

1. PART A - NUMERICAL METHOD

The one dimensional steady state transport equation

$$U \frac{\partial \phi}{\partial x} = \frac{\partial}{\partial x} \left( \Gamma \frac{\partial \phi}{\partial x} \right) + Q$$

can be discretized with central differences as

$$U \frac{\phi_{i+1} - \phi_{i-1}}{2\Delta x} - \underbrace{\frac{\left( \Gamma \frac{\partial \phi}{\partial x} \right)_{i+1/2} - \left( \Gamma \frac{\partial \phi}{\partial x} \right)_{i-1/2}}{\Delta x}}_b = Q_i. \quad (1)$$

The first derivatives in the numerator of  $b$  can be written as

$$\left( \Gamma \frac{\partial \phi}{\partial x} \right)_{i+1/2} = \Gamma_{i+1/2} \frac{\phi_{i+1} - \phi_i}{\Delta x} \quad \text{and} \quad \left( \Gamma \frac{\partial \phi}{\partial x} \right)_{i-1/2} = \Gamma_{i-1/2} \frac{\phi_i - \phi_{i-1}}{\Delta x}. \quad (2)$$

Substituting eq. (2) into eq. (1) and rearranging gives

$$\begin{aligned} U \frac{\phi_{i+1} - \phi_{i-1}}{2\Delta x} - \frac{\Gamma_{i+1/2} \frac{\phi_{i+1} - \phi_i}{\Delta x} - \Gamma_{i-1/2} \frac{\phi_i - \phi_{i-1}}{\Delta x}}{\Delta x} &= Q_i \\ U \frac{\phi_{i+1} - \phi_{i-1}}{2\Delta x} - \frac{\Gamma_{i+1/2} \phi_{i+1} - (\Gamma_{i+1/2} + \Gamma_{i-1/2}) \phi_i + \Gamma_{i-1/2} \phi_{i-1}}{(\Delta x)^2} &= Q_i \\ \left( \frac{U}{2\Delta x} - \frac{\Gamma_{i+1/2}}{(\Delta x)^2} \right) \phi_{i+1} + \left( \frac{\Gamma_{i+1/2} + \Gamma_{i-1/2}}{(\Delta x)^2} \right) \phi_i - \left( \frac{U}{2\Delta x} + \frac{\Gamma_{i-1/2}}{(\Delta x)^2} \right) \phi_{i-1} &= Q_i. \end{aligned} \quad (3)$$

Equation (3) can be cast as the system of linear equations

$$\underbrace{\begin{bmatrix} 1 & & & \\ -\left( \frac{U}{2\Delta x} + \frac{\Gamma_{1/2}}{(\Delta x)^2} \right) & \frac{\Gamma_{3/2} + \Gamma_{1/2}}{(\Delta x)^2} & \frac{U}{2\Delta x} - \frac{\Gamma_{3/2}}{(\Delta x)^2} & \\ & \ddots & \ddots & \\ & & -\left( \frac{U}{2\Delta x} + \frac{\Gamma_{N-3/2}}{(\Delta x)^2} \right) & \frac{\Gamma_{N-1/2} + \Gamma_{N-3/2}}{(\Delta x)^2} & \frac{U}{2\Delta x} - \frac{\Gamma_{N-1/2}}{(\Delta x)^2} \\ & & & 1 \end{bmatrix}}_A \underbrace{\begin{pmatrix} \phi_0 \\ \phi_1 \\ \vdots \\ \phi_{N-1} \\ \phi_N \end{pmatrix}}_{\Phi} = \underbrace{\begin{pmatrix} 1 \\ Q_1 \\ \vdots \\ Q_{N-1} \\ 0 \end{pmatrix}}_b$$

