3D Simulation of Sedimentation in Suspensions of Rod-Like Particles

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Overview

Mathematical Model for the Sedimentation of Rod-Like Particles

Coupling of a kinetic Smoluchowski equation with Navier-Stokes equation

$$
\begin{aligned}
\partial_t f + \nabla_{\boldsymbol{x}} \cdot (\boldsymbol{u} f) + \nabla_{\boldsymbol{n}} \cdot (P_{\boldsymbol{n}^\perp} \nabla_{\boldsymbol{x}} \boldsymbol{u} \boldsymbol{n} f) - \nabla_{\boldsymbol{x}} \cdot ((I + \boldsymbol{n} \otimes \boldsymbol{n}) \boldsymbol{e}_3 f) \\
= D_r \Delta_n f, \\
\mathrm{Re}\left(\partial_t \boldsymbol{u} + (\boldsymbol{u} \cdot \nabla_{\boldsymbol{x}})\, \boldsymbol{u}\right) = \Delta_{\boldsymbol{x}} \boldsymbol{u} - \nabla_{\boldsymbol{x}} p - \delta \left(\int_{S^{d-1}} f d\boldsymbol{n} \right) \boldsymbol{e}_3, \\
\nabla_{\boldsymbol{x}} \cdot \boldsymbol{u} = 0,
\end{aligned}
$$

where $f = f(\boldsymbol{x}, t, \boldsymbol{n})$ represents the particle distribution of rod-like particles as a function of time t, space $\boldsymbol{x} \in \mathbb{R}^3$ and orientation $\boldsymbol{n} \in S^2$. D_r, δ and Re are non-dimensional parameters.

Helzel & Tzavaras, 2017

2D: Coupled System for Rectilinear Flow

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

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

2D: Coupled System for Rectilinear Flow

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

The system of hierarchy of moment equations is given as

$$\partial_t Q + A\partial_x Q + B\partial_y Q = D(w_x, w_y)Q + D_r EQ, \tag{2}$$

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

Figure 1: 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.

Figure 2: Solution structure of c_0^0 with $N = 7$.

Status of Project

So far...

- Derive and approximate hierarchies of moment equations for the coupled kinetic-fluid model with f on S^2
  - 1D Shear Flow
  - 2D Rectilinear Flow

Now

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

- Extension to the 3D case: moment equations for the coupled kinetic–fluid model with f on S^2

Overview

Approximation of Coupled Shear Flow Problem

Consider

$$\begin{aligned} &\partial_t Q(x,t) + A\partial_x Q(x,t) = D(w_x)Q(x,t) + D_r EQ(x,t) \\ &\partial_t w = \partial_{xx} w + \delta(\bar{\rho} - 2\sqrt{\pi}c_0^0(x,t)). \end{aligned} \tag{3}$$

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 (Dahm et al.)

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.

1D Wave Propagation Algorithm (LeVeque et al.)

We consider the hyperbolic system

$$q_t + f(q)_x = 0, \quad q \in \mathbb{R}^m$$

- Discretize the domain into cells $[x_{i-1/2}, x_{i+1/2}]$.
- At each interface $x_{i+1/2}$, solve the Riemann problem:

$$q(x,0) = \begin{cases} q_i, & x < x_{i+1/2}, \\ q_{i+1}, & x > x_{i+1/2}. \end{cases}$$

- Decompose the jump into waves along eigenvectors of $A = f'(q)$:

$$q_{i+1} - q_i = \sum_{p=1}^{m} \alpha^p r^p, \quad W^p = \alpha^p r^p, \text{ travelling with } s^p.$$

- Define fluctuations:

$$\mathcal{A}^+ \Delta q_{i-1/2} = \sum_{p:s^p>0} s^p W^p, \quad \mathcal{A}^- \Delta q_{i+1/2} = \sum_{p:s^p<0} s^p W^p$$

- Update cell averages:

$$Q_i^{n+1} = Q_i^n - \frac{\Delta t}{\Delta x}\left(\mathcal{A}^+ \Delta q_{i-1/2} + \mathcal{A}^- \Delta q_{i+1/2}\right)$$

Multidimensional Wave Propagation (2D and 3D)

General system:

