the behavior of the original system in the limit of large timescale separation. We are able to obtain a reduced system to first order in the small parameter. The leading order represents the no-slip behavior, while the small-parameter term represents the slip. In practice, where only the no-slip condition is important, it may sometimes be useful to use only the leading-order term. In this case, the

small-parameter term can be used for error estimation. Further, we will explore the results in the limit when the excess mass is negligible to that of the displaced fluid, and obtain results that agrees with previous work based on Itō calculus [2].

Our approach utilizes a generic framework and thus generalizes many of the previous techniques, while also allowing for possible extensions. Importantly, we present our reduction procedure systematically, so that the same approach may be used for other similar frameworks. In particular, we demonstrate how to reduce "fast" degrees of freedom that follow an Ornstein-Uhlenbeck process. We also demonstrate how our procedure may be used to further reduce the system of consideration in the limit of high viscosity, while incorporating conditions like incompressibility.

Our analysis relies on writing the Backward Kolmogorov equation (BKE) and using an asymptotic reduction, similar to [38, 36, 40]. These methods are rigorously established in [44, 32].

3.2 Navier-Stokes Equation for the Fluid

We will use the Eulerian coordinate system to describe the fluid. We will denote the Eulerian coordinates by $\mathbf{x}$.

For an incompressible Newtonian fluid [14], the equation of motion is

$$\rho \frac{d\mathbf{u}}{dt} = \rho \left(\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} \right) = -\nabla p + \mu \nabla^2 \mathbf{u} + \mathbf{f} \tag{1}$$

Here, $\mathbf{u} = \mathbf{u}(\mathbf{x}, t)$ is the velocity field of the fluid, $-\nabla p$ is the stress due to the pressue in the fluid, $\mu \nabla^2 \mathbf{u}$ is the viscjosity present in the fluid, and $\mathbf{f}$ represents other forces on the fluid. μ is the dynamic viscosity, which is constant for Newtonian fluids. We will assume the fluid density ρ is constant.

We can interpret pressure p as the Lagrangian multiplier corresponding to the incompressibility constraint $\nabla \cdot \mathbf{u} = 0$. This will be useful since we will be able to impose the incompressibility condition after the asymptotic reduction is complete.

In practice, a numerical method like Chorin's projection method [13] should be used to simulate the behavior of the system. In this method, the Hodge decomposition is used to separate $d\mathbf{u}/dt$

into a divergence-free and curl-free components. An intermediate fluid velocity is calculated using the all terms but the pressure gradient. From the incompressibility condition, a Poisson equation for the new pressure can be constructed and the new pressure can be extracted. The new velocity field, which is divergence-free, can be recovered from the pressure.

3.3 Generic Formulation: Eulerian-Lagrangian Descriptions

Here, we begin the discussion the SELM framework we will use to model fluid-strucutre interactions based on [2]. In this section, we leave out thermal fluctuations. This can be interpreted as the behavior of the model in the zero diffusion limit, or more intuitively in the zero temperature limit. We will return to thermal fluctuations later. We will motivate our approach later when considering the immersed boundary method.

We would like to be able to use both the Eulerian reference frame and a Lagrangian reference frame to describe the dynamics of the fluid and some structure, respectively. We will use $\mathbf{X}(t)$ to describe the configuration of the structure, and define the velocity of the structure $\mathbf{v} = d\mathbf{X}/dt$. Notice this treatment allows us to use any generalized set of coordinates that may be convenient to describe the structure (throughout the paper, we assume the configuration variable is N-dimensional).

We will use linear operators $\Gamma, \Lambda, \Upsilon$ to model the fluid-structure coupling. The Γ operator describes how a structure depends on the fluid flow while Λ is used to attribute a spatial location for the viscous interactions between the structure and fluid. $-\Upsilon$ is a negative definite dissipative operator describing the viscous interactions coupling the structure to the fluid in the structure configuration space. We assume throughout that this dissipative operator is symmetric, $\Upsilon = \Upsilon^T$.

The linear operators are assumed to have dependence only on the configuration degrees of freedom $\Gamma = \Gamma[\mathbf{X}]$, $\Lambda = \Lambda[\mathbf{X}]$. We assume further that Υ does not have any dependence on $\mathbf{X}$.

Later, we will further discuss restrictions on the operators Γ and Λ that are sufficient for energy conservation in the appropriate limiting regimes.

Using λ and ζ for the Lagrangian constraints on the fluid and structure, and $\mathcal{L}$ for the dissipative operator in the fluid, we may write

$$\rho \frac{d\mathbf{u}}{dt} = \mathcal{L}\mathbf{u} + \Lambda[\Upsilon(\mathbf{v} - \Gamma\mathbf{u})] + \lambda \tag{2}$$

$$m\frac{d\mathbf{v}}{dt} = -\Upsilon\left(\mathbf{v} - \Gamma\mathbf{u}\right) - \nabla_{\mathbf{X}}\Phi[\mathbf{X}] + \zeta \tag{3}$$

$$\frac{d\mathbf{X}}{dt} = \mathbf{v}. \tag{4}$$

To account for the mechanics of structures, $\Phi[\mathbf{X}]$ denotes the potential energy of the configuration $\mathbf{X}$. The total energy associated with this fluid-structure system is given by

$$E[\mathbf{u}, \mathbf{v}, \mathbf{X}] = \int_\Omega \frac{1}{2}\rho|\mathbf{u}(\mathbf{y})|^2 d\mathbf{y} + \frac{1}{2}m\mathbf{v}^2 + \Phi[\mathbf{X}]. \tag{5}$$

The first two terms give the kinetic energy of the fluid and structures. The last term gives the potential energy of the structures.

3.4 Conditions on Coupling Operators

As we shall discuss, it is natural to consider coupling operators Λ and Γ which are adjoint in the sense

$$\int_{\mathcal{S}} (\Gamma\mathbf{u})(\mathbf{q}) \cdot \mathbf{v}(\mathbf{q}) d\mathbf{q} = \int_\Omega \mathbf{u}(\mathbf{x}) \cdot (\Lambda\mathbf{v})(\mathbf{x}) d\mathbf{x} \tag{6}$$

for any $\mathbf{u}$ and $\mathbf{v}$. The $\mathcal{S}$ and Ω denote the spaces used to parameterize respectively the structures and the fluid. We denote such an adjoint by $\Lambda = \Gamma^T$ or $\Gamma = \Lambda^T$.

When the structure has N degrees of freedom, the integral over $\mathcal{S}$ can be written

$$\sum_i^N (\Gamma[\mathbf{X}]\mathbf{u})_i v_i = (\Gamma\mathbf{u}) \cdot \mathbf{v} \tag{7}$$

We will now show this adjoint condition has the important consequence that the fluid-structure coupling conserves energy when $\Upsilon \to \infty$ in the inviscid and zero temperature limit.

First, observe the condition on the coupling $\Upsilon \to \infty$ implies $\mathbf{v} = \Gamma\mathbf{u}$. Differentiating the energy

in time gives

$$\frac{dE}{dt} = \int_\Omega \mathbf{u} \cdot \dot{\mathbf{u}} d\mathbf{y} + m\mathbf{v} \cdot \dot{\mathbf{v}} + \nabla_{\mathbf{X}} \Phi \cdot \mathbf{v} \tag{8}$$

$$= \int_\Omega \mathbf{u} \cdot \{\Lambda[\Upsilon(\mathbf{v} - \Gamma\mathbf{u})]\} d\mathbf{y} - \mathbf{v} \cdot [\Upsilon(\mathbf{v} - \Gamma\mathbf{u})] = 0. \tag{9}$$

3.5 Example: Immersed Boundary Method

One specific instance of the formulation developed here is the immersed boundary method, which is used to model the interaction of fluids with elastic structures, such as membranes. The immersed boundary method was developed by Charles Peskin to model fluid flow in the heart [46].

We assume the structure is made of N particles. We will assume that the position of each particle is described in the Eulerian coordinate system, so that the coordinate of the i^{th} particle $\mathbf{X}_i$ is a vector with three components. call $\mathbf{v}_i = d\mathbf{X}_i/dt$. With this notation, $\mathbf{X} = [\mathbf{X}_1\ \mathbf{X}_2\ ...\ \mathbf{X}_N]^T$ is a vector of dimension $3N$. The behavior of the structure is controlled by the potential function $\Phi[\mathbf{X}]$.

To see the immersed boundary method fits our model, consider

$$\left(\Lambda[\mathbf{X}]\mathbf{v}\right)(\mathbf{x}) = \sum_i^N \delta_a(\mathbf{x} - \mathbf{X}_i)\mathbf{v}_i \tag{10}$$

$$\Gamma[\mathbf{X}](\mathbf{u}) = \left[\int_\Omega \delta_a(\mathbf{x} - \mathbf{X}_1)\mathbf{u}(\mathbf{x})d\mathbf{x}\ ...\ \int_\Omega \delta_a(\mathbf{x} - \mathbf{X}_N)\mathbf{u}(\mathbf{x})d\mathbf{x}\right]^T \tag{11}$$

In this method, δ_a is some approximation to the δ-function over a volume of radius a, called the Peskin δ-function. To understand these equations intuitively, consider a fixed structure $\mathbf{X}$. The first equation can be interpreted as follows: At the point $\mathbf{x}$, the fluid will experience the flow of nearby structure particles. The second equation has a similar interpretation: Each particle will experience the flow of nearby fluid.

We will show our choice for Λ and Γ satisfy the adjoint condition. For any $\mathbf{u}$ and $\mathbf{v}$,

$$\left(\Gamma[\mathbf{X}]\mathbf{u}\right) \cdot \mathbf{v} = \sum_i^N \left(\int_\Omega \delta_a(\mathbf{x} - \mathbf{X}_i)\mathbf{u}(\mathbf{x})d\mathbf{x}\right) \cdot \mathbf{v}_i = \int_\Omega \mathbf{u}(\mathbf{x}) \cdot \sum_i^N \delta_a(\mathbf{x} - \mathbf{X_i})\mathbf{v}_i d\mathbf{x} \tag{12}$$

$$= \int_\Omega \mathbf{u}(\mathbf{x}) \cdot \left(\Lambda[\mathbf{X}]\mathbf{v}\right)(\mathbf{x})d\mathbf{x}. \tag{13}$$

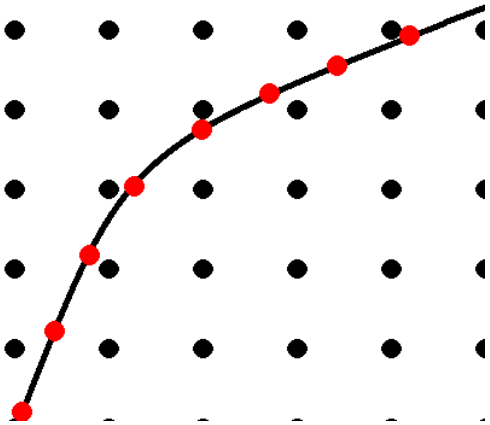

Figure 1: An Illustration of the Immsersed Boundary Method. The black dots represent points in the fluid, while the red dots represent points in the structure.

For Stokes flow in particular, we also set

$$\Upsilon = 6\pi\mu R. \tag{14}$$

Here, the R is the hydrodynamic radius of the particles in the structure. For more details see [2, 5, 46].

3.6 Thermal Fluctuations

In this paper, we are particularly interested in regimes where diffusion is important to the fluid-structure system. One application in the sciences where the study of diffusion is particularly important is cellular biology. Diffusion is known to be partially responsible for the transport of certain molecules inside of cells and between cells' interior and exterior [50], as well as the cilia or flagellum of certain microorganisms [34, 49].

We begin with an order-of-magnitude approximation to motivate physically when diffusion is important. The energy associated with a degree of freedom of a particle is k_BT by the Equipartition Theorem. By dimensional analysis, we see the speed due to diffusion alone is close to $\sqrt{k_BT/m}$. Precisely, an integration with the Boltzmann weight shows the mean of the magnitude of the velocities is $\sqrt{8k_BT/\pi m}$. For example, for a molecule of mass 10^6amu at $T = 300K$, the thermal speed is about $2m/s$.

In many microfluidics applications, diffusion will have an important role, and often will even allow for the advective term $\mathbf{u}\cdot\nabla\mathbf{u}$ to be neglected if the flow rate of the fluid is sufficiently small.

In our analysis, we will neglect the advective flow for simplicity. Effectively, the small constant is the Péclet number $Pe_L = LU/D$, where L is the characteristic length of the structure, U the advective velocity, and D the diffusion coefficient. [45]

3.7 Fluctuation-Dissipation Principle

In order to find the form of the noise terms, we will need to make certain assumptions about our system. Specifically, we will assume the noise terms are Gaussian and δ-correlated in time and have mean zero:

$$\left\langle \mathbf{f}_{\text{thm}}(t_1)\mathbf{f}_{\text{thm}}^T(t_2)\right\rangle = C\delta(t_1 - t_2) \tag{15}$$

$$\langle \mathbf{f}_{\text{thm}}(t)\rangle = 0 \tag{16}$$

In practice, a Gaussian with some small standard deviation will replace the δ-function. The above assumptions on the noise terms are inspired by the the central limit theorem. It states that the sum over many small random contributions is effectively a Gaussian. In the type of system considered here, these random contributions result from collisions due to the molecules colliding with the structure.

To find the form of C we will apply the fluctuation dissipation principle from statistical mechanics [31]. For this theorem to hold, we will also need to assume the system does not deviate far from equilibrium. This theorem states that for a system with velocity $\mathbf{v}$, mass m, a linear friction operator Υ, and noise $\mathbf{f}_{\text{thm}}$ satisfying

$$m\mathbf{v} = -\Upsilon\mathbf{v} + \mathbf{f}_{\text{thm}}, \tag{17}$$

C will have the value $2k_BT\Upsilon$.

Using similar notation as above, we will represent our system with thermal fluctuations as follows:

$$\rho\frac{d\mathbf{u}}{dt} = \mathcal{L}\mathbf{u} + \Lambda[\Upsilon(\mathbf{v} - \Gamma\mathbf{u})] + \mathbf{f}_{\text{thm}} + \lambda \tag{18}$$

$$m\frac{d\mathbf{v}}{dt} = -\Upsilon\left(\mathbf{v} - \Gamma\mathbf{u}\right) - \nabla_{\mathbf{X}}\Phi[\mathbf{X}] + \mathbf{F}_{\text{thm}} + \zeta \tag{19}$$

$$\frac{d\mathbf{X}}{dt} = \mathbf{v}. \tag{20}$$

Applying the fluctuation dissipation principle, we obtain

$$\langle \mathbf{f}_{\text{thm}}(\mathbf{x},s)\mathbf{f}^T_{\text{thm}}(\mathbf{y},t)\rangle = -(2k_BT)\,(\mathcal{L}-\Lambda\Upsilon\Gamma)\,\delta^3(\mathbf{x}-\mathbf{y})\delta(t-s) \quad (21)$$

$$\langle \mathbf{F}_{\text{thm}}(s)\mathbf{F}^T_{\text{thm}}(t)\rangle = (2k_BT)\,\Upsilon\,\delta(t-s) \quad (22)$$

$$\langle \mathbf{f}_{\text{thm}}(\mathbf{x},s)\mathbf{F}^T_{\text{thm}}(t)\rangle = -(2k_BT)\,\Lambda\Upsilon\,\phi(\mathbf{x})\delta(t-s). \quad (23)$$

Here, $\langle\phi(\mathbf{x})\phi(\mathbf{y})\rangle = \delta^3(\mathbf{x}-\mathbf{y})$. Notice that $\mathbf{f}_{\text{thm}}$ is a field in Eulerian space. We would like the noise terms to be uncorrelated in space as well as time, so we impose a spatial δ-correlation on $\mathbf{f}_{\text{thm}}$. This is important to remember in order to obtain consistency in the units, as we will see later when we non-dimensionalize the equations.

