Numerical Methods for a solution to the Heat Equation: Finite Differences

Consider the 1-D heat equation.

$$\frac{\partial T}{\partial t} = \alpha\left(\frac{\partial^2 T}{\partial x^2}\right) + \frac{f(t,x)}{\rho\hat{C}_p} - \frac{a(t,x)}{\rho\hat{C}_p}T$$

$$\frac{\partial T}{\partial t} = \alpha\left(\frac{\partial^2 T}{\partial x^2}\right) + F(t,x) - A(t,x)T$$

Our plan is to divide our 1-D space into m spatial increments, each of width $\frac{L}{m}$. If we are interested in observing the heat transfer from time t_o to t_f, then we can divide that time into n equal temporal increments, each of width $\frac{t_f - t_o}{n}$. See Figure One.

At the first step, you know all of the temperatures at time= t_o, 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 temperatures 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 $T(t_o,\{x\})$ and $T(t,x_o)$ 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 $T(t,x_o)$ and $T(t,x_m)$. In general we want to obtain $T(t_{j+1},\{x\})$ from $T(t_j,\{x\})$ and $T(t,x_o)$ 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

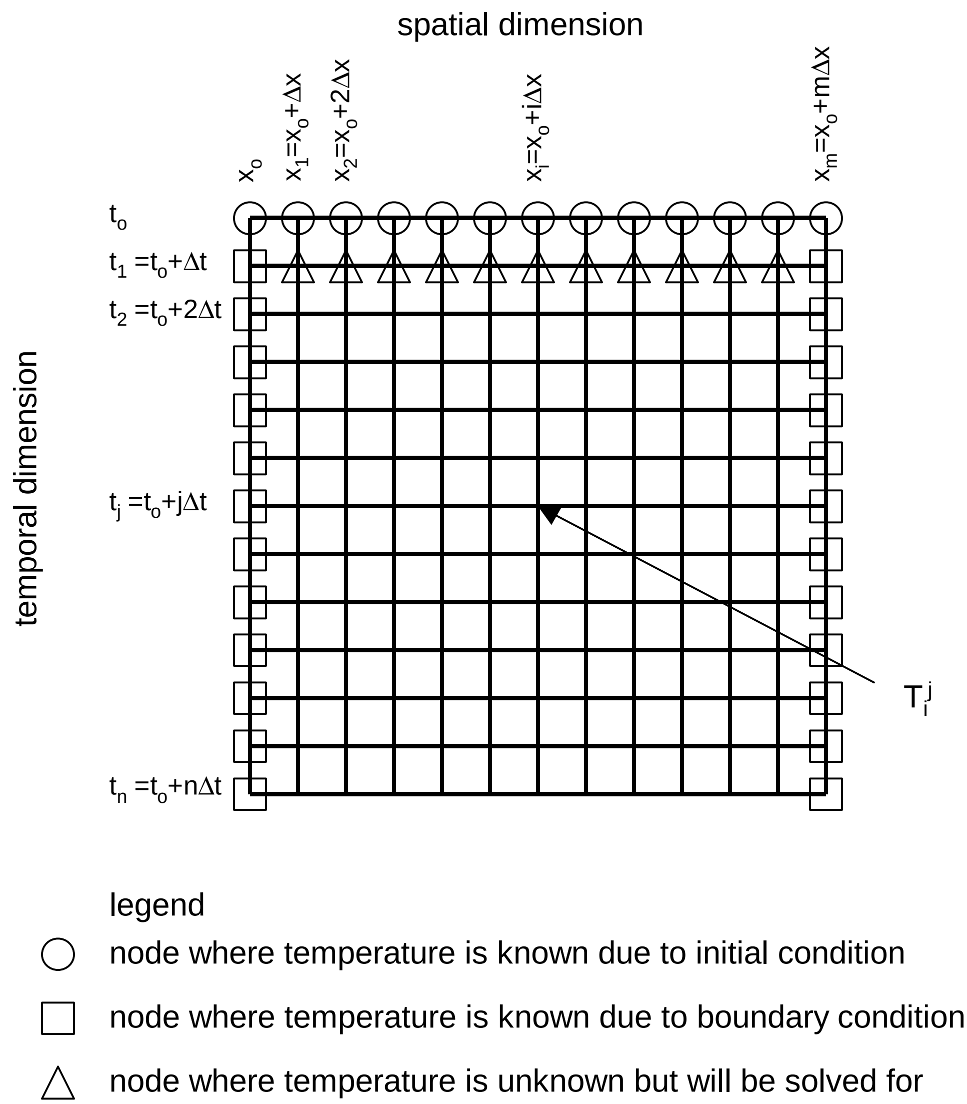

Figure One. Schematic of the spatial and temporal discretization. Case I. Two Dirichlet Boundary Conditions.

