Mean field surrogate model of a dilute and chaotic particle suspension

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We present a mean field approximation for a dilute suspension of small particles, which accounts for a non-homogeneous particle distribution and small inertial effects of the particle phase. The model consists of the momentum equation for the fluid coupled to a transport equation for the probability density function on the particle phase space. Apart from the well-known particle extra stress tensor first presented by Batchelor (1970), the fluid equation contains additional force terms resulting from inertia and hydrodynamic interaction of the particles. A brief sketch of the main derivation steps is presented.

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1 Mean field model

In [7] we derived a macroscopic model for the behavior of a dilute particle suspension, which accounts for small inertial particle effects. The model is based on the asymptotic approach for a single inertia-free particle by Junk and Illner [5], where the suspended bodies are characterized by the size ratio $\epsilon \ll 1$. By introducing a scaled density ratio $\rho_e = \epsilon^r \rho, r \geq 1$ with $\rho = p_0/\rho_f$ ratio of particle to fluid density, our extended approach allowed for the classification of different particle regimes (light-weighted, normal, heavy). The resulting asymptotic particle model was combined with the averaging framework by Batchelor [1] for the derivation of effective stresses. Because of the assumption of ergodicity, which is inherent in [1], it is unclear whether the description is also reasonable for non-homogeneous particle distributions in space. By applying the kinetic approach of [2] to the asymptotic particle model, we come up with a novel suspension model which covers the one in [7], is valid for non-homogeneous particle distributions and poses an approximation to the full suspension problem.

In the following we present and discuss our new mean field model. Consider an open domain $\Omega \subset \mathbb{R}^3$ with boundary $\partial \Omega$ and a time interval $(0, T), T > 0$, the macroscopic suspension velocity and pressure are given by $(u_0, p_0) : \Omega \times (0, T) \rightarrow \mathbb{R}^3 \times \mathbb{R}$ and the particle probability density function (pdf) by $\psi : \Omega \times SO(3) \times (0, T) \rightarrow \mathbb{R}^+_0$ on the particle phase space $\Omega \times SO(3)$. The mean field description of a dilute particle suspension consists of the momentum balance of the fluid in $\Omega$, where

\[
\text{Re}(\partial_t u_0 + u_0 \cdot \nabla u_0) = \nabla \cdot S[u_0, p_0] + \text{Re} \text{Fr}^{-2} \epsilon_0 + \phi_e \nabla \cdot \Sigma[\psi, u_0] + \phi_e |\Omega| (\rho_e - 1) \psi \Omega \nabla \cdot S[u_0, p_0]
\] (1a)

with the mass conservation realized by the solenoidality condition for $u_0$, coupled with a transport equation for the particle pdf

\[
\partial_t \psi + (u_0 + \epsilon F_v \cdot \nabla) \psi - \mathcal{L}[B(F_v u_0)](\psi) = (\text{div}_C \mathcal{L}[B(F_v u_0)] - \epsilon \nabla \cdot F_v u_0) \psi
\] (1b)

in $\Omega \times SO(3)$. The model is complemented with suitable initial and boundary conditions on $\partial \Omega$ for $u_0, \psi$. For a smooth function $M : SO(3) \rightarrow \mathbb{R}^{3 \times 3}$ with $M(R)$ skew-symmetric, $\mathcal{L}[M]$ denotes the vector field associated with the left Lie derivative on $SO(3)$, [3], i.e., for any smooth function $\theta : SO(3) \rightarrow \mathbb{R}$

\[
(\mathcal{L}[M](\theta))(R) = \frac{d}{dt} \theta(\exp(-\tau M(R)) \cdot R) \bigg|_{\tau=0}.
\]