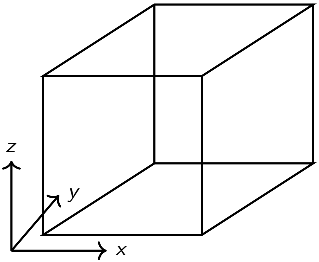
$$q_t + f(q)_x + g(q)_y + h(q)_z = 0$$

Key ideas:

- **1D Riemann problems at cell faces:** Solve along the normal direction of each cell face.
- **Wave decomposition:** Decompose jumps into waves W^p with speeds s^p.
- **Fluctuations:**

$$\mathcal{A}^{\pm}\Delta q, \quad \mathcal{B}^{\pm}\Delta q, \quad \mathcal{C}^{\pm}\Delta q$$

- **Transverse propagation:**
  - 2D: Waves in x-direction generate waves in y, and vice versa.
  - 3D: Each wave generates transverse waves along in the other two directions.



3D Transverse and Double Transverse Propagation

In 3D: every wave generates transverse and double–transverse contributions in the other directions

Examples of Transverse Interactions

- $x \to y$ (transverse)
- $x \to z$ (transverse)
- $x \to y \to z$ (double transverse)
- $y \to x \to z$, etc.

Update Scheme

$$
\begin{aligned}
Q^{n+1}_{i,j,k} = Q^{n}_{i,j,k} &- \frac{\Delta t}{\Delta x}\left(\mathcal{A}^{+}\Delta q_{i-1/2,j,k} + \mathcal{A}^{-}\Delta q_{i+1/2,j,k}\right) \\
&- \frac{\Delta t}{\Delta y}\left(\mathcal{B}^{+}\Delta q_{i,j-1/2,k} + \mathcal{B}^{-}\Delta q_{i,j+1/2,k}\right) \\
&- \frac{\Delta t}{\Delta z}\left(\mathcal{C}^{+}\Delta q_{i,j,k-1/2} + \mathcal{C}^{-}\Delta q_{i,j,k+1/2}\right).
\end{aligned}
$$

Overview

Coupled System for a Three-Dimensional Flow

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

$$
\begin{aligned}
&\sin\theta\partial_t f(x,y,t,\phi,\theta) + \partial_x(\cos\phi\sin\theta\cos\theta f) + \partial_y(\sin\phi\sin\theta\cos\theta f) - \partial_z((1+\cos^2\theta)f)\\
&= -\partial_\theta\left((w_x\sin^3\theta\cos\phi + w_y\sin\phi\sin^3\theta - w_z\cos\theta\sin^2\theta)f\right) D_r\left(\partial_\phi\left(\frac{1}{\sin\theta}\partial_\phi f\right) + \partial_\theta(\sin\theta\partial_\theta f)\right)\\
&Re\partial_t w(x,y,t) = \partial_{xx}w + \partial_{yy}w + \partial_{yy}z + \delta\left(\bar{\rho} - \int_0^{2\pi}\int_0^{\pi} f\sin\theta d\theta d\phi\right).
\end{aligned}
\tag{4}
$$

Coupled System for a Three-Dimensional Flow

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

$$\sin\theta \partial_t f(x, y, t, \phi, \theta) + \partial_x(\cos\phi \sin\theta \cos\theta f) + \partial_y(\sin\phi \sin\theta \cos\theta f) - \partial_z((1 + \cos^2\theta) f)$$
$$= -\partial_\theta \left((w_x \sin^3\theta \cos\phi + w_y \sin\phi \sin^3\theta - w_z \cos\theta \sin^2\theta) f \right) D_r \left(\partial_\phi \left(\frac{1}{\sin\theta} \partial_\phi f \right) + \partial_\theta(\sin\theta \partial_\theta f) \right)$$
$$Re \partial_t w(x, y, t) = \partial_{xx} w + \partial_{yy} w + \partial_{yy} z + \delta \left(\bar{\rho} - \int_0^{2\pi} \int_0^{\pi} f \sin\theta d\theta d\phi \right). \tag{4}$$

The system of hierarchy of moment equations is given as

$$\partial_t Q + A \partial_x Q + B \partial_y Q + C \partial_z Q = D(w_x, w_y, w_z) Q + D_r E Q, \tag{5}$$

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 $A, B, C, D, E \in \mathbb{R}^{(N+1)(2N+1)x(N+1)(2N+1)}$.

