Chapter 10

A Review

10.1 Introductory Remarks

The fundamental concepts of computational fluid dynamics were introduced in the previous chapters. Various aspects of numerical schemes were explored with regard to simple partial differential equations. In all cases up to Chapter 8, the investigations were limited to a single equation. In the upcoming chapters the concepts are extended to systems of equations. Before proceeding further, however, it is beneficial to review and summarize the content of the previous chapters.

10.2 Classification of Partial Differential Equations

Partial differential equations (PDEs) can be classified into different categories, where within each category they may be classified further into subcategories. The numerical procedure used to solve a partial differential equation very much depends on the classification of the governing equation. A brief review of the classification of partial differential equations is provided in the following subsections.

10.2.1 Linear and Nonlinear PDEs

(a) Linear PDE: There is no product of the dependent variable and/or product of its derivatives within the equation.

(b) Nonlinear PDE: The equation contains a product of the dependent variable and/or a product of the derivatives.

10.2.2 Classification Based on Characteristics

(I) First-order PDE: Almost all first-order PDEs have real characteristics, and therefore behave much like hyperbolic equations of second order.

(II) Second-order PDE: A second-order PDE in two independent variables, x and y, may be expressed in a general form as

$$A\frac{\partial^2\phi}{\partial x^2}+B\frac{\partial^2\phi}{\partial x\partial y}+C\frac{\partial^2\phi}{\partial y^2}+D\frac{\partial\phi}{\partial x}+E\frac{\partial\phi}{\partial y}+F\phi+G=0 \tag{10-1}$$

The equation is classified according to the expression (B^2-4AC) as follows :

$$\left(B^2-4AC\right)\begin{cases}<0\rightarrow\text{elliptic equation}\\=0\rightarrow\text{parabolic equation}\\>0\rightarrow\text{hyperbolic equation}\end{cases}$$

The following criteria may be stated with regard to each category defined above:

(a) Elliptic equations

- No real characteristic lines exist
- A disturbance propagates in all directions
- Domain of solution is a closed region
- Boundary conditions must be specified on the boundaries of the domain

(b) Parabolic equations

- Only one characteristic line exists
- A disturbance propagates along the characteristic line
- Domain of solution is an open region
- An initial condition and two boundary conditions are required

(c) Hyperbolic equations

- Two characteristic lines exist
- A disturbance propagates along the characteristic lines
- Domain of solution is an open region
- Two initial conditions along with two boundary conditions are required

(III) System of First-Order PDEs

A system of first-order PDEs may be expressed in a vector form as

$$\frac{\partial\Phi}{\partial t}+[A]\frac{\partial\Phi}{\partial x}+[B]\frac{\partial\Phi}{\partial y}+\Psi=0 \tag{10-2}$$

where the vector Φ contains the dependent variables. The system is classified according to the eigenvalues of coefficient matrices $[A]$ and $[B]$. If the eigenvalues of matrix $[A]$ are all real and distinct, the system is classified as hyperbolic in t and x. If the eigenvalues of $[A]$ are complex, the system is elliptic in t and x. Similarly, the system is classified with respect to the independent variables t and y based on the eigenvalues of matrix $[B]$.

For a steady equivalent of (10-2), given by

$$[A]\frac{\partial \Phi}{\partial x} + [B]\frac{\partial \Phi}{\partial y} + \Psi = 0 \tag{10-3}$$

the classification is as follows:

$$H \begin{cases} < 0 \rightarrow \text{elliptic} \\ = 0 \rightarrow \text{parabolic} \\ > 0 \rightarrow \text{hyperbolic} \end{cases}$$

where

$$H = R^2 - 4PQ$$

and

$$P = |A|, \quad Q = |B|$$

For a system composed of two equations, R is given by

$$R = \begin{vmatrix} a_1 & a_4 \\ b_1 & b_4 \end{vmatrix} + \begin{vmatrix} a_3 & a_2 \\ b_3 & b_2 \end{vmatrix}$$

where

$$[A] = \begin{bmatrix} a_1 & a_2 \\ b_1 & b_2 \end{bmatrix} \quad \text{and} \quad [B] = \begin{bmatrix} a_3 & a_4 \\ b_3 & b_4 \end{bmatrix}$$

(IV) System of Second-Order PDEs

The classification of a system of second-order PDEs is facilitated if the second-order PDEs are reduced to their equivalent first-order PDEs. Subsequently, the system is classified as previously seen. The procedure could be cumbersome. For specific details and examples, Section 1.9 should be reviewed.

10.3 Boundary Conditions

A set of specific information with regard to the dependent variable and/or its derivative must be specified along the boundaries of the domain. This set of information is known as the *boundary condition* and may be categorized as follows.

(a) The Dirichlet boundary condition: The value of the dependent variable along the boundary is specified.

(b) The Neumann boundary condition: The normal gradient of the dependent variable along the boundary is specified.

(c) The Mixed boundary condition: A combination of the Dirichlet and the Neumann type boundary conditions is specified.

10.4 Finite Difference Equations

The partial derivatives appearing in the differential equations are replaced by approximate algebraic expressions to provide an equivalent algebraic equation known as the *finite difference equation.* Subsequently, the finite difference equation is solved within a domain which has been discretized into equally spaced grids. Finite difference equations commonly used for the solution of parabolic, elliptic, and hyperbolic equations are reviewed in this section.