3.8 Total Momentum Formalism

Before we further discuss our tools and analysis, we will replace the field equation for the fluid with a field equation describing the total fluid-structure momentum density. This description is more convenient to work with in practice since it results in simplifications in the stochastic driving fields [2]. Primarily, the two noise terms in the stochastic differential equations involved become uncorrelated, simplifying the analysis. For this purpose we define

$$\mathbf{p}(\mathbf{x},t) = \rho\mathbf{u}(\mathbf{x},t) + \Lambda[m\mathbf{v}(t)](\mathbf{x}). \quad (24)$$

The operator Λ is used to give the distribution in space of the momentum associated with the structures for given configuration $\mathbf{X}(t)$. Using this approach, the fluid-structure dynamics are described by

$$\frac{d\mathbf{p}}{dt} = \rho^{-1}\mathcal{L}\,(\mathbf{p}-\Lambda[m\mathbf{v}]) + \Lambda[-\nabla_{\mathbf{X}}\Phi(\mathbf{X})] + (\nabla_{\mathbf{X}}\Lambda[m\mathbf{v}])\cdot\mathbf{v} + \lambda + \mathbf{g}_{\text{thm}} \quad (25)$$

$$m\frac{d\mathbf{v}}{dt} = -\Upsilon\mathbf{v} + \rho^{-1}\Upsilon\Gamma(\mathbf{p}-\mathbf{\Lambda}[\mathbf{mv}]) - \nabla_{\mathbf{X}}\Phi(\mathbf{X}) + \zeta + \mathbf{F}_{\text{thm}} \quad (26)$$

$$\frac{d\mathbf{X}}{dt} = \mathbf{v} \quad (27)$$

where $\mathbf{g}_{\text{thm}} = \mathbf{f}_{\text{thm}} + \Lambda[\mathbf{F}_{\text{thm}}]$. The third term in the first equation arises from the dependence of Λ on the configuration of the structures, $\Lambda[m\mathbf{v}] = (\Lambda[X])[m\mathbf{v}]$. The Lagrange multipliers for imposed constraints are denoted by λ, ζ. For the constraints, we use rather liberally the notation with the Lagrange multipliers denoted here not necessarily assumed to be equal to

the previous definition. The stochastic driving fields are again Gaussian with mean zero and δ-correlation in time. The stochastic driving fields have the covariance structure given by

$$\langle \mathbf{g}_{\text{thm}}(\mathbf{X}, s)\mathbf{g}^T_{\text{thm}}(\mathbf{Y}, t)\rangle = -(2k_BT)\,\mathcal{L}\,\delta^3(\mathbf{X}-\mathbf{Y})\delta(t-s) \tag{28}$$

$$\langle \mathbf{F}_{\text{thm}}(s)\mathbf{F}^T_{\text{thm}}(t)\rangle = (2k_BT)\,\Upsilon\,\delta(t-s) \tag{29}$$

$$\langle \mathbf{g}_{\text{thm}}(\mathbf{X}, s)\mathbf{F}^T_{\text{thm}}(t)\rangle = 0. \tag{30}$$

This formulation has the convenient feature that the stochastic driving fields become independent. This is a consequence of using the field for the total momentum for which the dissipative exchange of momentum between the fluid and structure no longer arises. In the equations for the total momentum, the only source of dissipation remaining occurs from the stresses of the fluid.

3.9 Itō Calculus

In order to better handle the noise terms, we will use stochastic calculus. For a rigorous introduction to the subject, see the book by Øksendal [43]. In order to proceed with the current discussion, we will summarize some important points.

First, it is possible to construct a stochastic process called (a version of) Brownian motion B_t. A stochastic process is a family of random variables parameterized in time, each a function from some probability space to Euclidean space (the position of the particle). In particular, B_t induces a probability distribution which describes a particle travelling from point x to y in time t with a probability density $p(t, x, y) = (\frac{1}{2\pi t})^{n/2} e^{-\frac{|x-y|^2}{2t}}$.

Brownian motion has the important consequence of having independent time increments, meaning two increments of B_t that do not overlap in time are uncorrelated. These are the properties make Brownian motion an ideal choice for rigorously studying the thermal fluctuations in our system.

We will describe our dynamical system using a particular stochastic process:

$$X_t = X_0 + \int_0^t b(s, X_s)ds + \int_0^t \sigma(s, X_s)dB_s \tag{31}$$

The last term above is an Itō integral, which can be constructred using

$$\int_S^T \sigma(s, X_s) dB_s = \lim_{k\to\infty} \sum_{j=0}^{k-1} \sigma(t_j, X_j) \Delta B_j. \tag{32}$$

The form we will use for the Itō process is

$$dX_t = bdt + \sigma dB_t, \text{ or } \frac{dX_t}{dt} = b + \sigma \frac{dB_t}{dt}. \tag{33}$$

In our analysis, the left-hand side of our equations will be interpreted as the left-hand side of the equation above. The term b will represent all of the deterministic terms (terms other then thermal fluctuations), and the term with σ will represent the thermal fluctuations.

3.10 Kolmogorov Theorems

We will assume here that the behavior of the system can be approximated using a finite number of degrees of freedom. It will be important in our analysis to use a description of stochastic differential equations which links their time evolution to partial differential equations. Physically, this description arises when considering the time evolution of the probability density of the system in phase space. This is closely related to the Fokker-Plank equation [25].

Define the infinitesimal generator $\mathcal{A}$ of a stochastic process X_t by

$$\mathcal{A}f(x) = \lim_{t\to 0} \frac{E^x[f(X_t)] - f(x)}{t} \tag{34}$$

The set of functions $f : \mathbb{R}^n \to \mathbb{R}$ for which the limit exists at each $x \in \mathbb{R}^n$ is denoted by $\mathcal{D}_{\mathcal{A}}$.

For the stochastic process X_t described by $dX_t = b(X_t)dt + \sigma(X_t)dB_t$ and $f \in C_0^2(\mathbb{R}^n)$, the infinitesimal operator has the form

$$\mathcal{A}f(x) = \sum_i b_i(x)\partial_{x_i} f + \frac{1}{2}\sum_{i,j} (\sigma\sigma^T)_{i,j}(x)\partial_{x_i}\partial_{x_j} f. \tag{35}$$

The same description can be achieved more rigorously using theorems from Stochastic calculus. In particular, it will be important in our analysis to use Kolmogorov's Backward Equation. It states the following [43]: suppose $f \in C_0^2(\mathbb{R}^n)$ and define $u(t, x) = E^x[f(X_t)]$, where E^x is the

expected value starting at x. Then:

a) $u(t,\cdot) \in \mathcal{D}_{\mathcal{A}}$ for all $t > 0$ and

$$\partial_t u = \mathcal{A}u \qquad \text{for } t > 0, x \in \mathbb{R}^n \tag{36}$$

$$u(0,x) = f(x) \qquad \text{for } x \in \mathbb{R}^n. \tag{37}$$

b. If $w(t,x) \in C^{1,2}(\mathbb{R} \times \mathbb{R}^n)$ is bounded and satisfies 36, 37, then $w(t,x) = u(t,x)$.

The upshot of the theorem is that the stochastic process can be essentially described by the PDE. Thus, we will be able to carry out an analysis on the PDE description to give a new infinitesimal operator which will yield a new stochastic process.

4 Dimensional Analysis and Conventions

For the SELM dynamics, it is natural to consider the time-scale on which the velocity of a particle relaxes or decorrelates. This gives the time-scale $\tau_v = m/\Upsilon_0$. The Υ_0 can be interpreted as the characteristic strength of the momentum-exchange coupling and m is the excess mass of the immersed structure. This is similar to the time-scale that often arises when considering the reduction of the Langevin equations to the Smoluchowski equations [52, 25]. Another important time-scale is the duration for a fluid parcel to move the distance ℓ when it has kinetic energy on the order $k_B T$. We define this time-scale as $\tau_k = \sqrt{m_0 \ell^2 / k_B T}$, where ℓ is a characteristic of the length scale of the fluid parcel and $m_0 = \rho \ell^3$ characterizes the mass of the fluid parcel. These scales provide a natural way to characterize the strength of the momentum-exchange. In particular, we consider the relative time-scale on which the structure momentum decorrelates in time relative to moving a significant displacement in space. For this purpose, we introduce our first non-dimensional group

$$\epsilon = \tau_v / \tau_k. \tag{38}$$

When ϵ becomes small this indicates the coupling has become strong.

To obtain a second non-dimensional group that characterizes the contributions of inertial effects, we consider the magnitude of the excess mass associated with the immersed structure. This is compared to the comparable mass of fluid that occupies a volume of comparable size to the

immersed structure. The ratio of these masses define our second non-dimensional group

$$\kappa^{-1} = m/\rho\ell^3. \tag{39}$$

We denote $m_0 = \rho\ell^3$. When κ^{-1} is small this indicates the inertia from the excess mass density of the immersed structure is negligible relative to that of the displaced fluid.

Finally, we note that the potential Φ may vary in scale depending on the application. For this reason we introduce a third timescale to characterize the potential $\Phi = \Phi_0\bar{\Phi}$,

$$\alpha = \Phi_0/k_BT. \tag{40}$$

Using this dimensional group will help separate the inertial effects due to the excess mass from the contributions due to the potential in both the Eulerian and Lagrangian frames.

We further impose the condition that $\alpha\kappa = O(1)$. As we will see, this is important in capturing the coupling forces on the structure over the forces due to the structures own potential.

By the Buckingham-Π Theorem [11] all parameters of the physical system can be expressed in terms of these three non-dimensional groups ϵ, κ^{-1}, α. For this purpose, we first express the parameters in terms of intermediate characteristic scales by :

$$t = \tau_k\bar{t}, \qquad \mathbf{X} = \ell\bar{\mathbf{X}}, \qquad \mathbf{v} = v_0\bar{\mathbf{v}} = \frac{\ell}{\tau_k}\bar{\mathbf{v}}, \tag{41}$$

$$\mathbf{p} = p_0\bar{\mathbf{p}} = \frac{m_0}{\tau_k\ell^2}\bar{\mathbf{p}}, \qquad \Lambda = \Lambda_0\bar{\Lambda} = \frac{1}{\ell^3}\bar{\Lambda}, \qquad \mathcal{L} = \mathcal{L}_0\bar{\mathcal{L}} = \frac{m_0}{\ell^3\tau_k}\bar{\mathcal{L}}. \tag{42}$$

The stochastic driving fields present some interesting considerations to obtain an appropriate non-dimensionalization. We express the stochastic terms by scalings of the form

$$\mathbf{g}_{\text{thm}}(\mathbf{X}, s) = g_0\bar{\mathbf{g}}_{\text{thm}} = g_0 D_{-\bar{\mathcal{L}}}\bar{\xi}\left(\frac{\mathbf{X}}{\ell}, \frac{s}{\tau_k}\right), \tag{43}$$

$$\mathbf{F}_{\text{thm}}(s) = F_0\bar{\mathbf{F}}_{\text{thm}} = F_0 D_{\bar{\Upsilon}}\bar{\eta}\left(\frac{s}{\tau_k}\right). \tag{44}$$

The $\bar{\xi}$ and $\bar{\eta}$ denote Gaussian random fields having mean zero and unit covariances

$$\langle\bar{\xi}(\bar{\mathbf{X}}, \bar{s})\bar{\xi}^T(\bar{\mathbf{Y}}, \bar{t})\rangle = \delta(\bar{\mathbf{X}} - \bar{\mathbf{Y}})\delta(\bar{s} - \bar{t}), \tag{45}$$

$$\langle\bar{\eta}(\bar{s})\bar{\eta}^T(\bar{t})\rangle = \delta(\bar{s} - \bar{t}). \tag{46}$$

This allows for the characteristic strengths of the stochastic driving fields to be expressed as

$$g_0{}^2 = \frac{k_B T}{\ell^3 \tau_k}\mathcal{L}_0, \qquad F_0{}^2 = \frac{k_B T}{\tau_k}\Upsilon_0, \qquad 2D_A D_A{}^T = A. \tag{47}$$

In our notation, D_A denotes the square root of the operator $\frac{1}{2}A$ which is assumed to be positive semi-definite. The D_A is an operator defined with the same domain and range as A. We also find it convenient to define at this stage the Reynold's number which is given by

$$Re = \rho \ell U/\mu \tag{48}$$

where U is a characteristic velocity scale.

4.1 Summary of Non-Dimensional Equations

The SELM equations 25– 27 can be expressed non-dimensionally using the characteristic scales introduced earlier in the section.

$$\frac{d\bar{\mathbf{p}}}{dt} = \bar{\mathcal{L}}\left(\bar{\mathbf{p}} - \kappa^{-1}\bar{\Lambda}[\bar{\mathbf{v}}]\right) + \alpha\bar{\Lambda}[-\nabla_{\bar{X}}\bar{\Phi}(\bar{\mathbf{X}})] + \kappa^{-1}\left(\nabla_{\bar{X}}\bar{\Lambda}[\bar{\mathbf{v}}]\right)\cdot\bar{\mathbf{v}} + \bar{\mathbf{g}}_{\rm thm} \tag{49}$$

$$\frac{d\bar{\mathbf{v}}}{dt} = -\frac{1}{\epsilon}\bar{\Upsilon}C_1(\bar{\mathbf{v}} - \bar{\mathbf{v}}_0) - \kappa\alpha\nabla_{\bar{X}}\bar{\Phi}(\bar{\mathbf{X}}) + \sqrt{\frac{1}{\epsilon}}\sqrt{\kappa}\bar{\mathbf{F}}_{\rm thm} \tag{50}$$

$$\frac{d\bar{\mathbf{X}}}{dt} = \bar{\mathbf{v}} \tag{51}$$

where

$$C_1 = (I + \kappa^{-1}\bar{\Gamma}\bar{\Lambda}) \tag{52}$$

$$\bar{\mathbf{v}}_0 = C_1^{-1}\bar{\Gamma}\bar{\mathbf{p}}. \tag{53}$$

The thermal fluctuations are given by the stochastic driving fields with covariances

$$\langle\bar{\mathbf{g}}_{\rm thm}(s)\bar{\mathbf{g}}^T_{\rm thm}(t)\rangle = -2\bar{\mathcal{L}}\,\delta(t-s) \tag{54}$$

$$\langle\bar{\mathbf{F}}_{\rm thm}(s)\bar{\mathbf{F}}^T_{\rm thm}(t)\rangle = 2\bar{\Upsilon}\,\delta(t-s) \tag{55}$$

$$\langle\bar{\mathbf{g}}_{\rm thm}(s)\bar{\mathbf{F}}^T_{\rm thm}(t)\rangle = 0. \tag{56}$$

As discussed in Section 4.2, the constraints are handled implicitly throughout. Our assumption $\kappa\alpha = O(1)$ is made to guarantee that the potential term in 50 contributes at order one.

4.2 Handling Constraints : Incompressibility and Solenoidal Decomposition

The structure equations depend on the total momentum field $\mathbf{p}$ only through $\mathbf{u} = \mathbf{p} - \Lambda[m\mathbf{v}]$ which is constrained to be solenoidal (incompressible). As a consequence, if we apply the operator $\mathscr{P}$ that projects any field to its solenoidal part we have $\mathbf{u} = \mathscr{P}\mathbf{u} = \mathscr{P}\mathbf{p} - \mathscr{P}\Lambda[m\mathbf{v}]$. This well-known approach for expressing the incompressibility of hydrodynamic equations [13] yields the following closed set of equations for SELM

$$\begin{aligned}
\frac{d(\mathscr{P}\mathbf{p})}{dt} &= \mathscr{P}\left[\rho^{-1}\mathcal{L}\left(\mathbf{p} - \Lambda[m\mathbf{v}]\right) + \Lambda[-\nabla_{\mathbf{X}}\Phi(\mathbf{X})] + (\nabla_{\mathbf{X}}\Lambda[m\mathbf{v}])\cdot\mathbf{v} + \mathbf{g}_{\text{thm}}\right] && (57)\\
m\frac{d\mathbf{v}}{dt} &= -\Upsilon\mathbf{v} + \rho^{-1}\Upsilon\Gamma\mathscr{P}(\mathbf{p} - \Lambda[m\mathbf{v}]) - \nabla_{\mathbf{X}}\Phi(\mathbf{X}) + \mathbf{F}_{\text{thm}} && (58)\\
\frac{d\mathbf{X}}{dt} &= \mathbf{v}. && (59)
\end{aligned}$$

We remark that only the dynamics of $\mathscr{P}\mathbf{p}$ need be explicitly retained, since the non-solenoidal components play no role in the fluid-structure dynamics. The equations take the same identical form as equations 25–27 when making the substitutions

$$\tilde{\mathbf{p}} = \mathscr{P}\mathbf{p}, \qquad \tilde{\mathcal{L}} = \mathscr{P}\mathcal{L}, \qquad \tilde{\Lambda} = \mathscr{P}\Lambda, \qquad \tilde{\Gamma} = \Gamma\mathscr{P}. \tag{60}$$

Similarly, the covariance structure of $\mathbf{g}_{\text{thm}}$ takes the same form when making these substitutions. Consequently, to avoid clutter in the notation, we shall not explicitly distinguish the incompressible case when carrying out the reductions. Instead, the procedure outlined above shall be assumed throughout the paper. We remark that the presentation can also be simplified with respect to the constraint terms for the microstructures. These can be handled readily by simply using an appropriate choice of generalized coordinates obeying the constraints. Again, we shall not explicitly distinguish this case and instead simply utilize this convention throughout the paper.

In practice, the fluid-structure dynamics given by equations 25 – 27 can exhibit a broad range of spatial/temporal scales. In the case of well-separated time-scales we shall aim to derive effective dynamical equations in terms of only those degrees of freedom and dynamics that evolve on the

slower time-scales. Such reduced equations are useful both in gaining insights into the physics of such fluid-structure interactions when subject to thermal fluctuations and in the development of efficient computational methods simulations. To characterize these important dynamical scales and different limiting physical regimes, we perform a dimension analysis of the SELM equations.

