

Chapter 2

Finite Difference Method

2.1 Classification of Partial Differential Equations

For analysing the equations for fluid flow problems, it is convenient to consider the case of a second-order differential equation given in the general form as

$$A \frac{\partial^2 \phi}{\partial x^2} + B \frac{\partial^2 \phi}{\partial x \partial y} + C \frac{\partial^2 \phi}{\partial y^2} + D \frac{\partial \phi}{\partial x} + E \frac{\partial \phi}{\partial y} + F \phi = G(x, y) \quad (2.1)$$

In the coefficients A, B, C, D, E and F are either constants or functions of only (x, y) (do not contain ϕ or its derivatives), it is said to be a linear equation, otherwise it is a non-linear equation. An important subclass of non-linear equations is quasilinear equations. In this case, the coefficients may contain ϕ or its first derivative but not the second (highest) derivative. If $G = 0$, the aforesaid equation is homogeneous, otherwise it is non-homogeneous.

Again for the above mentioned equation

- if $B^2 - 4AC = 0$, the equation is parabolic
- if $B^2 - 4AC < 0$, the equation is elliptic
- if $B^2 - 4AC > 0$, the equation is hyperbolic

The unsteady Navier-Stokes equations are elliptic in space and parabolic in time. At steady-state, the Navier-Stokes equations are elliptic. In elliptic problems, the boundary conditions must be applied on all confining surfaces. These are boundary value problems. A physical problem may be steady or unsteady. In the following text, we shall discuss mathematical aspects of some of the equations that describe fluid flow and heat transfer problems.

The Laplace equations and the Poisson equations are generally associated with the steady-state problems. These are elliptic equations and can be written

2.2 Computational Fluid Dynamics

respectively as

$$\frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2} = 0 \quad (2.2)$$

$$\frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2} + S = 0 \quad (2.3)$$

The velocity potential in steady, inviscid, incompressible, and irrotational flows satisfies the Laplace equation. The temperature distribution for steady-state, constant-property, two-dimensional conduction satisfies the Laplace equation if no volumetric heat source is present in the domain of interest and the Poisson equation if a volumetric heat source is present.

The parabolic equation in conduction heat transfer is of the form

$$\frac{\partial \phi}{\partial t} = B \frac{\partial^2 \phi}{\partial x^2} \quad (2.4)$$

The one-dimensional unsteady conduction problem is governed by this equation when t and x are identified as the time and space variables, respectively ϕ denotes the temperature and B is the thermal diffusivity. The boundary conditions at the two ends and an initial condition are needed to solve such equations. The unsteady conduction problem in two- dimensions is governed by an equation of the form

$$\frac{\partial \phi}{\partial t} = B \left(\frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2} \right) + S \quad (2.5)$$

Here t denotes the time variable, and a source term S is included. By comparing the highest derivatives in any two of the independent variables, with the help of the conditions given earlier, it can be concluded that Eq. (2.5) is parabolic in time and elliptic in space. An initial condition and two conditions for the extreme ends in each spacial coordinate is required to solve this equation.

Fluid flow problems generally have nonlinear terms due to the inertia or acceleration component in the momentum equation. These terms are called advection terms. The energy equation has nearly similar terms, usually called the convection terms, which involve the motion of the flow field. For unsteady two-dimensional problems, the appropriate equations can be represented as

$$\frac{\partial \phi}{\partial t} + u \frac{\partial \phi}{\partial x} + v \frac{\partial \phi}{\partial y} = B \left(\frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2} \right) + S \quad (2.6)$$

where ϕ denotes velocity, temperature or some other transported property, u and v are velocity components, B is the diffusivity for momentum or heat, and S is a source term. The pressure gradients in the momentum or the volumetric heating in the energy equation can be appropriately substituted in S . Eq. (2.6) is parabolic in time and elliptic in space. However, for very high-speed flows, the terms on the left side dominate, the second-order terms on the right hand side become trivial, and the equation becomes hyperbolic in time and space.

2.1.1 Boundary and Initial Conditions

In addition to the governing differential equations, the formulation of the problem requires a complete specification of the geometry of interest and appropriate boundary conditions. An arbitrary domain and bounding surfaces are sketched in Fig. 2.1. The conservation equations are to be applied within the domain. The number of boundary conditions required is generally determined by the order of the highest derivatives appearing in each independent variable in the governing differential equations.