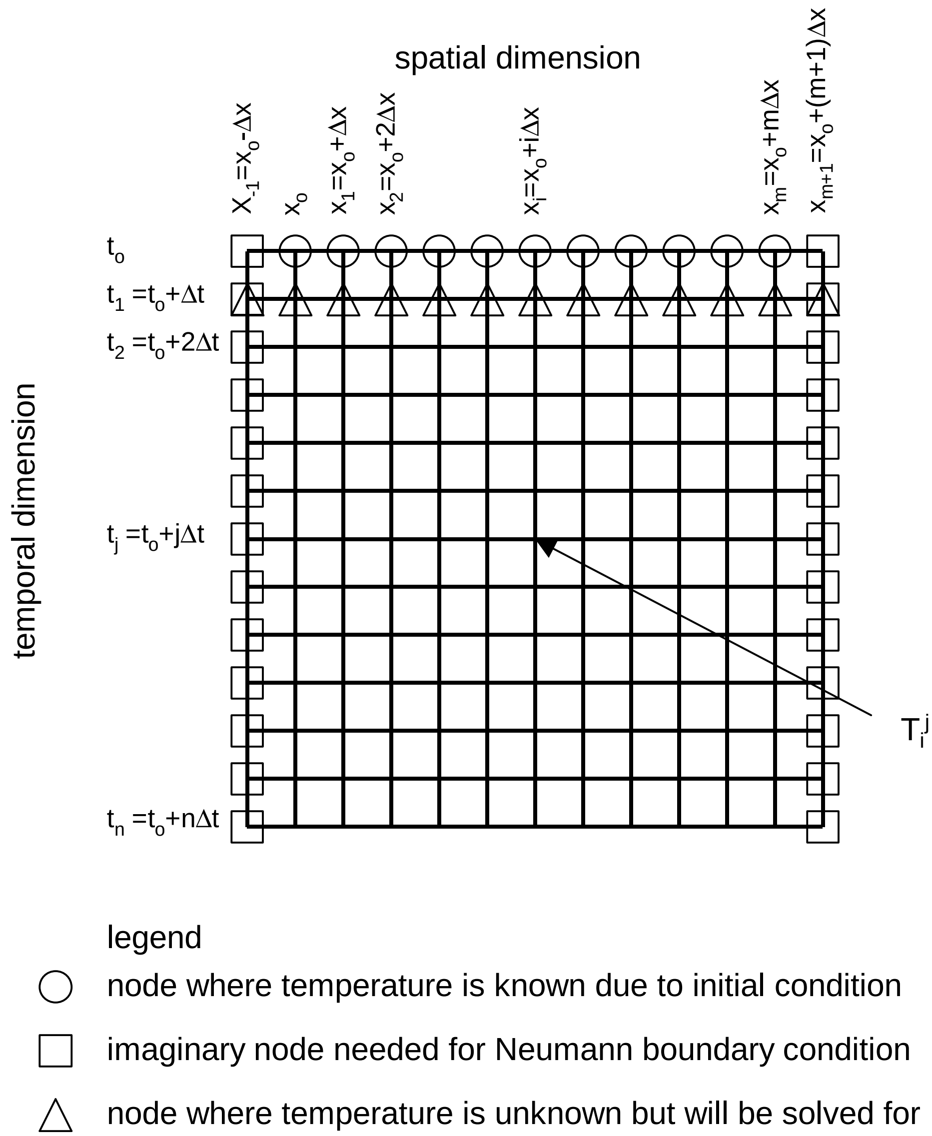

Figure Two. Schematic of the spatial and temporal discretization. Case II. Two Neumann Boundary Conditions.

Derivation of the Crank-Nicolson Equations

For any given point i in space, we can make a finite approximation of the partial derivative with respect to time.

