Derivation and Numerical Simulations of a Coupled Moment System for Modeling Sedimentation in Suspensions of Rod-Like Particles

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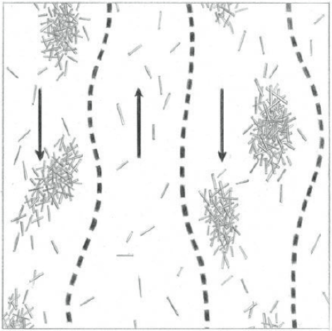
Overview

Guazzelli et al examined a dilute suspension of rod-like particles influenced by gravity.

- In an initially homogeneous suspension, rod-like particles form clusters where they are denser.
- The clusters create downward flows balanced by upward flows.
- Particles in a cluster mostly align with gravity, occasionally flipping.



Mathematical Model for the Sedimentation of Rod-Like Particles

Coupling of a kinetic Smoluchowski equation with Navier-Stokes equation

$$\begin{aligned}
\partial_t f + \nabla_{\boldsymbol{x}} \cdot (\boldsymbol{u} f) + \nabla_{\boldsymbol{n}} \cdot (P_{\boldsymbol{n}^\perp} \nabla_{\boldsymbol{x}} \boldsymbol{u} \boldsymbol{n} f) - \nabla_{\boldsymbol{x}} \cdot ((I + \boldsymbol{n} \otimes \boldsymbol{n}) e_3 f) \\
= D_r \Delta_n f + \gamma \nabla_{\boldsymbol{x}} \cdot (I + \boldsymbol{n} \otimes \boldsymbol{n}) \nabla_{\boldsymbol{x}} f, \\
\sigma = \int_{S^{d-1}} (\mathrm{d}\ \boldsymbol{n} \otimes \boldsymbol{n} - I) f d\boldsymbol{n}, \\
\mathrm{Re}\,(\partial_t \boldsymbol{u} + (\boldsymbol{u} \cdot \nabla_{\boldsymbol{x}})\, \boldsymbol{u}) = \Delta_{\boldsymbol{x}} \boldsymbol{u} - \nabla_{\boldsymbol{x}} p + \delta \gamma \nabla_{\boldsymbol{x}} \cdot \sigma - \delta \int_{S^{d-1}} f d\boldsymbol{n}\, e_3, \\
\nabla_{\boldsymbol{x}} \cdot \boldsymbol{u} = 0,
\end{aligned}$$

where $f = f(\boldsymbol{x}, t, \boldsymbol{n}), \boldsymbol{x} \in \mathbb{R}^3, \boldsymbol{n} \in S^2$ is a density distribution function of particle orientation. D_r, γ, δ and Re are non-dimensional parameters.

Helzel & Tzavaras, 2017

Here we consider the case $\gamma = 0$.

Status of Project

So far...

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

Dahm, Helzel, MMS 2022, Dahm, Giesselmann, Helzel, JCP 2024

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Dahm, Helzel, MMS 2022, Dahm, Giesselmann, Helzel, JCP 2024

Now

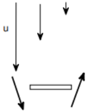
- Derive and approximate hierarchies of moment equations for the coupled kinetic-fluid model with f on S^2.

Overview

For a *shear flow* assume $\boldsymbol{u} = (0, 0, w(x,t))^T$, $f = f(x,t,\phi,\theta)$.

We have

$$\begin{aligned}
&\sin\theta\partial_t f(x,t,\phi,\theta) + \partial_x(\cos\phi\cos\theta\sin^2\theta f)\\
&\qquad + \partial_\theta\left(w_x\sin^3\theta\cos\phi f\right) = D_r\left(\partial_\phi\left(\frac{1}{\sin\theta}\partial_\phi f\right) + \partial_\theta(\sin\theta\partial_\theta f)\right),\\
&\qquad Re\partial_t w(x,t) = \partial_{xx} w + \delta\left(\bar{\rho} - \int_0^{2\pi}\int_0^{\pi} f\sin\theta\, d\theta\, d\phi\right).
\end{aligned} \tag{1}$$