4.3 Other Conventions

Since $\bar{\eta}(\cdot)$ and $\bar{\xi}(\bar{\mathbf{X}}, \cdot)$ are Gaussian processes with 0 mean and δ-correlation, we are technically using the mathematical objects

$$\bar{\eta}(\bar{t}) = \frac{dB_{\bar{t}}}{d\bar{t}}, \qquad \bar{\xi}(\bar{\mathbf{X}}, \bar{t}) = \phi(\bar{\mathbf{X}}) \frac{dB_{\bar{t}}^{(\bar{\mathbf{X}})}}{d\bar{t}}, \tag{61}$$

where

$$\langle \phi(\bar{\mathbf{X}}) \phi^T(\bar{\mathbf{Y}}) \rangle = \delta^3(\bar{\mathbf{X}} - \bar{\mathbf{Y}}). \tag{62}$$

This gurantees that the terms have the required properties, since the distributions of Wiener process are Gaussian and δ-correlated in time [43]. Above, the superscript $\bar{\mathbf{X}}$ distinguishes the different Weiner processes at each spatial point.

For the purposes of our analysis, we will approximate $\mathbf{p}$ as a function of a finite number of spatial points. However, since the number of points we use is arbitrary, the dynamics of the system may be approximated arbitrarily well, assuming the system is sufficiently well-behaved.

Moreover, during our analysis we will use the convention $\mathbf{p} = \mathbf{p}(t)$. We can establish an implicit spatial dependence of $\mathbf{p}$ by using a greater dimension for the range of $\mathbf{p}$. For example, if we would like to use N points, we could use $\mathbf{p}_i^k(t)$ where k = 1, ..., N corresponds to the spatial point and i is the corresponding component of $\mathbf{p}$ at each point.

With the new convention, there is no need to include ϕ because of our discretization scheme. Thus the noise due to $\mathbf{g}_{\text{thm}}$ can be labeled as $D_{-\mathcal{L}} \frac{d\hat{B}_t}{dt}$.

5 Summary of Results

This gives an overview of the SELM formalism and the associated stochastic differential equations. We remark that each of these regimes were motivated by a rather specific limit. Non-dimensional analysis of the equations can also be carried out and other limits considered to motivate working with such reduced equations.

For the purpose of summarizing some of the useful results, we present the reduced equations with dimensions.

The first regime we consider corresponds to the case when the coupling strength becomes strong for the momentum-exchange between the immersed structures and the fluid. This corresponds to the limit $\epsilon \to 0$. We summarize the leading order behavior in this section, as well as the first order terms in ϵ that result from the reduction. For the leading order terms, we then consider the case when the the immersed structures have an excess mass density that becomes small relative to the surrounding fluid. This corresponds to the limit $\kappa^{-1} \to 0$. Finally, we consider the case when in response to stresses the hydrodynamics relax rapidly relative to the motions of the microstructures. This corresponds to the small Reynold's number limit $Re \to 0$. Next, we give a summary of our results for the effective equations in each of these physical regimes. We then provide our detailed perturbation analysis and derivations of each of these equations in Section 6 and Section 7.

5.1 Limit of Strong Coupling : Summary of Reduced Equations

In the limit $\epsilon \to 0$ the fluid and the microstructures become strongly coupled and momentum is exchanged rapidly. In terms of the physical parameters this occurs when the momentum coupling parameter satisfies $\Upsilon_0 >> \sqrt{m_0 k_B T/\ell^2}$. In this regime we obtain the effective inertial dynamics

$$\begin{aligned} \frac{d\mathbf{p}}{dt} &= \rho^{-1}\mathcal{L}\left(\mathbf{p} - \Lambda[m\mathbf{v}_0]\right) - \Lambda\nabla_{\mathbf{X}}\Phi(\mathbf{X}) + \left(\nabla_{\mathbf{X}}\Lambda[m\mathbf{v}_0]\right)\cdot\mathbf{v}_0 \\ &+ k_B T\nabla_{\mathbf{X}}\Lambda : C_1^{-1} + \lambda + \mathbf{g}_{\text{thm}} + \theta_p \qquad (63) \\ \frac{d\mathbf{X}}{dt} &= \mathbf{v}_0 + \theta_X. \qquad (64) \end{aligned}$$

In the notation, the double dot product should be interpreted as $\partial_{X_k}\Lambda_{ij}(C_1^{-1})_{jk}$. The $\mathbf{v}_0$ denotes the effective velocity of the microstructures to leading order

$$\mathbf{v}_0 = \rho^{-1}C_1^{-1}\Gamma\mathbf{p} \tag{65}$$

$$C_1 = I + \rho^{-1}m\Gamma\Lambda. \tag{66}$$

The thermal fluctuations are taken into account through the Gaussian stochastic driving field $\mathbf{g}_{\text{thm}}$ with mean zero and covariance

$$\langle \mathbf{g}_{\text{thm}}(s)\mathbf{g}_{\text{thm}}^T(t)\rangle = -(2k_BT)\,\mathcal{L}\,\delta(t-s). \tag{67}$$

The θ terms represent higher-order terms at the next order in ϵ. For the strong coupling limit they capture the leading order correction from slip effects between the fluid and structures in this regime. These terms could be useful in capturing the permeation of fluid through a structure within the fluid such as a porous membrane. These terms are given explicitly in section 7.2.

5.2 Strong Coupling Limit: Reduced Equations in Terms of Effective Fluid Velocity $\mathbf{u}$

The effective fluid velocity field $\bar{\mathbf{u}}$ is obtained from the total momentum field $\mathbf{p}$ by

$$\bar{\mathbf{u}} = \rho^{-1}\left(\mathbf{p} - \Lambda[m(\mathbf{v}_0 + \theta_X)]\right). \tag{68}$$

The $\mathbf{v}_0$ is given in Section 5.1 and θ_X is given in Section 7.2. The effective fluid-structure dynamics are

$$\rho\frac{d\bar{\mathbf{u}}}{dt} = \mathcal{L}\bar{\mathbf{u}} + k_BT\nabla_{\mathbf{X}}\Lambda : C_1^{-1} - \Lambda\frac{d}{dt}[m\mathbf{v}_0] - \Lambda\nabla_{\mathbf{X}}\Phi(\mathbf{X}) + \theta_p + \lambda + \mathbf{g}_{\text{thm}} \tag{69}$$

$$\frac{d\mathbf{X}}{dt} = \mathbf{v}_0 + \theta_X = \Gamma\bar{\mathbf{u}} + C_1\theta_X \tag{70}$$

and

$$\langle \mathbf{g}_{\text{thm}}(s)\mathbf{g}_{\text{thm}}^T(t)\rangle = -(2k_BT)\,\mathcal{L}\,\delta(t-s). \tag{71}$$

The $\mathbf{v}_0$ can be interpreted as the effective velocity of the microstructures

$$\mathbf{v}_0 \quad = \quad \Gamma\bar{\mathbf{u}} + \rho^{-1} m \Gamma\Lambda\theta_X. \tag{72}$$

The higher-order correction due to the fluid slip is given by θ_X of Section 7.2. These equations were obtained by using the following terms that can be differentiated and combined to yield

$$(\nabla_{\mathbf{X}}\Lambda[m\mathbf{v}_0]) \cdot \mathbf{v}_0 - \frac{d}{dt}(\Lambda[m\mathbf{v}_0]) \tag{73}$$

$$= (\nabla_{\mathbf{X}}\Lambda[m\mathbf{v}_0]) \cdot \mathbf{v}_0 - (\nabla_{\mathbf{X}}\Lambda[m\mathbf{v}_0]) \cdot \mathbf{v}_0 - \Lambda\frac{d}{dt}[m\mathbf{v}_0] = \Lambda\frac{d}{dt}[m\mathbf{v}_0]. \tag{74}$$

We remark that the effective fluid equations 69 capture the hydrodynamic response to shear stresses within the fluid, structure related body forces, and the inertia of the immersed microstructures. The stochastic fields yield the thermal fluctuations. Interestingly, there are also higher order inertial effects that arise for a finite ϵ (non-infinite Υ) from the weakly permitted slip of a structure relative to the background fluid flow. This latter term can be thought of as the momentum response to an applied body force to a microstructure, for detailed expressions see Section 7.2.

Another interesting feature of the analysis is that it had to be performed using the total momentum density field (as opposed to directly on the fluid velocity field). This has the nice feature that the noise is decoupled between the Eulerian and Lagrangian frames. This has the important consequence that the fluid velocity does not behave as an appropriate "slow variable" in the strong coupling limit. Instead it is the total momentum density that serves the role of a suitable "slow variable." We found it a bit curious and counter-intuitive that after such an analysis we can again express the reduced equations in terms of the fluid velocity $\bar{\mathbf{u}}$. What should be realized is that while the instantaneous fluid velocity degrees of freedom were inadequate in the reduction analysis, upon performing the limit, their interpretation takes on a slightly different meaning as a consequence of subtle features of the averaging that was performed. In fact, this subtle point that the mathematical analysis systematically handles, can indeed be understood intuitively. In particular, one should realize that the fluid velocity $\bar{\mathbf{u}}$ attributed from $\mathbf{p}$ in equation 68 should no longer be viewed as the "instantaneous" fluid velocity. Instead, one should view it intuitively as an effective fluid velocity obtained by appropriately averaging over

an intermediate time-scale that is larger than the momentum exchange time-scale but shorter than the other dynamical time-scales. We can view our transformation to the total momentum density field and our systematic reduction analysis as a precise way to take just such a limit.

The fluid-structure equations 69– 72 greatly simplify in the limit when the excess body mass becomes negligible relative to the displaced fluid.

5.3 Limit of Negligible Excess Mass : Summary of Reduced Equations

When the excess mass associated with the microstructure relative to the local displaced fluid is small, this corresponds to the limit $\kappa \to \infty$, see equation 39. We approach this limit when the excess mass parameter satisfies $m << \rho\ell^3$. This results in the reduced fluid-structure equations

$$\begin{aligned}
\rho\frac{d\mathbf{u}}{dt} &= \mathcal{L}\mathbf{u} - \Lambda\nabla_{\mathbf{X}}\Phi(\mathbf{X}) + k_BT\nabla_{\mathbf{X}}\cdot\Lambda + \lambda + \theta_p + \mathbf{f}_{\text{thm}} && (75)\\
\frac{d\mathbf{X}}{dt} &= \Gamma\mathbf{u} + \theta_X && (76)\\
\left\langle \mathbf{f}_{\text{thm}}(t)\mathbf{f}_{\text{thm}}(s)^T \right\rangle &= -2k_BT\mathcal{L}\delta(t-s). && (77)
\end{aligned}$$

A derivation of these equations is given in Section 7.4.

In this limit, the inertial terms in equations 69– 70 disappear. This is very similar to the physical regime that is treated by the *Stochastic Immersed Boundary Method* (SIB) in [5]. However, the systematic reduction analysis we perform here in Section 7.1 shows that there is an important drift term that is missing in the original SIB formulation [5]. This corresponds to the term $k_BT\nabla_{\mathbf{X}}\Lambda : C_1^{-1}$ in equation 69 which becomes when $m = 0$ the term $k_BT\nabla_{\mathbf{X}}\cdot\Lambda$ in equation 75. This important drift term arises from the generalized coordinates (non-conjugate configuration and momentum in the Hamiltonian sense) that is used to describe the mechanics of the fluid-structure system. The consequence of this is that within the phase-space there is an induced metric factor in the generalized Louiville theorem for the dynamical system, see [2].

We remark that in the zero excess mass limit with $m = 0$ there is no longer a distinction between formulating the equations of motion in terms of the total momentum field or the fluid velocity equations since $\mathbf{p} = \rho\mathbf{u}$. Approximate fluid-structure methods, such as the Immersed Boundary

Method [46] treat precisely this physical regime. Our results suggest that in the mechanics we should interpret the immersed structures in the IB approach as assumed to be effectively density matched with that of the surrounding fluid flow so that the excess mass $m = 0$. Furthermore, any inertial effects of the immersed structures are modeled through the effective kernel functions involved in the velocity averaging / force-spreading and arise from the corresponding dynamics of the overlapping local fluid elements [46, 2, 5]. To model further inertial effects of structures, some recent extensions of IB have been introduced in [29, 6].

5.4 Limit of Rapid Hydrodynamic Relaxation : Summary of Reduced Equations

We consider the regime where the hydrodynamics rapidly equilibrate to a quasi-steady state in response to body forces. This corresponds to the limit when the Reynold's number $Re = \rho \ell U/\mu \ll 1$ is small. In terms of the fluid viscosity this requires μ is large in the sense $\mu >> \rho \ell U$. The ρ is the fluid density. The U is a characteristic velocity and ℓ a characteristic length-scale associated with the microstructures. We consider the case when the limit $\epsilon \to 0$ taken, so that slip corrections are neglected. This results in the reduced equations

$$\frac{d\mathbf{X}}{dt} = H_{\text{SELM}}[-\nabla_{\mathbf{X}}\Phi(\mathbf{X})] + (\nabla_{\mathbf{X}} \cdot H_{\text{SELM}})k_B T + \mathbf{h}_{\text{thm}} \tag{78}$$

$$H_{\text{SELM}} = \Gamma(\mathscr{P}\mathcal{L})^{-1}\Lambda \tag{79}$$

$$\langle \mathbf{h}_{\text{thm}}(s), \mathbf{h}^T_{\text{thm}}(t) \rangle = 2k_B T H_{\text{SELM}} \delta(t-s). \tag{80}$$

We define $\mathcal{L} = \mu\Delta$. In this regime the fluid degrees of freedom are eliminated entirely and replaced by the effective hydrodynamic coupling tensor H_{SELM}. Interestingly, the metric factors arising in the inertial regime from the generalized fluid-structure coordinates used for the description of the mechanical system manifests as the term $(\nabla_{\mathbf{X}} \cdot H_{\text{SELM}})k_B T$. This drift-divergence term is essential for the microstructure dynamics to have invariant the Gibbs-Boltzmann distribution with detailed balance.

6 Stochastic Reduction Method : Singular Perturbation of Backward Kolmogorov Equations

I would especially like to thank Paul J. Atzberger for his substantial contribution to this section.

We derive the reduced equations using a method based on a singular perturbation analysis of the Backward-Kolmogorov Equations (BKE) [38, 40, 32, 44]. See section 3.10 for a statement of the theorem. In the case of strong coupling, we use the process $\mathbf{Z}(t) = (\mathbf{X}(t), \mathbf{p}(t), \mathbf{v}(t))$, where the process starts as $\mathbf{Z}(0) = \mathbf{z}$. In particular, consider the stochastic process satisfying

$$d\mathbf{Z}(t) = \mathbf{a}(\mathbf{Z}(t))dt + \mathbf{b}(\mathbf{Z}(t))d\mathbf{W}_t. \tag{81}$$

The corresponding infinitesimal generator is

$$\mathcal{A} \quad = \quad \mathbf{a} \cdot \frac{\partial}{\partial \mathbf{z}} + \frac{1}{2}\mathbf{b}\mathbf{b}^T : \frac{\partial^2}{\partial \mathbf{z}^2}. \tag{82}$$

We shall use this to obtain the reduction by performing a singular perturbation analysis of the BKE to yield a limiting form for the infinitesimal generator $\tilde{\mathcal{A}} = \tilde{\mathbf{a}} \cdot \partial/\partial \mathbf{z} + \frac{1}{2}\tilde{\mathbf{b}}\tilde{\mathbf{b}}^T : \partial^2/\partial \mathbf{z}^2$. This determines a reduced stochastic process $\tilde{\mathbf{Z}}(t)$ satisfying $d\tilde{\mathbf{Z}}(t) = \tilde{\mathbf{a}}(\tilde{\mathbf{Z}}(t))dt + \tilde{\mathbf{b}}(\tilde{\mathbf{Z}}(t))d\tilde{\mathbf{W}}_t$ which approximates the full stochastic dynamics of equation 81. We remark that a distinct advantage of using the BKE over the Fokker-Planck Equations (FPE) is that our approximation will not be required to satisfy additional constraints, such as ensuring the equation conserves the total probability density. The adjoint of an approximated FPE differential operator is not always a valid infinitesimal generator. In contrast when making approximations of the BKE, the obtained second order differential operator has the plausible form for an infinitesimal generator [43].

To obtain a specific limiting regime, we require that terms be identified that split the dynamics of the infinitesimal generator into "slow" and "fast" parts

$$\mathcal{A}_\epsilon = L_{slow} + L_{fast}. \tag{83}$$

As the notation suggests, the splitting is meant to separate the degrees of freedom of the system into two classes $\mathbf{z} = (\mathbf{z}_s, \mathbf{z}_f)$. The $\mathbf{z}_s$ are those that exhibit relatively "slow" temporal dynamics.

The $\mathbf{z}_f$ are those degrees of freedom that exhibit relatively "fast" temporal dynamics. The L_{slow} contains only the terms of the infinitesimal generator that involves derivatives with respect to the "slow" degrees of freedom. Similarly, the L_{fast} contains only the terms governing the "fast" degrees of freedom. These notions are defined more precisely for the SELM dynamics in Section 7.