10.4.1 Parabolic Equations

Various finite difference formulations are reviewed for the one-dimensional parabolic equations initially and, subsequently, extended to multi-dimensional problems.

10.4.1.1 One-Space Dimension

The simple diffusion equation is used in this section to review various finite difference equations. The model equation is given by

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

where α is assumed to be a constant and hence a linear equation. To facilitate the review process, various aspects of each finite difference formulation such as the order of accuracy, amplification factor, stability requirement, and the corresponding modified equation are summarized. In the formulations to follow, the diffusion number is designated by d, which is defined by

$$d = \alpha \frac{\Delta t}{(\Delta x)^2}$$

Scheme:	FTCS explicit
Formulation:	$u_i^{n+1} = u_i^n + d\left(u_{i+1}^n - 2u_i^n + u_{i-1}^n\right)$
Order:	$O\left[(\Delta t),\ (\Delta x)^2\right]$
Amplification Factor:	$G = 1 + 2d(\cos\theta - 1)$
Stability Requirement:	$d \le \frac{1}{2}$
Modified Equation:	$\frac{\partial u}{\partial t} = \alpha\frac{\partial^2 u}{\partial x^2} + \left[-\frac{1}{2}\alpha^2(\Delta t) + \frac{1}{12}\alpha(\Delta x)^2\right]\frac{\partial^4 u}{\partial x^4} + \left[\frac{1}{3}\alpha^3(\Delta t)^2\frac{\partial^4 u}{\partial x^4} - \frac{1}{12}\alpha^2(\Delta t)(\Delta x)^2 + \frac{1}{360}\alpha(\Delta x)^2\right]\frac{\partial^6 u}{\partial x^6} + \ldots$
Special Considerations:	None

Scheme:	DuFort-Frankel explicit
Formulation:	$u_i^{n+1} = \frac{1-2d}{1+2d}u_i^{n-1} + \frac{2d}{1+2d}\left(u_{i+1}^n + u_{i-1}^n\right)$
Order:	$O\left[(\Delta t)^2,\ (\Delta x)^2,\ \left(\frac{\Delta t}{\Delta x}\right)^2\right]$
Amplification Factor:	$G = \frac{1}{1+2d}\left[2d\cos\theta \pm (1 - 4d^2\mathrm{Sin}^2\theta)^{\frac{1}{2}}\right]$
Stability Requirement:	Unconditionally stable
Modified Equation:	$\frac{\partial u}{\partial x} = \alpha\frac{\partial^2 u}{\partial x^2} + \left[\frac{1}{12}\alpha(\Delta x^2) - \alpha^3\left(\frac{\Delta t}{\Delta x}\right)^2\right]\frac{\partial^4 u}{\partial x^4} + \left[-\frac{1}{3}\alpha^3(\Delta t)^2 + \frac{1}{360}\alpha(\Delta x)^4 + 2\alpha^5\left(\frac{\Delta t}{\Delta x}\right)^4\right]\frac{\partial^6 u}{\partial x^6} + \ldots$
Special Considerations:	Requires two sets of data to proceed

Scheme:	Laasonen implicit
Formulation:	$du_{i-1}^{n+1} - (1+2d)u_i^{n+1} + du_{i-1}^{n} = u_i^n$
Order:	$O\left[(\Delta t),\ (\Delta x)^2\right]$
Amplification Factor:	$G = \dfrac{1}{1+2d(1-\mathrm{Cos}\theta)}$
Stability Requirement:	Unconditionally stable
Modified Equation:	$\dfrac{\partial u}{\partial t} = \alpha\dfrac{\partial^2 u}{\partial x^2} + \left[\dfrac{1}{2}\alpha^2(\Delta t) + \dfrac{1}{12}\alpha(\Delta x)^2\right]\dfrac{\partial^4 u}{\partial x^4} + \left[\dfrac{1}{3}\alpha^3(\Delta t)^2 + \dfrac{1}{12}\alpha^2(\Delta t)(\Delta x)^2 + \dfrac{1}{360}\alpha(\Delta x)^4\right]\dfrac{\partial^6 u}{\partial x^6} + \ldots$
Special Considerations:	Requires solution of a tridiagonal system

Scheme:	Crank-Nicolson implicit
Formulation:	$\dfrac{1}{2}du_{i+1}^{n+1} - (1+d)u_i^{n+1} + \dfrac{1}{2}du_{i-1}^{n+1} = -\dfrac{1}{2}u_{i+1}^{n} + (d-1)u_i^n - \dfrac{1}{2}du_{i-1}^{n}$
Order:	$O\left[(\Delta t)^2,\ (\Delta x)^2\right]$
Amplification Factor:	$G = \dfrac{1-d(1-\mathrm{Cos}\theta)}{1+d(1-\mathrm{Cos}\theta)}$
Stability Requirement:	Unconditionally stable
Modified Equation:	$\dfrac{\partial u}{\partial x} = \alpha\dfrac{\partial^2 u}{\partial x^2} + \left[\dfrac{1}{12}\alpha(\Delta x)^2\right]\dfrac{\partial^4 u}{\partial x^4} + \left[\dfrac{1}{12}\alpha^3(\Delta t)^2 + \dfrac{1}{360}\alpha(\Delta x)^4\right]\dfrac{\partial^6 u}{\partial x^6} + \ldots$
Special Considerations:	Requires solution of a tridiagonal system

