MA5232 Assignment 1

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1 Introduction

The problem is to find numerical solutions to the following system of partial differential equations defined on $\Omega := (-1,1) \times (-1,1) \times (-1,1)$:

$$\frac{\partial F_1}{\partial x} = \sigma(\frac{1}{6} \sum_{i=1}^{6} F_i - F_1),$$

$$-\frac{\partial F_2}{\partial x} = \sigma(\frac{1}{6} \sum_{i=1}^{6} F_i - F_2),$$

$$\frac{\partial F_3}{\partial y} = \sigma(\frac{1}{6} \sum_{i=1}^{6} F_i - F_3),$$

$$-\frac{\partial F_4}{\partial y} = \sigma(\frac{1}{6} \sum_{i=1}^{6} F_i - F_4),$$

$$\frac{\partial F_5}{\partial z} = \sigma(\frac{1}{6} \sum_{i=1}^{6} F_i - F_5),$$

$$-\frac{\partial F_6}{\partial z} = \sigma(\frac{1}{6} \sum_{i=1}^{6} F_i - F_6),$$

where $\sigma = 0.1, 1, 10, 100$, respectively. The prescribed boundary conditions are:

$$F_1(-1,y,z) = F_b(y,z), F_3(x,-1,z) = F_b(x,z), F_5(x,y,-1) = F_b(x,y),$$

$$F_2(1,y,z) = F_4(x,1,z) = F_6(x,y,1) = 0,$$

where

$$F_b(p,q) = \begin{cases} 1 & |p| \le 0.2 \text{ and } |q| \le 0.2 \\ 0 & \text{otherwise} \end{cases}$$

In general, there does not exist a closed-form solution for such a system, and hence numerical approximated solution is what can be sought for.

In the class a similar 2-dimensional problem has been discussed, and this assignment extend to a 3-dimensional problem, which needs some adjustments to the code for that problem, and demands more computational power. In view of this regard, the method used is Symmetric Gauss-Seidel (SGS) method with Newton iteration, which has a faster convergence. This method has convergent result for all required σ . On the other hand, the source iteration method, and the time evolution method has a slow convergence for large σ (such as $\sigma = 100$), fixed-point iteration method, and SGS method with fixed-point iteration, might diverge for large σ . For the time being, I do not attempt the SGS with synthetic method, which could be a decent choice for this problem.

2 Rationale of SGS with Newton iteration

Given the problem space Ω , the step size (or the number of mesh points) along each axis should be determined first. Then, if using A, B, C, D, E, F to represent the (3-dimensional) discretization matrix for F_1 to F_6 , respectively, boundary conditions can be fed into these matrices at corresponding positions.¹ Then SGS method gives six equations:

$$\frac{A_{ijk} - A_{i-1,j,k}}{\Delta x} = \sigma * \left(\frac{1}{6}(A_{ijk} + B_{ijk} + C_{ijk} + D_{ijk} + E_{ijk} + F_{ijk}) - A_{ijk}\right),$$

$$-\frac{B_{i+1,j,k} - B_{ijk}}{\Delta x} = \sigma * \left(\frac{1}{6}(A_{ijk} + B_{ijk} + C_{ijk} + D_{ijk} + E_{ijk}^{+}F_{ijk}) - B_{ijk}\right),$$

$$\frac{C_{i+1,j,k} - C_{ijk}}{\Delta y} = \sigma * \left(\frac{1}{6}(A_{ijk} + B_{ijk} + C_{ijk} + D_{ijk} + E_{ijk} + F_{ijk}) - C_{ijk}\right),$$

$$-\frac{D_{i+1,j,k} - D_{ijk}}{\Delta y} = \sigma * \left(\frac{1}{6}(A_{ijk} + B_{ijk} + C_{ijk} + D_{ijk} + E_{ijk} + F_{ijk}) - D_{ijk}\right),$$

$$\frac{E_{i+1,j,k} - E_{ijk}}{\Delta z} = \sigma * \left(\frac{1}{6}(A_{ijk} + B_{ijk} + C_{ijk} + D_{ijk} + E_{ijk} + F_{ijk}) - E_{ijk}\right),$$

$$-\frac{F_{i+1,j,k} - F_{ijk}}{\Delta z} = \sigma * \left(\frac{1}{6}(A_{ijk} + B_{ijk} + C_{ijk} + D_{ijk} + E_{ijk} + F_{ijk}) - F_{ijk}\right),$$

where X_{ijk} denotes the (i, j, k) entry of the 3-dimensional matrix X.

However, since the step size in the numerical simulation cannot be arbitrarily small, there would be a residual term in each of the above six equations. In order to reduce residuals, there would be a forward scan (that is, from the first entry not prescribed by boundary conditions to the last such one) and a backward scan to examine the component-wise residual. If such residue is larger than a tolerance value, Newton iteration would be applied to update the corresponding entry of the discretization matrix and hence reduce residuals.

3 Numerical settings

Since the problem space is a direct product of three (-1,1) intervals and

$$length((-1,1)) = 2,$$

a discretization of 100 evenly-spaced mesh points (hence step size 0.02) inside each interval would be sufficient. Therefore, the problem space Ω is discretized into 100^3 points. Boundary conditions, given by functions of two variables, are evaluated at corresponding grid points. There is a need to compute the norm of matrices, as the method produces matrices with entries representing the residual. The residual of matrices are calculated using Frobenius norm.

For this problem, tolerance of convergence (threshold) is set as 10^{-5} across all σ values examined.

