Structure-Preserving Multi-Scale Methods for Complex Fluids

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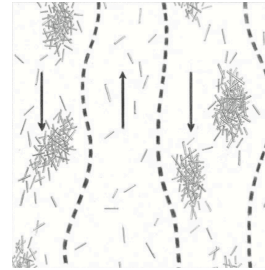
FOR 5409 – Project **B3**

Mathematical Model for the Sedimentation of Rod-Like Particles

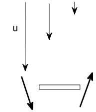
Bulk Coupling of a Kinetic Equation with the Navier-Stokes Equation

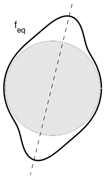
$$\partial_t f + \nabla_{\mathbf{x}} \cdot (\mathbf{u} f) + \nabla_{\mathbf{n}} \cdot (P_{\mathbf{n}^\perp} \nabla_{\mathbf{x}} \mathbf{u} \mathbf{n} f) - \nabla_{\mathbf{x}} \cdot ((I + \mathbf{n} \otimes \mathbf{n}) \, \mathbf{e}_3 f)$$
$$= D_r \Delta_{\mathbf{n}} f + \gamma \nabla_{\mathbf{x}} \cdot (I + \mathbf{n} \otimes \mathbf{n}) \nabla_{\mathbf{x}} f$$
$$\sigma = \int_{S^{d-1}} (d\mathbf{n} \otimes \mathbf{n} - I) \, f \, d\mathbf{n}$$
$$Re \, (\partial_t \mathbf{u} + (\mathbf{u} \cdot \nabla_{\mathbf{x}}) \, \mathbf{u}) = \Delta_{\mathbf{x}} \mathbf{u} - \nabla_{\mathbf{x}} p + \delta \gamma \nabla_{\mathbf{x}} \cdot \sigma - \delta \int_{S^{d-1}} f \, d\mathbf{n} \mathbf{e}_3$$
$$\nabla_{\mathbf{x}} \cdot \mathbf{u} = 0$$



Guazzelli & Morris

$f = f(t, \mathbf{x}, \mathbf{n})$: density distribution function of particle orientation





Helzel & Tzavaras, MMS 2017

A Hierarchy of Moment Equations for a Simplified Model

We illustrate our ideas for a simplified flow problem with $\mathbf{u} = (0, 0, w(x,t))^T$ and $f = f(t, x, \theta)$. Using $\gamma = 0$ we obtain the coupled system

$$\partial_t f(t,x,\theta) + \partial_\theta \left(w_x \cos^2\theta f \right) - \partial_x \left(\sin\theta \cos\theta f \right) = D_r \partial_{\theta\theta} f$$

$$Re \partial_t w = \partial_{xx} w + \delta \left(\bar{\rho} - \int_0^{2\pi} f \, d\theta \right)$$

Hierarchy of moment equations:

$$\begin{aligned}
\partial_t \rho(x,t) &= \partial_x S_1 \\
\partial_t C_\ell(x,t) &= \frac{1}{4} \partial_x \left(S_{\ell+1} - S_{\ell-1} \right) - \frac{\ell}{2} w_x \left(S_{\ell-1} + 2S_\ell + S_{\ell+1} \right) - 4\ell^2 D_r C_\ell, \quad \ell = 1, 2, \ldots \\
\partial_t S_\ell(x,t) &= \frac{1}{4} \partial_x \left(C_{\ell-1} - C_{\ell+1} \right) + \frac{\ell}{2} w_x \left(C_{\ell-1} + 2C_\ell + C_{\ell+1} \right) - 4\ell^2 D_r S_\ell, \quad \ell = 1, 2, \ldots.
\end{aligned}$$

Definition of moments:

$$\rho(x,t) := \int_0^{2\pi} f(x,t,\theta) \, d\theta, \; C_\ell(x,t) := \frac{1}{2} \int_0^{2\pi} \cos(2\ell\theta) f(x,t,\theta) \, d\theta, \; S_\ell(x,t) := \frac{1}{2} \int_0^{2\pi} \sin(2\ell\theta) f(x,t,\theta) \, d\theta, \quad \ell = 1, 2 \ldots$$

joint with PhD student S. Dahm

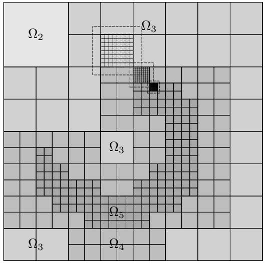
Challenges and Exemplary Work Packages

- Investigate hierarchy of moment equations for simplified shear flow problem with f on S^1
  - Transform high dimensional scalar PDE (in space and orientation) into a lower dimensional system of PDEs (in space)
  - Investigate accuracy of moment closure system

- Derive and explore hierarchies of moment equations for higher dimensional situations, in particular for f on S^2

- Develop interface coupling techniques, which allow the use of a different number of moments in different regions of the domain

  Use of forestClaw grid structure and solver (joint with D. Calhoun)



- Construction of structure preserving methods
  - preserve positivity of f and ρ
  - Investigate how the entropy structure of the kinetic model relates to the entropy structure of the moment system.

