Stochastic Immersed Boundary Method Incorporating Thermal Fluctuations

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We give a brief introduction to the stochastic immersed boundary method which allows for simulation of small length-scale physical systems in which elastic structures interact with a fluid flow in the presence of thermal fluctuations. The conventional immersed boundary method is extended to account for thermal fluctuations by introducing stochastic forcing terms in the fluid equations. This gives a system of stiff SPDE's for which standard numerical approaches perform poorly. We discuss a numerical method derived using stochastic calculus to overcome the stiff features of the equations. We then discuss results which indicate that the method captures physical features predicted by statistical mechanics for small length-scale systems. The stochastic immersed boundary method holds promise as a numerical approach in simulating microscopic mechanical systems in which thermal fluctuations play a fundamental role. A more detailed discussion of this work is given in [1, 2, 3].

1 Stochastic Immersed Boundary Method

1.1 Time Dependent Stokes Flow

For a fluid flow modeled by the time dependent Stokes equations the stochastic immersed boundary method is given by:

$$\rho\frac{\partial \mathbf{u}(\mathbf{x},t)}{\partial t} = \mu\Delta\mathbf{u}(\mathbf{x},t) - \nabla p(\mathbf{x},t) + \mathbf{f}_S(\mathbf{x},t) + \mathbf{f}_T(\mathbf{x},t) \quad (1)$$

$$\nabla\cdot\mathbf{u}(\mathbf{x},t) = 0 \quad (2)$$

$$\frac{d\mathbf{X}^{[j]}}{dt} = \int \delta_a(\mathbf{y}-\mathbf{X}^{[j]})\mathbf{u}(\mathbf{y},t)dy \quad (3)$$

$$\mathbf{f}_S(\mathbf{x},t) = \mathbf{F}^{[j]}\delta_a(\mathbf{x}-\mathbf{X}^{[j]}) \quad (4)$$

The term p is the pressure, ρ is the fluid density, μ is the dynamic viscosity. The force density $\mathbf{f}_S$ accounts for momentum transferred to the fluid by elastic deformations of immersed structures. The force density $\mathbf{f}_T$ is a Gaussian random field δ-correlated in time which accounts for the thermal fluctuations of the fluid-structure system. Structures are modeled by M control points $\mathbf{X}^{[j]}$ along with a force interaction law. The force acting on the j^{th} control point is denoted by $\mathbf{F}^{[j]}(\{\mathbf{X}^{[j']}\})$. The structure dynamics are given by equation 3, which corresponds to advection of the control points with the local fluid velocity. The term $\delta_a(\mathbf{x})$ approximates the Dirac δ-function. In the immersed boundary method the δ_a functions are taken so that they integrate to one and vanish outside a disk of radius a. This gives a brief formulation of the equations of the stochastic immersed boundary method. We now discuss the extension of the conventional immersed boundary method to account for thermal fluctuations.

1.2 Thermal Fluctuations

To account for thermal fluctuations an appropriate choice must be made for the stochastic forcing of the fluid-structure system. It is shown in [3] that in order for the model to be consistent with the principles of statistical mechanics only the fluid degrees of freedom should be stochastically forced. The spatial covariance structure of the Gaussian random field $\mathbf{f}_T$ is determined from the *fluctuation-dissipation principle* of statistical mechanics which relates equilibrium fluctuations of the system to the dissipative mechanism of the dynamics. For brevity we shall discuss only the case in which the equations above have been spatially discretized by finite differencing on a uniform periodic mesh, with L denoting the approximation of the Laplacian Δ. Let $C = \langle\mathbf{u}\mathbf{u}^T\rangle$, $G = \langle\mathbf{f}_T\mathbf{f}_T^T\rangle$ denote covariance matrices, respectively, for the equilibrium fluctuations of $\mathbf{u}$ and the Gaussian random field $\mathbf{f}_T$. The *fluctuation-dissipation principle* then requires covariance structure: $G = LC^T + CL^T$. At equilibrium the system has Gibbs-Boltzmann statistics with probability density $\Psi(\mathbf{u}) = \exp(-E[\mathbf{u}]/k_BT)$. Since the energy of the fluid is given by the kinetic energy $E[\mathbf{u}] = \sum_{\mathbf{m}}\rho|\mathbf{u}_{\mathbf{m}}|^2\Delta x^3$ summed over the mesh, the covariance matrix for the equilibrium fluctuations is given by $C = (k_BT/\rho\Delta x^3)I$. This determines the spatial covariance structure G of the Gaussian random field $\mathbf{f}_T$. See [3] for a more in depth discussion.

