STOCHASTIC REDUCTIONS FOR INERTIAL FLUID-STRUCTURE INTERACTIONS SUBJECT TO THERMAL FLUCTUATIONS

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Abstract. We investigate the dynamics of elastic microstructures that interact with a fluid flow when subject to thermal fluctuations. We perform analysis to obtain systematically simplified descriptions of the mechanics in the limiting regimes when (i) the coupling forces that transfer momentum between the fluid and microstructures is strong, (ii) the mass of the microstructures is small relative to the displaced mass of the fluid, and (iii) the response to stresses results in hydrodynamics that relax rapidly to a quasi-steady-state relative to the motions of the microstructure. We derive effective equations using a singular perturbation analysis of the Backward Kolmogorov equations of the stochastic process. Our continuum mechanics description is based on the Stochastic Eulerian Lagrangian Method (SELM) which provides a framework for approximation of the fluid-structure interactions when subject to thermal fluctuations. We perform a dimension 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 into the physical accuracy of SELM descriptions in comparison with classical results. The reduced equations also elimintate rapid time-scales from the dynamics and provide possible approaches for the development of more efficient computational methods for simulations of fluid-structure interactions when subject to thermal fluctuations.

Key words. Fluid-Structure Interaction, Fluctuating Hydrodynamics, Stochastic Mode Reduction, Stochastic Eulerian Lagrangian Method.

Last update to manuscript was on May 20, 2013; 9:59pm.

1. Introduction.

Many applications involve the mechanics of spatially extended elastic bodies that interact with a fluid. For instance, elastic bodies may represent the polymers of a complex fluid [12, 4], the individual or collective behaviors of amphiphilic molecules of a lipid bilayer membrane [18, 23, 8], the cilia or flagellum driving the swimming of microorganisms [22, 31], or the components of micro-mechanical devices [32, 19]. In such systems thermal fluctuations often play an important role. Even in the absence of fluctuations, the mechanics of fluid-structure interactions pose a number of difficult and long-standing challenges. The mechanics can exhibit rich behaviors through the interplay of the fluid flow which can drive deformations of the elastic structures while at the same time the elastic stresses of the deformed bodies can feedback to resist flow of the fluid or even drive flows. This can result in complicated long-range coupling between the motions of different bodies or the motions between different parts of a single spatially extended body. When subject to thermal fluctuations that drive spontaneous flows, this manifests as diffusive motions with long-range correlations between immersed microstructures. In continuum mechanics it is natural to consider descriptions for these interactions in which explicit boundary conditions are formulated at the interface between the elastic body with the fluid (i.e. the traction stress and kinematic conditions). However, in practice this approach is often intractable for physical analysis and prohibitively expensive in computational simulations.

To obtain more tractable descriptions, while still capturing essential features of the mechanics, many approximations of the fluid-structure interactions have been developed. These include the Immersed Boundary Method [30, 2], Arbitrary Lagrangian-Eulerian Methods [6, 13], Stokesian-Brownian Dynamics [5], Lattice-Boltzmann Method [15, 14], and Force Coupling Method [27, 10]. While these approximations may perform adequately in the de-

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terministic setting, when introducing the thermal fluctuations the approximations can often introduce unphysical dissipation, spurious drifts, and other artifacts affecting the propagation of fluctuations throughout the mechanical system. The Stochastic Eulerian Lagrangian Method (SELM) has been introduced in [1] to provide a framework for the development of approximate fluid-structure coupling schemes that are amenable to thermal fluctuations. Provided a few criteria are satisfied by the approximate fluid-structure coupling method employed, SELM provides an approach to formulate equations of motion for the fluid-structure system and to introduce stochastic driving fields that yield equilibrium fluctuations having Gibbs-Boltzmann statistics and stochastic dynamics satisfying detailed balance [1].

The SELM equations are formulated at the level of inertial fluid-structure interactions and allow for the case of slip between the microstructure and fluid. However, many of the widely used approximation methods for fluid-structure interactions are formulated in other physical regimes of interest, such as in the limit with strong fluid-structure coupling with no-slip, small body mass, or rapid hydrodynamic relaxation (small Reynold's number) [1]. A primary objective of our present work is to develop reductions of the SELM equations that are directly applicable to these regimes and to compare the reduced descriptions with well-known results in fluid mechanics and statistical mechanics. Some of this work was partially carried out in our prior paper [1]. In this prior work, we proposed reduced equations based on formal calculations carried out on an intuitive level using results from the Ito Calculus [28]. The focus of the current work is (i) to develop a more systematic and reliable approach to reduce the SELM equations, (ii) to characterize precisely the physical regimes and limits using a dimension analysis of the SELM equations, and (iii) to consider an important, but previously unexplored, limit for SELM equations in which the fluid-structure coupling forces that exchange momentum between the microstructures and the fluid becomes strong to yield no-slip. One potentially important use of these reductions is to eliminate sources of numerical stiffness by providing equations that can be handled more efficiently in simulations of fluid-structure interactions when subject to thermal fluctuations.

Our approach is based on a singular perturbation analysis of the Backward Kolmogorov equation (BKE) carried out using methods similar to those in [25, 24, 26] and rigorously established in [29, 21]. To perform reductions of fluid-structure mechanics, we show it is important to reformulate the system in terms of a total momentum density field which eliminates a fluid-structure momentum exchange time-scale from the problem since the total field includes both the local fluid momentum and local microstructure momentum. As a starting point in our analysis we present this formulation of the fluid-structure mechanics based on the Stochastic Eulerian Lagrangian Method (SELM) in Section 2. We present dimension analysis of the SELM equations to identify non-dimensional groups and to characterize precisely the limiting physical regimes in Section 3. We then summarize our main results for those readers primarily interested in the final reduced equations in Section 4. The general singular perturbation analysis we use for the the Backward Kolmogorov equations is developed in Section 5. We present the details of the derivations for each of the reduced equations for the different limiting physical regimes in Section 6. These results present in a few physical regimes of broad interest a general approach for the development of approximate models of the fluid-structure interaction when subject to thermal fluctuations.

2. Stochastic Eulerian Lagrangian Method : Inertial Regime. To account for the fluid-structure interactions subject to thermal fluctuations, we introduce the fluctuating hydrodynamic equations

$$\rho \frac{d\mathbf{u}}{dt} = \mu \Delta \mathbf{u} - \nabla p + \Lambda[\Upsilon(\mathbf{v} - \Gamma \mathbf{u})] + \mathbf{f}_{\text{thm}} \tag{2.1}$$

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

coupled to the elastic structure equations

$$m\frac{d\mathbf{v}}{dt} = -\Upsilon(\mathbf{v} - \Gamma\mathbf{u}) - \nabla_{\mathbf{X}}\Phi[\mathbf{X}] + \mathbf{F}_{\text{thm}} \tag{2.3}$$

$$\frac{d\mathbf{X}}{dt} = \mathbf{v}. \tag{2.4}$$

The thermal fluctuations are given by the Gaussian stochastic fields $\mathbf{f}_{\text{thm}}$ and $\mathbf{F}_{\text{thm}}$ with mean zero and covariances

$$\langle \mathbf{f}_{\text{thm}}(s)\mathbf{f}^T_{\text{thm}}(t)\rangle = -\left(2k_BT\right)\left(\mu\Delta - \Lambda\Upsilon\Gamma\right)\delta(t-s) \tag{2.5}$$

$$\langle \mathbf{F}_{\text{thm}}(s)\mathbf{F}^T_{\text{thm}}(t)\rangle = \left(2k_BT\right)\Upsilon\,\delta(t-s) \tag{2.6}$$

$$\langle \mathbf{f}_{\text{thm}}(s)\mathbf{F}^T_{\text{thm}}(t)\rangle = -\left(2k_BT\right)\Lambda\Upsilon\,\delta(t-s). \tag{2.7}$$

In the notation, the $\mathbf{a}\mathbf{b}^T$ denotes the tensor product of vector fields $\mathbf{a}$ and $\mathbf{b}$, k_BT the thermal energy, $\delta(t-s)$ the Dirac delta function, and $\langle\cdot\rangle$ a probability expectation of the random fields. The fluid velocity is given by $\mathbf{u}$, the structure configuration and velocities by $\mathbf{X}(\mathbf{q})$ and $\mathbf{v}(\mathbf{q})$ with $\mathbf{q}$ the parameterization of the structure. In the case of a finite collection of particles, the positions and velocities are given by $\mathbf{X}(\mathbf{q})$, $\mathbf{v}(\mathbf{q})$ indexed over the integers. The Φ denotes the potential energy associated with the structure configuration. The ρ denotes the fluid density, μ the dynamic fluid viscosity, and m the particle excess mass relative to the fluid (the precise interpretation of course depends on the specific choice of coupling operators). The p denotes the pressure that serves as the Lagrange multiplier to enforce the incompressibility condition $\nabla\cdot\mathbf{u} = 0$.

To provide a model of the fluid-structure interactions, momentum is transferred between the fluid and the structures by the terms $-\Upsilon(\mathbf{v}-\Gamma\mathbf{u})$ and $\Lambda[\Upsilon(\mathbf{v}-\Gamma\mathbf{u})]$. The first term accounts for the drag that the fluid exerts on the structures as they move. The second term accounts for the spatial distribution of the equal-and-opposite forces to the drag that are exerted by the structures on the fluid-body. The operators Λ, Γ serve to transfer information between the Eulerian and Lagrangian descriptions. The Γ determines from the state of the fluid a local reference velocity to which to compare in determining the local drag exerted on the structures. The Λ accounts for how the equal-and-opposite drag force exerted by the structures are distributed spatially within the fluid body. A number of natural conditions arise on these operators to ensure that dissipation in the coupling occurs only through the Υ-drag and not as a consequence of interconversion between the Eulerian and Lagrangian reference frames. This requires the condition that the operators satisfy the adjoint condition $\Lambda = \Gamma^T$, see [30, 1]. Another natural condition to ensure the drag is dissipative is that the operator Υ is positive semi-definite. The general formulation given in 2.1 – 2.7 is referred to throughout as the Stochastic Eulerian Lagrangian Method. For more details concerning the motivation of these equations and their derivation, see [1].

In practice, many different choices can be made for the coupling operators Λ, Γ, and Υ. For the purposes of our analysis, we leave this choice general. However, for concreteness we mention that a common approach is to use local Stokesian drag and the fluid-structure coupling scheme of the *Immersed Boundary Method* [30]. This would give the specific coupling operators

$$\left(\Gamma\mathbf{u}\right)(\mathbf{q}) = \int \delta_a(\mathbf{y} - \mathbf{X}(\mathbf{q}))\mathbf{u}(\mathbf{x},t)d\mathbf{y} \tag{2.8}$$

$$\left(\Lambda\mathbf{F}(\mathbf{q})\right)(\mathbf{y}) = \delta_a(\mathbf{y} - \mathbf{X}(\mathbf{q}))\mathbf{F}(\mathbf{q}) \tag{2.9}$$

$$\Upsilon = 6\pi\mu R. \tag{2.10}$$

The δ_a is a special kernel function localized around the structure designed to have desirable numerical properties that preserve to a good approximation translation invariance of the structure dynamics despite the breaking of this symmetry by the numerical discretization lattice of the fluid. We refer to the specific choice given [30] as the Peskin δ-function. In

the notation, the R is the hydrodynamic radius attributed to the effective local size of the structure. More general coupling schemes can also be developed to which our presented analysis is applicable. For more details on how these fluid-structure approaches are used in practice, see [1, 2, 30].

