Chapter 3
Numerical Solution of Heat Conduction and Diffusion Problems

1 Introduction

Recall that the mathematical expressions of heat conduction and diffusion problems are almost identical. In the case of heat conduction the problem consists in finding the function $T(r, t)$ for $r \in \Omega$ and $t > 0$ which satisfies

$$\rho C_v \frac{\partial T}{\partial t} = \nabla \cdot (k\nabla T) + g(r, t)$$

subject to

$$T = T_0 = f(r)$$

at $t = 0$ for all $r \in \Omega$ and

$$\alpha T + \beta \frac{\partial T}{\partial n} = \gamma$$

on $\partial \Omega$ for $t > 0$, where $\Omega$ is the region of space under analysis and $\partial \Omega$ is its boundary surface. Further, $g, f, \alpha, \beta$ and $\gamma$ are given quantities and the coefficients $\alpha, \beta$ and $\gamma$ can have different values along different portions of the boundary surface.

In the case of substance diffusion the problem consists in finding the function $c(r, t)$ for $r \in \Omega$ and $t > 0$ which satisfies

$$\frac{\partial c}{\partial t} = \nabla \cdot (D \nabla c) + g(r, t)$$

subject to

$$c = c_0 = f(r)$$
at \( t = 0 \) for all \( \mathbf{r} \in \Omega \) and
\[
\alpha c + \beta \frac{\partial c}{\partial n} = \gamma
\]
on \( \partial \Omega \) for \( t > 0 \), where \( \Omega \) is the region of space under analysis and \( \partial \Omega \) is its boundary surface. Further, \( g, f, \alpha, \beta \) and \( \gamma \) are given quantities and the coefficients \( \alpha, \beta \) and \( \gamma \) can have different values along different portions of the boundary surface.

Errors are always involved in performing any numerical computation. Round-off errors appear whenever computing takes place using a finite number of digits. This is the case when using modern computing machines. Truncation error is the error that exists even in the absence of round-off error and is the result of neglecting higher order terms in the finite difference approximations obtained from Taylor series expansions. Successful numerical work requires attention to issues of accuracy and error control.

The presentation below is comprehensive but brief. It includes descriptions of the finite difference method, the finite volume method and the finite element method. Finite difference and finite volume methodologies are emphasized since they are readily implemented and are also commonly used approaches to the analysis of real-world heat and mass transfer problems in engineering systems.

## 2 Finite Difference Method

The simplest numerical technique to apply for the solution of the heat/diffusion equation is the finite difference method. The basic idea behind the finite difference method is to replace the various derivatives appearing in the mathematical formulation of the problem by suitable approximations on a finite difference mesh of nodes.

The simplest derivation of finite difference formulae makes use of Taylor series. The Taylor series expansions of a function \( y(x) \) about a point \( x \) are:
\[
y(x + \Delta x) = y(x) + \Delta xy'(x) + \frac{\Delta x^2}{2!} y''(x) + \frac{\Delta x^3}{3!} y'''(x) + \ldots
\]
and
\[
y(x - \Delta x) = y(x) - \Delta xy'(x) + \frac{\Delta x^2}{2!} y''(x) - \frac{\Delta x^3}{3!} y'''(x) + \ldots
\]
where \( \Delta x \) is the mesh spacing.

Solving the first equation above for \( y'(x) \) gives
\[
y'(x) = \frac{y(x + \Delta x) - y(x)}{\Delta x} - \frac{\Delta x^2}{2} y''(x) - \frac{\Delta x^3}{6} y'''(x) + \ldots
\]
and solving the second one
\[
y'(x) = \frac{y(x) - y(x - \Delta x)}{\Delta x} + \frac{\Delta x^2}{2} y''(x) - \frac{\Delta x^3}{6} y'''(x) + \ldots
\]
Finally, from the first two equations

\[ y'(x) = \frac{y(x + \Delta x) - y(x - \Delta x)}{2\Delta x} - \frac{\Delta x^2}{6}y''(x) + \ldots \]

These are called respectively the forward, backward and central approximations to the derivative of \( y(x) \). Note that the second term on the right hand side in the first two equations above is proportional to \( \Delta x \) while the same second term in the third equation is proportional to \( \Delta x^2 \). Therefore, the first two equations are regarded as leading to first-order accurate approximations to the derivative while the last formula leads to a second-order accurate approximation.

Note that the neglect of higher order terms in the above formulae for \( y'(x) \) produces various approximation schemes for the derivative.

Second order derivative approximations can be similarly obtained. For example, expanding \( y(x \pm \Delta x) \) about \( x \)

\[ y(x + 2\Delta x) = y(x) + 2\Delta xy'(x) + 2\Delta x^2 y''(x) + \frac{4}{3}\Delta x^3 y'''(x) + \ldots \]

and

\[ y(x - 2\Delta x) = y(x) - 2\Delta xy'(x) + 2\Delta x^2 y''(x) - \frac{4}{3}\Delta x^3 y'''(x) + \ldots \]

Eliminating \( y'(x) \) gives

\[ y''(x) = \frac{y(x + \Delta x) - 2y(x) + y(x - \Delta x)}{\Delta x^2} - \frac{1}{12}\Delta x^2 y'''(x) + \ldots \]

Neglecting the higher order terms produces the central difference approximation to \( y''(x) \). Note that this leads to a second-order accurate approximation of the second derivative.

Finite difference approximations of derivatives for functions involving more than one independent variable are readily obtained. For instance, consider the function of two independent variables \( u(x, t) \). Introduce a mesh of \( N \) nodes in space \( x_i = (i - 1)\Delta x \) where \( \Delta x = L/(N - 1) \) is the mesh spacing, with \( i = 1, 2, \ldots, N \), the following discrete approximation is readily obtained for \( \partial^2 u / \partial x^2 \) at each time level \( j \)

\[ \frac{\partial^2 u}{\partial x^2} \approx \frac{u_{i-1,j} - 2u_{i,j} + u_{i+1,j}}{\Delta x^2} \]

Where \( u_{i,j} \approx u(x_i, t_j) \).

Similarly, introducing a mesh of \( M \) nodes in time \( t_j = (j - 1)\Delta t \) with \( j = 1, 2, \ldots, M \) the following discrete approximations are readily obtained for \( \partial u / \partial t \) at each space node \( i \),

\[ \frac{\partial u}{\partial t} \approx \frac{u_{i,j+1} - u_{i,j}}{\Delta t} \]
i.e. the forward finite difference formula,
\[ \frac{\partial u}{\partial t} \approx \frac{u_{i,j} - u_{i,j-1}}{\Delta t} \]
i.e. the backward finite difference formula and
\[ \frac{\partial u}{\partial t} \approx \frac{u_{i,j+1} - u_{i,j-1}}{2\Delta t} \]
i.e. the central finite difference formula. The forward and backward formulae are only first order accurate while the central difference formula is second order accurate.

Finite difference formula analogous to the original differential equation are then easily constructed. For instance, for the one-dimensional steady state heat equation with constant internal heat generation and thermal conductivity
\[ \frac{d}{dx}\left(\frac{dT}{dx}\right) + g/k = 0 \]
one readily obtains the analog
\[ \frac{T_{i-1} - 2T_i + T_{i+1}}{\Delta x^2} + \frac{g}{k} = 0 \]
Now for steady state heat conduction in a rectangle with constant thermal conductivity and without internal heat generation (Laplace’s equation)
\[ \frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} = 0 \]
the finite difference method with \( \Delta x = \Delta y \) yields the easily remembered useful formula
\[ T_{i,j} = \frac{1}{4}[T_{i-1,j} + T_{i+1,j} + T_{i,j-1} + T_{i,j+1}] \]
which gives \( T_{i,j} \) as the average of the temperatures of neighboring nodes.

