Numerical Solution with Spectral Method for Smoluchowski Equation on S^2

Bella My Phuong Quynh Duong

Heinrich-Heine University Düsseldorf

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Overview

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- Focus on a system of partial differential equations which couples a kinetic equation to a macroscopic flow equation. This system model (given by Helzel & Tzavaras) a sedimentation process in suspension of rigid rod-like particles.

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The update of the source term is equivalent to a spectral method ([1]).

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Overview

Mathematical Model for the Sedimentation of Rod-Like Particles [4]

Coupling of a Smoluchowski Equation and a Navier-Stokes Equation

$$
\begin{aligned}
\partial_t f + \nabla_x \cdot (\boldsymbol{u} f) + \nabla_{\boldsymbol{n}} \cdot (P_{\boldsymbol{n}^\perp} \nabla_x \boldsymbol{u} \boldsymbol{n} f) - \nabla_x \cdot ((I + \boldsymbol{n} \otimes \boldsymbol{n}) e_3 f) \\
= D_r \Delta_n f + \gamma \nabla_x \cdot (I + \boldsymbol{n} \otimes \boldsymbol{n}) \nabla_x f, \\
\sigma = \int_{S^{d-1}} (\mathrm{d}\ \boldsymbol{n} \otimes \boldsymbol{n} - I) f d\boldsymbol{n}, \\
\mathrm{Re}\, (\partial_t \boldsymbol{u} + (\boldsymbol{u} \cdot \nabla_x)\, \boldsymbol{u}) = \Delta_x \boldsymbol{u} - \nabla_x p + \delta \gamma \nabla_x \cdot \sigma - \delta \int_{S^{d-1}} f d\boldsymbol{n}\, e_3, \\
\nabla_x \cdot \boldsymbol{u} = 0,
\end{aligned}
$$

where $f = f(t; x; n), x \in \mathbb{R}^d, n \in S^{d-1}, t \in \mathbb{R}$ is a density distribution function of particle orientation. D_r, γ, δ and Re are non-dimensional values.

Consider

$$\partial_t f + \nabla_x \cdot (\boldsymbol{u} f) + \nabla_{\boldsymbol{n}} \cdot (P_{\boldsymbol{n}^\perp} \nabla_x \boldsymbol{u} \boldsymbol{n} f) - \nabla_x \cdot ((I + \boldsymbol{n} \otimes \boldsymbol{n}) e_3 f) \\ = D_r \Delta_n f + \gamma \nabla_x \cdot (I + \boldsymbol{n} \otimes \boldsymbol{n}) \nabla_x f. \tag{1}$$

Rewrite the equation (1) in spherical coordinates ([2], [3]) and it follows

$$\sin\theta \partial_t f + \partial_\phi \left(a(\phi,\theta) f\right) + \partial_\theta \left(b(\phi,\theta) f\right) = D_r \left(\partial_\phi \left(\frac{1}{\sin\theta} \partial_\phi f \right) + \partial_\theta \left(\sin\theta \partial_\theta f \right) \right), \tag{2}$$

with $\phi \in [0, 2 \cdot \pi]$ and $\theta \in [0, \pi]$. Solving the Smoluchoswki equation (2) on S^2 by using a spectral method, which is based on the ansatz

$$f(\phi,\theta,t) = f_0(t) \cdot P_0^0 + \sum_{n=1}^{\infty} \sum_{i=-n}^{n} c_{2n}^i(t) \cdot P_{2n}^i(\phi,\theta), \tag{3}$$

where $P_{2n}^i(\phi,\theta)$ are harmonic polynomial basis functions.

Harmonic polynomial basis functions

Let $P_n^i(\phi, \theta)$ with $n = 0, ..., \infty$ and $i = n, ..., -n$ be the basis function

$$TODO$$

The scalar product of any two basis functions over sphere is defined as follows

$$< P_n^i, P_m^l >_{S^2} = \int_0^{2\pi} \int_0^{\pi} P_n^i(\phi, \theta) \cdot P_m^l(\phi, \theta) \cdot \sin(\theta) d\theta d\phi.$$

Properties of harmonic polynomial basis functions

Property 1

Let $P_n^i(\phi, \theta)$ and $P_m^l(\phi, \theta)$ are two different harmonic polynomial basis functions. Then

$$< P_n^i, P_m^l >_{S^2} = 0,$$

for $i \neq l$ or $n \neq m$.