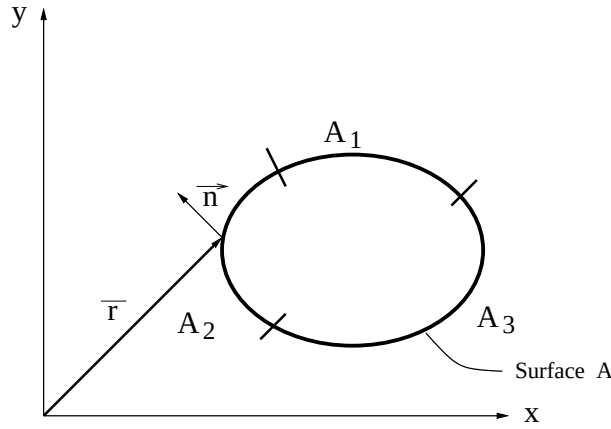


Figure 2.1: Schematic sketch of an arbitrary domain.

The unsteady problems governed by a first derivative in time will require initial condition in order to carry out the time integration. The diffusion terms require two spatial boundary conditions for each coordinate in which a second derivative appears.

The spatial boundary conditions in flow and heat transfer problems are of three general types. They may be stated

$$\phi = \phi_1(r) \quad \in A_1 \quad (2.7)$$

$$\frac{\partial \phi}{\partial n} = \phi_2(r) \quad \in A_2 \quad (2.8)$$

$$a(r)\phi + b(r)\frac{\partial \phi}{\partial n} = \phi_3(r) \quad \in A_3 \quad (2.9)$$

where A_1 , A_2 and A_3 denote three separate zones on the bounding surface in Fig. 2.1. The boundary conditions on ϕ in Eqns. (2.7) to (2.9) are usually referred to as Dirichlet, Neumann and mixed boundary conditions, respectively. The boundary conditions are linear in the dependant variable ϕ .

In Eqns. (2.7) to (2.8), $\vec{r} = \vec{r}(x, y)$ is a vector denoting position on the boundary,

2.4 Computational Fluid Dynamics

$\frac{\partial}{\partial n}$ is the directional derivative normal to the boundary, and $\phi_1, \phi_2, \phi_3, a$, and b are arbitrary functions. The normal derivative may be expressed as

$$\begin{aligned}\frac{\partial \phi}{\partial n} &= \vec{n} \cdot \nabla \phi \\ &= (n_x \hat{i} + n_y \hat{j}) \cdot \left(\frac{\partial \phi}{\partial x} \hat{i} + \frac{\partial \phi}{\partial y} \hat{j} \right) \\ &= n_x \frac{\partial \phi}{\partial x} + n_y \frac{\partial \phi}{\partial y}\end{aligned}\tag{2.10}$$

Here, $\vec{n}$ is the unit vector normal to the boundary, ∇ is the nabla operator, $[\cdot]$ denotes the dot product, (n_x, n_y) are the direction-cosine components of $\vec{n}$ and $(\hat{i}, \hat{j})$ are the unit vectors aligned with the (x, y) coordinates.

2.2 Finite Differences

Analytical solutions of partial differential equations provide us with closed-form expressions which depict the variation of the dependant variables in the domain. The numerical solutions, based on finite differences, provide us with the values at discrete points in the domain which are known as grid points. Consider Fig. 2.2, which shows a domain of calculation in the $x - y$ plane. Let us assume that the spacing of the grid points in the x -direction is uniform, and given by Δx . Likewise, the spacing of the points in the y -direction is also uniform, and given by Δy . It is not necessary that Δx or Δy be uniform. We could imagine unequal spacing in both directions, where different values of Δx between each successive pairs of grid points are used. The same could be presumed for Δy as well. However, often, problems are solved on a grid which involves uniform spacing in each direction, because this simplifies the programming, and often results in higher accuracy. In some class of problems, the numerical calculations are performed on a transformed computational plane which has uniform spacing in the transformed-independent-variables, but non-uniform spacing in the physical plane. These typical aspects will be discussed later in the Chapter on grid generation. In the present chapter we shall consider uniform spacing in each coordinate direction. According to our consideration, Δx and Δy are constants, but it is not mandatory that Δx be equal to Δy .

Let us once again refer to Fig. 2.2. The grid points are identified by an index i which increases in the positive x -direction, and an index j , which increases in the positive y -direction. If (i, j) is the index of point P in Fig. 2.2, then the point immediately to the right is designated as $(i + 1, j)$ and the point immediately to the left is $(i - 1, j)$. Similarly the point directly above is $(i, j + 1)$, and the point directly below is $(i, j - 1)$. The basic philosophy of finite difference methods is to replace the derivatives of the governing equations with algebraic difference quotients. This will result in a system of algebraic equations which can be solved for the dependant variables at the discrete grid points in the flow field. Let us

now look at some of the common algebraic difference quotients in order to be acquainted with the methods related to discretization of the partial differential equations.