Now for transient diffusion in the one dimensional case with constant diffusivity
\[ \frac{\partial c}{\partial t} = D \frac{\partial^2 c}{\partial x^2} \]
the FD formula obtained using forward differencing in time is
\[ \frac{c_{i,j+1} - c_{i,j}}{\Delta t} = D \frac{c_{i-1,j} - 2c_{i,j} + c_{i+1,j}}{\Delta x^2} \]
where \( \Delta x \) is the mesh spacing in the \( x \) direction and \( c_{i,j} \approx c(x_i, t_j) \).
The corresponding FD formula obtained using backward differencing in time is
\[
\frac{c_{i,j}^{n+1} - c_{i,j}^n}{\Delta t} = D \frac{c_{i-1,j}^{n+1} - 2c_{i,j}^{n+1} + c_{i+1,j}^{n+1}}{\Delta x^2}
\]

The above is easily generalized to three dimensions. For instance, the finite difference analog of the equation
\[
\frac{\partial c}{\partial t} = D \left( \frac{\partial^2 c}{\partial x^2} + \frac{\partial^2 c}{\partial y^2} + \frac{\partial^2 c}{\partial z^2} \right)
\]
obtained using forward differencing in time is
\[
\frac{c_{i,j,k}^{n+1} - c_{i,j,k}^n}{\Delta t} = D \left[ \frac{c_{i-1,j,k}^{n+1} - 2c_{i,j,k}^{n+1} + c_{i+1,j,k}^{n+1}}{\Delta x^2} + \frac{c_{i,j-1,k}^{n+1} - 2c_{i,j,k}^{n+1} + c_{i,j+1,k}^{n+1}}{\Delta y^2} + \frac{c_{i,j,k-1}^{n+1} - 2c_{i,j,k}^{n+1} + c_{i,j,k+1}^{n+1}}{\Delta z^2} \right]
\]
where \(\Delta x, \Delta y\) and \(\Delta z\) are the mesh spacings in the \(x, y\) and \(z\) directions, respectively and \(c_{i,j,k,n} \approx c(x_i, y_j, z_k, t_n)\).

Generalizations to other coordinate systems are also straightforward. Consider the heat conduction equation in a solid cylinder of radius \(R\) with azimuthal and independent of \(z\)
\[
\frac{\partial T}{\partial t} = \alpha \left[ \frac{\partial}{\partial r} \left( r \frac{\partial T}{\partial r} \right) \right]
\]
Introducing a mesh of \(N\) nodes along the \(r\)–direction, \(r_i\) with \(i = 1, 2, ..., N\) and \(\Delta r = R/(N - 1)\) and a mesh of nodes in time \(t_j\), with \(j = 1, 2, ..., \) spacing \(\Delta t\), and forward differencing in time, a finite difference analog is
\[
\frac{T_{i,j}^{n+1} - T_{i,j}^n}{\Delta t} = \alpha \frac{r_{i+1/2}(T_{i+1,j}^{n+1} - T_{i,j}^n) - r_{i-1/2}(T_{i,j} - T_{i-1,j}^{n+1})}{r_i \Delta r}
\]
where \(r_{i+1/2}\) is a radial position located halfway between \(r_{i+1}\) and \(r_i\), \(r_{i-1/2}\) is a radial position located halfway between \(r_i\) and \(r_{i-1}\) and \(T_{i,j} \approx T(r_i, t_j)\).

If backward differencing in time is used instead, the result is
\[
\frac{T_{i,j}^{n+1} - T_{i,j}^n}{\Delta t} = \alpha \frac{r_{i+1/2}(T_{i+1,j}^{n+1} - T_{i,j}^n) - r_{i-1/2}(T_{i,j}^{n+1} - T_{i-1,j}^{n+1})}{r_i \Delta r}
\]
As a final example consider the diffusion equation in a solid sphere of radius \(R\) with azimuthal and poloidal symmetry
\[
\frac{\partial c}{\partial t} = \frac{D}{r^2} \left[ \frac{\partial}{\partial r} \left( r^2 \frac{\partial c}{\partial r} \right) \right]
\]
Introducing a mesh of $N$ nodes along the $r-$direction, $r_i$ with $i = 1, 2, ..., N$ and $\Delta r = R/(N - 1)$ and a mesh of nodes in time $t_j$, with $j = 1, 2, ..., $ spacing $\Delta t$, and forward differencing in time, a finite difference analog is

$$\frac{c_{i,j} - c_{i,j}}{\Delta t} = D \left( r_{i+1/2}^2 \left( \frac{c_{i,j+1} - c_{i,j}}{\Delta r} \right) - r_{i-1/2}^2 \left( \frac{c_{i,j} - c_{i,j-1}}{\Delta r} \right) \right)$$

where $c_{i,j} \approx c(r_i, t_j)$.

If backward differencing in time is used instead, the result is

$$\frac{c_{i,j} - c_{i,j}}{\Delta t} = D \left( r_{i+1/2}^2 \left( \frac{c_{i,j+1} - c_{i,j}}{\Delta r} \right) - r_{i-1/2}^2 \left( \frac{c_{i,j} - c_{i,j+1}}{\Delta r} \right) \right)$$

Since in every case one equation is obtained for each node and each equation relates the approximate value of $T$ or $c$ at the node with those of neighboring nodes, the result is a system of interlinked simultaneous algebraic equations. This is a feature common to all numerical methods employed to solve the heat and diffusion equations.

3 Finite Volume Method

An alternative discretization method is based on the idea of regarding the computation domain as subdivided into a collection of finite volumes. In this view, each finite volume is represented by a line in 1D, an area in 2D and a volume in 3D. Nodes, located inside each finite volume, become the locus of computational values. In rectangular cartesian coordinates in 2D the simplest finite volumes are rectangles. For each node, the rectangle faces are formed by drawing perpendiculars through the midpoints between contiguous nodes. Discretization equations are obtained by integrating the original partial differential equation over the span of each finite volume. The method is easily extended to nonlinear problems.

3.1 Steady State Conduction in a Slab with Internal Heat Generation

The problem of steady state heat transport through the thickness $L$ of a large slab with constant internal heat generation $g$ is described by the following form of the heat or diffusion equation

$$\frac{d}{dx} \left( k \frac{dT}{dx} \right) + g = 0$$

To implement the finite volume method first subdivide the thickness of the slab into a collection of $N$ adjoining segments of thickness not necessarily of uniform size (finite volumes) and place a node inside each volume. Thus, an arbitrary node will be called $P$, its size is $\Delta x$ and the nodes to its left and right, respectively $W$ and $E$. 

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Note that two different types of nodes result. While *interior* nodes are surrounded by finite volume on both sides, *boundary* nodes contain material only on one side. Here we shall concentrate on the derivation of discrete equations for the interior nodes. Those for the boundary nodes will be discussed later.

The distance between nodes $W$ and $P$ is $\delta x_w$ and that between $P$ and $E$, $\delta x_e$. The locations of the finite volume boundaries corresponding to node $P$ will be denoted by $w$ and $e$. Finally, the distance between $P$ and $e$ is called $\delta x_{e-}$ and that between $e$ and $E$ is $\delta x_{e+}$. If $P$ is located in the center of the finite volume then $\delta x_{e-} = \delta x_{e+} = \frac{1}{2}\delta x_e$.

To implement the finite volume method we now integrate the above equation over the span of the finite volume associated with node $P$, i.e. from $x_w$ to $x_e$

$$\int_w^e d(k \frac{dT}{dx}) + \int_w^e g dx = (k \frac{dT}{dx})_e - (k \frac{dT}{dx})_w + g \Delta x = 0$$

Next, approximate the derivatives by piecewise linear profiles to give

$$k_e \frac{T_E - T_P}{\delta x_e} - k_w \frac{T_P - T_W}{\delta x_w} + g \Delta x = 0$$

where the conductivities at the finite volume faces are calculated as the harmonic means of the values at the neighboring nodes, i.e.

$$k_e = \left[ \frac{1 - \delta x_{e+}/\delta x_e}{k_P} + \frac{\delta x_{e+}/\delta x_e}{k_E} \right]^{-1}$$

and

$$k_w = \left[ \frac{1 - \delta x_{w+}/\delta x_w}{k_W} + \frac{\delta x_{w+}/\delta x_w}{k_P} \right]^{-1}$$

Rearranging one obtains the algebraic equation

$$a_P T_P = a_E T_E + a_W T_W + b$$

where the coefficients are given by

$$a_E = \frac{k_e}{\delta x_e}$$

$$a_W = \frac{k_w}{\delta x_w}$$

$$a_P = a_E + a_W$$

and

$$b = g \Delta x$$
One algebraic equation like the above, relating the values of \( T \) at three contiguous nodes, is obtained for each of the \( N \) nodes. Adding the this set the discrete equations associated with the boundary nodes one obtains a consistent set of interlinked simultaneous algebraic equations which must be solved to give the values of \( T \) for all nodal locations.