Role within Research Unit and Outlook

- Contribution to *Coupling of Models*
  - interface coupling of moment equations with different numbers of moments
  - prototyp of a model with hierarchy of moment equations
- Contribution to *Structure Preservation*
- Strong interactions with Project **B4**
  - compare moment cascade / hierarchy
  - possible usage of maximum entropy
- Strong interaction with Project **C2**
  - Implementation of coupling concepts;
- Collaboration with A.E. Tzavaras, G. Gassner, R. Abgrall

Outlook

- Increase complexity of the model (semi-dilute, concentrated regime)
- Consideration of more realistic flow situations
- Investigate relations between spectral methods for kinetic equations and moment approximations collaboration with K. Kormann

First Steps towards Considerations of the Full Model with f on S^2

From previous studies of the simplified model we know that the system of moment equations has the form of a hyperbolic system with source term.

The update of the source term is equivalent with a spectral method for the kinetic Smoluchowski equation.

Consider

$$\partial_t f + \nabla_{\mathbf{n}} \cdot (P_{\mathbf{n}^\perp} \nabla_{\mathbf{x}} \mathbf{u}_{ext} \mathbf{n} f) = D_r \Delta_{\mathbf{n}} f \tag{1}$$

Ansatz for spectral method:

$$f(\phi, \theta, t) = f_0(t) P_0^0 + \sum_{i=-2}^{2} c_{2,i}(t) P_2^i + \sum_{i=-4}^{4} c_{4,i}(t) P_4^i(t) + \sum_{i=-6}^{6} c_{6,i}(t) P_6^i(t) + \dots \tag{2}$$

where P_{2k}^j are harmonic polynomial basis functions, i.e. eigenfunctions of the Laplace Beltrami operator

0th order	2nd order
$P_0^0 = 1$	$P_2^{-2} = \sin^2(\theta)\cos(2\phi)$ $P_2^{-1} = \sin(\theta)\cos(\theta)\cos(\phi)$ $P_2^0 = \cos^2(\theta) - \frac{1}{3}$ $P_2^1 = \sin(\theta)\cos(\theta)\sin(\phi)$ $P_2^2 = \sin^2(\theta)\sin(2\phi)$

- By inserting (2) in (1) we derive a system of ODEs for the coefficients $f_0(t), c_{2,-2}(t), \dots, c_{2,2}(t), c_{4,-4}(t), \dots, c_{4,4}(t), \dots$
- We close the system by ignoring higher order basis functions

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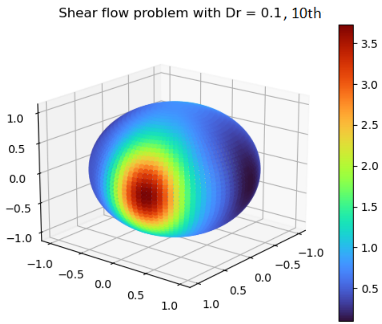
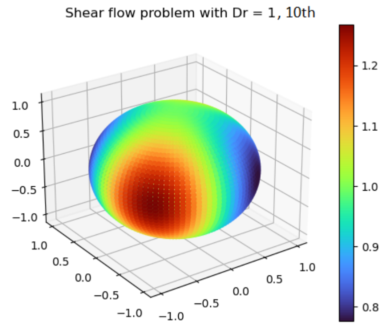
Results for shear flow

Consider externally imposed shear flow

$$\mathbf{u}_{ext} = \begin{pmatrix} u(y) \\ 0 \\ 0 \end{pmatrix}, \quad \nabla_{\mathbf{x}} \mathbf{u}_{ext} = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

Steady state solution of the Smoluchowski equation approximated at $t = 10$ using different values of D_r





For smaller values of D_r particles align stronger. An accurate approximation of the kinetic equation requires a larger number of basis functions. Here spherical harmonics up to order 10 are used.