MA5232 Assignment 1

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Contents

Problem 1

Let $\Omega = (-1,+1)^3 \subseteq \mathbb{R}^3$. Let $A, B, C, D, E, F : \Omega \to R$ be sufficiently smooth functions. Let $S = A + B + C + D + E + F$. Consider the 3D equations defined on $\Omega = (-1,+1)^3$

$$
\begin{aligned}
\frac{\partial A}{\partial x} &= \sigma\left(\frac{1}{6}S - A\right)\\
-\frac{\partial B}{\partial x} &= \sigma\left(\frac{1}{6}S - B\right)\\
\frac{\partial C}{\partial y} &= \sigma\left(\frac{1}{6}S - C\right)\\
-\frac{\partial D}{\partial y} &= \sigma\left(\frac{1}{6}S - D\right)\\
\frac{\partial E}{\partial z} &= \sigma\left(\frac{1}{6}S - E\right)\\
-\frac{\partial F}{\partial z} &= \sigma\left(\frac{1}{6}S - F\right)
\end{aligned}
$$

The boundary conditions are

$$
\begin{aligned}
A(-1,y,z) &= \phi(y,z)\\
C(x,-1,z) &= \phi(x,z)\\
E(x,y,-1) &= \phi(x,y)\\
B(1,y,z) &= D(x,1,z) = F(x,y,1) = 0
\end{aligned}
$$

where $\phi(p,q) = \begin{cases} 1 & \text{if } |p| \leq 0.2 \text{ and } |q| \leq 0.2 \\ 0 & \text{otherwise} \end{cases}$

Solve this system of equations numerically for $\sigma = 0.1, 1, 10, 100$. Assume $\sigma = 1/\epsilon$. Consider the time-dependent equations

$$
\begin{aligned}
\frac{\partial A}{\partial t} + \frac{\partial A}{\partial x} &= \sigma\left(\frac{1}{6}S - A\right)\\
\frac{\partial B}{\partial t} - \frac{\partial B}{\partial x} &= \sigma\left(\frac{1}{6}S - B\right)\\
\frac{\partial C}{\partial t} + \frac{\partial C}{\partial y} &= \sigma\left(\frac{1}{6}S - C\right)\\
\frac{\partial D}{\partial t} - \frac{\partial D}{\partial y} &= \sigma\left(\frac{1}{6}S - D\right)\\
\frac{\partial E}{\partial t} + \frac{\partial E}{\partial z} &= \sigma\left(\frac{1}{6}S - E\right)\\
\frac{\partial F}{\partial t} - \frac{\partial F}{\partial z} &= \sigma\left(\frac{1}{6}S - F\right)
\end{aligned}
$$

Derive the equation of S that approximates the system A, B, C, D, E, F up to the first order

1 NUMERICAL METHODS

The numerical method consists of the following steps:

1. Discretizing Ω into grid
2. Using upwind method to approximate $\frac{\partial U}{\partial w}$ for $U = A, B, C, D, E, F$ and $w = x, y, z$
3. Decoupling the system of equations

1.1 DISCRETIZING Ω INTO GRID

By symmetry of the equations, we will discretize Ω into grid of $n \times n \times n$ cells where the distance between centers of two adjacent cells is $h = 2/n$

1.2 UPWIND METHOD

Let $U_{i,j,k}$ denote the value of A, B, C, D, E, F at cell (i, j, k). Since we know the boundary of A at $x = -1$ and B at $x = +1$, we will approximate

$$\begin{aligned}\frac{\partial A}{\partial x} &\approx \frac{A_{i,j,k} - A_{i-1,j,k}}{h} \\ -\frac{\partial B}{\partial x} &\approx \frac{B_{i,j,k} - B_{i+1,j,k}}{h}\end{aligned}$$

Similarly for C, D, E, F, we have

$$\begin{aligned}\frac{\partial C}{\partial y} &\approx \frac{C_{i,j,k} - C_{i,j-1,k}}{h} \\ -\frac{\partial D}{\partial y} &\approx \frac{D_{i,j,k} - D_{i,j+1,k}}{h} \\ \frac{\partial E}{\partial z} &\approx \frac{E_{i,j,k} - E_{i,j,k-1}}{h} \\ -\frac{\partial F}{\partial z} &\approx \frac{F_{i,j,k} - F_{i,j,k+1}}{h}\end{aligned}$$