For the special case of constant thermal properties and finite volumes of uniform size \( (\delta x_e = \delta x_w = \Delta x) \), the above is easily rearranged as

\[
\frac{T_E - 2T_P + T_W}{\Delta x^2} + \frac{g}{k} = 0
\]

which coincides with the FD formula obtained before.

### 3.2 Transient Diffusion in a Slab

Now we apply the finite volume method to the discretization of a transient problem. Consider the problem of determining \( c(x, t) \) for the slab \( x \in [0, L] \) and \( t > 0 \) such that

\[
\frac{\partial c}{\partial t} = \frac{\partial}{\partial x} \left( D \frac{\partial c}{\partial x} \right)
\]

subject to

\[
c(x, 0) = c_0(x)
\]

and

\[
c(0, t) = c(L, t) = 0
\]

Subdivide the slab into a collection of \( N \) adjacent segments of thickness \( (\text{finite volumes}) \) and introduce a set of \( N + 1 \) nodes (one inside each volume and one on each boundary). The positions of nodes are then labelled from left to right in the form of a sequence \( x_1, x_2, x_3, ..., x_i, ...x_{N+1} \). To discretize time simply select time intervals of duration \( \Delta t \) at which the calculations will be performed. Uniform time intervals will be assumed here. As before, we focus on the derivation of the discretized heat equation for all the interior volumes.

Consider now an arbitrary finite volume of size \( \Delta x \). Its representative node is locate at \( x_P \) and its boundaries are located at \( x_w \) and \( x_e \). The two contiguous nodes to the left and right of node \( P \) are \( W \) and \( E \) and their locations are \( x_W \) and \( x_E \). Introduce again the various mesh spacings as in the steady case \( \delta x_e, \delta x_{e+}, \delta x_{e-}, \delta x_w, \delta x_{w+}, \delta x_{w-} \) and \( \Delta x \).

Integrate now the diffusion equation over the span of the finite volume (i.e. from \( x \) to \( x + \Delta x \)) and also over the time interval from \( t \) to \( t + \Delta t \), i.e.

\[
\int_t^{t+\Delta t} \int_x^{x+\Delta x} \frac{\partial c}{\partial t} \, dx \, dt = \int_t^{t+\Delta t} \int_x^{x+\Delta x} \frac{\partial}{\partial x} \left( D \frac{\partial c}{\partial x} \right) dx \, dt = \int_t^{t+\Delta t} \int_x^{x+\Delta x} \frac{\partial}{\partial x} \left( D \frac{\partial c}{\partial x} \right) dx \, dt
\]
The double integration on the left hand side is straightforward and yields
\[ \int_{t}^{t+\Delta t} \int_{x_{w}}^{x_{e}} \frac{\partial c}{\partial t} \, dx \, dt = \Delta x (c_{P} - c_{P}^{o}) \]
where \( c_{P} \) is the value of \( c \) at \( P \) at time \( t + \Delta t \) and \( c_{P}^{o} \) is the value of \( c \) at \( P \) at time \( t \).

On the right hand side, the space integration is performed first and the resulting derivatives are approximated from a piecewise linear profile to yield
\[ \int_{t}^{t+\Delta t} \int_{x_{w}}^{x_{e}} \partial \left( D \frac{\partial u}{\partial x} \right) \, dt = \int_{t}^{t+\Delta t} \left[ (D \frac{\partial c}{\partial x})|_{e} - (D \frac{\partial c}{\partial x})|_{w} \right] dt = \int_{t}^{t+\Delta t} \left[ D_{e} \frac{c_{E} - c_{P}}{\delta x_{e}} - D_{w} \frac{c_{P} - c_{W}}{\delta x_{w}} \right] dt \]

To complete the process and important decision must be made when carrying out the time integration. A very general proposition is to assume that the integral is given by time-weighed averages as follows
\[ \int_{t}^{t+\Delta t} c_{P} \, dt = [\theta c_{P} + (1 - \theta) c_{P}^{o}] \Delta t \]
\[ \int_{t}^{t+\Delta t} c_{E} \, dt = [\theta c_{E} + (1 - \theta) c_{E}^{o}] \Delta t \]
and
\[ \int_{t}^{t+\Delta t} c_{W} \, dt = [\theta c_{W} + (1 - \theta) c_{W}^{o}] \Delta t \]
where the weighing factor \( \theta \) is a pure number with \( 0 \leq \theta \leq 1 \).

Introducing the above, the integrated heat/diffusion equation then finally becomes
\[ \frac{\Delta x}{\Delta t} (c_{P} - c_{P}^{o}) = \theta \left[ \frac{D_{e} (c_{E} - c_{P})}{\delta x_{e}} - \frac{D_{w} (c_{P} - c_{W})}{\delta x_{w}} \right] + (1 - \theta) \left[ \frac{D_{e} (c_{E}^{o} - c_{P}^{o})}{\delta x_{e}} - \frac{D_{w} (c_{P}^{o} - c_{W}^{o})}{\delta x_{w}} \right] \]

Rearrangement gives
\[ a_{P} c_{P} = a_{E} [\theta c_{E} + (1 - \theta) c_{E}^{o}] + a_{W} [\theta c_{W} + (1 - \theta) c_{W}^{o}] + a_{F}^{o} - (1 - \theta) a_{E} - (1 - \theta) a_{W} c_{P}^{o} \]
where
\[ a_{E} = \frac{D_{e}}{\delta x_{e}} \]
\[ a_W = \frac{D_w}{\delta x_w} \]

\[ a_P^0 = \frac{\Delta x}{\Delta t} \]

and

\[ a_P = \theta a_E + \theta a_W + a_P^0 \]

The result for the corresponding heat conduction problem is almost identical except for the fact that \( k \)'s must be used instead of \( D \)'s and the coefficient \( a_P^0 = \rho C_p \Delta x/\Delta t \).

Note that if finite volumes of uniform size are used with nodes at their midpoints, transport properties are assumed constant and \( \theta = 0 \) is assumed, the above reduces, after some rearrangement to

\[ \frac{c_P - c_P^0}{\Delta t} = D \frac{c_W^0 - 2c_P^0 + c_E^0}{\Delta x^2} \]

which is identical to the result obtained earlier using the finite difference method with forward differencing in time.

### 3.3 Transient Conduction in Multidimensional Systems

Consider the problem of estimating the temperature \( T(x, y, z, t) \) in a three-dimensional brick \( x \in [0, X], y \in [0, Y], z \in [0, Z] \) undergoing transient heat conduction with constant internal heat generation. The heat equation for this case is

\[ \rho C_p \frac{\partial T}{\partial t} = \frac{\partial}{\partial x} \left( k \frac{\partial T}{\partial x} \right) + \frac{\partial}{\partial y} \left( k \frac{\partial T}{\partial y} \right) + \frac{\partial}{\partial z} \left( k \frac{\partial T}{\partial z} \right) + g \]

subject to specified conditions at the boundaries of the domain.

