

## Derivation of a Numerical Method for solving a single linear parabolic PDE

### I. FORMULATION.

Linear parabolic partial differential equations are, in their most general form, given by:

$$d \frac{\partial T}{\partial t} = \nabla \cdot [c(\nabla T)] - aT - \underline{b} \cdot \nabla T + f \quad (\text{I.1})$$

where the functions,  $\underline{a}, \underline{b}, c, d, f$  are known functions of  $t, x, y, z$  and the temperature,  $T$ , is an unknown function of  $t, x, y, z$ . In order to approximate this creature using a finite difference scheme we recognize that

$$\nabla \cdot [c(\nabla T)] = c \nabla \cdot \nabla T + \nabla T \cdot \nabla c = c \nabla^2 T + \nabla T \cdot \nabla c = c \nabla^2 T + \nabla c \cdot \nabla T \quad (\text{I.2})$$

and rewrite this as:

$$d \frac{\partial T}{\partial t} = c \nabla^2 T + \nabla c \cdot \nabla T - aT - \underline{b} \cdot \nabla T + f \quad (\text{I.3})$$

$$d \frac{\partial T}{\partial t} = c \nabla^2 T - aT + (\nabla c - \underline{b}) \cdot \nabla T + f \quad (\text{I.4})$$

For purposes of brevity only, we will consider the case with variation only in one spatial dimension. The extension to three dimensions is straightforward. Our most general parabolic PDE becomes in one spatial dimension

$$d \frac{\partial T}{\partial t} = c \frac{\partial^2 T}{\partial x^2} - aT + \left( \frac{\partial c}{\partial x} - b_x \right) \frac{\partial T}{\partial x} + f \quad (\text{I.5})$$

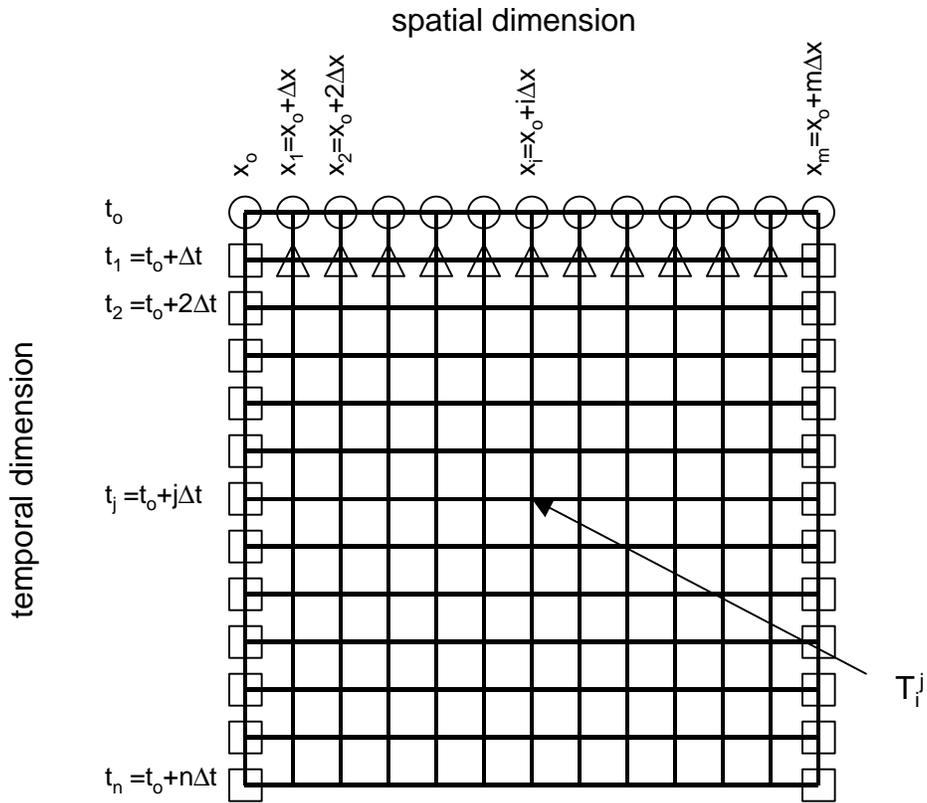
We now need to know the functional forms of  $\underline{a}, \underline{b}, c, d, f, \nabla c$ , which must be given. In many problems, most of these functions are constants and, often the constants are unity or zero. However, in order to write a code that solves any parabolic PDE, it is for this general formulation that we derive a finite-difference method.

