

# Modeling and Simulations of Sedimentation in Suspensions of Rod-Like Particles

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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  $\mathbf{n} \in S^2$ .  $D_r, \delta$  and  $\text{Re}$  are non-dimensional parameters.

Helzel & Tzavaras, 2017

# Outline of the Project

## Goal

- Reduce the high-dimensional kinetic equation (in space and orientation) to a lower-dimensional system of moment equations (in space).
- Derive and approximate hierarchies of moment equations for the coupled kinetic-fluid model with  $f$  on  $S^2$

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## Our Approach

Investigate different coupled flow situations

- externally imposed velocity field ✓
- coupled problems:
  - 1D shear flow ✓
  - 2D rectilinear flow ✓
  - 3D flow with periodic boundary conditions

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# Shear Flow

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

Consider *Shear Flow*, i.e. assume  $\mathbf{u} = (0, 0, w(x, t))^T$ ,  $f = f(x, t, \phi, \theta)$ .



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Consider *Shear Flow*, i.e. assume  $\mathbf{u} = (0, 0, w(x, t))^T$ ,  $f = f(x, t, \phi, \theta)$ .

In spherical coordinates and for the given velocity field  $\mathbf{u}$ , we get

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

# Derivation of Moment Equations

Consider approximation of the form

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

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

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

- Projection to the basis functions

The system of moment equations has the general form

$$\partial_t Q + A \partial_x Q = D(w_x) Q + D_r E Q, \quad (3)$$

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  $A, D, E \in \mathbb{R}^{(N+1)(2N+1) \times (N+1)(2N+1)}$ . For  $N = 1$  the matrix  $A$  has the form

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

# Rectilinear Flow

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

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

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$$Re \partial_t w(x, y, t) = \partial_{xx} w + \partial_{yy} w + \delta \left( \bar{\rho} - \int_0^{2\pi} \int_0^\pi f \sin \theta d\theta d\phi \right).$$

The moment equations have the general form

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

For  $N = 1$ :

$$B = \left[ \begin{array}{c|cccccc} 0 & 0 & 0 & 0 & \frac{\sqrt{15}}{15} & 0 \\ \hline 0 & 0 & 0 & 0 & -\frac{1}{7} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{1}{7} \\ 0 & 0 & 0 & 0 & \frac{\sqrt{3}}{21} & 0 \\ \hline \frac{\sqrt{15}}{15} & -\frac{1}{7} & 0 & \frac{\sqrt{3}}{21} & 0 & 0 \\ \hline 0 & 0 & \frac{1}{7} & 0 & 0 & 0 \end{array} \right].$$

# 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

$$\begin{aligned} & \sin \theta \partial_t f(x, y, t, \phi, \theta) + \partial_x (\cos \phi \sin \theta \cos \theta f) + \partial_y (\sin \phi \sin \theta \cos \theta f) - \partial_z ((1 + \cos^2 \theta) f) \\ &= -\partial_\theta ((w_x \sin^3 \theta \cos \phi + w_y \sin \phi \sin^3 \theta - w_z \cos \theta \sin^2 \theta) f) D_r \left( \partial_\phi \left( \frac{1}{\sin \theta} \partial_\phi f \right) + \partial_\theta (\sin \theta \partial_\theta f) \right) \\ & Re \partial_t w(x, y, t) = \partial_{xx} w + \partial_{yy} w + \partial_{yy} z + \delta \left( \bar{\rho} - \int_0^{2\pi} \int_0^\pi f \sin \theta d\theta d\phi \right). \end{aligned} \tag{6}$$

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The moment equations have the general form

$$\partial_t Q + A \partial_x Q + B \partial_y Q + C \partial_z Q = D(w_x, w_y, w_z) Q + D_r E Q. \quad (7)$$