Given a basis of the skew-symmetric matrices $B_i, i = 1, 2, 3, \text{holds} \mathcal{L}[M(R)] = \sum_{i=1}^3 \alpha_i(R) \mathcal{L}[B_i]$, with smooth coefficients $\alpha_i$. The divergence operator of $\mathcal{L}$ is set as $\text{div}_C(\mathcal{L}[M])(R) = \sum_{i=1}^3 (\mathcal{L}[B_i](\alpha_i))(R)$. Moreover, $\nabla$ and $\nabla \cdot$ denote the gradient and divergence operators in $\mathbb{R}^3$, and $B : \mathbb{R}^3 \rightarrow \mathbb{R}^{3 \times 3}$ is the unique mapping which fulfills $B(\psi \cdot x = \psi \cdot x$ for all $\psi, x \in \mathbb{R}^3$. By $\psi_\Omega(x, t) = \int_{SO(3)} \psi(x, R, t) dR$ we denote the marginal pdf over $\Omega$ with the Haar measure $dR$ on $SO(3)$.

The model (1) is characterized by the following parameters: Reynolds number Re (ratio of inertial and viscous forces in the fluid), Froude number Fr (ratio of inertial and gravitational forces in the fluid with $\epsilon_0$ the gravitational direction), and volume fraction $\phi_e$ (ratio of the total particle volume and the total volume $|\Omega|$). The function $F_v[u_0] = (F_v[u_0], F_v[u_0]) : \Omega \times SO(3) \times (0, T) \rightarrow \mathbb{R}^6$ depends on the chosen inertial particle regime and geometry. The Newtonian stress tensor is $S[u_0, p_0] = -p_0 I + 2 \mathbf{E}[u_0]$ with the symmetric deformation gradient $\mathbf{E}[u_0] = 0.5(\nabla u_0 + \nabla u_0^T)$. The integral operators $U[\psi, u_0]$ and $H[\psi, u_0]$ are mean values of hydrodynamic interaction terms with respect to the density $\psi$. Similarly, $\Sigma$ is an integral operator which depends on $\psi$. In case of a homogeneous suspension in space, i.e., $\psi(x, R, t) = |\Omega|^{-1}\psi(R, t)$, $\Sigma$ becomes the well-known particle stress tensor derived by Batchelor in [1].

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The model is meaningful under the following assumptions: The hydrodynamic interaction is small and thus the disturbance fields generated by the particles cancel each other out instead of having an amplifying effect. Additionally, the particle number is chosen as $N_e = \epsilon^{-1/2}$ in accordance with the condition $N_e \ll \epsilon^{-1}$ in [4], which implies $\phi_k = \epsilon \phi / 2$. Lastly, due to the source term on the right-hand side of (1b), $\psi$ is a probability density only if

$$\int_{\Omega \times SO(3)} \left( \text{div}_C(\mathcal{L}[B(F_{\nu}(u_0)]) - \epsilon \nabla \cdot F_{\nu}(u_0) \right) \psi \, d\mathbf{R} = 0, \quad \text{for all } t \geq 0.$$  

(2)

The model inherits effects of the different inertial particle regimes as seen by the presence of $\rho$, in (1a). It also adresses small hydrodynamic interaction via the terms associated to $U, H$. An important observation is that the latter appear in (1a) of order $O(\epsilon^{3/2})$ compared to the one of the particle extra stress tensor $\Sigma$ that is of $O(\epsilon^{5/2})$. This indicates that their omission in [7] due to the ergodicity assumption neglects a major contribution to the overall dynamics in the non-homogeneous case.

To illustrate (1b) and the condition (2) we use the example of spherical particles, i.e., the particle shape $\bar{E}$ is given as the unit ball. In case of the heavy particle regime ($r = -1$), $F$ is then $F[u_0] = (-\rho \frac{2}{3} \text{Re}(\partial_t u_0 + u_0 \cdot \nabla u_0), -\frac{1}{2} \nabla \times u_0)$ and is independent of $\mathbf{R}$. Therefore, $\text{div}_C(\mathcal{L}[B(F_{\nu})]) = 0$, but $\nabla \cdot F_{\nu} = \epsilon \rho \text{Re}([|E| u_0]_F^2 - 0.5 ||\nabla \times u_0||^2_2)$, where $||.||_F$ is the Frobenius norm and $||.||_2$ the Euclidean vector norm. For $\epsilon > 0$, condition (2) then demands that the mean square shear rate magnitude is balanced by the mean square vorticity magnitude. In case of the normal or light-weighted regime ($r \geq 0$), $F[u_0] = (0, \frac{1}{2} \nabla \times u_0)$ and (2) holds true.