Our plan is to divide our space dimensions each into  $m$  spatial increments, each of width  $\frac{L}{m}$ . If we are interested in observing the heat transfer from time  $t_0$  to  $t_f$ , then we can divide that time into  $n$  equal temporal increments, each of width  $\frac{t_f - t_0}{n}$ . See Figure One.

At the first step, you know all of the function values,  $T$ , at time= $t_0$ , because these are given by the initial condition. Let's first consider the case where we have 2 Dirichlet boundary conditions. In that case, we also know the values (temperatures, if we assume we are solving the heat equation) at the beginning and end of the rod for all time. Then what we next want is the temperatures for all interior nodes (all nodes but the 2 nodes with temperatures defined by the boundary conditions at the first time increment,  $t_1$ . If we can get  $T(t_1, \{x\})$  from  $T(t_0, \{x\})$  and  $T(t, x_0)$  and  $T(t, x_m)$ , then we have a formulation which will allow us to incrementally solve the P.D.E through time. Where we could then obtain  $T(t_2, \{x\})$  from  $T(t_1, \{x\})$  and  $T(t, x_0)$  and  $T(t, x_m)$ . In general we want to obtain  $T(t_{j+1}, \{x\})$  from  $T(t_j, \{x\})$  and  $T(t, x_0)$  and  $T(t, x_m)$ .

We will derive one such method, a method known as the Crank-Nicolson method.

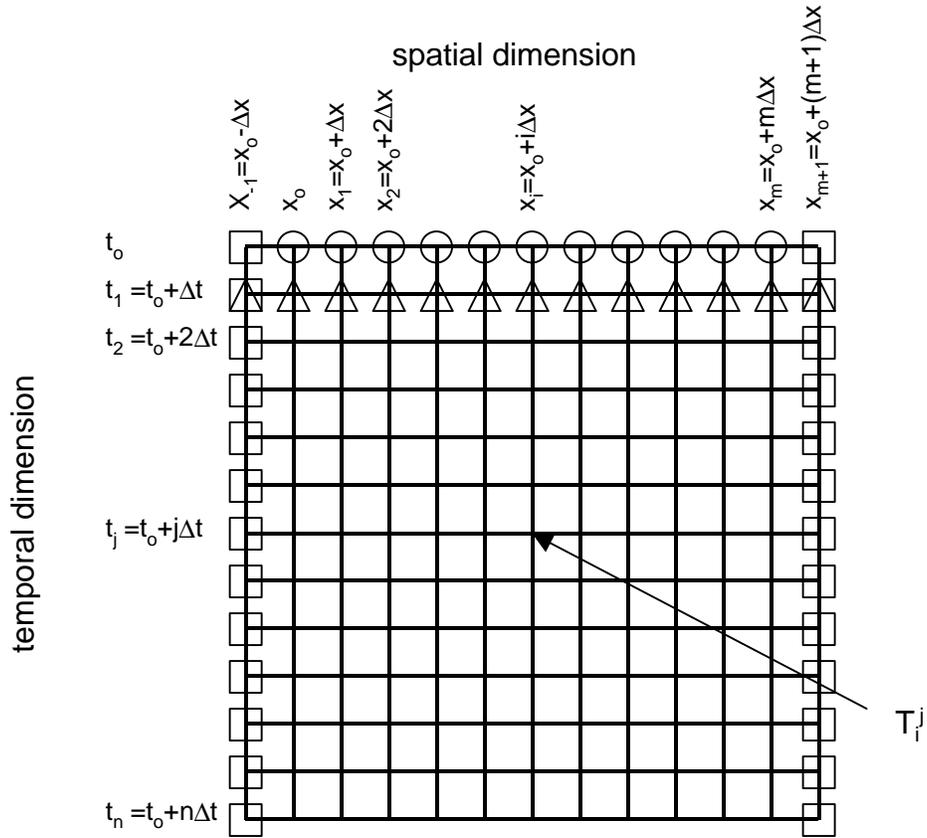
A comment on notation: we will write  $T(t_j, x_i)$  as  $T_i^j$  so that  
 $j$  superscripts designate temporal increments  
 $i$  subscripts designate spatial increments



legend

- node where temperature is known due to initial condition
- node where temperature is known due to boundary condition
- △ node where temperature is unknown but will be solved for