For  $N = 1$ :

$$C = \left[ \begin{array}{c|ccc} -\frac{4}{3} & 0 & 0 & -\frac{2\sqrt{5}}{15} & 0 & 0 \\ \hline 0 & -\frac{8}{7} & 0 & 0 & 0 & 0 \\ 0 & 0 & -\frac{10}{7} & 0 & 0 & 0 \\ -\frac{2\sqrt{5}}{15} & 0 & 0 & -\frac{32}{21} & 0 & 0 \\ 0 & 0 & 0 & 0 & -\frac{10}{7} & 0 \\ 0 & 0 & 0 & 0 & 0 & -\frac{8}{7} \end{array} \right].$$



# 1D Wave Propagation Algorithm (LeVeque et al.)

We consider the linear hyperbolic system

$$q_t + Aq_x = 0, \quad q \in \mathbb{R}^m$$

- 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  $A$ :

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

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- 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)

**Linear hyperbolic system:**

$$q_t + Aq_x + Bq_y + Cq_z = 0$$

**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:**

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

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- **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

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

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# Approximation of Coupled Shear Flow Problem

Consider

$$\begin{aligned}\partial_t Q(x, t) + A\partial_x Q(x, t) &= D(w_x)Q(x, t) + D_rEQ(x, t) \\ \partial_t w &= \partial_{xx} w + \delta(\bar{\rho} - 2\sqrt{\pi}c_0^0(x, t)).\end{aligned}\tag{8}$$

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.	$\Delta t$ 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  $w$ .

# Coupled Problems

- externally imposed velocity field ✓
- 1D shear flow ✓
- 2D rectilinear flow ✓
- 3D flow with periodic boundary conditions



# Numerical Result for externally imposed velocity field

Consider the drift-diffusion term

$$\partial_t Q(x, t) = D(w_x)Q(x, t) + D_r EQ(x, t),$$

with  $w_x = 1$ .

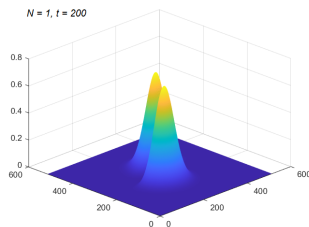
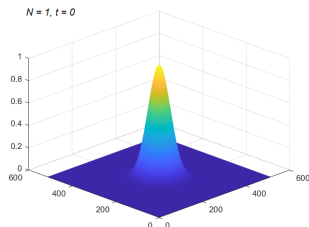


**Figure 1:** Numerical solution of the drift-diffusion term with constant externally imposed velocity gradient corresponding to shear flow using different values of  $D_r$ .

# Numerical Result for externally imposed velocity field

Approximations of the two-dimensional hyperbolic system

$$\partial_t Q(x, t) + A \partial_x Q(x, t) + B \partial_y Q(x, t) = D(w_x, w_y) Q(x, t) + D_r E Q(x, t).$$



**Figure 2:** Solution structure of  $c_0^0$  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.

# Coupled Problems

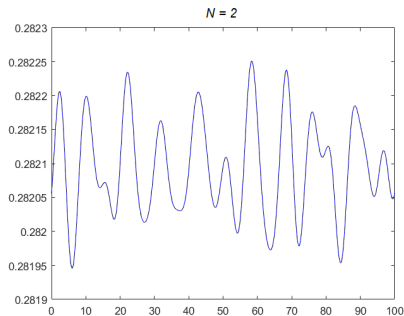
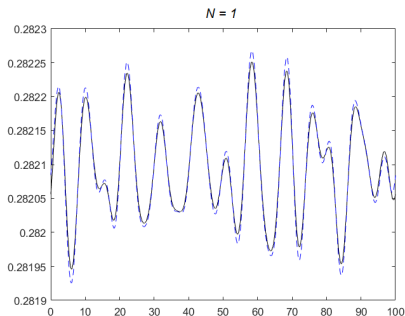
- externally imposed velocity field ✓
- 1D shear flow ✓
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- 3D flow with periodic boundary conditions

# Numerical Result for Shear Flow

Let

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

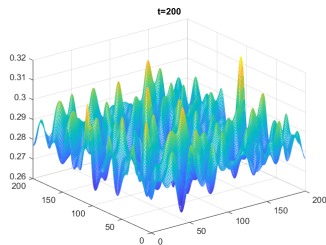
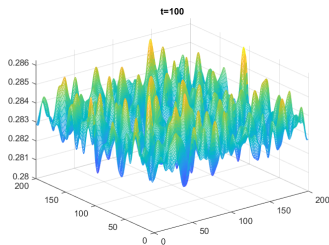
where  $\eta(x)$  is a random variable taking values in the interval  $\pm \frac{1}{2}$ .