10.4.1.2 Multi-Space Dimensions

The review of multi-dimensional problems will be limited to two-space dimensions. The procedure to three-space dimensions is similar. However, it is cautioned that the extension may not be trivial, and certain formulations which may have been unconditionally stable in two-space dimensions may become only conditionally stable in three-space dimensions. The model equation used is the diffusion equation in two-space dimensions given by

$$\frac{\partial u}{\partial t} = \alpha \left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} \right)$$

Scheme:	FTCS explicit
Formulation:	$u_{i,j}^{n+1} = u_{i,j}^n + d_x(u_{i+1,j}^n - 2u_{i,j}^n + u_{i-1,j}^n) + d_y \left(u_{i,j+1}^n - 2u_{i,j}^n + u_{i,j-1}^n\right)$
Order:	$O\left[(\Delta t),\ (\Delta x)^2,\ (\Delta y)^2\right]$
Stability Requirement:	$(d_x + d_y) \leq \frac{1}{2}$

Scheme:	ADI
Formulation:	$-\left(\frac{1}{2}d_x\right) u_{i-1,j}^{n+\frac{1}{2}} + (1+d_x) u_{i,j}^{n+\frac{1}{2}} - \left(\frac{1}{2}d_x\right) u_{i+1,j}^{n+\frac{1}{2}} = \left(\frac{1}{2}d_y\right) u_{i,j+1}^n + (1-d_y) u_{i,j}^n + \left(\frac{1}{2}d_y\right) u_{i,j-1}^n$
and	$-\left(\frac{1}{2}d_y\right) u_{i,j-1}^{n+1} + (1+d_y) u_{i,j}^{n+1} - \left(\frac{1}{2}d_y\right) u_{i,j+1}^{n+1} = \left(\frac{1}{2}d_x\right) u_{i+1,j}^{n+\frac{1}{2}} + (1-d_x) u_{i,j}^{n+\frac{1}{2}} + \left(\frac{1}{2}d_x\right) u_{i-1,j}^{n+\frac{1}{2}}$
Order:	$O\left[(\Delta t)^2,\ (\Delta x)^2,\ (\Delta y)^2\right]$
Amplification Factor:	$G = \frac{[1 - d_x(1 - \text{Cos}\theta_x)]\ [1 - d_y(1 - \text{Cos}\theta_y)]}{[1 + d_x(1 - \text{Cos}\theta_x)]\ [1 + d_y(1 - \text{Cos}\theta_y)]}$
Stability Requirement:	Unconditionally stable

Scheme:	Fractional step
Formulation:	$d_x u_{i+1,j}^{n+\frac{1}{2}} - (1+2d_x)u_{i,j}^{n+\frac{1}{2}} + d_x u_{i-1,j}^{n+\frac{1}{2}}$
	$= -d_x u_{i+1,j}^{n} + (2d_x - 1)u_{i,j}^{n} - d_x u_{i-1,j}^{n}$
and	$d_y u_{i,j+1}^{n+1} - (1+2d_y)u_{i,j}^{n+1} + d_y u_{i,j-1}^{n+1}$
	$= -d_y u_{i,j+1}^{n+\frac{1}{2}} + (2d_y - 1)u_{i,j}^{n+\frac{1}{2}} - d_y u_{i,j-1}^{n+\frac{1}{2}}$
Order:	$O\left[(\Delta t)^2,\ (\Delta x)^2,\ (\Delta y)^2\right]$
Stability Requirement:	Unconditionally stable

10.4.2 Elliptic Equations

The model equation utilized to represent various finite difference equations is the Poisson equation expressed in two-space dimensions given by

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = 0$$

Only iterative schemes which are usually the most efficient schemes to solve elliptic equations are reviewed in this section. In the formulations to follow, the ratio of stepsizes is designated by β, i.e., $\beta = \dfrac{\Delta x}{\Delta y}$.

Scheme:	Point Gauss-Seidel (PGS)
Formulation:	$u_i^{k+1} = \dfrac{1}{2(1+\beta^2)}\left[u_{i+1,j}^{k} + u_{i-1,j}^{k+1} + \beta\left(u_{i,j+1}^{k} + u_{i,j-1}^{k+1}\right)\right]$
Order:	$O\left[(\Delta x)^2,\ (\Delta y)^2\right]$

Scheme:	Line Gauss-Seidel (LGS)
Formulation: (x direction)	$u_{i-1,j}^{k+1} - 2(1+\beta^2)u_{i,j}^{k+1} + u_{i+1,j}^{k+1} = -\beta u_{i,j+1}^{k} - \beta^2 u_{i,j-1}^{k+1}$
Order:	$O\left[(\Delta x)^2,\ (\Delta y)^2\right]$
Modified Equation:	$\dfrac{\partial^2 u}{\partial x^2} + \dfrac{\partial^2 u}{\partial y^2} = -\dfrac{1}{12}(\Delta x)^2\dfrac{\partial^4 u}{\partial x^4} - \dfrac{1}{12}(\Delta y)^2\dfrac{\partial^4 u}{\partial y^4} + \ldots$