¹in the code, A_i is used to denote the corresponding matrix for F_i , $1 \le i \le 6$.

4 Numerical solutions

The numerical solutions presented by figures are as follows:

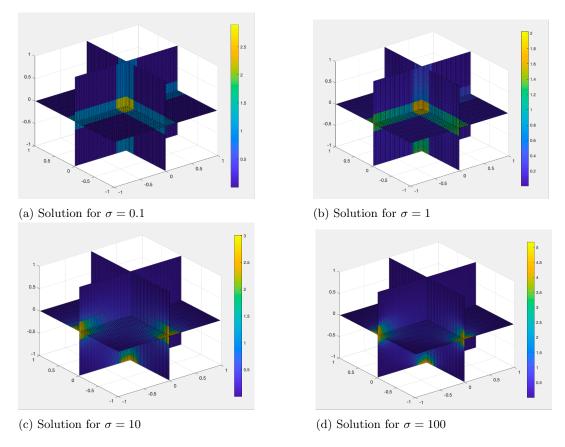


Figure 1: Plots of numerical solutions for different σ

To interpret these solutions, firstly, notice that at the beginning in the x=-1 plane, the value is one in a square centered at (-1,0,0) with side length 0.4, and similarly for y=-1 and z=-1 planes. Remaining positions inside Ω has value zero at the start. Then, as the system evolves, the 'energy' (non-zero values) tend to spread in the space, and as Figure 1 shows, as σ increases, it becomes harder for 'energy' to spread: for example, when $\sigma=0.1$, the 'energy' spreads to the region around the origin very fast, whereas for $\sigma=100$, the 'energy' spreads out but decays very fast, so it does not reach the origin.

5 Convergence of the method

Below is a summary of the number of iterations needed to 'converge' (residual less than 10^{-5}) for different σ :

σ	iterations	
0.1	2	
	6	
1	•	
10	88	
100	1319	

Table 1: Number of iterations to converge for different σ

Clearly, the number of iterations needed increases as σ increases. As σ increases, the update tends to be slower and the residual would be larger during the scan process, and thus it takes more time to

converge.

Next have a look of how the method converges as more iterations are processed, as in the following Figure 2:

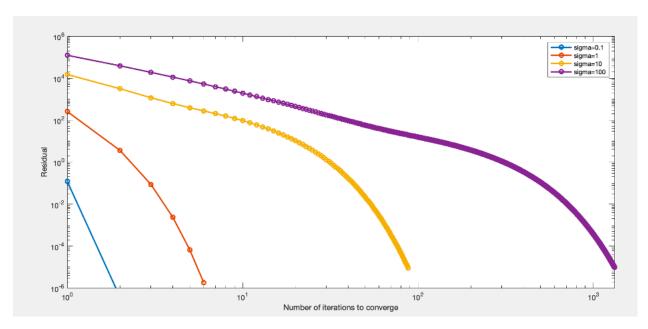


Figure 2: Convergence of SGS with Newton iteration (convergence threshold: 10^{-5})

Since different σ 's have varying scale of number of iterations needed to converge, as well as different beginning residual values, for better visualization, both x- and y-axis have been changed to log scale, and y starts at 10^{-6} . For each σ , residual decreases significantly during the first several iterations, and then the decrease slows down.

The next section is MATLAB code for this problem. A separate MATLAB code file would be submitted. Also, I have commented the code for plotting the convergence against number of iterations to avoid replacing the numerical solution plot.

