

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 , Γ , 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 Φ using TDMA

When U , Γ , or Q depend on the value of ϕ 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

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.

Algorithm 1 Tridiagonal Matrix Algorithm

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

2. PART B - LINEAR PROBLEMS

3. PART C - NON-LINEAR PROBLEMS