

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

Bella My Phuong Quynh Duong, Christiane Helzel

Heinrich-Heine University Düsseldorf

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Overview

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Mathematical Model for the Sedimentation of Rod-Like Particles

Coupling of a kinetic Smoluchowski equation with Navier-Stokes equation

$$\begin{aligned}\partial_t f + \nabla_{\mathbf{x}} \cdot (\mathbf{u} f) + \nabla_{\mathbf{n}} \cdot (P_{\mathbf{n}^\perp} \nabla_{\mathbf{x}} \mathbf{u} n f) - \nabla_{\mathbf{x}} \cdot ((I + \mathbf{n} \otimes \mathbf{n}) \mathbf{e}_3 f) \\ = D_r \Delta_{\mathbf{n}} f,\end{aligned}$$

$$\text{Re} (\partial_t \mathbf{u} + (\mathbf{u} \cdot \nabla_{\mathbf{x}}) \mathbf{u}) = \Delta_{\mathbf{x}} \mathbf{u} - \nabla_{\mathbf{x}} p - \delta \left(\int_{S^{d-1}} f d\mathbf{n} \right) \mathbf{e}_3,$$

$$\nabla_{\mathbf{x}} \cdot \mathbf{u} = 0,$$

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

Helzel & Tzavaras, 2017

2D: Coupled System for Rectilinear Flow

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

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

2D: Coupled System for Rectilinear Flow

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

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

The system of hierarchy of moment equations is given as

$$\partial_t Q + A \partial_x Q + B \partial_y Q = D(w_x, w_y) Q + D_r E Q, \quad (2)$$

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

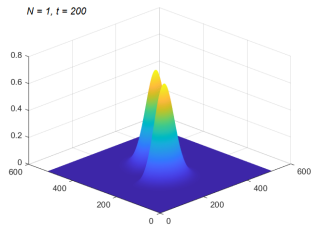
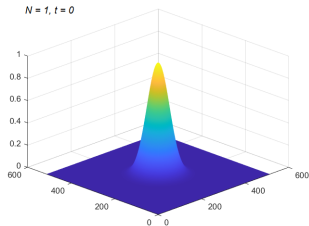


Figure 1: Numerical results for c_0^0 at different times using $D_r = 1$ and $w_x = w_y = 1$ for $x < 50$ and $w_x = w_y = -1$ otherwise. A cluster with higher particle density splits into two, each moving in opposite directions.

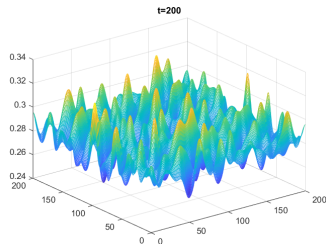
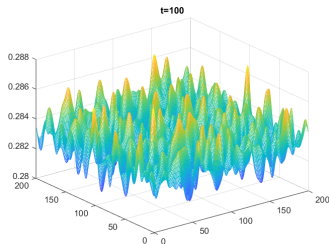


Figure 2: Solution structure of c_0^0 with $N = 7$.

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

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Approximation of Coupled Shear Flow Problem

Consider

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

1.	$\frac{1}{2}\Delta t$ step on $\partial_t Q(x, t) = (D(w_x(x, t_n)) + D_rE)Q(x, t)$
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 $\partial_t Q(x, t) = (D(w_x(x, t_{n+1})) + D_rE)Q(x, t)$

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:

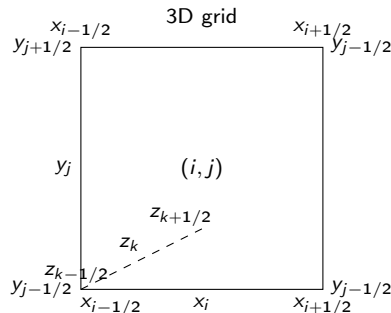
$$q_t + f(q)_x + g(q)_y + h(q)_z = 0$$

Key ideas:

- **1D Riemann problems at cell interfaces:** Solve along the normal direction of each cell interface.
- **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

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

Update Scheme

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

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Coupled System for a Three-Dimensional Flow

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

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

Coupled System for a Three-Dimensional Flow

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

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

The system of hierarchy of moment equations is given as

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

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

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

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 $cfl \leq 0.45$ for method (1,1,1) and $cfl \leq 0.9$ for method (2,2,2).

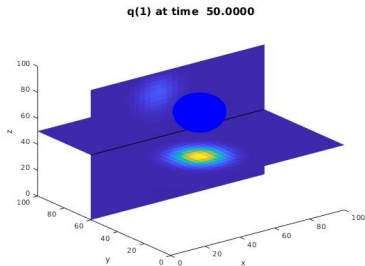
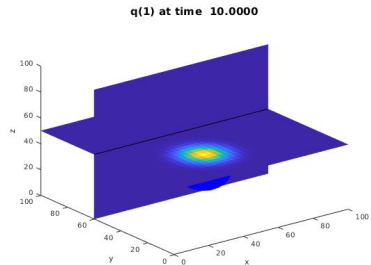
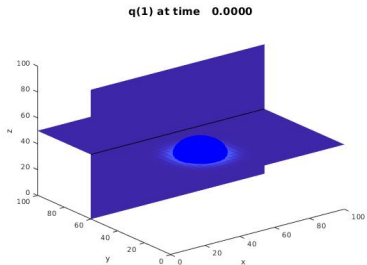


Figure 3: Numerical results for c_0^0 at different times using $D_r = 1$, $w_x = w_y = 1$ and $w_z = 0$.

Conclusion

- TODO
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