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Hyperbolic Systems of Moment Equations Describing Sedimentation in Suspensions of Rod-Like Particles

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1 The Mathematical Model

We consider a mathematical model, which describes sedimentation in dilute suspensions of rod-like particles. The model was derived by Helzel and Tzavaras [4] and is based on work of Doi and Edwards [1]. In non-dimensional form, the multiscale model is given as

$$
\begin{aligned}
\partial_t f + \nabla_x \cdot (\boldsymbol{u} f) &+ \nabla_n \cdot (P_{\boldsymbol{n}^\perp} \nabla_{\boldsymbol{x}} \boldsymbol{u} \boldsymbol{n} f) - \nabla_x \cdot ((I + \boldsymbol{n} \otimes \boldsymbol{n}) \boldsymbol{e}_3 f) \\
&= D_r \Delta_n f + \gamma \nabla_x \cdot (I + \boldsymbol{n} \otimes \boldsymbol{n}) \nabla_x f, \\
\sigma &= \textstyle\int_{S^{d-1}} (d\boldsymbol{n} \otimes \boldsymbol{n} - I) f d\boldsymbol{n}, \\
Re\,(\partial_t \boldsymbol{u} + (\boldsymbol{u} \cdot \nabla_x) \boldsymbol{u}) &= \Delta_x \boldsymbol{u} - \nabla_x p + \delta\gamma \nabla_x \cdot \sigma - \delta \int_{S^{d-1}} f d\boldsymbol{n} \boldsymbol{e}_3, \\
\nabla_x \cdot u &= 0.
\end{aligned}
\tag{1}
$$

The probability distribution function $f = f(t, \boldsymbol{x}, \boldsymbol{n})$ models the time-dependent probability that a rod with center of mass at the macroscopic position $\boldsymbol{x} \in \mathbb{R}^d$ has at time $t \in \mathbb{R}^+$ an axis in the area element $d\boldsymbol{n}$, where $\boldsymbol{n} \in S^{d-1}$ is a director on the unit sphere embedded in $\mathbb{R}^d$. The physical application we are interested in assumes $d = 3$. $\boldsymbol{u}(\boldsymbol{x}, t)$ describes the velocity and $p = p(t, \boldsymbol{x})$ the pressure of the solvent. Experimental work of Guazzelli et al. [2] shows that the interaction between particles and fluid leads to complex flow structures, for example the clustering of sedimenting particles of an initially well stirred suspension.
A direct numerical simulation of the coupled model (1) is cumbersome due to the high dimensionality of the problem. Therefore, we develop a new numerical method which is based on a hierarchy of moment equations derived from the full model.

2 Hierarchy of Moment Equations for Shear Flow

In order to simplify the studies, we restrict our considerations to a simplified model on S^1 for a shear flow problem. We assume $f = f(t, x, \theta)$ and $\boldsymbol{u} = (0, 0, w(t, x))^T$. For $\gamma = 0$ and an equilibrated flow, we obtain the coupled system of the form

$$
\begin{aligned}
\partial_t f + \partial_\theta (w_x \cos^2 \theta f) - \partial_x (\sin\theta \cos\theta f) &= D_r \partial_{\theta\theta} f, \\
Re \partial_t w &= \partial_{xx} w + \delta \left(\bar{\rho} - \int_0^{2\pi} f d\theta \right).
\end{aligned}
\tag{2}
$$

We define the quantities

$$
\rho(\boldsymbol{x}, t) := \int_0^{2\pi} f(\boldsymbol{x}, t, \theta) d\theta, \quad C_l(\boldsymbol{x}, t) := \frac{1}{2} \int_0^{2\pi} \cos(2l\theta) f(\boldsymbol{x}, t, \theta) d\theta, \quad S_l(\boldsymbol{x}, t) := \frac{1}{2} \int_0^{2\pi} \sin(2l\theta) f(\boldsymbol{x}, t, \theta) d\theta, \quad l = 1, 2, \ldots
$$

