Structure-Preserving Multi-Scale Methods for Complex Fluids

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FOR 5409 – Project **B3**

Experiment: Sedimentation of a suspension of fibers

B.Metzger and É.Guazzelli

Experimental observations by Guazzelli et al.

- Starting from a well stired suspension, packets of particles form after some time. These packets seem to have a mesoscopic equilibrium width, suggesting that the density of particles acquires variations of a characteristic length scale.
- Within such a cluster, individual particles are aligned with the direction of gravity during most of the time, occasionally they flip.
- The average settling speed in a suspension is larger than the sedimentation speed of a single particle oriented in the direction of gravity.

Our Goal: Mathematical modeling and numerical simulation of the sedimentation process of suspensions of rod-like particels

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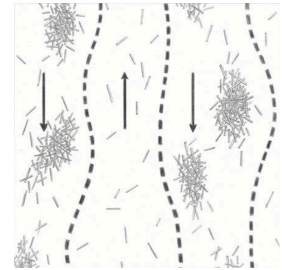
Mathematical Model for the Sedimentation of Rod-Like Particles

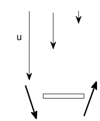
Bulk Coupling of a Kinetic Equation with the Navier-Stokes Equation

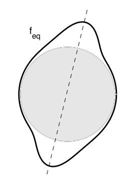
$$\partial_t f + \nabla_{\mathbf{x}} \cdot (\mathbf{u} f) + \nabla_{\mathbf{n}} \cdot (P_{\mathbf{n}^\perp} \nabla_{\mathbf{x}} \mathbf{u} \mathbf{n} f) - \nabla_{\mathbf{x}} \cdot ((I + \mathbf{n} \otimes \mathbf{n})\, \mathbf{e}_3 f)$$
$$= D_r \Delta_{\mathbf{n}} f + \gamma \nabla_{\mathbf{x}} \cdot (I + \mathbf{n} \otimes \mathbf{n})\, \nabla_{\mathbf{x}} f$$
$$\sigma = \int_{S^{d-1}} (d\mathbf{n} \otimes \mathbf{n} - I)\, f \, d\mathbf{n}$$
$$Re\,(\partial_t \mathbf{u} + (\mathbf{u} \cdot \nabla_{\mathbf{x}})\, \mathbf{u}) = \Delta_{\mathbf{x}} \mathbf{u} - \nabla_{\mathbf{x}} p + \delta\gamma \nabla_{\mathbf{x}} \cdot \sigma - \delta \int_{S^{d-1}} f \, d\mathbf{n} \mathbf{e}_3$$
$$\nabla_{\mathbf{x}} \cdot \mathbf{u} = 0$$



Guazzelli & Morris

$f = f(t, \mathbf{x}, \mathbf{n})$: density distribution function of particle orientation





Helzel & Tzavaras, MMS 2017

Status of Project: Comparison with Work Packages

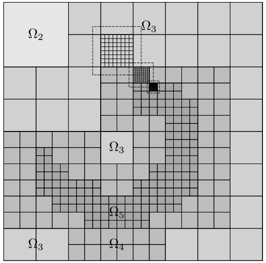
- Investigate hierarchy of moment equations for simplified shear flow problem with f on S^1
  - Transform high dimensional scalar PDE (in space and orientation) into a lower dimensional system of PDEs (in space)
  - Investigate accuracy of moment closure system

  Dahm, Helzel, MMS 2022, Dahm, Giesselmann, Helzel, JCP 2024 $\surd$

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

- Develop interface coupling techniques, which allow the use of a different number of moments in different regions of the domain

  Use of forestClaw grid structure and solver (joint with D. Calhoun)



- Construction of structure preserving methods
  - preserve positivity of f and ρ
  - Investigate how the entropy structure of the kinetic model relates to the entropy structure of the moment system.