We have the system of equations

$$\begin{aligned}\frac{A_{i,j,k} - A_{i-1,j,k}}{h} &= \sigma\left(\frac{1}{6}S_{i,j,k} - A_{i,j,k}\right) \\ \frac{B_{i,j,k} - B_{i+1,j,k}}{h} &= \sigma\left(\frac{1}{6}S_{i,j,k} - B_{i,j,k}\right) \\ \frac{C_{i,j,k} - C_{i,j-1,k}}{h} &= \sigma\left(\frac{1}{6}S_{i,j,k} - C_{i,j,k}\right) \\ \frac{D_{i,j,k} - D_{i,j+1,k}}{h} &= \sigma\left(\frac{1}{6}S_{i,j,k} - D_{i,j,k}\right) \\ \frac{E_{i,j,k} - E_{i,j,k-1}}{h} &= \sigma\left(\frac{1}{6}S_{i,j,k} - E_{i,j,k}\right) \\ \frac{F_{i,j,k} - F_{i,j,k+1}}{h} &= \sigma\left(\frac{1}{6}S_{i,j,k} - F_{i,j,k}\right)\end{aligned}$$

So that we can iteratively calculate the value of A, C, E from small indices to large indices and B, D, F from large indices to small indices

1.3 DECOUPLING THE SYSTEM OF EQUATIONS

EXPLICIT METHOD

In explicit method, in each iteration, we calculate the right hand side using previous calculated values, at t-th iteration, we calculate the next value as follows:

$$
\begin{aligned}
\frac{A_{i,j,k}^{(t)} - A_{i-1,j,k}^{(t)}}{h} &= \sigma\left(\frac{1}{6}S_{i,j,k}^{(t-1)} - A_{i,j,k}^{(t-1)}\right) \\
\frac{B_{i,j,k}^{(t)} - B_{i+1,j,k}^{(t)}}{h} &= \sigma\left(\frac{1}{6}S_{i,j,k}^{(t-1)} - B_{i,j,k}^{(t-1)}\right) \\
\frac{C_{i,j,k}^{(t)} - C_{i,j-1,k}^{(t)}}{h} &= \sigma\left(\frac{1}{6}S_{i,j,k}^{(t-1)} - C_{i,j,k}^{(t-1)}\right) \\
\frac{D_{i,j,k}^{(t)} - D_{i,j+1,k}^{(t)}}{h} &= \sigma\left(\frac{1}{6}S_{i,j,k}^{(t-1)} - D_{i,j,k}^{(t-1)}\right) \\
\frac{E_{i,j,k}^{(t)} - E_{i,j,k-1}^{(t)}}{h} &= \sigma\left(\frac{1}{6}S_{i,j,k}^{(t-1)} - E_{i,j,k}^{(t-1)}\right) \\
\frac{F_{i,j,k}^{(t)} - F_{i,j,k+1}^{(t)}}{h} &= \sigma\left(\frac{1}{6}S_{i,j,k}^{(t-1)} - F_{i,j,k}^{(t-1)}\right)
\end{aligned}
$$

In particular, $A_{i,j,k}^{(t)} = A_{i-1,j,k}^{(k)} + h\sigma\left(\frac{1}{6}S_{i,j,k}^{(t-1)} - A_{i,j,k}^{(t-1)}\right)$. Similarly for B, C, D, E, F.