2.1. Reformulation in Terms of the Total Momentum Density Field. For our analysis it is useful to reformulate the equations in terms of a total momentum density field. This field accounts simultaneously for both the momentum of the fluid and structures at a given location in space. For this purpose we define the *total momentum density field*

$$\mathbf{p}(\mathbf{x},t) = \rho\mathbf{u}(\mathbf{x},t) + \Lambda\left[m\mathbf{v}(t)\right]. \tag{2.11}$$

Also for convenience, and to treat more general approaches for the fluid-structure system, we introduce the operator $\mathcal{L} = \mu\Delta$ in place of the Newtonian stress term. We only assume $\mathcal{L}$ is negative semi-definite throughout. This allows for fluid-structure interactions to be expressed in terms of $\mathbf{p}, \mathbf{v}, \mathbf{X}$ as

$$\frac{d\mathbf{p}}{dt} = \rho^{-1}\mathcal{L}\left(\mathbf{p} - \Lambda[m\mathbf{v}]\right) + \Lambda[-\nabla_{\mathbf{X}}\Phi(\mathbf{X})] + (\nabla_{\mathbf{X}}\Lambda[m\mathbf{v}])\cdot\mathbf{v} + \lambda + \mathbf{g}_{\text{thm}} \tag{2.12}$$

$$m\frac{d\mathbf{v}}{dt} = -\Upsilon\mathbf{v} + \rho^{-1}\Upsilon\Gamma(\mathbf{p} - \Lambda[m\mathbf{v}]) - \nabla_{\mathbf{X}}\Phi(\mathbf{X}) + \zeta + \mathbf{F}_{\text{thm}} \tag{2.13}$$

$$\frac{d\mathbf{X}}{dt} = \mathbf{v}. \tag{2.14}$$

The thermal fluctuations are given by the Gaussian stochastic fields with covariance

$$\langle \mathbf{g}_{\text{thm}}(s)\mathbf{g}^T_{\text{thm}}(t)\rangle = -\left(2k_BT\right)\mathcal{L}\,\delta(t-s) \tag{2.15}$$

$$\langle \mathbf{F}_{\text{thm}}(s)\mathbf{F}^T_{\text{thm}}(t)\rangle = \left(2k_BT\right)\Upsilon\,\delta(t-s) \tag{2.16}$$

$$\langle \mathbf{g}_{\text{thm}}(s)\mathbf{F}^T_{\text{thm}}(t)\rangle = 0. \tag{2.17}$$

The λ and ζ are Lagrange multipliers enforcing holonomic constraints on the system (such as incompressibility of the fluid or rigid-body restrictions on deformations of the structures). The stochastic driving field for the total momentum is related to the stochastic driving fields of the fluid and structures in equations 2.1 and 2.3 by $\mathbf{g}_{\text{thm}} = \mathbf{f}_{\text{thm}} + \Lambda[\mathbf{F}_{\text{thm}}]$, see [1].

An important technical issue is that the total momentum field $\mathbf{p}$ itself need not be incompressible (solenoidal) as a consequence of the somewhat arbitrary way momentum of the structures is spatial distributed by $\Lambda\left[m\mathbf{v}(t)\right]$. This will require some care in our calculations to ensure that the incompressibility constraint is satisfied by the corresponding fluid velocity field $\mathbf{u}$. We handle this technical point by considering a decomposition of the total momentum field into a solenoidal part and non-solenoidal part. An important feature is that only the solenoidal part of the total momentum field plays a significant role in the coupled fluid-structure equations 2.12 – 2.14.

2.2. 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 $\wp$ that projects any field to its solenoidal part we have $\mathbf{u} = \wp\mathbf{u} = \wp\mathbf{p} - \wp\Lambda[m\mathbf{v}]$. This well-known approach for expressing the incompressibility of hydrodynamic equations [9] yields the following closed set of equations for SELM

$$\frac{d(\wp\mathbf{p})}{dt} = \wp\left[\rho^{-1}\mathcal{L}\left(\mathbf{p} - \Lambda[m\mathbf{v}]\right) + \Lambda[-\nabla_{\mathbf{X}}\Phi(\mathbf{X})] + (\nabla_{\mathbf{X}}\Lambda[m\mathbf{v}])\cdot\mathbf{v} + \mathbf{g}_{\text{thm}}\right] \tag{2.18}$$

$$m\frac{d\mathbf{v}}{dt} = -\Upsilon\mathbf{v} + \rho^{-1}\Upsilon\Gamma\wp(\mathbf{p} - \Lambda[m\mathbf{v}]) - \nabla_{\mathbf{X}}\Phi(\mathbf{X}) + \mathbf{F}_{\text{thm}} \tag{2.19}$$

$$\frac{d\mathbf{X}}{dt} = \mathbf{v}. \tag{2.20}$$

We remark that only the dynamics of $\wp\mathbf{p}$ 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 2.12–2.14 when making the substitutions

$$\tilde{\mathbf{p}} = \wp\mathbf{p}, \qquad \tilde{\mathcal{L}} = \wp\mathcal{L}, \qquad \tilde{\Lambda} = \wp\Lambda, \qquad \tilde{\Gamma} = \Gamma\wp. \tag{2.21}$$

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 2.12 – 2.14 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.

3. Dimension Analysis.

To investigate behaviors of the fluid-structure system it is useful to introduce characteristic scales that can be employed to non-dimensionalize the dynamic equations 2.12 – 2.14. The Buckingham Π-theorem provides a useful guide by stating that for a physical system with M parameters and m fundamental physical units the system can be characterized completely by $M-m$ non-dimensional groups $\Pi_1, \cdots, \Pi_{M-m}$ [7]. For the SELM equations there are $M = 7$ distinct parameters $\rho, \mu, m, T, \Phi, \Upsilon, \Gamma$ (note that $\Gamma = \Lambda^T$) and $m = 4$ fundamental physical units *mass, length, time, temperature*. From the Buckingham Π-theorem, we have that SELM is characterized by three non-dimensional groups Π_1, Π_2, Π_3. In principle, There are many possible choices that can be made for these non-dimensional groups. We have found it useful to make the specific choice with this first group characterizing the strength of the coupling that exchanges momentum between the fluid and structures. For the second group, we choose a parameter that characterizes the inertial contributions arising from the differences in density between the fluid and the structures. To define these more precisely, we introduce for SELM some natural characteristic scales for length, time, and mass.

3.1. Characteristic Scales.

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 [34, 17]. 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_BT. We define this time-scale as $\tau_k = \sqrt{m_0\ell^2/k_BT}$, 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

$$\epsilon = \tau_v/\tau_k, \quad \text{with } \Pi_1 = \epsilon. \tag{3.1}$$

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

$$\kappa^{-1} = m/\rho\ell^3 = m/m_0, \quad \text{with } \Pi_2 = \kappa^{-1}. \tag{3.2}$$

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 $\Phi = \Phi_0\bar{\Phi}$,

$$\alpha = \Phi_0/k_BT, \quad \text{with } \Pi_3 = \alpha. \tag{3.3}$$

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 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 :

$$t = \tau_k\bar{t}, \qquad \mathbf{X} = \ell\bar{\mathbf{X}}, \qquad \mathbf{v} = v_0\bar{\mathbf{v}} = \frac{\ell}{\tau_k}\bar{\mathbf{v}}, \tag{3.4}$$

$$\mathbf{p} = p_0\bar{\mathbf{p}} = \frac{m_0}{\tau_k\ell^2}\bar{\mathbf{p}}, \qquad \Lambda = \Lambda_0\bar{\Lambda} = \frac{1}{\ell^3}\bar{\Lambda}, \qquad \mathcal{L} = \mathcal{L}_0\bar{\mathcal{L}} = \frac{m_0}{\ell^3\tau_k}\bar{\mathcal{L}}. \tag{3.5}$$

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

$$\mathbf{g}_{\text{thm}}(\mathbf{X}, s) = g_0\bar{\mathbf{g}}_{\text{thm}} = g_0 D_{-\bar{\mathcal{L}}}\bar{\xi}\left(\frac{\mathbf{X}}{\ell}, \frac{s}{\tau_k}\right), \tag{3.6}$$

$$\mathbf{F}_{\text{thm}}(s) = F_0\bar{\mathbf{F}}_{\text{thm}} = F_0 D_{\bar{\Upsilon}}\bar{\eta}\left(\frac{s}{\tau_k}\right). \tag{3.7}$$

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

$$\langle\bar{\xi}(\bar{\mathbf{X}}, \bar{s})\bar{\xi}^T(\bar{\mathbf{Y}}, \bar{t})\rangle = \delta(\bar{\mathbf{X}} - \bar{\mathbf{Y}})\delta(\bar{s} - \bar{t}), \tag{3.8}$$

$$\langle\bar{\eta}(\bar{s})\bar{\eta}^T(\bar{t})\rangle = \delta(\bar{s} - \bar{t}). \tag{3.9}$$

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

$$g_0{}^2 = \frac{k_BT}{\ell^3\tau_k}\mathcal{L}_0, \qquad F_0{}^2 = \frac{k_BT}{\tau_k}\Upsilon_0, \qquad 2D_AD_A{}^T = A. \tag{3.10}$$

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

$$Re = \rho\ell U/\mu \tag{3.11}$$

where U is a characteristic velocity scale.

3.2. Summary of Non-Dimensional Equations. The SELM equations 2.12–2.14 can be expressed non-dimensionally using the characteristic scales of Section 3.1 as

$$\frac{d\bar{\mathbf{p}}}{dt} = \bar{\mathcal{L}}\left(\bar{\mathbf{p}} - \kappa^{-1}\bar{\Lambda}[\bar{\mathbf{v}}]\right) + \alpha\bar{\Lambda}[-\nabla_{\bar{X}}\bar{\Phi}(\bar{\mathbf{X}})] + \kappa^{-1}\left(\nabla_{\bar{X}}\bar{\Lambda}[\bar{\mathbf{v}}]\right)\cdot\bar{\mathbf{v}} + \bar{\mathbf{g}}_{\text{thm}} \tag{3.12}$$

$$\frac{d\bar{\mathbf{v}}}{dt} = -\frac{1}{\epsilon}\bar{\Upsilon}C_1(\bar{\mathbf{v}} - \bar{\mathbf{v}}_0) - \kappa\alpha\nabla_{\bar{X}}\bar{\Phi}(\bar{\mathbf{X}}) + \sqrt{\frac{1}{\epsilon}}\sqrt{\kappa}\bar{\mathbf{F}}_{\text{thm}} \tag{3.13}$$

$$\frac{d\bar{\mathbf{X}}}{dt} = \bar{\mathbf{v}} \tag{3.14}$$

where

$$C_1 = (I + \kappa^{-1}\bar{\Gamma}\bar{\Lambda}) \tag{3.15}$$

$$\bar{\mathbf{v}}_0 = C_1^{-1}\bar{\Gamma}\bar{\mathbf{p}}. \tag{3.16}$$

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

$$\langle\bar{\mathbf{g}}_{\text{thm}}(s)\bar{\mathbf{g}}^T_{\text{thm}}(t)\rangle = -2\bar{\mathcal{L}}\,\delta(t-s) \tag{3.17}$$

$$\langle\bar{\mathbf{F}}_{\text{thm}}(s)\bar{\mathbf{F}}^T_{\text{thm}}(t)\rangle = 2\bar{\Upsilon}\,\delta(t-s) \tag{3.18}$$

$$\langle\bar{\mathbf{g}}_{\text{thm}}(s)\bar{\mathbf{F}}^T_{\text{thm}}(t)\rangle = 0. \tag{3.19}$$

As discussed in Section 2.2, the constraints are handled implicitly throughout. Our assumption $\kappa\alpha = O(1)$ is made to guarantee that the potential term in 3.13 contributes at order one.

