MA5232 Assignment Part 1

Symmetric Gauss Seidel method applied to Photon diffusion

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1 Introduction

The objective of this assignment is to approximate the steady-state solution of the following light-scattering problem.

$$
\begin{aligned}
\partial_x F_1 &= \sigma \left(\frac{1}{6} \sum_{i=1}^{6} F_i - F_1 \right) \\
-\partial_x F_2 &= \sigma \left(\frac{1}{6} \sum_{i=1}^{6} F_i - F_2 \right) \\
\partial_y F_3 &= \sigma \left(\frac{1}{6} \sum_{i=1}^{6} F_i - F_3 \right) \\
-\partial_y F_4 &= \sigma \left(\frac{1}{6} \sum_{i=1}^{6} F_i - F_4 \right) \\
\partial_z F_5 &= \sigma \left(\frac{1}{6} \sum_{i=1}^{6} F_i - F_5 \right) \\
-\partial_z F_6 &= \sigma \left(\frac{1}{6} \sum_{i=1}^{6} F_i - F_6 \right)
\end{aligned}
$$

The quantities F_i stand for the number of photons travelling in a given direction in a given region of the domain, given as $\Omega = (-1, 1)^3$, at the steady state. In this model only six different directions are considered. F_1 counts the number of photons moving in the positive x direction, F_2 counts the number moving in the negative x direction. Similarly, F_3 and F_4 count the numbers in the positive and negative y directions, and F_5 and F_6 count the numbers in the positive and negative z directions respectively. σ is a constant scattering coefficient relating to how densely filled the domain is with matter, and the terms on the right-hand-side are the source and loss terms that occur when a photon scatters off of a matter particle.

The boundary conditions are given as follows.

$$
\begin{aligned}
F_1(-1, y, z) &= 1, \quad y, z \in (-0.2, 0.2) \\
F_3(x, -1, z) &= 1, \quad x, z \in (-0.2, 0.2) \\
F_5(x, y, -1) &= 1, \quad x, y \in (-0.2, 0.2)
\end{aligned}
$$

All the other boundary values are zero.

2 Numerical Scheme

The finite volume method is the basic scheme used to solve the problem numerically. For this purpose, we divide the domain into a homogeneous 100 x 100 x 100 grid of cubes with side lengths $h = 0.02$.

Since the left-hand-side of the equations represents a transport term, the upwind scheme is used in deriving the following numerical method.

$$
\begin{aligned}
\frac{F_{1,ijk}-F_{1,i-1,jk}}{h} &= \sigma\left(-\frac{5}{6}F_{1,ijk}+\frac{1}{6}F_{2,ijk}+\frac{1}{6}F_{3,ijk}+\frac{1}{6}F_{4,ijk}+\frac{1}{6}F_{5,ijk}+\frac{1}{6}F_{6,ijk}\right)\\
-\frac{F_{2,i+1,jk}-F_{2,ijk}}{h} &= \sigma\left(+\frac{1}{6}F_{1,ijk}-\frac{5}{6}F_{2,ijk}+\frac{1}{6}F_{3,ijk}+\frac{1}{6}F_{4,ijk}+\frac{1}{6}F_{5,ijk}+\frac{1}{6}F_{6,ijk}\right)\\
\frac{F_{3,i,j-1,k}-F_{3,ijk}}{h} &= \sigma\left(+\frac{1}{6}F_{1,ijk}+\frac{1}{6}F_{2,ijk}-\frac{5}{6}F_{3,ijk}+\frac{1}{6}F_{4,ijk}+\frac{1}{6}F_{5,ijk}+\frac{1}{6}F_{6,ijk}\right)\\
-\frac{F_{4,i,j+1,k}-F_{4,ijk}}{h} &= \sigma\left(+\frac{1}{6}F_{1,ijk}+\frac{1}{6}F_{2,ijk}+\frac{1}{6}F_{3,ijk}-\frac{5}{6}F_{4,ijk}+\frac{1}{6}F_{5,ijk}+\frac{1}{6}F_{6,ijk}\right)\\
\frac{F_{5,ijk}-F_{5,ij,k-1}}{h} &= \sigma\left(+\frac{1}{6}F_{1,ijk}+\frac{1}{6}F_{2,ijk}+\frac{1}{6}F_{3,ijk}+\frac{1}{6}F_{4,ijk}-\frac{5}{6}F_{5,ijk}+\frac{1}{6}F_{6,ijk}\right)\\
-\frac{F_{6,ij,k+1}-F_{6,ijk}}{h} &= \sigma\left(+\frac{1}{6}F_{1,ijk}+\frac{1}{6}F_{2,ijk}+\frac{1}{6}F_{3,ijk}+\frac{1}{6}F_{4,ijk}+\frac{1}{6}F_{5,ijk}-\frac{5}{6}F_{6,ijk}\right)
\end{aligned}
$$