This splitting provides a useful stationary probability distribution $\Psi(\mathbf{z}_f|\mathbf{z}_s)$ for the "fast" degrees of freedom $\mathbf{Z}_f(t)$ when evolving under dynamics with the "slow" degrees of freedom held fixed $\mathbf{Z}_s = \mathbf{z}_s$. This is given by solving the steady-state FPE for the fast degrees of freedom which can be expressed using the adjoint of the generator as a solution of

$$L_2^*\Psi = 0 \tag{84}$$

$$\int \Psi d\mathbf{z}_f = 1. \tag{85}$$

More precisely, we shall consider in our analysis for the "fast" degrees of freedom generators of the general form

$$L_{fast} = \frac{1}{\epsilon}\left(L_2 + \epsilon\tilde{L}_2\right). \tag{86}$$

The L_2 represents the leading order contribution to the generator L_{fast} and is used to determine the invariant distribution Ψ. Often we have $\tilde{L}_2 = 0$, but as we shall discuss, for many cases of interest this term is non-zero making an interesting contribution to the reduced effective stochastic dynamics.

For the "slow" degrees of freedom, we find it convenient to split the generator as

$$L_{slow} = \bar{L}_1 + L_1 \tag{87}$$

where

$$\bar{L}_1 = \int \Psi(\mathbf{z}_f|\mathbf{z}_s) L_{slow} d\mathbf{z}_f \tag{88}$$

$$L_1 = L_{slow} - \bar{L}_1. \tag{89}$$

This splitting ensures that L_1 generates a stochastic process having mean zero. As we shall

discuss, if $\bar{L}_1$ is a non-zero operator then it captures the leading order dynamics. The L_1 then contributes at the next order. These conventions allow for the infinitesimal generator to be expressed as

$$\begin{aligned} \mathcal{A}_\epsilon &= \bar{L}_1 + \epsilon L_\epsilon & (90) \\ L_\epsilon &= \frac{1}{\epsilon}\left(L_1 + \tilde{L}_2\right) + \frac{1}{\epsilon^2} L_2. & (91) \end{aligned}$$

As we shall show, the operator L_ϵ contributes effectively as order one in the limit $\epsilon \to 0$ and hence the scaling and notation chosen.

To make this more precise, we perform the perturbation using the expansion

$$u(\mathbf{z}, t) = u_0(\mathbf{z}, t) + u_1(\mathbf{z}, t)\epsilon + u_2(\mathbf{z}, t)\epsilon^2 \cdots + u_n(\mathbf{z}, t)\epsilon^n + \cdots . \quad (92)$$

We shall seek ultimately a partial differential equation (BKE) for the first two orders

$$\bar{u}(\mathbf{z}_s, t) = u_0(\mathbf{z}_s, t) + \bar{u}_1(\mathbf{z}_s, t)\epsilon \quad (93)$$

where $\bar{u}_1(\mathbf{z}_s, t) = \int \Psi(\mathbf{z}_f|\mathbf{z}_s) u_1(\mathbf{z}, t) d\mathbf{z}_f$. By comparing orders when plugging equation 92 into the BKE given by $\frac{\partial}{\partial t} = \mathcal{A}_\epsilon$ and using 90 we obtain

$$\begin{aligned} O\left(\epsilon^{-1}\right) : L_2 u_0 &= 0 & (94) \\ O\left(1\right) : \frac{\partial u_0}{\partial t} &= \bar{L}_1 u_0 + L_1 u_0 + \tilde{L}_2 u_0 + L_2 u_1 & (95) \\ O\left(\epsilon\right) : \frac{\partial u_1}{\partial t} &= \bar{L}_1 u_1 + L_1 u_1 + \tilde{L}_2 u_1 + L_2 u_2. & (96) \end{aligned}$$

We assume throughout that the stochastic process generated by L_2 is ergodic on the space of $\mathbf{z}_f$ so that $\dim \ker\{L_2^*\} = 1$. The order $O\left(\epsilon^{-1}\right)$ can be interpreted as the steady-state of the Backward-Kolmogorov equation of a stochastic process $\hat{\mathbf{Z}}_f(t)$ generated by L_2. This suggests that $u_0(\mathbf{z}) = \lim_{t\to\infty} E^{\mathbf{z}}\left[f(\hat{\mathbf{Z}}_f(t)\right] = E^{\mathbf{z}_s}\left[f(\hat{\mathbf{Z}}_f)\right] = u_0(\mathbf{z}_s)$, where $\hat{\mathbf{Z}}_f(t)$ is the process started with $\hat{\mathbf{Z}}_f(t) = \mathbf{z}_f$. By ergodicity the long-term behavior of $\hat{\mathbf{Z}}_f(t)$ would be independent of the initial condition and the latter expectation is to be taken with respect to Ψ satisfying equation 84. This gives that $u_0 = u_0(\mathbf{z}_s)$ with the only dependence on $\mathbf{z}_s$. Throughout we take u_0 only depending on $\mathbf{z}_s$ which ensures the order $O\left(\epsilon^{-1}\right)$ is always satisfied since L_2 only involves derivatives with respect to $\mathbf{z}_f$. The order $O\left(1\right)$ can be used to solve for u_1 in terms of

u_0 by

$$L_2 u_1 \quad = \quad \frac{\partial u_0}{\partial t} - \bar{L}_1 u_0 - L_1 u_0. \tag{97}$$

We used that $\tilde{L}_2 u_0 = 0$ since $u_0 = u_0(\mathbf{z}_s)$ and $\tilde{L}_2$ only involves derivatives in $\mathbf{z}_f$. The solvability of equation 97 requires the right-hand side of the equation be in the range of the operator L_2. A well known condition for this is that the right-hand side be orthogonal to all elements of the null-space of L_2^*. In other words, the $\overline{\text{range}\{L_2\}} = \overline{\text{ker}\{L_2^*\}^\perp}$, where $\perp$ denotes the orthogonal compliment of a set under the standard L^2-inner product, see [51]. By our ergodicity assumption the kernel only has one dimension and the solvability can be represented by the condition

$$\int \Psi \left(\frac{\partial}{\partial t} - \bar{L}_1 - L_1 \right) d\mathbf{z}_f u_0 = 0. \tag{98}$$

The Ψ is the stationary probability density satisfying equation 84. This yields the BKE for the leading order

$$\frac{\partial u_0}{\partial t} = \bar{L}_1 u_0. \tag{99}$$

This follows since by definition $\int \Psi L_1 d\mathbf{z}_f = 0$ and the $\bar{L}_1 = \int \Psi \bar{L}_1 d\mathbf{z}_f$ since it has already been averaged with respect to the probability distribution. The condition for the existence of the solution u_1 in the asymptotic expansion expressed in equation 97 provides the equation 99 for the leading order u_0. Using equation 97, the order u_1 can be expressed as

$$u_1 \quad = \quad L_2^{-1} \left(\frac{\partial u_0}{\partial t} - (\bar{L}_1 + L_1) u_0 \right) = -L_2^{-1} L_1 u_0. \tag{100}$$

The final expression comes from the relationship of the partial derivative $\partial u_0 / \partial t$ and the operator $\bar{L}_1$ given by equation 99. Now at the order $O(\epsilon)$ a very similar argument can be made to ensure the solvability of u_2. This yields

$$\frac{\partial \bar{u}_1}{\partial t} \quad = \quad - \int \Psi \left(\bar{L}_1 + L_1 + \tilde{L}_2 \right) L_2^{-1} L_1 d\mathbf{z}_f u_0 \tag{101}$$

where $\bar{u}_1(\mathbf{z}_s, t) = \int \Psi(\mathbf{z}_f | \mathbf{z}_s) u_1(\mathbf{z}, t) d\mathbf{z}_f$. This provides a closed set of differential equations for the first two orders u_0, $\bar{u}_1$ approximating the solution of the BKE in the $\epsilon \to 0$ limit, see equations 99 and 101.

It is convenient to express this approximation by deriving a set of closed equations for $\bar{u} = u_0 + \epsilon \bar{u}_1$. We have that

$$\frac{\partial \bar{u}}{\partial t} = \bar{L}_1 u_0 + \epsilon \left(- \int \Psi \left(\bar{L}_1 + L_1 + \tilde{L}_2 \right) L_2^{-1} L_1 d\mathbf{z}_f \right) u_0. \tag{102}$$

To express this in terms of $\bar{u}$ it is useful to notice that

$$\bar{u} = \left(\mathcal{I} - \epsilon \int \Psi L_2^{-1} L_1 d\mathbf{z}_f \right) u_0. \tag{103}$$

By inverting this operator and expanding to leading orders in ϵ we have

$$u_0 = \left(\mathcal{I} + \epsilon \int \Psi L_2^{-1} L_1 d\mathbf{z}_f + \epsilon^2 (\cdots) + \cdots \right) \bar{u} \tag{104}$$

By neglecting orders greater than ϵ we have

$$\bar{L}_1 u_0 \quad = \quad \bar{L}_1 \bar{u} + \epsilon \bar{L}_1 \int \Psi L_2^{-1} L_1 d\mathbf{z}_f \bar{u}. \tag{105}$$

This gives the final set of closed reduced equations

$$\frac{\partial \bar{u}}{\partial t} \quad = \quad \left(\bar{L}_1 + \epsilon \bar{L}_0 \right) \bar{u} \tag{106}$$

$$\bar{L}_0 \quad = \quad - \int \Psi \left(L_1 + \tilde{L}_2 \right) L_2^{-1} L_1 d\mathbf{z}_f. \tag{107}$$

This follows by using equation 105 in equation 102 and canceling common terms. This derivation provides a unified expression consistent with the methods used in [37, 38, 40] and the rigorous results obtained in [32, 44]. This provides a BKE with generator $\tilde{\mathcal{A}} = \bar{L}_1 + \epsilon \bar{L}_0$ approximating the full BKE of the system. Interestingly, the term L_ϵ of equation 91 is approximated in the final set of equations by $\bar{L}_0$ which contributes only as order one in ϵ, "$L_\epsilon \to \bar{L}_0$." The operator $\tilde{\mathcal{A}}$ provides the infinitesimal generator for the reduced stochastic process $\tilde{\mathbf{Z}}(t)$ approximating the full stochastic process $\mathbf{Z}(t)$ given by equation 81. The equations 106 and 107 establishes our systematic reduction procedure to approximate the full stochastic dynamics.

7 Derivation of the Non-Dimensional Reduced Equations

The details are now presented for the derivation of the various reduced equations in the different limits of strong coupling, small body excess mass, and rapid hydrodynamic relaxation. These regimes are identified precisely through non-dimensionalization of the equations and definition of precise non-dimensional groups. The reduced equations are obtained by decomposing the infinitesimal generator into fast and slow components and applying the singular perturbation analysis presented in Section 6. A central challenge is to compute the effective averaged infinitesimal generator which involves inversion of the fast component operator L_2. We identify an appropriate decomposition and show how to perform inversion of L_2 to obtain an explicit expression for the reduced equation in each regime.

7.1 Limit of Strong Coupling : Derivation of Reduced Equations

We derive the reduced equations in the regime when the coupling for the momentum exchange between the fluid and the microstructures becomes strong $\epsilon \to 0$. In this regime the momentum coupling parameter satisfies $\Upsilon_0 >> \sqrt{m_0 k_B T/\ell^2}$, see equation 38. This corresponds to the physical regime where the momentum exchange between the fluid and microstructure degrees of freedom occurs rapidly. This reduction eliminates this rapid time-scale from the dynamics of the fluid-structure system.

7.1.1 Splitting of the Infinitesimal Generator into Slow and Fast Parts

To handle the infinitesimal generator in this regime, it is very useful to make the change of variable in the velocity $\tilde{\mathbf{v}} = \mathbf{v} - \mathbf{v_0}$. Specifically, we define

$$\mathbf{v}_0 = C_1^{-1}\Gamma\mathbf{p} \tag{108}$$

$$C_1 = (I + \kappa^{-1}\Gamma\Lambda). \tag{109}$$

It will be convenient to introduce

$$C = \kappa^{-1}C_1. \tag{110}$$

This serves to center up to terms of order ϵ the equation 50 and allows for the equations to be put into the convenient form

$$\frac{d\mathbf{p}}{dt} = \mathcal{L}\left(\mathbf{p} - \kappa^{-1}\Lambda[\mathbf{v}]\right) + \alpha\Lambda[-\nabla_X\Phi(\mathbf{X})] + \kappa^{-1}\left(\nabla_X\Lambda[\mathbf{v}]\right)\cdot(\mathbf{v}) + \mathbf{g}_{\text{thm}} \tag{111}$$

$$\frac{d\tilde{\mathbf{v}}}{dt} = \frac{d\mathbf{v}}{dt} - \frac{d\mathbf{v_0}}{dt} = -\frac{1}{\epsilon}\Upsilon C_1\tilde{\mathbf{v}} + \sqrt{\frac{1}{\epsilon}}\sqrt{\kappa}\mathbf{F}_{\text{thm}} - \alpha\kappa\nabla_X\Phi(\mathbf{X}) - \nabla_{\mathbf{X},\mathbf{p}}\mathbf{v_0}\cdot\frac{d}{dt}(\mathbf{X},\mathbf{p}) \tag{112}$$

$$\frac{d\mathbf{X}}{dt} = \mathbf{v}. \tag{113}$$

The infinitesimal generator of this fluid-structure system is split into the parts

$$\mathcal{A} = L_{slow} + L_{fast} \tag{114}$$

where

$$L_{slow} = \left[\mathcal{L}\left(\mathbf{p} - \kappa^{-1}\Lambda[\mathbf{v}]\right) + \alpha\Lambda[-\nabla_{\mathbf{X}}\Phi(\mathbf{X})] + \kappa^{-1}\left(\nabla_{\mathbf{X}}\Lambda[\mathbf{v}]\right)\cdot\mathbf{v}\right]\cdot\nabla_{\mathbf{p}} \tag{115}$$

$$-\mathcal{L} : \nabla^2_{\mathbf{p}} + \mathbf{v}\cdot\nabla_{\mathbf{X}} \tag{116}$$

$$L_{fast} = [-\Upsilon C_1\tilde{\mathbf{v}}]\cdot\nabla_{\tilde{\mathbf{v}}} + \kappa\Upsilon : \nabla^2_{\tilde{\mathbf{v}}} - \alpha\kappa\nabla_{\mathbf{X}}\Phi(\mathbf{X})\cdot\nabla_{\tilde{\mathbf{v}}} - \mathcal{A}\left[\nabla_{\mathbf{X},\mathbf{p}}\mathbf{v_0}\cdot\frac{d}{dt}(\mathbf{X},\mathbf{p})\right]. \tag{117}$$

The slow degrees of freedom are identified as $\mathbf{z}_s = (\mathbf{X},\mathbf{p})$ and the fast degrees of freedom as $\mathbf{z}_f = \tilde{\mathbf{v}}$.

We split further the fast operator

$$L_{fast} = L_2 + \tilde{L}_2 \tag{118}$$

with

$$L_2 = [-\Upsilon C_1\tilde{\mathbf{v}}]\cdot\nabla_{\tilde{\mathbf{v}}} + \kappa\Upsilon : \nabla^2_{\tilde{\mathbf{v}}} \tag{119}$$

$$\tilde{L}_2 = -\alpha\kappa\nabla_{\mathbf{X}}\Phi(\mathbf{X})\cdot\nabla_{\tilde{\mathbf{v}}} - \mathcal{A}\left[\nabla_{\mathbf{X},\mathbf{p}}\mathbf{v_0}\cdot\frac{d}{dt}(\mathbf{X},\mathbf{p})\right]. \tag{120}$$

The Einstein summation convention for repeated indices is used throughout. We denote by $A : B = A_{ij}B_{ij}$. The notation $\mathcal{A}\left[\nabla_{\mathbf{X},\mathbf{p}}\mathbf{v_0}\cdot\frac{d}{dt}(\mathbf{X},\mathbf{p})\right]$ is introduced to denote compactly the terms of the infinitesimal generator associated with the $\nabla_{\mathbf{X},\mathbf{p}}\mathbf{v_0}\cdot\frac{d}{dt}(\mathbf{X},\mathbf{p})$ contribution in the $\tilde{\mathbf{v}}$ equations. The $\tilde{L}_2$ will be expressed more explicitly later. For now, we remark that because of

the stochastic contribution of the term $d\mathbf{p}/dt$, the differential operator $\tilde{L}_2$ when fully expressed is second order in $\tilde{\mathbf{v}}$.

In the perturbation analysis, it is sufficient to know L_2 to determine the stationary probability distribution satisfying equation 84 for the fast degrees of freedom.

$$\Psi(\tilde{\mathbf{v}}) = \frac{\sqrt{\det C}}{(2\pi)^{N/2}} \exp\left[-\frac{1}{2}\tilde{\mathbf{v}}^T C \tilde{\mathbf{v}}\right]. \tag{121}$$

This is a Gaussian distribution. The C is given in equation 110. The N denotes the number of degrees of freedom for a configuration of the microstructures. This solution intuitively corresponds to the Gibbs-Boltzmann distribution of $\mathbf{z}_f$ when holding the $\mathbf{z}_s$ degrees of freedom fixed, see Section 6.