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1.3 Numerical Method

For spatial discretization on a uniform periodic mesh the following numerical scheme is used to update the Fourier modes $\hat{\mathbf{u}}_{\mathbf{k}}$ of the fluid and to update the immersed structure control points $\mathbf{X}^{[j]}$ from time step n to $n+1$:

$$\hat{\mathbf{u}}_{\mathbf{k}}^{n+1} = e^{-\alpha_{\mathbf{k}}\Delta t}\hat{\mathbf{u}}_{\mathbf{k}}^{n} + \frac{1}{\rho\alpha_{\mathbf{k}}}\left(1-e^{-\alpha_{\mathbf{k}}\Delta t}\right)\wp_{\mathbf{k}}^{\perp}\hat{\mathbf{f}}_{S,\mathbf{k}}^{n} + \wp_{\mathbf{k}}^{\perp}\hat{\boldsymbol{\Xi}}_{\mathbf{k}}^{n} \tag{5}$$

$$\mathbf{X}^{n+1,[j]} = \mathbf{X}^{n,[j]} + \sum_{\mathbf{m}} \delta_a(\mathbf{x}_{\mathbf{m}} - \mathbf{X}^{n,[j]})\boldsymbol{\Gamma}_{\mathbf{m}}^{n}\Delta x^3 \tag{6}$$

$$\boldsymbol{\Gamma}_{\mathbf{m}}^{n} = \sum_{\mathbf{k}} \hat{\boldsymbol{\Gamma}}_{\mathbf{k}}^{n}\cdot\exp\left(i2\pi\mathbf{k}\cdot\mathbf{m}/N\right) \tag{7}$$

$$\hat{\boldsymbol{\Gamma}}_{\mathbf{k}}^{n} = \hat{\mathbf{H}}_{\mathbf{k}} + c_{1,\mathbf{k}}\wp_{\mathbf{k}}^{\perp}\hat{\boldsymbol{\Xi}}_{\mathbf{k}}^{n} + c_{2,\mathbf{k}}\wp_{\mathbf{k}}^{\perp}\hat{\mathbf{G}}_{\mathbf{k}} \tag{8}$$

$$\hat{\mathbf{H}}_{\mathbf{k}} = \frac{1-\exp\left(-\alpha_{\mathbf{k}}\Delta t\right)}{\alpha_{\mathbf{k}}}\hat{\mathbf{u}}_{\mathbf{k}}^{n} + \left(\frac{\Delta t}{\alpha_{\mathbf{k}}} + \left(\frac{1}{\alpha_{\mathbf{k}}}\right)^2\left(\exp\left(-\alpha_{\mathbf{k}}\Delta t\right)-1\right)\right)\rho^{-1}\wp_{\mathbf{k}}^{\perp}\hat{\mathbf{f}}_{S,\mathbf{k}}^{n} \tag{9}$$

$$c_{1,\mathbf{k}} = \frac{1}{\alpha_{\mathbf{k}}}\tanh\left(\frac{\alpha_{\mathbf{k}}\Delta t}{2}\right), \text{ and } c_{2,\mathbf{k}} = \sqrt{\left(\frac{2D_{\mathbf{k}}}{\alpha_{\mathbf{k}}^3}\right)\left(\alpha_{\mathbf{k}}\Delta t - 2\tanh\left(\frac{\alpha_{\mathbf{k}}\Delta t}{2}\right)\right)}. \tag{10}$$