6 MATLAB Code

```
function [iter_arr, res_arr, A1, A2, A3, A4, A5, A6] = a1_code(Nx, Ny, Nz, sigma
      , f1, f2, f3, f4, f5, f6, thres)
  %A_i: discretization matrix for F_i; f_i: boundary condition for F_i
  dx = 2 / Nx; dy = 2 / Ny; dz = 2 / Nz;
  x = linspace(-1+dx/2, 1-dx/2, Nx); %row vector
  y = linspace(-1+dy/2, 1-dy/2, Ny);
  z = linspace(-1+dz/2, 1-dz/2, Nz);
  [X, Y, Z] = meshgrid(x, y, z);
  A1 = zeros(Nx+2, Ny+2, Nz+2); A2 = A1; A3 = A1; A4 = A1; A5 = A1; A6 = A1
  n_{iter} = 0;
10
11
  % Boundary conditions
12
  [X_xy, Y_xy] = meshgrid(x,y); [X_xz, Z_xz] = meshgrid(x,z); [Y_yz, Z_yz] = meshgrid(x,y);
      (y,z);
  A1b = f1(Y_yz, Z_yz); A2b = f2(Y_yz, Z_yz); A3b = f3(X_xz, Z_xz); A4b = f4(
      X_xz, Z_xz; A5b=f5(X_xy, Y_xy); A6b=f6(X_xy, Y_xy);
  A1(1,2:end-1,2:end-1) = A1b'; A2(end,2:end-1,2:end-1) = A2b';
 A3(2:end-1,1,2:end-1) = A3b'; A4(2:end-1,end,2:end-1) = A4b';
```

```
A5(2:end-1,2:end-1,1) = A5b'; A6(2:end-1,2:end-1,end) = A6b';
17
18
                % Residual
19
                 resA1 = -(A1(2:Nx+1,2:Ny+1,2:Nz+1) - A1(1:Nx,2:Ny+1,2:Nz+1)) / dx + sigma
                                                  * ((1/6)*(A1(2:Nx+1,2:Ny+1,2:Nz+1) + A2(2:Nx+1,2:Ny+1,2:Nz+1) + A3(2:Nz+1) + A3(2
                                          Nx+1,2:Ny+1,2:Nz+1 + A4(2:Nx+1,2:Ny+1,2:Nz+1)+A5(2:Nx+1,2:Ny+1,2:Nz+1)+A5(2:Nx+1,2:Ny+1,2:Nz+1)+A5(2:Nx+1,2:Ny+1,2:Nz+1)+A5(2:Nx+1,2:Ny+1,2:Nz+1)+A5(2:Nx+1,2:Ny+1,2:Nz+1)+A5(2:Nx+1,2:Ny+1,2:Nz+1)+A5(2:Nx+1,2:Ny+1,2:Nz+1)+A5(2:Nx+1,2:Ny+1,2:Nz+1)+A5(2:Nx+1,2:Ny+1,2:Nz+1)+A5(2:Nx+1,2:Ny+1,2:Nz+1)+A5(2:Nx+1,2:Ny+1,2:Nz+1)+A5(2:Nx+1,2:Ny+1,2:Nz+1)+A5(2:Nx+1,2:Ny+1,2:Nz+1)+A5(2:Nx+1,2:Ny+1,2:Nz+1)+A5(2:Nx+1,2:Ny+1,2:Nz+1)+A5(2:Nx+1,2:Ny+1,2:Nz+1)+A5(2:Nx+1,2:Ny+1,2:Nz+1)+A5(2:Nx+1,2:Ny+1,2:Nz+1)+A5(2:Nx+1,2:Ny+1,2:Nz+1)+A5(2:Nx+1,2:Ny+1,2:Nz+1)+A5(2:Nx+1,2:Ny+1,2:Nz+1)+A5(2:Nx+1,2:Ny+1,2:Nz+1)+A5(2:Nx+1,2:Nz+1)+A5(2:Nx+1,2:Nz+1)+A5(2:Nx+1,2:Nz+1)+A5(2:Nx+1,2:Nz+1)+A5(2:Nx+1,2:Nz+1)+A5(2:Nx+1,2:Nz+1)+A5(2:Nx+1,2:Nz+1)+A5(2:Nx+1,2:Nz+1)+A5(2:Nx+1,2:Nz+1)+A5(2:Nx+1,2:Nz+1)+A5(2:Nx+1,2:Nz+1)+A5(2:Nx+1,2:Nz+1)+A5(2:Nx+1,2:Nz+1)+A5(2:Nx+1,2:Nz+1)+A5(2:Nx+1,2:Nz+1)+A5(2:Nx+1,2:Nz+1)+A5(2:Nx+1,2:Nz+1)+A5(2:Nx+1,2:Nz+1)+A5(2:Nx+1,2:Nz+1)+A5(2:Nx+1,2:Nz+1)+A5(2:Nx+1,2:Nz+1)+A5(2:Nx+1,2:Nz+1)+A5(2:Nx+1,2:Nz+1)+A5(2:Nx+1,2:Nz+1)+A5(2:Nx+1,2:Nz+1)+A5(2:Nx+1,2:Nz+1)+A5(2:Nx+1,2:Nz+1)+A5(2:Nx+1,2:Nz+1)+A5(2:Nx+1,2:Nz+1)+A5(2:Nx+1,2:Nz+1)+A5(2:Nx+1,2:Nz+1)+A5(2:Nx+1,2:Nz+1)+A5(2:Nx+1,2:Nz+1)+A5(2:Nx+1,2:Nz+1)+A5(2:Nx+1,2:Nz+1)+A5(2:Nx+1,2:Nz+1)+A5(2:Nx+1,2:Nz+1)+A5(2:Nx+1,2:Nz+1)+A5(2:Nx+1,2:Nz+1)+A5(2:Nx+1,2:Nz+1)+A5(2:Nx+1,2:Nz+1)+A5(2:Nx+1,2:Nz+1)+A5(2:Nx+1,2:Nz+1)+A5(2:Nx+1,2:Nz+1)+A5(2:Nx+1,2:Nz+1)+A5(2:Nx+1,2:Nz+1)+A5(2:Nx+1,2:Nz+1)+A5(2:Nx+1,2:Nz+1)+A5(2:Nx+1,2:Nz+1)+A5(2:Nx+1,2:Nz+1)+A5(2:Nx+1,2:Nz+1)+A5(2:Nx+1,2:Nz+1)+A5(2:Nx+1,2:Nz+1)+A5(2:Nx+1,2:Nz+1)+A5(2:Nx+1,2:Nx+1,2:Nx+1)+A5(2:Nx+1,2:Nx+1,2:Nx+1)+A5(2:Nx+1,2:Nx+1,2:Nx+1,2:Nx+1)+A5(2:Nx+1,2:Nx+1,2:Nx+1,2:Nx+1)+A5(2:Nx+1,2:Nx+1,2:Nx+1,2:Nx+1,2:Nx+1,2:Nx+1,2:Nx+1,2:Nx+1,2:Nx+1,2:Nx+1,2:Nx+1,2:Nx+1,2:Nx+1,2:Nx+1,2:Nx+1,2:Nx+1,2:Nx+1,2:Nx+1,2:Nx+1,2:Nx+1,2:Nx+1,2:Nx+1,2:Nx+1,2:Nx+1,2:Nx+1,2:Nx+1,2:Nx+1,2:Nx+1,2:Nx+1,2:Nx+1,2:Nx+1,2:Nx+1,2:Nx+1,2:Nx+1,2:Nx+1,2:Nx+1,2:Nx+1,2:Nx+1,2:Nx+1,2:Nx+1,2:Nx+1,2:Nx+1,2:Nx+1,2:Nx+1,2:Nx+1,2:Nx+1,2:Nx+1,2:Nx+1,2:Nx+1,2:Nx+1,2:Nx+1,
                                          +1)+A6 (2:Nx+1,2:Ny+1,2:Nz+1))-A1 (2:Nx+1,2:Ny+1,2:Nz+1));
                 resA2 = (A2(3:Nx+2,2:Ny+1,2:Nz+1) - A2(2:Nx+1,2:Ny+1,2:Nz+1)) / dx +
                                          sigma * ((1/6)*(A1(2:Nx+1,2:Ny+1,2:Nz+1) + A2(2:Nx+1,2:Ny+1,2:Nz+1) +
                                          A3(2:Nx+1,2:Ny+1,2:Nz+1) + A4(2:Nx+1,2:Ny+1,2:Nz+1) + A5(2:Nx+1,2:Ny+1,2:Ny+1,2:Nz+1) + A5(2:Nx+1,2:Ny+1,2:Nz+1) + A5(2:Nx+1,2:Nz+1,2:Nz+1) + A5(2:Nx+1,2:Nz+1,2:Nz+1) + A5(2:Nx+1,2:Nz+1,2:Nz+1,2:Nz+1) + A5(2:Nx+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1,2:Nz+1
                                           +1,2:Nz+1)+A6(2:Nx+1,2:Ny+1,2:Nz+1)-A2(2:Nx+1,2:Ny+1,2:Nz+1));
           resA3 = -(A3(2:Nx+1,2:Ny+1,2:Nz+1) - A3(2:Nx+1,1:Ny,2:Nz+1)) / dy + sigma
                                                  * ((1/6)*(A1(2:Nx+1,2:Ny+1,2:Nz+1) + A2(2:Nx+1,2:Ny+1,2:Nz+1) + A3(2:Nx+1,2:Nz+1) + A3(2:Nz+1) + A3(2:Nz+1)