We split further the slow operator by

$$L_{slow} = \bar{L}_1 + L_1 \tag{122}$$

with

$$\begin{aligned} \bar{L}_1 &= \left(\mathcal{L}(\mathbf{p} - \kappa^{-1}\Lambda\mathbf{v}_0) + \nabla_{\mathbf{X}}\Lambda : C_1^{-1} + \kappa^{-1}(\nabla_{\mathbf{X}}\Lambda[\mathbf{v}_0]) \cdot \mathbf{v}_0 - \alpha\Lambda\nabla_{\mathbf{X}}\Phi(\mathbf{X})\right) \cdot \nabla_{\mathbf{p}} \quad (123) \\ &+ \mathbf{v}_0 \cdot \nabla_{\mathbf{X}} - \mathcal{L} : \nabla^2_{\mathbf{p}} \\ L_1 &= L_{slow} - \bar{L}_1. \quad (124) \end{aligned}$$

The $\bar{L}_1$ is obtained by averaging L_{slow} with respect to Ψ. This splits the operator into a part L_1 that averages to zero and a part $\bar{L}_1$ that may have a non-zero average. The presented splittings into "slow" and "fast" parts provide the required decomposition of the infinitesimal generators for our perturbation analysis.

We remark that the $\bar{L}_1$ operator describes the leading order dynamics for strong-coupling case considered. That is, the no-slip dynamics may already be recovered from $\bar{L}_1$ without determining the next-order terms. The next-order dynamics will be captured by the L_0 term given by 107.

7.1.2 Generic Formulation for Inverting the L_2 Operator

To obtain the reduced stochastic process including the ϵ-order term, we must determine the operator

$$L_0 = -\int \Psi(L_1 + \tilde{L}_2)L_2^{-1}L_1 d\mathbf{z}_f. \tag{125}$$

An often challenging step in determining L_0 is to perform the inverse of L_2 to find $w = -L_2^{-1}L_1u_0$. While in simple cases the resulting equation $L_2w = -L_1u_0$ can be solved directly, we take a more general approach

We use that L_2 has the form

$$L_2 \;=\; -(\Upsilon C\tilde{\mathbf{v}})_i\frac{\partial}{\partial\tilde{v}_i} + \Upsilon_{ij}\frac{\partial^2}{\partial\tilde{v}_i\partial\tilde{v}_j}.$$

This can be put into an even more convenient form by choosing a change of basis for the velocity vector $\tilde{\mathbf{v}}$ so that the matrices diagonalize and the operator is the sum $L_2 = \sum_i L_2^{(i)}$ where $L_2^{(i)}$ only involves independently the i^{th} coordinate of velocity. For this purpose, we introduce the change of variable $\boldsymbol{\alpha} = C^{1/2}\tilde{\mathbf{v}}$, where the square root $C^{1/2}$ is ensured to exist since C is symmetric and positive semi-definite. This allows us to express the operator as

$$L_2 \;=\; A_{nm}\left(-\alpha_m\partial_{\alpha_n} + \partial_{\alpha_m}\partial_{\alpha_n}\right) \tag{126}$$

$$A \;=\; C^{1/2}\Upsilon C^{1/2}. \tag{127}$$

Since A is symmetric there is a unitary operator Q for a a change of basis that diagonalizes the operator to yield $D = Q^TAQ$ with $D_{ij} = \delta_{ij}d_i$, $\boldsymbol{\beta} = Q^T\boldsymbol{\alpha}$. This gives

$$L_2 \;=\; \sum L_2^{(i)} \tag{128}$$

$$L_2^{(i)} \;=\; d_i\left(-\beta_i\partial_{\beta_i} + \partial_{\beta_i}^2\right). \tag{129}$$

We remark that the cumulative change of variable used is $\boldsymbol{\beta} = Q^TC^{1/2}\tilde{\mathbf{v}}$. We find it convenient also to introduce $\hat{Q} = C^{-1/2}Q$. Now we will see how this change of variable will allow us to invert L_2.

We recall the Hermite equation $-up'(\beta) + p''(\beta) = -\lambda p(\beta)$, whose eigenfunctions are the (prob-

abilists') Hermite polynomials $He_\lambda(\beta)$ with eigenvalues λ corresponding to the degree of the polynomial. We see that for each i, the Hermite polynomials $He_\lambda(\beta_i)$ are eigenfunctions of $L_2^{(i)}$ with eigenvalues λD_i. Thus $\Pi_k He_{\lambda_k}(\beta_k)$ is an eigenfunction of L_2 with eigenvalue $-\sum_k \lambda_k D_k$. Moreover, any non-trivial product $\Pi_k He_{\lambda_k}(\beta_k)$ (i.e. at least some $\lambda_k \neq 0$), is in $\mathcal{R}(L_2)$, since its corresponding eigenvalue is non-zero.

Next, we will see that any polynomial $p(\beta)$ that satisfies the solvability condition $\overline{p(\beta)} = 0$ can be written as a sum of non-trivial polynomials of the form $\Pi_k He_{\lambda_k}(\beta_k)$. Consider the vector space $\mathcal{V}_1$ of such polynomials up to degree M. The solvability condition on p determines exactly one dimension, since a constant can be added to any polynomial to satisfy the solvability condition.

Let $\mathcal{V}_2$ be the vector space generated by linear combinations of non-trivial polynomials of degree up to M of the form $\Pi_k He_{\lambda_k}(\beta_k)$. Since the non-trivial Hermitian polynomials are orthogonal to constants, the non-triviality condition on the elements in $\mathcal{V}_2$ implies they satisfy the solvability condition $\overline{\Pi_k He_{\lambda_k}(\beta_k)} = 0$. Thus $\mathcal{V}_2$ is a subspace of $\mathcal{V}_1$. We see $\dim \mathcal{V}_1 = \sum_{d=1}^{M} \binom{N+d-1}{d} = \dim \mathcal{V}_2$, so we conclude $\mathcal{V}_1 = \mathcal{V}_2$. Thus we can express $p(\beta)$ as a linear combination of non-trivial terms $\Pi_k He_{\lambda_k}(\beta_k)$. In practice, Gaussian elimination could be used to write $p(\beta)$ in this form, starting with the highest-degree monomials and working downwards.

Now, since a non-trivial term $\Pi_k He_{\lambda_k}(\beta_k)$ is an eigenfunction of L_2, we see

$$L_2^{-1}[\Pi_k He_{\lambda_k}(\beta_k)] = -\left[\sum_k \lambda_k D_k\right]^{-1} \Pi_k He_{\lambda_k}(\beta_k). \tag{130}$$

Thus, noting L_2^{-1} is linear, the change of basis allows us to find $L_2^{-1} p(\beta)$.

For convenience, we list here the first few Hermite Polynomials

$$H_0(\beta) = 1 \tag{131}$$

$$H_1(\beta) = \beta \tag{132}$$

$$H_2(\beta) = \beta^2 - 1. \tag{133}$$

A few useful inversion formulas of which we shall make use include

$$L_2^{-1}\beta_i = -D_{ij}^{-1}\beta_j = -d_i^{-1}\beta_i \tag{134}$$

$$L_2^{-1}\beta_i\beta_j = -\left(d_i + d_j\right)^{-1}\beta_i\beta_j, \quad i \neq j \tag{135}$$

$$L_2^{-1}\left(\beta_i^2 - 1\right) = -(2d_i)^{-1}\left(\beta_i^2 - 1\right). \tag{136}$$

In some of the calculations it is helpful to use the tensor notation $D_{ij}^{-1} = d_i^{-1}\delta_{ij}$ and to combine equation 135 and 136 to obtain

$$L_2^{-1}\left(\beta_i\beta_j - \delta_{ij}\right) = -\left(d_i + d_j\right)^{-1}\left(\beta_i\beta_j - \delta_{ij}\right) = -E_{ij}\left(\beta_i\beta_j - \delta_{ij}\right) \tag{137}$$

where $E_{ij} = (d_i + d_j)^{-1}$.

7.1.3 Representation of the Operators under the Change of Variable for Strong Coupling

To succinctly carry-out the calculation of the effective infinitesimal generator, it is helpful to introduce some notation for the change of variable we use from $\tilde{\mathbf{v}}$ to $\boldsymbol{\beta}$. To summarize the notation we introduced so far we had

$$A \equiv C^{1/2}\Upsilon C^{1/2}, \tag{138}$$

$$D = Q^T A Q \text{ (Q unitarily diagonalizes A)}, \tag{139}$$

$$\hat{Q} \equiv C^{1/2}Q, \text{ so that } D = \hat{Q}^T\Upsilon\hat{Q} \tag{140}$$

$$\boldsymbol{\beta} \equiv \hat{Q}^T\tilde{\mathbf{v}}. \tag{141}$$

To account for the drift contributions to the slow variable in a form amenable to Hermite polynomials of order 0, 1, and 2 we introduce respectively

$$T \equiv \mathbf{v}_0 \boxtimes \left[\mathcal{L}\left(\mathbf{p} - \kappa^{-1}\Lambda[\mathbf{v}_0]\right) - \alpha\Lambda[\nabla_X\Phi(\mathbf{X})] + \nabla_{\mathbf{X}}\Lambda : C_1^{-1} + \kappa^{-1}(\nabla_{\mathbf{X}}\Lambda[\mathbf{v}_0])\cdot\mathbf{v}_0\right] \tag{142}$$

$$R \equiv \mathcal{I}_{N\times N} \boxtimes B, \quad \text{with} \tag{143}$$

$$B \equiv \kappa^{-1}\left[-\mathcal{L}\Lambda(\cdot) + (\nabla_{\mathbf{X}}\Lambda(\cdot))\cdot\mathbf{v}_0 + \nabla_{\mathbf{X}}(\Lambda\mathbf{v}_0)\cdot(\cdot)\right] \tag{144}$$

$$S \equiv 0_{N\times N\times N} \boxtimes \kappa^{-1}\nabla_{\mathbf{X}}\Lambda. \tag{145}$$

The notation $\boxtimes$ is introduced to "glue-together" two tensors along the first index, so that for A_{ijk} with $1 \leq i \leq N$ and B_{ijk} with $1 \leq i \leq M$ we define the new tensor $C = A \boxtimes B$ by $C_{ijk} = A_{ijk}$ when $1 \leq i \leq N$ and $C_{ijk} = B_{(i-N)jk}$ when $N+1 \leq i \leq N+M$. We call $\boxtimes$ the "glue-product." The $0_{N\times N\times N}$ denotes a 3-tensor of zeros and $\mathcal{I}_{N\times N}$ the identity 2-tensor. The order of coordinates in 145 is understood to be $(\nabla_{\mathbf{X}}\Lambda)_{ijk} = \partial_{X_k}\Lambda_{ij}$. It will be useful in $\tilde{L}_2$ to introduce the modified noise term

$$V \quad = 0_{N\times N} \boxtimes -C_1^{-1}\Gamma\mathcal{L}\Lambda C_1^{-1}. \tag{146}$$

where $0_{N\times N}$ denotes a 2-tensor of zeros. Here, C_1 is the same as in 109. We also use

$$\mathbf{y} \equiv \mathbf{z_s} = (\mathbf{X}, \mathbf{p}). \tag{147}$$

This allows for the slow operator of equation 124 to be expressed succinctly as

$$L_1 \quad = \quad \left[R_{ij}\tilde{v}_j + S_{ijk}(\tilde{v}_k\tilde{v}_j - \overline{\tilde{v}_k\tilde{v}_j})\right]\frac{\partial}{\partial y_i}. \tag{148}$$

Ultimately, this operator will be expressed in terms of a change of variable from $\tilde{\mathbf{v}}$ to $\boldsymbol{\beta}$. This makes it useful to make also the change of variable for R and S, which is given by

$$\hat{R}_{ij} = R_{ik}\hat{Q}_{kj} \qquad\qquad \hat{S}_{ijk} = S_{ilm}\hat{Q}_{lj}\hat{Q}_{mk}. \tag{149}$$

We then have for the fast operator an expression in terms of $\boldsymbol{\beta}$

$$L_1 \quad = \quad \left[\hat{R}_{ij}\beta_j + \hat{S}_{ijk}(\beta_k\beta_j - \delta_{kj})\right]\frac{\partial}{\partial y_i} = L_1^{(1)} + L_1^{(2)} \quad \text{where} \tag{150}$$

$$L_1^{(1)} \quad = \quad \hat{R}_{ij}\beta_j\frac{\partial}{\partial y_i}, \qquad L_1^{(2)} = \hat{S}_{ijk}(\beta_k\beta_j - \delta_{kj})\frac{\partial}{\partial y_i}. \tag{151}$$

In the interest of computing the $\mathcal{A}[\nabla_{\mathbf{y}}\mathbf{v}_0 \cdot \frac{d\mathbf{y}}{dt}]$ appearing in $\tilde{L}_2$, it is useful to express

$$\frac{d\mathbf{y}}{dt} \quad = \quad U(\tilde{\mathbf{v}}) + \mathbf{g}_{\text{thm}}, \quad \text{with} \tag{152}$$

$$U(\tilde{\mathbf{v}}) \quad = \quad T_i + R_{ij}\tilde{v}_j + S_{ijk}(\tilde{v}_k\tilde{v}_j - \overline{\tilde{v}_k\tilde{v}_j}) \tag{153}$$

$$\langle \mathbf{g}_{\text{thm}}(s), \mathbf{g}_{\text{thm}}^T(t)\rangle \quad = \quad 0_{N\times N} \boxtimes -2\mathcal{L}\delta(t-s). \tag{154}$$

This allows for the fast operator to be expressed in terms of $\boldsymbol{\beta}$ as

$$\begin{aligned}
\tilde{L}_2 &= \left[-\alpha\kappa\nabla_{\mathbf{X}}\Phi(\mathbf{X}) - \nabla_{\mathbf{y}}\mathbf{v_0}\cdot U(\tilde{\mathbf{v}}) \right]\cdot\nabla_{\tilde{\mathbf{v}}} - V : \Delta^2_{\tilde{\mathbf{v}}} && (155)\\
&= \left[-\alpha\kappa\nabla_{\mathbf{X}}\Phi(\mathbf{X}) - \nabla_{\mathbf{y}}\mathbf{v_0}\cdot U(\tilde{\mathbf{v}}) \right]\cdot\hat{Q}\nabla_{\boldsymbol{\beta}} - \hat{Q}^T V\hat{Q} : \Delta^2_{\boldsymbol{\beta}} && (156)\\
&= \left[\tilde{T}_i + \tilde{R}_{ij}\beta_j + \tilde{S}_{ijk}(\beta_k\beta_j - \delta_{kj}) \right]\cdot\nabla_{\boldsymbol{\beta}} + \tilde{V} : \Delta^2_{\boldsymbol{\beta}}. && (157)
\end{aligned}$$

In these expressions we define

$$\begin{aligned}
\tilde{T} &= \hat{Q}^T(-\alpha\kappa\nabla_{\mathbf{X}}\Phi(\mathbf{X}) - \nabla_{\mathbf{y}}\mathbf{v_0}\cdot T) && (158)\\
\tilde{R} &= \hat{Q}^T(-\nabla_{\mathbf{y}}\mathbf{v_0}\cdot R) && (159)\\
\tilde{S} &= \hat{Q}^T(-\nabla_{\mathbf{y}}\mathbf{v_0}\cdot S) && (160)\\
\tilde{V} &= -\hat{Q}^T V\hat{Q}. && (161)
\end{aligned}$$

We take the convention that the dot products above are all taken between the first components in the gradient terms and the R, S, and T tensors. We further take the convention that each Q^T multiplies along the first component index of the tensor.

Finally, we split $\tilde{L}_2$ for convenience in later integral expressions into several components that each involve a different degree polynomial in $\boldsymbol{\beta}$. We label these using the convention that a derivative contributes "negatively" to the degree while a variable in $\boldsymbol{\beta}$ contributes "positively" to the degree. This gives the decomposition

$$\tilde{L}_2 = \sum \tilde{L}_2^{(i)} \qquad (162)$$

with

$$\begin{aligned}
\tilde{L}_2^{(-2)} &= \tilde{V}_{ij}\partial^2_{\beta_{ij}} & \tilde{L}_2^{(-1)} &= \tilde{T}_i\partial_{\beta_i}\\
\tilde{L}_2^{(0)} &= \tilde{R}_{ij}\beta_j\partial_{\beta_i} & \tilde{L}_2^{(1)} &= \tilde{S}_{ijk}(\beta_k\beta_j - \delta_{kj})\partial_{\beta_i}. && (163)
\end{aligned}$$

These conventions provide useful notation to succinctly express the consequences of the change of variable from $\tilde{\mathbf{v}}$ to $\boldsymbol{\beta}$.