2 Derivation procedure

In the following we sketch the main ideas behind the derivation of (1), for all technical details we refer to [8]. In a fully coupled three-dimensional fluid-particle system for a dilute suspension, which interacts only by hydrodynamic forces, the behavior of the fluid velocity $u$ and $N_e$ suspended particles can be modeled by the incompressible Navier-Stokes equations in $\Omega = \Omega \setminus \cup_{i=1}^{N_e} \mathbb{E}^i_{\nu}$ with no-slip condition on $\partial \Omega$, as well as by the kinematic equations for the particles’ centers of mass $c^i$ and rotations $\mathbb{R}^i$ and their dynamic balances for the linear and angular momenta. The particle domains $\mathbb{E}^i_{\nu}$ are given as the accordingly rotated, scaled and translated particle shapes $\mathbb{E}$. The particles are assumed to be separated by a minimal distance $\nu = N_e^{-1/3}$. We assume that the particle velocities and accelerations possess regular expansions in $\epsilon$, while the velocity and pressure of the fluid are given as a global and a local part, i.e., $u = u_0 + u_{loc}$ for the velocity. We set $u_{loc}$ as the superposition of every particle disturbance field, which has a regular expansion in $\epsilon$, $u_{loc} = \sum_{k=1}^{\infty} \sum_{i=1}^{N_e} \epsilon^k \mathbb{R}^i \cdot u_{loc,k}^i$. By plugging the expansions into the particle related equations and using appropriate Taylor expansions for $u_0$, while assuming that the latter is sufficiently smooth, we find balance laws for the asymptotic coefficients such that a desired approximation order is reached.

In fact, we find the following approximation of the particle motion

$$\frac{d}{dt} c^i = u_0(c^i, t) + \epsilon F_0(c^i, \mathbb{R}^i, t) + O(\epsilon^2), \quad \frac{d}{dt} \mathbb{R}^i = B(F_{\nu}(c^i, \mathbb{R}^i, t)) + O(\epsilon),$$  

(3)

with $F = (F_{\nu}, F_0)$ found as advection term in (1b). At the same time, the local disturbance fields $u_{loc,k}^i$ are solutions of homogeneous stationary Stokes equations in $\mathbb{R}^3 \setminus \mathbb{E}$ decaying at infinity and with boundary conditions depending on $u_0$. The assumption of a small hydrodynamic interaction then reads as $\sum_{i=1}^{N_e} \mathbb{R}^i \cdot u_{loc,k}^i \leq C \epsilon$ for any $x \in \Omega$ with $||x - c^i|| > \nu$. As the next step, we apply the mean field approach proposed by [2] by interpreting the system of equations (3) as characteristic equations of a transport equation for the empirical measure of $c^i, \mathbb{R}^i$ on the particle phase space. The transport equation can then be extended to more regular Borel measures on $\Omega \times SO(3)$ and is given as (1b) in case of a first order approximation and an absolutely continuous measure with respect to the product of Lebesgue measure on $\Omega$ and the Haar measure on $SO(3)$. Finally, we insert the velocity expansions also into the momentum balance of $u$. In order to get well-defined operators on the complete domain $\Omega$, we expand the local disturbance fields $u_{loc,k}^i$ by their boundary conditions onto $\mathbb{E}$ and the Newtonian stresses by Lagrangian multipliers to the rigid body motion constraint as proposed by [6]. By using suitable approximations, we come up with the resulting momentum equation (1a) which is coupled to (1b).

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