                                          Nx+1,2:Ny+1,2:Nz+1) + A4(2:Nx+1,2:Ny+1,2:Nz+1)+A5(2:Nx+1,2:Ny+1,2:Nz+1)
                                          +1)+A6 (2:Nx+1,2:Ny+1,2:Nz+1))-A3 (2:Nx+1,2:Ny+1,2:Nz+1));
                 res A4 = (A4(2:Nx+1,3:Ny+2,2:Nz+1) - A4(2:Nx+1,2:Ny+1,2:Nz+1)) / dy +
                                          sigma * ((1/6)*(A1(2:Nx+1,2:Ny+1,2:Nz+1) + A2(2:Nx+1,2:Ny+1,2:Nz+1) +
                                          A3(2:Nx+1,2:Ny+1,2:Nz+1) + A4(2:Nx+1,2:Ny+1,2:Nz+1) + A5(2:Nx+1,2:Ny+1,2:Nz+1) + A5(2:Nx+1,2:Ny+1,2:Nz+1) + A5(2:Nx+1,2:Nz+1) + A5(2:Nx+1,2:Nz+1
                                           +1,2:Nz+1)+A6(2:Nx+1,2:Ny+1,2:Nz+1)-A4(2:Nx+1,2:Ny+1,2:Nz+1));
              res A5 = -(A5(2:Nx+1,2:Ny+1,2:Nz+1) - A5(2:Nx+1,2:Ny+1,1:Nz)) / dz + sigma
                                                 * ((1/6)*(A1(2:Nx+1,2:Ny+1,2:Nz+1) + A2(2:Nx+1,2:Ny+1,2:Nz+1) + A3(2:Nz+1) + A3(2
                                          Nx+1,2:Ny+1,2:Nz+1 + A4(2:Nx+1,2:Ny+1,2:Nz+1)+A5(2:Nx+1,2:Ny+1,2:Nz+1)
                                          +1)+A6(2:Nx+1,2:Ny+1,2:Nz+1))-A5(2:Nx+1,2:Ny+1,2:Nz+1));
                 resA6 = (A6(2:Nx+1,2:Ny+1,3:Nz+2) - A6(2:Nx+1,2:Ny+1,2:Nz+1)) / dz +
                                          sigma * ((1/6)*(A1(2:Nx+1,2:Ny+1,2:Nz+1) + A2(2:Nx+1,2:Ny+1,2:Nz+1) +
                                          A3(2:Nx+1,2:Ny+1,2:Nz+1) + A4(2:Nx+1,2:Ny+1,2:Nz+1) + A5(2:Nx+1,2:Ny+1,2:Nz+1) + A5(2:Nx+1,2:Ny+1,2:Nz+1) + A5(2:Nx+1,2:Nz+1) + A5(2:Nx+1,2:Nz+1
                                           +1,2:Nz+1)+A6(2:Nx+1,2:Ny+1,2:Nz+1))-A6(2:Nx+1,2:Ny+1,2:Nz+1));
26
                   res = \!\! norm(resA1 \;, \; 'fro')^2 \; + \; norm(resA2 \;, \; 'fro')^2 \; + \; norm(resA3 \;, \; 'fro')^2 \; + \; norm(resA3 \;, \; 'fro')^2 \; + \; norm(resA3 \;, \; 'fro')^3 \; + \; norm(resA3 \;, \; 'fro
27
                                          \operatorname{norm}(\operatorname{res} A4, '\operatorname{fro}')^2 + \operatorname{norm}(\operatorname{res} A5, '\operatorname{fro}')^2 + \operatorname{norm}(\operatorname{res} A6, '\operatorname{fro}')^2;
                   res_arr = [];
28
                   iter_arr = [];
30
                    while res > thres && n_iter < 8000
31
                                                n_Newton_iter = 0;
32
                                                n_nonlin_{eqs} = 0;
33
                                                count=0;
                                                 for i=2:Nx+1
36
                                                                             for j=2:Ny+1
37
                                                                                                        for k=2:Nz+1
                                                                                                                                     count = count + 1;
39
                                                                                                                                     resA1 = -(A1(i,j,k) - A1(i-1,j,k)) / dx + sigma * ...
                                                                                                                                                                    ((1/6)*(A1(i,j,k) + A2(i,j,k) + A3(i,j,k) + A4(i,j,k))
41
                                                                                                                                                                                               + A5(i,j,k)+A6(i,j,k))-A1(i,j,k));
                                                                                                                                     resA2 = (A2(i+1,j,k) - A2(i,j,k)) / dx + sigma * ...
42
                                                                                                                                                                   ((1/6)*(A1(i,j,k) + A2(i,j,k) + A3(i,j,k) + A4(i,j,k))
43
                                                                                                                                                                                              + A5(i,j,k)+A6(i,j,k))-A2(i,j,k);
                                                                                                                                     resA3 = -(A3(i,j,k) - A3(i,j-1,k)) / dy + sigma * ...
