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Brownian dynamics of rigid particles in an incompressible fluctuating fluid by a meshfree method

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ABSTRACT

A meshfree Lagrangian method for the fluctuating hydrodynamic equations (FHEs) with fluid-structure interactions is presented. Brownian motion of the particle is investigated by direct numerical simulation of the fluctuating hydrodynamic equations. In this framework a bidirectional coupling has been introduced between the fluctuating fluid and the solid object. The force governing the motion of the solid object is solely due to the surrounding fluid particles. Since a meshfree formulation is used, the method can be extended to many real applications involving complex fluid flows. A three-dimensional implementation is presented. In particular, we observe the short and long-time behavior of the velocity autocorrelation function (VACF) of Brownian particles and compare it with the analytical expression. Moreover, the Stokes-Einstein relation is reproduced to ensure the correct long-time behavior of Brownian dynamics.

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1. Introduction

The dynamics of small rigid particles immersed in a fluid presents an important and challenging problem, in particular, for micro/nano scale objects in small scale geometries. The dynamics of small rigid particle can be influenced by the inherent thermal fluctuation in the fluid. As one approaches smaller scales, thermal fluctuations play an essential role in the description of the fluid flow, see for example [1,2] or [3–5] for more recent works.

This study focuses on Brownian motion of particles immersed in an incompressible fluid. The average motion of the surrounding fluid yields a hydrodynamic force on the particles. Moreover, a random force is also experienced by the immersed particles due to the thermal fluctuation in the fluid. The average motion of fluid is modeled by the Navier–Stokes equations. The thermal fluctuations can either be described on a microscopic level using methods like molecular dynamics or they can be included in the continuum description of the fluid by additional stochastic fluxes. If one concentrates on a continuum field description, the resulting equations of motion for the fluctuating fluid turn out to be stochastic partial differential equations (SPDEs). Such equations, including an additional stochastic stress tensor in the Navier-Stokes equations, have been proposed by Landau and Lifshitz [6]. These equations are termed the Landau-Lifshitz Navier-Stokes (LLNS) equations. Initially, the LLNS equations have been presented for fluctuations around an equilibrium state of the system, but later on, their validity for non-equilibrium systems has also been shown [7] and verified by molecular simulations [8,9].

Early work in the context of numerical approximation of the LLNS equations has been done by Garcia et al. [10]. The authors have developed a simple scheme for the stochastic heat conduction equation and the linearized one-dimensional LLNS equations. Later on in [11] a centered scheme based on a finite-volume discretization, combined with the third-order Runge–Kutta (RK3) temporal integrator, has been introduced for the compressible LLNS equations. Afterward, a systematic approach for the analysis of this grid based finite-volume approximation for the LLNS equations and related SPDEs has been discussed by Donev et al. [12]. The extension of this numerical solver for the LLNS equations to binary mixtures and staggered schemes for the fluctuating hydrodynamic equations have been presented in [13,14]. A meshfree Lagrangian formulation for the 1D LLNS equations for compressible fluids has been presented by the present authors in [15] and the results have been compared to the above-mentioned FVM-based RK3 scheme from [11].

In the context of fluid–structure interactions, Brownian dynamics of immersed particles due to the surrounding fluctuating fluid

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has been studied. in [16,17], using the coupling of the equations of motion for the particles with the fluctuating hydrodynamic equations. There, inertia terms in the governing equations have been neglected and the resultant time independent problem has been solved with a numerical approach using a fixed grid spatial discretization. A hybrid Eulerian–Lagrangian approach for the inertial coupling of point particle with fluctuating compressible fluids has been presented by Usabiaga et al. [18]. Subsequently, an inertial coupling method for particles in an incompressible fluctuating fluid has been reported in [19]. In this work, the equations of motion of the suspended particle are directly coupled with an incompressible finite-volume solver for the LLNS equations [14]. The authors have also discussed the Stokes-Einstein relation for fluid-structure systems at moderate Schmidt number, see [20]. They have modeled the particle through a source term in the momentum equation and dealt with the full incompressible fluctuating hydrodynamic equations. In this work, a very efficient coupling of the fluctuating fluid with particles and a finite-volume approximation of the coupled model have been proposed. The short and long-time behavior of Brownian dynamics has been captured very well. Moreover, the authors were able to handle a wide range of Schmidt numbers in their proposed approximation, which has been a difficult task for many numerical approximations. An immersed boundary approach has been reported by Atzberger [21] for fluid-structure interaction with thermal fluctuations using a grid-based method and extended to complex geometries in [22]. The fluctuating hydrodynamics approach has also been used to analyze the Brownian motion of nanoparticles in an incompressible fluid, compare Uma et al. [23].

