Introduction

Mathematical Model

Let me start with a quick recap of the mathematical model we're using for the sedimentation in suspensions of rod-like particles. Here the kinetic Smoluchowski equation is coupled to the Navier-Stokes equation.

The function f(x,t,n) describes how the particles are distributed in space and orientation over time. We also have some non-dimensional parameters: Dr for rotational diffusion, δ which measures the relative importance of buoyancy vs. viscous stresses and Re a Reynolds number based on the sedimentation velocity.

The first equation tells us how the particle distribution evolves, thats means it describes the transport, the orientation of the particles and how the particles sediment depending on their orientation. The second equation is the Navier-Stokes equation with an additional buoyancy term.

This formulation is a simplified model follows the work of Helzel and Tzavaras from 2017.

- More in Details

The second in the first equation describe the transport of the particles due to the macroscopic velocity u.
The third term describes the rotation of the particles due to a macroscopic velocity gradient.
The fourth term describes how particles sediment depending on their orientation.

The terms on the right hand side of the first equation describe rotational as well as translational diffusion of the particles.

Status of Project

So far, we have derived and approximated hierarchies of moment equations for the coupled kinetic-fluid model with f on S2. This has been done for one-dimensional shear flows and two-dimensional rectilinear flows. The one-dimensional shear flow we have done it last year. And the two-dimensional flow we started last year and we also finished it last year.

Currently, we are working on the full three-dimensional case, deriving moment equations for the coupled kinetic-fluid model.

Derivation of Moment Equations and their Approximation

Shear Flow

Looking at the equations, the red terms describe the transport along the x and y directions, while the blue terms describes for rotational effects caused by the velocity gradients and rotational diffusion.

We consider the velocity of this form u, the velocity depends on the x-direction and time.
The flow occurs in z-direction. And in this case f is also a function of one variable, which we denote by x.

Derivation of Moment Equations

Now we derive approximations of the coupled model using hierarchies of moment equations.
We consider approximations of the form which we can see in eq (3).
We only consider the even order (bc the particles are symmetric).

The moment equations are derived by inserting the ansatz into our kinetic equation and then we do a projection to the basis functions.

The system of moment equations has the general form:

E is a diagonal matrix.

- Derivation: A Closer Look

Term Laplace-Operator:
From the properties this term corresponds to the Laplace-Beltrami operator*sin(theta). So after we insert the ansatz for f into this term, we get sin()*eigenvalue*ansatz. And if we then multiply with this corresponding ansatz, then almost all terms will be omitted. And as the result Dr*eigenvalue*coefficient.

Term [1]:
When we multiply term 1 with P0 then we get the time derivative for f0. If we multiply it with P22, then we get the time derivative for c22. So after we insert the ansatz for f in term [1], we get the time derivative of these coefficients. Bc the function c doesnt depend on \phi and \theta, we take this out of the integral. And this expression is the L2-inner product. Bc of the time I will only explain this term [2] in details.

Term [2]:
Short: The term cos(phi)cos(theta)… is a multiple one of the second order basis functions. That is the reason why we get in the first row and in the first column here an entry and other entries are zero. For N=1, the matrix A has the form. The term cos φ cos θ sin θ is a multiple one of the second order basis functions.

Let‘s consider the projection of products of spherical harmonics to spherical harmonic basis function. The first row means that we multiply the ansatz with P00. And we will get the entry [1,3]. We get here an entry bc we insert the ansatz w this term cos φ cos θ sin θ and project it to P00. Assume: Set f^N to P00. Then multiply this ansatz with the basisfct up to order two, we will get this entry [3,1].

For $N=2$:
Block $A_{1,2}$: If we use in our ansatz the basis functions up to order 4, and then multiply them by the basis functions of up to order 2, we will get the Block $A_{1,2}$.
Block $A_{1,2}^T$: If we use up to order 2 in order Ansatz and multiply it w basis function order 4, we get the Block $A_{1,2}^T$, which is the transport of $A_{1,2}$.
If more base functions are used, we always have three additional blocks.

Note that the number of moments depends on the size N via $(N+1)(2N+1)$.

Moreover the Matrix A is symmetric, therefore the system is hyperbolic.

Remaining terms:
We follow the same procedure. We insert our Ansatz and then project onto all the basis functions used in the Ansatz. In this case, however, the calculations are more extensive because we need to compute the derivative of θ. This leads to the matrix $D*Q$.

Rectilinear Flow

Now, we consider a two-dimensional simplified flow situation is rectilinear flow, the velocity has only a component in the z-direction, so $u=(0,0,w(x,y,t))$.

Here we get a hyperbolic system.
Gleichung (6): Here the source term didnt change, on the left hand side we get additional a Matrix B, which results from the spatial transport in the y-direction.