                                                                                                                                                                   ((1/6)*(A1(i,j,k) + A2(i,j,k) + A3(i,j,k) + A4(i,j,k))
45
                                                                                                                                                                                              + A5(i,j,k)+A6(i,j,k))-A3(i,j,k);
                                                                                                                                     resA4 = (A4(i, j+1,k) - A4(i, j,k)) / dy + sigma * ...
46
                                                                                                                                                                    ((1/6)*(A1(i,j,k) + A2(i,j,k) + A3(i,j,k) + A4(i,j,k))
                                                                                                                                                                                              + A5(i,j,k)+A6(i,j,k))-A4(i,j,k));
                                                                                                                                      resA5 = -(A5(i,j,k)-A5(i,j,k-1)) / dz + sigma * ...
48
                                                                                                                                                                   ((1/6)*(A1(i,j,k) + A2(i,j,k) + A3(i,j,k) + A4(i,j,k)
49
```

```
+ A5(i,j,k)+A6(i,j,k))-A5(i,j,k));
                        resA6 = (A6(i,j,k+1)-A6(i,j,k)) / dz + sigma * ...
50
                              ((1/6)*(A1(i,j,k) + A2(i,j,k) + A3(i,j,k) + A4(i,j,k))
51
                                   + A5(i,j,k)+A6(i,j,k))-A6(i,j,k);
                         res = sqrt(resA1^2 + resA2^2 + resA3^2 + resA4^2 + resA5^2)
52
                              + resA6^2;
53
                         n_nonlin_eqs = n_nonlin_eqs + 1;
54
                         while res > thres * 1e-3
56
                              Jac = [1/dx - sigma/6 + sigma, -sigma/6, -sigma/6, -
                                  \operatorname{sigma}/6, -\operatorname{sigma}/6, -\operatorname{sigma}/6;
                                   -\operatorname{sigma}/6, 1/\operatorname{dx} - \operatorname{sigma}/6 + \operatorname{sigma}, -\operatorname{sigma}/6, -\operatorname{sigma}/6
                                       \operatorname{sigma}/6, -\operatorname{sigma}/6, -\operatorname{sigma}/6;
                                   -sigma/6, -sigma/6, 1/dy - sigma/6 + sigma, -
59
                                       \operatorname{sigma}/6, -\operatorname{sigma}/6, -\operatorname{sigma}/6;
                                   -\operatorname{sigma}/6, -\operatorname{sigma}/6, -\operatorname{sigma}/6, 1/\operatorname{dy} - \operatorname{sigma}/6 +
60
                                       sigma, -sigma/6, -sigma/6;
                                   -\operatorname{sigma}/6, -\operatorname{sigma}/6, -\operatorname{sigma}/6, -\operatorname{sigma}/6, 1/\operatorname{dz}
61
                                       sigma/6 + sigma, -sigma/6;
                                   -\operatorname{sigma}/6, -\operatorname{sigma}/6, -\operatorname{sigma}/6, -\operatorname{sigma}/6, -\operatorname{sigma}/6,
62
                                         1/dz - sigma/6 + sigma;
63
                              dsol = Jac \setminus [resA1; resA2; resA3; resA4; resA5;
64
                                  resA6];
                              A1(i, j, k) = A1(i, j, k) + dsol(1);
66
                              A2(i,j,k) = A2(i,j,k) + dsol(2);
                              A3(i,j,k) = A3(i,j,k) + dsol(3);
                              A4(i, j, k) = A4(i, j, k) + dsol(4);
                              A5(i, j, k) = A5(i, j, k) + dsol(5);
70
                              A6(i, j, k) = A6(i, j, k) + dsol(6);
72
73
                              resA1 = -(A1(i,j,k) - A1(i-1,j,k)) / dx + sigma * ...
74
                                   ((1/6)*(A1(i,j,k) + A2(i,j,k) + A3(i,j,k) + A4(i,j,k))
75
                                       j, k) + A5(i, j, k)+A6(i, j, k))-A1(i, j, k);
                              resA2 = (A2(i+1,j,k) - A2(i,j,k)) / dx + sigma * ...
76
                                   ((1/6)*(A1(i,j,k) + A2(i,j,k) + A3(i,j,k) + A4(i,j,k))
77