SEMI-IMPLICIT METHOD

In implicit method, we calculate the right hand side using the current iteration values. However, this at least requires solving a system of 6 equations. Moreover, since the direction of upwind are different between A and B, the number of equations we need to solve is proportional to number of cells. Hence, we use the semi-implicit method as follows: in each iteration of calculating U, we will use the current value of U and previous values of all other terms

$$
\begin{aligned}
\frac{A_{i,j,k}^{(t)} - A_{i-1,j,k}^{(t)}}{h} &= \frac{1}{6}\sigma\left(S_{i,j,k}^{(t-1)} - A_{i,j,k}^{(t-1)} - 5A_{i,j,k}^{(t)}\right) \\
\frac{B_{i,j,k}^{(t)} - B_{i+1,j,k}^{(t)}}{h} &= \frac{1}{6}\sigma\left(S_{i,j,k}^{(t-1)} - B_{i,j,k}^{(t-1)} - 5B_{i,j,k}^{(t)}\right) \\
\frac{C_{i,j,k}^{(t)} - C_{i,j-1,k}^{(t)}}{h} &= \frac{1}{6}\sigma\left(S_{i,j,k}^{(t-1)} - C_{i,j,k}^{(t-1)} - 5C_{i,j,k}^{(t)}\right) \\
\frac{D_{i,j,k}^{(t)} - D_{i,j+1,k}^{(t)}}{h} &= \frac{1}{6}\sigma\left(S_{i,j,k}^{(t-1)} - D_{i,j,k}^{(t-1)} - 5D_{i,j,k}^{(t)}\right) \\
\frac{E_{i,j,k}^{(t)} - E_{i,j,k-1}^{(t)}}{h} &= \frac{1}{6}\sigma\left(S_{i,j,k}^{(t-1)} - E_{i,j,k}^{(t-1)} - 5E_{i,j,k}^{(t)}\right) \\
\frac{F_{i,j,k}^{(t)} - F_{i,j,k+1}^{(t)}}{h} &= \frac{1}{6}\sigma\left(S_{i,j,k}^{(t-1)} - F_{i,j,k}^{(t-1)} - 5F_{i,j,k}^{(t)}\right)
\end{aligned}
$$

In particular,

$$
A_{i,j,k}^{(t)} = \frac{A_{i-1,j,k}^{(t)} + \frac{1}{6}h\sigma(S_{i,j,k}^{(t-1)} - A_{i,j,k}^{(t-1)})}{\left(1 + \frac{5}{6}h\sigma\right)}
$$

2 NUMERICAL SETTINGS

We divided Ω into $100 \times 100 \times 100$ grid cells ($n = 100$) and set value of A, B, C, D, E, F into 0 initially. Then, we update A, B, C, D, E, F iteratively using the previously described method until residue is less than $\epsilon = 1e - 6$ where the residue is calculated by

$$
\begin{aligned}
r_{i,j,k} = &\left(-\frac{A^{(t)}_{i,j,k} - A^{(t)}_{i-1,j,k}}{h} + \sigma\left(\frac{1}{6}S^{(t-1)}_{i,j,k} - A^{(t-1)}_{i,j,k}\right)\right)^2 \\
&+\left(-\frac{B^{(t)}_{i,j,k} - B^{(t)}_{i+1,j,k}}{h} + \sigma\left(\frac{1}{6}S^{(t-1)}_{i,j,k} - B^{(t-1)}_{i,j,k}\right)\right)^2 \\
&+\left(-\frac{C^{(t)}_{i,j,k} - C^{(t)}_{i,j-1,k}}{h} + \sigma\left(\frac{1}{6}S^{(t-1)}_{i,j,k} - C^{(t-1)}_{i,j,k}\right)\right)^2 \\
&+\left(-\frac{D^{(t)}_{i,j,k} - D^{(t)}_{i,j+1,k}}{h} + \sigma\left(\frac{1}{6}S^{(t-1)}_{i,j,k} - D^{(t-1)}_{i,j,k}\right)\right)^2 \\
&+\left(-\frac{E^{(t)}_{i,j,k} - E^{(t)}_{i,j,k-1}}{h} + \sigma\left(\frac{1}{6}S^{(t-1)}_{i,j,k} - E^{(t-1)}_{i,j,k}\right)\right)^2 \\
&+\left(-\frac{F^{(t)}_{i,j,k} - F^{(t)}_{i,j,k+1}}{h} + \sigma\left(\frac{1}{6}S^{(t-1)}_{i,j,k} - F^{(t-1)}_{i,j,k}\right)\right)^2
\end{aligned}
$$

and $r = \frac{\sum_{i,j,k} r_{i,j,k}}{6n^3}$. Informally, r is about the square of the difference between left hand side and right hand side.