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For the shear flow problem (2), we obtain the following infinit system of moment equations

$$\begin{aligned} \partial_t \rho &= \partial_x S_l \\ \partial_t C_l &= \frac{1}{4}\partial_x (S_{l+1} - S_{l-1}) - \frac{l}{2} w_x (S_{l-1} + 2S_l + S_{l+1}) - 4l^2 D_r C_l, \quad l = 1, 2, .. \\ \partial_t S_l &= \frac{1}{4}\partial_x \left(C_{l+1}(x,t) - C_{l-1}\right) + \frac{l}{2} w_x \left(C_{l-1} + 2C_l + C_{l+1}\right) - 4l^2 D_r S_l, \quad l = 1, 2, ... \end{aligned} \tag{3}$$

In practical computations we need to consider a fixed number of moment equations, i.e. we use $l = 1, ..., N$. In order to close the system, we set $C_{N+1} = S_{N+1} = 0$. The system of moment equations allows us to approximate the high dimensional scalar Smoluchowski equation with a lower dimensional system of partial differential equations. While the original system is a time-dependent partial differential equation in space and orientation, the system of moment equations depends only on space and time. In addition, we can adaptively adjust the level of detail used in the mathematical model and the numerical method. The closed system of moment equations is considered together with the flow equation

$$Re \partial_t w(\boldsymbol{x}, t) = \partial_{xx} w + \delta(\bar{\rho} - \rho(\boldsymbol{x}, t)). \tag{4}$$

3 Hyperbolic Structure of the One-Dimensional System of Moment Equations for Shear Flow

The system of moment equations can be written in the form

$$\partial_t Q(x,t) + A \partial_x Q(x,t) = \phi(Q(x,t)), \tag{5}$$

where $Q(x,t) = (\rho, C_1, S_1, ..., C_N, S_N)^T$ represents the vector of moments and $A \in \mathbb{R}^{(2N+1)\times(2N+1)}$ has the components

$$a_{1,3} := -1, \quad a_{3,1} := -\tfrac{1}{8},$$

$$\begin{pmatrix} a_{2(N-j)-2,2(N-j)-2} & \cdots & a_{2(N-j)-2,2(N-j)+1} \\ \vdots & & \vdots \\ a_{2(n-j)+1,2(N-j)-2} & \cdots & a_{2(N-j)+1,2(N-j)+1} \end{pmatrix} := \begin{pmatrix} 0 & 0 & 0 & -\frac{1}{4} \\ 0 & 0 & \frac{1}{4} & 0 \\ 0 & \frac{1}{4} & 0 & 0 \\ -\frac{1}{4} & 0 & 0 & 0 \end{pmatrix} \quad j = 0, ..., N-2.$$

All other entries are equal to zero. To proof the hyperbolicity of the moment system (5) for general N, we use a similarity transformation.

4 Numerical Discretisation of the Moment System

A splitting method is used to split the macroscopic flow equation (4) from the discretisation of the moment equations (5). The standard approach to approximate systems of the form (5) is to use an operator splitting approach which separately solves the homogenous hyperbolic system $\partial_t Q(x,t) + A\partial_x Q(x,t) = 0$ and the system of ordinary differential equations $\partial_t Q(x,t) = \phi(Q(x,t))$. We use LeVeque's Wave Propagation Algorithm, see for example [6], to solve the hyperbolic system with a high-resolution finite volume method. Strang splitting is used to incorporate the source term. We compare the discretisation of the lower dimensional model with a direct numerical method for the full model (2) and show that the hyperbolic system of moment equations can be interpreted as an approximation of the original problem.

In [5], we also derive a hierarchy of moment equations for a two-dimensional flow problem. We use a similarity transformation to proof that the two-dimensional system of moment equations is hyperbolic.

References

[1] M. Doi and S. Edwards. The Theory of Polymer Dynamics. *Oxford University Press.* 1986.

[2] E. Guazzelli and E. Hinch. Fluctuations and instability in sedimentation *Ann. Rev. Fluid Mech., 43, pp. 87-116.* 2011.

[3] C. Helzel and A. E. Tzavaras. A Kinetic Model for the sedimentation of rod-like particles. *Multiscale Model. Simul., 15, pp. 500-536.* 2017.

[4] S. Dahm and C. Helzel. Hyperbolic Systems of Moment Equations Describing Sedimentation in Suspensions of Rod-Like Particles. *Submitted for publication.* 2021.

[5] R. J. LeVeque. Wave Propagation Algorithms for Multi-Dimensional Hyperbolic Systems *J. Comput. Phys., 131, pp. 327-353.* 1997.