Overview

Ansatz for Derivation of Moment Equations

Consider approximation of the form

$$f(\mathbf{x}, t, \phi, \theta) \approx f^N(\mathbf{x}, t, \phi, \theta) := \sum_{n=0}^{N} \sum_{i=-2n}^{2n} c_{2n}^i(\mathbf{x}, t) \cdot P_{2n}^i(\phi, \theta), \tag{2}$$

where $P_{2n}^i(\phi, \theta)$, $n = 0, \dots, N$, $i = -2n, \dots, 2n$

- are harmonic polynomial basis functions, i.e., the eigenfunctions of the Laplace-Beltrami operator with the eigenvalue $-2n(2n+1)$

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- are harmonic polynomial basis functions, i.e., the eigenfunctions of the Laplace-Beltrami operator with the eigenvalue $-2n(2n+1)$
- form an orthonormal basis, wrt. the L_2-inner product on the sphere

$$(g, h)_{S^2} := \int_0^{2\pi} \int_0^{\pi} g(\phi, \theta) h(\phi, \theta) \cdot \sin(\theta) d\theta d\phi,$$

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$$(g,h)_{S^2} := \int_0^{2\pi} \int_0^{\pi} g(\phi,\theta) h(\phi,\theta) \cdot \sin(\theta) d\theta d\phi,$$

- every square integrable function on S^2 can be expressed as a linear combination of spherical harmonics $f(\phi,\theta) = \sum_{n=0}^{\infty} \sum_{i=-n}^{n} c_n^i \cdot P_n^i(\phi,\theta)$.

Derivation of Moment Equations

We derive the moment equations by

- Insert ansatz $f^N = \sum_{n=0}^{N} \sum_{i=-2n}^{2n} c_{2n}^i(x,t) \cdot P_{2n}^i(\phi,\theta)$ into kinetic equation

$$\sin\theta \partial_t f^N(x,t,\phi,\theta) + \partial_x(\cos\phi\cos\theta\sin^2\theta f^N)$$
$$= -\partial_\theta\left(w_x \sin^3\theta\cos\phi f^N\right) + D_r\left(\partial_\phi\left(\frac{1}{\sin\theta}\partial_\phi f^N\right) + \partial_\theta(\sin\theta\partial_\theta f^N)\right)$$

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- Multiply consecutively with all basis functions used in the ansatz and integrate the resulting equations over the sphere

The system of moment equations has the general form

$$\partial_t Q + A\partial_x Q = D(w_x)Q + D_r EQ, \qquad (3)$$

where $Q = (c_0^0(x,t), c_2^{-2}(x,t), \ldots, c_{2N}^{2N}(x,t))^T$ represents the vector of the moments and $A, D, E \in \mathbb{R}^{(N+1)(2N+1)x(N+1)(2N+1)}$.

Derivation: A Closer Look

Consider

$$\underbrace{\sin\theta\partial_t f^N(x,t,\phi,\theta)}_{[1]} + \underbrace{\partial_x(\cos\phi\cos\theta\sin^2\theta f^N)}_{[2]}$$
$$= -\partial_\theta\left(w_x\sin^3\theta\cos\phi f^N\right) + D_r\left(\partial_\phi\left(\frac{1}{\sin\theta}\partial_\phi f^N\right) + \partial_\theta(\sin\theta\partial_\theta f^N)\right)$$