Scheme:	Point Successive Over-Relaxation (PSOR)
Formulation:	$u_{i,j}^{k+1} = (1-\omega)u_{i,j}^{k} + \frac{\omega}{2(1+\beta^2)}\left[u_{i+1,j}^{k} + u_{i-1,j}^{k+1} + \beta^2\left(u_{i,j}^{k} + u_{i,j-1}^{k+1}\right)\right]$
Order:	$O\left[(\Delta x)^2, (\Delta y)^2\right]$
Special Considerations:	The range of relaxation parameter is $1 \leq \omega < 2$

Scheme:	Line Successive Over-Relaxation (LSOR)
Formulation: (x direction)	$\omega u_{i-1,j}^{k+1} - 2\left(1+\beta^2\right)u_{i,j}^{k+1} + \omega u_{i+1,j}^{k+1} = -(1-\omega)\left[2(1+\beta^2)\right]u_{i,j}^{k} - \omega\beta^2\left(u_{i,j+1}^{k} + u_{i,j-1}^{k+1}\right)$
Special Considerations:	The range of relaxation parameter is $1 \leq \omega < 2$

Scheme:	ADI
Formulation:	$u_{i-1,j}^{k+\frac{1}{2}} - 2(1+\beta^2)u_{i,j}^{k+\frac{1}{2}} + u_{i+1,j}^{k+\frac{1}{2}} = -\beta^2\left(u_{i,j+1}^{k} + u_{i,j-1}^{k+\frac{1}{2}}\right)$
and	$\beta^2 u_{i,j-1}^{k+1} - 2(1+\beta^2)u_{i,j}^{k+1} + \beta^2 u_{i,j+1}^{k+1} = -u_{i+1,j}^{k+\frac{1}{2}} - u_{i-1,j}^{k+1}$

Scheme:	ADI with relaxation parameter
Formulation:	$\omega\, u_{i-1,j}^{k+\frac{1}{2}} - 2(1+\beta^2)u_{i,j}^{k+\frac{1}{2}} + \omega\, u_{i+1,j}^{k+\frac{1}{2}} = -(1-\omega)\left[2\left(1+\beta^2\right)\right]u_{i,j}^{k} - \omega\,\beta^2\left(u_{i,j+1}^{k} + u_{i,j-1}^{k+\frac{1}{2}}\right)$
and	$\omega\,\beta^2 u_{i,j-1}^{k+1} - 2(1+\beta^2)u_{i,j}^{k+1} + \omega\,\beta^2 u_{i,j+1}^{k+1} = (1-\omega)\left[2\left(1+\beta^2\right)\right]u_{i,j}^{k+\frac{1}{2}} - \omega\left(u_{i+1,j}^{k+\frac{1}{2}} + u_{i-1,j}^{k+1}\right)$

10.4.3 Hyperbolic Equations

Investigation of various finite difference equations is easily accomplished with regard to linear hyperbolic equations. Subsequently, the conclusions may be extended to nonlinear hyperbolic equations. With that in mind, the review of the formulations is performed sequentially in two parts.

10.4.3.1 Linear Equations

The wave equation given by

$$\frac{\partial u}{\partial t} = -a\frac{\partial u}{\partial x}, \quad a > 0$$

is used to review linear hyperbolic equations. Note that the speed of sound, a, in the equation above is assumed to be a constant and, hence, a linear equation. The parameter, $a\frac{\Delta t}{\Delta x}$, defined as the Courant number and designated by c, will be used in the formulations to follow.

Scheme:	First upwind differencing
Formulation:	$u_i^{n+1} = u_i^n - c\left(u_i^n - u_{i-1}^n\right)$
Order:	$O\left[(\Delta t),\ (\Delta x)\right]$
Amplification Factor:	$G = 1 - c(1 - \text{Cos}\,\theta) - i(c\text{Sin}\,\theta)$
Stability Requirement:	$c \leq 1$
Modified Equation:	$\frac{\partial u}{\partial t} = -a\frac{\partial u}{\partial x} + \frac{1}{2}a\Delta x(1-c)\frac{\partial^2 u}{\partial x^2} - \frac{1}{6}a(\Delta x)^2(2c^2 - 3c + 1)\frac{\partial^3 u}{\partial x^3} + \ldots$

Scheme:	Lax
Formulation:	$u_i^{n+1} = \frac{1}{2}\left(u_{i+1}^n + u_{i-1}^n\right) - \frac{1}{2}c\left(u_{i+1}^n - u_{i-1}^n\right)$
Order:	$O\left[(\Delta t),\ \frac{(\Delta x^2)}{(\Delta t)}\right]$
Amplification Factor:	$G = \text{Cos}\,\theta - i(c\text{Sin}\,\theta)$
Stability Requirement:	$c \leq 1$
Modified Equation:	$\frac{\partial u}{\partial t} = a\frac{\partial u}{\partial x} + \frac{1}{2}a(\Delta x)\left(\frac{1}{c} - c\right)\frac{\partial^2 u}{\partial x^2} + \frac{1}{3}a(\Delta x)^2(1 - c^2)\frac{\partial^3 u}{\partial x^3} + \ldots$