                                       j,k) + A5(i,j,k)+A6(i,j,k)-A2(i,j,k);
                              resA3 = -(A3(i,j,k) - A3(i,j-1,k)) / dy + sigma * ...
                                   ((1/6)*(A1(i,j,k) + A2(i,j,k) + A3(i,j,k) + A4(i,j,k))
79
                                       j, k) + A5(i, j, k)+A6(i, j, k))-A3(i, j, k);
                              resA4 = (A4(i, j+1,k) - A4(i, j,k)) / dy + sigma * ...
80
                                   ((1/6)*(A1(i,j,k) + A2(i,j,k) + A3(i,j,k) + A4(i,j,k))
                                       j, k) + A5(i, j, k) + A6(i, j, k) - A4(i, j, k);
                              resA5 = -(A5(i,j,k)-A5(i,j,k-1))/dz + sigma * ...
                                   ((1/6)*(A1(i,j,k) + A2(i,j,k) + A3(i,j,k) + A4(i,j,k))
83
                                       j, k) + A5(i, j, k) + A6(i, j, k) - A5(i, j, k);
                              resA6 = (A6(i,j,k+1)-A6(i,j,k))/dz + sigma * ...
84
                                   ((1/6)*(A1(i,j,k) + A2(i,j,k) + A3(i,j,k) + A4(i,j,k))
85
                                       j, k) + A5(i, j, k) + A6(i, j, k) - A6(i, j, k);
                              res = sqrt(resA1^2 + resA2^2 + resA3^2 + resA4^2 +
86
                                  resA5^2 + resA6^2;
```

```
89
                                  n_Newton_iter = n_Newton_iter + 1;
90
                                  if (res > 1e+8)
92
                                        error ("The Newton iteration fails to converge.");
93
                                 end
                            end
                      end
96
                end
          end
98
           for i=Nx+1:-1:2
100
                for j=Ny+1:-1:2
101
                      for k=Nz+1:-1:2
102
                            {\rm res} A \, 1 \, = \, - (A \, 1 \, (\, i \, , j \, , k \, ) \, - \, A \, 1 \, (\, i \, - 1, j \, , k \, ) \, ) \  \, / \  \, dx \, + \, sigma \, * \, \, \ldots
                                  ((1/6)*(A1(i,j,k) + A2(i,j,k) + A3(i,j,k) + A4(i,j,k))
104
                                        + A5(i,j,k)+A6(i,j,k))-A1(i,j,k);
                            resA2 = (A2(i+1,j,k) - A2(i,j,k)) / dx + sigma * ...
105
                                  ((1/6)*(A1(i,j,k) + A2(i,j,k) + A3(i,j,k) + A4(i,j,k))
106
                                        + A5(i,j,k)+A6(i,j,k))-A2(i,j,k));
                            resA3 = -(A3(i,j,k) - A3(i,j-1,k)) / dy + sigma * ...
107
                                  ((1/6)*(A1(i,j,k) + A2(i,j,k) + A3(i,j,k) + A4(i,j,k))
108
                                        + A5(i,j,k)+A6(i,j,k))-A3(i,j,k);
                            {\rm res} \, A4 \, = \, \left( \, A4 \, (\, i \, , \, j + 1, k \, ) \, \, - \, \, A4 \, (\, i \, , \, j \, , k \, ) \, \, \right) \, \, / \, \, {\rm dy} \, + \, {\rm sigma} \, \, * \, \, \ldots
109
                                  ((1/6)*(A1(i,j,k) + A2(i,j,k) + A3(i,j,k) + A4(i,j,k)
110
                                        + A5(i,j,k)+A6(i,j,k))-A4(i,j,k);
                            resA5 = -(A5(i,j,k)-A5(i,j,k-1))/dz + sigma * ...
111
                                  ((1/6)*(A1(i,j,k) + A2(i,j,k) + A3(i,j,k) + A4(i,j,k))
                                        + A5(i,j,k)+A6(i,j,k))-A5(i,j,k);
                            resA6 = (A6(i,j,k+1)-A6(i,j,k))/dz + sigma *
113
                                  ((1/6)*(A1(i,j,k) + A2(i,j,k) + A3(i,j,k) + A4(i,j,k)
114
                                        + A5(i,j,k)+A6(i,j,k))-A6(i,j,k);
                            res = sqrt(resA1^2 + resA2^2 + resA3^2 + resA4^2 + resA5^2)
115
                                  + \operatorname{resA6^{2}};
116
117
                            n_nonlin_eqs = n_nonlin_eqs + 1;
                            while res > 1e-3 * thres
119
                                 Jac = [1/dx - sigma/6 + sigma, -sigma/6, -sigma/6, -
120
                                      sigma/6, -sigma/6, -sigma/6;
                                         -\operatorname{sigma}/6, 1/\operatorname{dx} - \operatorname{sigma}/6 + \operatorname{sigma}, -\operatorname{sigma}/6, -\operatorname{sigma}/6
121
                                              \operatorname{sigma}/6, -\operatorname{sigma}/6, -\operatorname{sigma}/6;
                                        -\operatorname{sigma}/6, -\operatorname{sigma}/6, 1/\operatorname{dy} - \operatorname{sigma}/6 + \operatorname{sigma}, -