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For $k = 0,\ldots,N$, $l = -2k,\ldots,2k$ we obtain for term [1]

$$\int_0^{2\pi}\int_0^{\pi}\sin\theta\partial_t\left(\sum_{n=0}^{N}\sum_{i=-2n}^{2n} c_{2n}^i(x,t)\cdot P_{2n}^i(\phi,\theta)\right)P_{2k}^l(\phi,\theta)$$
$$= \sum_{n=0}^{N}\sum_{i=-2n}^{2n}\partial_t c_{2n}^i(x,t)\int_0^{2\pi}\int_0^{\pi}\sin\theta P_{2n}^i(\phi,\theta)P_{2k}^l(\phi,\theta)d\phi d\theta$$
$$= \sum_{n=0}^{N}\sum_{i=-2n}^{2n}\partial_t c_{2n}^i(x,t)(P_{2n}^i(\phi,\theta)P_{2k}^l(\phi,\theta))_{S^2} = \sum_{n=0}^{N}\sum_{i=-2n}^{2n}\partial_t c_{2n}^i(x,t)\cdot\delta_{n,k}\delta_{i,l}$$
$$= \partial_t c_{2k}^l(x,t)$$

Derivation: A Closer Look

Consider

$$\underbrace{\sin\theta\partial_t f^N(x,t,\phi,\theta)}_{[1]}+\underbrace{\partial_x(\cos\phi\cos\theta\sin^2\theta f^N)}_{[2]}$$
$$= -\partial_\theta\left(w_x\sin^3\theta\cos\phi f^N\right)+D_r\left(\partial_\phi\left(\frac{1}{\sin\theta}\partial_\phi f^N\right)+\partial_\theta(\sin\theta\partial_\theta f^N)\right)$$

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$$=\sum_{n=0}^{N}\sum_{i=-2n}^{2n}\partial_t c_{2n}^i(x,t)(P_{2n}^i(\phi,\theta)P_{2k}^l(\phi,\theta))_{S^2}=\sum_{n=0}^{N}\sum_{i=-2n}^{2n}\partial_t c_{2n}^i(x,t)\cdot\delta_{n,k}\delta_{i,l}$$
$$=\partial_t c_{2k}^l(x,t)$$

This corresponds to this term $\partial_t Q + A\partial_x Q = D(w_x)Q + D_r EQ$.

Consider term [2]

$$\underbrace{\sin\theta\partial_t f^N(x,t,\phi,\theta)}_{[1]} + \underbrace{\partial_x(\cos\phi\cos\theta\sin^2\theta f^N)}_{[2]}$$

$$= -\partial_\theta\left(w_x \sin^3\theta\cos\phi f^N\right) + D_r\left(\partial_\phi\left(\frac{1}{\sin\theta}\partial_\phi f^N\right) + \partial_\theta(\sin\theta\partial_\theta f^N)\right)$$

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This represents the term $\partial_t Q + A\partial_x Q = D(w_x)Q + D_r EQ$

For $N = 1$ the matrix A has the form

$$\left[\begin{array}{c:c} A_{0,0} & A_{0,1} \\ \hdashline A_{0,1}^T & A_{1,1} \end{array}\right] = \left[\begin{array}{c:ccccc} 0 & 0 & \frac{1}{\sqrt{15}} & 0 & 0 & 0 \\ \hdashline 0 & 0 & \frac{1}{7} & 0 & 0 & 0 \\ \frac{1}{\sqrt{15}} & \frac{1}{7} & 0 & \frac{\sqrt{3}}{21} & 0 & 0 \\ 0 & 0 & \frac{\sqrt{3}}{21} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{1}{7} \\ 0 & 0 & 0 & 0 & \frac{1}{7} & 0 \end{array}\right].$$

For N = 2 the symmetric matrix A has the structure

$$\left[\begin{array}{c|c|c} A_{0,0} & A_{0,1} & \\ \hline A_{0,1}^T & A_{1,1} & A_{1,2} \\ \hline & A_{1,2}^T & A_{2,2} \end{array}\right].$$

For any N the system of moment equations is hyperbolic.

Now consider the remaining terms:

$$\sin\theta\partial_t f^N(x,t,\phi,\theta) + \partial_x(\cos\phi\cos\theta\sin^2\theta f^N)$$
$$= \underbrace{-\partial_\theta\left(w_x\sin^3\theta\cos\phi f^N\right)}_{[3]} + \underbrace{D_r\left(\partial_\phi\left(\frac{1}{\sin\theta}\partial_\phi f^N\right) + \partial_\theta(\sin\theta\partial_\theta f^N)\right)}_{[4]}.$$

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- Term [4] corresponds to the Laplace-Beltrami operator, resulting in $D_r EQ$, where the matrix E is a diagonal matrix with the Laplace-Beltrami eigenvalues.