Here, $F_{r,ijk}$ represents the value of F_r averaged over the cell i, j, k, where the indices range from 1 to 100 for the x, y and z directions separately.

This system of equations has 6×10^6 unknowns. We want to solve it iteratively, but in an efficient manner. To do this, we use the Symmetric Gauss-Seidel method. The idea is to cover the cells one by one in a systematic order, so that in each computation some of the terms of the current iteration can be used. First, we do a forward scan, back to front, left to right, and bottom to top:

$$
\begin{aligned}
\frac{F^{(m+1)}_{1,ijk}-F^{(m+1)}_{1,i-1,jk}}{h} &= \sigma\left(-\frac{5}{6}F^{(m+1)}_{1,ijk}+\frac{1}{6}F^{(m+1)}_{2,ijk}+\frac{1}{6}F^{(m+1)}_{3,ijk}+\frac{1}{6}F^{(m+1)}_{4,ijk}+\frac{1}{6}F^{(m+1)}_{5,ijk}+\frac{1}{6}F^{(m+1)}_{6,ijk}\right)\\
-\frac{F^{(m)}_{2,i+1,jk}-F^{(m+1)}_{2,ijk}}{h} &= \sigma\left(+\frac{1}{6}F^{(m+1)}_{1,ijk}-\frac{5}{6}F^{(m+1)}_{2,ijk}+\frac{1}{6}F^{(m+1)}_{3,ijk}+\frac{1}{6}F^{(m+1)}_{4,ijk}+\frac{1}{6}F^{(m+1)}_{5,ijk}+\frac{1}{6}F^{(m+1)}_{6,ijk}\right)\\
\frac{F^{(m+1)}_{3,ijk}-F^{(m+1)}_{3,i,j-1,k}}{h} &= \sigma\left(+\frac{1}{6}F^{(m+1)}_{1,ijk}+\frac{1}{6}F^{(m+1)}_{2,ijk}-\frac{5}{6}F^{(m+1)}_{3,ijk}+\frac{1}{6}F^{(m+1)}_{4,ijk}+\frac{1}{6}F^{(m+1)}_{5,ijk}+\frac{1}{6}F^{(m+1)}_{6,ijk}\right)\\
-\frac{F^{(m)}_{4,i,j+1,k}-F^{(m+1)}_{4,ijk}}{h} &= \sigma\left(+\frac{1}{6}F^{(m+1)}_{1,ijk}+\frac{1}{6}F^{(m+1)}_{2,ijk}+\frac{1}{6}F^{(m+1)}_{3,ijk}-\frac{5}{6}F^{(m+1)}_{4,ijk}+\frac{1}{6}F^{(m+1)}_{5,ijk}+\frac{1}{6}F^{(m+1)}_{6,ijk}\right)\\
\frac{F^{(m+1)}_{5,ijk}-F^{(m+1)}_{5,ij,k-1}}{h} &= \sigma\left(+\frac{1}{6}F^{(m+1)}_{1,ijk}+\frac{1}{6}F^{(m+1)}_{2,ijk}+\frac{1}{6}F^{(m+1)}_{3,ijk}+\frac{1}{6}F^{(m+1)}_{4,ijk}-\frac{5}{6}F^{(m+1)}_{5,ijk}+\frac{1}{6}F^{(m+1)}_{6,ijk}\right)\\
-\frac{F^{(m)}_{6,ij,k+1}-F^{(m+1)}_{6,ijk}}{h} &= \sigma\left(+\frac{1}{6}F^{(m+1)}_{1,ijk}+\frac{1}{6}F^{(m+1)}_{2,ijk}+\frac{1}{6}F^{(m+1)}_{3,ijk}+\frac{1}{6}F^{(m+1)}_{4,ijk}+\frac{1}{6}F^{(m+1)}_{5,ijk}-\frac{5}{6}F^{(m+1)}_{6,ijk}\right)
\end{aligned}
$$