4. Stochastic Reduction. In a few limiting physical regimes, we derive effective fluid-structure dynamics from the inertial SELM equations 2.12– 2.14. 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 $Re \to 0$. We give a summary of our results for the effective equations in each of these physical regimes in Section 4. We then provide our detailed perturbation analysis and derivations of each of these equations in Section 5 and Section 6.

4.1. 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

$$\begin{aligned}\frac{d\mathbf{p}}{dt} &= \rho^{-1}\mathcal{L}\left(\mathbf{p} - \Lambda[m\mathbf{v}_0]\right) - \Lambda\nabla_{\mathbf{X}}\Phi(\mathbf{X}) + \left(\nabla_{\mathbf{X}}\Lambda[m\mathbf{v}_0]\right)\cdot\mathbf{v}_0 \\ &\quad + k_B T\nabla_{\mathbf{X}}\Lambda : C_1^{-1} + \lambda + \mathbf{g}_{\text{thm}} + \theta_p \end{aligned}\tag{4.1}$$

$$\frac{d\mathbf{X}}{dt} = \mathbf{v}_0 + \theta_X. \tag{4.2}$$

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

$$\mathbf{v}_0 = \rho^{-1}C_1^{-1}\Gamma\mathbf{p} \tag{4.3}$$

$$C_1 = I + \rho^{-1}m\Gamma\Lambda. \tag{4.4}$$

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

$$\langle \mathbf{g}_{\text{thm}}(s)\mathbf{g}^T_{\text{thm}}(t)\rangle = -\,(2k_BT)\,\mathcal{L}\,\delta(t-s). \tag{4.5}$$

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 6.2.

4.2. Limit of Strong Coupling : Reduced Equations in Terms of the Effective Fluid Velocity u. The effective fluid velocity field $\bar{\mathbf{u}}$ is obtained from the total momentum field $\mathbf{p}$ by

$$\bar{\mathbf{u}} = \rho^{-1}\left(\mathbf{p} - \Lambda[m(\mathbf{v}_0 + \theta_X)]\right). \tag{4.6}$$

The $\mathbf{v}_0$ is given in Section 4.1 and θ_X is given in Section 6.2. The effective fluid-structure dynamics are

$$\rho\frac{d\bar{\mathbf{u}}}{dt} = \mathcal{L}\bar{\mathbf{u}} + k_BT\nabla_{\mathbf{X}}\Lambda : C_1^{-1} - \Lambda\frac{d}{dt}[m\mathbf{v}_0] - \Lambda\nabla_{\mathbf{X}}\Phi(\mathbf{X}) + \theta_p + \lambda + \mathbf{g}_{\text{thm}} \tag{4.7}$$

$$\frac{d\mathbf{X}}{dt} = \mathbf{v}_0 + \theta_X = \Gamma\bar{\mathbf{u}} + C_1\theta_X \tag{4.8}$$

and

$$\langle \mathbf{g}_{\text{thm}}(s)\mathbf{g}^T_{\text{thm}}(t)\rangle = -\,(2k_BT)\,\mathcal{L}\,\delta(t-s). \tag{4.9}$$

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

$$\mathbf{v}_0 = \Gamma\bar{\mathbf{u}} + \rho^{-1}m\Gamma\Lambda\theta_X. \tag{4.10}$$

The higher-order correction due to the fluid slip is given by θ_X of Section 6.2. These equations were obtained by using the following terms that can be differentiated and combined to yield

$$(\nabla_{\mathbf{X}}\Lambda[m\mathbf{v}_0])\cdot\mathbf{v}_0 - \frac{d}{dt}(\Lambda[m\mathbf{v}_0]) \tag{4.11}$$

$$= (\nabla_{\mathbf{X}}\Lambda[m\mathbf{v}_0])\cdot\mathbf{v}_0 - (\nabla_{\mathbf{X}}\Lambda[m\mathbf{v}_0])\cdot\mathbf{v}_0 - \Lambda\frac{d}{dt}[m\mathbf{v}_0] = \Lambda\frac{d}{dt}[m\mathbf{v}_0]. \tag{4.12}$$

We remark that the effective fluid equations 4.7 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 6.2.

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) since in the strong coupling limit the momentum exchange between the fluid and microstructures becomes increasingly rapid as the coupling strength increases, see Section 2.1. 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 4.6 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 4.7– 4.10 greatly simplify in the limit when the excess body mass becomes negligible relative to the displaced fluid.

4.3. 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 3.2. We approach this limit when the excess mass parameter satisfies $m << \rho\ell^3$. This results in the reduced fluid-structure equations

$$\rho\frac{d\mathbf{u}}{dt} = \mathcal{L}\mathbf{u} - \Lambda\nabla_{\mathbf{X}}\Phi(\mathbf{X}) + k_BT\nabla_{\mathbf{X}}\cdot\Lambda + \lambda + \theta_p + \mathbf{f}_{\text{thm}} \tag{4.13}$$

$$\frac{d\mathbf{X}}{dt} = \Gamma\mathbf{u} + \theta_X \tag{4.14}$$

$$\left\langle \mathbf{f}_{\text{thm}}(t)\mathbf{f}_{\text{thm}}(s)^T \right\rangle = -2k_BT\mathcal{L}\delta(t-s). \tag{4.15}$$

A derivation of these equations is given in Section 6.4.

In this limit, the inertial terms in equations 4.7– 4.8 disappear. This is very similar to the physical regime that is treated by the *Stochastic Immersed Boundary Method* (SIB) in [2]. However, the systematic reduction analysis we perform here in Section 6.1 shows that there is an important drift term that is missing in the original SIB formulation [2]. This corresponds to the term $k_BT\nabla_{\mathbf{X}}\Lambda : C_1^{-1}$ in equation 4.7 which becomes when $m = 0$ the term $k_BT\nabla_{\mathbf{X}}\cdot\Lambda$ in equation 4.13. 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 [1].

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 [30] 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 [30, 1, 2]. To model further inertial effects of structures, some recent extensions of IB have been introduced in [20, 3].

4.4. 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

$$\frac{d\mathbf{X}}{dt} = H_{\text{SELM}}[-\nabla_{\mathbf{X}}\Phi(\mathbf{X})] + (\nabla_{\mathbf{X}} \cdot H_{\text{SELM}})k_BT + \mathbf{h}_{\text{thm}} \tag{4.16}$$

$$H_{\text{SELM}} = \Gamma(\wp\mathcal{L})^{-1}\Lambda \tag{4.17}$$

$$\langle \mathbf{h}_{\text{thm}}(s), \mathbf{h}^T_{\text{thm}}(t)\rangle = 2k_BTH_{\text{SELM}}\delta(t-s). \tag{4.18}$$

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 $(\nabla_{\mathbf{X}} \cdot H_{\text{SELM}})k_BT$. This drift-divergence term is essential for the microstructure dynamics to have invariant the Gibbs-Boltzmann distribution with detailed balance.

5. Stochastic Reduction Method : Singular Perturbation of Backward Kolmogorov Equations. We derive the reduced equations using a method based on a singular perturbation analysis of the Backward-Kolmogorov Equations (BKE) [25, 26, 21, 29]. The BKE are given by

$$\frac{\partial u}{\partial t} = \mathcal{A}u \tag{5.1}$$

$$u(0, \mathbf{z}) = f(\mathbf{z}). \tag{5.2}$$

The $u(t, \mathbf{z}) = E^{\mathbf{z}}[f(\mathbf{Z}(t))]$ with $\mathbf{Z}(t) = (\mathbf{X}(t), \mathbf{p}(t), \mathbf{v}(t))$ [28]. The $E^{\mathbf{z}}[\cdots]$ denotes taking expectation when the stochastic process starts with $\mathbf{Z}(0) = \mathbf{z}$. The $\mathcal{A}$ is the infinitesimal generator of the stochastic process $\mathbf{Z}(t)$. The f is assumed to be a C^2 smooth function with compact support. An important connection is that the statistics of the stochastic process are determined by the expectations taken over the class of functions f. This provides a mapping between the infinitesimal generator $\mathcal{A}$ that appears in the BKE and the underlying stochastic process $\mathbf{Z}(t)$. In particular, consider the stochastic process satisfying

$$d\mathbf{Z}(t) = \mathbf{a}(\mathbf{Z}(t))dt + \mathbf{b}(\mathbf{Z}(t))d\mathbf{W}_t. \tag{5.3}$$

The Stochastic Differential Equation (SDE) is to be given the the Ito interpretation [28]. The corresponding infinitesimal generator is

$$\mathcal{A} = \mathbf{a} \cdot \frac{\partial}{\partial \mathbf{z}} + \frac{1}{2}\mathbf{b}\mathbf{b}^T : \frac{\partial^2}{\partial \mathbf{z}^2}. \tag{5.4}$$

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 5.3. 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 [28].

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

$$\mathcal{A}_\epsilon = L_{slow} + L_{fast}. \tag{5.5}$$

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 6.

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

$$L_2^*\Psi = 0 \tag{5.6}$$

$$\int \Psi d\mathbf{z}_f = 1. \tag{5.7}$$

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

$$L_{fast} = \frac{1}{\epsilon}\left(L_2 + \epsilon\tilde{L}_2\right). \tag{5.8}$$

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

$$L_{slow} = \bar{L}_1 + L_1 \tag{5.9}$$

where

$$\bar{L}_1 = \int \Psi(\mathbf{z}_f|\mathbf{z}_s)L_{slow}d\mathbf{z}_f \tag{5.10}$$

$$L_1 = L_{slow} - \bar{L}_1. \tag{5.11}$$

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

$$\mathcal{A}_\epsilon = \bar{L}_1 + \epsilon L_\epsilon \tag{5.12}$$

$$L_\epsilon = \frac{1}{\epsilon}\left(L_1 + \tilde{L}_2\right) + \frac{1}{\epsilon^2}L_2. \tag{5.13}$$

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

$$u(\mathbf{z},t) = u_0(\mathbf{z},t) + u_1(\mathbf{z},t)\epsilon + u_2(\mathbf{z},t)\epsilon^2 \cdots + u_n(\mathbf{z},t)\epsilon^n + \cdots. \tag{5.14}$$

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

$$\bar{u}(\mathbf{z}_s,t) = u_0(\mathbf{z}_s,t) + \bar{u}_1(\mathbf{z}_s,t)\epsilon \tag{5.15}$$

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 5.14 into 5.1 and using 5.12 we obtain

$$O\left(\epsilon^{-1}\right) : L_2u_0 = 0 \tag{5.16}$$

$$O\left(1\right) : \frac{\partial u_0}{\partial t} = \bar{L}_1u_0 + L_1u_0 + \tilde{L}_2u_0 + L_2u_1 \tag{5.17}$$

$$O\left(\epsilon\right) : \frac{\partial u_1}{\partial t} = \bar{L}_1u_1 + L_1u_1 + \tilde{L}_2u_1 + L_2u_2. \tag{5.18}$$

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 5.6. 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 $O(1)$ can be used to solve for u_1 in terms of u_0 by

$$L_2 u_1 = \frac{\partial u_0}{\partial t} - \bar{L}_1 u_0 - L_1 u_0. \tag{5.19}$$

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 5.19 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 $\overline{\text{range}\{L_2\}} = \overline{\ker\{L_2^*\}^\perp}$, where $\perp$ denotes the orthogonal compliment of a set under the standard L^2-inner product, see [33]. By our ergodicity assumption the kernel only has one dimension and the solvability can be represented by the condition

$$\int \Psi \left(\frac{\partial}{\partial t} - \bar{L}_1 - L_1\right) d\mathbf{z}_f u_0 = 0. \tag{5.20}$$

The Ψ is the stationary probability density satisfying equation 5.6. This yields the BKE for the leading order

$$\frac{\partial u_0}{\partial t} = \bar{L}_1 u_0. \tag{5.21}$$

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 5.19 provides the equation 5.21 for the leading order u_0. Using equation 5.19, the order u_1 can be expressed as

$$u_1 = L_2^{-1}\left(\frac{\partial u_0}{\partial t} - (\bar{L}_1 + L_1)u_0\right) = -L_2^{-1} L_1 u_0. \tag{5.22}$$

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 5.21. Now at the order $O(\epsilon)$ a very similar argument can be made to ensure the solvability of u_2. This yields

$$\frac{\partial \bar{u}_1}{\partial t} = -\int \Psi \left(\bar{L}_1 + L_1 + \tilde{L}_2\right) L_2^{-1} L_1 d\mathbf{z}_f u_0 \tag{5.23}$$

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 5.21 and 5.23.