Figure One. Schematic of the spatial and temporal discretization. Case I. Two Dirichlet Boundary Conditions.



legend

- node where temperature is known due to initial condition
- imaginary node needed for Neumann boundary condition
- △ node where temperature is unknown but will be solved for

Figure Two. Schematic of the spatial and temporal discretization. Case II. Two Neumann Boundary Conditions.

## II. DISCRETIZATION.

Derivation of the Crank-Nicolson finite difference equations

### A. The Parabolic partial differential equation.

The Crank-Nicolson finite difference equations provide estimates that are second order in space and time. The Crank-Nicolson is an implicit method.

Let  $j$  superscripts designate temporal increments and let  $i$  subscripts designate spatial increments. For purposes of brevity only, we will consider the case with variation only in one spatial dimension. The extension to three dimensions is straightforward. Our most general parabolic PDE becomes in one spatial dimension

$$d \frac{\partial T}{\partial t} = c \frac{\partial^2 T}{\partial x^2} - aT + \left( \frac{\partial c}{\partial x} - b_x \right) \frac{\partial T}{\partial x} + f \quad (\text{II.1})$$

In order to get an approximation that is second order in time, we recast this equation as

$$\frac{\partial T}{\partial t} = \frac{1}{d} \left[ c \frac{\partial^2 T}{\partial x^2} - aT + \left( \frac{\partial c}{\partial x} - b_x \right) \frac{\partial T}{\partial x} + f \right] = K(x, t, T) \quad (\text{II.2})$$

Looking at it in this light, we can obtain a new estimate of the temperature, one increment ahead in time, namely

$$\left( \frac{\partial T}{\partial t} \right)_i \approx \frac{T_i^{j+1} - T_i^j}{t_{j+1} - t_j} = \frac{T_i^{j+1} - T_i^j}{\Delta t} \quad (\text{II.3})$$

This statement is true at any given point  $i$  in space. It is a can make a forward finite difference formula of the partial derivative with respect to time. Now what is also true by the second-order Runge-Kutta method is that:

$$\left( \frac{\partial T}{\partial t} \right)_i \approx \frac{1}{2} \left[ K(x_i, t_{j+1}, T_i^{j+1}) + K(x_i, t_{j+1}, T_i^j) \right] = \frac{1}{2} \left[ K_i^{j+1} + K_i^j \right] \quad (\text{II.4})$$

so that:

$$T_i^{j+1} = T_i^j + \frac{\Delta t}{2} \left[ K_i^{j+1} + K_i^j \right] \quad (\text{II.5})$$

This is the formula for the second order Runge-Kutta. Ordinarily, we wouldn't know the temperature needed to evaluate  $K_i^{j+1}$  (and we would be forced to approximate it) but we shall see that we can formulate the problem in a linear fashion so that we can implicitly solve the right and left-hand sides of this equation simultaneously, without further approximation.

To continue, we need to evaluate the right hand side of equation (II.4). For any given point  $j$  in time, we can make a finite approximation of the partial derivative with respect to space (centered finite difference formula).

$$\left(\frac{\partial T}{\partial x}\right)_i^j \approx \frac{T_{i+1}^j - T_{i-1}^j}{x_{i+1} - x_{i-1}} = \frac{T_{i+1}^j - T_{i-1}^j}{2\Delta x} \quad (\text{II.6})$$

Moreover, we can use that same formula, again to obtain the second derivative of the temperature with respect to space. (Forward finite difference formula for first derivative with backward finite difference formula for second derivative gives centered finite difference formula.)

