# Modeling and Simulations 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

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

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 $\boldsymbol{n} \in S^2$. $D_r, \delta$ and $Re$ 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

# Overview

# Shear Flow

$$\partial_t f + \nabla_{\boldsymbol{x}} \cdot (\boldsymbol{u} f) - \nabla_{\boldsymbol{x}} \cdot ((I + \boldsymbol{n} \otimes \boldsymbol{n}) e_3 f) = -\nabla_{\boldsymbol{n}} \cdot (P_{\boldsymbol{n}^\perp} \nabla_{\boldsymbol{x}} \boldsymbol{u} \boldsymbol{n} f) + D_r \Delta_n f,$$

$$\mathrm{Re}\left(\partial_t \boldsymbol{u} + (\boldsymbol{u} \cdot \nabla_{\boldsymbol{x}})\, \boldsymbol{u}\right) = \Delta_{\boldsymbol{x}} \boldsymbol{u} - \nabla_{\boldsymbol{x}} p - \delta \left( \int_{S^{d-\mathbf{1}}} f d\boldsymbol{n} \right) \boldsymbol{e_3}$$

$$\nabla_{\boldsymbol{x}} \cdot \boldsymbol{u} = 0.$$

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

# Shear Flow

$$\partial_t f + \nabla_{\boldsymbol{x}} \cdot (\boldsymbol{u} f) - \nabla_{\boldsymbol{x}} \cdot ((I + \boldsymbol{n} \otimes \boldsymbol{n}) e_3 f) = -\nabla_{\boldsymbol{n}} \cdot (P_{\boldsymbol{n}^\perp} \nabla_{\boldsymbol{x}} \boldsymbol{u} \boldsymbol{n} f) + D_r \Delta_n f,$$
$$\mathrm{Re}\left(\partial_t \boldsymbol{u} + (\boldsymbol{u} \cdot \nabla_{\boldsymbol{x}})\, \boldsymbol{u}\right) = \Delta_{\boldsymbol{x}} \boldsymbol{u} - \nabla_{\boldsymbol{x}} p - \delta \left( \int_{S^{d-\mathbf{1}}} f d\boldsymbol{n} \right) \boldsymbol{e}_3$$
$$\nabla_{\boldsymbol{x}} \cdot \boldsymbol{u} = 0.$$

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

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

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

# Derivation of Moment Equations

Consider approximation of the form

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

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

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

- Projection to the basis functions

The system of moment equations has the general form

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

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

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

# Rectilinear Flow

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

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

# Rectilinear Flow

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

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

The moment equations have the general form

$$\partial_t Q + A\partial_x Q + B\partial_y Q = D(w_x, w_y)Q + D_r EQ. \tag{5}$$

For $N = 1$:

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

# 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

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

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The moment equations have the general form

$$\partial_t Q + A\partial_x Q + B\partial_y Q + C\partial_z Q = D(w_x, w_y, w_z)Q + D_r EQ. \tag{7}$$

For $N = 1$:

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

# 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:**

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

# Multidimensional Wave Propagation (2D and 3D)

**Linear hyperbolic system:**

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**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

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

## Update Scheme

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

# Overview

# Approximation of Coupled Shear Flow Problem

Consider

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

| | |
|---|---|
| 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. | $\Delta t$ 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 $\partial_t Q(x,t) = (D(w_x(x,t_{n+1})) + D_r E)Q(x,t)$ |

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 $w$.

# 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

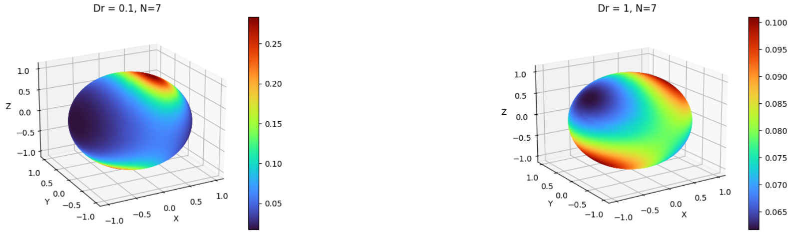



Figure 1: Numerical solution of the drift-diffusion term with constant externally imposed velocity gradient corresponding to shear flow using different values of $D_r$.

# Numerical Result for externally imposed velocity field


Figure 2: 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.

# Coupled Problems

- externally imposed velocity field ✓
- 1D shear flow ✓
- 2D rectilinear flow ✓
- 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 $\pm\frac{1}{2}$.