                                              \operatorname{sigma}/6, -\operatorname{sigma}/6, -\operatorname{sigma}/6;
                                        -\operatorname{sigma}/6, -\operatorname{sigma}/6, -\operatorname{sigma}/6, 1/\operatorname{dy} - \operatorname{sigma}/6 +
123
                                              sigma, -sigma/6, -sigma/6;
                                        -\operatorname{sigma}/6, -\operatorname{sigma}/6, -\operatorname{sigma}/6, -\operatorname{sigma}/6, 1/\operatorname{dz}
124
                                              sigma/6 + sigma, -sigma/6;
                                        -sigma/6, -sigma/6, -sigma/6, -sigma/6, -sigma
125
                                              /6, 1/dz - sigma/6 + sigma;
                                  dsol = Jac \setminus [resA1; resA2; resA3; resA4; resA5;
127
                                      resA6];
128
                                 A1(i, j, k) = A1(i, j, k) + dsol(1);
129
                                 A2(i,j,k) = A2(i,j,k) + dsol(2);
130
```

```
A3(i,j,k) = A3(i,j,k) + dsol(3);
131
                                                  A4(i, j, k) = A4(i, j, k) + dsol(4);
132
                                                  A5(i,j,k) = A5(i,j,k) + dsol(5);
133
                                                  A6(i, j, k) = A6(i, j, k) + dsol(6);
134
135
136
                                                  resA1 = -(A1(i,j,k) - A1(i-1,j,k)) / dx + sigma * ...
                                                           ((1/6)*(A1(i,j,k) + A2(i,j,k) + A3(i,j,k) + A4(i,j,k))
138
                                                                 j, k) + A5(i, j, k)+A6(i, j, k))-A1(i, j, k);
                                                  resA2 = (A2(i+1,j,k) - A2(i,j,k)) / dx + sigma * ...
139
                                                           ((1/6)*(A1(i,j,k) + A2(i,j,k) + A3(i,j,k) + A4(i,j,k))
                                                                 {\rm j}\,\,,{\rm k}\,) \,\,+\,\, {\rm A5}\,({\rm\,i}\,\,,{\rm j}\,\,,{\rm k}\,) + {\rm A6}\,({\rm\,i}\,\,,{\rm j}\,\,,{\rm k}\,)\,) - {\rm A2}\,({\rm\,i}\,\,,{\rm j}\,\,,{\rm k}\,)\,)\,;
                                                  resA3 = -(A3(i,j,k) - A3(i,j-1,k)) / dy + sigma * ...
141
                                                           ((1/6)*(A1(i,j,k) + A2(i,j,k) + A3(i,j,k) + A4(i,j,k))
142
                                                                 j, k) + A5(i, j, k) + A6(i, j, k) - A3(i, j, k);
                                                  resA4 = (A4(i, j+1,k) - A4(i, j,k)) / dy + sigma * ...
143
                                                           ((1/6)*(A1(i,j,k) + A2(i,j,k) + A3(i,j,k) + A4(i,j,k))
144
                                                                  j, k) + A5(i, j, k) + A6(i, j, k) - A4(i, j, k);
                                                  resA5 = -(A5(i,j,k)-A5(i,j,k-1))/dz + sigma * ...
                                                           ((1/6)*(A1(i,j,k) + A2(i,j,k) + A3(i,j,k) + A4(i,j,k))
146
                                                                 j, k) + A5(i, j, k) + A6(i, j, k) - A5(i, j, k);
                                                  resA6 = (A6(i,j,k+1)-A6(i,j,k))/dz + sigma * ...
147
                                                           ((1/6)*(A1(i,j,k) + A2(i,j,k) + A3(i,j,k) + A4(i,j,k))
148
                                                                 j, k) + A5(i, j, k) + A6(i, j, k) - A6(i, j, k);
149
                                                  res = sqrt(resA1^2 + resA2^2 + resA3^2 + resA4^2 +
                                                         resA5^2 + resA6^2;
                                                  n_Newton_iter = n_Newton_iter + 1;
152
                                                  if (res > 1e+8)
154
                                                           error ("The Newton iteration fails to converge.");
                                                  end
156
                                         end
                                 end
158
                        end
159
               end
160
161
               res A1 = -(A1(2:Nx+1,2:Ny+1,2:Nz+1) - A1(1:Nx,2:Ny+1,2:Nz+1)) / dx +
162