The finite volume formulation regards the brick as composed of a set of adjoining volumes each containing a node. The dimensions of the typical volume are \( \Delta x \times \Delta y \times \Delta z \) and the typical node \( P \) has six neighbors \( E, W, N, S, T \) and \( B \). Proceeding exactly as above, the finite volume method produces the following result (with \( \theta = 1 \))

\[ a_P T_P = a_E T_E + a_W T_W + a_N T_N + a_S T_S + a_T T_T + a_B T_B + b \]

where

\[ a_E = \frac{k_e \Delta y \Delta z}{\delta x_e} \]

\[ a_W = \frac{k_w \Delta y \Delta z}{\delta x_w} \]
\[ a_N = \frac{k_i \Delta z \Delta x}{\delta y_n} \]

\[ a_S = \frac{k_w \Delta z \Delta x}{\delta y_s} \]

\[ a_T = \frac{k_i \Delta x \Delta y}{\delta z_t} \]

\[ a_B = \frac{k_i \Delta x \Delta y}{\delta z_b} \]

\[ a_P = \rho C_p \frac{\Delta x \Delta y \Delta z}{\Delta t} \]

\[ b = g \Delta x \Delta y \Delta z + a_P^0 T_P^0 \]

and

\[ a_P = a_E + a_W + a_N + a_S + a_T + a_B + a_P^0 \]

Note that all the above expressions can all be generically written as

\[ a_P T_P = \sum a_{nb} T_{nb} + b \]

where the summation contains just \( T_E \) and \( T_W \) in the case of uni-dimensional systems, contains \( T_E, T_W, T_N \) and \( T_S \) in the case of 2D systems and all \( T_E, T_W, T_N, T_S, T_T \) and \( T_B \) in the case of three dimensional systems.

The discrete equation derived using the FV method can be rearranged for \( \theta = 1 \) to produce a very appealing and physically meaningful expression. Consider two dimensional systems. The generic discrete form of the conservation equation is

\[ \lambda_P (\phi_P - \phi_P^0) \frac{\Delta V}{\Delta t} = J_w A_w - J_e A_e + J_s A_s - J_n A_n + g \Delta V \]

where the dependent variable \( \phi \) is the temperature \( T \), for heat transfer and the concentration \( c \), for mass transfer. Further, the \( J_i \)'s are the fluxes of the transported quantity and the \( A_i \)'s are the cross-sectional areas of the finite volume faces through which the transported quantity enters/leaves the finite volume. Therefore the products \( J_i A_i \) are the rates of transport of energy or mass through the various control volume faces. Moreover, \( \lambda = \rho C_p \) for heat transfer and \( \theta = 1 \) for mass transfer. The transport rates are given as

\[ J_e A_e = \left[ \frac{\delta x_e^-}{\Gamma_P} + \frac{\delta x_e^+}{\Gamma_E} \right]^{-1} (\phi_P - \phi_E) A_e \]
\[ J_w A_w = \left[ \left( \frac{\delta x_w^-}{\Gamma_W} \right) + \left( \frac{\delta x_w^+}{\Gamma_P} \right) \right]^{-1} (\phi_W - \phi_P) A_w \]

\[ J_n A_n = \left[ \left( \frac{\delta y_n^-}{\Gamma_P} \right) + \left( \frac{\delta y_n^+}{\Gamma_N} \right) \right]^{-1} (\phi_P - \phi_N) A_n \]

\[ J_s A_s = \left[ \left( \frac{\delta y_s^-}{\Gamma_S} \right) + \left( \frac{\delta y_s^+}{\Gamma_P} \right) \right]^{-1} (\phi_S - \phi_P) \]

where \( \Gamma_i = k_i \) for heat transfer and \( = D \) for mass transfer.

Many special forms can be obtained by simplification of the above. For instance, for a rectangle with constant thermal properties, without internal heat generation at steady state and using \( \Delta x = \Delta y \) one obtains

\[ T_P = \frac{1}{4} [T_E + T_W + T_N + T_S] \]

which is identical to the expression obtained before using the method of finite differences.

### 4 Finite Element Method

Consider the problem of multi-dimensional steady state heat conduction with internal heat generation and constant thermal properties

\[ \nabla^2 T = -\frac{g}{k} \]

inside the domain \( \Omega \), and subject to \( T = 0 \) at the boundary. Intimately associated with this boundary value problem is the following **energy functional** \( I \)

\[ I(v) = \int_{\Omega} \left[ \frac{1}{2} |\nabla v|^2 - \frac{g}{k} v \right] dx dy \]

where \( v \) are functions among which the solution of the original heat conduction problem is included. It can be shown that the solution of the boundary value problem above is the function \( T(r) = v(r) \) that produces the minimum value of the energy functional \( I \), i.e.

\[ \delta I(T) = 0 \]

and this function must clearly come from the set of functions which satisfy the stated boundary conditions.

Discretization in the finite element method is obtained by subdividing the computational domain into subdomains (finite elements), commonly triangles, rectangles, tetrahedra or
rectangular parallelepipeds (bricks). The vertices in each of these geometries are called nodes. The methods seeks an approximation inside each element of the form

\[ T(\mathbf{r}) = \sum_{i=1}^{m} c_i \phi_i(\mathbf{r}) \]

where the \( \phi_i(\mathbf{r}) \) are known linearly independent piecewise polynomials called the shape functions and the \( c_i \) are unknown coefficients actually representing the values of \( T \) at the given nodal locations. The finite element method determines the specific values of these coefficients which minimize the functional \( I \). (i.e. \( \frac{\partial I}{\partial c_i} = 0 \)).

Minimization of \( I \) with respect to the \( c_i \)'s produces a set of simultaneous linear algebraic equations of the form

\[ A \mathbf{c} = \mathbf{b} \]

where \( \mathbf{c} = (c_1, c_2, ..., c_m)^T \) is the solution vector and \( \mathbf{b} = (b_1, b_2, ..., b_m)^T \) is the forcing vector. Solution of the above system using standard techniques yields the desired approximation.

To illustrate the practical implementation of the finite element methodology we now consider the case of one-dimensional steady heat conduction with internal heat generation inside a slab, i.e.

\[ \frac{d}{dx}(k \frac{dT}{dx}) + g = 0 \quad (1) \]

in \( 0 \leq x \leq 1 \) subject to the boundary conditions

\[ T(0) = 0 \quad (2) \]

and

\[ T(1) = 0 \quad (3) \]

In the Galerkin formulation of the finite element method, the domain \( 0 \leq x \leq 1 \) is first subdivided into a set of \( n \) intervals (finite elements) of size \( \Delta x \) connected at their ends (nodes). For each node \( i \), introduce the following shape function of position

\[ \phi_i(x) = \begin{cases} 0 & 0 \leq x \leq x_{i-1} \\ N_1(x) & x_{i-1} \leq x \leq x_i \\ N_2(x) & x_i \leq x \leq x_{i+1} \\ 0 & x_{i+1} \leq x \leq 1 \end{cases} \quad (4) \]

where

\[ N_1(x) = \frac{x - x_{i-1}}{\Delta x} \quad (5) \]

and

\[ N_2(x) = \frac{x_{i+1} - x}{\Delta x} \quad (6) \]
The function $\phi_i$ is continuous and zero everywhere except for the interval $x_{i-1} \leq x \leq x_{i+1}$, on which it consists of two linear segments with a maximum value of 1 attained at $x = x_i$. As a set, these functions possess the very interesting property that any continuous piecewise-linear function of position, such as $T(x)$, can be represented by the linear combination

$$T(x) \approx \sum_{j=1}^{n} c_j \phi_j(x) \quad (7)$$

where the coefficients $c_j$ are the values of $T$ at the nodes $j = 1, 2, ..., n$, i.e. $c_j = T_j$.