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

$$\frac{\partial \bar{u}}{\partial t} = \bar{L}_1 u_0 + \epsilon \left(-\int \Psi \left(\bar{L}_1 + L_1 + \tilde{L}_2\right) L_2^{-1} L_1 d\mathbf{z}_f\right) u_0. \tag{5.24}$$

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

$$\bar{u} = \left(\mathcal{I} - \epsilon \int \Psi L_2^{-1} L_1 d\mathbf{z}_f\right) u_0. \tag{5.25}$$

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

$$u_0 = \left(\mathcal{I} + \epsilon \int \Psi L_2^{-1} L_1 d\mathbf{z}_f + \epsilon^2 (\cdots) + \cdots \right) \bar{u} \tag{5.26}$$

By neglecting orders greater than ϵ we have

$$\bar{L}_1 u_0 = \bar{L}_1 \bar{u} + \epsilon \bar{L}_1 \int \Psi L_2^{-1} L_1 d\mathbf{z}_f \bar{u}. \tag{5.27}$$

This gives the final set of closed reduced equations

$$\frac{\partial \bar{u}}{\partial t} = \left(\bar{L}_1 + \epsilon \bar{L}_0 \right) \bar{u} \tag{5.28}$$

$$\bar{L}_0 = - \int \Psi \left(L_1 + \tilde{L}_2 \right) L_2^{-1} L_1 d\mathbf{z}_f. \tag{5.29}$$

This follows by using equation 5.27 in equation 5.24 and canceling common terms. This derivation provides a unified expression consistent with the methods used in [24, 25, 26] and the rigorous results obtained in [21, 29]. This provides a BKE with generator $\tilde{\mathcal{A}} = \bar{L}_1 + \epsilon \bar{L}_0$ approximating the full BKE given in equation 5.1. Interestingly, the term L_ϵ of equation 5.13 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 5.3. The equations 5.28 and 5.29 establishes our systematic reduction procedure to approximate the full stochastic dynamics.

6. 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 4. 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.

6.1. 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 3.1. 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.

6.1.1. 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

$$\mathbf{v}_0 = C_1^{-1} \Gamma \mathbf{p} \tag{6.1}$$

$$C_1 = (I + \kappa^{-1} \Gamma \Lambda). \tag{6.2}$$

It will be convenient to introduce

$$C = \kappa^{-1} C_1. \tag{6.3}$$

This serves to center up to terms of order ϵ the equation 3.13 and allows for the equations to be put into the convenient form

$$\frac{d\mathbf{p}}{dt} = \mathcal{L}\left(\mathbf{p} - \kappa^{-1}\Lambda[\mathbf{v}]\right) + \alpha\Lambda[-\nabla_X \Phi(\mathbf{X})] + \kappa^{-1}\left(\nabla_X \Lambda[\mathbf{v}]\right)\cdot(\mathbf{v}) + \mathbf{g}_{\text{thm}} \tag{6.4}$$

$$\frac{d\tilde{\mathbf{v}}}{dt} = \frac{d\mathbf{v}}{dt} - \frac{d\mathbf{v_0}}{dt} = -\frac{1}{\epsilon}\Upsilon C_1 \tilde{\mathbf{v}} + \sqrt{\frac{1}{\epsilon}}\sqrt{\kappa}\mathbf{F}_{\text{thm}} - \alpha\kappa\nabla_X\Phi(\mathbf{X}) - \nabla_{\mathbf{X},\mathbf{p}}\mathbf{v_0}\cdot\frac{d}{dt}(\mathbf{X},\mathbf{p}) \tag{6.5}$$

$$\frac{d\mathbf{X}}{dt} = \mathbf{v}. \tag{6.6}$$

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

$$\mathcal{A} = L_{slow} + L_{fast} \tag{6.7}$$

where

$$L_{slow} = \left[\mathcal{L}\left(\mathbf{p} - \kappa^{-1}\Lambda[\mathbf{v}]\right) + \alpha\Lambda[-\nabla_{\mathbf{X}}\Phi(\mathbf{X})] + \kappa^{-1}\left(\nabla_{\mathbf{X}}\Lambda[\mathbf{v}]\right)\cdot\mathbf{v}\right]\cdot\nabla_{\mathbf{p}} \tag{6.8}$$

$$-\mathcal{L}:\nabla^2_{\mathbf{p}} + \mathbf{v}\cdot\nabla_{\mathbf{X}} \tag{6.9}$$

$$L_{fast} = [-\Upsilon C_1\tilde{\mathbf{v}}]\cdot\nabla_{\tilde{\mathbf{v}}} + \kappa\Upsilon:\nabla^2_{\tilde{\mathbf{v}}} - \alpha\kappa\nabla_{\mathbf{X}}\Phi(\mathbf{X})\cdot\nabla_{\tilde{\mathbf{v}}} - \mathcal{A}\left[\nabla_{\mathbf{X},\mathbf{p}}\mathbf{v_0}\cdot\frac{d}{dt}(\mathbf{X},\mathbf{p})\right]. \tag{6.10}$$

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

$$L_{fast} = L_2 + \tilde{L}_2 \tag{6.11}$$

with

$$L_2 = [-\Upsilon C_1\tilde{\mathbf{v}}]\cdot\nabla_{\tilde{\mathbf{v}}} + \kappa\Upsilon:\nabla^2_{\tilde{\mathbf{v}}} \tag{6.12}$$

$$\tilde{L}_2 = -\alpha\kappa\nabla_{\mathbf{X}}\Phi(\mathbf{X})\cdot\nabla_{\tilde{\mathbf{v}}} - \mathcal{A}\left[\nabla_{\mathbf{X},\mathbf{p}}\mathbf{v_0}\cdot\frac{d}{dt}(\mathbf{X},\mathbf{p})\right]. \tag{6.13}$$

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 5.6 for the fast degrees of freedom

$$\Psi(\tilde{\mathbf{v}}) = \frac{\sqrt{\det C}}{(2\pi)^{N/2}}\exp\left[-\frac{1}{2}\tilde{\mathbf{v}}^T C\tilde{\mathbf{v}}\right]. \tag{6.14}$$

This is a Gaussian distribution. The C is given in equation 6.3. 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 5.

We split further the slow operator by

$$L_{slow} = \bar{L}_1 + L_1 \tag{6.15}$$

with

$$\bar{L}_1 = \left(\mathcal{L}(\mathbf{p} - \kappa^{-1}\Lambda\mathbf{v}_0) + \nabla_{\mathbf{X}}\Lambda : C_1^{-1} + \kappa^{-1}(\nabla_{\mathbf{X}}\Lambda[\mathbf{v}_0])\cdot\mathbf{v}_0 - \alpha\Lambda\nabla_{\mathbf{X}}\Phi(\mathbf{X})\right)\cdot\nabla_{\mathbf{p}} \tag{6.16}$$

$$+ \mathbf{v}_0\cdot\nabla_{\mathbf{X}} - \mathcal{L}:\nabla^2_{\mathbf{p}}$$

$$L_1 = L_{slow} - \bar{L}_1. \tag{6.17}$$

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 5.29.

6.1.2. Inverting the L_2 Operator. To obtain the reduced stochastic process including the ϵ-order term, we must determine the operator

$$L_0 = -\int \Psi(L_1 + \tilde{L}_2)L_2^{-1}L_1 d\mathbf{z}_f. \tag{6.18}$$

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 by representing the action of the inverse operator over an orthonormal basis determined from solving a related Sturm-Louiville problem [35], see Appendix A. To apply this 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

$$L_2 = A_{nm}\left(-\alpha_m \partial_{\alpha_n} + \partial_{\alpha_m}\partial_{\alpha_n}\right) \tag{6.19}$$

$$A = C^{1/2}\Upsilon C^{1/2}. \tag{6.20}$$

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

$$L_2 = \sum L_2^{(i)} \tag{6.21}$$

$$L_2^{(i)} = d_i\left(-\beta_i\partial_{\beta_i} + \partial^2_{\beta_i}\right). \tag{6.22}$$

We remark that the cumulative change of variable used is $\boldsymbol{\beta} = Q^T C^{1/2}\tilde{\mathbf{v}}$. We find it convenient also to introduce $\hat{Q} = C^{-1/2}Q$. We can now express the inverse problem in terms of Sturm-Louiville operators, see Appendix A. This is achieved by introducing a factor to define a new operator

$$\hat{L}_2 = e^{-\frac{1}{2}\boldsymbol{\beta}^2}L_2. \tag{6.23}$$

The inverse problem that needs to be solved becomes

$$\hat{L}_2 w = \tilde{f}(\beta)\mu(\beta) \tag{6.24}$$

where $\mu(\beta) = e^{-\frac{1}{2}\boldsymbol{\beta}^2}$ and $\tilde{f} = -L_1u_0$. This gives the eigenvalue problem

$$\sum_i d_i\mu(\beta)\left(-\beta_i\partial_{\beta_i} + \partial^2_{\beta_i}\right)\phi_{\mathbf{k}}(\boldsymbol{\beta}) = \lambda_{\mathbf{k}}\mu(\beta)\phi_{\mathbf{k}}(\boldsymbol{\beta}). \tag{6.25}$$

The separated form of the differential operator allows for the solution to be represented in the separated form $\phi_{\mathbf{k}}(\boldsymbol{\beta}) = \prod_i \phi_{k_i}(\beta_i)$ with $k_i = [\mathbf{k}]_i$, $\beta_i = [\boldsymbol{\beta}]_i$. The equation 6.25 can be

decomposed into distinct Sturm-Louiville problems for the eigenfunctions $\phi_{k_i}(\beta_i)$ by using $p_i(\beta_i) = d_i e^{-\frac{1}{2}\boldsymbol{\beta_i}^2}$, see Appendix A. After some algebra, each of these eigenvalue problems have the general form

$$\phi_k''(\beta) - \beta\phi_k'(\beta) = \tilde{\lambda}_k \phi_k(\beta). \tag{6.26}$$