Property 2

Let P_n^i be the normalized harmonic polynomial basis functions. Then

$$< P_n^i, P_n^i >_{S^2} = 1.$$

Property 3

The spherical harmonic function are the eigenfunctions of Laplace-Beltrami operator with the eigenvalues $(-n(n+1), n \in \mathbb{N}_0)$(see [5])

$$\Delta_{S^2} P_n^i = -n(n+1)P_n^i.$$

Spectral method

Recall the Smochluchowski equation on S^2

$$\underbrace{\sin\theta\partial_t f}_{(1)} + \underbrace{\partial_\phi\left(a(\phi,\theta)f\right) + \partial_\theta\left(b(\phi,\theta)f\right)}_{(2)} = \underbrace{D_r\left(\partial_\phi\left(\frac{1}{\sin\theta}\partial_\phi f\right) + \partial_\theta\left(\sin\theta\partial_\theta f\right)\right)}_{(3)} \tag{4}$$

and the ansatz

$$f(\phi,\theta,t) = f_0(t)\cdot P_0^0 + \sum_{n=1}^{\infty}\sum_{i=-n}^{n} c_{2n}^i(t)\cdot P_{2n}^i(\phi,\theta). \tag{5}$$

The Laplace Beltrami operator ([3]) on the unit sphere S^2 is given by

$$\Delta_{S^2} f = \frac{1}{\sin^2\theta}\partial_{\phi\phi} f + \frac{1}{\sin\theta}\partial_\theta\left(\sin\theta\partial_\theta f\right). \tag{6}$$

From property 3 and the equation (6), it follows for the term (3)

$$\Delta_{S^2} P_{2n}^i = -n(n+1)P_{2n}^i.$$

For the term (1) and (2), we inserting (5) in (4), multiplying with each basis function and integrate it over S^2. We derive a system of ODEs for the coefficients

$$\begin{pmatrix} f_0 \\ c_2^{-2} \\ \vdots \\ c_{2n}^i \end{pmatrix}' = A \begin{pmatrix} f_0 \\ c_2^{-2} \\ \vdots \\ c_{2n}^i \end{pmatrix}, \tag{7}$$

with $A \in \mathbb{R}^{cnxcn}$

$$cn = \begin{cases} \text{order} \;\; = 2: & cn = 2 \cdot \text{order} + 2 \\ \text{order} \;\; = \text{even}: & c2 = 6 \\ & cn = c2 \\ & cn = c2 + \sum_{i=4}^{order}(2i+1) \end{cases}$$

Example: Shear flow

Example: Shear flow

Consider the Smoluchowski equation (4) with the velocity gradient

$$\vec{u} = \begin{pmatrix} u(x,y,z) \\ v(x,y,z) \\ w(x,y,z) \end{pmatrix}, \nabla_x \vec{u}_{\mathrm{ext}} = \begin{pmatrix} u_x & u_y & u_z \\ v_x & v_y & v_z \\ w_x & w_y & w_z \end{pmatrix} = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}.$$

With the given velocity gradient it follows

$$\begin{aligned} &\partial_t \left(\sin\theta f\right) + \partial_\theta \left(\sin\phi \cos\phi \sin^2\theta \cos\theta f\right) + \partial_\phi \left(-\sin\theta \sin^2\phi f\right) \\ &= D_r \left(\partial_\theta \left(\sin\theta \partial_\theta f\right) + \partial_\phi \left(\frac{1}{\sin\theta} \partial_\phi f\right)\right). \end{aligned} \tag{8}$$

Consider the ansatz with the zeroth order

$$f(\phi,\theta,t) = f_0(t) \cdot P_0^0. \tag{9}$$

Insert the ansatz (9) in (8)

$$\partial_t (f_0(t) \cdot P_0^0) + \frac{1}{\sin\theta} \left(\partial_\theta(\ldots) + \partial_\phi(\ldots)\right) = \frac{1}{\sin\theta} D_r \left(\ldots\right). \tag{10}$$

We know

$$\Delta_{S^2} P_0^0(\phi,\theta) = \frac{1}{\sin\theta} D_r(\dots) = \lambda_{2n,i} \cdot P_0^0(\phi,\theta),$$

where $\lambda_{2n,i}$ is the corresponding eigenvalue.
Since $P_0^0(\phi,\theta) = 1$ does not depend on ϕ and θ, the partial derivatives will be zero

$$\Delta_{S^2} P_0^0(\phi,\theta) = 0. \tag{11}$$

Consider the rest of the equation (10)

$$\underbrace{\partial_t(f_0(t) \cdot P_0^0)}_{(1)} + \underbrace{\frac{1}{\sin\theta}\left(\partial_\theta(\sin\phi\cos\phi\sin^2\theta\cos\theta \cdot f_0(t) \cdot P_0^0) + \partial_\phi(-\sin\theta\sin^2\phi \cdot f_0(t) \cdot P_0^0)\right)}_{(2)}.$$