7.1.4 Computing the Effective Infinitesimal Generator for Strong Coupling

To obtain the effective infinitesimal generator $\bar{L} = \bar{L}_1 + \epsilon L_0$ we must still compute $L_0 = -\int \Psi(L_1 + \tilde{L}_2)L_2^{-1}L_1 d\mathbf{z}$. We start by expressing the probability distribution Ψ from equation 121 in terms of the variable $\boldsymbol{\beta}$ and use the associated Jacobian to obtain

$$\Psi(\boldsymbol{\beta}) = (2\pi)^{-N/2} \exp\left[-\frac{1}{2}\boldsymbol{\beta}^2\right]. \tag{164}$$

To determine the operator is useful to split into the parts $L_0 = \sum_{ij} I_{ij} + \sum_{ij} J_{ij}$ with

$$I_{ij} = -\int \Psi(\boldsymbol{\beta}) L_1^{(i)} L_2^{-1} L_1^{(j)} d\boldsymbol{\beta} \tag{165}$$

$$J_{ij} = -\int \Psi(\boldsymbol{\beta}) \tilde{L}_2^{(i)} L_2^{-1} L_1^{(j)} d\boldsymbol{\beta}. \tag{166}$$

The operators $L_1^{(i)}$ and $\tilde{L}_2^{(i)}$ are defined in equations 150 and 163. In practice, the terms I_{11} and I_{22} are the only I_{ij} needed to determine L_0 since the $I_{ij} = 0$ when $i \neq j$. This is a consequence of odd degree monomials in β averaging to zero under the probability distribution. Similarly, the only terms J_{ij} that are non-zero and needed to determine L_0 are $J_{-2,2}, J_{0,2}, J_{-1,1}, J_{1,1}$.

A useful feature of our decomposition is that the operators involve terms that are at most a degree two multinomial in the variables β_i. From the inversion formulas established in equations 134– 136 and the decomposition of L_1 we have

$$I_{11} = -\int_{\mathbb{R}^N} \psi(\beta) \hat{R}_{nm} \beta_m \partial_{y_n} L_2^{-1} [\hat{R}_{ij} \beta_j \partial_{y_i}] d\beta \tag{167}$$

$$= \int_{\mathbb{R}^N} \psi(\beta) \hat{R}_{nm} \beta_m \partial_{y_n} [\hat{R}_{ij} D_{jk}^{-1} \beta_k \partial_{y_i}] d\beta = \hat{R}_{nk} D_{jk}^{-1} \partial_{y_n} [\hat{R}_{ij} \partial_{y_i}]. \tag{168}$$

We used the specific inversion formula 134 to obtain that $L_2^{-1}[\hat{R}_{ij}\beta_j\partial_{y_i}] = [\hat{R}_{ij}D_{jk}^{-1}\beta_k\partial_{y_i}]$. We can reverse the change of variable to express this in terms of the original variables $(\mathbf{X}, \mathbf{p})$ as

$$I_{11} = R_{nr} C_{rs}^{-\frac{1}{2}} Q_{sk} D_{jk}^{-1} \partial_{y_n} [R_{ip} C_{pq}^{-\frac{1}{2}} Q_{qj} \partial_{y_i}] = R_{nr} \Upsilon_{rp}^{-1} \partial_{y_n} [R_{ip} \partial_{y_i}] \tag{169}$$

$$= R_{nr} \Upsilon_{rp}^{-1} R_{pi}^T \partial^2_{y_n y_i} + \Upsilon_{np}^{-1} [\partial_{X_n} B_{ip}] \partial_{p_i} \tag{170}$$

$$= (R\Upsilon^{-1}R^T) : \nabla^2_{\mathbf{y}} + [(\nabla_{\mathbf{X}} B) : \Upsilon^{-1}] \cdot \nabla_{\mathbf{p}} \tag{171}$$

$$= \Upsilon^{-1} : \nabla^2_{\mathbf{X}} + (B\Upsilon^{-1}B^T) : \nabla^2_{\mathbf{p}} + [(\nabla_{\mathbf{X}} B) : \Upsilon^{-1}] \cdot \nabla_{\mathbf{p}}. \tag{172}$$

To obtain this result, we used that R is a function of $\mathbf{X}$ but not $\mathbf{p}$. We also used that the first N rows of R are constant (and correspond to $\mathcal{I}$). The B is defined in equation 144.

We next compute I_{22}. From equation 145, we denote $\hat{S}_{ijk} = S_{imn}\hat{Q}_{mj}\hat{Q}_{nk}$. To avoid confusion in the notation for the indices m and n, we denote this sum explicitly. This gives

$$I_{22} = -\int_{\mathbb{R}^N} \psi(\beta) L_1^{(2)} L_2^{-1} L_1^{(2)} d\beta \tag{173}$$

$$= -\int_{\mathbb{R}^N} \psi(\beta) \hat{S}_{ijk}(\beta_j\beta_k - \delta_{jk})\partial_{y_i} L_2^{-1}[\hat{S}_{lmn}(\beta_m\beta_n - \delta_{mn})\partial_{y_l}] d\beta \tag{174}$$

$$= \int_{\mathbb{R}^N} \psi(\beta) \hat{S}_{ijk}(\beta_j\beta_k - \delta_{jk})\partial_{y_i} \left[\sum_{mn} \hat{S}_{lmn} E_{mn}(\beta_m\beta_n - \delta_{mn})\partial_{y_l}\right] d\beta \tag{175}$$

$$= \sum_{mn} \hat{S}^{(2)}_{ijk}\hat{S}^{(2)}_{lmn} E_{mn} \int_{\mathbb{R}^N} \psi(\beta)(\beta_j\beta_k - \delta_{jk})\left[(\beta_m\beta_n - \delta_{mn})\right] d\beta \partial^2_{p_i p_l}. \tag{176}$$

The inversion formula 137 was used to obtain $L_2^{-1}(\beta_m\beta_n - \delta_{mn}) = E_{mn}(\beta_m\beta_n - \delta_{mn})$. Another important point to mention is that $\hat{S}_{ijk}$ only yields non-zero terms when $i > N$. This follows since the indices with $i < N$ involve contributions to the $\mathbf{X}$ equations which are zero and were represented using our glue-product in equation 145. For this reason it is convenient to use the notation for $\hat{S}$ above, $A^{(2)}_{ijk} = A_{(i-N)jk}$ for $i > N$.

To integrate the expressions against Ψ, we find it useful to introduce an integration by parts in the variable β_j

$$\int_{\mathbb{R}^N} \psi(\beta)\beta_j\beta_k\beta_m\beta_n d\beta \tag{177}$$

$$= \frac{1}{(2\pi)^{N/2}} \int_{\mathbb{R}^{N-1}} \left(\int_{\mathbb{R}} \beta_j e^{-\frac{1}{2}\beta_j^2} \beta_k\beta_m\beta_n d\beta_j\right) e^{-\frac{1}{2}\sum_{a\neq j}\beta_a^2} d\beta^{/j} \tag{178}$$

$$= \frac{1}{(2\pi)^{N/2}} \int_{\mathbb{R}^N} e^{-\frac{1}{2}\beta_j^2} \partial_{\beta_j}(\beta_k\beta_m\beta_n) d\beta_j e^{-\frac{1}{2}\sum_{a\neq j}\beta_a^2} d\beta^{/j} \tag{179}$$

$$= \delta_{jk}\delta_{mn} + \delta_{jm}\delta_{kn} + \delta_{jn}\delta_{km}. \tag{180}$$

The $d\beta^{/j} = d\beta_1 \cdots d\beta_{j-1} d\beta_{j+1} \cdots d\beta_N$ denotes the differential excluding dw_j. Using this result we obtain

$$\int_{\mathbb{R}^N} \psi(\beta)(\beta_j\beta_k - \delta_{jk})(\beta_m\beta_n - \delta_{mn}) d\beta \tag{181}$$

$$= \delta_{jk}\delta_{mn} + \delta_{jm}\delta_{kn} + \delta_{jn}\delta_{km} - 2\delta_{jk}\delta_{mn} + \delta_{jk}\delta_{mn} \tag{182}$$

$$= \delta_{jm}\delta_{kn} + \delta_{jn}\delta_{km}. \tag{183}$$

This yields

$$I_{22} = \sum_{mn} \hat{S}^{(2)}_{ijk} \hat{S}^{(2)}_{lmn} E_{mn} (\delta_{jm}\delta_{kn} + \delta_{jn}\delta_{km}) \partial^2_{p_i p_l} \tag{184}$$

$$= \sum_{mn} (\hat{S}^{(2)}_{imn} \hat{S}^{(2)}_{lmn} + \hat{S}^{(2)}_{imn} \hat{S}^{(2)}_{lnm}) E_{mn} \partial^2_{p_i p_l}. \tag{185}$$

Since the terms $\partial^2_{p_i p_l} = \partial^2_{p_l p_i}$ are equal we can write the differential operator as

$$I_{22} = \sum_{mn} (\hat{S}^{(2)}_{imn} \hat{S}^{(2)}_{lmn} + \frac{1}{2} \hat{S}^{(2)}_{imn} \hat{S}^{(2)}_{lnm} + \frac{1}{2} \hat{S}^{(2)}_{lmn} \hat{S}^{(2)}_{inm}) E_{mn} \partial^2_{p_i p_l}. \tag{186}$$

This gives $\frac{1}{2} A_{il} \partial^2_{p_i p_l}$ with a tensor A that is symmetric in the indices i, l. This allows for the operator to be expressed as

$$I_{22} = \frac{1}{2} [\sigma \sigma^T]_{il} \partial^2_{p_i p_l} = \frac{1}{2} \sigma \sigma^T : \nabla^2_{\mathbf{p}} \tag{187}$$

where σ is a square root factor for $A = \sigma \sigma^T$.

To determine the specific form of σ, we consider for fixed indices m and n

$$\mathcal{W}_{ilmn} = \hat{S}^{(2)}_{imn} \hat{S}^{(2)}_{lmn} + \hat{S}^{(2)}_{imn} \hat{S}^{(2)}_{lnm} = S^{(2)}_{iab} S^{(2)}_{lcd} \hat{Q}_{am} \hat{Q}_{bn} (\hat{Q}_{cm} \hat{Q}_{dn} + \hat{Q}_{cn} \hat{Q}_{dm}). \tag{188}$$

Using the form 188 in 185, we have

$$I_{22} = S^{(2)}_{iab} S^{(2)}_{lcd} \left[\sum_{mn} \hat{Q}_{am} \hat{Q}_{bn} E_{mn} (\hat{Q}_{cm} \hat{Q}_{dn} + \hat{Q}_{cn} \hat{Q}_{dm}) \right] \partial^2_{p_i p_l}. \tag{189}$$

By interchanging m and n and averaging the original and new forms of I_{22} we find

$$I_{22} = \frac{1}{2} S^{(2)}_{iab} S^{(2)}_{lcd} \left[\sum_{mn} (\hat{Q}_{am} \hat{Q}_{bn} + \hat{Q}_{an} \hat{Q}_{bm}) E_{mn} (\hat{Q}_{cm} \hat{Q}_{dn} + \hat{Q}_{cn} \hat{Q}_{dm}) \right] \partial^2_{p_i p_l}. \tag{190}$$

This gives

$$\sigma_{i,\{m,n\}} = S^{(2)}_{iab} (\hat{Q}_{am} \hat{Q}_{bn} + \hat{Q}_{an} \hat{Q}_{bm}) \sqrt{E_{mn}}. \tag{191}$$

We remark that the summation convention is assumed on the indices a, b, but not m, n. This provides an explicit form for the factor $A = \sigma \sigma^T$ required in equation 191. This result is useful since it provides an explicit form in the reduced equations for any general choice that is made

for the coupling operator Υ.

Next, we can compute the integrals J_{ij}. Recalling the function on which the operator is applied depends only on the slow variables, we may apply the derivative in $\tilde{L}_2$ only on the fast variables appearing on $L_2^{-1}L_1$. We find

$$J_{-2,2} = -\int_{\mathbb{R}^N} \psi(\beta)\tilde{L}_2^{(-2)}L_2^{-1}L_1^{(2)}d\beta \tag{192}$$

$$= \int_{\mathbb{R}^N} \psi(\beta)\tilde{V}_{ij}\partial^2_{\beta_{ij}}\left[\sum_{mn}\hat{S}_{lmn}E_{mn}(\beta_m\beta_n - \delta_{mn})\partial_{y_l}\right]d\beta \tag{193}$$

$$= \int_{\mathbb{R}^N} \psi(\beta)\tilde{V}_{ij}\left[\sum_{mn}\hat{S}_{lmn}E_{mn}(\delta_{jm}\delta_{ni} + \delta_{mi}\delta_{jn})\partial_{y_l}\right]d\beta \tag{194}$$

$$= \left[\sum_{mn}\hat{S}_{lmn}E_{mn}(\tilde{V}_{nm} + \tilde{V}_{mn})\partial_{y_l}\right] \tag{195}$$

$$= -\frac{1}{2}S_{lab}\left[\sum_{mn}(\hat{Q}_{am}\hat{Q}_{bn} + \hat{Q}_{an}\hat{Q}_{bm})E_{mn}(\hat{Q}_{cm}\hat{Q}_{dn} + \hat{Q}_{dm}\hat{Q}_{cn})\right]V_{cd}\partial_{y_l} \tag{196}$$

$$= -\frac{1}{2}S_{lab}\Xi^{cd}_{ab}V_{cd}\partial_{y_l} = -\frac{1}{2}(S:\Xi:V)\cdot\nabla_{\mathbf{y}} = -\frac{1}{2}(S^{(2)}:\Xi:V)\cdot\nabla_{\mathbf{p}} \tag{197}$$

Here,

$$\Xi^{cd}_{ab} = \sum_{mn}(\hat{Q}_{am}\hat{Q}_{bn} + \hat{Q}_{an}\hat{Q}_{bm})E_{mn}(\hat{Q}_{cm}\hat{Q}_{dn} + \hat{Q}_{dm}\hat{Q}_{cn}) \tag{198}$$

The notation $A:\Xi:B = A_{ij}\Xi^{kl}_{ij}B_{kl}$, where the iterated sum over i,j is taken over the last two coordinates of A, while the sum over k,l is taken over the first two coordinates of B. We remark with this notation we can write

$$\sigma\sigma^T = S^{(2)}:\Xi:(S^{(2)})^T = \kappa^{-2}\nabla_{\mathbf{X}}\Lambda:\Xi:(\nabla_{\mathbf{X}}\Lambda)^T. \tag{199}$$

Next,

$$J_{0,2} = -\int_{\mathbb{R}^N} \psi(\beta)\tilde{L}_2^{(0)}L_2^{-1}L_1^{(2)}d\beta \tag{200}$$

$$= \int_{\mathbb{R}^N} \psi(\beta)\tilde{R}_{ij}\beta_j\partial_{\beta_i}\left[\sum_{mn}\hat{S}_{lmn}E_{mn}(\beta_m\beta_n - \delta_{mn})\partial_{y_l}\right]d\beta \tag{201}$$

$$= \int_{\mathbb{R}^N} \psi(\beta)\tilde{R}_{ij}\left[\sum_{mn}\hat{S}_{lmn}E_{mn}(\delta_{mi}\beta_j\beta_n + \beta_m\beta_j\delta_{ni})\partial_{y_l}\right]d\beta \tag{202}$$

$$= \tilde{R}_{ij}\left[\sum_{mn}\hat{S}_{lmn}E_{mn}(\delta_{mi}\delta_{jn} + \delta_{mj}\delta_{ni})\partial_{y_l}\right] \tag{203}$$

$$= \frac{1}{2}S_{lab}\left[\sum_{mn}(\hat{Q}_{am}\hat{Q}_{bn} + \hat{Q}_{an}\hat{Q}_{bm})E_{mn}(\tilde{R}_{mn} + \tilde{R}_{nm})\right]\partial_{y_l} \tag{204}$$

$$= S_{lab}\left[\sum_{mn}(\hat{Q}_{am}\hat{Q}_{bn} + \hat{Q}_{an}\hat{Q}_{bm})E_{mn}\tilde{R}_{mn}\right]\partial_{y_l} \tag{205}$$

$$= \sum_{nm}\sigma_{l,\{m,n\}}\omega_{mn}\partial_{p_l} = Z\cdot\nabla_{\mathbf{p}} \tag{206}$$

We label the tensors

$$\omega_{mn} = \sqrt{E_{mn}}\tilde{R}_{mn} \qquad\qquad Z_i = \sum_{nm}\sigma_{i,\{m,n\}}\omega_{mn}. \tag{207}$$

$$J_{-1,1} = -\int_{\mathbb{R}^N} \psi(\beta)\tilde{L}_2^{(-1)}L_2^{-1}L_1^{(1)}d\beta = \int_{\mathbb{R}^N} \psi(\beta)\tilde{T}_i\partial_{\beta_i}[\hat{R}_{lj}D_{jk}^{-1}\beta_k\partial_{y_l}]d\beta \tag{208}$$

$$= \int_{\mathbb{R}^N} \psi(\beta)\tilde{T}_i[\hat{R}_{lj}D_{ji}^{-1}\partial_{y_l}]d\beta = \tilde{T}_i\hat{R}_{lj}D_{ji}^{-1}\partial_{y_l} \tag{209}$$

$$= -[R\Upsilon^{-1}(\alpha\kappa\nabla_{\mathbf{X}}\Phi(\mathbf{X}) + \nabla_{\mathbf{y}}\mathbf{v_0}\cdot T)]\cdot\nabla_{\mathbf{y}} \tag{210}$$

$$= -[\Upsilon^{-1}(\alpha\kappa\nabla_{\mathbf{X}}\Phi(\mathbf{X}) + \nabla_{\mathbf{y}}\mathbf{v_0}\cdot T)]\cdot\nabla_{\mathbf{X}} \tag{211}$$

$$-[B\Upsilon^{-1}(\alpha\kappa\nabla_{\mathbf{X}}\Phi(\mathbf{X}) + \nabla_{\mathbf{y}}\mathbf{v_0}\cdot T)]\cdot\nabla_{\mathbf{p}} \tag{212}$$

$$J_{1,1} = -\int_{\mathbb{R}^N} \psi(\beta)\tilde{L}_2^{(1)}L_2^{-1}L_1^{(1)}d\beta \tag{213}$$

$$= \int_{\mathbb{R}^N} \psi(\beta)\tilde{S}_{inm}(\beta_n\beta_m - \delta_{nm})[\hat{R}_{lj}D_{ji}^{-1}\partial_{y_l}]d\beta = 0 \tag{214}$$

$$\tag{215}$$

The last integral is 0 since $\overline{\beta_n\beta_m} = \delta_{nm}$.