The parameter m is the iteration counter. Note, that this is an isolated system of 6 unknowns. All the values with $i-1, j-1, k-1$ indices have been computed in a previous cell during the current iteration, so we can use these values in computing the solution of the current cell. For the values with $i+1, j+1, k+1$ indices we have to use the previous iteration's results. To deal with this asymmetry we alternate between using this scheme and the following backward scan during each iteration:

$$
\begin{aligned}
\frac{F_{1,ijk}^{(m+1)} - F_{1,i-1,jk}^{(m)}}{h} &= \sigma\left(-\frac{5}{6}F_{1,ijk}^{(m+1)} + \frac{1}{6}F_{2,ijk}^{(m+1)} + \frac{1}{6}F_{3,ijk}^{(m+1)} + \frac{1}{6}F_{4,ijk}^{(m+1)} + \frac{1}{6}F_{5,ijk}^{(m+1)} + \frac{1}{6}F_{6,ijk}^{(m+1)}\right) \\
-\frac{F_{2,i+1,jk}^{(m+1)} - F_{2,ijk}^{(m+1)}}{h} &= \sigma\left(+\frac{1}{6}F_{1,ijk}^{(m+1)} - \frac{5}{6}F_{2,ijk}^{(m+1)} + \frac{1}{6}F_{3,ijk}^{(m+1)} + \frac{1}{6}F_{4,ijk}^{(m+1)} + \frac{1}{6}F_{5,ijk}^{(m+1)} + \frac{1}{6}F_{6,ijk}^{(m+1)}\right) \\
\frac{F_{3,ijk}^{(m+1)} - F_{3,i,j-1,k}^{(m)}}{h} &= \sigma\left(+\frac{1}{6}F_{1,ijk}^{(m+1)} + \frac{1}{6}F_{2,ijk}^{(m+1)} - \frac{5}{6}F_{3,ijk}^{(m+1)} + \frac{1}{6}F_{4,ijk}^{(m+1)} + \frac{1}{6}F_{5,ijk}^{(m+1)} + \frac{1}{6}F_{6,ijk}^{(m+1)}\right) \\
-\frac{F_{4,i,j+1,k}^{(m+1)} - F_{4,ijk}^{(m+1)}}{h} &= \sigma\left(+\frac{1}{6}F_{1,ijk}^{(m+1)} + \frac{1}{6}F_{2,ijk}^{(m+1)} + \frac{1}{6}F_{3,ijk}^{(m+1)} - \frac{5}{6}F_{4,ijk}^{(m+1)} + \frac{1}{6}F_{5,ijk}^{(m+1)} + \frac{1}{6}F_{6,ijk}^{(m+1)}\right) \\
\frac{F_{5,ijk}^{(m+1)} - F_{5,ij,k-1}^{(m)}}{h} &= \sigma\left(+\frac{1}{6}F_{1,ijk}^{(m+1)} + \frac{1}{6}F_{2,ijk}^{(m+1)} + \frac{1}{6}F_{3,ijk}^{(m+1)} + \frac{1}{6}F_{4,ijk}^{(m+1)} - \frac{5}{6}F_{5,ijk}^{(m+1)} + \frac{1}{6}F_{6,ijk}^{(m+1)}\right) \\
-\frac{F_{6,ij,k+1}^{(m+1)} - F_{6,ijk}^{(m+1)}}{h} &= \sigma\left(+\frac{1}{6}F_{1,ijk}^{(m+1)} + \frac{1}{6}F_{2,ijk}^{(m+1)} + \frac{1}{6}F_{3,ijk}^{(m+1)} + \frac{1}{6}F_{4,ijk}^{(m+1)} + \frac{1}{6}F_{5,ijk}^{(m+1)} - \frac{5}{6}F_{6,ijk}^{(m+1)}\right)
\end{aligned}
$$

Now, all the $i-1, j-1, k-1$ values need to be taken from the previous iteration, and the $i+1, j+1, k+1$ are known.