It is

$$\partial_t\left(f_0(t) \cdot P_0^0\right) = f_0'(t).$$

Let $z(\phi,\theta) := (2)$

Project the solution $z(\phi,\theta)$ onto all polynomials to find out which polynomial are needed

$$\int_0^{2\pi}\int_0^{\pi} z(\phi,\theta)\cdot P_2^{-2}(\phi,\theta)\,\sin\theta d\theta d\phi \overset{Maple}{=} 0$$
$$\int_0^{2\pi}\int_0^{\pi} z(\phi,\theta)\cdot P_2^{-1}(\phi,\theta)\,\sin\theta d\theta d\phi \overset{Maple}{=} 0$$
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$$\int_0^{2\pi}\int_0^{\pi} z(\phi,\theta)\cdot P_2^{2}(\phi,\theta)\,\sin\theta d\theta d\phi \overset{Maple}{=} -\frac{\sqrt{15}}{5}$$

It follows

$$f_0(t) \cdot P_0^0 \cdot \frac{1}{\sin\theta}\left(\partial_\theta\left(\sin\phi\cos\phi\sin^2\theta\cos\theta\right) + \partial_\phi\left(-\sin\theta\sin^2\phi\right)\right) = f_0(t)\left[-\frac{\sqrt{15}}{2}P_2^2\right]. \quad (12)$$

Together we have

$$f_0'(t) - \frac{\sqrt{15}}{2}f_0(t)P_2^2(\phi,\theta) = 0 \cdot P_0^0(\phi,\theta)D_r.$$

For the ansatzfunction with higher order, the calculation is done in the same way. As an example we obtain an ODE system with ansatzfunction of the $2nd$. order

$$\begin{pmatrix} f_0'(t) \\ c_2^{-2} \\ c_2^{-1} \\ c_2^0 \\ c_2^1 \\ c_2^2 \end{pmatrix} = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -6D_r & 0 & 0 & 0 & 1 \\ 0 & 0 & -6D_r & 0 & 5/7 & 0 \\ 0 & 0 & 0 & -6D_r & 0 & -\frac{\sqrt{3}}{7} \\ 0 & 0 & -2/7 & 0 & -6D_r & 0 \\ \frac{\sqrt{15}}{5} & 1 & 0 & -\frac{\sqrt{3}}{7} & 0 & -6D_r \end{pmatrix} \cdot \begin{pmatrix} f_0 \\ c_2^{-2} \\ c_2^{-1} \\ c_2^0 \\ c_2^1 \\ c_2^2 \end{pmatrix} \tag{13}$$

Overview

Shear flow on S^2

Shear flow on S^2

Consider the externally imposed shear flow

$$\mathbf{u} = \begin{pmatrix} u(y) \\ 0 \\ 0 \end{pmatrix}, \quad \nabla_x \mathbf{u} = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \tag{14}$$

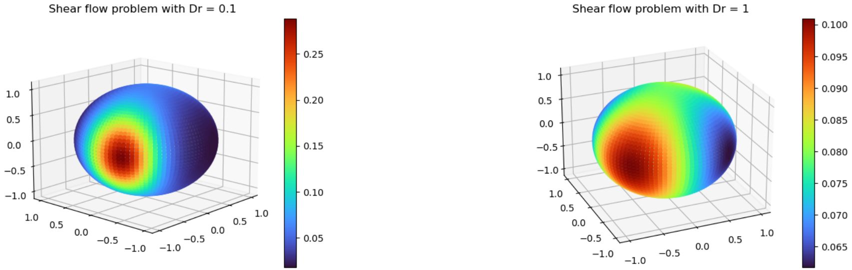


Figure 1: Steady state solution of the Smoluchowski equation approximated at $T = 10$ using different values of D_r.