Coupled System for a Three-Dimensional Flow

Now we extend the coupled system to a full three-dimensional flow. Here, the fluid velocity has only a z-component, $u=(0,0,w(x,y,z,t))$, but the particle distribution f depends on all three spatial coordinates and the orientation angles ϕ and θ.

Similarly to the 2D case, we can derive a hierarchy of moment equations. Here, Q is the vector of moments and the matrices A, B, C, D, and E are the matrices .

1D Wave Propagation Algorithm (LeVeque et al.)

Let me briefly explain the wave propagation algorithm used in step 5.

We consider a hyperbolic system of the form $q_t+f(q)_x=0$, where q is a vector of conserved quantities. The domain is divided into discrete cells, and at each interface we solve a Riemann problem, which is a local initial value problem with a jump between neighboring cells.

The jump is decomposed into waves along the eigenvectors of the Jacobian A, and each wave travels at a characteristic speed sp. We then define fluctuations, A^+ and A^-, which correspond to waves moving to the right and left, respectively.

Finally, the cell averages are updated using these fluctuations, which ensures that information propagates correctly along the characteristics of the system.

Multidimensional Wave Propagation (2D and 3D)

When we extend the wave propagation algorithm to multiple dimensions, the idea is similar. For a system $q_t+f(q)_x+g(q)_y+h(q)_z=0$, we solve one-dimensional Riemann problems at the faces of each cell along the normal direction.

We decompose the jumps into waves and compute fluctuations in each direction, denoted $A^\pm,B^\pm,C^\pm$.

An important feature of multidimensional wave propagation is transverse effects: in 2D, a wave moving in the x-direction can generate waves in the y-direction, and vice versa. In 3D, each wave generates transverse waves in the other two directions. On the right, you can see a schematic of a 3D cell with axes x, y, and z.

3D Transverse and Double Transverse Propagation

In 3D, every wave generates not only transverse contributions but also double-transverse contributions along the other directions. For example, a wave in the x-direction can propagate into the y-direction, the z-direction, or even sequentially into y and then z. Similar interactions occur for waves originating in y or z directions.

The update scheme for the 3D case combines all these contributions. Each cell is updated based on the fluctuations in x, y, and z directions. This ensures that the multidimensional effects of wave propagation are properly captured, which is essential for accurately simulating the coupled shear flow problem.

Approximation of Coupled Shear Flow Problem

Moving on, we now focus on the coupled shear flow problem and its numerical approximation.

To solve this system, we use a splitting algorithm, shown here in the table. Step 1, 5 and 9, we use a Strang Splitting Algorithm for our moment equations and between these steps we use the Strang Splitting for the second equation. For the hyperbolic system in step 5 we use wave propagation.

For the 2d and 3d we have to adapt the step 2-4 and 6-8 (dyyw&dzzw).

But the coefficients c^0_0, which is the density, is always there also in 2d and 3d case.

- Details

In between those substeps the velocity is evolved. For the evolution of w we used simple second order accurate finite difference methods. The evolution of the source term (i.e., line 1 and 9) is performed with a higher-order Runge-Kutta method.

Numerical Result for externally imposed velocity field

1D-Case

We can solve for any fixed velocity field on the sphere.

We consider here the numerical solution for a fixed w_x.

Blau = niedrige Dichte (weniger Partikel sind in diese Richtung ausgerichtet).

Rot = hohe Dichte (mehr Partikel sind in diese Richtung ausgerichtet).

For a larger Dr=1, by using N=1 moment equations we can see that the solution structure has already a good approximation as N=6.

N = 1: 6 moment equations

N = 6: 91 moment equations

N = 7: 120 moment equations

2D-Case

In this simulation, we set Dr=1 and imposed velocity gradients wx=wy=1 in one region and −1 elsewhere. You can see that an initial cluster splits into two, each moving in opposite directions

The homogeneous hyperbolic system $\partial_t Q + A\partial_x Q + B\partial_y Q = 0$ describes a horizontal transport which depends on the orientation of the particles. For rectilinear flow this is a horizontal transport in the $x - y$ plane. For our test problem this transport moves the particles along the diagonal of the domain out of the cluster. This causes the initial cluster of particles to split into two clusters which slowly move away from each other as shown in Figure.

Over time (t=200), this piecewise constant flow velocity causes the particles located on the left side of the system ($x<50$) to drift to the right and upwards, while the particles on the right side ($x \geq 50$) drift to the left and downwards. As the velocities in the two areas are opposite, two separate clusters are formed as the particles in the two areas move in opposite directions.
The splitting into two clusters is caused by the piecewise constant velocity distribution. The particles located in the areas $x<50$ and $x \geq 50$ have different and opposite velocities, which causes the particles to move in opposite directions and ultimately form two separate clusters.

