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# Spatially adaptive stochastic methods for fluid–structure interactions subject to thermal fluctuations in domains with complex geometries

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ABSTRACT

We develop stochastic mixed finite element methods for spatially adaptive simulations of fluid–structure interactions when subject to thermal fluctuations. To account for thermal fluctuations, we introduce a discrete fluctuation–dissipation balance condition to develop compatible stochastic driving fields for our discretization. We perform analysis that shows our condition is sufficient to ensure results consistent with statistical mechanics. We show the Gibbs–Boltzmann distribution is invariant under the stochastic dynamics of the semi-discretization. To generate efficiently the required stochastic driving fields, we develop a Gibbs sampler based on iterative methods and multigrid to generate fields with $O(N)$ computational complexity. Our stochastic methods provide an alternative to uniform discretizations on periodic domains that rely on Fast Fourier Transforms. To demonstrate in practice our stochastic computational methods, we investigate within channel geometries having internal obstacles and no-slip walls how the mobility/diffusivity of particles depends on location. Our methods extend the applicability of fluctuating hydrodynamic approaches by allowing for spatially adaptive resolution of the mechanics and for domains that have complex geometries relevant in many applications.



## 0. Introduction

We develop general computational methods for applications involving the microscopic mechanics of spatially extended elastic bodies within a fluid that are subjected to thermal fluctuations. Motivating applications include the study of the microstructures of complex fluids [17], lipid bilayer membranes [28,33,49], and micro-mechanical devices [29,38]. Even in the deterministic setting, the mechanics of fluid–structure interactions pose a number of difficult and long-standing challenges owing to the rich behaviors that can arise from the interplay of the fluid flow and elastic stresses of the microstructures [19,43]. To obtain descriptions tractable for analysis and simulations, approximations are often introduced into the fluid–structure coupling. For deterministic systems, many spatially adaptive numerical methods have been developed for approximate fluid–structure interactions [2,25,26,30,36,40]. In the presence of thermal fluctuations, additional challenges

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arise from the need to capture in computational methods the appropriate propagation of fluctuations throughout the discretized system to obtain results consistent with statistical mechanics. In practice, challenges arise from the very different dissipative properties of the discrete operators relative to their continuum differential counterparts. These issues have important implications for how stochastic fluctuations should be handled in the discrete setting. Even when it is possible to formulate stochastic driving fields in a well-founded manner consistent with statistical mechanics, these Gaussian random fields have often many degrees of freedom and non-trivial spatial correlations that can be difficult to sample without significant computational expense. Many finite difference methods on uniform periodic meshes have been developed for fluctuating hydrodynamics [6,7,9,16,18,42,48]. One of the main reasons that fluctuating hydrodynamics is treated on uniform periodic domains is so that stochastic driving fields can be generated using Fast Fourier Transforms (FFTs) [6,7]. Here, we take a different approach by developing stochastic methods based on Finite Element Methods for fluctuating hydrodynamics and provide an alternative to Fast Fourier Transforms for the generation of stochastic driving fields. Our approach allows for non-uniform spatially adaptive discretizations on non-periodic domains with geometries more naturally encountered in many applications.

We develop Finite Element Methods with properties that facilitate the introduction of stochastic driving fields and their efficient generation. We show our discretization approach provides operators that satisfy certain symmetry and commutation conditions that are important when subject to the incompressibility constraint for how thermal fluctuations propagate throughout the discrete system. We formulate the stochastic equations for our fluid–structure system subject to thermal fluctuations in Section 1. We introduce for a given spatial discretization our general procedure for deriving compatible stochastic driving fields that model the thermal fluctuations in a manner consistent with statistical mechanics in Section 2. To obtain the stochastic driving fields with the required spatial correlation structure, we develop stochastic iterative methods based on multigrid to generate the Gaussian random fields with computational complexity $O(N)$ in Section 3. We present validation of our stochastic numerical methods with respect to the hydrodynamic coupling and thermal fluctuations in Section 5. To demonstrate our approach in practice, we present simulations of a few example systems in Section 6.

Overall, our approach extends the range of problems that can be treated numerically with fluctuating hydrodynamic methods by allowing for arbitrary geometries with walls having no-slip boundary conditions and by allowing for spatially adaptive resolution. Many of the central ideas used for our numerical approximation of the fluctuating hydrodynamic equations should also be applicable in the approximation of other parabolic Stochastic Partial Differential Equations (SPDEs). We expect our stochastic numerical methods for fluctuating hydrodynamics to be useful in applications where the domain geometry plays an important role.

## 1. Fluid–structure hydrodynamics and fluid–structure interactions

We describe the mechanics of fluid–structure interactions subject to thermal fluctuations using the Stochastic Eulerian Lagrangian Method (SELM) [6]. In the inertial regime this is given by momentum equations for the fluid coupled to momentum equations for the microstructures [6]. We consider here the regime in which the fluid–structure coupling is strong and the microstructures are mass density matched with the fluid [4,6]. This regime is closely related to the Stochastic Immersed Boundary Method [4,7,14,37]. In this regime, we use the time-dependent Stokes equations for the fluid coupled to an equation of motion for the microstructures

$$\begin{aligned} &\rho\frac{\partial \boldsymbol{u}}{\partial t} = \mu\Delta\boldsymbol{u} - \nabla p + \boldsymbol{f}_s + \boldsymbol{f}_{thm} \quad \text{in } \Omega \\ &\nabla\cdot\boldsymbol{u} = 0 \quad \text{in } \Omega \\ &\boldsymbol{u}|_{\partial\Omega} = 0. \end{aligned} \tag{1.1}$$

The elastic microstructures with configuration $\mathbf{X}$ are given by the following equation of motion and coupling condition that models the bidirectional coupling between the fluid and microstructures

$$\frac{d\mathbf{X}}{dt} = \Gamma\mathbf{u} \tag{1.2}$$

$$\boldsymbol{f}_s = \Lambda\big[-\nabla\Phi(\mathbf{X})\big]. \tag{1.3}$$

The thermal fluctuations are taken into account by the Gaussian random field $\boldsymbol{f}_{thm}$ which when decomposed into a mean and fluctuating part $\boldsymbol{f}_{thm} = \bar{\boldsymbol{f}}_{thm} + \tilde{\boldsymbol{f}}_{thm}$ has the form

$$\bar{\boldsymbol{f}}_{thm} = \langle\boldsymbol{f}_{thm}\rangle = k_B T\nabla_{\mathbf{X}}\cdot\Lambda \tag{1.4}$$

$$\big\langle\tilde{\boldsymbol{f}}_{thm}(s,\mathbf{x})\tilde{\boldsymbol{f}}_{thm}^T(t,\mathbf{y})\big\rangle = 2\mu\Delta C(\mathbf{x}-\mathbf{y})\delta(t-s) \tag{1.5}$$

$$C(\mathbf{x}-\mathbf{y}) = k_B T\rho^{-1}\delta(\mathbf{x}-\mathbf{y}). \tag{1.6}$$

These stochastic driving fields were derived for the mechanical system using the SELM framework in [6]. A notable difference with the original formulation of the Stochastic Immersed Boundary Method (SIBM) is the presence of the thermal drift term in Eq. (1.4) which arises from the more systematic treatment through stochastic averaging to obtain in this regime