The β is now simply a scalar variable. In this case, we have the well-known Sturm-Louiville equations for the Hermite Orthogonal Polynomials [35]. The eigenvalues can be shown to be the non-negative integers. We denote the k^{th} Hermite Polynomial by $H_k(\beta)$ and the eigenvalue by $\tilde{\lambda}_k = k \geq 0$ with $k \in \mathbb{Z}^+$. For equation 6.25 this gives the eigenfunctions $\phi_{\mathbf{k}}(\boldsymbol{\beta}) = \prod_i H_{k_i}(\beta_i)$ and the eigenvalues $\lambda_{\mathbf{k}} = \sum_i d_i \tilde{\lambda}_{k_i} = \sum_i d_i k_i$. The action of the inverse operator on a basis element can then be expressed as

$$L_2^{-1}\phi_{\mathbf{k}} = -\left[\sum_i d_i k_i\right]^{-1} \phi_{\mathbf{k}}. \tag{6.27}$$

In the case that $\tilde{f} = -L_1 u_0$ is a polynomial of finite degree in $\mathbf{z}_f$ the inverse is also a finite degree polynomial. For the low degree polynomials that arise from the SELM dynamics these results provide a particularly useful inversion procedure. For convenience, we list here the first few Hermite Polynomials

$$H_0(\beta) = 1 \tag{6.28}$$
$$H_1(\beta) = \beta \tag{6.29}$$
$$H_2(\beta) = \beta^2 - 1. \tag{6.30}$$

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

$$L_2^{-1}\beta_i = -D_{ij}^{-1}\beta_j = -d_i^{-1}\beta_i \tag{6.31}$$
$$L_2^{-1}\beta_i\beta_j = -\left(d_i + d_j\right)^{-1}\beta_i\beta_j, \qquad i \neq j \tag{6.32}$$
$$L_2^{-1}\left(\beta_i^2 - 1\right) = -(2d_i)^{-1}\left(\beta_i^2 - 1\right). \tag{6.33}$$

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 6.32 and 6.33 to obtain

$$L_2^{-1}\left(\beta_i\beta_j - \delta_{ij}\right) = -\left(d_i + d_j\right)^{-1}\left(\beta_i\beta_j - \delta_{ij}\right) = -E_{ij}\left(\beta_i\beta_j - \delta_{ij}\right) \tag{6.34}$$

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

6.1.3. 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 β. To summarize the notation we introduced so far we had

$$A \equiv C^{1/2}\Upsilon C^{1/2}, \tag{6.35}$$
$$D = Q^T A Q \text{ (Q unitarily diagonalizes A)}, \tag{6.36}$$
$$\hat{Q} \equiv C^{1/2}Q, \text{ so that } D = \hat{Q}^T\Upsilon\hat{Q} \tag{6.37}$$
$$\boldsymbol{\beta} \equiv \hat{Q}^T\tilde{\mathbf{v}}. \tag{6.38}$$

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

$$T \equiv \mathbf{v}_0 \boxtimes \left[\mathcal{L}\left(\mathbf{p} - \kappa^{-1}\Lambda[\mathbf{v}_0]\right) - \alpha\Lambda[\nabla_X\Phi(\mathbf{X})] + \nabla_{\mathbf{X}}\Lambda : C_1^{-1} + \kappa^{-1}(\nabla_{\mathbf{X}}\Lambda[\mathbf{v}_0])\cdot\mathbf{v}_0\right] \tag{6.39}$$
$$R \equiv \mathcal{I}_{N\times N} \boxtimes B, \quad \text{with} \tag{6.40}$$
$$B \equiv \kappa^{-1}\left[-\mathcal{L}\Lambda(\cdot) + (\nabla_{\mathbf{X}}\Lambda(\cdot))\cdot\mathbf{v}_0 + \nabla_{\mathbf{X}}(\Lambda\mathbf{v}_0)\cdot(\cdot)\right] \tag{6.41}$$
$$S \equiv 0_{N\times N\times N} \boxtimes \kappa^{-1}\nabla_{\mathbf{X}}\Lambda. \tag{6.42}$$

The notation $\boxtimes$ is introduced to "glue-together" two tensors along the first index, so that for A_{ijk} with $1 \le i \le N$ and B_{ijk} with $1 \le i \le M$ we define the new tensor $C = A \boxtimes B$ by $C_{ijk} = A_{ijk}$ when $1 \le i \le N$ and $C_{ijk} = B_{(i-N)jk}$ when $N+1 \le i \le N+M$. 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 6.42 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

$$V = 0_{N\times N} \boxtimes -C_1^{-1}\Gamma\mathcal{L}\Lambda C_1^{-1}. \tag{6.43}$$

where $0_{N\times N}$ denotes a 2-tensor of zeros. Here, C_1 is the same as in 6.2. We also use

$$\mathbf{y} \equiv \mathbf{z_s} = (\mathbf{X}, \mathbf{p}). \tag{6.44}$$

This allows for the slow operator of equation 6.17 to be expressed succinctly as

$$L_1 = \left[R_{ij}\tilde{v}_j + S_{ijk}(\tilde{v}_k\tilde{v}_j - \overline{\tilde{v}_k\tilde{v}_j})\right]\frac{\partial}{\partial y_i}. \tag{6.45}$$

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

$$\hat{R}_{ij} = R_{ik}\hat{Q}_{kj} \qquad\qquad \hat{S}_{ijk} = S_{ilm}\hat{Q}_{lj}\hat{Q}_{mk}. \tag{6.46}$$

We then have for the fast operator an expression in terms of β

$$L_1 = \left[\hat{R}_{ij}\beta_j + \hat{S}_{ijk}(\beta_k\beta_j - \delta_{kj})\right]\frac{\partial}{\partial y_i} = L_1^{(1)} + L_1^{(2)} \quad \text{where} \tag{6.47}$$

$$L_1^{(1)} = \hat{R}_{ij}\beta_j\frac{\partial}{\partial y_i}, \qquad L_1^{(2)} = \hat{S}_{ijk}(\beta_k\beta_j - \delta_{kj})\frac{\partial}{\partial y_i}. \tag{6.48}$$

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

$$\frac{d\mathbf{y}}{dt} = U(\tilde{\mathbf{v}}) + \mathbf{g}_{\text{thm}}, \quad \text{with} \tag{6.49}$$

$$U(\tilde{\mathbf{v}}) = T_i + R_{ij}\tilde{v}_j + S_{ijk}(\tilde{v}_k\tilde{v}_j - \overline{\tilde{v}_k\tilde{v}_j}) \tag{6.50}$$

$$\langle \mathbf{g}_{\text{thm}}(s), \mathbf{g}_{\text{thm}}^T(t)\rangle = 0_{N\times N} \boxtimes -2\mathcal{L}\delta(t-s). \tag{6.51}$$

This allows for the fast operator to be expressed in terms of β as

$$\tilde{L}_2 = \left[-\alpha\kappa\nabla_{\mathbf{X}}\Phi(\mathbf{X}) - \nabla_{\mathbf{y}}\mathbf{v_0}\cdot U(\tilde{\mathbf{v}})\right]\cdot\nabla_{\tilde{\mathbf{v}}} - V : \Delta^2_{\tilde{\mathbf{v}}} \tag{6.52}$$

$$= \left[-\alpha\kappa\nabla_{\mathbf{X}}\Phi(\mathbf{X}) - \nabla_{\mathbf{y}}\mathbf{v_0}\cdot U(\tilde{\mathbf{v}})\right]\cdot\hat{Q}\nabla_{\boldsymbol{\beta}} - \hat{Q}^T V\hat{Q} : \Delta^2_{\boldsymbol{\beta}} \tag{6.53}$$

$$= \left[\tilde{T}_i + \tilde{R}_{ij}\beta_j + \tilde{S}_{ijk}(\beta_k\beta_j - \delta_{kj})\right]\cdot\nabla_{\boldsymbol{\beta}} + \tilde{V} : \Delta^2_{\boldsymbol{\beta}}. \tag{6.54}$$

In these expressions we define

$$\tilde{T} = \hat{Q}^T(-\alpha\kappa\nabla_{\mathbf{X}}\Phi(\mathbf{X}) - \nabla_{\mathbf{y}}\mathbf{v_0}\cdot T) \tag{6.55}$$

$$\tilde{R} = \hat{Q}^T(-\nabla_{\mathbf{y}}\mathbf{v_0}\cdot R) \tag{6.56}$$

$$\tilde{S} = \hat{Q}^T(-\nabla_{\mathbf{y}}\mathbf{v_0}\cdot S) \tag{6.57}$$

$$\tilde{V} = -\hat{Q}^T V\hat{Q}. \tag{6.58}$$

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 β contributes "positively" to the degree. This gives the decomposition

$$\tilde{L}_2 = \sum \tilde{L}_2^{(i)} \tag{6.59}$$

with

$$\begin{aligned} \tilde{L}_2^{(-2)} &= \tilde{V}_{ij}\partial^2_{\beta_{ij}} & \tilde{L}_2^{(-1)} &= \tilde{T}_i\partial_{\beta_i} \\ \tilde{L}_2^{(0)} &= \tilde{R}_{ij}\beta_j\partial_{\beta_i} & \tilde{L}_2^{(1)} &= \tilde{S}_{ijk}(\beta_k\beta_j - \delta_{kj})\partial_{\beta_i}. \end{aligned} \tag{6.60}$$

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

6.1.4. 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 6.14 in terms of the variable $\boldsymbol{\beta}$ and use the associated Jacobian to obtain

$$\Psi(\boldsymbol{\beta}) = (2\pi)^{-N/2}\exp\left[-\frac{1}{2}\boldsymbol{\beta}^2\right]. \tag{6.61}$$

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

$$I_{ij} = -\int \Psi(\boldsymbol{\beta})L_1^{(i)}L_2^{-1}L_1^{(j)}d\boldsymbol{\beta} \tag{6.62}$$

$$J_{ij} = -\int \Psi(\boldsymbol{\beta})\tilde{L}_2^{(i)}L_2^{-1}L_1^{(j)}d\boldsymbol{\beta}. \tag{6.63}$$

The operators $L_1^{(i)}$ and $\tilde{L}_2^{(i)}$ are defined in equations 6.47 and 6.60. 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 6.31– 6.33 and the decomposition of L_1 we have

$$I_{11} = -\int_{\mathbb{R}^N} \psi(\beta)\hat{R}_{nm}\beta_m\partial_{y_n}L_2^{-1}[\hat{R}_{ij}\beta_j\partial_{y_i}]d\beta \tag{6.64}$$

$$= \int_{\mathbb{R}^N} \psi(\beta)\hat{R}_{nm}\beta_m\partial_{y_n}[\hat{R}_{ij}D^{-1}_{jk}\beta_k\partial_{y_i}]d\beta = \hat{R}_{nk}D^{-1}_{jk}\partial_{y_n}[\hat{R}_{ij}\partial_{y_i}]. \tag{6.65}$$

We used the specific inversion formula 6.31 to obtain that $L_2^{-1}[\hat{R}_{ij}\beta_j\partial_{y_i}] = [\hat{R}_{ij}D^{-1}_{jk}\beta_k\partial_{y_i}]$. We can reverse the change of variable to express this in terms of the original variables $(\mathbf{X}, \mathbf{p})$ as

$$I_{11} = R_{nr}C^{-\frac{1}{2}}_{rs}Q_{sk}D^{-1}_{jk}\partial_{y_n}[R_{ip}C^{-\frac{1}{2}}_{pq}Q_{qj}\partial_{y_i}] = R_{nr}\Upsilon^{-1}_{rp}\partial_{y_n}[R_{ip}\partial_{y_i}] \tag{6.66}$$

$$= R_{nr}\Upsilon^{-1}_{rp}R^T_{pi}\partial^2_{y_n y_i} + \Upsilon^{-1}_{np}[\partial_{X_n}B_{ip}]\partial_{p_i} \tag{6.67}$$

$$= (R\Upsilon^{-1}R^T) : \nabla^2_{\mathbf{y}} + [(\nabla_{\mathbf{X}}B) : \Upsilon^{-1}]\cdot\nabla_{\mathbf{p}} \tag{6.68}$$

$$= \Upsilon^{-1} : \nabla^2_{\mathbf{X}} + (B\Upsilon^{-1}B^T) : \nabla^2_{\mathbf{p}} + [(\nabla_{\mathbf{X}}B) : \Upsilon^{-1}]\cdot\nabla_{\mathbf{p}}. \tag{6.69}$$

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 6.41.