Each time step the structure force density $\mathbf{f}_S$ and its discrete Fourier transform $\hat{\mathbf{f}}_{S,\mathbf{k}}$ are computed. Next the Gaussian random variables $\hat{\boldsymbol{\Xi}}_{\mathbf{k}}^{n}$ and $\boldsymbol{\Gamma}_{\mathbf{m}}^{n}$ are generated. The random variable $\hat{\boldsymbol{\Xi}}_{\mathbf{k}}^{n}$ has mean 0 and variance $\sigma_{\mathbf{k}}^2 = (D_{\mathbf{k}}/\alpha_{\mathbf{k}})\left(1-\exp\left(-2\alpha_{\mathbf{k}}\Delta t\right)\right)$. The Fourier representation of the central difference discretization of the Laplacian is given by $\alpha_{\mathbf{k}} = (2\mu/\rho\Delta x^2)\sum_{j=1}^{3}(1-\cos(2\pi\mathbf{k}^{(j)}/N)))$. From the constraint that the velocity field must be real-valued and the *fluctuation-dissipation principle* we obtain $D_{\mathbf{k}} = \alpha_{\mathbf{k}}k_BT/\rho L^3$ for $\mathbf{k}\in\mathcal{K}$ and $D_{\mathbf{k}} = \alpha_{\mathbf{k}}k_BT/2\rho L^3$ for $\mathbf{k}\notin\mathcal{K}$ with the set of self-conjugate modes denoted by $\mathcal{K}$ = $\{\ \mathbf{k}\mid \mathbf{k}^{(j)}=0$ or $\mathbf{k}^{(j)}=N/2,\ j=1,2,3\ \}$. To enforce incompressibility each Fourier mode is projected by $\wp_{\mathbf{k}}^{\perp} = \mathcal{I} - (\hat{\mathbf{g}}_{\mathbf{k}}\hat{\mathbf{g}}_{\mathbf{k}}^T/|\hat{\mathbf{g}}_{\mathbf{k}}|^2)$ with $\hat{\mathbf{g}}_k^{(j)} = \sin(2\pi\mathbf{k}^{(j)}/N)/\Delta x$. The $\hat{\boldsymbol{\Xi}}_{\mathbf{k}}^{n}$ then accounts for the contributions to $\hat{\mathbf{u}}_{\mathbf{k}}$ of the thermal fluctuations of the fluid over the time step. Next the structure control points $\mathbf{X}^{[j]}$ are updated by generating the Gaussian random variable $\boldsymbol{\Gamma}_{\mathbf{m}}^{n}$ which accounts for the contributions of the thermal fluctuations of the fluid to the structure dynamics over the time step. This can be shown to enter as the time integral of the fluid velocity, $\boldsymbol{\Gamma}_{\mathbf{m}}^{n} = \int_{t_n}^{t_{n+1}}\sum_{\mathbf{k}}\hat{\mathbf{u}}_{\mathbf{k}}(s)\exp\left(i2\pi\mathbf{k}\cdot\mathbf{m}/N\right)ds$. An important consideration in generating the random variables is to take into account the correlations between $\boldsymbol{\Gamma}_{\mathbf{m}}^{n}$ and $\hat{\boldsymbol{\Xi}}_{\mathbf{k}}^{n}$, which both account for the same underlying thermal fluctuations of the fluid. The correct correlations can be obtained by using equation 8, in which an independent standard Gaussian $\hat{\mathbf{G}}_{\mathbf{k}}$ is generated and linearly combined with the previously generated random variables used to update the fluid modes. For a discussion of the derivation of the numerical method see [1].

2 Conclusion

In formulating the stochastic immersed boundary method a number of approximations were introduced, both at the level of the physical model for fluid-structure interactions and through the spatial and temporal numerical discretizations. A number of checks can be performed to verify whether the method is consistent with statistical mechanics and adequate to capture physical phenomena for microscopic systems. In [1] it was found that while only the fluid is stochastically forced, both independent and interacting particles diffusing in a conservative force field have Gibbs-Boltzmann equilibrium statistics. While particles are represented by the function δ_a in the immersed boundary method the diffusivities were computed both analytically and from numerical simulations and found to have the correct scaling in the physical parameters. In [2] it was also found that the immersed boundary framework can be used to capture osmotic phenomena occurring in microscopic systems. These results indicate that the method holds promise as a numerical approach in simulating microscopic mechanical systems in which thermal fluctuations play a fundamental role. For a more in depth discussion of this work see [1, 2, 3].

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References

[1] P. J. ATZBERGER, P, R. KRAMER, AND C. S. PESKIN, *A Stochastic Immersed Boundary Method for Fluid-Structure Interactions at Microscopic Length Scales*, J. Comp. Phys., Vol. 224, Iss. 2, (2007).

[2] P. J. ATZBERGER, P, R. KRAMER, *Theoretical Framework for Microscopic Osmotic Phenomena*, Phys. Rev. E, 75, 1, (2007).

[3] P, R. KRAMER, C. S. PESKIN, AND P. J. ATZBERGER, *On the Foundations of the Stochastic Immersed Boundary Method*, (to appear in Computational Mechanics).