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- Term [4] corresponds to the Laplace-Beltrami operator, resulting in $D_r EQ$, where the matrix E is a diagonal matrix with the Laplace-Beltrami eigenvalues.
- Term [3]: We apply the same approach by inserting the ansatz for f and projecting onto the polynomials, resulting in $D(w_x)Q$.

The system of moment equations: $\partial_t Q + A\partial_x Q = D(w_x)Q + D_r EQ$.

Overview

Approximation of Coupled Shear Flow Problem

Consider

$$\begin{aligned}
&\partial_t Q(x,t) + \partial_x Q(x,t) = D(w_x)Q(x,t) + D_r EQ(x,t) \\
&\partial_t w = \partial_{xx} w + \delta(\bar{\rho} - 2\sqrt{\pi} c_0^0(x,t)).
\end{aligned} \tag{4}$$

Approximation of Coupled Shear Flow Problem

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$$\begin{aligned} \partial_t Q(x,t) + \partial_x Q(x,t) &= D(w_x)Q(x,t) + D_r E Q(x,t) \\ \partial_t w &= \partial_{xx} w + \delta(\bar{\rho} - 2\sqrt{\pi} c_0^0(x,t)). \end{aligned} \tag{4}$$

1.	$\frac{1}{2}\Delta t$ step on $\partial_t Q(x,t) = (D(w_x(x,t_n)) + D_r E)Q(x,t)$
2.	$\frac{1}{4}\Delta t$ step on $\partial_t w(x,t) = \delta(\bar{\rho} - 2\sqrt{\pi} c_0^0(x,t))$
3.	$\frac{1}{2}\Delta t$ step on $\partial_t w(x,t) = \partial_{xx} w(x,t)$
4.	$\frac{1}{4}\Delta t$ step on $\partial_t w(x,t) = \delta(\bar{\rho} - 2\sqrt{\pi} c_0^0(x,t))$
5.	Δt step on $\partial_t Q(x,t) + A\partial_x Q(x,t) = 0$
6.	$\frac{1}{4}\Delta t$ step on $\partial_t w(x,t) = \delta(\bar{\rho} - 2\sqrt{\pi} c_0^0(x,t))$
7.	$\frac{1}{2}\Delta t$ step on $\partial_t w(x,t) = \partial_{xx} w(x,t)$
8.	$\frac{1}{4}\Delta t$ step on $\partial_t w(x,t) = \delta(\bar{\rho} - 2\sqrt{\pi} c_0^0(x,t))$
9.	$\frac{1}{2}\Delta t$ step on $\partial_t Q(x,t) = (D(w_x(x,t_{n+1})) + D_r E)Q(x,t)$

Table 1: Splitting algorithm for solving the coupled shear flow problem ([1])

We use an ODE solver for $1. + 9.$, LeVeque's high resolution wave propagation algorithm for 5. and finite difference methods for the evolution of w.