Wave Propagation and Error Analysis

Wave propagation parameters (LeVeque et al.): The scheme can be characterized by three integers (m_1, m_2, m_3):

- m_1: Correction wave (1 = not included, 2 = included)
- m_2: Transverse propagation (0 = none, 1 = increment only, 2 = increment + correction)
- m_3: Double-transverse propagation (0 = none, 1 = increment only, 2 = increment + correction)

Error computation: On a coarse grid, define

$$E(h) = U(h) - U(h/2), \quad E(h/2) = U(h/2) - U(h/4)$$

Accuracy Analysis

Let

$$r = \sqrt{(x-40)^2 + (y-30)^2 + (z-50)^2}, \quad c_0^0(x,y,k,0) = \exp(-0.01\, r^2)$$

be the initial value.

Method	Grid	N=1		N=2		N=7	
		L_1 Error	EOC	L_1 Error	EOC	L_1 Error	EOC
(1,1,1)	32	$5.57 \cdot 10^{-4}$	-	$5.47 \cdot 10^{-4}$	-	$5.01 \cdot 10^{-4}$	-
	64	$3.54 \cdot 10^{-4}$	0.65	$3.40 \cdot 10^{-4}$	0.68	$2.93 \cdot 10^{-4}$	0.77
	128	$1.79 \cdot 10^{-4}$	0.98	$1.80 \cdot 10^{-4}$	0.91	-	-
(2,2,2)	32	$1.79 \cdot 10^{-4}$	-	$2.00 \cdot 10^{-4}$	-	$1.83 \cdot 10^{-4}$	-
	64	$4.66 \cdot 10^{-5}$	1.94	$5.45 \cdot 10^{-5}$	1.86	$4.82 \cdot 10^{-5}$	1.92
	128	$1.17 \cdot 10^{-5}$	1.99	$1.38 \cdot 10^{-5}$	1.98	-	-

Table: Accuracy analysis for the component c_0^0 of the coupled 3D flow problem ($D_r = 1$). The time step was limited by the CFL condition, with *cfl* ≤ 0.45 for method (1,1,1) and *cfl* ≤ 0.9 for method (2,2,2).

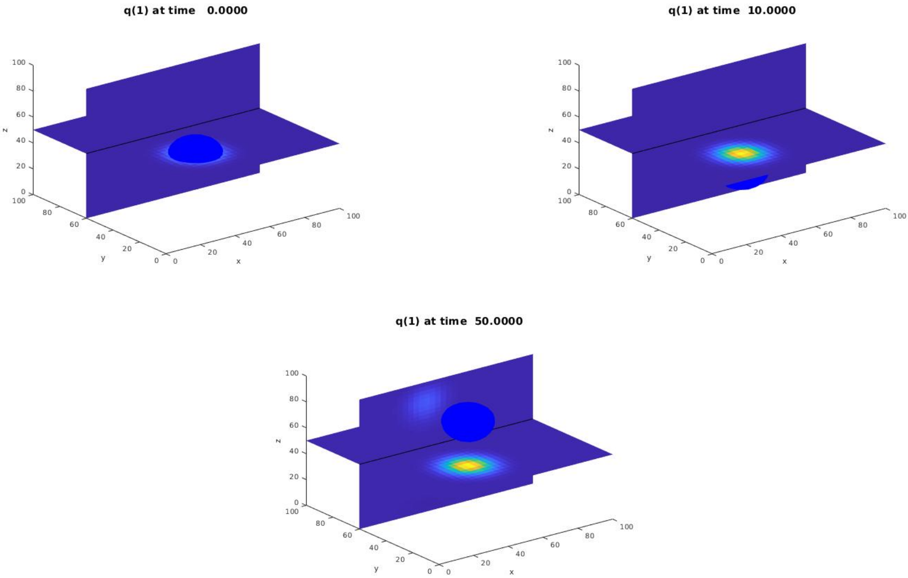


Figure 3: Numerical results for c_0^0 at different times using $D_r = 1$, $w_x = w_y = 1$ and $w_z = 0$.

Conclusion

- TODO
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