Scheme:	Midpoint Leapfrog
Formulation:	$u_i^{n+1} = u_i^{n-1} - c\left(u_{i+1}^n - u_{i-1}^n\right)$
Order:	$O\left[(\Delta t)^2,\ (\Delta x)^2\right]$
Amplification Factor:	$G = \pm\left[1 - c^2\text{Sin}^2\,\theta\right]^{\frac{1}{2}} - i(c\text{Sin}\,\theta)$
Stability Requirement:	$c \le 1$
Modified Equation:	$\frac{\partial u}{\partial t} = -a\frac{\partial u}{\partial x} - \frac{1}{6}a(\Delta x)^2\left(1 - c^2\right)\frac{\partial^3 u}{\partial x^3} + \ldots$
Special Considerations:	Requires two sets of data for the solution to proceed

Scheme:	Lax-Wendroff
Formulation:	$u_i^{n+1} = u_i^n - \frac{1}{2}c\left(u_{i+1}^n - u_{i-1}^n\right) + \frac{1}{2}c^2\left(u_{i+1}^n - 2u_i^n + u_{i-1}^n\right)$
Order:	$O\left[(\Delta t)^2,\ (\Delta x)^2\right]$
Amplification Factor:	$G = 1 - c^2(1 - \text{Cos}\,\theta) - i(c\,\text{Sin}\,\theta)$
Stability Requirement:	$c \le 1$
Modified Equation:	$\frac{\partial u}{\partial t} = -a\frac{\partial u}{\partial x} - \frac{1}{6}a(\Delta x)^2\left(1 - c^2\right)\frac{\partial^3 u}{\partial x^3} - \frac{1}{8}a(\Delta x)^3 c(1 - c^2)\frac{\partial^4 u}{\partial x^4} + \ldots$

Scheme:	BTCS implicit
Formulation:	$\frac{1}{2}c\,u_{i-1}^{n+1} - u_i^{n+1} - \frac{1}{2}c\,u_{i+1}^{n+1} = -u_i^n$
Order:	$O\left[(\Delta t)\ ,\ (\Delta x)^2\right]$
Amplification Factor:	$G = \frac{1 - i(c\,\text{Sin}\,\theta)}{1 + c^2\,(\text{Sin}^2\,\theta\,)}$
Stability Requirement:	*None*
Modified Equation:	$\frac{\partial u}{\partial t} = -a\frac{\partial u}{\partial x} + \frac{1}{2}a^2(\Delta t)\frac{\partial^2 u}{\partial x^2} - \left[\frac{1}{6}a(\Delta x)^2 + \frac{1}{3}a^3(\Delta t)^2\right]\frac{\partial^3 u}{\partial x^3} + \ldots$

Scheme:	Crank-Nicolson
Formulation:	$\frac{1}{4}c\,u_{i+1}^{n+1} - u_i^{n+1} - \frac{1}{4}c\,u_{i-1}^{n+1} = u_i^n - \frac{1}{4}c\left(u_{i+1}^n - u_{i-1}^n\right)$
Order:	$O\left[(\Delta t)^2\ ,\ (\Delta x)^2\right]$
Amplification Factor:	$G = \frac{1 - 0.5i(c\,\text{Sin}\,\theta)}{1 + 0.5i\,(c\,\text{Sin}\,\theta\,)}$
Stability Requirement:	None
Modified Equation:	$\frac{\partial u}{\partial t} = -a\frac{\partial u}{\partial x} - \frac{1}{6}a\,(\Delta x)^2\left(1 + \frac{1}{2}c^2\right)\frac{\partial^3 u}{\partial x^3}\cdots$

Scheme:	Lax-Wendroff
Formulation:	$u_{i+\frac{1}{2}}^{n+\frac{1}{2}} = \frac{1}{2}\left(u_{i+1}^n + u_i^n\right) - \frac{1}{2}c\left(u_{i+1}^n - u^{n_i}\right)$
and	$u_i^{n+1} = u_i^n - c\left(u_{i+\frac{1}{2}}^{n+\frac{1}{2}} - u_{i-\frac{1}{2}}^{n+\frac{1}{2}}\right)$
Order:	$O\,[(\Delta t)^2\ ,\ (\Delta x)^2]$
Stability Requirement:	$c \leq 1$

Scheme:	MacCormack
Formulation:	$u_i^* = u_i^n - c\left(u_{i+1}^n - u_i^n\right)$
and	$u_i^{n+1} = \frac{1}{2}\left[u_i^n + u_i^* - c\left(u_i^* - u_i^*\right)\right]$
Order:	$O\left[(\Delta t)^2\ ,\ (\Delta x)^2\right]$
Stability Requirement:	$c \leq 1$

10.4.3.2 Nonlinear Equations

The inviscid Burgers equation is used to review various schemes for the solution of hyperbolic equations. Recall that the model equation is given by

$$\frac{\partial u}{\partial t} = -u\frac{\partial u}{\partial x} = -\frac{\partial E}{\partial x}$$

where $E = \frac{1}{2}u^2$. Now, the Courant number is defined as $c = u\frac{\Delta t}{\Delta x}$.