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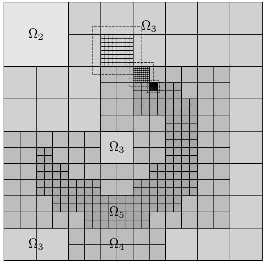

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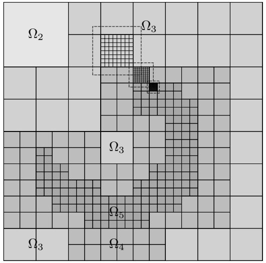

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Coupled model in spherical coordinates

$$
\begin{aligned}
\sin\theta\partial_t f(t,\mathbf{x},\phi,\theta) &+ \partial_x\left((u+\cos\phi\cos\theta\sin\theta)\sin\theta f\right) + \partial_y\left((v+\sin\phi\sin\theta\cos\theta)\sin\theta f\right)\\
&+ \partial_z\left(\left(w-(\cos^2\theta+1)\right)\sin\theta f\right)\\
&+ \partial_\phi(c_\phi f) + \partial_\theta(\sin\theta c_\theta f) = D_r\left(\partial_\phi\left(\frac{1}{\sin\theta}\partial_\phi f\right) + \partial_\theta\left(\sin\theta\partial_\theta f\right)\right)\\
Re\left(\partial_t\vec{u}(t,\mathbf{x}) + (\vec{u}\cdot\nabla_{\vec{x}})\,\vec{u}\right) &= \Delta_{\vec{x}}\vec{u} - \nabla_{\vec{x}}p - \delta\int_0^{2\pi}\int_0^{\pi} f\sin\theta\,\mathrm{d}\theta\mathrm{d}\phi\,\vec{e}_3\\
\nabla_{\vec{x}}\cdot\vec{u} &= 0\,.
\end{aligned}
$$

with

$$
\begin{aligned}
c_\phi &= -(u_x-v_y)\sin\phi\cos\phi\sin\theta - (u_y\sin\phi - v_x\cos\phi)\sin\phi\cos\theta\\
&\quad + (u_z\sin\phi - v_z\cos\phi)\cos\theta\\
\sin\theta c_\theta &= \sin\theta\Big[\left(u_x\cos^2\phi + v_y\sin^2\phi - w_z\right)\sin\theta\cos\theta + (u_y+v_x)\sin\phi\cos\phi\sin\theta\cos\theta\\
&\quad - (u_z\cos\phi + v_z\sin\phi)\cos^2\theta + (w_x\cos\phi + w_y\sin\phi)\sin^2\theta\Big].
\end{aligned}
$$

$\phi\in[0,2\pi]$, $\theta\in[0,\pi]$, $\mathbf{x}\in\mathbb{R}^3$

Simplified Flows

Shear flow: $\mathbf{u} = (0, 0, w(t, x))^T$, $f = f(t, x, \phi, \theta)$

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

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

Rectilinear flow $\mathbf{u} = (0, 0, w(t, x, y))^T$, $f = f(t, x, y, \phi, \theta)$

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

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Ansatz for Derivation of Moment Equations

$$f(t,\mathbf{x},\phi,\theta) \approx f^N(t,\mathbf{x},\phi,\theta) := \sum_{\ell=0}^{N} \sum_{m=-2\ell}^{2\ell} c_{2\ell,m}(t,\mathbf{x}) Y_{2\ell,m}(\phi,\theta).$$

$Y_{2\ell,m}$, $\ell = 0,\dots,N$, $m = -2\ell,\dots,2\ell$ are real valued spherical harmonic basis functions of even order.

Properties:

- Every square integrable function on S^2 can be expressed as linear combination of spherical harmonics $f(\theta,\phi) = \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} c_{l,m} Y_{\ell,m}(\theta,\phi)$ and the coefficients can be computed by projecting f onto each basis.
- The basis functions are orthogonal with respect to the standard $L_2(S^2)$ inner product $(f,g)_{L_2(S^2)} = \int_0^{2\pi} \int_0^{\pi} f(\phi,\theta) g(\phi,\theta) \sin\theta \mathrm{d}\theta \mathrm{d}\phi$
- $Y_{2\ell,m}$ is an eigenfunction of the Laplace Beltrami operator with eigenvalue $-2\ell(2\ell+1)$, i.e.