By combining the above results $L_0 = I_{11} + I_{22} + J_{-2,2} + J_{0,2} + J_{-1,1} + J_{1,1}$ from equations 169, 190, 192, 200, 208, and 213 we obtain the operator

$$L_0 = \Upsilon^{-1} : \nabla^2_{\mathbf{X}} + [(\nabla_{\mathbf{X}} B) : \Upsilon^{-1}] \cdot \nabla_{\mathbf{p}} + \frac{1}{2} M : \nabla^2_{\mathbf{p}} \tag{216}$$

$$- \left(\frac{1}{2} S^{(2)} : \Xi : V - Z + B\Upsilon^{-1}(\alpha\kappa \nabla_{\mathbf{X}} \Phi(\mathbf{X}) + \nabla_{\mathbf{y}} \mathbf{v_0} \cdot T) \right) \cdot \nabla_{\mathbf{p}} \tag{217}$$

$$- [\Upsilon^{-1}(\alpha\kappa \nabla_{\mathbf{X}} \Phi(\mathbf{X}) + \nabla_{\mathbf{y}} \mathbf{v_0} \cdot T)] \cdot \nabla_{\mathbf{X}} \tag{218}$$

The $M = \sigma\sigma^T + 2(B\Upsilon^{-1}B^T)$.

These results combined with the $\bar{L}_1$ given in equation 123 gives the final reduced operator $L_0 = \bar{L}_1 + \epsilon L_0$. While the $\bar{L}_1$ operator yields the reduced stochastic process in the strong coupling limit given in equations 63 and 64, the terms due to effects of order ϵ are captured in the operator L_0.

We may be interested in the limit of L_0 in the negligible mass limit ($\kappa^{-1} \to 0$). In this case it is important to remember to make certain assumptions about the relationship of the non-dimensional constants κ, ϵ, and α. In particular, we recall the requirement $\kappa\alpha = O(1)$, which implies $\epsilon << (\kappa\alpha)^{-1}$. This avoids the blow-up of the potential terms in L_0 when we wish to take $\kappa^{-1} \to 0$.

7.2 Strong Coupling with Weak Slip: Higher Order Terms in ϵ

We now consider the next order correction terms in ϵ. These first-order terms contain contributions that can be interpreted in the strong coupling regime as the weak leading-order slip-effects between the fluid and structures. Such effects are known to arise in small-scale systems from hydrophobic effects or a break-down of the continuum hypothesis (non-negligible Knudsen number) [33, 15]. In the SELM formulation the precise form of the slip arises from the choice of coupling operators Λ and Γ. To capture weak slip effects, these terms could possibly be used to incorporate leading-order slip effects for analysis or for computational simulations without suffering the rapid dynamics over short time-scales associated with the strong coupling.

For the SELM formulation, it is convenient to express the effective "slip terms" θ_p and θ_X in

Section 5.1 by decomposition into the parts

$$\theta_p = \Theta^p + \Theta^p_{\text{thm}} \tag{219}$$

$$\theta_X = \Theta^X + \Theta^X_{\text{thm}}. \tag{220}$$

These were computed using the non-dimensional conventions. It is most convenient to combine the dimensions to the resulting non-dimensional ϵ-order terms, as dictated by the units of each equation. That is, we multiply

$$\Theta^p = \Theta^p_0 \bar{\Theta}^p, \qquad \Theta^X = \Theta^X_0 \bar{\Theta}^X. \qquad \Theta^p_{\text{thm}} = \Theta^p_0 \bar{\Theta}^p_{\text{thm}}, \qquad \Theta^X_{\text{thm}} = \Theta^X_0 \bar{\Theta}^X_{\text{thm}} \tag{221}$$

where

$$\Theta^p_0 = \left(\frac{m_0}{\tau_k \ell^2}\right), \qquad\qquad \Theta^X_0 = \left(\frac{\ell}{\tau_k}\right). \tag{222}$$

The non-dimensional ϵ-order corrections to the drift are given by

$$\bar{\Theta}^p = \epsilon\left((\nabla_{\mathbf{X}} B) : \Upsilon^{-1} - \frac{1}{2} S^{(2)} : \Xi : V + Z - B\Upsilon^{-1}(\alpha\kappa\nabla_{\mathbf{X}}\Phi(\mathbf{X}) + \nabla_{\mathbf{y}}\mathbf{v_0}\cdot T)\right) \tag{223}$$

$$\bar{\Theta}^X = \epsilon\left(-\Upsilon^{-1}(\alpha\kappa\nabla_{\mathbf{X}}\Phi(\mathbf{X}) + \nabla_{\mathbf{y}}\mathbf{v_0}\cdot T)\right). \tag{224}$$

In our notation, the constituent terms $\bar{\Theta}$ are understood to have no dimensions. The non-dimensional ϵ-order corrections to the noise are given by:

$$\left\langle \bar{\Theta}^p_{\text{thm}}(\bar{s})(\bar{\Theta}^p_{\text{thm}})^T(\bar{t})\right\rangle = \epsilon\left(\sigma\sigma^T + 2(B\bar{\Upsilon}^{-1}B^T)\right)\delta(\bar{t}-\bar{s}), \tag{225}$$

$$\left\langle \bar{\Theta}^X_{\text{thm}}(\bar{s})(\bar{\Theta}^X_{\text{thm}})^T(t)\right\rangle = 2\epsilon\bar{\Upsilon}^{-1}\,\delta(\bar{t}-\bar{s}). \tag{226}$$

The Ξ is given in equation 198, Z is given in equation 207, and σ is given in equation 199. The T, B, S, and V are defined in equations 142, 144, 145, and 146. A derivation of these equations is given in Section 7.1. In the notation $A : \Xi : B = A_{ij}\Xi^{kl}_{ij}B_{kl}$, where the indices i, j iterate through the last two coordinates of A, while k, l iterate through the first two coordinates of B.

7.3 Limit of Negligible Excess Mass : Derivation of Reduced Equations

To obtain the reduced equations in the limit of negligible excess mass, we consider the limit $\kappa \to \infty$, with the limit $\epsilon \to 0$ assumed to be already taken for simplicity. This corresponds to the physical regime with $m << m_0 = \rho\ell^3$ with the coupling very strong.

We begin with the $\bar{L}_1$ operator, which describes the dynamics for the limit $\epsilon \to 0$ taken. This operator is given by equation 123. In the limit $\kappa^{-1} \to 0$ we find

$$\bar{L}_1 \quad = \quad (\mathcal{L}\mathbf{p} + \nabla_{\mathbf{X}}\Lambda : \mathcal{I} - \Lambda\nabla_{\mathbf{X}}\Phi(\mathbf{X})) \cdot \nabla_{\mathbf{p}} + \mathbf{v}_0 \cdot \nabla_{\mathbf{X}} - \mathcal{L} : \nabla^2_{\mathbf{p}} \tag{227}$$

Equations 108–109 simplify to

$$\mathbf{v}_0 = \Gamma\mathbf{u}. \tag{228}$$

We write

$$\nabla_{\mathbf{X}}\Lambda : \mathcal{I} = \mathrm{tr}[\nabla_{\mathbf{X}}\Lambda] = \nabla_{\mathbf{X}} \cdot \Lambda. \tag{229}$$

We obtain 75–77 by adding the units to the non-dimensional variables and writing the equation in its dynamical form.

7.3.1 Special Case of Stokes Drag

In the special case when the Stokes drag is used for coupling $\Upsilon = \Upsilon_0\mathcal{I}$ and $C = C_0\mathcal{I}$, the expressions for the strong coupling regime simplify. In this case, we have $D = \Upsilon_0 C_0 \mathcal{I}$ and $Q = \mathcal{I}$. This gives that $E = \frac{1}{2}\Upsilon_0^{-1}C_0^{-1}\mathcal{I}$. The reduced equations are given by

$$\frac{1}{2}\sigma\sigma^T = (\Upsilon_0 C_0 \kappa^2)^{-1}[(\nabla_{\mathbf{X}}\Lambda) : (\nabla_{\mathbf{X}}\Lambda)^T] : \nabla^2_{\mathbf{p}} \tag{230}$$

$$\sigma_{i,\{m,n\}} = \sqrt{2}(\Upsilon_0 C_0 \kappa^2)^{-1/2}(\nabla_{\mathbf{X}}\Lambda)_{inm}. \tag{231}$$

We note that B, S, and σ are proportional to κ^{-1}, and thus appear only when inertial contributions are important. We see that even in the case considered here the contributions due to inertial terms in higher order are non-trivial. The inertial terms contribute at first order in ϵ

both to the effective total momentum equations and to the configuration equations.

Consider $\Phi(\mathbf{X}) = 0$ for simplicity. Taking $\kappa^{-1} \to 0$, we obtain the contribution with no inertial dynamics:

$$L_0 = \Upsilon_0^{-1}[\mathrm{tr}\nabla_{\mathbf{X}}^2] + \Upsilon_0^{-1}(\nabla_{\mathbf{y}}\mathbf{v_0} \cdot T) \cdot \nabla_{\mathbf{X}}. \tag{232}$$

7.4 Limit of Rapid Hydrodynamic Relaxation : Derivation of Reduced Equations

We now consider the regime where the hydrodynamics relaxes rapidly relative to the time-scale of the microstructure motions. We consider the regime with small Reynold's number $Re = \rho LU/\mu \ll 1$, where U is a characteristic flow velocity, $L = \ell$ a characteristic length-scale, and μ the fluid viscosity.

To handle the important incompressibility constraint on the fluid, we now introduce a projection operator approach to handle the Lagrange multiplier λ in

$$\rho\frac{d\mathbf{u}}{dt} = \mathcal{L}\mathbf{u} - \Lambda\nabla_{\mathbf{X}}\Phi(\mathbf{X}) + k_BT\nabla_{\mathbf{X}} \cdot \Lambda + \mathbf{f}_{\mathrm{thm}} + \lambda \tag{233}$$

$$\frac{d\mathbf{X}}{dt} = \Gamma\mathbf{u}. \tag{234}$$

The λ acts as a constraint force density that enforces $\nabla \cdot \mathbf{u} = 0$. This can be written in terms of a projection operator as

$$\lambda = -(\mathcal{I} - \mathscr{P})(\mathcal{L}\mathbf{u} - \Lambda\nabla_{\mathbf{X}}\Phi(\mathbf{X}) + k_BT\nabla_{\mathbf{X}} \cdot \Lambda + \mathbf{f}_{\mathrm{thm}}). \tag{235}$$

The projection operator is given by $\mathscr{P} = \mathcal{I} - \nabla\Delta^{-1}\nabla\cdot$. This gives

$$\rho\frac{d\mathbf{u}}{dt} = \mathscr{P}[\mathcal{L}\mathbf{u} - \Lambda\nabla_{\mathbf{X}}\Phi(\mathbf{X}) + k_BT\nabla_{\mathbf{X}} \cdot \Lambda + \mathbf{f}_{\mathrm{thm}}] \tag{236}$$

$$\frac{d\mathbf{X}}{dt} = \Gamma\mathbf{u}. \tag{237}$$

We assume that $\mathscr{P}\mathcal{L} = \mathcal{L}\mathscr{P}$ and make use of the properties $\mathscr{P}^2 = \mathscr{P}$ and $\mathscr{P} = \mathscr{P}^T$. We can

express this in non-dimensionalized form with $\epsilon = Re$ as

$$\frac{d\mathbf{u}}{dt} = \mathscr{P}\left[\frac{1}{\epsilon}\mathcal{L}\mathbf{u} - \Lambda\nabla_{\mathbf{X}}\Phi(\mathbf{X}) + \nabla_{\mathbf{X}}\cdot\Lambda + \sqrt{\frac{1}{\epsilon}}\mathbf{f}_{\text{thm}}\right] \tag{238}$$

$$\frac{d\mathbf{X}}{dt} = \Gamma\mathbf{u}. \tag{239}$$

The infinitesimal generator is given by

$$\mathcal{A} = \frac{1}{\epsilon}[\mathscr{P}\mathcal{L}\mathbf{u} + \epsilon\mathscr{P}(-\Lambda\nabla_{\mathbf{X}}\Phi(\mathbf{X}) + \nabla_{\mathbf{X}}\cdot\Lambda)]\cdot\nabla_{\mathbf{u}} - \frac{1}{\epsilon}(\mathscr{P}\mathcal{L}) : \nabla^2_{\mathbf{u}} + [\Gamma\mathbf{u}]\cdot\nabla_{\mathbf{X}}. \tag{240}$$

To apply our perturbation analysis introduced in Section 6, we split the operator as

$$\mathcal{A} = L_{slow} + L_{fast} \tag{241}$$

with

$$L_{slow} = \bar{L}_1 + L_1 \tag{242}$$

$$L_{fast} = L_2 + \tilde{L}_2. \tag{243}$$

In this regime we have

$$\bar{L}_1 = 0 \tag{244}$$

$$L_1 = (\Gamma\mathbf{u})\cdot\nabla_{\mathbf{X}} \tag{245}$$

$$L_2 = (\mathscr{P}\mathcal{L}\mathbf{u})\cdot\nabla_{\mathbf{u}} - (\mathscr{P}\mathcal{L}) : \nabla^2_{\mathbf{u}} \tag{246}$$

$$\tilde{L}_2 = \mathscr{P}(-\Lambda\nabla_{\mathbf{X}}\Phi(\mathbf{X}) + \nabla_{\mathbf{X}}\cdot\Lambda)\cdot\nabla_{\mathbf{u}}. \tag{247}$$

We remark that each of the coefficients of L_2 and $\tilde{L}_2$ are in the range of $\mathscr{P}$. Using the linearity of $\mathscr{P}$ and $\mathcal{L}$ we may interpret the derivatives $\nabla_{\mathbf{u}}$ as $\nabla_{\mathscr{P}\mathbf{u}}$ and complete the reduction with the fast variable in the space $u \in \mathcal{S}$. The $\mathcal{S}$ denotes our space of solenoidal vector fields. Given the specific form of L_2, the inverse operator can be expressed as

$$L_2^{-1}\mathbf{u} = \mathcal{L}^{-1}\mathbf{u}, \qquad \text{for } u \in \mathcal{S}. \tag{248}$$

This allows us to carry out readily the inverse

$$L_1 L_2^{-1} L_1 = L_1 L_2^{-1}[(\Gamma \mathbf{u}) \cdot \nabla_{\mathbf{X}}] = L_1[(\Gamma \mathcal{L}^{-1} \mathbf{u}) \cdot \nabla_{\mathbf{X}}] \tag{249}$$

$$= (\Gamma \mathbf{u}) \cdot \nabla_{\mathbf{X}}[(\Gamma \mathcal{L}^{-1} \mathbf{u}) \cdot \nabla_{\mathbf{X}}], \qquad \text{for } u \in \mathcal{S}. \tag{250}$$

We still need to evaluate $\int_{u \in \mathcal{S}} \psi(\mathbf{u}) L_1 L_2^{-1} L_1$. An important feature is that the covariance structure of ψ is the identity in the space $\mathcal{S}$ because the operator coefficients on the first and second order terms in L_2 are identical. It is useful to rewrite the inverse as

$$L_1 L_2^{-1} L_1 = (\Gamma \mathbf{u}) \cdot \nabla_{\mathbf{X}}[(\Gamma \mathcal{L}^{-1} \mathbf{u}) \cdot \nabla_{\mathbf{X}}] \tag{251}$$

$$= \nabla_{\mathbf{X}} \cdot \{(\Gamma \mathbf{u})[(\Gamma \mathcal{L}^{-1} \mathbf{u}) \cdot \nabla_{\mathbf{X}}]\} - (\nabla_{\mathbf{X}} \cdot (\Gamma \mathbf{u}))[(\Gamma \mathcal{L}^{-1} \mathbf{u}) \cdot \nabla_{\mathbf{X}}]. \tag{252}$$