The present work distinguishes itself from the existing literature in its approach. An explicit coupling has been used between the fluctuating fluid and the solid structure, and a numerical approximation based on a meshfree formulation is used for the LLNS equations. In general, meshfree methods are an alternative to classical methods for problems with time-varying fluid domains such as problems with bodies suspended in a fluid, where one can avoid re-meshing during the time evolution. We note that a meshfree method termed “Smoothed dissipative particle dynamics (SDPD)” has been presented in [24] which incorporates thermal fluctuations. The SDPD is a combination of meshfree smoothed particle hydrodynamics (SPH) [25] and dissipative particle dynamics (DPD) [26]. In this approach, the SPH discretization of the Navier-Stokes equations is performed, and then thermal fluctuations are treated in the same way as in DPD. On the contrary, the present meshfree method is a formulation which is based on a direct numerical discretization of the stochastic partial differential equation. In the method the continuum constitutive model with a stochastic stress tensor is considered, and then a numerical approximation for the stochastic partial differential equations is employed. An extension of the SDPD method including the conservation of angular momentum has been presented by Müller et al. [27] to tackle fluid problems where angular momentum conservation is essential. Moreover, we note, that in [24] a rotational friction force governing particle spin interactions is included. In the present work, we focus on the Brownian motion of a particle due to inherent fluctuations of the surrounding fluid. Problems, where the conservation of angular momentum of the fluid particles is required, are left for future work. The other important distinguishing feature of the present work, is the use of an incompressible fluid solver instead of a compressible one as done in [24,28,29]. This allows treating the Brownian motion of a particle inside a liquid considered in the present work. We note that a compressible fluid needs to be considered if one want to focus on the interaction between ultrasound waves and colloidal particles, as studied by Usabiaga et al. [18]. For a compressible solver for the fluctuating hydrodynamics equations in one dimension developed by the present authors we refer to [15]. The coupling of a suspended particle with a fluctuating compressible fluid is left to future work.

In the present work we consider a fully Lagrangian meshfree particle method [30,31]. The computational domain is approximated by moving grid points or particles. We note that a particle management procedure has to be added in the method, see [30,31] for details. The suitability of the method, for fluid-structure interaction with highly flexible structures in the case of regular flow fields has been shown by Tiwari et al. [32]. In this paper, we have extended this meshfree method to the coupling of rigid particles with fluctuating fluids. For validation, the Brownian motion of particles has been investigated. We have computed the velocity autocorrelation function (VACF) of the Brownian particle and compared it with the theoretical result, as given for example in [33]. A rigid sphere immersed in the incompressible fluctuating fluid has been considered to validate the numerical results.

2. Governing equations

We consider a rigid sphere inside an incompressible fluctuating fluid. Let $\Omega \subset \mathbb{R}^3$ denote the entire computational domain including both fluid and rigid body, the domain of the rigid body is denoted by P. A neutrally buoyant rigid particle is considered to demonstrate the Brownian motion of an immersed particle due to the inherent fluctuations in the fluid.

The governing equations for the motion of the incompressible fluctuating fluid are given by

$$\frac{d\mathbf{x}}{dt} = \mathbf{u} \qquad \text{in } \Omega \setminus P, \tag{1}$$

$$\rho_f \frac{d\mathbf{u}}{dt} = \nabla \cdot \boldsymbol{\sigma} \qquad \text{in } \Omega \setminus P, \tag{2}$$

$$\nabla \cdot \mathbf{u} = 0 \qquad \text{in } \Omega \setminus P, \tag{3}$$

where $\mathbf{x}$ stands for the position vector of the fluid particle, ρ_f denotes the density of the fluid. $\frac{d}{dt} = \frac{\partial}{\partial t} + \mathbf{u}.\nabla$ defines the material derivative. The stress tensor $\boldsymbol{\sigma}$ is given by

$$\boldsymbol{\sigma} = -pI + \mu[\nabla\mathbf{u} + (\nabla\mathbf{u})^T] + \widetilde{\mathbf{S}}, \tag{4}$$

where p is the pressure and μ is the dynamic viscosity of the surrounding fluid. $\widetilde{\mathbf{S}}$ stands for the stochastic stress tensor, which models the inherent molecular fluctuations in the fluid. The required stochastic properties of $\widetilde{\mathbf{S}}$ have been derived by Landau and Lifshitz [6] in the spirit of a fluctuation-dissipation balance principle, described as

$$\langle \widetilde{S}_{ij}(\mathbf{x}, t) \rangle = 0, \tag{5a}$$

$$\begin{aligned} \langle \widetilde{S}_{ik}(\mathbf{x}, t)\widetilde{S}_{lm}(\mathbf{x}', t') \rangle &= 2k_B T \mu(\delta_{il}\delta_{km} + \delta_{im}\delta_{kl}) \\ &\quad \times \delta(\mathbf{x} - \mathbf{x}')\delta(t - t'), \end{aligned} \tag{5b}$$

where k_B is the Boltzmann constant, T is the temperature of the fluid and $\langle\rangle$ is used for the ensemble averages. It has to be noted that originally these expressions have been derived for compressible fluids, but Eq. (5) is the corresponding approximation for an incompressible fluids.

We note that the non-linear LLNS equations define an ill-posed problem. It has to be noticed that the stochastic forcing in the LLNS equations is the divergence of a white noise process, rather than the more common external fluctuations modeled through white noise which have been discussed in [34–36]. $\widetilde{\mathbf{S}}$ cannot be defined pointwise either in space and time, therefore $\nabla \cdot \widetilde{\mathbf{S}}$ cannot be given a precise mathematical interpretation. Further mathematical problems arise with the interpretation of the non-linear term $\mathbf{u} \cdot \nabla\mathbf{u}$. An approach to deal with these issues is to consider a regularization of the stochastic stress tensor, which is typically the source

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