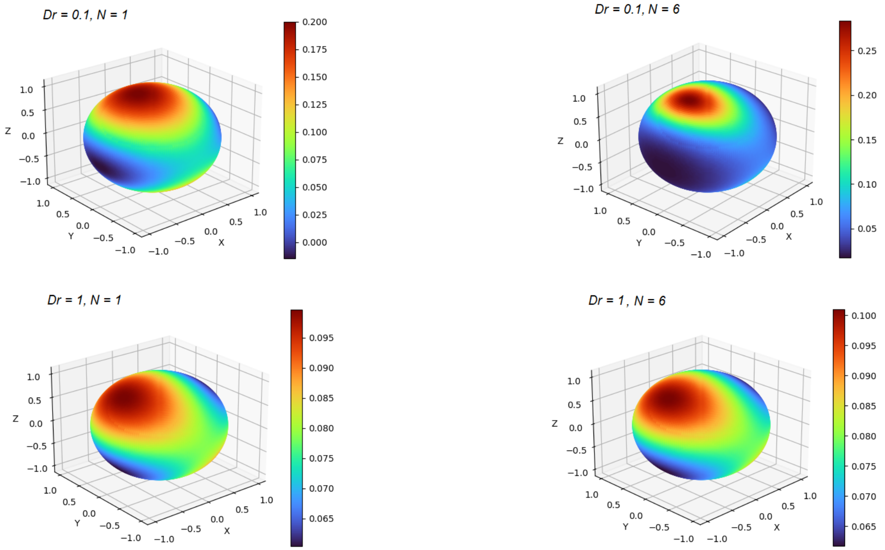

Figure 1: Numerical solution of the drift-diffusion term with constant externally imposed velocity gradient corresponding to shear flow using different values of D_r and $N = 1, 6$.

Accuracy Study

Let $c_0^0(x,0) = exp(-(x-50)^2)/(2 \cdot \sqrt{\pi})$ be the initial value.

	$\mathrm{N}=1$		$\mathrm{N}=2$		$\mathrm{N}=3$	
grid	$L1$-Error	EOC	$L1$-Error	EOC	$L1$-Error	EOC
256	$2.7197 \cdot 10^{-1}$		$1.9174 \cdot 10^{-2}$		$1.6585 \cdot 10^{-1}$	
512	$1.0421 \cdot 10^{-1}$	1.38	$6.4197 \cdot 10^{-2}$	1.57	$5.4157 \cdot 10^{-2}$	1.61
1024	$3.0275 \cdot 10^{-2}$	1.78	$1.7984 \cdot 10^{-2}$	1.83	$1.5270 \cdot 10^{-2}$	1.82
2048	$7.6037 \cdot 10^{-3}$	1.99	$4.4721 \cdot 10^{-3}$	2.0	$3.6918 \cdot 10^{-3}$	2.04

Table 2: Accuracy study for the component c_0^0 of the coupled problem for shear flow using $D_r = 1$. The reference solution, computed on a grid with 8192 cells, uses the same number of moment equations as the coarse solution. In all computations the time step was limited by a CFL condition with $cfl \leq 0.8$.

Accuracy Study

	N = 1		N = 2		N = 3	
grid	$L1$-Error	EOC	$L1$-Error	EOC	$L1$-Error	EOC
256	$1.1624 \cdot 10^{-2}$		$2.6060 \cdot 10^{-3}$		$6.0421 \cdot 10^{-3}$	
512	$1.2524 \cdot 10^{-2}$	-0.10	$1.1655 \cdot 10^{-3}$	1.16	$1.1655 \cdot 10^{-3}$	2.37
1024	$1.3168 \cdot 10^{-2}$	-0.07	$3.1649 \cdot 10^{-3}$	-1.44	$8.0673 \cdot 10^{-4}$	0.53
2048	$1.3310 \cdot 10^{-2}$	-0.01	$3.4125 \cdot 10^{-3}$	-0.10	$5.5722 \cdot 10^{-4}$	0.53

Table 3: Accuracy analysis for the component c_0^0 of the coupled problem for shear flow using $D_r = 0.01$. The reference solution, computed on a grid with 8192 cells using $N = 6$. In all computations the time step was limited by a CFL condition with $cfl \leq 0.8$.

	N = 4		N = 5	
grid	$L1$-Error	EOC	$L1$-Error	EOC
256	$5.9343 \cdot 10^{-3}$		$6.2261 \cdot 10^{-3}$	
512	$2.1285 \cdot 10^{-3}$	1.47	$2.3204 \cdot 10^{-3}$	1.42
1024	$6.1323 \cdot 10^{-4}$	1.79	$6.8919 \cdot 10^{-4}$	1.75
2048	$2.4303 \cdot 10^{-4}$	1.33	$1.7118 \cdot 10^{-4}$	2.0

Table 4: Accuracy analysis for the component c_0^0 of the coupled problem for shear flow using $D_r = 0.01$. The reference solution, computed on a grid with 8192 cells using $N = 6$. In all computations the time step was limited by a CFL condition with $cfl \leq 0.8$.