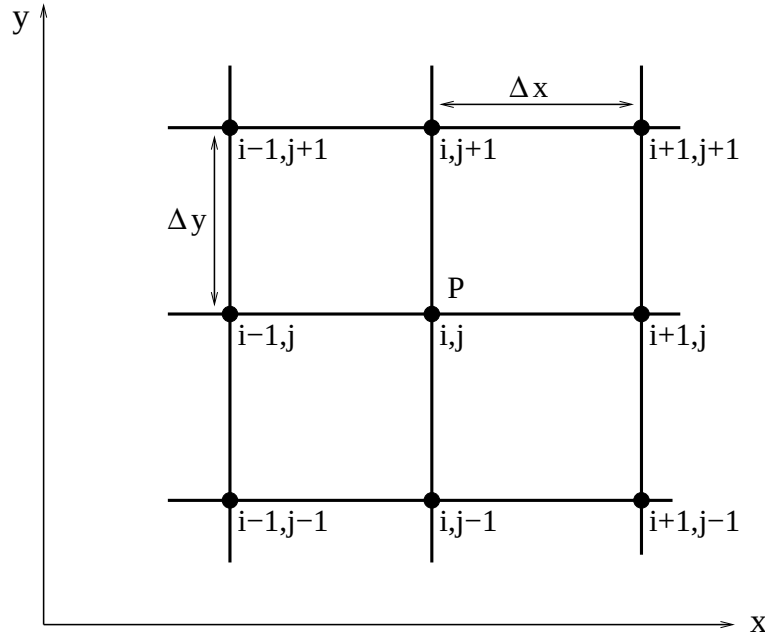


Figure 2.2: Discrete grid points.

2.2.1 Elementary Finite Difference Quotients

Finite difference representations of derivatives are derived from Taylor series expansions. For example, if $u_{i,j}$ is the x -component of the velocity $u_{i+1,j}$ at point $(i+1, j)$ can be expressed in terms of Taylor series expansion about point (i, j) as

$$u_{i+1,j} = u_{i,j} + \left(\frac{\partial u}{\partial x} \right)_{i,j} \Delta x + \left(\frac{\partial^2 u}{\partial x^2} \right)_{i,j} \frac{(\Delta x)^2}{2} + \left(\frac{\partial^3 u}{\partial x^3} \right)_{i,j} \frac{(\Delta x)^3}{6} + \dots \quad (2.11)$$

Mathematically, Eq. (2.11) is an exact expression for $u_{i+1,j}$ if the series converges. In practice, Δx is small and any higher-order term of Δx is smaller than Δx . Hence, for any function $u(x)$, Eq. (2.11) can be truncated after a finite number of terms. For example, if terms of magnitude $(\Delta x)^3$ and higher order are neglected, Eq. (2.11) becomes

$$u_{i+1,j} \approx u_{i,j} + \left(\frac{\partial u}{\partial x} \right)_{i,j} \Delta x + \left(\frac{\partial^2 u}{\partial x^2} \right)_{i,j} \frac{(\Delta x)^2}{2} \dots \quad (2.12)$$

2.6 Computational Fluid Dynamics

Eq. (2.12) is second-order accurate, because terms of order $(\Delta x)^3$ and higher have been neglected. If terms of order $(\Delta x)^2$ and higher are neglected, Eq. (2.12) is reduced to

$$u_{i+1,j} \approx u_{i,j} + \left(\frac{\partial u}{\partial x} \right)_{i,j} \Delta x \quad (2.13)$$

Eq. (2.13) is first-order accurate. In Eqns. (2.12) and (2.13) the neglected higher-order terms represent the truncation error. Therefore, the truncation errors for Eqns. (2.12) and (2.13) are

$$\sum_{n=3}^{\infty} = \left(\frac{\partial^n u}{\partial x^n} \right)_{i,j} \frac{(\Delta x)^n}{n!}$$

and

$$\sum_{n=2}^{\infty} = \left(\frac{\partial^n u}{\partial x^n} \right)_{i,j} \frac{(\Delta x)^n}{n!}$$

It is now obvious that the truncation error can be reduced by retaining more terms in the Taylor series expansion of the corresponding derivative and reducing the magnitude of Δx .

Let us once again return to Eq. (2.11) and solve for $(\partial u / \partial x)_{i,j}$ as:

$$\left(\frac{\partial u}{\partial x} \right)_{i,j} = \frac{u_{i+1,j} - u_{i,j}}{\Delta x} - \left(\frac{\partial^2 u}{\partial x^2} \right)_{i,j} \frac{\Delta x}{2} - \left(\frac{\partial^3 u}{\partial x^3} \right)_{i,j} \frac{(\Delta x)^2}{6} + \dots$$

or

$$\left(\frac{\partial u}{\partial x} \right)_{i,j} = \frac{u_{i+1,j} - u_{i,j}}{\Delta x} + \mathcal{O}(\Delta x) \quad (2.14)$$