$$\frac{1}{\sin^2\theta}\partial_\phi^2 Y_{2\ell,m} + \frac{1}{\sin\theta}\partial_\theta\left(\sin\theta\,\partial_\theta Y_{2\ell,m}\right) = -2\ell(2\ell+1)Y_{2\ell,m}.$$

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Derivation of Moment Equations for Shear Flow

Insert f^N into kinetic equation:

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

Multiply equation subsequently with basis functions $Y_{2k,m}\in\{Y_{0,0},Y_{2,-2},\dots,Y_{2,2},Y_{4,-4},\dots,Y_{2N,2N}\}$ and integrate in ϕ and θ over $[0,2\pi]\times[0,\pi]$.

We obtain a **System of moment equations:**

$$\partial_t\mathbf{Q}+A\partial_x\mathbf{Q}=D(w_x)\mathbf{Q}+D_rE\mathbf{Q}$$

with $\mathbf{Q}=(c_{00}(t,x),c_{2,-2}(t,x),\dots,c_{2N,2N}(t,x))^T$ and $A,D,E\in\mathbb{R}^{(N+1)(2N+1)\times(N+1)(2N+1)}$

Example: $N=1$: 6 moment equations, $N=6$: 91 moment equations

Some Details on the Derivation ...

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

For $k = 0,\ldots,N, n = -2k,\ldots,2k$ we obtain

$$
\begin{aligned}
&\int_0^{2\pi}\int_0^{\pi}\sin\theta\partial_t\left(\sum_{\ell=0}^{N}\sum_{m=-2\ell}^{2\ell} c_{2\ell,m}(t,\mathbf{x})Y_{2\ell,m}(\theta,\phi)\right)Y_{2k,n}\mathrm{d}\phi\mathrm{d}\theta\\
&=\sum_{\ell=0}^{N}\sum_{m=-2\ell}^{2\ell}\partial_t c_{2\ell,m}(t,x)\int_0^{2\pi}\int_0^{\pi}\sin\theta Y_{2\ell,m}Y_{2k,n}\mathrm{d}\phi\mathrm{d}\theta\\
&=\sum_{\ell=0}^{N}\sum_{m=-2\ell}^{2\ell}\partial_t c_{2\ell,m}(t,x)\left(Y_{2\ell,m},Y_{2k,n}\right)_{L_2(S^2)} = \sum_{\ell=0}^{N}\sum_{m=-2\ell}^{2\ell}\partial_t c_{2\ell,m}(t,x)\delta_{\ell,k}\delta_{m,n} = \partial_t c_{2k,n}(t,x).
\end{aligned}
$$

$$
\partial_t\mathbf{Q} + A\partial_x\mathbf{Q} = D(w_x)\mathbf{Q} + D_r E\mathbf{Q}
$$

Some Details on the Derivation ...

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

The term $\cos\phi\cos\theta\sin\theta$ is a scalar multiple of $Y_{2,-1}$. Thus, we consider the projection of products of sherical harmonics to spherical harmonic basis functions.

$$\partial_t\mathbf{Q} + A\partial_x\mathbf{Q} = D(w_x)\mathbf{Q} + D_r E\mathbf{Q}$$

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

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

Some Details on the Derivation ...

$$\partial_t \mathbf{Q} + A\partial_x \mathbf{Q} = D(w_x)\mathbf{Q} + D_r E \mathbf{Q}$$

For $N = 2$ the symmetric matrix A has the structure

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

For every N the system of moment equations is hyperbolic.