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

Similarly, for any given point j in time, we can make a finite approximation of the partial derivative with respect to space.

$$\left(\frac{\partial T}{\partial x}\right)^j \approx \frac{T_{i+1}^j - T_i^j}{x_{i+1} - x_i} = \frac{T_{i+1}^j - T_i^j}{\Delta x}$$

Moreover, we can use that same formula, again to obtain the second derivative with respect to space.

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

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

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

This gives the second spatial derivative at time j. But our goal is to find the temperature profile at time j+1. In order to estimate the temperature at time j+1 from the temperature at time j, we ought to use a second derivative that is an average over the second spatial derivatives at both times:

$$\frac{\partial^2 T}{\partial x^2} \approx \frac{1}{2}\left[\left(\frac{\partial^2 T}{\partial x^2}\right)^j + \left(\frac{\partial^2 T}{\partial x^2}\right)^{j+1}\right]$$

$$\frac{\partial^2 T}{\partial x^2} \approx \frac{1}{2}\left[\frac{T_{i+1}^{j} - 2T_{i}^{j} + T_{i-1}^{j}}{\Delta x^2} + \frac{T_{i+1}^{j+1} - 2T_{i}^{j+1} + T_{i-1}^{j+1}}{\Delta x^2}\right]$$

So now we have an estimate for the second spatial derivative as a function of the temperatures at time j and j+1.

Lastly, we need an approximation for the temperature itself. The temperature at point i used for the calculation of the temperature at the same point but ahead one step in time is the average of the temperatures at both times.

$$T_i \approx \frac{1}{2}\left[T_i^j + T_i^{j+1}\right]$$

We can substitute into our 1-D heat equation, the approximations for the time partial, space partial, and temperature to obtain:

$$\frac{T_i^{j+1} - T_i^j}{\Delta t} = \alpha\left(\frac{1}{2}\left[\frac{T_{i+1}^{j} - 2T_{i}^{j} + T_{i-1}^{j}}{\Delta x^2} + \frac{T_{i+1}^{j+1} - 2T_{i}^{j+1} + T_{i-1}^{j+1}}{\Delta x^2}\right]\right) + F - A\frac{1}{2}\left[T_i^j + T_i^{j+1}\right]$$

Multiply through by $2\Delta t$:

$$2T_i^{j+1} - 2T_i^j = \frac{\alpha\Delta t}{\Delta x^2}\left(T_{i+1}^{j} - 2T_{i}^{j} + T_{i-1}^{j} + T_{i+1}^{j+1} - 2T_{i}^{j+1} + T_{i-1}^{j+1}\right) + 2\Delta t F - A\Delta t\left[T_i^j + T_i^{j+1}\right]$$

Now define $\lambda = \alpha\frac{\Delta t}{\Delta x^2}$

Rearrange, grouping like terms

$$-\lambda T_{i-1}^{j+1} + (2 + 2\lambda + A\Delta t)T_i^{j+1} - \lambda T_{i+1}^{j+1} = \lambda T_{i-1}^{j} + (2 - 2\lambda - A\Delta t)T_i^{j} + \lambda T_{i+1}^{j} + 2\Delta t F$$

We could write this equation for every interior node. (We don’t need to write it for exterior nodes because we already know the temperatures there from the Dirichlet boundary conditions.)

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. How do we solve that? Using linear algebra. In fact, we can write the above equation as:

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

This is a system of equations of the standard form:

$$\underline{\underline{A}}\,\underline{x} = \underline{b}$$

with a solution

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

so long as the determinant of the J matrix is non-zero.

Size of the matrix:

If there are m spatial intervals, there are m+1 spatial nodes. For 2 Dirichlet boundary conditions, if there are m spatial nodes, then there are m=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.

For 2 Neumann boundary conditions, there are m=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 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.

For 1 Dirichlet, and 1 Neumann BC, there are m=m+2 spatial nodes. The temperature at all but one of these nodes are unknown. Thus there are m+1 unknown temperatures. The $\underline{\underline{J}}$ matrix is a matrix of dimension m+1 by m+1.

The right hands 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.