In Eq. (2.14) the symbol $\mathcal{O}(\Delta x)$ is a formal mathematical nomenclature which means “terms of order of Δx ”, expressing the order of magnitude of the truncation error. The first-order-accurate difference representation for the derivative $(\partial u / \partial x)_{i,j}$ expressed by Eq. (2.14) can be identified as a **first-order forward** difference. We now consider a Taylor series expansion for $u_{i-1,j}$, about $u_{i,j}$

$$u_{i-1,j} = u_{i,j} + \left(\frac{\partial u}{\partial x} \right)_{i,j} (-\Delta x) + \left(\frac{\partial^2 u}{\partial x^2} \right)_{i,j} \frac{(-\Delta x)^2}{2} + \left(\frac{\partial^3 u}{\partial x^3} \right)_{i,j} \frac{(-\Delta x)^3}{6} + \dots$$

or

$$u_{i-1,j} = u_{i,j} - \left(\frac{\partial u}{\partial x} \right)_{i,j} (\Delta x) + \left(\frac{\partial^2 u}{\partial x^2} \right)_{i,j} \frac{(\Delta x)^2}{2} - \left(\frac{\partial^3 u}{\partial x^3} \right)_{i,j} \frac{(\Delta x)^3}{6} + \dots \quad (2.15)$$

Solving for $(\partial u / \partial x)_{i,j}$, we obtain

$$\left(\frac{\partial u}{\partial x} \right)_{i,j} = \frac{u_{i,j} - u_{i-1,j}}{\Delta x} + \mathcal{O}(\Delta x) \quad (2.16)$$

Eq. (2.16) is a **first-order backward** expression for the derivative $(\partial u/\partial x)$ at grid point (i, j) .

Subtracting Eq. (2.15) from (2.11)

$$u_{i+1,j} - u_{i-1,j} = 2\left(\frac{\partial u}{\partial x}\right)_{i,j}(\Delta x) + \left(\frac{\partial^3 u}{\partial x^3}\right)_{i,j} \frac{(\Delta x)^3}{3} + \dots \quad (2.17)$$

and solving for $(\partial u/\partial x)_{i,j}$ from Eq. (2.17) we obtain

$$\left(\frac{\partial u}{\partial x}\right)_{i,j} = \frac{u_{i+1,j} - u_{i-1,j}}{2\Delta x} + \mathcal{O}(\Delta x)^2 \quad (2.18)$$

Eq. (2.18) is a **second-order central** difference for the derivative $(\partial u/\partial x)$ at grid point (i, j) .

In order to obtain a finite-difference for the second-order partial derivative $(\partial^2 u/\partial x^2)_{i,j}$, add Eq. (2.11) and (2.15). This produces

$$u_{i+1,j} + u_{i-1,j} = 2u_{i,j} + \left(\frac{\partial^2 u}{\partial x^2}\right)_{i,j}(\Delta x)^2 + \left(\frac{\partial^4 u}{\partial x^4}\right)_{i,j} \frac{(\Delta x)^4}{12} + \dots \quad (2.19)$$

Solving Eq. (2.19) for $(\partial^2 u/\partial x^2)_{i,j}$, we obtain

$$\left(\frac{\partial^2 u}{\partial x^2}\right)_{i,j} = \frac{u_{i+1,j} - 2u_{i,j} + u_{i-1,j}}{(\Delta x)^2} + \mathcal{O}(\Delta x)^2 \quad (2.20)$$

Eq. (2.20) is a second-order central difference form for the derivative $(\partial^2 u/\partial x^2)$ at grid point (i, j) .

Difference quotients for the y -derivatives are obtained in exactly the similar way. The results are analogous to the expressions for the x -derivatives.

$$\begin{aligned} \left(\frac{\partial u}{\partial y}\right)_{i,j} &= \frac{u_{i,j+1} - u_{i,j}}{\Delta y} + \mathcal{O}(\Delta y) && \text{[Forward difference]} \\ \left(\frac{\partial u}{\partial y}\right)_{i,j} &= \frac{u_{i,j} - u_{i,j-1}}{\Delta y} + \mathcal{O}(\Delta y) && \text{[Backward difference]} \\ \left(\frac{\partial u}{\partial y}\right)_{i,j} &= \frac{u_{i,j+1} - u_{i,j-1}}{2\Delta y} + \mathcal{O}(\Delta y)^2 && \text{[Central difference]} \\ \left(\frac{\partial^2 u}{\partial y^2}\right)_{i,j} &= \frac{u_{i,j+1} - 2u_{i,j} + u_{i,j-1}}{(\Delta y)^2} + \mathcal{O}(\Delta y)^2 && \text{[Central difference of second} \\ &&& \text{derivative]} \end{aligned}$$

It is interesting to note that the central difference given by Eq. (2.20) can be interpreted as a forward difference of the first order derivatives, with backward differences in terms of dependent variables for the first-order derivatives. This is because

$$\left(\frac{\partial^2 u}{\partial x^2}\right)_{i,j} = \left[\frac{\partial}{\partial x} \left(\frac{\partial u}{\partial x} \right) \right]_{i,j} = \frac{\left(\frac{\partial u}{\partial x}\right)_{i+1,j} - \left(\frac{\partial u}{\partial x}\right)_{i,j}}{\Delta x}$$