The question remains, how the small linear system of equations occurring in each cell should be solved. We could use direct methods, or iterative methods to solve it, but in this particular problem there is a faster way.

Looking back at the original set of equations, it becomes clear that the total number of photons is conserved during scattering. If we consider a spatially homogeneous version of the model, we could see that in the steady state, one sixth of the total number of photons must be equal to the number of photons travelling in each specific direction. This inspires us to look at the problem in a more holistic manner. Indeed, if we sum all of the equations in scheme of the forward scan, the right-hand-side completely cancels out, and we obtain the following simple expression for the total number of photons in cell ijk:

$$
M_{ijk}^{(m+1)} \equiv \sum_{r=1}^{6} F_{r,ijk}^{(m+1)} = F_{1,i-1,jk}^{(m+1)} + F_{2,i+1,jk}^{(m)} + F_{3,i,j-1,k}^{(m+1)} + F_{4,i,j+1,k}^{(m)} + F_{5,ij,k-1}^{(m+1)} + F_{6,ij,k+1}^{(m)}
$$

All of the values on the right-hand-side are known by virtue of the scanning direction or by use of the previous iteration. When doing similar for the backward scan, we obtain the following expression:

$$
M_{ijk}^{(m+1)} \equiv \sum_{r=1}^{6} F_{r,ijk}^{(m+1)} = F_{1,i-1,jk}^{(m)} + F_{2,i+1,jk}^{(m+1)} + F_{3,i,j-1,k}^{(m)} + F_{4,i,j+1,k}^{(m+1)} + F_{5,ij,k-1}^{(m)} + F_{6,ij,k+1}^{(m+1)}
$$

Once the total number of photons is explicitly computed, the individual systems can be further decoupled and all of the variables may be computed directly via a single equation. First, for the forward scan:

$$
\begin{aligned}
\left(\frac{1}{h}+\sigma\right)F_{1,ijk}^{(m+1)} &= \sigma\left(\frac{1}{6}M_{ijk}^{(m+1)}\right)+\frac{1}{h}F_{1,i-1,jk}^{(m+1)}\\
\left(\frac{1}{h}+\sigma\right)F_{2,ijk}^{(m+1)} &= \sigma\left(\frac{1}{6}M_{ijk}^{(m+1)}\right)+\frac{1}{h}F_{2,i+1,jk}^{(m)}\\
\left(\frac{1}{h}+\sigma\right)F_{3,ijk}^{(m+1)} &= \sigma\left(\frac{1}{6}M_{ijk}^{(m+1)}\right)+\frac{1}{h}F_{3,i,j-1,k}^{(m+1)}\\
\left(\frac{1}{h}+\sigma\right)F_{4,ijk}^{(m+1)} &= \sigma\left(\frac{1}{6}M_{ijk}^{(m+1)}\right)+\frac{1}{h}F_{4,i,j+1,k}^{(m)}\\
\left(\frac{1}{h}+\sigma\right)F_{5,ijk}^{(m+1)} &= \sigma\left(\frac{1}{6}M_{ijk}^{(m+1)}\right)+\frac{1}{h}F_{5,ij,k-1}^{(m+1)}\\
\left(\frac{1}{h}+\sigma\right)F_{6,ijk}^{(m+1)} &= \sigma\left(\frac{1}{6}M_{ijk}^{(m+1)}\right)+\frac{1}{h}F_{6,ijk,k+1}^{(m)}
\end{aligned}
$$