Furthermore, the set of functions $\phi_i$ possess the fundamental property of orthogonality i.e.

$$\int_0^1 \phi_i \phi_j dx = \begin{cases} 0 & j \leq i - 2 \\ \Delta x/6 & j = i - 1 \\ \Delta x/3 & j = i \\ \Delta x/6 & j = i + 1 \\ 0 & j \geq i + 2 \end{cases} \quad (8)$$

The Galerkin method requires consideration of the scalar product of the (approximated) energy equation with the shape functions, i.e.

$$\int_0^1 \left( \frac{d}{dx} \left( k \frac{dT}{dx} \right) + g \right) \phi_i(x) dx = 0 \quad (9)$$

Integrating the first term by parts and noting the behavior of the shape functions at the boundary nodes, one obtains,

$$\int_0^1 \left( -k \frac{dT}{dx} \frac{d\phi_i}{dx} + g \phi_i \right) dx = 0 \quad (10)$$

Since the same value of the integral is obtained if one integrates first over the interval $[x_{i-1}, x_{i+1}]$ for all $i$ and then adds up all the resulting integrals one can write

$$\sum_{i=1}^{n} \int_{x_{i-1}}^{x_{i+1}} \left( -k \frac{dT}{dx} \frac{d\phi_i}{dx} + g \phi_i \right) dx = 0 \quad (11)$$

Performing the integration over $[x_{i-1}, x_{i+1}]$ with the given $\phi_i$’s (and the approximation $T(x) = \sum_{j=1}^{n} c_j \phi_j(x)$) one obtains,

$$\int_{x_{i-1}}^{x_i} \frac{d}{dx} \left( k \frac{dT}{dx} \frac{d\phi_i}{dx} \right) dx = \begin{cases} 0 & j \neq i \\ -k \frac{T_i - T_{i-1}}{\Delta x} & j = i \end{cases} \quad (12)$$

and

$$\int_{x_i}^{x_{i+1}} \frac{d}{dx} \left( k \frac{dT}{dx} \frac{d\phi_i}{dx} \right) dx = \begin{cases} 0 & j \neq i \\ k \frac{T_{i+1} - T_i}{\Delta x} & j = i \end{cases} \quad (13)$$
and
\[ \int_{x_{i-1}}^{x_{i+1}} g \phi_i \, dx = \int_{x_{i-1}}^{x_i} g N_1 \, dx + \int_{x_i}^{x_{i+1}} g N_2 \, dx = g \Delta x \] (14)

Therefore, the integrated energy equation is
\[ \frac{k}{(\Delta x)^2} (-T_{i-1} + 2T_i - T_{i+1}) = g \] (15)

for \( i = 1, 2, 3, \ldots, n \). Note this is exactly the same result obtained using the finite difference or the finite volume methods.

This result can be written using matrix notation as
\[ Ac = b \] (16)

which is simply a tridiagonal system of linear algebraic equations where \( A \) is the global stiffness matrix,
\[ A = \begin{pmatrix}
  K_{11}^i & 0 & 0 & \cdots \\
  K_{21}^i & (K_{22}^i + K_{11}^i) & K_{12}^i & \cdots \\
  0 & K_{22}^i & (K_{22}^i + K_{11}^i) & K_{12}^i & \cdots \\
  0 & 0 & K_{22}^i & (K_{22}^i + K_{11}^i) & K_{12}^i & \cdots \\
  \cdots & \cdots & \cdots & \cdots & \cdots & \cdots 
\end{pmatrix} \] (17)

The entries \( K_{11}^i, K_{12}^i, K_{21}^i, \) and \( K_{22}^i \) are the components of the element stiffness matrices for the \( i \)-th element
\[ K^i = \begin{pmatrix}
  K_{11}^i & K_{12}^i \\
  K_{21}^i & K_{22}^i 
\end{pmatrix} = \frac{k}{(\Delta x)^2} \begin{pmatrix}
  1 & -1 \\
  -1 & 1 
\end{pmatrix} \] (18)

Further, \( c = T \) is the vector of nodal temperatures,
\[ c = \begin{pmatrix}
  T_1 \\
  T_2 \\
  \vdots \\
  T_n 
\end{pmatrix} \] (19)

and \( b \) is the force vector.
\[ b = \begin{pmatrix}
  0 \\
  g \\
  \vdots \\
  g \\
  0 
\end{pmatrix} \] (20)

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Note that the simplest way to handle the boundary conditions in this problem consists of resetting the values of all the entries in the first and last rows of the stiffness matrix to zero (except for the first entry in the first row and last entry in the last row, which should be set to 1), together with resetting the first and last elements of the force vector to zero (the specified temperatures at the boundaries).

As a specific illustration of the development of the finite element formulation for transient problems consider the problem of one-dimensional, transient heat conduction without internal heat generation through a plane wall of thickness \( L = 1 \) with constant thermal properties. The heat equation is

\[
\frac{\partial T}{\partial t} = \alpha \frac{\partial^2 T}{\partial x^2} \tag{21}
\]

The problem is to be solved subject to the initial condition

\[
T(x,0) = T_0 \tag{22}
\]

and the boundary conditions

\[
T(0,t) = T(1,t) = 0 \tag{23}
\]

The Galerkin finite element method subdivides the domain \( 0 \leq x \leq 1 \) into a set of \( n \) intervals (finite elements) of size \( \Delta x \) connected at their ends (nodes). For each node \( i \), introduce the following shape function of position

\[
\phi_i(x) = \begin{cases} 
0 & 0 \leq x \leq x_{i-1} \\
N_1(x) & x_{i-1} \leq x \leq x_i \\
N_2(x) & x_i \leq x \leq x_{i+1} \\
0 & x_{i+1} \leq x \leq 1 
\end{cases} \tag{24}
\]

where

\[
N_1(x) = \frac{x - x_{i-1}}{\Delta x} \tag{25}
\]

and

\[
N_2(x) = \frac{x_{i+1} - x}{\Delta x} \tag{26}
\]

The function \( \phi_i \) is continuous and zero everywhere except for the interval \( x_{i-1} \leq x \leq x_{i+1} \), on which it consists of two linear segments with a maximum value of 1 attained at \( x = x_i \). The set of \( N_i \)'s is used to construct a linear combination to approximate \( T(x,t) \) as follows

\[
T(x,t) = \sum_{j=1}^{n} c_j(t) \phi_j(x) = \sum_{j=1}^{n} T_j(t) N_j(x) \tag{27}
\]

where the Fourier coefficients \( T_j \) are the values of \( T \) at the nodes \( j = 1, 2, ..., n \). Note that the Galerkin formulation separates the dependency of the problem on \( t \) from that of \( x \) through the use of the shape functions.
Furthermore, the set of functions $N_i$ possess an orthogonality property such that

$$
\int_0^1 N_i N_j dx = \begin{cases} 
0 & j \leq i - 2 \\
\Delta x/6 & j = i - 1 \\
\Delta x/3 & j = i \\
\Delta x/6 & j = i + 1 \\
0 & j \geq i + 2 
\end{cases}
$$

(28)

The Galerkin method is based in the weighed minimization of the residual $R = T_t - \alpha T_{xx}$ by constructing the scalar product $(R, N_i)$ of the (approximated) energy equation with the shape functions, i.e.

$$
(R, N_i) = \int_0^1 \int_0^t \left[ \frac{\partial T}{\partial t} - \alpha \frac{\partial^2 T}{\partial x^2} \right] N_i(x) dx dt = 0
$$

(29)

Note that the scalar product now involves integration over time as well as over space.

The same value of the integral is obtained if one first integrates over the interval $[x_{i-1}, x_{i+1}]$, for all $i$ and then collects all the resulting integrals, i.e.

$$
\sum_{i=1}^n \int_{x_{i-1}}^{x_{i+1}} \int_0^t \left[ \frac{\partial T}{\partial t} - \alpha \frac{\partial^2 T}{\partial x^2} \right] N_i(x) dx dt = 0
$$

(30)

Given the dependencies on $x$ and $t$, this can be written as

$$
\sum_{i=1}^n \int_{x_{i-1}}^{x_{i+1}} \int_0^t \left[ \frac{dT_j}{dt} N_j(x) N_i(x) - T_j(t) \alpha \frac{d^2 N_j(x)}{dx^2} N_i(x) \right] dx dt = 0
$$

(31)

This can now be written using matrix notation as a set of ordinary differential equations

$$
A \frac{d\vec{T}}{dt} + B \vec{T} = 0
$$

(32)

where $\vec{T}$ is the vector of nodal temperatures

$$
\vec{T} = (T_1, T_2, ..., T_n)^T
$$

(33)

and $A$ and $B$ are matrices defined by the scalar products

$$
A = a_{ij} = (N_j, N_i)
$$

(34)

and

$$
B = b_{ij} = (-\alpha \frac{d^2 N_j(x)}{dx^2}, N_i)
$$

(35)

In order to solve the resulting system of ordinary differential equations, consider the following generic implicit approximation with parameter $\theta$ such that $0 \leq \theta \leq 1$,

$$
A \left( \frac{\vec{T}_{t+\Delta t} - \vec{T}_t}{\Delta t} \right) + B(\theta \vec{T}_{t+\Delta t} + (1 - \theta) \vec{T}_t) = 0
$$

(36)

For any value of $\theta$, a system of algebraic equations has to be solved. As in the steady case, introduction of the boundary conditions requires modification of the finite element equations for the boundary nodes.
5 Boundary Conditions

Special care is required to handle more general boundary conditions. As an example consider the situation where the following condition applies at \( x = 0 \)

\[
\frac{\partial c}{\partial x} = \beta c + g
\]

where \( \beta \) and \( g \) can be functions of time. To derive a discrete equation for the node located at \( x = 0 \) one introduces a fictitious node located at \( x = 0 - h \) and uses centered differences to write

\[
\frac{c_{0+h,j} - c_{0-h,j}}{2h} = \beta c_{0,j} + g
\]

The fictitious node value \( c_{0-h,j} \) is then eliminated by combining the above with the corresponding finite difference formula (explicit, implicit or semi-implicit) which is assumed valid up to \( x = 0 - h \). The result is the algebraic equation for \( c_{0,j} \).