$$\left(\frac{\partial^2 T}{\partial x^2}\right)_i^j \approx \frac{\left(\frac{\partial T}{\partial x}\right)_{i+1}^j - \left(\frac{\partial T}{\partial x}\right)_i^j}{x_{i+1} - x_i} = \frac{\left(\frac{\partial T}{\partial x}\right)_{i+1}^j - \left(\frac{\partial T}{\partial x}\right)_i^j}{\Delta x} \quad (\text{II.7})$$

We can substitute our formula for the first spatial derivative into that for the second spatial derivative.

$$\left(\frac{\partial^2 T}{\partial x^2}\right)_i^j \approx \frac{\left(\frac{T_{i+1}^j - T_i^j}{\Delta x}\right) - \left(\frac{T_i^j - T_{i-1}^j}{\Delta x}\right)}{\Delta x} = \frac{T_{i+1}^j - 2T_i^j + T_{i-1}^j}{\Delta x^2} \quad (\text{II.8})$$

This gives the second spatial derivative at time  $j$ . We can then obtain the two functions,  $K_i^{j+1}$  and  $K_i^j$  which we require to obtain the temperatures at the new time.

$$K_i^j = \frac{1}{d_i^j} \left[ c_i^j \left( \frac{T_{i+1}^j - 2T_i^j + T_{i-1}^j}{\Delta x^2} \right) - a_i^j T_i^j + \left( \left( \frac{\partial c}{\partial x} \right)_i^j - b_{x_i}^j \right) \left( \frac{T_{i+1}^j - T_{i-1}^j}{2\Delta x} \right) + f_i^j \right] \quad (\text{II.9})$$

$$K_i^{j+1} = \frac{1}{d_i^{j+1}} \left[ c_i^{j+1} \left( \frac{T_{i+1}^{j+1} - 2T_i^{j+1} + T_{i-1}^{j+1}}{\Delta x^2} \right) - a_i^{j+1} T_i^{j+1} + \left( \left( \frac{\partial c}{\partial x} \right)_i^{j+1} - b_{x_i}^{j+1} \right) \left( \frac{T_{i+1}^{j+1} - T_{i-1}^{j+1}}{2\Delta x} \right) + f_i^{j+1} \right] \quad (\text{II.10})$$

Define

$$A = \frac{\Delta t a}{2d}, \quad B = \frac{\Delta t}{4d\Delta x} \left( \frac{\partial c}{\partial x} - b_x \right), \quad C = \frac{\Delta t}{2d\Delta x^2} c, \quad D = 1, \quad \text{and} \quad F = \frac{\Delta t f}{2d}$$

so that we can rewrite equations (II.9) and (II.10) as

$$K_i^j = \frac{2}{\Delta t} \left[ C_i^j (T_{i+1}^j - 2T_i^j + T_{i-1}^j) - A_i^j T_i^j + B_i^j (T_{i+1}^j - T_{i-1}^j) + F_i^j \right] \quad (\text{II.9b})$$

$$K_i^{j+1} = \frac{2}{\Delta t} \left[ C_i^{j+1} (T_{i+1}^{j+1} - 2T_i^{j+1} + T_{i-1}^{j+1}) - A_i^{j+1} T_i^{j+1} + B_i^j (T_{i+1}^{j+1} - T_{i-1}^{j+1}) + F_i^{j+1} \right] \quad (\text{II.10b})$$

Group like temperatures in equations (II.9b) and (II.10b)

$$K_i^j = \frac{2}{\Delta t} \left[ (C_i^j - B_i^j) T_{i-1}^j + (-2C_i^j - A_i^j) T_i^j + (C_i^j + B_i^j) T_{i+1}^j + F_i^j \right] \quad (\text{II.9c})$$

$$K_i^{j+1} = \frac{2}{\Delta t} \left[ (C_i^{j+1} - B_i^{j+1}) T_{i-1}^{j+1} + (-2C_i^{j+1} - A_i^{j+1}) T_i^{j+1} + (C_i^{j+1} + B_i^{j+1}) T_{i+1}^{j+1} + F_i^{j+1} \right] \quad (\text{II.10c})$$