I. For Dirichlet Boundary Conditions (with m interior nodes, and 2 exterior nodes)

A. Calculate Jacobian

1. First exterior node, node 1
   Not included in the Jacobian because this is not an unknown.
   The temperature here is given by the boundary condition.
2. Last exterior node, node m+1
   Not included in the Jacobian because this is not an unknown.
   The temperature here is given by the boundary condition.
3. First interior node, node 2 but unknown 1
   $$J(1,1) = (2 + 2\lambda + A\Delta t)$$
   $$J(1,2) = -\lambda$$
4. Last interior node, node m but unknown m-1
   $$J(1, m-2) = -\lambda$$
   $$J(1, m-1) = (2 + 2\lambda + A\Delta t)$$
5. All other nodes i

$$J(1,i-1) = -\lambda$$
$$J(1,i) = (2 + 2\lambda + A\Delta t)$$
$$J(1,i+1) = -\lambda$$

Let $J_{diag} = (2 + 2\lambda + A\Delta t)$
so that the Jacobian looks like:

$$\underline{\underline{J}} = \begin{bmatrix} J_{diag} & -\lambda & 0 & 0 & 0 & 0 \\ -\lambda & J_{diag} & -\lambda & 0 & 0 & 0 \\ 0 & -\lambda & J_{diag} & -\lambda & 0 & 0 \\ 0 & 0 & -\lambda & J_{diag} & -\lambda & 0 \\ 0 & 0 & 0 & -\lambda & J_{diag} & -\lambda \\ 0 & 0 & 0 & 0 & -\lambda & J_{diag} \end{bmatrix}$$

This is a matrix of known quantities. It is a constant matrix unless A is a function of time.

B. Calculate Residual
1. First exterior node, node 1
   Not included in the Jacobian because this is not an unknown.
   The temperature here is given by the boundary condition.
2. Last exterior node, node m+1
   Not included in the Jacobian because this is not an unknown.
   The temperature here is given by the boundary condition.
3. First interior node, node i=2 but unknown 1
$$R(1) = \lambda T_1^j + (2 - 2\lambda - A\Delta t)T_2^j + \lambda T_3^j + 2\Delta tF + \lambda T_1^{j+1}$$
4. Last interior node, node i=m but unknown m-1
$$R(m-1) = \lambda T_{m-1}^j + (2 - 2\lambda - A\Delta t)T_m^j + \lambda T_{m+1}^j + 2\Delta tF + \lambda T_{m+1}^{j+1}$$
5. All other nodes
$$R(i) = \lambda T_{i-1}^j + (2 - 2\lambda - A\Delta t)T_i^j + \lambda T_{i+1}^j + 2\Delta tF$$

Let $R_{diag} = (2 - 2\lambda - A\Delta t)$
so that the Residual looks like:

$$\underline{R} = \begin{bmatrix} \lambda T_1^j + R_{diag} T_2^j + \lambda T_3^j + 2\Delta t F + \lambda T_1^{j+1} \\ \lambda T_{i-1}^j + R_{diag} T_i^j + \lambda T_{i+1}^j + 2\Delta t F \\ \ldots \\ \lambda T_{i-1}^j + R_{diag} T_i^j + \lambda T_{i+1}^j + 2\Delta t F \\ \lambda T_{m-1}^j + R_{diag} T_m^j + \lambda T_{m+1}^j + 2\Delta t F + \lambda T_{m+1}^{j+1} \end{bmatrix}$$

This is a vector of known quantities.

II. For Pure Neumann Boundary Conditions (with m intervals, m+3 nodes, m+3 unknowns)

A pure Neumann Boundary condition is a boundary condition of the form:

$$\frac{dT}{dx}(x = 0, t) = g(t) \neq g(T)$$

where the boundary condition can be a function of time but is not a function of temperature.

The approximation we make for this first spatial derivative is that

$$\left[\frac{dT}{dx}(x = 0, t)\right]^{j+1} = g(t_{j+1}) = \frac{T_{i+1}^{j+1} - T_{i-1}^{j+1}}{2\Delta x}$$

This equation can be rearranged to fit into the Jacobian as:

$$T_{i+1}^{j+1} - T_{i-1}^{j+1} = 2\Delta x g(t_{j+1})$$

A. Calculate Jacobian

1. First exterior node (an imaginary node)

$$J(1,1) = 1.0$$
$$J(1,3) = -1.0$$

2. Last exterior node (an imaginary node)

$$J(1, m+3) = 1.0$$
$$J(1, m+1) = -1.0$$

3. All other nodes i

$$J(1, i-1) = -\lambda$$
$$J(1, i) = (2 + 2\lambda + A\Delta t)$$
$$J(1, i+1) = -\lambda$$