2.8 Computational Fluid Dynamics

or

$$\left(\frac{\partial^2 u}{\partial x^2}\right)_{i,j} = \left[\left(\frac{u_{i+1,j} - u_{i,j}}{\Delta x}\right) - \left(\frac{u_{i,j} - u_{i-1,j}}{\Delta x}\right)\right] \frac{1}{\Delta x}$$

or

$$\left(\frac{\partial^2 u}{\partial x^2}\right)_{i,j} = \frac{u_{i+1,j} - 2u_{i,j} + u_{i-1,j}}{(\Delta x)^2}$$

The same approach can be made to generate a finite difference quotient for the mixed derivative $(\partial^2 u / \partial x \partial y)$ at grid point (i, j) . For example,

$$\frac{\partial^2 u}{\partial x \partial y} = \frac{\partial}{\partial x} \left(\frac{\partial u}{\partial y} \right) \quad (2.21)$$

In Eq. (2.21), if we write the x -derivative as a central difference of y -derivatives, and further make use of central differences to find out the y -derivatives, we obtain

$$\begin{aligned} \frac{\partial^2 u}{\partial x \partial y} &= \frac{\partial}{\partial x} \left(\frac{\partial u}{\partial y} \right) = \frac{\left(\frac{\partial u}{\partial y}\right)_{i+1,j} - \left(\frac{\partial u}{\partial y}\right)_{i-1,j}}{2(\Delta x)} \\ \left(\frac{\partial^2 u}{\partial x \partial y}\right) &= \left[\left(\frac{u_{i+1,j+1} - u_{i+1,j-1}}{2(\Delta y)}\right) - \left(\frac{u_{i-1,j+1} - u_{i-1,j-1}}{2(\Delta y)}\right)\right] \frac{1}{2(\Delta x)} \\ \left(\frac{\partial^2 u}{\partial x \partial y}\right) &= \frac{1}{4\Delta x \Delta y} (u_{i+1,j+1} + u_{i-1,j-1} - u_{i+1,j-1} - u_{i-1,j+1}) + \mathcal{O}[(\Delta x)^2, (\Delta y)^2] \end{aligned} \quad (2.22)$$

Combinations of such finite difference quotients for partial derivatives form finite difference expressions for the partial differential equations. For example, the Laplace equation $\nabla^2 u = 0$ in two dimensions, becomes

$$\frac{u_{i+1,j} - 2u_{i,j} + u_{i-1,j}}{(\Delta x)^2} + \frac{u_{i,j+1} - 2u_{i,j} + u_{i,j-1}}{(\Delta y)^2} = 0$$

or

$$u_{i+1,j} + u_{i-1,j} + \lambda^2(u_{i,j+1} + u_{i,j-1}) - 2(1 + \lambda^2)u_{i,j} = 0 \quad (2.23)$$

where λ is the mesh aspect ratio $(\Delta x)/(\Delta y)$. If we solve the Laplace equation on a domain given by Fig. 2.2, the value of $u_{i,j}$ will be

$$u_{i,j} = \frac{u_{i+1,j} + u_{i-1,j} + \lambda^2(u_{i,j+1} + u_{i,j-1})}{2(1 + \lambda^2)} \quad (2.24)$$

It can be said that many other forms of difference approximations can be obtained for the derivatives which constitute the governing equations for fluid flow and heat transfer. The basic procedure, however, remains the same. In order to appreciate some more finite difference representations see Tables 2.1 and 2.2. Interested readers are referred to Anderson, Tannehill and Pletcher (1984) for more insight into different kind of discretization methods.

2.3 Basic Aspects of Finite-Difference Equations

Here we shall look into some of the basic aspects of difference equations. Consider the following one dimensional unsteady state heat conduction equation. The dependent variable u (temperature) is a function of x and t (time) and α is a constant known as thermal diffusivity.

$$\frac{\partial u}{\partial t} = \alpha \frac{\partial^2 u}{\partial x^2} \quad (2.25)$$

It is to be noted that Eq. (2.25) is classified as a parabolic partial differential equation.

If we substitute the time derivative in Eq. (2.25) with a forward difference, and a spatial derivative with a central difference (usually called FTCS, **F**orward **T**ime **C**entral **S**pace method of discretization), we obtain

$$\frac{u_i^{n+1} - u_i^n}{\Delta t} = \alpha \left[\frac{u_{i+1}^n - 2u_i^n + u_{i-1}^n}{(\Delta x)^2} \right] \quad (2.26)$$

In Eq. (2.26), the index for time appears as a superscript, where n denotes conditions at time t , $(n+1)$ denotes conditions at time $(t + \Delta t)$, and so on. The subscript denotes the grid point in the spatial dimension.