Substitute equations (II.9c) and (II.10c) into (II.5) to obtain

$$T_i^{j+1} = T_i^j + \left[ \begin{array}{l} (C_i^j - B_i^j) T_{i-1}^j + (-2C_i^j - A_i^j) T_i^j + (C_i^j + B_i^j) T_{i+1}^j + F_i^j + \\ (C_i^{j+1} - B_i^{j+1}) T_{i-1}^{j+1} + (-2C_i^{j+1} - A_i^{j+1}) T_i^{j+1} + (C_i^{j+1} + B_i^{j+1}) T_{i+1}^{j+1} + F_i^{j+1} \end{array} \right] \quad (\text{II.11})$$

Group like temperatures, placing all unknown temperatures (at time  $j+1$ ) on the right-hand side and all known temperatures (at time  $j$ ) on the left-hand side.

$$\begin{aligned}
& -\left(C_i^{j+1} - B_i^{j+1}\right) T_{i-1}^{j+1} + \left(1 + 2C_i^{j+1} + A_i^{j+1}\right) T_i^{j+1} - \left(C_i^{j+1} + B_i^{j+1}\right) T_{i+1}^{j+1} \\
& = \left(C_i^j - B_i^j\right) T_{i-1}^j + \left(1 - 2C_i^j - A_i^j\right) T_i^j + \left(C_i^j + B_i^j\right) T_{i+1}^j + F_i^j + F_i^{j+1}
\end{aligned} \tag{II.12}$$

If we define  $J_{\text{diag}} = (1 + 2C + A)$ ,  $J_{\text{hi}} = -(C + B)$ ,  $J_{\text{lo}} = -(C - B)$  and  $R_{\text{diag}} = (1 - 2C - A)$  then we can rewrite equation (II.12) as

$$J_{\text{lo},i}^{j+1} T_{i-1}^{j+1} + J_{\text{diag},i}^{j+1} T_i^{j+1} + J_{\text{hi},i}^{j+1} T_{i+1}^{j+1} = -J_{\text{lo},i}^j T_{i-1}^j + R_{\text{diag},i}^j T_i^j - J_{\text{hi},i}^j T_{i+1}^j + F_i^j + F_i^{j+1} \tag{II.13}$$

These equations hold for all interior nodes. We will deal with nodes affected by the boundary conditions shortly. When we have Dirichlet boundary conditions, an interior node is any node except those at the boundary. When we have Neumann boundary conditions, we are forced to add an imaginary node on each side of the system. Thus an interior node is any node except those two imaginary nodes (but including the nodes that would be the boundary if we had Dirichlet boundary conditions).

This format is linear in unknowns,  $\left\{ T^{j+1} \right\}$ . We should take careful notice of this

equation. (1) All our unknown temperatures (the temperatures at time  $j+1$  are on the left hand side of the equation). (2) Moreover, they appear in a linear fashion on the LHS. (3) All the variables on the RHS are known quantities. Clearly this is going to give us a system of linear, algebraic equations. We solve this system of equations using the rules of linear algebra. In fact, we can write the above equation as:

$$\underline{J} \underline{T}^{j+1} = \underline{R} \tag{II.14}$$

This is a system of equations of the standard form:

$$\underline{A} \underline{x} = \underline{b} \tag{II.15}$$

with a solution

$$\underline{T}^{j+1} = \underline{J}^{-1} \underline{R} \tag{II.16}$$

so long as the determinant of the  $J$  matrix is non-zero. We will call the matrix on the left-hand side of equation (II.14) the Jacobian and we will call the vector on the right-hand side of equation (II.14) the residual.

Size of the matrix:

If there are  $m$  spatial intervals, there are  $m+1$  spatial nodes, numbered by the variable  $i$  from 0 to  $m$ . For 2 Dirichlet boundary conditions, if there are  $m$  spatial nodes, then there are  $m-1$  interior nodes, thus there are  $m-1$  unknown temperatures. The  $\underline{\underline{J}}$  matrix is a matrix of dimension  $m-1$  by  $m-1$ , with an index  $k$  bounded by  $1 \leq k \leq m-1$  corresponding to spatial nodes  $1 \leq i \leq m-1$ .