Shear flow: Stability analysis

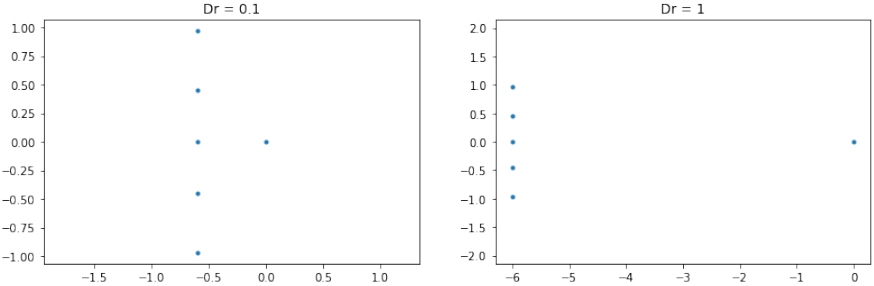


Figure 2: Eigenvalue of matrix A with basis functions of $2nd$. order

Proposition 1

Spectral method for $2nd$. order is stable with for both small and large D_r.

Shear flow: Stability analysis

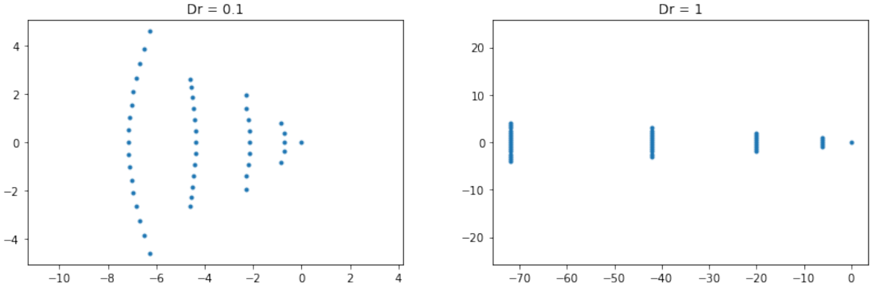


Figure 3: Eigenvalue of matrix A with basis functions of $8th$. order

Proposition 2

Sprectal method for $8th$. order is stable with for both small and large D_r.

Elongational flow

Elongational flow

Consider the externally imposed velocity gradient

$$\nabla_{\vec{x}} \vec{u}_{\mathrm{ext}} = \begin{pmatrix} 2 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix}.$$

The exact steady-state solution has the form

$$f_{\mathrm{exact}}(\phi, \theta) = C_1 \exp\left(-\frac{3}{2D_{\mathrm{r}}}\left(1 - \cos^2(\phi)\sin^2(\theta)\right)\right), \tag{15}$$

with the constants $C_1 = 2.30121384511755303190$ for $D_r = 0.1$.

Figure 4: Exact steady state solution with different D_r

Elongational flow

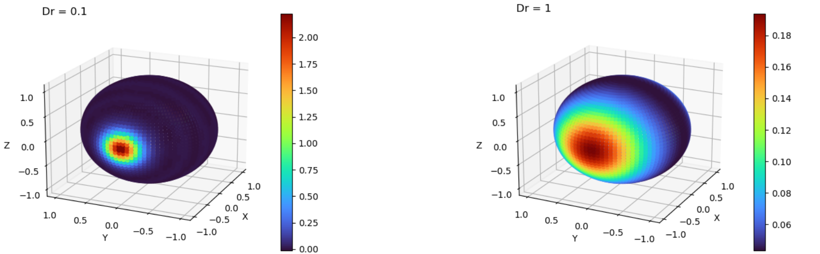


Figure 5: Numerical solution on S^2 with basis functions of $14th$. order

Convergence Study

For the convergence study, the maximum norm error is used

$$E_{max} = max\left|U_{exact} - U_{approx}\right|.$$

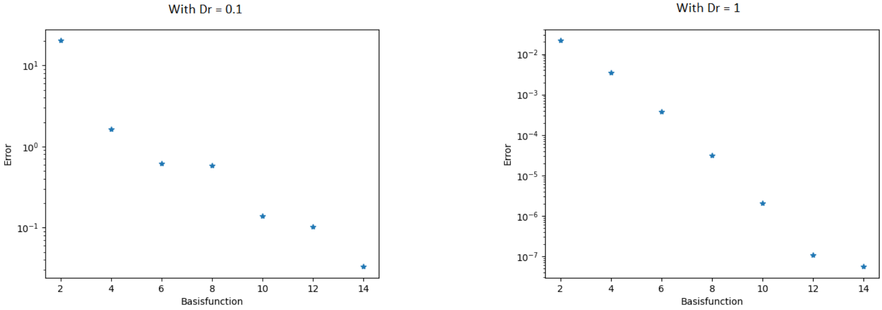
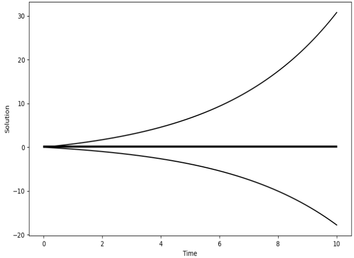
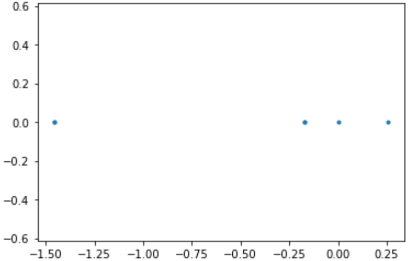