We next compute I_{22}. From equation 6.42, 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

$$I_{22} = -\int_{\mathbb{R}^N} \psi(\beta) L_1^{(2)} L_2^{-1} L_1^{(2)} d\beta \tag{6.70}$$

$$= -\int_{\mathbb{R}^N} \psi(\beta)\hat{S}_{ijk}(\beta_j\beta_k - \delta_{jk})\partial_{y_i} L_2^{-1}[\hat{S}_{lmn}(\beta_m\beta_n - \delta_{mn})\partial_{y_l}] d\beta \tag{6.71}$$

$$= \int_{\mathbb{R}^N} \psi(\beta)\hat{S}_{ijk}(\beta_j\beta_k - \delta_{jk})\partial_{y_i}\left[\sum_{mn} \hat{S}_{lmn}E_{mn}(\beta_m\beta_n - \delta_{mn})\partial_{y_l}\right] d\beta \tag{6.72}$$

$$= \sum_{mn} \hat{S}^{(2)}_{ijk}\hat{S}^{(2)}_{lmn}E_{mn}\int_{\mathbb{R}^N} \psi(\beta)(\beta_j\beta_k - \delta_{jk})\left[(\beta_m\beta_n - \delta_{mn})\right] d\beta\partial^2_{p_ip_l}. \tag{6.73}$$

The inversion formula 6.34 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 6.42. For this reason it is convenient to use the notation for $\hat{S}$ above, $A^{(2)}_{ijk} = A^{(2)}_{(i-N)jk}$ for $i > N$.

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

$$\int_{\mathbb{R}^N} \psi(\beta)\beta_j\beta_k\beta_m\beta_n d\beta \tag{6.74}$$

$$= \frac{1}{(2\pi)^{N/2}}\int_{\mathbb{R}^{N-1}}\left(\int_{\mathbb{R}} \beta_j e^{-\frac{1}{2}\beta_j^2}\beta_k\beta_m\beta_n d\beta_j\right) e^{-\frac{1}{2}\sum_{a\neq j}\beta_a^2} d\beta^{/j} \tag{6.75}$$

$$= \frac{1}{(2\pi)^{N/2}}\int_{\mathbb{R}^N} e^{-\frac{1}{2}\beta_j^2}\partial_{\beta_j}(\beta_k\beta_m\beta_n) d\beta_j e^{-\frac{1}{2}\sum_{a\neq j}\beta_a^2} d\beta^{/j} \tag{6.76}$$

$$= \delta_{jk}\delta_{mn} + \delta_{jm}\delta_{kn} + \delta_{jn}\delta_{km}. \tag{6.77}$$

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

$$\int_{\mathbb{R}^N} \psi(\beta)(\beta_j\beta_k - \delta_{jk})(\beta_m\beta_n - \delta_{mn}) d\beta \tag{6.78}$$

$$= \delta_{jk}\delta_{mn} + \delta_{jm}\delta_{kn} + \delta_{jn}\delta_{km} - 2\delta_{jk}\delta_{mn} + \delta_{jk}\delta_{mn} \tag{6.79}$$

$$= \delta_{jm}\delta_{kn} + \delta_{jn}\delta_{km}. \tag{6.80}$$

This yields

$$I_{22} = \sum_{mn} \hat{S}^{(2)}_{ijk}\hat{S}^{(2)}_{lmn}E_{mn}(\delta_{jm}\delta_{kn} + \delta_{jn}\delta_{km})\partial^2_{p_ip_l} \tag{6.81}$$

$$= \sum_{mn}(\hat{S}^{(2)}_{imn}\hat{S}^{(2)}_{lmn} + \hat{S}^{(2)}_{imn}\hat{S}^{(2)}_{lnm})E_{mn}\partial^2_{p_ip_l}. \tag{6.82}$$

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

$$I_{22} = \sum_{mn}(\hat{S}^{(2)}_{imn}\hat{S}^{(2)}_{lmn} + \frac{1}{2}\hat{S}^{(2)}_{imn}\hat{S}^{(2)}_{lnm} + \frac{1}{2}\hat{S}^{(2)}_{lmn}\hat{S}^{(2)}_{inm})E_{mn}\partial^2_{p_ip_l}. \tag{6.83}$$

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

$$I_{22} = \frac{1}{2}[\sigma\sigma^T]_{il}\partial^2_{p_ip_l} = \frac{1}{2}\sigma\sigma^T : \nabla^2_{\mathbf{p}} \tag{6.84}$$

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

$$\mathcal{W}_{ilmn} = \hat{S}^{(2)}_{imn}\hat{S}^{(2)}_{lmn} + \hat{S}^{(2)}_{imn}\hat{S}^{(2)}_{lnm} = S^{(2)}_{iab}S^{(2)}_{lcd}\hat{Q}_{am}\hat{Q}_{bn}(\hat{Q}_{cm}\hat{Q}_{dn} + \hat{Q}_{cn}\hat{Q}_{dm}). \tag{6.85}$$

Using the form 6.85 in 6.82, we have

$$I_{22} = S^{(2)}_{iab}S^{(2)}_{lcd}\left[\sum_{mn}\hat{Q}_{am}\hat{Q}_{bn}E_{mn}(\hat{Q}_{cm}\hat{Q}_{dn} + \hat{Q}_{cn}\hat{Q}_{dm})\right]\partial^2_{p_ip_l}. \tag{6.86}$$

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

$$I_{22} = \frac{1}{2}S^{(2)}_{iab}S^{(2)}_{lcd}\left[\sum_{mn}(\hat{Q}_{am}\hat{Q}_{bn} + \hat{Q}_{an}\hat{Q}_{bm})E_{mn}(\hat{Q}_{cm}\hat{Q}_{dn} + \hat{Q}_{cn}\hat{Q}_{dm})\right]\partial^2_{p_ip_l}. \tag{6.87}$$

This gives

$$\sigma_{i,\{m,n\}} = S^{(2)}_{iab}(\hat{Q}_{am}\hat{Q}_{bn} + \hat{Q}_{an}\hat{Q}_{bm})\sqrt{E_{mn}}. \tag{6.88}$$

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 6.88. 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

$$\begin{aligned}
J_{-2,2} &= -\int_{\mathbb{R}^N}\psi(\beta)\tilde{L}_2^{(-2)}L_2^{-1}L_1^{(2)}d\beta && (6.89)\\
&= \int_{\mathbb{R}^N}\psi(\beta)\tilde{V}_{ij}\partial^2_{\beta_{ij}}\left[\sum_{mn}\hat{S}_{lmn}E_{mn}(\beta_m\beta_n - \delta_{mn})\partial_{y_l}\right]d\beta && (6.90)\\
&= \int_{\mathbb{R}^N}\psi(\beta)\tilde{V}_{ij}\left[\sum_{mn}\hat{S}_{lmn}E_{mn}(\delta_{jm}\delta_{ni} + \delta_{mi}\delta_{jn})\partial_{y_l}\right]d\beta && (6.91)\\
&= \left[\sum_{mn}\hat{S}_{lmn}E_{mn}(\tilde{V}_{nm} + \tilde{V}_{mn})\partial_{y_l}\right] && (6.92)\\
&= -\frac{1}{2}S_{lab}\left[\sum_{mn}(\hat{Q}_{am}\hat{Q}_{bn} + \hat{Q}_{an}\hat{Q}_{bm})E_{mn}(\hat{Q}_{cm}\hat{Q}_{dn} + \hat{Q}_{dm}\hat{Q}_{cn})\right]V_{cd}\partial_{y_l} && (6.93)\\
&= -\frac{1}{2}S_{lab}\Xi^{cd}_{ab}V_{cd}\partial_{y_l} = -\frac{1}{2}(S : \Xi : V)\cdot\nabla_{\mathbf{y}} = -\frac{1}{2}(S^{(2)} : \Xi : V)\cdot\nabla_{\mathbf{p}} && (6.94)
\end{aligned}$$

Here,

$$\Xi^{cd}_{ab} = \sum_{mn}(\hat{Q}_{am}\hat{Q}_{bn} + \hat{Q}_{an}\hat{Q}_{bm})E_{mn}(\hat{Q}_{cm}\hat{Q}_{dn} + \hat{Q}_{dm}\hat{Q}_{cn}) \tag{6.95}$$

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

$$\sigma\sigma^T = S^{(2)} : \Xi : (S^{(2)})^T = \kappa^{-2}\nabla_{\mathbf{X}}\Lambda : \Xi : (\nabla_{\mathbf{X}}\Lambda)^T \tag{6.96}$$

Next,

$$J_{0,2} = -\int_{\mathbb{R}^N} \psi(\beta)\tilde{L}_2^{(0)} L_2^{-1} L_1^{(2)} d\beta \tag{6.97}$$

$$= \int_{\mathbb{R}^N} \psi(\beta)\tilde{R}_{ij}\beta_j\partial_{\beta_i}\left[\sum_{mn}\hat{S}_{lmn}E_{mn}(\beta_m\beta_n - \delta_{mn})\partial_{y_l}\right] d\beta \tag{6.98}$$

$$= \int_{\mathbb{R}^N} \psi(\beta)\tilde{R}_{ij}\left[\sum_{mn}\hat{S}_{lmn}E_{mn}(\delta_{mi}\beta_j\beta_n + \beta_m\beta_j\delta_{ni})\partial_{y_l}\right] d\beta \tag{6.99}$$

$$= \tilde{R}_{ij}\left[\sum_{mn}\hat{S}_{lmn}E_{mn}(\delta_{mi}\delta_{jn} + \delta_{mj}\delta_{ni})\partial_{y_l}\right] \tag{6.100}$$

$$= \frac{1}{2}S_{lab}\left[\sum_{mn}(\hat{Q}_{am}\hat{Q}_{bn} + \hat{Q}_{an}\hat{Q}_{bm})E_{mn}(\tilde{R}_{mn} + \tilde{R}_{nm})\right]\partial_{y_l} \tag{6.101}$$

$$= S_{lab}\left[\sum_{mn}(\hat{Q}_{am}\hat{Q}_{bn} + \hat{Q}_{an}\hat{Q}_{bm})E_{mn}\tilde{R}_{mn}\right]\partial_{y_l} \tag{6.102}$$

$$= \sum_{nm}\sigma_{l,\{m,n\}}\omega_{mn}\partial_{p_l} = Z\cdot\nabla_{\mathbf{p}} \tag{6.103}$$