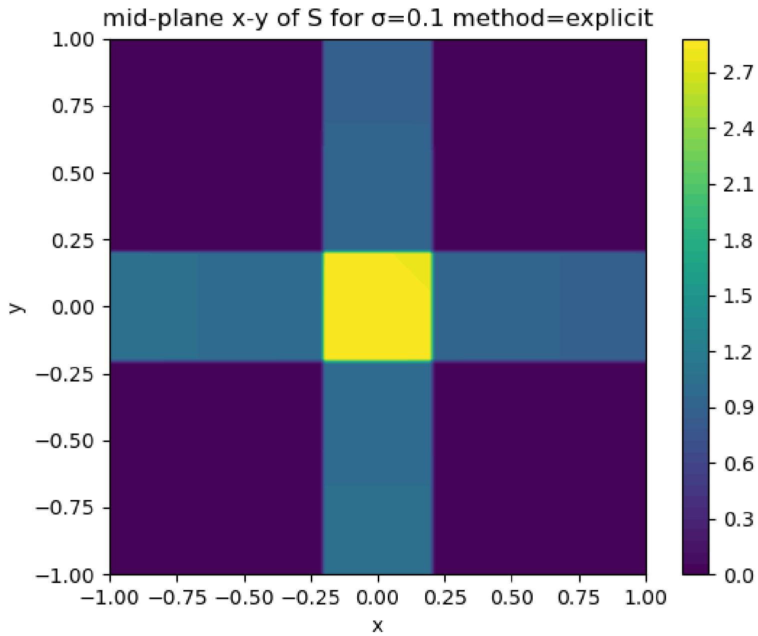
3 NUMERICAL RESULTS

3.1 EXPLICIT METHOD

$\sigma = 0.1$

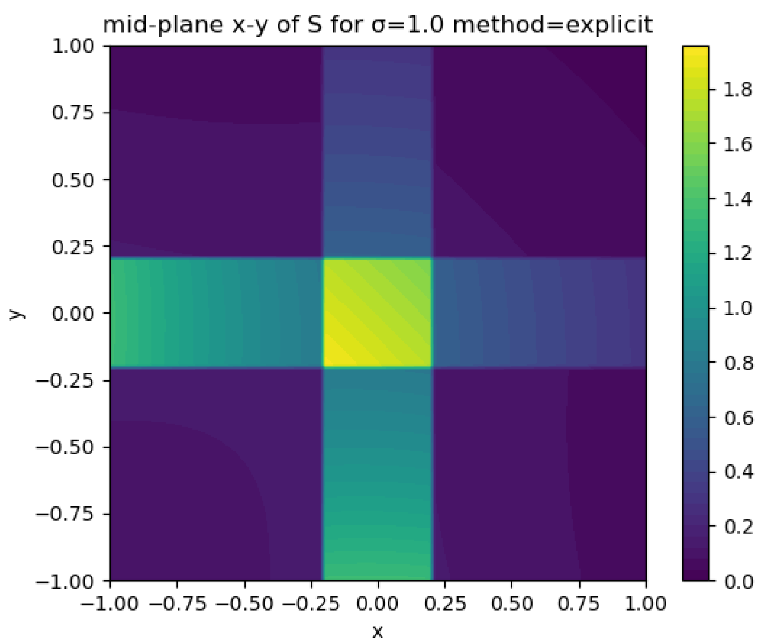
When $\sigma = 0.1$, the explicit method converged, the midplane $x - y$ is shown in the figure below

Figure 1: explicit method for $\sigma = 0.1$



When $\sigma = 1$, the explicit method converged, the midplane $x - y$ is shown in the figure below