Scheme:	Lax
Formulation:	$u_i^{n+1} = \frac{1}{2}\left(u_{i+1}^n + u_{i-1}^n\right) - \frac{1}{2}\frac{\Delta t}{\Delta x}\left(E_{i+1}^n - E_{i-1}^n\right)$
Order:	$O\left[(\Delta t)\ ,\ (\Delta x)^2\right]$
Amplification Factor:	$G = \text{Cos}\,\theta - i(c\,\text{Sin}\,\theta)$
Stability Requirement:	$\left\lvert u_{\max}\frac{\Delta t}{\Delta x}\right\rvert \leq 1$

Scheme:	Lax-Wendroff
Formulation:	$u_i^{n+1} = u_i^n - \frac{1}{2}\frac{\Delta t}{\Delta x}\left(E_{i+1}^n - E_{i-1}^n\right) + \frac{1}{4}\left(\frac{\Delta t}{\Delta x}\right)^2$
	$\left[\left(u_{i+1}^n + u_i^n\right)\left(E_{i+1}^n - E_i^n\right) - \left(u_i^n + u_{i-1}^n\right)\left(E_i^n - E_{i-1}^n\right)\right]$
Amplification Factor:	$G = 1 - 2c^2(1 - \text{Cos}\,\theta) - 2i(c\,\text{Sin}\,\theta)$
Stability Requirement:	$\left\lvert u_{\max}\frac{\Delta t}{\Delta x}\right\rvert \leq 1$

Scheme:	MacCormack
Formulation:	$u_i^* = u_i^n - \frac{\Delta t}{\Delta x}\left(E_{i+1}^n - E_i^n\right)$
and	$u_i^{n+1} = \frac{1}{2}\left[u_i^n + u_i^* - \frac{\Delta t}{\Delta x}\left(E_i^* - E_{i-1}^*\right)\right]$
Order:	$O\left[(\Delta t)^2\ ,\ (\Delta x)^2\right]$

10.5 Stability Analysis

The error introduced in the finite difference equations due to the truncation of the higher order terms in the Taylor series expansion may grow unbounded, producing an unstable solution. The control of errors within the solution is of primary concern for any numerical scheme. To establish the necessary requirements, a stability analysis must be performed. Among various methods available for stability analysis are: (1) The discrete perturbation stability analysis, (2) The von Neumann (or Fourier) stability analysis, and (3) The matrix method. It should be noted that direct stability analysis of a nonlinear, multi-dimensional, coupled system of equations is usually cumbersome. In most cases, expressions are proposed which are based on the stability analysis of simple model equations complimented and reinforced by numerical experimentation. Thus, one encounters the suggested stability requirement for a particular scheme which resembles those of simple model equations, but includes some modifications based on numerical experimentations.

To review the limitations and conclusions provided from the von Neumann stability analysis, the summary stated in Chapter 4 is repeated at this point.

1. The von Neumann stability analysis can be applied to linear equations only.
2. The influence of the boundary conditions on the stability of the solution is not included.
3. For a scalar PDE which is approximated by a two-level FDE, the mathematical requirement is imposed on the amplification factor G as follows:
   (a) if G is real, then $|G| \leq 1$
   (b) if G is complex, then $|G|^2 \leq 1$, where $|G|^2 = G\overline{G}$
4. For a scalar PDE which is approximated by a three-level FDE, the amplification factor is a matrix. In this case, the requirement is imposed on the eigenvalues of G as follows:

(a) if λ is real, then $|\lambda| \leq 1$

(b) if λ is complex, then $|\lambda|^2 \leq 1$

5. The method can be easily extended to multi-dimensional problems.

6. The procedure can be used for stability analysis of a system of linear PDEs. The requirement is imposed on the largest eigenvalue of the amplification matrix.

7. Benchmark values for the stability of unsteady one-dimensional problems may be established as follows:

   (a) For most explicit formulations:

      I. Courant number, $c \leq 1$

      II. Diffusion number, $d \leq \frac{1}{2}$

      III. Cell Reynolds number, $Re_c \leq (2/c)$

   (b) For implicit formulation, most are unconditionally stable.

8. For multi-dimensional problems with equal grid spacing in all spatial directions, the stated benchmark values are adjusted usually by dividing them by the number of spatial dimensions.

9. On occasions where the amplification factor is a difficult expression to analyze, graphical solution along with some numerical experimentation will facilitate the analysis.