**Figure 3:** 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).

# Coupled Problems

- externally imposed velocity field ✓
- 1D shear flow ✓
- 2D rectilinear flow ✓
- 3D flow with periodic boundary conditions



Solution structure of  $c_0^0$  with  $N=1$ .

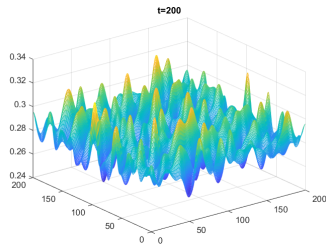
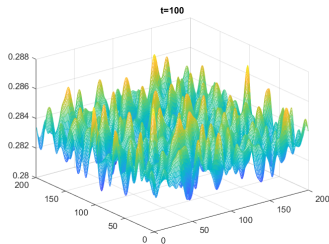


Figure 4: Solution structure of  $c_0^0$  with  $N=7$ .

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# 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

Consider approximations of the three-dimensional hyperbolic system

$$\partial_t Q + A Q_x + B Q_y + C Q_z = (D(w_x, w_y, w_z) + DrE)Q \quad (9)$$

with externally imposed velocity gradient  $w_x = 1 = w_y$  and  $w_z = 0$ .

Let

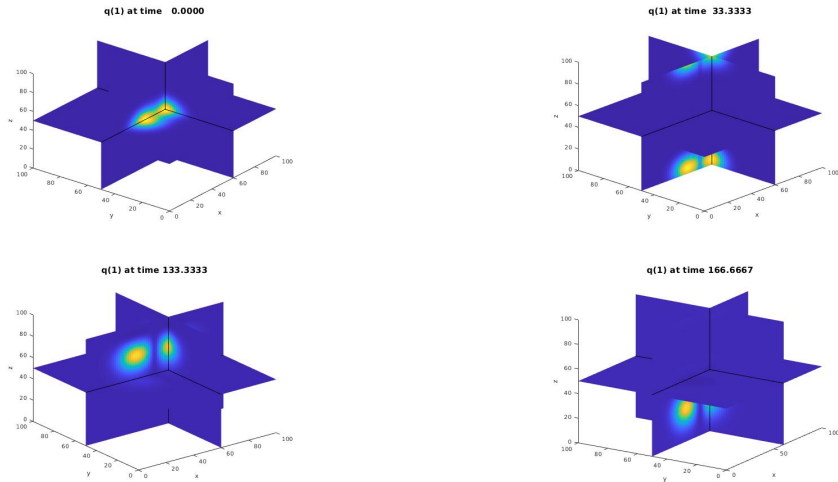
$$r = \sqrt{(x - 40)^2 + (y - 30)^2 + (z - 50)^2}, \quad c_0^0(x, y, k, 0) = \exp(-0.01 r^2)$$

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 (9) using  $D_r = 1$ . 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).

# Numerical Result for externally imposed velocity field



**Figure 5:** Evolution of  $c_0^0$  at different times, showing two Gaussian clusters transported in opposite directions by a piecewise constant velocity field ( $w_x = w_y = 1$  for  $x < 50$ ,  $w_x = w_y = -1$  otherwise, and  $w_z = 0$  everywhere).

# Conclusion

- Derive and approximate moment systems for the kinetic Smochulowski equation with  $f$  on  $S^2$
- High-resolution wave propagation methods (LeVeque) were successfully adapted to 1D, 2D, and 3D moment systems.
- Numerical tests:
  - Drift vs. diffusion effects visible
  - Clustering and splitting in flow fields
- Outlook: simulations in fully coupled 3D flows and accuracy analysis.