Alternatively, finite volume methods can be used to derive accurate and physically meaningful approximative equations for complex boundary conditions. This approach is sometimes preferred since it does not require consideration of auxiliary nodes.

An simple and convenient finite volume formulation of the boundary conditions is obtained by assuming that a certain amount of volume is associated with node 1. Consider heat conduction in a rectangular plate with constant internal heat generation and focus on the boundary conditions applied on the vertical edge located at \( x = 0 \). Consider the three contiguous nodes 1, 2 and 3. Node 1 is located at the boundary \( (x_1 = 0) \), node 2 is at a distance \( \Delta x \) from node 1 (i.e. \( x_2 = \Delta x \) and node 3 is at a distance \( \Delta x \) from node 2 (i.e. \( x_3 = x_2 + \Delta x \)). The associated finite volumes are as follows. Node 1 has volume on only one side \( (x > 0) \) and it value is \( \Delta x/2 \). The volumes of the finite volumes associated with nodes 2 and 3 are \( \Delta x \).

Let the heat flux at the boundary be specified by the boundary conditions and be given as \( q_1 \). Under steady state conditions, a discrete heat balance on the finite volume associated with node 1 yields

\[
q_1 + g \frac{\Delta x}{2} = -k_1 \frac{T_2 - T_1}{\Delta x}
\]

Under transient conditions, since the volume associated with the boundary node is finite, there is energy accumulation producing a time dependent change in its temperature and the appropriate form of the energy balance becomes

\[
q_1 + g \frac{\Delta x}{2} = -k_1 \frac{T_2^o - T_1^o}{\Delta x} + \rho C_p \frac{\Delta x}{2} \frac{T_1 - T_1^o}{\Delta t}
\]

where \( T_1^o \) and \( T_2^o \) are the temperatures at nodes 1 and 2 at the previous time step and \( T_1 \) is the temperature at node 1 at the next time step.
The above expressions produce an equation defining the value of $T_1$. Equations analogous to the above can be readily derived for all other boundaries. Such equations are added to the set obtained for all interior nodes and the system solved using standard techniques.

An alternative finite volume formulation equivalent to the one above has been incorporated in the research code CONDUCT. Consider again heat conduction in a rectangular plate and focus on the boundary conditions applied on the vertical edge located at $x = 0$. The finite volume closest to that edge is associated with three nodes. Node 1, located at the boundary, node 2, located inside the first finite volume at a distance $\delta$ from node 1, and node 3, located a distance $\delta x + \delta x_+$ away from node 2. Note that node 1 has the special feature of being located on the boundary of the first finite volume. This practice thus assumes that the finite volume associated with node 1 has volume of zero. Also, the right hand boundary of the finite volume is located a distance $\delta$ from node 2 (i.e. $2\delta = \Delta x$). If uniform mesh spacing were used in this scheme, the distance between nodes 1 and 2 would be half of that between any other pair of contiguous nodes.

A first approximation to the flux at the boundary of the finite volume, $q_2$ is given by

$$q_2 = \frac{k_2}{\delta}(T_1 - T_2)$$

A more accurate approximation is obtained by incorporating $T_3$. This is done by approximating the flux at a point $x$, $q$ between nodes 1 and 2 by the relationship

$$q = q_2 + \frac{q_3 - q_2}{2\delta} x$$

Rearrangement produces the following expression

$$q_2 = \frac{4}{3}\left[\frac{k_2}{\delta} \frac{T_1 - T_2}{\delta}\right] - \frac{1}{3} q_3$$

where

$$q_3 = \left[\left(\frac{\delta x}{k_2}\right) + \left(\frac{\delta x_+}{k_3}\right)\right]^{-1}(T_2 - T_3)$$

The above expressions can then be used to compute the value of $T_1$ for many different types of boundary conditions.

When a multidimensional problem exhibits cylindrical or spherical symmetry it can be represented as a one dimensional problem in polar coordinates. For example for radially symmetric diffusion from rods or spheres

$$\frac{\partial c}{\partial t} = \frac{D}{r^{\gamma}} \frac{\partial}{\partial r} \left(r^{\gamma} \frac{\partial c}{\partial r}\right) = c_t = D[c_{rr} + \frac{\gamma}{r} c_r]$$

where $\gamma = 1$ for systems with cylindrical symmetry and $\gamma = 2$ for systems with spherical symmetry. Subscript notation for derivatives is used for simplicity.
All ideas presented before can be directly applied here with little modification. However, special care is required to handle the symmetry condition at the origin $r = 0$. For symmetry, it is required that

$$\frac{\partial c}{\partial r} = 0$$

By means of a Maclaurin expansion one can show that at the origin, the following form of the diffusion equation is valid (when one has symmetry at the origin),

$$c_t = (\gamma + 1) D c_{rr}$$

These expressions can then be readily discretized to obtain finite difference formulae for the point at the origin.

If no symmetry can be assumed the following expressions can be used instead to approximate the Laplacian,

$$\nabla^2 c \approx \frac{4(c_{M,j} - c_{0,j})}{\Delta r^2}$$

for cylindrical systems and

$$\nabla^2 c \approx \frac{6(c_{M,j} - c_{0,j})}{\Delta r^2}$$

for spherical systems. Here $c_{M,j}$ is the nearest-neighbor mean value of $c$ obtained by averaging over all nearest neighbor nodes to the node at the origin. The above approximations can then be used in the original PDE to obtain finite difference formulae for $c_{0,j}$.

6 Computational Schemes

We can now use the discrete formulae given above to obtain numerical approximations to heat conduction and diffusion equations. Steady state problems in two dimensions are examined first followed by one-dimensional transient problems.

6.1 Steady State Problems

The 2D steady state energy equation with internal heat generation in rectangular Cartesian coordinates is

$$\frac{\partial}{\partial x} \left( k \frac{\partial T}{\partial x} \right) + \frac{\partial}{\partial y} \left( k \frac{\partial T}{\partial y} \right) + g(x, y) = 0$$

If $k$ and $g$ are assumed constant this becomes Poisson’s equation

$$\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} + \frac{g}{k} = 0$$
Furthermore, if \( g = 0 \) this reduces to Laplace’s equation

\[
\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} = 0
\]

In practice, these equations must be solved subject to suitable boundary conditions to obtain the function \( T(x, y) \).

As mentioned before, finite difference methods readily yield approximate solutions. Consider Laplace’s equation in a rectangular plate of width \( X \) and height \( Y \) subject to Dirichlet conditions as follows

\[
T(x, 0) = 0
\]
\[
T(0, y) = 0
\]
\[
T(X, y) = 0
\]

and

\[
T(x, Y) = y(x)
\]

Create a finite difference mesh of points \( x_i, i = 1, 2, 3, ..., N \) and \( y_j, j = 1, 2, 3, ..., M \). Nodes \((x_1, y_j), (x_N, y_j), (x_i, y_1)\) and \((x_i, y_M)\) are boundary nodes while the rest are interior nodes. The value of \( T \) at a specific nodal location \((x_i, y_j)\), will be denoted by \( T(x_i, y_j) \) and its numerical approximation will be \( T_{i,j} \).