However, there must be a truncation error for the equation because each one of the finite-difference quotients has been taken from a truncated series. Considering Eqns. (2.25) and (2.26), and looking at the truncation errors associated with the difference quotients we can write

$$\begin{aligned} \frac{\partial u}{\partial t} - \alpha \frac{\partial^2 u}{\partial x^2} &= \frac{u_i^{n+1} - u_i^n}{\Delta t} - \alpha \frac{u_{i+1}^n - 2u_i^n + u_{i-1}^n}{(\Delta x)^2} \\ &+ \left[- \left(\frac{\partial^2 u}{\partial t^2} \right)_i \frac{(\Delta t)}{2} + \alpha \left(\frac{\partial^4 u}{\partial x^4} \right)_i \frac{(\Delta x)^2}{12} + \dots \right] \end{aligned} \quad (2.27)$$

In Eq. (2.27), the terms in the square brackets represent truncation error for the complete equation. It is evident that the truncation error (TE) for this representation is $\mathcal{O}[\Delta t, (\Delta x)^2]$.

With respect to Eq. (2.27), it can be said that as $\Delta x \rightarrow 0$ and $\Delta t \rightarrow 0$, the truncation error approaches zero. Hence, in the limiting case, the difference equation also approaches the original differential equation. Under such circumstances, the finite difference representation of the partial differential equation is said to be *consistent*.

2.3.1 Consistency

A finite difference representation of a partial differential equation (PDE) is said to be consistent if we can show that the difference between the PDE and its finite difference (FDE) representation vanishes as the mesh is refined, i.e.,

$$\lim_{\text{mesh} \rightarrow 0} (PDE - FDE) = \lim_{\text{mesh} \rightarrow 0} (TE) = 0$$

Table 2.1: Difference Approximations for Derivatives

$\left(\frac{\partial^3 u}{\partial x^3}\right)_{i,j}$	$= \frac{u_{i+2,j} - 2u_{i+1,j} + 2u_{i-1,j} - u_{i-2,j}}{2h^3} + \mathcal{O}(h^2)$
$\left(\frac{\partial^4 u}{\partial x^4}\right)_{i,j}$	$= \frac{u_{i+2,j} - 4u_{i+1,j} + 6u_{i,j} - 4u_{i-1,j} + u_{i-2,j}}{h^4} + \mathcal{O}(h^2)$
$\left(\frac{\partial^2 u}{\partial x^2}\right)_{i,j}$	$= \frac{-u_{i+3,j} + 4u_{i+2,j} - 5u_{i+1,j} + 2u_{i,j}}{h^2} + \mathcal{O}(h^2)$
$\left(\frac{\partial u}{\partial x}\right)_{i,j}$	$= \frac{-u_{i+2,j} + 8u_{i+1,j} - 8u_{i-1,j} + u_{i-2,j}}{12h} + \mathcal{O}(h^4)$
$\left(\frac{\partial^2 u}{\partial x^2}\right)_{i,j}$	$= \frac{-u_{i+2,j} + 16u_{i+1,j} - 30u_{i,j} + 16u_{i-1,j} - u_{i-2,j}}{12h^2} + \mathcal{O}(h^4)$
h	$= \text{grid spacing in } x\text{-direction}$

Table 2.2: Difference Approximations for Mixed Partial Derivatives

$\left(\frac{\partial^2 u}{\partial x \partial y}\right)_{i,j}$	$= \frac{1}{\Delta x} \left(\frac{u_{i+1,j} - u_{i+1,j-1}}{\Delta y} - \frac{u_{i,j} - u_{i,j-1}}{\Delta y} \right) + \mathcal{O}(\Delta x, \Delta y)$
$\left(\frac{\partial^2 u}{\partial x \partial y}\right)_{i,j}$	$= \frac{1}{\Delta x} \left(\frac{u_{i,j+1} - u_{i,j}}{\Delta y} - \frac{u_{i-1,j+1} - u_{i-1,j}}{\Delta y} \right) + \mathcal{O}(\Delta x, \Delta y)$
$\left(\frac{\partial^2 u}{\partial x \partial y}\right)_{i,j}$	$= \frac{1}{\Delta x} \left(\frac{u_{i+1,j+1} - u_{i+1,j-1}}{2\Delta y} - \frac{u_{i,j+1} - u_{i,j-1}}{2\Delta y} \right) + \mathcal{O}[(\Delta x), (\Delta y)^2]$
$\left(\frac{\partial^2 u}{\partial x \partial y}\right)_{i,j}$	$= \frac{1}{2\Delta x} \left(\frac{u_{i+1,j+1} - u_{i+1,j-1}}{2\Delta y} - \frac{u_{i-1,j+1} - u_{i-1,j-1}}{2\Delta y} \right) + \mathcal{O}[(\Delta x)^2, (\Delta y)^2]$
$\left(\frac{\partial^2 u}{\partial x \partial y}\right)_{i,j}$	$= \frac{1}{2\Delta x} \left(\frac{u_{i+1,j} - u_{i+1,j-1}}{\Delta y} - \frac{u_{i-1,j} - u_{i-1,j-1}}{\Delta y} \right) + \mathcal{O}[(\Delta x)^2, (\Delta y)]$