Let $J_{diag} = (2 + 2\lambda + A\Delta t)$
so that the Jacobian looks like:

$$\underline{\underline{J}} = \begin{bmatrix} -1 & 0 & 1 & 0 & 0 & 0 \\ -\lambda & J_{diag} & -\lambda & 0 & 0 & 0 \\ 0 & -\lambda & J_{diag} & -\lambda & 0 & 0 \\ 0 & 0 & -\lambda & J_{diag} & -\lambda & 0 \\ 0 & 0 & 0 & -\lambda & J_{diag} & -\lambda \\ 0 & 0 & 0 & -1 & 0 & 1 \end{bmatrix}$$

This is a matrix of known quantities. It is a constant matrix unless A is a function of time.

B. Calculate Residual

1. First exterior node (the imaginary boundary condition)

$$R(1) = 2\Delta x g_{bc1}(t_{j+1})$$

2. Last exterior node (the imaginary boundary condition)

$$R(m+3) = 2\Delta x g_{bc2}(t_{j+1})$$

3. All other nodes

$$R(i) = \lambda T_{i-1}^{j} + (2 - 2\lambda - A\Delta t)T_{i}^{j} + \lambda T_{i+1}^{j} + 2\Delta t F$$

Let $R_{diag} = (2 - 2\lambda - A\Delta t)$
so that the Residual looks like:

$$\underline{R} = \begin{bmatrix} 2\Delta x g_{bc1}(t_{j+1}) \\ \lambda T_{i-1}^{j} + R_{diag} T_{i}^{j} + \lambda T_{i+1}^{j} + 2\Delta t F \\ \cdots \\ \lambda T_{i-1}^{j} + R_{diag} T_{i}^{j} + \lambda T_{i+1}^{j} + 2\Delta t F \\ 2\Delta x g_{bc2}(t_{j+1}) \end{bmatrix}$$

II. For Mixed Boundary Conditions (with m intervals, m+3 nodes, m+3 unknowns)

A mixed (generalized Neumann) boundary condition is a boundary condition of the form:

$$\frac{dT}{dx}(x = 0, t) = g(t) - q(t)T$$

where the boundary condition can be a function of time but is not a function of temperature.

The approximation we make for this first spatial derivative is that

$$\left[\frac{dT}{dx}(x=0,t)\right]^{j+1} = g(t_{j+1}) - q(t_{j+1})T_i^{j+1} = \frac{T_{i+1}^{j+1} - T_{i-1}^{j+1}}{2\Delta x}$$

This equation can be rearranged to fit into the Jacobian as:

$$T_{i+1}^{j+1} - T_{i-1}^{j+1} = 2\Delta x g(t_{j+1}) - 2\Delta x q(t_{j+1})T_i^{j+1}$$

$$-T_{i-1}^{j+1} + 2\Delta x q(t_{j+1})T_i^{j+1} + T_{i+1}^{j+1} = 2\Delta x g(t_{j+1})$$

A. Calculate Jacobian

1. First exterior node (now an imaginary node)

   $J(1,1) = -1.0$

   $J(1,2) = 2\Delta x q(t_{j+1})$

   $J(1,3) = 1.0$

2. Last exterior node (now an imaginary node)

   $J(1,m+1) = -1.0$

   $J(1,m+2) = 2\Delta x q(t_{j+1})$

   $J(1,m+3) = 1.0$

3. All other nodes i

   $J(1,i-1) = -\lambda$

   $J(1,i) = (2 + 2\lambda + A\Delta t)$

   $J(1,i+1) = -\lambda$

Let $J_{diag} = (2 + 2\lambda + A\Delta t)$
so that the Jacobian looks like:

$$\underline{\underline{J}} = \begin{bmatrix} -1 & 2\Delta x q(t_{j+1}) & 1 & 0 & 0 & 0 \\ -\lambda & J_{diag} & -\lambda & 0 & 0 & 0 \\ 0 & -\lambda & J_{diag} & -\lambda & 0 & 0 \\ 0 & 0 & -\lambda & J_{diag} & -\lambda & 0 \\ 0 & 0 & 0 & -\lambda & J_{diag} & -\lambda \\ 0 & 0 & 0 & -1 & 2\Delta x q(t_{j+1}) & 1 \end{bmatrix}$$

This is a matrix of known quantities. It is a constant matrix unless A is a function of time.

B. Calculate Residual

The residual is the same as in the pure Neumann boundary condition case.