Approximation of Coupled Shear Flow Problem

$$\partial_t \mathbf{Q}(t,x) + A\partial_x \mathbf{Q} = D(w_x(t,x))\mathbf{Q} + D_r E\mathbf{Q}$$
$$\partial_t w(t,x) = \partial_{xx} w + \delta\left(\bar\rho - 2\sqrt{\pi}c_{0,0}(t,x)\right),$$

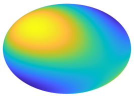
Splitting algorithm for coupled shear flow problem:

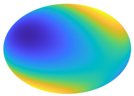
1: $\frac{1}{2}\Delta t$ step on	$\partial_t Q(t,x) = (D(w_x(t_n,x)) + D_r E)Q(t,x)$.
2: $\frac{1}{4}\Delta t$ step on	$\partial_t w(t,x) = \delta(\bar\rho - 2\sqrt{\pi}c_{0,0}(t,x)$.
3: $\frac{1}{2}\Delta t$ step on	$\partial_t w(x,t) = \partial_{xx} w(t,x)$.
4: $\frac{1}{4}\Delta t$ step on	$\partial_t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

We solve the hyperbolic system using LeVeque's wave propagation algorithm and the other subproblems using appropriate finite difference methods. The resulting splitting scheme is second order accurate.

Simulation of Coupled Shear Flow Problem: Cluster Formation

Consider initial values of the form $c_{0,0}(0,x) = \frac{1}{2\sqrt{\pi}}(1 + 10^{-4}\eta(x))$, where η describes random values between $\pm\frac{1}{2}$; all other variables are initially equal to zero, $D_r = 0.1$





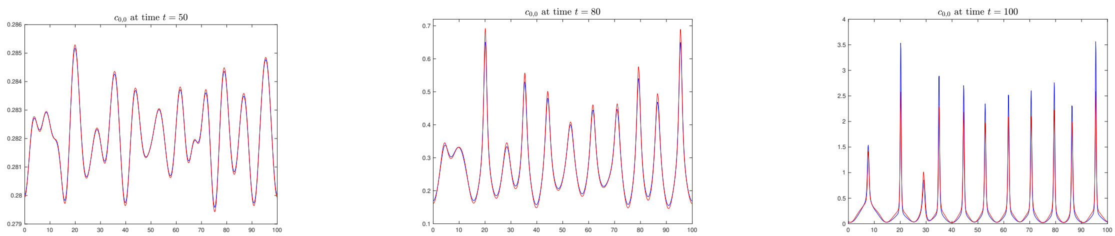


Figure: Numerical results showing the formation of clusters with higher density. Red curve using $N = 1$, blue curve using $N = 6$, all computations used 1024 grid cells.

Current Work in Progress: Coupled System for Rectilinear Flow

Preliminary results for two-dimensional system of moment equations with externally imposed velocity $\mathbf{u} = (0, 0, w(x, y))^T$:

$$\partial_t \mathbf{Q}(t, x, y) + A\partial_x \mathbf{Q} + B\partial_y \mathbf{Q} = \left(D(w_x, w_y) + D_r E\right) \mathbf{Q}$$

with $\mathbf{Q}(t, x, y) = (c_{0,0}(t, x, y), c_{2,-2}(t, x, y), \ldots, c_{2N,2N}(t, x, y))^T$ and externally imposed velocity.

Consider the two-dimensional system of moment equations on $[0, 100] \times [0, 100]$ using $N = 1$, $D_r = 1$ and $w_x = w_y = 1$ for $x < 50$ and $w_x = w_y = -1$ otherwise.

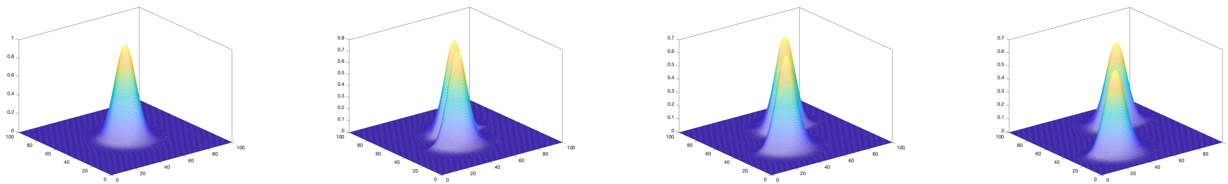


Figure: Numerical results for $c_{0,0}$ at different times. An initial cluster with higher particle density splits into two clusters that move in oposite directions.