And then for the backward scan:

$$
\begin{aligned}
\left(\frac{1}{h}+\sigma\right)F_{1,ijk}^{(m+1)} &= \sigma\left(\frac{1}{6}M_{ijk}^{(m+1)}\right)+\frac{1}{h}F_{1,i-1,jk}^{(m)}\\
\left(\frac{1}{h}+\sigma\right)F_{2,ijk}^{(m+1)} &= \sigma\left(\frac{1}{6}M_{ijk}^{(m+1)}\right)+\frac{1}{h}F_{2,i+1,jk}^{(m+1)}\\
\left(\frac{1}{h}+\sigma\right)F_{3,ijk}^{(m+1)} &= \sigma\left(\frac{1}{6}M_{ijk}^{(m+1)}\right)+\frac{1}{h}F_{3,i,j-1,k}^{(m)}\\
\left(\frac{1}{h}+\sigma\right)F_{4,ijk}^{(m+1)} &= \sigma\left(\frac{1}{6}M_{ijk}^{(m+1)}\right)+\frac{1}{h}F_{4,i,j+1,k}^{(m+1)}\\
\left(\frac{1}{h}+\sigma\right)F_{5,ijk}^{(m+1)} &= \sigma\left(\frac{1}{6}M_{ijk}^{(m+1)}\right)+\frac{1}{h}F_{5,ij,k-1}^{(m)}\\
\left(\frac{1}{h}+\sigma\right)F_{6,ijk}^{(m+1)} &= \sigma\left(\frac{1}{6}M_{ijk}^{(m+1)}\right)+\frac{1}{h}F_{6,ijk,k+1}^{(m+1)}
\end{aligned}
$$

This leads to a completely explicit iterative scheme using the Symmetric Gauss-Seidel method for the outer iterations over the cells and a direct computation of the variables within the cells.

3 Results

For the simulations, a threshold value of 10^{-5} was used for the error, which was taken as the L^2-norm of the difference between the left-hand-side and the right-hand-side of all the equations summed over all the cells.

Four different simulations were run, each for a different value of the scattering coefficient σ, ranging from 0.1 to 100. Figures 1 to 4 depict the solutions upon reaching the desired accuracy. We can see that σ reflects how densely the domain is filled with matter particles, as we get more and more scattering of the photons with higher σ values.

To conclude, Figures 5 and 6 show the convergence rate of the respective simulations. One forward and one backward scan has been counted as a single iteration. In each case we can observe an exponential decay of the error, as the vertical axis is logarithmic. The problem clearly becomes more difficult to solve for larger σ. For $\sigma = 0.1$, it took only three iterations to reach the desired threshold, whereas it took over 2000 iterations for $\sigma = 100$. This was to be expected, as a higher σ means more interactions for the photons, and therefore a more complex scattering behaviour.

