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Mean field models for interacting ellipsoidal particles

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ABSTRACT

We consider a mean field hierarchy of models for large systems of interacting ellipsoids suspended in an incompressible fluid. The models range from microscopic to macroscopic mean field models. The microscopic model is based on three ingredients. Starting from a Langevin type model for rigid body interactions, we use a Jefferys type term to model the influence of the fluid on the ellipsoids and a simplified interaction potential between the ellipsoids to model the interaction between the ellipsoids. A mean field equation and corresponding equations for the marginals of the distribution function are derived and a numerical comparison between the different levels of the model hierarchy is given. The results clearly justify the suitability of the proposed approximations for the example cases under consideration.

1. Introduction

Large systems of interacting ellipsoidal shaped particles have attracted the attention of researchers from many different fields. For example, such systems are used to describe polymers and liquid crystals in the chemical sciences [1–3]. The movement of ellipsoidal particles suspended in a fluid is also used in process engineering to describe the physics inside a liquid–liquid extraction column [4–8]. A recent application of such models may be found in paper production processes [9–12].

Mathematically the movement of ellipsoidal particles can be described on a microscopic level by large systems of ordinary differential equation based on Newtonian laws of mechanics for translational and rotational motion of the ellipsoids. For ellipsoidal particles suspended in an incompressible viscous fluid, one can use the model of Jeffery (e.g. [13,14,3]), which describes the forces exerted by the fluid on an ellipsoid. In our work, the inter-particle interaction forces between ellipsoids are described via pairwise potentials for the particles and a random force. For the interaction potentials, we use potentials common in the literature for polymers [15–20], where the form of the ellipsoids is modeled with the help of Gaussian type functions. This leads to a Langevin-type microscopic model similar to the ones described in [21–23,3]. For the numerical treatment of large systems of hard interacting ellipsoids, we refer, for example, to [24].

For a very large number of particles, macroscopic equation for density, mean velocity, and other statistical quantities are expected to be a more efficient approximation of these models. In the present work we derive, via a mean field approximation, corresponding kinetic equation, which can be used in turn to derive hydrodynamic and scalar limit equations. This procedure has also been used for example in the case of self-organizing systems of particles or for the description of pedestrian or granular flows [25–28].

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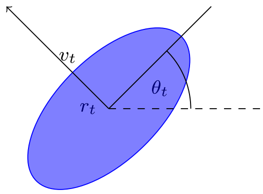

Fig. 2.1. Sketch of an ellipsoidal particle with position r_t, orientation angle θ_t and velocity v_t.

The paper is organized as follows: In Section 2 the microscopic model is introduced and the ellipsoidal interaction potential is constructed. From this, we derive the mean field limit equation in Section 3 and use different moment closure procedures for the derivation of different hydrodynamic limit equations in Section 4. In Section 5, we numerically compare the derived models with the microscopic model for several different examples and flow fields.

2. The microscopic model

We consider a microscopic Langevin-type model as in [3] to describe the motion of ellipsoidal particles suspended in an incompressible fluid in two space dimensions. The interaction of the fluid with the ellipsoids is described by a Jefferys type term [13,14]. Interactions of the ellipsoids with each other are described by a many-particle interaction potential similar to [16].

As illustrated in Fig. 2.1, each ellipsoidal particle is described by its position $r_t \in \mathbb{R}^2$, velocity $v_t \in \mathbb{R}^2$, orientation angle $\theta_t \in [0,\ 2\pi)$ and angular velocity $\omega_t \in \mathbb{R}$. The angle θ_t is given by the relative angle between the horizontal axis and the main axis of the ellipsoidal particle such that the angle $\theta_t = 0$ corresponds to the orientation $(1, 0)^\top$. The equations of motion for N particles $i = 1, \dots, N$ are

$$\begin{cases} dr_t^i &= v_t^i dt \\ dv_t^i &= \gamma(u - v_t^i)dt - \frac{1}{m}\frac{1}{N}\sum_{i\neq j} \nabla_{r_i} U(r_t^i, r_t^j, \theta_t^i, \theta_t^j)dt - \nabla_r V_1(r_t^i)dt - (A^2/2)v_t^i dt + AdW_t^{A,i} \\ d\theta_t^i &= \omega_t^i dt \\ d\omega_t^i &= \bar{\gamma}(g(\theta_t^i, u) - \omega_t^i)dt - \frac{1}{I_c}\frac{1}{N}\sum_{i\neq j} \nabla_{\theta_i} U(r_t^i, r_t^j, \theta_t^i, \theta_t^j)dt - \nabla_\theta V_2(\theta_t^i)dt - (B^2/2)\omega_t^i dt + BdW_t^{B,i}, \end{cases} \tag{2.1}$$

with appropriate initial conditions. Here u is the velocity of a stationary surrounding fluid and $g(\theta, u)$ is given by

$$g(\theta, u) = \frac{1}{2}\text{curl}(u) + \lambda \begin{pmatrix} -\sin\theta \\ \cos\theta \end{pmatrix}^\top \left(\frac{1}{2}(\nabla u + \nabla u^\top)\right)\begin{pmatrix} \cos\theta \\ \sin\theta \end{pmatrix}.$$

The first terms on the right hand side of the velocity and angular velocity equations describe the relaxation of the particles to the velocity of the fluid and to the rotation resulting from the velocity field, respectively. The speed of relaxation is determined by the parameters γ and $\bar{\gamma}$. The second terms model the repulsive interaction between the particles. The parameters m and I_c are the mass and the moment of inertia of the particles. The functions V_1, V_2 model an outer potential like for example gravitation or a magnetic field. The parameters A, B are nonnegative diffusion constants and $W^{A,i}$, $W^{B,i}$ are independent standard Brownian motions. The interaction potential is given by the following considerations.

There exist many different interaction potentials for ellipsoidal particles [15–20]. We use the soft potential as proposed by Berne [16]. It is obtained by overlapping two ellipsoidal Gaussians representing the mutual repulsion of two particles. This leads to

$$\tilde{U}(r, \bar{r}, \theta, \bar{\theta}) = a(\theta, \bar{\theta}) \exp\left(-(\bar{r} - r)\left(\gamma(\theta) + \gamma(\bar{\theta})\right)^{-1}(\bar{r} - r)\right),$$

where a and γ are defined by

$$a(\theta, \bar{\theta}) = \epsilon_0\left(1 - \lambda^2(\eta(\theta)\cdot\eta(\bar{\theta}))^2\right)^{-\frac{1}{2}}, \qquad \eta(\theta) = (\cos\theta, \sin\theta)^\top,$$

$$\gamma(\theta) = \left(l^2 - d^2\right)\eta(\theta)\otimes\eta(\bar{\theta}) + d^2\mathbb{1}, \qquad \lambda = \frac{l^2 - d^2}{l^2 + d^2}.$$

Here, $l = 2L$ and $d = 2D$ where L is the length and the D the width of the particle. The parameter ϵ_0 models the strength of the potential. To have compact support we slightly modify the potential and define

$$U(r, \bar{r}, \theta, \bar{\theta}) = a(\theta, \bar{\theta}) \exp\left(-\frac{(\bar{r} - r)\left(\gamma(\theta) + \gamma(\bar{\theta})\right)^{-1}(\bar{r} - r)}{1 - (\bar{r} - r)\left(\gamma(\theta) + \gamma(\bar{\theta})\right)^{-1}(\bar{r} - r)}\right). \tag{2.2}$$