For the interior nodes, a second order accurate finite difference approximation of Laplace’s equation is

\[
\frac{T_{i-1,j} - 2T_{i,j} + T_{i+1,j}}{\Delta x^2} + \frac{T_{i,j-1} - 2T_{i,j} + T_{i,j+1}}{\Delta y^2} = 0
\]

The equations for the boundary nodes are simply

\[
T(x_i, 0) = T_{i,1} = 0
\]

for \( i = 1, 2, ..., N \)

\[
T(0, y_j) = T_{1,j} = T(x_N, y_j) = T_{N,j} = 0
\]

and

\[
T(x_i, y_M) = T_{i,M} = f(x_i)
\]

The above is a system of \( N \times M \) simultaneous linear algebraic equations which must be solved to obtain the approximate values of the temperatures at the interior nodes.
Now we must proceed to the solution of the system of algebraic equations. To simplify, consider the case of the square plate \( X = Y \) with \( N = M \) and a uniform mesh with \( \Delta x = \Delta y = \Delta \). With this the finite difference equation for the interior node \((i, j)\) becomes

\[
T_{i-1,j} + T_{i,j-1} - 4T_{i,j} + T_{i+1,j} + T_{i,j+1} = 0
\]

This is the five point formula introduced earlier.

To obtain a banded matrix the mesh points must be relabeled sequentially from left to right and from top to bottom. The resulting system can be solved by Gaussian elimination if \( N \) and \( M \) are small and by SOR iteration when they are large.

Iteration methods can be used to solve this system of equations. These methods require an initial guess for \( T(x, y) \) and the final result must be independent of the guess. The iteration converges when the calculated temperature values at one iteration differ little from those obtained at the subsequent iteration.

In the Jacobi iteration method the interior nodes are visited sequentially and an improved guess of the value of \( T_{i,j} \) is calculated using the previous guess values of all neighboring nodes. If \( T_{i,j} \) represents the new value and \( T_{i,j}^o \) the old one the algorithm is

\[
T_{i,j} = \frac{T_{i-1,j}^o + T_{i,j-1}^o + T_{i+1,j}^o + T_{i,j+1}^o}{4}
\]

Note that in the Jacobi method, the temperature field is only updated once all the nodes have been visited.

Typically, nodes are visited from left to right and from bottom to top. I.e. \((2, 2), (3, 2), ..., (N-1, 2), (2, 3), (3, 3), ..., (N-1, M-1)\). Note that in this scheme, when visiting node \((i, j)\) nodes \((i-1, j)\) and \((i, j-1)\) would have already been visited (and improved guesses \( T_{i-1,j} \) and \( T_{i,j-1} \) would be available). Therefore, the Gauss-Seidel iteration uses calculated values as soon as they are available and the algorithm is

\[
T_{i,j} = \frac{T_{i-1,j} + T_{i,j-1} + T_{i+1,j} + T_{i,j+1}}{4}
\]

As a result of updating as the calculation proceeds, the Gauss-Seidel method converges at a faster rate than the Jacobi method.

It is possible to increase even more the speed of convergence by using the Successive Overrelaxation (SOR) method. First, note that the Gauss-Seidel algorithm can be rewritten as

\[
T_{i,j} = T_{i,j}^o + \frac{T_{i-1,j} + T_{i,j-1} - 4T_{i,j} + T_{i+1,j} + T_{i,j+1}}{4}
\]

The second term on the right hand side is the correction or displacement in the value of the temperature at node \((i, j)\) from \( T_{i,j}^o \) to \( T_{i,j} \).
The SOR method converges at a faster rate because larger corrections are done at each iteration, i.e.,

$$T_{i,j} = T^o_{i,j} + \omega \frac{T_{i-1,j} + T_{i,j-1} - 4T^o_{i,j} + T^o_{i+1,j} + T^o_{i,j+1}}{4}$$

where here the overrelaxation parameter $\omega$ is $1 \leq \omega \leq 2$.

6.2 Transient Problems: The Explicit Scheme

Consider the diffusion problem in a slab of thickness $L$

$$\frac{\partial c}{\partial t} = D \frac{\partial^2 c}{\partial x^2}$$

subject to suitable initial and boundary conditions. Using a forward difference in time to approximately represent the time rate of change of $c$ at nodal location $(x_i, t_j)$ yields

$$\frac{\partial c}{\partial t} \approx \frac{c(x_i, t_j + \Delta t) - c(x_i, t_j)}{\Delta t} = \frac{c_{i,j+1} - c_{i,j}}{\Delta t}$$

where $c_{i,j}$ is the numerical approximation to the value of $c(x_i, t_j)$.

A central difference approximation to the right hand side term around the same nodal location yields

$$D \frac{\partial^2 c}{\partial x^2} \approx D \frac{c(x_i + \Delta x, t_j) - 2c(x_i, t_j) + c(x_i - \Delta x, t_j)}{\Delta x^2} = D \frac{c_{i+1,j} - 2c_{i,j} + c_{i-1,j}}{\Delta x^2}$$

Substituting and rearranging gives the following explicit formula for the calculation of $c_{i,j+1}$ for all interior nodes $i$, i.e.

$$c_{i,j+1} = c_{i,j} + \frac{D\Delta t}{\Delta x^2}(c_{i+1,j} - 2c_{i,j} + c_{i-1,j})$$

If the problem to be solved involves the initial condition

$$c(x, 0) = c_0$$

and Dirichlet boundary conditions, for instance

$$c(0, t) = c(x_1, t_j) = c_1$$

and

$$c(L, t) = c(x_N, t_j) = c_N$$
The above equations completely define the values of $c$ at all the nodal locations. Since $c_{i,j}$, $c_{1,j}$ and $c_{N,j}$ are given, one computes only $c_{i,j+1}$ for $i = 2, 3, ..., N - 1$ and for all time levels $j + 1$.

An important limitation of the explicit scheme is that it is conditionally stable. It can be shown that the calculation of $c_{i,j}$ with the above method produces stable and physically meaningful results only as long as the Courant-Friedrichs-Lewy (CFL) condition is fulfilled, i.e. as long as

$$\frac{D\Delta t}{\Delta x^2} \leq \frac{1}{2}$$

### 6.3 Transient Problems: The Implicit Scheme

An alternative scheme is obtained using instead a central difference approximation to the right hand side term around the nodal location $(x_i, t_{j+1})$. This gives

$$\frac{\partial^2 c}{\partial x^2} \approx \frac{c(x_i + \Delta x, t_{j+1}) - 2c(x_i, t_{j+1}) + c(x_i - \Delta x, t_{j+1})}{\Delta x^2} = \frac{c_{i+1,j+1} - 2c_{i,j+1} + c_{i-1,j+1}}{\Delta x^2}$$

Substituting and rearranging gives the following implicit formula for the calculation of $c_{i,j+1}$ for all spatial nodes $i$ at time level $j + 1$, i.e.

$$-\frac{D\Delta t}{\Delta x^2}c_{i-1,j+1} + \left(2\frac{D\Delta t}{\Delta x^2} + 1\right)c_{i,j+1} - \frac{D\Delta t}{\Delta x^2}c_{i+1,j+1} = c_{i,j}$$

For given values of $c$ at the boundaries, the above formula constitutes a system of simultaneous algebraic equations the solution of which yields the desired values of $c_{i,j+1}$ for all $i = 2, 3, ..., N - 1$ and for all time levels $j + 1$.

Introducing the expressions

$$a_i = c_i = \frac{D\Delta t}{\Delta x^2}$$

$$b_i = 2\frac{D\Delta t}{\Delta x^2} + 1$$

and

$$d_i = c_{i,j}$$

the system of equations becomes

$$-a_i c_{i-1,j+1} + b_i c_{i,j+1} - c_i c_{i+1,j+1} = d_i$$
for \( i = 2, 3, ..., N - 1 \) for each and every time level \( j + 1 \) such that \( j = 1, 2, ..., M \). Recall that the values of \( c_{i,1} \) are given for all \( i \) by the initial condition of the problem.