Accuracy Study

	N = 1		N = 2		N = 3	
grid	$L1$-Error	EOC	$L1$-Error	EOC	$L1$-Error	EOC
256	$1.4093 \cdot 10^{-2}$		$8.4036 \cdot 10^{-3}$		$6.6520 \cdot 10^{-3}$	
512	$3.4409 \cdot 10^{-3}$	2.03	$2.0240 \cdot 10^{-3}$	2.05	$2.0034 \cdot 10^{-3}$	1.73
1024	$1.5602 \cdot 10^{-3}$	1.14	$4.3070 \cdot 10^{-4}$	2.23	$5.4486 \cdot 10^{-4}$	1.87
2048	$1.4673 \cdot 10^{-3}$	0.08	$1.2731 \cdot 10^{-4}$	1.75	$1.3623 \cdot 10^{-4}$	1.99

Table 5: Accuracy analysis for the component c_0^0 of the coupled problem for shear flow using $D_r = 0.05$. The reference solution, computed on a grid with 8192 cells using $N = 6$. In all computations the time step was limited by a CFL condition with $cfl \leq 0.8$.

	$\mathrm{N}=1$		$\mathrm{N}=2$		$\mathrm{N}=3$	
grid	$L1$-Error	EOC	$L1$-Error	EOC	$L1$-Error	EOC
256	$2.7228 \cdot 10^{-1}$		$1.9183 \cdot 10^{-1}$		$1.6589 \cdot 10^{-1}$	
512	$1.0452 \cdot 10^{-1}$	1.38	$3.1259 \cdot 10^{-2}$	2.61	$5.4197 \cdot 10^{-2}$	1.61
1024	$3.0596 \cdot 10^{-2}$	1.77	$1.8077 \cdot 10^{-2}$	0.79	$1.5310 \cdot 10^{-2}$	1.82
2048	$7.9252 \cdot 10^{-3}$	1.94	$4.5655 \cdot 10^{-3}$	1.98	$3.7315 \cdot 10^{-3}$	2.03

Table 6: Accuracy analysis for the component c_0^0 of the coupled problem for shear flow using $D_r = 1$. The reference solution, computed on a grid with 8192 cells using $N = 6$. All simulations employed a time step constrained by a CFL condition with $cfl \leq 0.8$.

Let

$$c_0^0(x,0) = (1 + (1 \cdot 10^{-4} \cdot \eta(x) - 5 \cdot 10^{-5}))/(2\sqrt{\pi}),$$

where $\eta(x)$ is a random variable taking values in the interval $\pm\frac{1}{2}$.

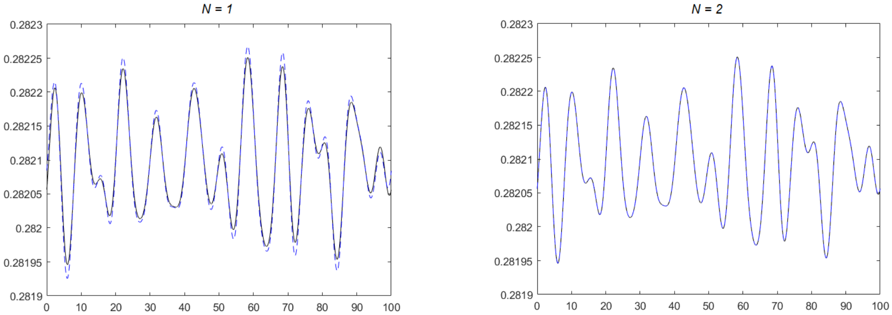

Figure 2: Approximation of the coupled problem for shear flow with $D_r = 0.05$. The plot shows the density at time $t = 30$ for $N = 1$ and $N = 2$ (blue line). A reference solution is calculated with $N = 6$ moment equations (black line).