10.6 Error Analysis

The truncation of terms in the approximation of a partial derivative could begin from an odd-order or an even-order derivative term. For example, one may approximate a first-order derivative by either

$$\frac{\partial u}{\partial x} = \frac{u_{i+1} - u_i}{\Delta x} + \frac{(\Delta x)}{2!}\frac{\partial^2 u}{\partial x^2} + \frac{(\Delta x)^2}{3!}\frac{\partial^3 u}{\partial x^3} + \ldots \tag{10-4}$$

or

$$\frac{\partial u}{\partial x} = \frac{u_{i+1} - u_{i-1}}{2\Delta x} + \frac{(\Delta x)^2}{3!}\frac{\partial^3 u}{\partial x^3} + \ldots \tag{10-5}$$

The approximation (10-4) may be truncated and expressed as

$$\frac{\partial u}{\partial x} = \frac{u_{i+1} - u_i}{\Delta x} + O(\Delta x)$$

where the dominant (or leading) error term includes a second-order derivative, i.e., even. The second expression given by (10-5) is written as

$$\frac{\partial u}{\partial x} = \frac{u_{i+1} - u_{i-1}}{2\Delta x} + O(\Delta x)^2$$

where the dominant error term now includes an odd derivative. The behavior of error associated with finite difference equations is strongly influenced by the dominant error term. To clarify the types of error introduced to the finite difference equations, a convective dominated equation, where physical viscosity is absent, will be used. Thus, consider the wave equation and two different finite difference equations given by

$$u_i^{n+1} = u_i^n - c(u_i^n - u_{i-1}^n) \qquad (10\text{-}6)$$

and

$$u_i^{n+1} = u_i^{n-1} - c(u_{i+1}^n - u_{i-1}^n) \qquad (10\text{-}7)$$

The FDEs are recognized as the first upwind differencing scheme and the midpoint leapfrog method. To identify the dominant error term of an FDE, the modified equation must be investigated. The corresponding modified equations for the FDEs given by (10-6) and (10-7) are, respectively:

$$\frac{\partial u}{\partial t} = -a\frac{\partial u}{\partial x} + \frac{1}{2}\alpha(\Delta x)(1-c)\frac{\partial^2 u}{\partial x^2} - \frac{1}{6}\alpha(\Delta x)^2\left(2c^2 - 3c + 1\right)\frac{\partial^3 u}{\partial x^3} + \ldots \qquad (10\text{-}8)$$

and

$$\frac{\partial u}{\partial t} = -a\frac{\partial u}{\partial x} + \frac{1}{6}\alpha(\Delta x)^2\left(c^2 - 1\right)\frac{\partial^3 u}{\partial x^3} + \ldots \qquad (10\text{-}9)$$

Observe that the dominant error terms in Equations (10-8) and (10-9) include second-order derivative and third-order derivative, respectively. Recall that, from a physical point of view, a second-order derivative is associated with diffusion. Indeed, the coefficient of the second-order derivative in Equation (10-8) is known as the *numerical viscosity*. Thus, it is obvious that the error associated with Equation (10-8) is dissipative and, hence, it is called *dissipation error*. On the other hand, an FDE scheme, where its corresponding modified equation possesses an odd-order derivative as the lead term in error, is associated with oscillations within the solution. Such an error is called *dispersion error*.

10.7 Grid Generation-Structured Grids

Finite difference equations are most efficiently solved in a rectangular domain (for 2-D applications and an equivalent hexahedral domain for 3-D applications) with equal grid spacings. Unfortunately, the majority of physical domains encountered are nonrectangular in shape. Thus, it is necessary to transform the nonrectangular physical domain to a rectangular computational domain where grid points are distributed at equal spacings. It is also important to note that the transformation allows the alignment of one of the coordinates along the body, thus facilitating the implementation of the boundary conditions. The objective of grid generation is then to identify the location of the grid points in the computational domain and the location of the corresponding grid points in the physical space. Furthermore, the metrics and Jacobian of transformation which are required for the solution of flow equations are computed within the grid generation routine.

Typically, grid generation schemes may be categorized as algebraic methods or differential methods. In the latter case, the scheme is based on the solution of a set of PDEs and may be subcategorized as either an elliptic, parabolic, or hyperbolic grid generation. Either category of grid generation scheme should include the following considerations.

1. A mapping which guarantees one-to-one correspondence ensuring grid lines of the same family do not cross each other;
2. Smoothness of the grid distribution;
3. Orthogonality or near orthogonality of the grid lines;
4. Options for grid clustering.

A brief summary of the advantages and disadvantages of each method is provided below.

1. Algebraic grids

   The advantages of this category of grid generators are:

   (a) They are very fast computationally;
   (b) Metrics may be evaluated analytically, thus avoiding numerical errors;
   (c) The ability to cluster grid points in different regions can be easily implemented.

   The disadvantages are:

   (a) Discontinuities at a boundary may propagate into the interior region which could lead to errors due to sudden changes in the metrics;
   (b) Smoothness and skewness may be difficult to control.

2. Elliptic grids

   The advantages of this class of grid generators are:

(a) Will provide smooth grid point distribution, i.e., if a boundary discontinuity point exists, it will be smoothed out in the interior domain;

(b) Numerous options for grid clustering and surface orthogonality are available;

(c) Method can be extended to 3-D problems.

The disadvantages of the method are:

(a) Computation time is large (compared to algebraic methods or hyperbolic grid generators);

(b) Specification of the forcing functions P and Q (or the constants used in these functions) is not easy;

(c) Metrics must be computed numerically.

3. Hyperbolic grids

The advantages of hyperbolic grid generators are:

(a) The grid system is orthogonal in two dimensions;

(b) Since a marching scheme is used for the solution of the system, computationally they are much faster compared to elliptic systems;

(c) Grid line spacing may be controlled by the cell area or arc-length functions.