For 2 Neumann boundary conditions, there are  $m+3$  spatial nodes. (This is because for Neumann boundary conditions, we create imaginary nodes at each end, in order to satisfy the boundary condition fluxes. See Figure Two. The additional nodes take  $i$  values of  $-1$  and  $m+1$ .) The temperature at all of these nodes are unknown. Thus there are  $m+3$  unknown temperatures. The  $\underline{\underline{J}}$  matrix is a matrix of dimension  $m+3$  by  $m+3$ , with an index  $k$  bounded by  $1 \leq k \leq m+3$  corresponding to spatial nodes  $-1 \leq i \leq m+1$ .

For 1 Dirichlet, and 1 Neumann BC, there are  $m+2$  spatial nodes, numbered by the variable  $i$  from 0 to  $m+1$ , if the Dirichlet node is at 0, numbered by the variable  $i$  from  $-1$  to  $m$ , if the Dirichlet node is at  $m$ . The temperature at all but one of these nodes (the Dirichlet node) are unknown. Thus there are  $m+1$  unknown temperatures. The  $\underline{\underline{J}}$  matrix is a matrix of dimension  $m+1$  by  $m+1$ , with an index  $k$  bounded by  $1 \leq k \leq m+1$  corresponding to spatial nodes  $0 \leq i \leq m+1$  or  $-1 \leq i \leq m$ .

The right hand side of the above equation is the residual. The left hand side is a tridiagonal matrix.

Below we consider the explicit forms of the Jacobian and residual.

### B. Dirichlet boundary conditions.

We will consider our Dirichlet Boundary conditions in their most general form as

$$T = h \quad (\text{II.17})$$

where  $h$  is a known functions of  $t, x$  in one spatial dimension and  $t, x, y, z$  in three dimensions. In terms of an unknown temperature at a discretized node, we have:

$$T_i^{j+1} = h_i^{j+1} = h(x_i, t_{j+1}) \quad (\text{II.18})$$

This equation will be used at the boundary nodes. This is in the same linear form as the finite-difference equations for the P.D.E., which is what we need since, ultimately, we need to solve them simultaneously.

### C. Neumann boundary conditions.

We will consider our Neumann Boundary conditions in their most general form as

$$p \frac{\partial T}{\partial x} = -qT + g \quad (\text{II.19})$$

where  $\mathbf{p}, \mathbf{q}, \mathbf{g}$  are known functions of  $\mathbf{t}, \mathbf{x}$  in one spatial dimension and  $\mathbf{t}, \mathbf{x}, \mathbf{y}, \mathbf{z}$  in three dimensions. We already have a formula for the first spatial derivative, namely

$$\left( \frac{\partial T}{\partial x} \right)_i^j \approx \frac{T_{i+1}^j - T_{i-1}^j}{x_{i+1} - x_{i-1}} = \frac{T_{i+1}^j - T_{i-1}^j}{2\Delta x} \quad (\text{II.6})$$

so our Neumann boundary condition becomes at time  $j+1$

$$p_i^{j+1} \left( \frac{T_{i+1}^{j+1} - T_{i-1}^{j+1}}{2\Delta x} \right) = -q_i^{j+1} T_i^{j+1} + g_i^{j+1} \quad (\text{II.20})$$

We define  $\mathbf{P} = \left( \frac{\mathbf{p}}{2\Delta x} \right)$  and obtain

$$P_i^{j+1} \left( T_{i+1}^{j+1} - T_{i-1}^{j+1} \right) = -q_i^{j+1} T_i^j + g_i^{j+1} \quad (\text{II.21})$$

We perform the same rearrangement as we did on the PDE, putting all unknown temperatures at time  $j+1$  on the left-hand side and all other temperatures on the right-hand side.

$$-P_i^{j+1} T_{i-1}^{j+1} + q_i^{j+1} T_i^j + P_i^{j+1} T_{i+1}^{j+1} = g_i^{j+1} \quad (\text{II.22})$$

This equation will be used for the imaginary spatial nodes created to handle Neumann boundary conditions. This is in the same linear form as the finite-difference equations for the P.D.E., which is what we need since, ultimately, we need to solve them simultaneously.