Numerical Result for Shear Flow

Here we consider approximations of the coupled problem Shear flow using systems of moment equations.

We started with almost constant density at some random noise and with these pictures we want to

illustrate how the cluster form. We show $c_{0,0}$ at t=30 using both N = 6 as well as N = 1. The Figure shows that using N=1 moment eqs, compared to the ref. sol. w. N=6 moment eqs., already provides a good approximation. With N=2 moment eqs. better.

Result for Two-Dimensional Case

The pictures shows the solution structure at different times, confirming the formation of clusters. In these computations we used N = 1, i.e. only six moment equations and N=7, i.e. 120 moment equations.

The pictures show the clustering behavior at time=100 and time=200.
The overall structure appears similiar in both cases for t=100. But over time we can see some different. Like in this picture we can see slightly more pronounced peaks.

Current Work in Progress

Now that we have discussed the numerical method in detail—including the 1D and multidimensional wave propagation algorithms, as well as the handling of transverse and double-transverse waves in 3D—we are ready to move on to the actual numerical simulations.

Using the framework we just described, we can solve the coupled moment-fluid system in three dimensions. This allows us to study how the particle distribution evolves over time under the influence of the fluid flow, rotational diffusion, and particle-fluid coupling.

Next, I will show some results from these 3D simulations, including accuracy studies and the temporal evolution of the particle moments.

Wave Propagation and Error Analysis

To solve this 3D system numerically, we use the multidimensional wave propagation algorithm introduced by LeVeque. The scheme can be characterized by three integers m1,m2,m3.

- m1 determines whether the correction wave is included or not.
- m2 specifies the transverse propagation.
- m3 determines whether double-transverse propagation is applied.

We also perform an error analysis by comparing solutions on different grid resolutions. On a coarse grid with spacing h, we define the error $E(h)=U(h)-U(h/2)$, and similarly $E(h/2)=U(h/2)-U(h/4)$. This allows us to estimate the convergence rate of the method.

Accuracy Analysis

Here, we present the accuracy results for the zeroth moment c00 of the 3D flow problem. The initial condition is a Gaussian bell-shaped distribution centered at $(x,y,z)=(40,30,50)$.

The table shows the L1 error and the estimated order of convergence for different grid sizes and for different numbers of moments N.

For the method with parameters (1,1,1), which is formally first-order, the convergence rate is below 1, while for the higher-order method (2,2,2), the error decreases nearly quadratically as we refine the grid. This confirms that the scheme achieves the expected accuracy.

The CFL condition was respected in all simulations, with $cfl \leq 0.45$ for the first-order method and $cfl \leq 0.9$ for the higher-order method.

Numerical Results

Finally, here are some numerical results for c00 over time. On the top, we show the initial distribution and its evolution at an intermediate time.

On the bottom, you can see the distribution at a later time. In this simulation, $Dr=1$, and we set the fluid gradients $wx=wy=1$ and $wz=0$.

You can observe how the initial cluster evolves and spreads under the influence of the fluid flow and rotational effects. These results illustrate that our 3D moment hierarchy, combined with the wave propagation algorithm, captures the key dynamics of the coupled system.

Conclusion

Drift vs. diffusion effects visible

- Bei kleinem Dr: Drift dominiert → Partikel richten sich stärker entlang der Strömung aus.
- Bei größerem Dr: Diffusion glättet die Verteilung → weniger Alignment, mehr isotrope Verteilung.
- Das konntest du z. B. bei den extern aufgeprägten Gradienten sehen, wo sich die Lösung je nach Dr unterschiedlich verhält.

Clustering and splitting in flow fields

- Bei Wechsel der Vorzeichen im Velocity Gradient (z. B. wx=wy=1 vs. −1): Ein anfänglicher Cluster teilt sich auf → zwei Gruppen bewegen sich in entgegengesetzte Richtungen.
- Im Scherfluss-Szenario entstehen Dichteanreicherungen („clusters“) durch Kopplung mit dem Fluidfeld.

Info

Später wird diese Struktur in die Momentengleichungen übertragen, wo der Drift über die Matrix

$D(\nabla x u)$) und die Diffusion über den Term DrE eingeht

Drift = deterministische Orientierung durch Strömung (Velocity-Gradient).

Diffusion = zufällige Orientierung durch Rotationsdiffusion.

Finally, the hyperbolic transport term in the system of moment equations 458 describes a spatial transport of particles due to their orientation.

The acceleration of gravity acts in the direction e3, where e3 is the unit vector in the upward direction.