                      sigma * ...
                        ((1/6)*(A1(2:Nx+1,2:Ny+1,2:Nz+1) + A2(2:Nx+1,2:Ny+1,2:Nz+1) + A3
163
                                (2:Nx+1,2:Ny+1,2:Nz+1) + A4(2:Nx+1,2:Ny+1,2:Nz+1)+A5(2:Nx+1,2:Nz+1)
                               Ny+1,2:Nz+1)+A6(2:Nx+1,2:Ny+1,2:Nz+1))-A1(2:Nx+1,2:Ny+1,2:Nz+1)
                               +1));
               res A2 = (A2(3:Nx+2,2:Ny+1,2:Nz+1) - A2(2:Nx+1,2:Ny+1,2:Nz+1)) / dx +
164
                      sigma * ...
                        ((1/6)*(A1(2:Nx+1,2:Ny+1,2:Nz+1) + A2(2:Nx+1,2:Ny+1,2:Nz+1) + A3
165
                                (2:Nx+1,2:Ny+1,2:Nz+1) + A4(2:Nx+1,2:Ny+1,2:Nz+1)+A5(2:Nx+1,2:Nz+1)
                               Ny+1,2:Nz+1)+A6(2:Nx+1,2:Ny+1,2:Nz+1))-A2(2:Nx+1,2:Ny+1,2:Nz+1)
                               +1));
               resA3 = -(A3(2:Nx+1,2:Ny+1,2:Nz+1) - A3(2:Nx+1,1:Ny,2:Nz+1)) / dy +
                      sigma * ...
                        ((1/6)*(A1(2:Nx+1,2:Ny+1,2:Nz+1) + A2(2:Nx+1,2:Ny+1,2:Nz+1) + A3
167
                                (2:Nx+1,2:Ny+1,2:Nz+1) + A4(2:Nx+1,2:Ny+1,2:Nz+1) + A5(2:Nx+1,2:Nz+1) + A5(2:Nx+1,2:
                               Ny+1,2:Nz+1)+A6(2:Nx+1,2:Ny+1,2:Nz+1))-A3(2:Nx+1,2:Ny+1,2:Nz+1)
                               +1));
```

```
res A4 = (A4(2:Nx+1,3:Ny+2,2:Nz+1) - A4(2:Nx+1,2:Ny+1,2:Nz+1)) / dy +
168
                        sigma * ...
                          ((1/6)*(A1(2:Nx+1,2:Ny+1,2:Nz+1) + A2(2:Nx+1,2:Ny+1,2:Nz+1) + A3
169
                                   (2:Nx+1,2:Ny+1,2:Nz+1) + A4(2:Nx+1,2:Ny+1,2:Nz+1) + A5(2:Nx+1,2:Nz+1) + A5(2:Nx+1,2:
                                 Ny+1,2:Nz+1)+A6(2:Nx+1,2:Ny+1,2:Nz+1))-A4(2:Nx+1,2:Ny+1,2:Nz+1)
                                 +1));
                res A5 = -(A5(2:Nx+1,2:Ny+1,2:Nz+1) - A5(2:Nx+1,2:Ny+1,1:Nz)) / dz +
170
                        sigma * ...
                          ((1/6)*(A1(2:Nx+1,2:Ny+1,2:Nz+1) + A2(2:Nx+1,2:Ny+1,2:Nz+1) + A3
171
                                  (2:Nx+1,2:Ny+1,2:Nz+1) + A4(2:Nx+1,2:Ny+1,2:Nz+1)+A5(2:Nx+1,2:Nz+1)
                                 Ny+1, 2:Nz+1)+A6(2:Nx+1, 2:Ny+1, 2:Nz+1))-A5(2:Nx+1, 2:Ny+1, 2:Nz+1)
                                 +1));
                res A6 = (A6(2:Nx+1,2:Ny+1,3:Nz+2) - A6(2:Nx+1,2:Ny+1,2:Nz+1)) / dz +
172
                        sigma * ...
                          ((1/6)*(A1(2:Nx+1,2:Ny+1,2:Nz+1) + A2(2:Nx+1,2:Ny+1,2:Nz+1) + A3
173
                                  (2:Nx+1,2:Ny+1,2:Nz+1) + A4(2:Nx+1,2:Ny+1,2:Nz+1)+A5(2:Nx+1,2:
                                 Ny+1\ ,2:Nz+1)+A6\left(\ 2:Nx+1\ ,2:Ny+1\ ,2:Nz+1\right))-A6\left(\ 2:Nx+1\ ,2:Ny+1\ ,2:Nz+1\right)
                                 +1));
                 res=norm(resA1, 'fro')^2 + norm(resA2, 'fro')^2 + norm(resA3, 'fro')
175
                         ^2 + \text{norm}(\text{resA4}, '\text{fro'})^2 + \text{norm}(\text{resA5}, '\text{fro'})^2 + \text{norm}(\text{resA6}, '
                         fro')^2;
176
177
                 x s lice = 0;
178
                 y s lice = 0;
                 z s lice = 0;
180
                 slice(X, Y, Z, A1(2:end-1, 2:end-1, 2:end-1) + A2(2:end-1, 2:end-1, 2:end-1) +
                        A3(2:end-1,2:end-1,2:end-1)+A4(2:end-1,2:end-1,2:end-1)+A5(2:end-1)
                         -1,2: end -1,2: end -1)+A6(2: end -1,2: end -1,2: end -1),...
                          xslice , yslice , zslice , 'nearest');
182
                 colorbar;
183
184
                pause (.1);
186
                 n_{iter} = n_{iter} + 1;
187
                 iter_arr = [iter_arr n_iter];
188
                 res_arr = [res_arr, res];
189
                 variableName=num2str(sigma);
190
                 display=['sigma=', variableName];
191
                %plot(iter_arr, res_arr, 'o-', 'LineWidth', 2, 'DisplayName', display);
                %xlabel('Number of iterations');
193
                %ylabel('Residual');
194
                %title('Convergence of the method');
195
                %grid on;
                %legend('show');
197
198
                 fprintf("Iter %d: Residual: %f, Averge number of Newton iterations: %
199
                         f\n", n_iter, res, n_Newton_iter/n_nonlin_eqs);
       end
200
       end
```

References

Zhenning Cai, MA5232 lecture slides
Zhenning Cai, MA5232 MATLAB codes for lectures