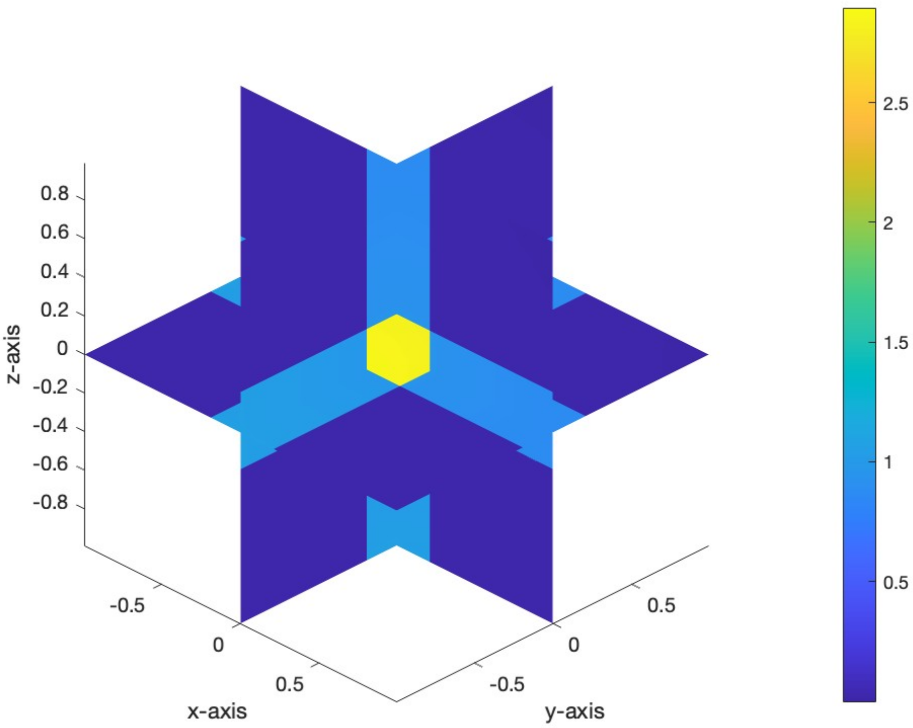

Figure 1: Solution for $\sigma = 0.1$

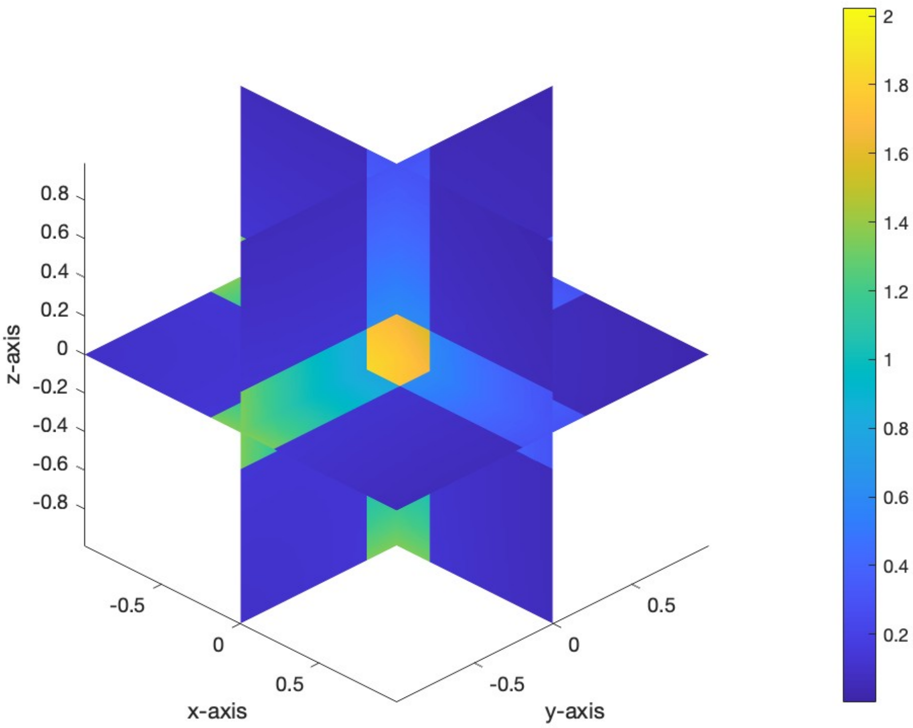

Figure 2: Solution for $\sigma = 1$