The averaging with respect to $\psi(\mathbf{u})$ can be computed readily in this form by passing the integral onto $\mathbf{u}$ inside each term. From the covariance structure of ψ we have the useful identities $\int u_i u_j \psi(\mathbf{u}) d\mathbf{u} = \delta_{ij}$ for $u \in \mathcal{S}$. By using these identities and that $\Gamma = \Lambda^T$, we have

$$\int_{u \in \mathcal{S}} \psi(\mathbf{u}) L_1 L_2^{-1} L_1 = \nabla_{\mathbf{X}} \cdot [(\Gamma \mathcal{L}^{-1} \mathscr{P} \Lambda) \cdot \nabla_{\mathbf{X}}] - (\Gamma \mathcal{L}^{-1} \mathscr{P} \nabla_{\mathbf{X}} \cdot \Lambda) \cdot \nabla_{\mathbf{X}} \tag{253}$$

$$= [\nabla_{\mathbf{X}} \cdot (\Gamma \mathcal{L}^{-1} \mathscr{P} \Lambda)] \cdot \nabla_{\mathbf{X}} + (\Gamma \mathcal{L}^{-1} \mathscr{P} \Lambda) : \nabla_{\mathbf{X}}^2 - (\Gamma \mathcal{L}^{-1} \mathscr{P} \nabla_{\mathbf{X}} \cdot \Lambda) \cdot \nabla_{\mathbf{X}}. \tag{254}$$

We can evaluate the remaining integral term in L_0 by

$$\int_{u \in \mathcal{S}} \psi(\mathbf{u}) \tilde{L}_2 L_2^{-1} L_1 \tag{255}$$

$$= \int_{u \in \mathcal{S}} \psi(\mathbf{u}) \mathscr{P}(-\Lambda \nabla_{\mathbf{X}} \Phi(\mathbf{X}) + \nabla_{\mathbf{X}} \cdot \Lambda) \cdot \nabla_{\mathbf{u}}[(\Gamma \mathcal{L}^{-1} \mathbf{u}) \cdot \nabla_{\mathbf{X}}] \tag{256}$$

$$= \int_{u \in \mathcal{S}} \psi(\mathbf{u})[(\Gamma \mathcal{L}^{-1} \mathscr{P}(-\Lambda \nabla_{\mathbf{X}} \Phi(\mathbf{X}) + \nabla_{\mathbf{X}} \cdot \Lambda)) \cdot \nabla_{\mathbf{X}}] \tag{257}$$

$$= (\Gamma \mathcal{L}^{-1} \mathscr{P}(-\Lambda \nabla_{\mathbf{X}} \Phi(\mathbf{X}) + \nabla_{\mathbf{X}} \cdot \Lambda)) \cdot \nabla_{\mathbf{X}}. \tag{258}$$

For the effective infinitesimal operator $\bar{L} = \bar{L}_1 + \epsilon L_0$, this gives

$$\bar{L} = -\epsilon \left(\int_{u \in \mathcal{R}(\mathscr{P})} \psi(\mathbf{u}) \tilde{L}_2 L_2^{-1} L_1 + \int_{u \in \mathcal{R}(\mathscr{P})} \psi(\mathbf{u}) L_1 L_2^{-1} L_1 \right) \tag{259}$$

$$= -\epsilon \Big\{ (\Gamma \mathcal{L}^{-1} \mathscr{P}[-\Lambda \nabla_{\mathbf{X}} \Phi(\mathbf{X}) + \nabla_{\mathbf{X}} \cdot \Lambda]) \cdot \nabla_{\mathbf{X}} \tag{260}$$

$$+ [\nabla_{\mathbf{X}} \cdot (\Gamma \mathcal{L}^{-1} \mathscr{P} \Lambda)] \cdot \nabla_{\mathbf{X}} + (\Gamma \mathcal{L}^{-1} \mathscr{P} \Lambda) : \nabla_{\mathbf{X}}^2 - (\Gamma \mathcal{L}^{-1} \mathscr{P} \nabla_{\mathbf{X}} \cdot \Lambda) \cdot \nabla_{\mathbf{X}} \Big\} \tag{261}$$

$$= \epsilon \Big\{ \Big[\Gamma(-\mathcal{L})^{-1} \mathscr{P}[-\Lambda \nabla_{\mathbf{X}} \Phi(\mathbf{X})] + [\nabla_{\mathbf{X}} \cdot (\Gamma(-\mathcal{L})^{-1} \mathscr{P} \Lambda)] \Big] \cdot \nabla_{\mathbf{X}} \tag{262}$$

$$+ (\Gamma(-\mathcal{L})^{-1} \mathscr{P} \Lambda) : \nabla_{\mathbf{X}}^2 \Big\}. \tag{263}$$

By letting $\tilde{H}_{\text{SELM}} = -\Gamma \mathcal{L}^{-1} \mathscr{P} \Lambda$, we can express this more compactly as

$$\bar{L} = \epsilon \Big\{ \Big[\tilde{H}_{\text{SELM}}(-\nabla_{\mathbf{X}} \Phi(\mathbf{X})) + \nabla_{\mathbf{X}} \cdot \tilde{H}_{\text{SELM}} \Big] \cdot \nabla_{\mathbf{X}} + \tilde{H}_{\text{SELM}} : \nabla_{\mathbf{X}}^2 \Big\}. \tag{264}$$

By converting expressions to have physical units, the reduced stochastic processes in the small Reynold's number limit is

$$\frac{d\mathbf{X}}{dt} = H_{\text{SELM}}[-\nabla_{\mathbf{X}} \Phi(\mathbf{X})] + (\nabla_{\mathbf{X}} \cdot H_{\text{SELM}}) k_B T + \mathbf{h}_{\text{thm}} \tag{265}$$

$$H_{\text{SELM}} = \Gamma(-\mathcal{L})^{-1} \mathscr{P} \Lambda \tag{266}$$

$$\langle \mathbf{h}_{\text{thm}}(s), \mathbf{h}_{\text{thm}}^T(t) \rangle = 2 k_B T H_{\text{SELM}} \delta(t - s). \tag{267}$$

The properties of $\mathscr{P}$ allow us to write $H_{\text{SELM}} = \Gamma \mathscr{P}^T (-\mathcal{L})^{-1} \mathscr{P} \Lambda$. This provides a convenient way to factor the hydrodynamic coupling tensor and generate stochastic driving fields. In particular, $H_{\text{SELM}} = Q^T Q$ with $Q = \Gamma \mathscr{P}^T \sqrt{(-\mathcal{L})^{-1}}$.

8 Conclusion

We have systematically reduced the dynamics of fluid structure interactions with thermal fluctuations in several limiting regimes of interest. In particular, we gave much attention to the case of strong coupling. Our approach allows for preserving the inertial dynamics, as well as weak slip effects if necessary. Our analysis shows that important terms arise in this description. We have also found the form of the equations when the excess mass of the immersed structures becomes negligible. Next, we also used our systematic technique to obtain effective equations

for the structure in the case of rapid hydrodynamic relaxation. Our results allow reducing the description of the dynamical system when timescales vary sufficiently to cause stiffness in numerical simulations. Our approach may also be readily applied to other regimes, making it useful for further applications.

References

[1] P. J. Atzberger, *A note on the correspondence of an immersed boundary method incorporating thermal fluctuations with stokesian-brownian dynamics*, Physica D-Nonlinear Phenomena, 226 (2007), pp. 144–150.

[2] P. J. Atzberger, *Stochastic eulerian lagrangian methods for fluid–structure interactions with thermal fluctuations*, Journal of Computational Physics, 230 (2011), pp. 2821–2837.

[3] P. J. Atzberger and P. R. Kramer, *Theoretical framework for microscopic osmotic phenomena.*, Phys Rev E Stat Nonlin Soft Matter Phys, 75 (2007), p. 061125.

[4] P. J. Atzberger and P. R. Kramer, *Error analysis of a stochastic immersed boundary method incorporating thermal fluctuations*, Mathematics and Computers in Simulation, 79 (2008), pp. 379–408.

[5] P. J. Atzberger, P. R. Kramer, and C. S. Peskin, *A stochastic immersed boundary method for fluid-structure dynamics at microscopic length scales*, Journal of Computational Physics, 224 (2007), pp. 1255–1292.

[6] D.-B. R. G. B. E. Balboa Usabiaga, F. and A. Donev, *Inertial coupling method for particles in an incompressible fluctuating fluid*, ArXiv e-prints, (2012).

[7] A. J. Banchio and J. F. Brady, *Accelerated stokesian dynamics: Brownian motion*, Journal of Chemical Physics, 118 (2003), pp. 10323–10332.

[8] J. B. Bell, A. L. Garcia, and S. A. Williams, *Computational fluctuating fluid dynamics*, ESAIM: Mathematical Modelling and Numerical Analysis., 44(5) (2010), pp. 1085–1105.

[9] D. C. Bottino and L. J. Fauci, *A computational model of ameboid deformation and locomotion*, European Biophysics Journal with Biophysics Letters, 27 (1998), pp. 532–539.

[10] J. F. Brady and G. Bossis, *Stokesian dynamics*, Annual review of fluid mechanics. Vol.20—Annual review of fluid mechanics. Vol.20, (1988), pp. 111–57.

[11] E. Buckingham, *On physically similar systems; illustrations of the use of dimensional equations*, Phys. Rev., 4 (1914), pp. 345–376.

[12] Y. Chen, N. Sharma, and N. Patankar, *Fluctuating Immersed Material (FIMAT) Dynamics for the Direct Simulation of the Brownian Motion of Particles*, vol. 81, Springer Netherlands, 2006.

[13] A. J. Chorin, *Numerical solution of navier-stokes equations*, Mathematics of Computation, 22 (1968), pp. 745–762.

[14] A. J. Chorin and J. E. Marsden, *A Mathematical Introduction to Fluid Mechanics*, Springer-Verlag, 3rd ed., 1993.

[15] E. Cunningham, *On the velocity of steady fall of spherical particles through fluid medium*, Proc. R. Soc. Lond. A, 83 (1910), pp. 357–365.

[16] B. Danowsky, P. Thompson, C. Farhat, T. Lieu, C. Harris, and J. Lechniak, *A complete aeroservoelastic model: Incorporation of oscillation-reduction-control into a high-order cfd/fem fighter aircraft model*, in AIAA Paper 2009-5708, AIAA Atmospherics Flight Mechanics Conference, Chicago, Illinois, August 10-13 2009.

[17] J. Donea, A. Huerta, J. Ponthot, and A. Rodriguez-Ferran, *Arbitrary lagrangian-eulerian methods*, Encyclopedia of Computational Mechanics, 1 (2004).

[18] E. Dowell and K. Hall, *Modeling of fluid-structure interaction*, Ann. Rev. Fluid Mech., 33 (2001), pp. 445–490.

[19] B. Duenweg and A. J. C. Ladd, *Lattice boltzmann simulations of soft matter systems*, arXiv, (2008).

[20] B. Dünweg, U. D. Schiller, and A. J. C. Ladd, *Statistical mechanics of the fluctuating lattice boltzmann equation*, Phys. Rev. E, 76 (2007), p. 036704.

[21] D. Floreano, J. Zufferey, M. Srinivasan, and C. Ellington, *Flying Insects and Robots*, Springer-Verlag, 2009.

[22] H. C. Fu, V. B. Shenoy, and T. R. Powers, *Role of slip between a probe particle and a gel in microrheology*, Phys. Rev. E, 78(6) (2008), p. 061503.

[23] Y. Fung, *An Introduction to the Theory of Aeroelasticity*, John Wiley, 1955.

[24] L. Gammaitoni, P. Hänggi, P. Jung, and F. Marchesoni, *Stochastic resonance: A remarkable idea that changed our perception of noise*, European Physical Journal B, 69(1) (2009), pp. 1–3.

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

[26] B. Griffith, X. Luo, D. McQueen, and C. Peskin., *Simulating the fluid dynamics of natural and prosthetic heart valves using the immersed boundary method.*, Int J Appl Mech., 1 (2009), pp. 137–177.

[27] C. W. Hirt, A. A. Amsden, and J. L. Cook, *Arbitrary lagrangian-eulerian computing method for all flow speeds*, Journal of Computational Physics, 14 (1974), pp. 227–253.

[28] D. L. Hu, B. Chan, and J. W. M. Bush, *The hydrodynamics of water strider locomotion*, letters to nature, 424 (2003), pp. 663–666.

[29] Y. Kim and C. S. Peskin, *Penalty immersed boundary method for an elastic boundary with mass*, Physics of Fluids, 19 (2007), p. 053103.

[30] P. R. Kramer, C. S. Peskin, and P. J. Atzberger, *On the foundations of the stochastic immersed boundary method*, Computer Methods in Applied Mechanics and Engineering, 197 (2008), pp. 2232–2249.

[31] R. Kubo, *The fluctuation-dissipation theorem*, Rep. Prog. Phys., 29(255) (1966), pp. 255–284.

[32] T. G. Kurtz, *A limit theorem for perturbed operator semigroups with applications to random evolutions*, Journal of Functional Analysis, 12 (1973), pp. 55–67.

[33] E. Lauga, M. Brenner, and H. Stone, *Microfluidics: The no-slip boundary condition. Handbook of Experimental Fluid Dynamics*, Springer, New-York, 2007.

[34] E. Lauga and T. R. Powers, *The hydrodynamics of swimming microorganisms*, 2009.

[35] S.-H. Lin, F.-Y. Hsiao, and C.-L. Chen, *Trajectory control of flapping-wing mav using vision-based navigation*, in American Control Conference, Baltimore, Maryland, USA, Jun. 30 - Jul. 2 2010.

[36] A. Majda and P. Kramer, *Stochastic mode reduction for particle-based simulation methods for complex microfluid systems*, SIAM J. Appl. Math., 64 (2004), pp. 401–422.

[37] ——, *Stochastic mode reduction for particle-based simulation methods for complex microfluid systems*, SIAM J. Appl. Math., 64 (2004), pp. 401–422.

[38] ——, *Stochastic mode reduction for the immersed boundary method*, SIAM Journal on Applied Mathematics, 64 (2004), pp. 369–400.

[39] A. J. Majda, I. Timofeyev, and E. V. Eijnden, *Models for stochastic climate prediction*, The National Academy of Sciences, 96(26) (1999), pp. 14687–14691.

[40] A. J. Majda, I. Timofeyev, and E. Vanden-Eijnden, *Systematic strategies for stochastic mode reduction in climate*, J. Atmos. Sci., 60 (2003), pp. 1705–1722.

[41] M. McDonnell and D. Abbott, *What is stochastic resonance? definitions, misconceptions, debates, and its relevance to biology*, Computational Biology, 5(5) (2009), p. e1000348.

[42] L. A. Miller and C. S. Peskin, *A computational fluid dynamics of 'clap and fling' in the smallest insects*, Journal of Experimental Biology, 208 (2005), pp. 195–212.

[43] B. Oksendal, *Stochastic Differential Equations: An Introduction*, Springer, 2000.

[44] G. C. Papanicolaou, *Some probabilistic problems and methods in singular perturbations*, Rocky Mountain J. Math., 6 (1976), p. 653–674.

[45] S. V. Patankar, *Numerical Heat Transfer and Fluid Flow*, New York: McGraw-Hill, 1980.

[46] C. S. Peskin, *The immersed boundary method*, Acta Numerica, 11 (2002), pp. 479–517.

[47] C. S. Peskin and D. M. McQueen, *Cardiac fluid-dynamics*, Critical Reviews in Biomedical Engineering, 20 (1992), pp. 451–9.

[48] A. C. Powell and D. Dussault, *Floating solids: combining phase field and fluid-structure interactions*, Applied Numerical Analysis and Computational Mathematics, 2 (2005), pp. 157–66.

[49] E. M. Purcell, *Life at low reynolds number*, American Journal of Physics, 45 (1977), pp. 3–10.

[50] A. Raman, J. Melcher, and R. Tung, *Cantilever dynamics in atomic force microscopy*, Nano Today, 3 (2008), pp. 20–27.

[51] M. Reed and B. Simon, *Functional Analysis*, Elsevier, 1980.

[52] L. E. Reichl, *A Modern Course in Statistical Physics*, John Wiley and Sons, 1998.

[53] M. Souli, A. Ouahsine, and L. Lewin, *Ale formulation for fluid-structure interaction problems*, Computer Methods in Applied Mechanics and Engineering, 190 (2000), pp. 659–675.

[54] T. M. Squires and S. R. Quake, *Microfluidics: Fluid physics at the nanoliter scale*, Rev. Mod. Phys., 77 (2005), pp. 977–1026.

[55] T. von Kármán, *Aerodynamics*, Theodore von Kármán, 1963.

[56] J. Young and S. Mitran, *A numerical model of cellular blebbing: A volume-conserving, fluid-structure interaction model of the entire cell*, J. Biomech., 43(2) (2010), p. 210.