The resulting system is tri-diagonal, the associated matrix is diagonally dominant and it is easily and efficiently solved by the Thomas algorithm.

The main idea in the Thomas algorithm is to first reduce the original tri-diagonal system of equations to a simple upper triangular form and then backsubstitute to determine the values of all the unknowns. Specifically, new variables \( \beta_i, S_i \) and \( D_i \) for \( i = 1, 2, 3, ..., N \) are introduced and computed as follows, first

\[
\beta_1 = \frac{d_1}{b_1}
\]

next, recursively for \( i = 2, 3, ..., N \)

\[
S_i = \frac{a_i}{b_{i-1}}
\]

\[
D_i = b_i - S_i c_{i-1}
\]

\[
\beta_i = d_i - S_i \beta_{i-1}
\]

Then, backsubstitution is performed to obtain the solution, first for \( i = N \)

\[
c_{N,j+1} = \frac{\beta_N}{D_N}
\]

and finally for \( i = N - 1, N - 2, ..., 2, 1 \) as follows

\[
c_{i,j+1} = \frac{(\beta_i - c_i c_{i+1,j+1})}{D_i}
\]

An advantage of the implicit scheme is that it is unconditionally stable. However, accuracy considerations preclude the use of large values of \( \Delta t \).

Consider the problem of transient heat conduction in a slab and recall the discrete fully implicit formula obtained when using the finite volume method

\[
a_P T_P = a_E T_E + a_W T_W + b
\]

where

\[
a_E = \frac{k_e}{\delta x_e},
\]

\[
a_W = \frac{k_w}{\delta x_w},
\]
Here the superscript \( \circ \) denotes time level \( t \) and the subscript \( P \) refers to the node located at \( x_i \). In this form, the implicit scheme leads to a tridiagonal system of algebraic equations which can be solved by the TDM algorithm described before.

### 6.4 The Semi-implicit Scheme

Still another possibility is to use weight averaging for the finite difference approximation of the right hand side term. Specifically, consider approximating the problem of diffusion in a slab using the method of finite differences. Recall that in this case the right hand side of the diffusion equation becomes

\[
\frac{\partial^2 c}{\partial x^2} \approx \frac{\theta c(x_i + \Delta x, t_{j+1}) - 2c(x_i, t_{j+1}) + c(x_i - \Delta x, t_{j+1})}{\Delta x^2} + (1 - \theta) \frac{c(x_i + \Delta x, t_j) - 2c(x_i, t_j) + c(x_i - \Delta x, t_j)}{\Delta x^2} = \\
= \theta \frac{c_{i+1,j+1} - 2c_{i,j+1} + c_{i+1,j+1}}{\Delta x^2} + (1 - \theta) \frac{c_{i,j} - 2c_{i,j} + c_{i+1,j}}{\Delta x^2}
\]

where \( 0 \leq \theta \leq 1 \).

Substituting and rearranging gives a semi-implicit formula for the calculation of \( c_{i,j+1} \) for all spatial nodes \( i \), i.e.

\[
-\frac{\theta D \Delta t}{\Delta x^2} c_{i-1,j+1} + (2\theta \frac{D \Delta t}{\Delta x^2} + 1)c_{i,j+1} - \frac{\theta D \Delta t}{\Delta x^2} c_{i+1,j+1} = \\
= c_{i,j} + (1 - \theta) \frac{D \Delta t}{\Delta x^2} (c_{i+1,j} - 2c_{i,j} + c_{i+1,j})
\]

The resulting system is also tridiagonal and it is also easily and efficiently solved by the Thomas algorithm. The scheme is also unconditionally stable. If \( \theta = \frac{1}{2} \) one obtains the Crank-Nicolson scheme.

Note that the above formula reduces to the explicit scheme when \( \theta = 0 \) and to the implicit scheme when \( \theta = 1 \).

Although the choice of \( \Delta x \) is arbitrary, the value of \( \Delta t \) may have to be selected based on stability or accuracy considerations.
Recall that the generic discrete expression of the energy balance produced by the finite volume method is

\[ a_P T_P = \sum a_{nb} T_{nb} + b \]

The Gauss-Seidel point by point method can be readily implemented to produce numerical approximations to the solution \( T_P \) for all nodes in a finite volume discretization. To do this rewrite the above equation as

\[ T_P = \frac{\sum a_{nb} T_{nb}^* + b}{a_P} \]

where \( T_{nb}^* \) stands for the nearest neighbor value of \( T \) currently existing in the storage memory of the computer. This is the most recently calculated value for those neighbors that have already been visited by the computational algorithm but is the value obtained in the previous iteration for those yet to be visited nodes. Convergence of the Gauss-Seidel method is assured if the associated matrix of coefficients is strictly diagonally dominant. A sufficient condition for convergence is then that

\[ \frac{\sum |a_{nb}|}{|a_P|} \leq 1 \]

The rate of convergence can be significantly improved by implementing the line by line iteration method. In this method one focuses on the nodes lying along a selected coordinate direction (say \( y \)). If the discrete equation is written such that only those nodes are regarded as unknowns at any given iteration step then the resulting system of equations only involves \( T_P, T_N \) and \( T_S \), i.e. it is a tridiagonal system. Systems of this form are solve very efficiently using the TDMA algorithm. The line by line iteration method then proceeds by visiting lines of nodes, one at a time, and solving for the all the \( T_P \)'s along the line using the most recent values of \( T_{nb} \) existing in the memory of the computer. The entire mesh is visited in this fashion until convergence is achieved. The result represents the value of \( T \) for all nodes at position \((x, y, z)\) and time \( t \).

7 Exercises

**Exercise 1.** Derive the equation for \( q_2 \) implemented in the code CONDUCT.

**Exercise 2.** Consider steady state heat conduction in a thin square plate of edge = 100 cm. The edges \( x = 0, x = l \) and \( y = 0 \) are maintained at \( u = 0 \) while at the edge \( y = d \) \( u(x, d) = 100 \). No heat flow along the \( z \) direction perpendicular to the plate. The required temperature \( u(x, y) \) satisfies

\[ \frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} = 0 \]
This problem is readily solved in closed form by separation of variables yielding

\[ T(x, y) = \sum_{n=1}^{\infty} c_n \sin\left(\frac{n\pi}{100} x\right) \frac{\sinh\left(\frac{n\pi}{100} y\right)}{\sinh(n\pi)} \]

with

\[ c_n = \begin{cases} 
0 & n \text{ even} \\
\frac{400}{n\pi} & n \text{ odd}
\end{cases} \]

Solve the above problem numerically using the finite difference method and compare your results against the analytical solution.

**Exercise 3.** Derive the finite difference formula analog to the transient 1D diffusion equation using the explicit scheme.

**Exercise 4.** Derive the finite difference formula analog to the transient 1D diffusion equation using the implicit scheme.

**Exercise 5.** Obtain the expressions for \(a_i, b_i, c_i\) and \(d_i\) for the C-N scheme applied to the diffusion equation.

**Exercise 6.** A large, 0.1 meter thick steel slab emerges from a rolling mill with a uniform temperature of 1000 degrees Celsius and is left to cool by convection into an environment at zero degrees Celsius. For this steel \(k = 50W/mK\), \(\rho = 7,900kg/m^3\) and \(C_p = 470J/kgK\). Assume the heat transfer coefficient is \(h = 250W/m^2K\). Investigate the cooling process by solving the problem numerically using a finite difference method and explicit, implicit and semi-implicit schemes. Compare your results against the analytical solution and investigate the sensitivity of the results to the mesh resolution.

**Exercise 7.** A solid pure iron cylinder with radius \(a = 0.01\) m is exposed to a carburizing environment which fixes the surface concentration of carbon to 1 percent \(c_S = 0.01\). For a temperature of 1000 degrees Celsius, \(D = 10^{-11}m^2/s\) is the diffusivity of carbon in the austenite phase of iron. Use the method of finite differences to map out the progress of this carburization treatment.

8 References