Figure 6: Error with respect to basisfunction with different D_r

Stability analysis



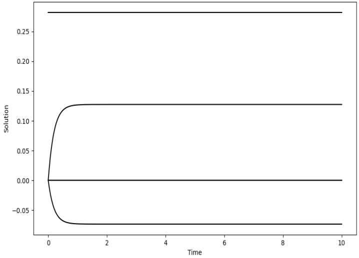
(a) Coefficients as function order



(b) Eigenwert of matrix A order

Figure 7: With $2nd$. order and $D_r = 0.1$

Stability analysis



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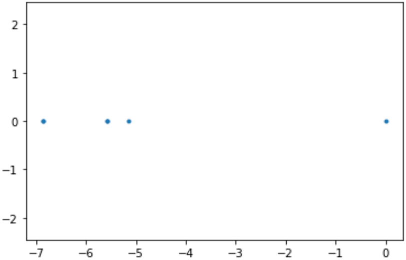
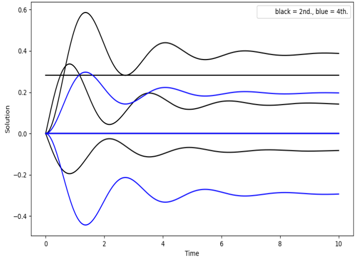


(b) Eigenwert of matrix A order

Figure 8: With $2nd$. order and $D_r = 1$



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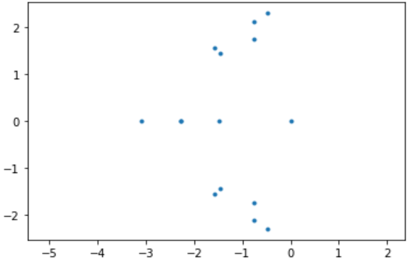
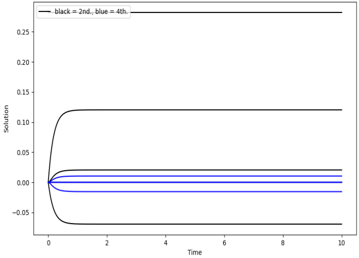


(b) Eigenwert of matrix A order

Figure 9: With $4th.$ order and $D_r = 0.1$

Stability analysis



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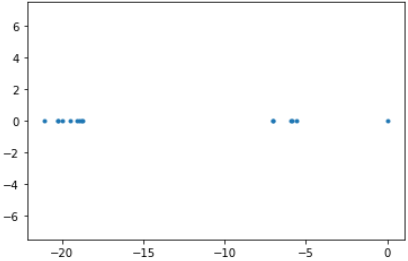
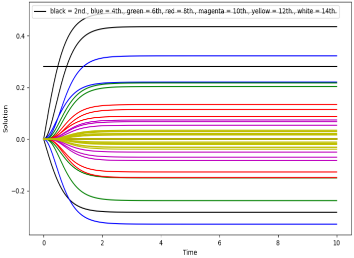


(b) Eigenwert of matrix A order

Figure 10: With $4th.$ order and $D_r = 1$

Stability analysis



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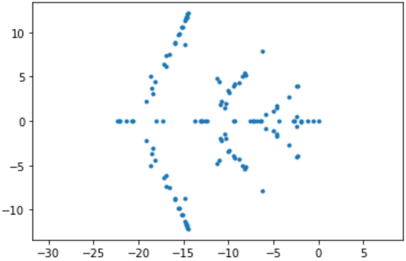

(b) Eigenwert of matrix A order

Figure 11: With $14th.$ order and $D_r = 0.1$

Conclusion

Finding

- For small D_r we have seen that the error was relatively large.
- The eigenvalue of the matrix A of the $2nd$. order ODE system for $D_r = 0.1$ has a positive real part $\rightarrow$ the ansatzfunction with $2nd$. order is unsuitable.
- The spectral method becomes stable when taking more approach functions for small D_r.

Thank you for listening!

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