### III. JACOBIANS AND RESIDUALS.

#### A. Dirichlet boundary conditions

1. Calculate Jacobian ( $k$  is the index inside the Jacobian matrix)

a. First exterior node ( $i=0$ )

Not included in the Jacobian because this is not an unknown.

The temperature here is given by the boundary condition.

b. Last exterior node ( $i=m$ )

Not included in the Jacobian because this is not an unknown.

The temperature here is given by the boundary condition.

c. First interior node ( $i=1$ ) ( $k=1$ )

$$J(1,1) = J_{\text{diag},1}^{j+1}$$

$$J(1,2) = J_{hi,1}^{j+1}$$

d. Last interior node ( $i=m-1$ ) ( $k=m-1$ )

$$J(m-1, m-2) = J_{lo, m-1}^{j+1}$$

$$J(m-1, m-1) = J_{diag, m-1}^{j+1}$$

e. All other nodes ( $1 < i < m-1$ ) ( $1 < k < m-1$ )

$$J(k, k-1) = J_{lo, i}^{j+1}$$

$$J(k, k) = J_{diag, i}^{j+1}$$

$$J(k, k+1) = J_{hi, j}^{j+1}$$

so that the Jacobian looks like:

$$J = \begin{bmatrix} J_{diag_1}^{j+1} & J_{hi_1}^{j+1} & 0 & 0 & 0 & 0 \\ J_{lo_2}^{j+1} & J_{diag_2}^{j+1} & J_{hi_2}^{j+1} & 0 & 0 & 0 \\ 0 & J_{lo_i}^{j+1} & J_{diag_i}^{j+1} & J_{hi_i}^{j+1} & 0 & 0 \\ 0 & 0 & J_{lo_i}^{j+1} & J_{diag_i}^{j+1} & J_{hi_i}^{j+1} & 0 \\ 0 & 0 & 0 & J_{lo, m-2}^{j+1} & J_{diag_{m-2}}^{j+1} & J_{hi, m-2}^{j+1} \\ 0 & 0 & 0 & 0 & J_{lo, m-1}^{j+1} & J_{diag_{m-1}}^{j+1} \end{bmatrix}$$

This is a tri-diagonal matrix of known functions of time and space.

#### A. Dirichlet boundary conditions

##### 2. Calculate Residual

a. First exterior node ( $i=0$ )

Not included in the Jacobian because this is not an unknown.

The temperature here is given by the boundary condition.

b. Last exterior node ( $i=m$ )

Not included in the Jacobian because this is not an unknown.

The temperature here is given by the boundary condition.

c. First interior node ( $i=1$ ) ( $k=1$ )

$$R(1) = -J_{lo, 1}^j T_0^j + R_{diag, 1}^j T_1^j - J_{hi, 1}^j T_2^j + F_1^j + F_1^{j+1} - J_{lo, 1}^{j+1} T_0^{j+1}$$

d. Last interior node ( $i=m-1$ ) ( $k=m-1$ )

$$R(m-1) = -J_{lo, m-1}^j T_{m-2}^j + R_{diag, m-1}^j T_{m-1}^j - J_{hi, m-1}^j T_m^j + F_{m-1}^j + F_{m-1}^{j+1} - J_{hi, m-1}^{j+1} T_m^{j+1}$$

e. All other nodes ( $1 < i < m-1$ ) ( $1 < k < m-1$ )

$$R(k) = -J_{lo, i}^j T_{i-1}^j + R_{diag, i}^j T_i^j - J_{hi, i}^j T_{i+1}^j + F_i^j + F_i^{j+1}$$

so that the Residual looks like:

$$\underline{R} = \begin{bmatrix} -J_{lo,1}^j T_0^j + R_{diag,1}^j T_1^j - J_{hi,1}^j T_2^j + F_1^j + F_1^{j+1} - J_{lo,1}^{j+1} T_0^{j+1} \\ -J_{lo,i}^j T_{i-1}^j + R_{diag,i}^j T_i^j - J_{hi,i}^j T_{i+1}^j + F_i^j + F_i^{j+1} \\ \dots \\ -J_{lo,i}^j T_{i-1}^j + R_{diag,i}^j T_i^j - J_{hi,i}^j T_{i+1}^j + F_i^j + F_i^{j+1} \\ -J_{lo,m-1}^j T_{m-2}^j + R_{diag,m-1}^j T_{m-1}^j - J_{hi,m-1}^j T_m^j + F_{m-1}^j + F_{m-1}^{j+1} - J_{hi,m-1}^{j+1} T_m^{j+1} \end{bmatrix}$$

This is a vector of known quantities.