Figure 2: explicit method for $\sigma = 1$

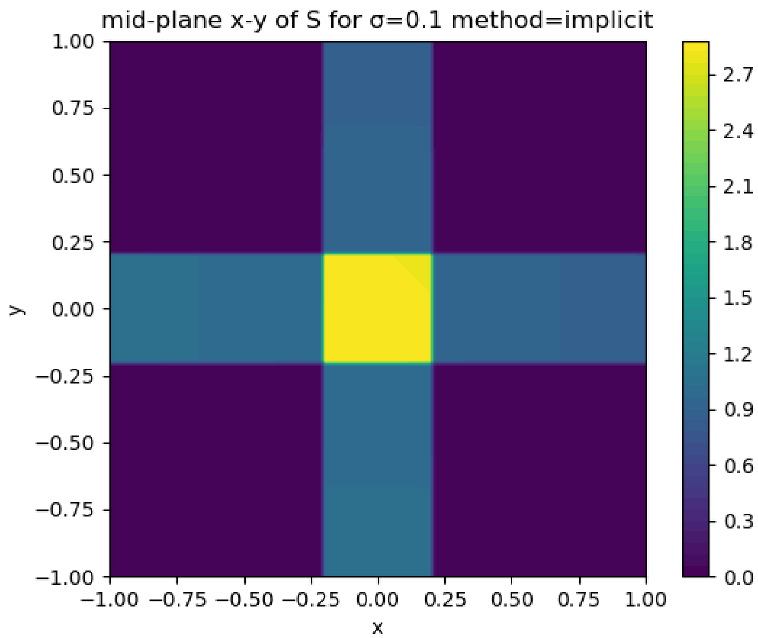


When $\sigma \geq 10$, the expliciti method failed to converge

3.2 SEMI-IMPLICIT METHOD

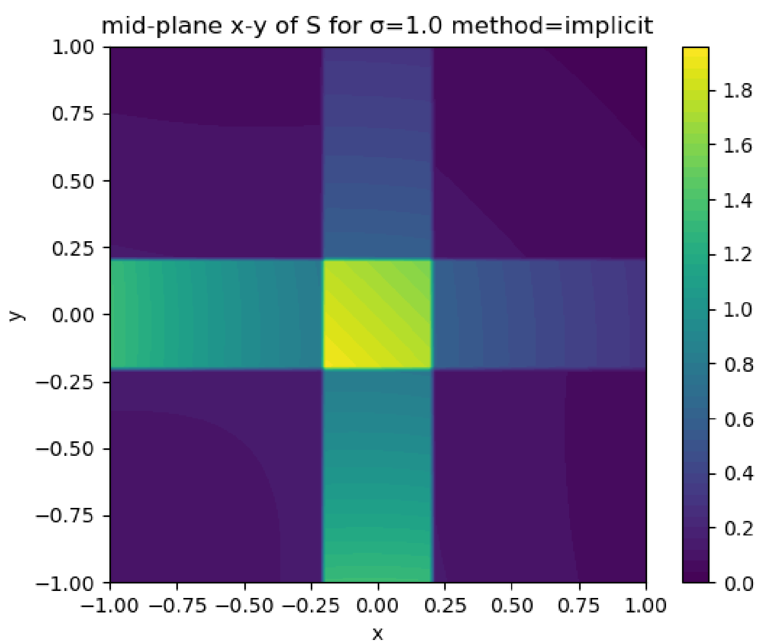
When $\sigma = 0.1$, the semi-implicit method converged, the midplane $x - y$ is shown in the figure below