A questionable scheme would be one for which the truncation error is $\mathcal{O}(\Delta t/\Delta x)$ and not explicitly $\mathcal{O}(\Delta t)$ or $\mathcal{O}(\Delta x)$ or higher orders. In such cases the scheme would not be formally consistent unless the mesh were refined in a manner such that $(\Delta t/\Delta x) \rightarrow 0$. Let us take Eq. (2.25) and the Dufort-Frankel (1953) differencing scheme. The FDE is

$$\frac{u_i^{n+1} - u_i^{n-1}}{2\Delta t} = \alpha \left[\frac{u_{i+1}^n - u_i^{n+1} - u_i^{n-1} + u_{i-1}^n}{(\Delta x)^2} \right] \quad (2.28)$$

Now the leading terms of truncated series form the truncation error for the complete equation:

$$\frac{\alpha}{12} \left(\frac{\partial^4 u}{\partial x^4} \right)_i (\Delta x)^2 - \alpha \left(\frac{\partial^2 u}{\partial t^2} \right)_i \left(\frac{\Delta t}{\Delta x} \right)^2 - \frac{1}{6} \left(\frac{\partial^3 u}{\partial t^3} \right)_i (\Delta t)^2$$

The above expression for truncation error is meaningful if $(\Delta t/\Delta x) \rightarrow 0$ together with $\Delta t \rightarrow 0$ and $\Delta x \rightarrow 0$. However, (Δt) and (Δx) may individually approach zero in such a way that $(\Delta t/\Delta x) = \beta$. Then if we reconstitute the PDE from FDE and TE, we shall obtain

$$\lim_{\Delta t, \Delta x \rightarrow 0} (PDE - FDE) = \lim_{mesh \rightarrow 0} (TE) = -\alpha\beta^2 \left(\frac{\partial^2 u}{\partial t^2} \right)$$

and finally PDE becomes

$$\frac{\partial u}{\partial t} + \alpha\beta^2 \frac{\partial^2 u}{\partial t^2} = \alpha \frac{\partial^2 u}{\partial x^2}$$

We started with a parabolic one and ended with a hyperbolic one!

So, DuFort-Frankel scheme is not consistent for the 1D unsteady state heat conduction equation unless $(\Delta t/\Delta x) \rightarrow 0$ together with $\Delta t \rightarrow 0$ and $\Delta x \rightarrow 0$.

2.3.2 Convergence

A solution of the algebraic equations that approximate a partial differential equation (PDE) is convergent if the approximate solution approaches the exact solution of the PDE for each value of the independent variable as the grid spacing tends to zero. The requirement is

$$u_i^n = \bar{u}(x_i, t_n) \quad \text{as } \Delta x, \Delta t \rightarrow 0$$

where, $\bar{u}(x_i, t_n)$ is the solution of the system of algebraic equations.

2.3.3 Explicit and Implicit Methods

The solution of Eq. (2.26) takes the form of a “marching” procedure (or scheme) in steps of time. We know the dependent variable at all x at a time level

2.12 Computational Fluid Dynamics

from given initial conditions. Examining Eq. (2.26) we see that it contains one unknown, namely u_i^{n+1} . Thus, the dependent variable at time $(t + \Delta t)$ is obtained directly from the known values of u_{i+1}^n , u_i^n and u_{i-1}^n .

$$\frac{u_i^{n+1} - u_i^n}{\Delta t} = \alpha \left[\frac{u_{i+1}^n - 2u_i^n + u_{i-1}^n}{(\Delta x)^2} \right] \quad (2.29)$$

This is a typical example of an explicit finite difference method.

Let us now attempt a different discretization of the original partial differential equation given by Eq. (2.25). Here we express the spatial differences on the right-hand side in terms of averages between n and $(n + 1)$ time level

$$\frac{u_i^{n+1} - u_i^n}{\Delta t} = \frac{\alpha}{2} \left[\frac{u_{i+1}^{n+1} + u_{i+1}^n - 2u_i^{n+1} - 2u_i^n + u_{i-1}^{n+1} + u_{i-1}^n}{(\Delta x)^2} \right] \quad (2.30)$$

The differencing shown in Eq. (2.30) is known as the Crank-Nicolson implicit scheme. The unknown u_i^{n+1} is not only expressed in terms of the known quantities at time level n , but also in terms of unknown quantities at time level $(n + 1)$. Hence Eq. (2.30) at a given grid point i , cannot itself result in a solution of u_i^{n+1} . Eq. (2.30) has to be written at all grid points, resulting in a system of algebraic equations from which the unknowns u_i^{n+1} for all i can be solved simultaneously. This is a typical example of an implicit finite-difference solution (Fig. 2.3). Since they deal with the solution of large systems of simultaneous linear algebraic equations, implicit methods usually require the handling of large matrices.