The disadvantages are:

(a) Boundary discontinuity may be propagated into the interior domain;

(b) Specifying the cell-area or arc-length functions must be handled carefully. A bad selection of these functions easily leads to undesirable grid systems.

Finally, the metrics and Jacobian of tranformation are given by the following expressions.

1. Two dimensions

$$\xi_x = J y_\eta$$
$$\xi_y = -J x_\eta$$
$$\eta_x = -J y_\xi$$
$$\eta_y = J x_\xi$$

where

$$J = \frac{1}{x_\xi y_\eta - y_\xi x_\eta}$$

2. Three dimensions

$$
\begin{aligned}
\xi_x &= J(y_\eta z_\zeta - y_\zeta z_\eta) \\
\xi_y &= J(x_\zeta z_\eta - x_\eta z_\zeta) \\
\xi_z &= J(x_\eta y_\zeta - x_\zeta y_\eta) \\
\eta_x &= J(y_\zeta z_\xi - y_\xi z_\zeta) \\
\eta_y &= J(x_\xi z_\zeta - x_\zeta z_\xi) \\
\eta_z &= J(x_\zeta y_\xi - x_\xi y_\zeta) \\
\zeta_x &= J(y_\xi z_\eta - y_\eta z_\xi) \\
\zeta_y &= J(x_\eta z_\xi - x_\xi z_\eta) \\
\zeta_z &- J(x_\xi y_\eta - x_\eta y_\xi) \\
\xi_t &= -(x_\tau \xi_x + y_\tau \xi_y + z_\tau \xi_z) \\
\eta_t &= -(x_\tau \eta_x + y_\tau \eta_y + z_\tau \eta_z) \\
\zeta_t &= -(x_\tau \zeta_x + y_\tau \zeta_y + z_\tau \zeta_z)
\end{aligned}
$$

where

$$
J = \frac{\partial(\xi\,,\eta\,,\zeta)}{\partial(x\,,y\,,z)} = \frac{1}{x_\xi(y_\eta z_\zeta - y_\zeta z_\eta) - x_\eta(y_\xi z_\zeta - y_\zeta z_\xi) + x_\zeta(y_\xi z_\eta - y_\eta z_\xi)}
$$

10.8 Transformation of the Equations From the Physical Space to Computational Space

The partial derivatives expressed in the physical space are related to the partial derivatives in the computational space by the following relations:

$$
\begin{aligned}
\frac{\partial}{\partial t} &= \frac{\partial}{\partial \tau} + \xi_t \frac{\partial}{\partial \xi} + \eta_t \frac{\partial}{\partial \eta} + \zeta_t \frac{\partial}{\partial \zeta} \\
\frac{\partial}{\partial x} &= \xi_x \frac{\partial}{\partial \xi} + \eta_x \frac{\partial}{\partial \eta} + \zeta_x \frac{\partial}{\partial \zeta} \\
\frac{\partial}{\partial y} &= \xi_y \frac{\partial}{\partial \xi} + \eta_y \frac{\partial}{\partial \eta} + \zeta_y \frac{\partial}{\partial \zeta} \\
\frac{\partial}{\partial x} &= \xi_z \frac{\partial}{\partial \xi} + \eta_z \frac{\partial}{\partial \eta} + \zeta_z \frac{\partial}{\partial \zeta}
\end{aligned}
$$

The Navier-Stokes equations in a flux vector form may be expressed in the physical space by

$$
\frac{\partial Q}{\partial t} + \frac{\partial E}{\partial x} + \frac{\partial F}{\partial y} + \frac{\partial G}{\partial z} = \frac{\partial E_v}{\partial x} + \frac{\partial F_v}{\partial y} + \frac{\partial G_v}{\partial z}
$$

can be transformed to the computational space and expressed by

$$
\frac{\partial \overline{Q}}{\partial \tau} + \frac{\partial \overline{E}}{\partial \xi} + \frac{\partial \overline{F}}{\partial \eta} + \frac{\partial \overline{G}}{\partial \zeta} = \frac{\partial \overline{E}_v}{\partial \xi} + \frac{\partial \overline{F}_v}{\partial \eta} + \frac{\partial \overline{G}}{\partial \zeta}
$$

where

$$\overline{Q} = \frac{Q}{J}$$

$$\overline{E} = \frac{1}{J}(\xi_t Q + \xi_x E + \xi_y F + \xi_z G)$$

$$\overline{F} = \frac{1}{J}(\eta_t Q + \eta_x E + \eta_y F + \eta_z G)$$

$$\overline{G} = \frac{1}{J}(\zeta_t Q + \zeta_x E + \zeta_y F + \zeta_z G)$$

$$\overline{E}_v = \frac{1}{J}(\xi_x E_v + \xi_y F_v + \xi_z G_v)$$

$$\overline{F}_v = \frac{1}{J}(\eta_x E_v + \eta_y F_v + \eta_z G_v)$$

$$\overline{G}_v = \frac{1}{J}(\zeta_x E_v + \zeta_y F_v + \zeta_z G_v)$$

The inviscid and viscous Jacobian matrices which are produced in the process of linearization of the equations are given in Chapter 11 for the Navier-Stokes, Thin-Layer Navier-Stokes, Euler, and Parabolized Navier-Stokes equations.