Figure 3: semi-implicit method for $\sigma = 0.1$



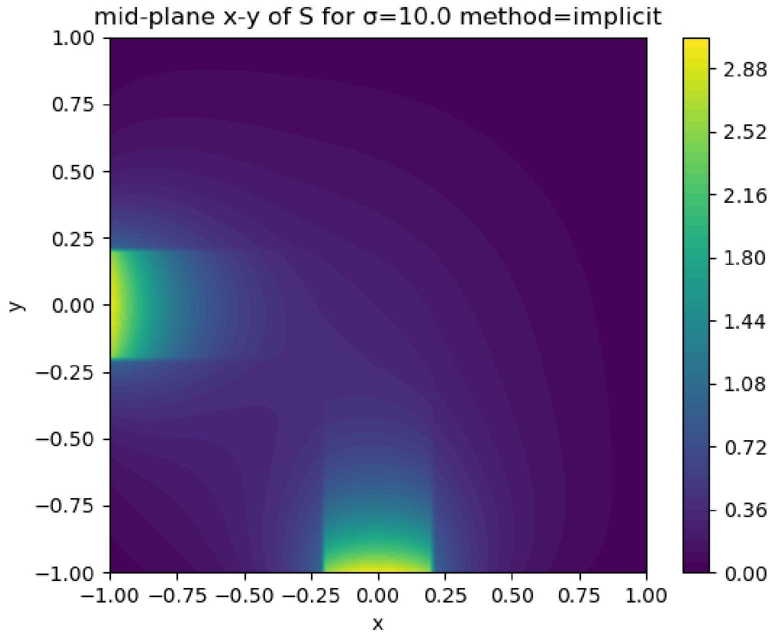
When $\sigma = 1$, the semi-implicit method converged, the midplane $x - y$ is shown in the figure below

Figure 4: semi-implicit method for $\sigma = 1$



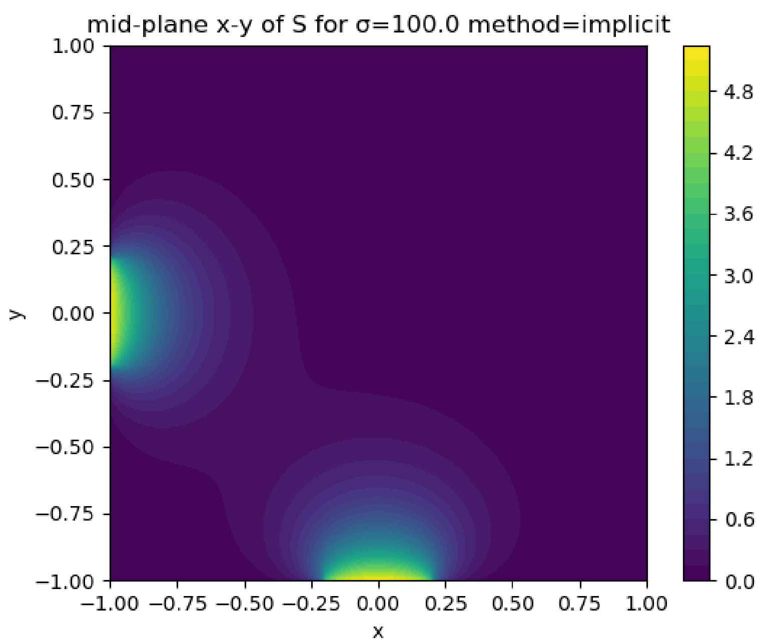
When $\sigma = 10$, the semi-implicit method converged, the midplane $x - y$ is shown in the figure below

Figure 5: semi-implicit method for $\sigma = 10$



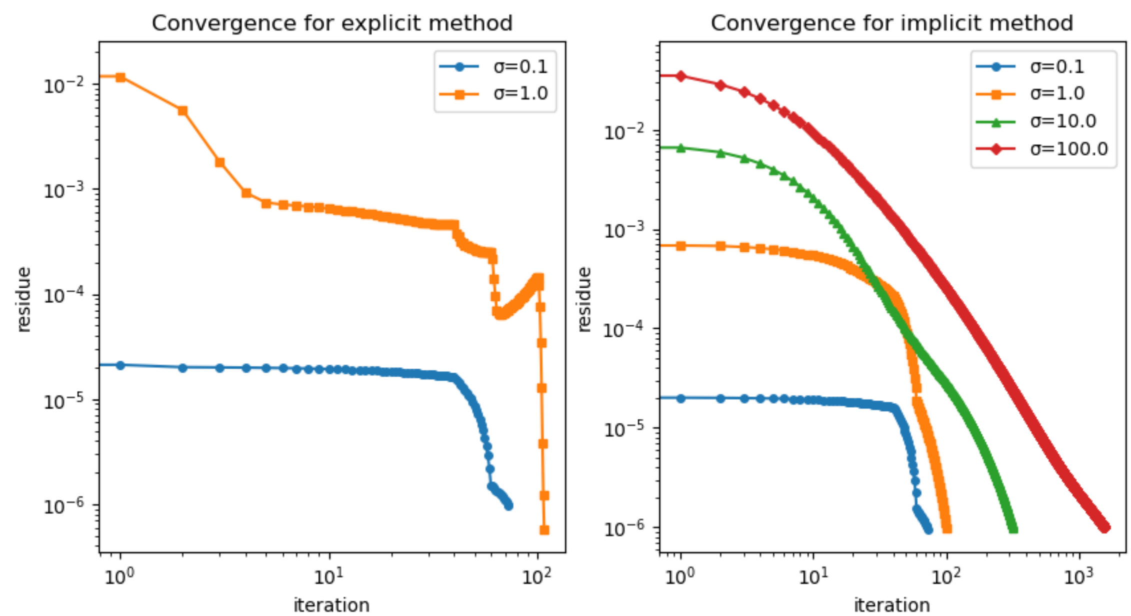
When $\sigma = 100$, the semi-implicit method converged, the midplane $x - y$ is shown in the figure below