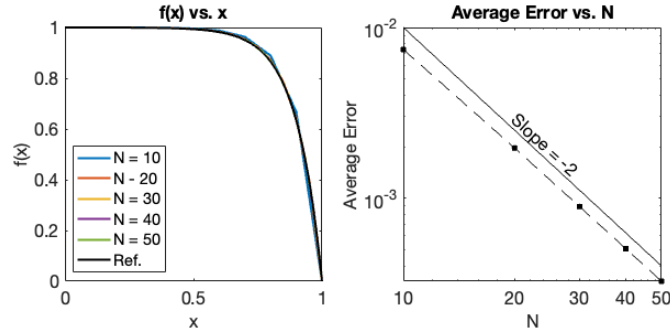
for a discretization at  $\{x_0, x_1, \dots, x_N\} = \{0, \Delta x, 2\Delta x, \dots, N\Delta x\}$ . The boundary conditions are given by  $\phi_{-1/2} = 1$  and  $\phi_{N+1/2} = 0$ .

For the cases in which  $U$ ,  $\Gamma$ , and  $Q$  are constant, the solution is found via the following steps:

- (1) Populate the matrix  $A$
- (2) Populate the vector  $b$
- (3) Solve  $A\Phi = b$  for the vector  $\Phi$  using TDMA

When  $U$ ,  $\Gamma$ , or  $Q$  depend on the value of  $\phi$  the problem becomes nonlinear and an iterative approach must be taken. For nonlinear problems, the solution is found via the following steps:

- (1) Make an initial guess for the vector  $\Phi^{(0)}$
- (2) Calculate  $U(\Phi^{(n)})$ ,  $\Gamma(\Phi^{(n)})$ , and  $Q(\Phi^{(n)})$
- (3) Populate the matrix  $A$
- (4) Populate the vector  $b$
- (5) Solve  $A\Phi^{(n+1)} = b$  for the vector  $\Phi^{(n+1)}$  using TDMA
- (6) Repeat steps 2 though 5 until convergence

FIGURE 1. Solution and average error for  $N = 10, 20, 30, 40, 50$ 

For this problem I will use a discretization of  $\phi(x) = 1 - x/L$  as an initial guess.

The tridiagonal matrix  $A$  is stored in an  $N + 1 \times 3$  to take advantage of its sparsity. The lower, center, and upper diagonal are stored in  $A_{1:N,0}$ ,  $A_{0:N,1}$ , and  $A_{0:N-1,2}$ . The tridiagonal linear solve using this data structure is given in algorithm 1.

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**Algorithm 1** Tridiagonal Matrix Algorithm
 

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Given:  $A$   $\triangleright N + 1 \times N + 1$   
 Given:  $x$   $\triangleright N + 1 \times 1$   
 Given:  $b$   $\triangleright N + 1 \times 1$

**for**  $i = 1 : N$  **do**  $\triangleright$  In place LU factorization  
      $w = A_{i,0}/A_{i-1,1}$   
      $A_{i,0} = A_{i,0} - wA_{i-1,1}$   
      $A_{i,1} = A_{i,0} - wA_{i-1,2}$   
      $A_{i,0} = w$   
**end for**

$y_0 = b_0$   $\triangleright$  Forward Substitution  
**for**  $i = 1 : N$  **do**  
      $y_i = b_i - A_{i,0}y_{i-1}$   
**end for**

$x_N = y_N/A_{N,1}$   $\triangleright$  Backward Substitution  
**for**  $i = N - 1 : -1 : 0$  **do**  
      $x_i = \frac{y_i - A_{i,2}x_{i+1}}{A_{i,1}}$   
**end for**

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## 2. PART B - LINEAR PROBLEMS

Figure 1 shows the solution, average error, and runtime for the case  $U = 1$ ,  $\Gamma = 0.1$ , and  $Q = 0$  with  $N = 10, 20, 30, 40, 50$ . The error decreases with increasing  $N$  as expected. The plot of average error versus  $N$  shows that the method is second-order-accurate. This is because the error decreases with a slope of two in loglog space. This order of accuracy is expected given that central differences were used to discretize the derivatives.

## 3. PART C - NON-LINEAR PROBLEMS