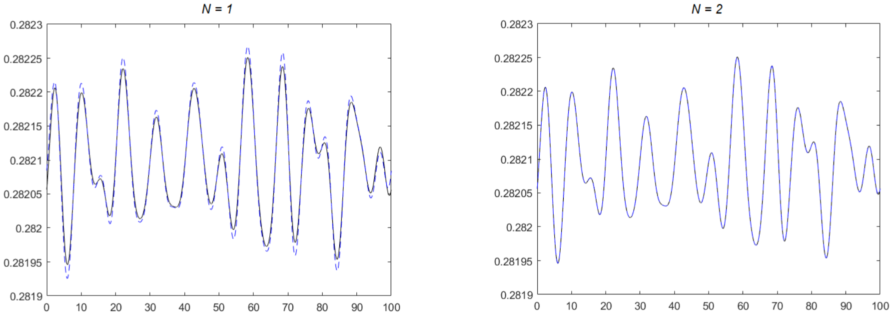
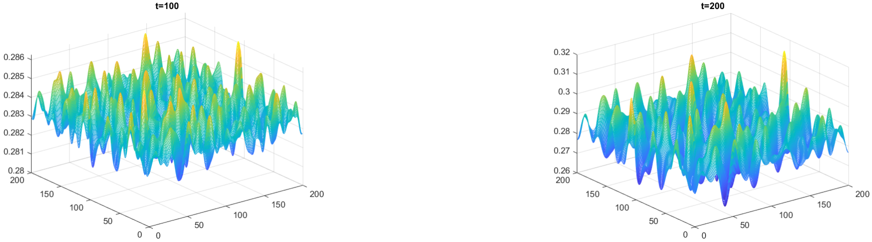



Figure 3: Approximation of the coupled problem for shear flow with $D_r = 0.05$. The plot shows the density at time $t = 30$ for $N = 1$ and $N = 2$ (blue line). A reference solution is calculated with $N = 6$ moment equations (black line).

# 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 $N = 1$.

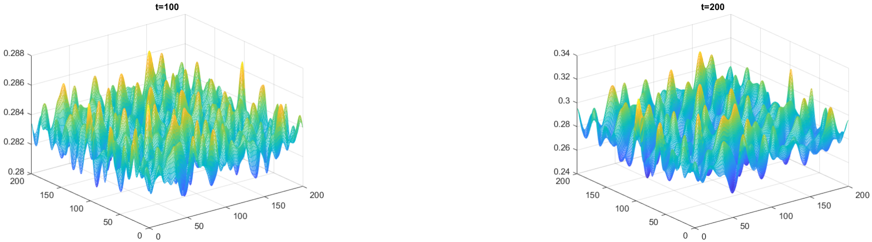



Figure 4: Solution structure of $c_0^0$ with $N = 7$.

# Overview

# 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

$$\partial_t Q + AQ_x + BQ_y + CQ_z = (D(wx, wy, wz) + DrE)Q \tag{9}$$

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).

# Example 1

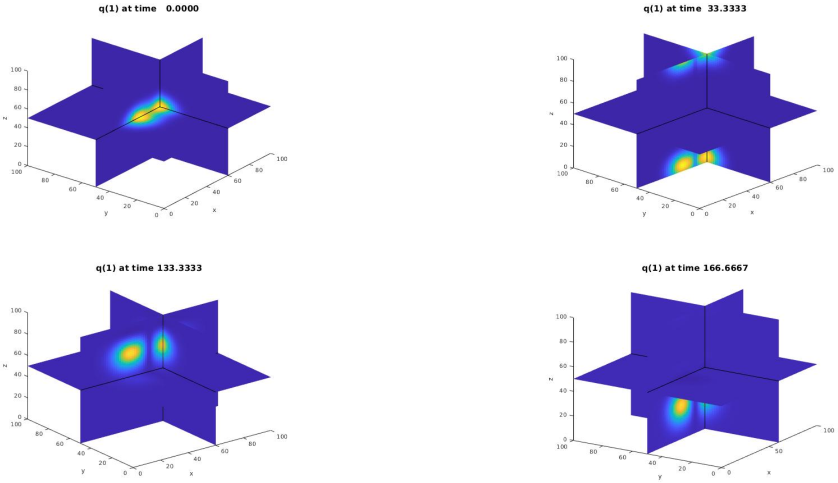



Figure 5: Evolution of $c_0^0$ at different times, showing two Gaussian clusters transported in opposite directions by a piecewise constant velocity field ($w_x = w_y = 1$ for $x < 50$, $w_x = w_y = -1$ otherwise, and $w_z = 0$ everywhere).

# Conclusion

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