We label the tensors

$$\omega_{mn} = \sqrt{E_{mn}}\tilde{R}_{mn} \qquad\qquad Z_i = \sum_{nm}\sigma_{i,\{m,n\}}\omega_{mn}. \tag{6.104}$$

$$J_{-1,1} = -\int_{\mathbb{R}^N}\psi(\beta)\tilde{L}_2^{(-1)}L_2^{-1}L_1^{(1)}d\beta = \int_{\mathbb{R}^N}\psi(\beta)\tilde{T}_i\partial_{\beta_i}[\hat{R}_{lj}D_{jk}^{-1}\beta_k\partial_{y_l}]d\beta \tag{6.105}$$

$$= \int_{\mathbb{R}^N}\psi(\beta)\tilde{T}_i[\hat{R}_{lj}D_{ji}^{-1}\partial_{y_l}]d\beta = \tilde{T}_i\hat{R}_{lj}D_{ji}^{-1}\partial_{y_l} \tag{6.106}$$

$$= -[R\Upsilon^{-1}(\alpha\kappa\nabla_{\mathbf{X}}\Phi(\mathbf{X}) + \nabla_{\mathbf{y}}\mathbf{v_0}\cdot T)]\cdot\nabla_{\mathbf{y}} \tag{6.107}$$

$$= -[\Upsilon^{-1}(\alpha\kappa\nabla_{\mathbf{X}}\Phi(\mathbf{X}) + \nabla_{\mathbf{y}}\mathbf{v_0}\cdot T)]\cdot\nabla_{\mathbf{X}} \tag{6.108}$$

$$-[B\Upsilon^{-1}(\alpha\kappa\nabla_{\mathbf{X}}\Phi(\mathbf{X}) + \nabla_{\mathbf{y}}\mathbf{v_0}\cdot T)]\cdot\nabla_{\mathbf{p}} \tag{6.109}$$

$$J_{1,1} = -\int_{\mathbb{R}^N}\psi(\beta)\tilde{L}_2^{(1)}L_2^{-1}L_1^{(1)}d\beta \tag{6.110}$$

$$= \int_{\mathbb{R}^N}\psi(\beta)\tilde{S}_{inm}(\beta_n\beta_m - \delta_{nm})[\hat{R}_{lj}D_{ji}^{-1}\partial_{y_l}]d\beta = 0 \tag{6.111}$$

$$\tag{6.112}$$

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 6.66, 6.87, 6.89, 6.97, 6.105, and 6.110 we obtain the operator

$$L_0 = \Upsilon^{-1} : \nabla_{\mathbf{X}}^2 + [(\nabla_{\mathbf{X}}B) : \Upsilon^{-1}]\cdot\nabla_{\mathbf{p}} + \frac{1}{2}M : \nabla_{\mathbf{p}}^2 \tag{6.113}$$

$$-\left(\frac{1}{2}S^{(2)} : \Xi : V - Z + B\Upsilon^{-1}(\alpha\kappa\nabla_{\mathbf{X}}\Phi(\mathbf{X}) + \nabla_{\mathbf{y}}\mathbf{v_0}\cdot T)\right)\cdot\nabla_{\mathbf{p}} \tag{6.114}$$

$$-[\Upsilon^{-1}(\alpha\kappa\nabla_{\mathbf{X}}\Phi(\mathbf{X}) + \nabla_{\mathbf{y}}\mathbf{v_0}\cdot T)]\cdot\nabla_{\mathbf{X}} \tag{6.115}$$

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

These results combined with the $\bar{L}_1$ given in equation 6.16 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 4.1 and 4.2, 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 $\kappa^{-1} \to 0$.

6.2. 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) [16, 11]. 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 4.1 by decomposition into the parts

$$\theta_p = \Theta^p + \Theta^p_{\text{thm}} \tag{6.116}$$

$$\theta_X = \Theta^X + \Theta^X_{\text{thm}}. \tag{6.117}$$

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

$$\Theta^p = \Theta^p_0 \bar{\Theta}^p, \qquad \Theta^X = \Theta^X_0 \bar{\Theta}^X. \qquad \Theta^p_{\text{thm}} = \Theta^p_0 \bar{\Theta}^p_{\text{thm}}, \qquad \Theta^X_{\text{thm}} = \Theta^X_0 \bar{\Theta}^X_{\text{thm}} \tag{6.118}$$

where

$$\Theta^p_0 = \left(\frac{m_0}{\tau_k \ell^2}\right), \qquad \Theta^X_0 = \left(\frac{\ell}{\tau_k}\right). \tag{6.119}$$

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

$$\bar{\Theta}^p = \epsilon\Big((\nabla_{\mathbf{X}} B) : \Upsilon^{-1} - \frac{1}{2} S^{(2)} : \Xi : V + Z - B\Upsilon^{-1}(\alpha\kappa\nabla_{\mathbf{X}}\Phi(\mathbf{X}) + \nabla_{\mathbf{y}}\mathbf{v_0}\cdot T)\Big) \tag{6.120}$$

$$\bar{\Theta}^X = \epsilon\left(-\Upsilon^{-1}(\alpha\kappa\nabla_{\mathbf{X}}\Phi(\mathbf{X}) + \nabla_{\mathbf{y}}\mathbf{v_0}\cdot T)\right). \tag{6.121}$$

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:

$$\left\langle \bar{\Theta}^p_{\text{thm}}(\bar{s})(\bar{\Theta}^p_{\text{thm}})^T(\bar{t})\right\rangle = \epsilon\left(\sigma\sigma^T + 2(B\bar{\Upsilon}^{-1}B^T)\right)\,\delta(\bar{t}-\bar{s}), \tag{6.122}$$

$$\left\langle \bar{\Theta}^X_{\text{thm}}(\bar{s})(\bar{\Theta}^X_{\text{thm}})^T(t)\right\rangle = 2\epsilon\bar{\Upsilon}^{-1}\,\delta(\bar{t}-\bar{s}). \tag{6.123}$$

The Ξ is given in equation 6.95, Z is given in equation 6.104, and σ is given in equation 6.96. The T, B, S, and V are defined in equations 6.39, 6.41, 6.42, and 6.43. A derivation of these equations is given in Section 6.1. 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.

6.3. 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 6.16. In the limit $\kappa^{-1} \to 0$ we find

$$\bar{L}_1 = (\mathcal{L}\mathbf{p} + \nabla_{\mathbf{X}}\Lambda : \mathcal{I} - \Lambda\nabla_{\mathbf{X}}\Phi(\mathbf{X})) \cdot \nabla_{\mathbf{p}} + \mathbf{v}_0 \cdot \nabla_{\mathbf{X}} - \mathcal{L} : \nabla^2_{\mathbf{p}} \tag{6.124}$$

Equations 6.1–6.2 simplify to

$$\mathbf{v}_0 = \Gamma\mathbf{u}. \tag{6.125}$$

We write

$$\nabla_{\mathbf{X}}\Lambda : \mathcal{I} = \mathrm{tr}[\nabla_{\mathbf{X}}\Lambda] = \nabla_{\mathbf{X}} \cdot \Lambda. \tag{6.126}$$

We obtain 4.13–4.15 by adding the units to the non-dimensional variables and writing the equation in its dynamical form.

6.3.1. 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

$$\frac{1}{2}\sigma\sigma^T = (\Upsilon_0 C_0 \kappa^2)^{-1}[(\nabla_{\mathbf{X}}\Lambda) : (\nabla_{\mathbf{X}}\Lambda)^T] : \nabla^2_{\mathbf{p}} \tag{6.127}$$

$$\sigma_{i,\{m,n\}} = \sqrt{2}(\Upsilon_0 C_0 \kappa^2)^{-1/2}(\nabla_{\mathbf{X}}\Lambda)_{inm}. \tag{6.128}$$

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:

$$L_0 = \Upsilon_0^{-1}[\mathrm{tr}\nabla^2_{\mathbf{X}}] + \Upsilon_0^{-1}(\nabla_{\mathbf{y}}\mathbf{v_0} \cdot T) \cdot \nabla_{\mathbf{X}}. \tag{6.129}$$

6.4. 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

$$\rho\frac{d\mathbf{u}}{dt} = \mathcal{L}\mathbf{u} - \Lambda\nabla_{\mathbf{X}}\Phi(\mathbf{X}) + k_B T\nabla_{\mathbf{X}} \cdot \Lambda + \mathbf{f}_{\mathrm{thm}} + \lambda \tag{6.130}$$

$$\frac{d\mathbf{X}}{dt} = \Gamma\mathbf{u}. \tag{6.131}$$

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

$$\lambda = -(\mathcal{I} - \wp)(\mathcal{L}\mathbf{u} - \Lambda\nabla_{\mathbf{X}}\Phi(\mathbf{X}) + k_B T\nabla_{\mathbf{X}} \cdot \Lambda + \mathbf{f}_{\mathrm{thm}}). \tag{6.132}$$

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

$$\rho\frac{d\mathbf{u}}{dt} = \wp[\mathcal{L}\mathbf{u} - \Lambda\nabla_{\mathbf{X}}\Phi(\mathbf{X}) + k_B T\nabla_{\mathbf{X}} \cdot \Lambda + \mathbf{f}_{\mathrm{thm}}] \tag{6.133}$$

$$\frac{d\mathbf{X}}{dt} = \Gamma\mathbf{u}. \tag{6.134}$$

We assume that $\wp\mathcal{L} = \mathcal{L}\wp$ and make use of the properties $\wp^2 = \wp$ and $\wp = \wp^T$. We can express this in non-dimensionalized form with $\epsilon = Re$ as

$$\frac{d\mathbf{u}}{dt} = \wp\left[\frac{1}{\epsilon}\mathcal{L}\mathbf{u} - \Lambda\nabla_{\mathbf{X}}\Phi(\mathbf{X}) + \nabla_{\mathbf{X}}\cdot\Lambda + \sqrt{\frac{1}{\epsilon}}\mathbf{f}_{\text{thm}}\right] \tag{6.135}$$

$$\frac{d\mathbf{X}}{dt} = \Gamma\mathbf{u}. \tag{6.136}$$

The infinitesimal generator is given by

$$\mathcal{A} = \frac{1}{\epsilon}[\wp\mathcal{L}\mathbf{u} + \epsilon\wp(-\Lambda\nabla_{\mathbf{X}}\Phi(\mathbf{X}) + \nabla_{\mathbf{X}}\cdot\Lambda)]\cdot\nabla_{\mathbf{u}} - \frac{1}{\epsilon}(\wp\mathcal{L}) : \nabla^2_{\mathbf{u}} + [\Gamma\mathbf{u}]\cdot\nabla_{\mathbf{X}}. \tag{6.137}$$

To apply our perturbation analysis introduced in Section 4, we split the operator as

$$\mathcal{A} = L_{slow} + L_{fast} \tag{6.138}$$

with

$$L_{slow} = \bar{L}_1 + L_1 \tag{6.139}$$

$$L_{fast} = L_2 + \tilde{L}_2. \tag{6.140}$$

In this regime we have

$$\bar{L}_1 = 0 \tag{6.141}$$

$$L_1 = (\Gamma\mathbf{u})\cdot\nabla_{\mathbf{X}} \tag{6.142}$$

$$L_2 = (\wp\mathcal{L}\mathbf{u})\cdot\nabla_{\mathbf{u}} - (\wp\mathcal{L}) : \nabla^2_{\mathbf{u}} \tag{6.143}$$

$$\tilde{L}_2 = \wp(-\Lambda\nabla_{\mathbf{X}}\Phi(\mathbf{X}) + \nabla_{\mathbf{X}}\cdot\Lambda)\cdot\nabla_{\mathbf{u}}. \tag{6.144}$$