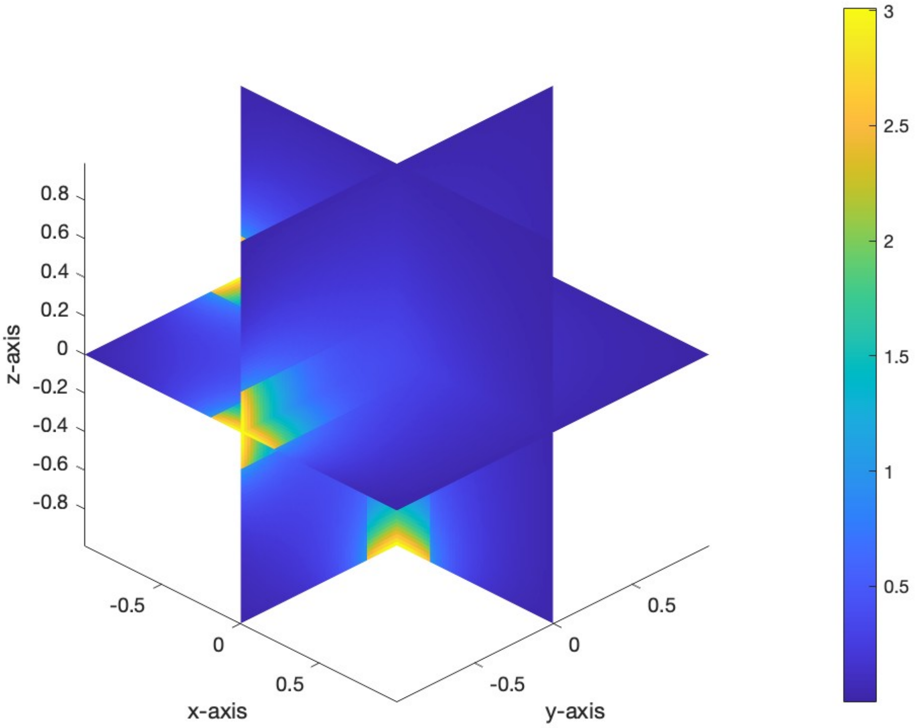

Figure 3: Solution for $\sigma = 10$

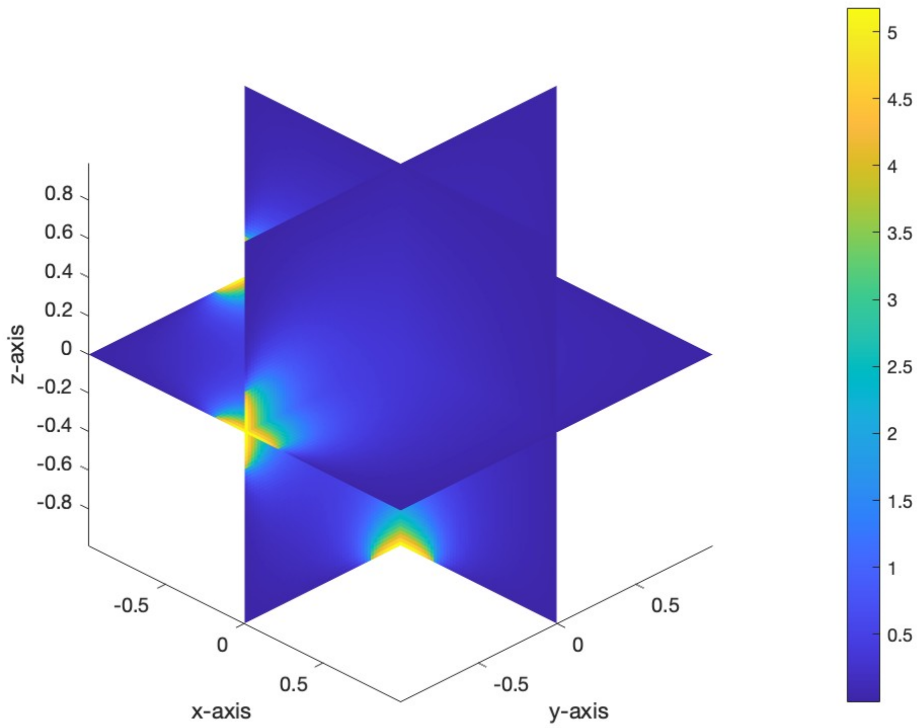

Figure 4: Solution for $\sigma = 100$