Generally, the following steps are followed in order to obtain a solution. Eq. (2.30) can be rewritten as

$$u_i^{n+1} - u_i^n = \frac{r}{2} [u_{i+1}^{n+1} + u_{i+1}^n - 2u_i^{n+1} - 2u_i^n + u_{i-1}^{n+1} + u_{i-1}^n] \quad (2.31)$$

where $r = \alpha(\Delta t)/(\Delta x)^2$ or

$$-r u_{i-1}^{n+1} + (2 + 2r)u_i^{n+1} - r u_{i+1}^{n+1} = r u_{i-1}^n + (2 - 2r)u_i^n + r u_{i+1}^n$$

or

$$-u_{i-1}^{n+1} + \left(\frac{2 + 2r}{r} \right) u_i^{n+1} - u_{i+1}^{n+1} = u_{i-1}^n + \left(\frac{2 - 2r}{r} \right) u_i^n + u_{i+1}^n \quad (2.32)$$

Eq. (2.32) has to be applied at all grid points, i.e., from $i = 1$ to $i = k + 1$. A system of algebraic equations will result (refer to Fig. 2.3).

$$\begin{aligned} \text{at } i = 2 & \quad -A + B(1)u_2^{n+1} - u_3^{n+1} = C(1) \\ \text{at } i = 3 & \quad -u_2^{n+1} + B(2)u_3^{n+1} - u_4^{n+1} = C(2) \\ \text{at } i = 4 & \quad -u_3^{n+1} + B(3)u_4^{n+1} - u_5^{n+1} = C(3) \\ & \quad \vdots \\ \text{at } i = k & \quad -u_{k-1}^{n+1} + B(k-1)u_k^{n+1} - D = C(k-1) \end{aligned}$$

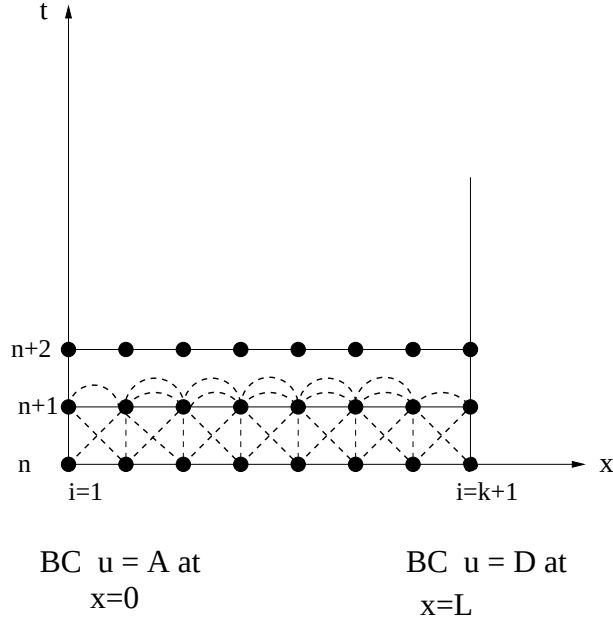


Figure 2.3: Crank Nicolson implicit scheme.

Finally the equations will be of the form:

$$\begin{bmatrix} B(1) & -1 & 0 & 0 & \dots & 0 \\ -1 & B(2) & -1 & 0 & \dots & 0 \\ 0 & -1 & B(3) & -1 & \dots & 0 \\ \vdots & & & & & \\ 0 & 0 & 0 & \dots & -1 & B(k-1) \end{bmatrix} \begin{bmatrix} u_2^{n+1} \\ u_3^{n+1} \\ u_4^{n+1} \\ \vdots \\ u_k^{n+1} \end{bmatrix} = \begin{bmatrix} (C(1) + A)^n \\ C(2)^n \\ C(3)^n \\ \vdots \\ (C(k-1) + D)^n \end{bmatrix} \quad (2.33)$$

Here, we express the system of equations in the form of $\mathbf{A}x = C$, where C is the right-hand side column vector (known), $\mathbf{A}$ the tridiagonal coefficient matrix (known) and x the solution vector (to be determined). Note that the boundary values at $i = 1$ and $i = k + 1$ are transferred to the known right-hand side.

For such a tridiagonal system, different solution procedures are available. In order to derive advantage of the zeros in the coefficient-matrix, the well known Thomas algorithm (1949) can be used (see appendix).