Figure 6: semi-implicit method for $\sigma = 100$



3.3 CONVERGENCE OF EXPLICIT METHOD AND SEMI-IMPLICIT METHOD

Figure 7: Residue over time for explicit method and semi-implicit method



4 APPROXIMATE MODEL TO SOLVE FOR S

From the original equation we have

$$\frac{\partial S}{\partial t} + \frac{\partial (A-B)}{\partial x} + \frac{\partial (C-D)}{\partial y} + \frac{\partial (E-F)}{\partial z} = 0 \tag{1}$$

When $\epsilon \to 0$, suppose the left hand side are of order $O(1)$, we can approximate A, B, C, D, E, F up to the first order as follows:

$$\begin{aligned}
A &= \frac{1}{6}S + \epsilon A_1 \\
B &= \frac{1}{6}S + \epsilon B_1 \\
C &= \frac{1}{6}S + \epsilon C_1 \\
D &= \frac{1}{6}S + \epsilon D_1 \\
E &= \frac{1}{6}S + \epsilon E_1 \\
F &= \frac{1}{6}S + \epsilon F_1
\end{aligned}$$

for some functions $A_1, B_1, C_1, D_1, E_1, F_1 : \Omega \times [0, \infty) \to \mathbb{R}$ sufficiently smooth. Then, the equation for A and B become

$$\begin{aligned}
\left(\frac{1}{6}\frac{\partial S}{\partial t} + \epsilon \frac{\partial A_1}{\partial t}\right) + \left(\frac{1}{6}\frac{\partial S}{\partial x} + \epsilon \frac{\partial A_1}{\partial x}\right) &= -A_1 \\
\left(\frac{1}{6}\frac{\partial S}{\partial t} + \epsilon \frac{\partial B_1}{\partial t}\right) - \left(\frac{1}{6}\frac{\partial S}{\partial x} + \epsilon \frac{\partial B_1}{\partial x}\right) &= -B_1
\end{aligned}$$

At order $O(1)$, we have

$$A_1 = -\frac{1}{6}\left(\frac{\partial S}{\partial t} + \frac{\partial S}{\partial x}\right)$$
$$B_1 = -\frac{1}{6}\left(\frac{\partial S}{\partial t} - \frac{\partial S}{\partial x}\right)$$
$$A - B = \epsilon(A_1 - B_1) = -\frac{1}{3}\epsilon\frac{\partial S}{\partial x}$$

Similar calculation gives

$$C - D = -\frac{1}{3}\epsilon\frac{\partial S}{\partial y}$$
$$E - F = -\frac{1}{3}\epsilon\frac{\partial S}{\partial z}$$

Plugging into equation 1, we have

$$\frac{\partial S}{\partial t} - \frac{1}{3}\epsilon\left(\frac{\partial^2 S}{\partial x^2} + \frac{\partial^2 S}{\partial y^2} + \frac{\partial^2 S}{\partial z^2}\right) = 0$$

which is a diffusion equation with boundary condition.