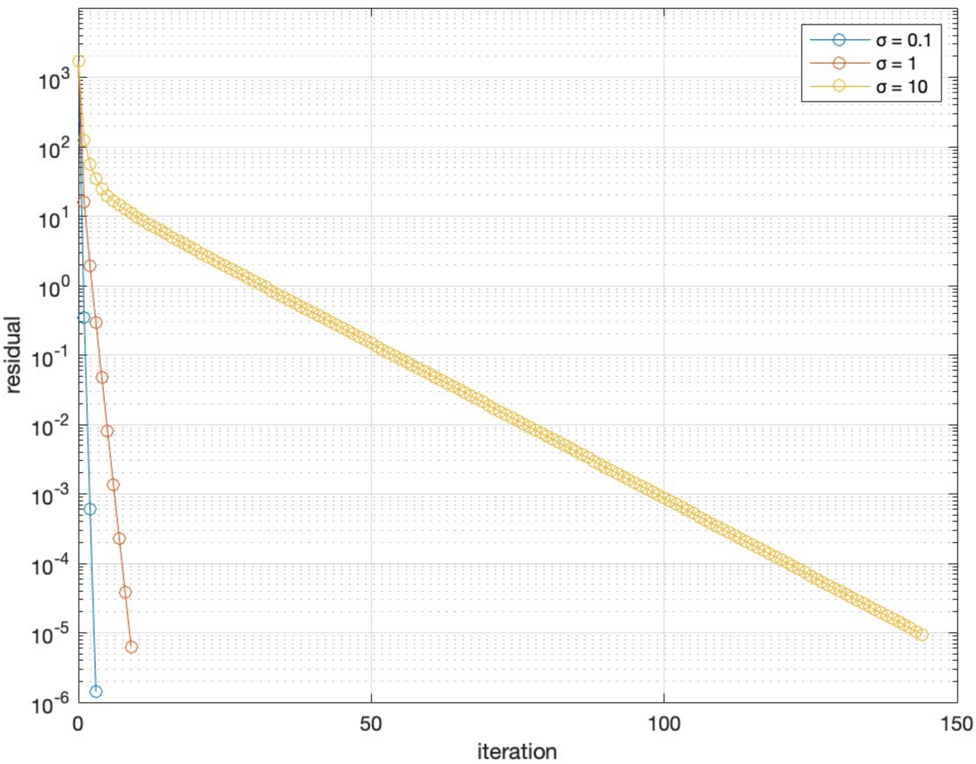

Figure 5: Convergence rates for $\sigma = 0.1, 1, 10$

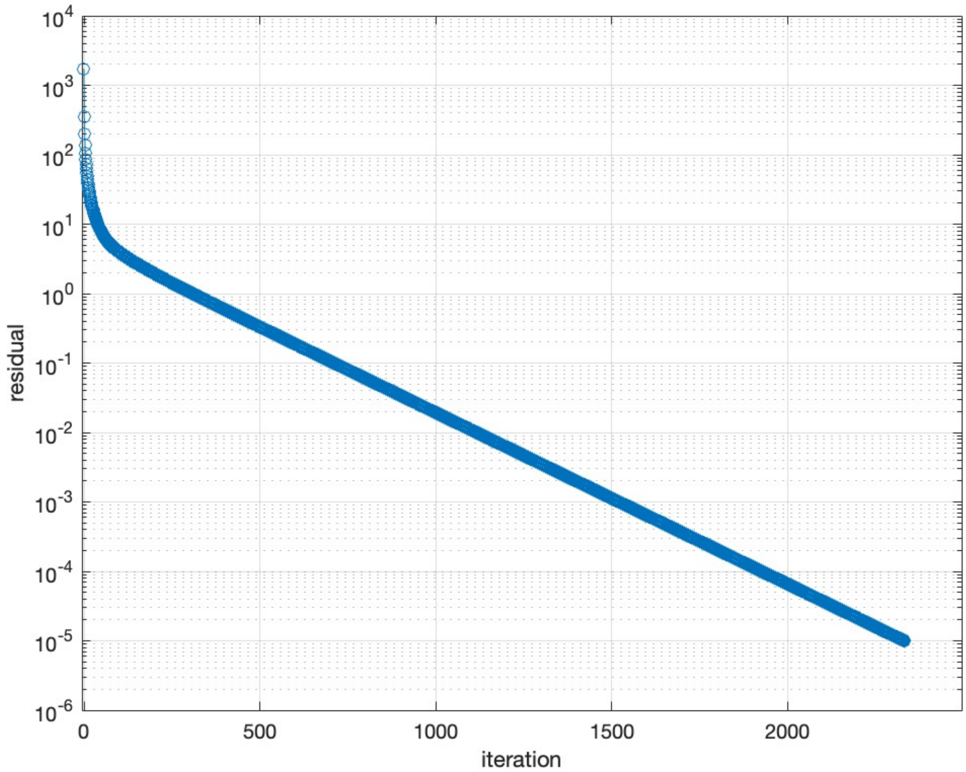

Figure 6: Convergence rate for $\sigma = 100$