### B. Neumann boundary conditions

1. Calculate Jacobian (k is the index inside the Jacobian matrix)

a. First exterior node (now an imaginary node) ( $i=-1$ ) ( $k=1$ )

$$J(1,1) = -P_0^{j+1}$$

$$J(1,2) = q_0^{j+1}$$

$$J(1,3) = P_0^{j+1}$$

b. Last exterior node (now an imaginary node) ( $i=m+1$ ) ( $k=m+3$ )

$$J(m+3,m+1) = -P_m^{j+1}$$

$$J(m+3,m+2) = q_m^{j+1}$$

$$J(m+3,m+3) = P_m^{j+1}$$

c. All other nodes ( $-1 < i < m+1$ ) ( $1 < k < m+3$ )

$$J(k,k-1) = J_{lo,i}^{j+1}$$

$$J(k,k) = J_{diag,i}^{j+1}$$

$$J(k,k+1) = J_{hi,i}^{j+1}$$

The Jacobian looks like:

$$\underline{\underline{J}} = \begin{bmatrix} -P_0^{j+1} & q_0^{j+1} & P_0^{j+1} & 0 & 0 & 0 \\ J_{lo0}^{j+1} & J_{diag_0}^{j+1} & J_{hi0}^{j+1} & 0 & 0 & 0 \\ 0 & J_{lo1}^{j+1} & J_{diag_1}^{j+1} & J_{hi1}^{j+1} & 0 & 0 \\ 0 & 0 & J_{lo_{m-1}}^{j+1} & J_{diag_{m-1}}^{j+1} & J_{hi_{m-1}}^{j+1} & 0 \\ 0 & 0 & 0 & J_{lo_m}^{j+1} & J_{diag_m}^{j+1} & J_{hi_m}^{j+1} \\ 0 & 0 & 0 & -P_m^{j+1} & q_m^{j+1} & P_m^{j+1} \end{bmatrix}$$

### B. Neumann boundary conditions

#### 2. Calculate Residual

- a. First exterior node ( $i=-1$ ) ( $k=1$ )

$$R(1) = g_0^{j+1}$$

- b. Last interior node ( $i=m+1$ ) ( $k=m+3$ )

$$R(m+3) = g_m^{j+1}$$

- c. All other nodes ( $-1 < i < m+1$ ) ( $1 < k < m+3$ )

$$R(k) = -J_{lo,i}^j T_{i-1}^j + R_{diag,i}^j T_i^j - J_{hi,i}^j T_{i+1}^j + F_i^j + F_i^{j+1}$$

so that the Residual looks like:

$$\underline{\underline{R}} = \begin{bmatrix} g_0^{j+1} \\ -J_{lo,0}^j T_{-1}^j + R_{diag,0}^j T_0^j - J_{hi,0}^j T_1^j + F_0^j + F_0^{j+1} \\ \cdot - J_{lo,i}^j T_{i-1}^j + R_{diag,i}^j T_i^j - J_{hi,i}^j T_{i+1}^j + F_i^j + F_i^{j+1} \cdot \\ -J_{lo,m}^j T_{m-1}^j + R_{diag,m}^j T_m^j - J_{hi,m}^j T_{m+1}^j + F_m^j + F_m^{j+1} \\ g_m^{j+1} \end{bmatrix}$$

This is a vector of known quantities.

### IV. SOLUTION.

With the Jacobian and Residual, we solve for the temperatures at the next time,  $j+1$ :

$$\underline{\underline{T}}^{j+1} = \underline{\underline{J}}^{-1} \underline{\underline{R}}$$

We can then repeat the calculation of the Jacobian and the residual and solve for the temperatures at time,  $j+2$ , and so on.