We remark that each of the coefficients of L_2 and $\tilde{L}_2$ are in the range of $\wp$. Using the linearity of $\wp$ and $\mathcal{L}$ we may interpret the derivatives $\nabla_{\mathbf{u}}$ as $\nabla_{\wp\mathbf{u}}$ 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

$$L_2^{-1}\mathbf{u} = \mathcal{L}^{-1}\mathbf{u}, \qquad \text{for } u \in \mathcal{S}. \tag{6.145}$$

This allows us to carry out readily the inverse

$$L_1 L_2^{-1} L_1 = L_1 L_2^{-1}[(\Gamma\mathbf{u})\cdot\nabla_{\mathbf{X}}] = L_1[(\Gamma\mathcal{L}^{-1}\mathbf{u})\cdot\nabla_{\mathbf{X}}] \tag{6.146}$$

$$= (\Gamma\mathbf{u})\cdot\nabla_{\mathbf{X}}[(\Gamma\mathcal{L}^{-1}\mathbf{u})\cdot\nabla_{\mathbf{X}}], \qquad \text{for } u \in \mathcal{S}. \tag{6.147}$$

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

$$L_1 L_2^{-1} L_1 = (\Gamma\mathbf{u})\cdot\nabla_{\mathbf{X}}[(\Gamma\mathcal{L}^{-1}\mathbf{u})\cdot\nabla_{\mathbf{X}}] \tag{6.148}$$

$$= \nabla_{\mathbf{X}}\cdot\{(\Gamma\mathbf{u})[(\Gamma\mathcal{L}^{-1}\mathbf{u})\cdot\nabla_{\mathbf{X}}]\} - (\nabla_{\mathbf{X}}\cdot(\Gamma\mathbf{u}))[(\Gamma\mathcal{L}^{-1}\mathbf{u})\cdot\nabla_{\mathbf{X}}]. \tag{6.149}$$

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

$$\int_{u\in\mathcal{S}} \psi(\mathbf{u}) L_1 L_2^{-1} L_1 = \nabla_{\mathbf{X}}\cdot[(\Gamma\mathcal{L}^{-1}\wp\Lambda)\cdot\nabla_{\mathbf{X}}] - (\Gamma\mathcal{L}^{-1}\wp\nabla_{\mathbf{X}}\cdot\Lambda)\cdot\nabla_{\mathbf{X}} \tag{6.150}$$

$$= [\nabla_{\mathbf{X}}\cdot(\Gamma\mathcal{L}^{-1}\wp\Lambda)]\cdot\nabla_{\mathbf{X}} + (\Gamma\mathcal{L}^{-1}\wp\Lambda) : \nabla^2_{\mathbf{X}} - (\Gamma\mathcal{L}^{-1}\wp\nabla_{\mathbf{X}}\cdot\Lambda)\cdot\nabla_{\mathbf{X}}. \tag{6.151}$$

We can evaluate the remaining integral term in L_0 by

$$\int_{u\in\mathcal{S}} \psi(\mathbf{u})\tilde{L}_2 L_2^{-1} L_1 \tag{6.152}$$

$$= \int_{u\in\mathcal{S}} \psi(\mathbf{u})\wp(-\Lambda\nabla_{\mathbf{X}}\Phi(\mathbf{X}) + \nabla_{\mathbf{X}}\cdot\Lambda)\cdot\nabla_{\mathbf{u}}[(\Gamma\mathcal{L}^{-1}\mathbf{u})\cdot\nabla_{\mathbf{X}}] \tag{6.153}$$

$$= \int_{u\in\mathcal{S}} \psi(\mathbf{u})[(\Gamma\mathcal{L}^{-1}\wp(-\Lambda\nabla_{\mathbf{X}}\Phi(\mathbf{X}) + \nabla_{\mathbf{X}}\cdot\Lambda))\cdot\nabla_{\mathbf{X}}] \tag{6.154}$$

$$= (\Gamma\mathcal{L}^{-1}\wp(-\Lambda\nabla_{\mathbf{X}}\Phi(\mathbf{X}) + \nabla_{\mathbf{X}}\cdot\Lambda))\cdot\nabla_{\mathbf{X}}. \tag{6.155}$$

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

$$\bar{L} = -\epsilon\left(\int_{u\in\mathcal{R}(\wp)} \psi(\mathbf{u})\tilde{L}_2 L_2^{-1} L_1 + \int_{u\in\mathcal{R}(\wp)} \psi(\mathbf{u}) L_1 L_2^{-1} L_1\right) \tag{6.156}$$

$$= -\epsilon\Big\{(\Gamma\mathcal{L}^{-1}\wp[-\Lambda\nabla_{\mathbf{X}}\Phi(\mathbf{X}) + \nabla_{\mathbf{X}}\cdot\Lambda])\cdot\nabla_{\mathbf{X}} \tag{6.157}$$

$$+ [\nabla_{\mathbf{X}}\cdot(\Gamma\mathcal{L}^{-1}\wp\Lambda)]\cdot\nabla_{\mathbf{X}} + (\Gamma\mathcal{L}^{-1}\wp\Lambda) : \nabla^2_{\mathbf{X}} - (\Gamma\mathcal{L}^{-1}\wp\nabla_{\mathbf{X}}\cdot\Lambda)\cdot\nabla_{\mathbf{X}}\Big\} \tag{6.158}$$

$$= \epsilon\Big\{\Big[\Gamma(-\mathcal{L})^{-1}\wp[-\Lambda\nabla_{\mathbf{X}}\Phi(\mathbf{X})] + [\nabla_{\mathbf{X}}\cdot(\Gamma(-\mathcal{L})^{-1}\wp\Lambda)]\Big]\cdot\nabla_{\mathbf{X}} \tag{6.159}$$

$$+ (\Gamma(-\mathcal{L})^{-1}\wp\Lambda) : \nabla^2_{\mathbf{X}}\Big\}. \tag{6.160}$$

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

$$\bar{L} = \epsilon\Big\{\Big[\tilde{H}_{\text{SELM}}(-\nabla_{\mathbf{X}}\Phi(\mathbf{X})) + \nabla_{\mathbf{X}}\cdot\tilde{H}_{\text{SELM}}\Big]\cdot\nabla_{\mathbf{X}} + \tilde{H}_{\text{SELM}} : \nabla^2_{\mathbf{X}}\Big\}. \tag{6.161}$$

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

$$\frac{d\mathbf{X}}{dt} = H_{\text{SELM}}[-\nabla_{\mathbf{X}}\Phi(\mathbf{X})] + (\nabla_{\mathbf{X}}\cdot H_{\text{SELM}})k_BT + \mathbf{h}_{\text{thm}} \tag{6.162}$$

$$H_{\text{SELM}} = \Gamma(-\mathcal{L})^{-1}\wp\Lambda \tag{6.163}$$

$$\langle\mathbf{h}_{\text{thm}}(s), \mathbf{h}^T_{\text{thm}}(t)\rangle = 2k_BTH_{\text{SELM}}\delta(t-s). \tag{6.164}$$

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

7. Conclusions. We have shown how to systematically reduce in different physical regimes the inertial dynamics of fluid-structure interactions subject to thermal fluctuations. We have shown in the limit of strong coupling between the fluid and microstructures important terms appear in the fluid equations that account for inertial effects. We have further shown that in the limit of small excess mass of immersed bodies relative to the displaced fluid, important thermal drift terms arise in the fluid equations arising from the generalized coordinates used in the mechanics (non-conjugate configuration and momentum coordinates). In the over-damped limit where the hydrodynamics relaxes rapidly on the time-scale of the microstructure motion, we have shown how the approximate fluid-structure coupling operators contribute to the effective hydrodynamic tensor that couples the motions of the microstructures. The presented reduction approach and reduced equations allow for removing sources of numerical stiffness and provide a promising approach for the development of efficient computational methods for simulations of fluid-structure interactions subject to thermal fluctuations.

8. Acknowledgements. The author P.J.A. and G.T. acknowledges support from research grant NSF CAREER DMS - 0956210 and DOE CM4. G.T also acknowledges undergraduate support from NSF REU DMS-0852065 and undergraduate support from the UCSB CCS program.

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Appendix A. Inverting L_2 : A General Method based on Sturm-Louiville Theory.

In the stochastic reduction procedure of Section 4 the operator L_2 needs to be inverted. In general, this presents one of the most significant challenges in determining the form of the reduced equations. Interestingly in the regimes we consider for the SELM stochastic dynamics, the L_2 operators can be related to Sturm-Louiville problems [35] and the inversions can be represented readily over a finite sum over elements of an orthonormal basis of known functions. We first develop this general theory and then show how it can be used as an effective method to invert the L_2 operators that arise in practice for the SELM stochastic dynamics.

The L_2 is an infinitesimal generator of a stochastic process and second order differential operator. We refer to it as a Sturm-Louiville operator (for short a SL-operator) if it has the specific form

$$L_2 = -\frac{\partial}{\partial z}\left[p(z)\frac{\partial}{\partial z}\right] + q(z) \tag{A.1}$$

where $p(z) > 0$ and $q(z) \geq 0$. In practice, not all of the infinitesimal generators we encounter will be SL-operators directly but with a change of variable and other related adjustments can be related to an operator of this form. The inverses we encounter are typically of the form $w = -L_2^{-1}L_1 u$ which amounts to finding a solution to the problem

$$L_2 w = f(z). \tag{A.2}$$

As we shall discuss the functions $f(z)$ that arise in practice often have special properties that we can utilize. The Sturm-Louiville property has the important consequence that an orthonormal basis of eigenfunctions can be constructed for this operator by solving

$$L_2\phi_n = \lambda_n \mu(z)\phi_n. \tag{A.3}$$

The μ is some fixed function with $\mu(z) > 0$ which serves to give a weighted inner product

$$\langle g(z), h(z)\rangle_\mu = \int g(z)\overline{h(z)}\mu(z)dz. \tag{A.4}$$

Since ϕ_n are eigenfunctions of L_2 in the sense of equation A.3, it is useful to express the inversion problem as

$$L_2 w = \tilde{f}(z)\mu(z) \tag{A.5}$$

where $\tilde{f}(z) = f(z)/\mu(z)$. The orthonormal basis can then be used to represent both w and $\tilde{f}$ as

$$\tilde{f}(z) = \sum_k \tilde{f}_k \phi_k(z) \tag{A.6}$$

$$w(z) = \sum_k w_k \phi_k(z) \tag{A.7}$$

$$\tilde{f}_k = \langle \tilde{f}(z), \phi_k(z) \rangle_\mu \tag{A.8}$$

$$w_k = \langle v(z), \phi_k(z) \rangle_\mu. \tag{A.9}$$

Plugging this into equation A.5 gives

$$\langle L_2 u, \phi_k(z) \rangle = w_k \lambda_k = \tilde{f}_k. \tag{A.10}$$

The $\langle \cdot, \cdot \rangle$ without the subscript denotes the usual unweighted L^2-inner-product. For the inverse $w = L_2^{-1} f$, this provides the following representation

$$w(z) = \sum_k w_k \phi_k(z) \tag{A.11}$$

$$w_k = \tilde{f}_k / \lambda_k. \tag{A.12}$$

Appendix B. 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.