Current Work in Progress: Coupled System for Rectilinear Flow

We consider $\boldsymbol{u} = (0, 0, w(x, y, t))^T$, $f(x, y, t, \phi, \theta)$. We get

$$
\begin{aligned}
&\sin\theta \partial_t f(x, y, t, \phi, \theta) + \partial_x(\cos\phi \sin\theta \cos\theta f) + \partial_y(\sin\phi \sin\theta \cos\theta f) \\
&+ \partial_\theta \left((w_x \sin^3\theta \cos\phi + w_y \sin\phi \sin^3\theta) f \right) = D_r \left(\partial_\phi \left(\frac{1}{\sin\theta} \partial_\phi f \right) + \partial_\theta (\sin\theta \partial_\theta f) \right) \\
&Re \partial_t w(x, y, t) = \partial_{xx} w + \partial_{yy} w + \delta \left(\bar{\rho} - \int_0^{2\pi} \int_0^{\pi} f \sin\theta d\theta d\phi \right).
\end{aligned} \tag{5}
$$

Current Work in Progress: Coupled System for Rectilinear Flow

We consider $\boldsymbol{u} = (0, 0, w(x, y, t))^T$, $f(x, y, t, \phi, \theta)$. We get

$$\begin{aligned}
&\sin\theta\partial_t f(x, y, t, \phi, \theta) + \partial_x(\cos\phi\sin\theta\cos\theta f) + \partial_y(\sin\phi\sin\theta\cos\theta f) \\
&+ \partial_\theta\left((w_x\sin^3\theta\cos\phi + w_y\sin\phi\sin^3\theta)f\right) = D_r\left(\partial_\phi\left(\frac{1}{\sin\theta}\partial_\phi f\right) + \partial_\theta(\sin\theta\partial_\theta f)\right) \\
&Re\partial_t w(x, y, t) = \partial_{xx}w + \partial_{yy}w + \delta\left(\bar{\rho} - \int_0^{2\pi}\int_0^{\pi} f\sin\theta d\theta d\phi\right).
\end{aligned} \tag{5}$$

The system of hierarchy of moment equations is given as

$$\partial_t Q + A\partial_x Q + B\partial_y Q = D(w_x, w_y)Q + D_r EQ. \tag{6}$$

Figure 3: Numerical solution of the drift-diffusion term for fixed w_x and w_y.

Figure 4: Numerical results for c_0^0 at different times using $D_r = 1$ and $w_x = w_y = 1$ for $x < 50$ and $w_x = w_y = -1$ otherwise. A cluster with higher particle density splits into two, each moving in opposite directions.

Literatur I

S. Dahm, J. Giesselmann, and C. Helzel.
Numerical discretisation of hyperbolic systems of moment equations describing sedimentation in suspensions of rod-like particles, 2024.

S. Dahm and C. Helzel.
Hyperbolic systems of moment equations describing sedimentation in suspensions of rod-like particles.
Multiscale Modeling & Simulation, 20(3):1002–1039, 2022.

É. Guazzelli and J. F. Morris.
A physical introduction to suspension dynamics. With illustrations by Sylvie Pic.
Camb. Texts Appl. Math. Cambridge: Cambridge University Press, 2012.

Literatur II

C. Helzel and F. Otto.
Multiscale simulations for suspensions of rod-like molecules.
J. Comput. Phys., 216(1):52–75, 2006.

C. Helzel and M. Schneiders.
Numerical approximation of the Smoluchowski equation using radial basis functions.
J. Comput. Math., 38(1):176–194, 2020.

C. Helzel and A. E. Tzavaras.
A kinetic model for the sedimentation of rod-like particles.
Multiscale Model. Simul., 15(1):500–536, 2017.

M. Morimoto.
Analytic functionals on the sphere, volume 178 of *Transl. Math. Monogr.*
Providence, RI: American Mathematical Society, 1998.