Chapter 3

Numerical Approximation

3.1 Introduction

Numerical procedures solve finite difference approximations to the governing differential equations. The flow volume is typically first discretized into a set of mesh points and then the derivative terms of the equations are approximated as the change in flow variable between two or more points of the mesh divided by the distance between the chosen mesh points. The accuracy of the approximations can be determined by Taylor series analysis. Difference operators are defined for convenience in presenting numerical procedures and the modified equation, the equation actually solved by the numerical method, is derived and discussed. Finally, the importance of solving the conservation law form of the equations is illustrated.

3.2 Numerical Approximation on an Equally Spaced Mesh

(i) Spatial first derivatives

$$\frac{\partial \phi}{\partial x} \simeq \begin{cases} \dfrac{\phi_{i+1}-\phi_{i-1}}{2\Delta x}, & \textit{Central Difference,} \\ \dfrac{\phi_{i+1}-\phi_{i}}{\Delta x}, & \textit{Forward Difference,} \\ \dfrac{\phi_{i}-\phi_{i-1}}{\Delta x}, & \textit{Backward Difference} \end{cases}$$

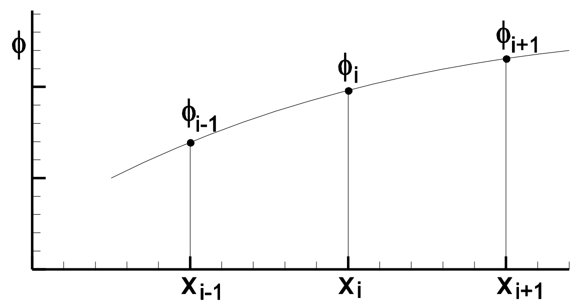

Figure 3.1 Equally spaced mesh

To analyze the above approximations for accuracy, it is convenient to expand each dependent flow variable appearing in the difference quotients about a common point using a Taylor series. Expanding about x_i we obtain the following representations.

$$\phi_{i+1} = \phi_i + \Delta x \left.\frac{\partial \phi}{\partial x}\right|_i + \frac{\Delta x^2}{2}\left.\frac{\partial^2 \phi}{\partial x^2}\right|_i + \frac{\Delta x^3}{3!}\left.\frac{\partial^2 \phi}{\partial x^2}\right|_i + \cdots$$

$$\phi_i = \phi_i$$

$$\phi_{i-1} = \phi_i - \Delta x \left.\frac{\partial \phi}{\partial x}\right|_i + \frac{\Delta x^2}{2}\left.\frac{\partial^2 \phi}{\partial x^2}\right|_i - \frac{\Delta x^3}{3!}\left.\frac{\partial^2 \phi}{\partial x^2}\right|_i + \cdots$$

By direct substitution, we obtain for the central difference approximation

$$\frac{\phi_{i+1}-\phi_{i-1}}{2\Delta x}=\left.\frac{\partial\phi}{\partial x}\right|_i+\frac{\Delta x^2}{3!}\left.\frac{\partial^3\phi}{\partial x^3}\right|_i+\cdots\text{, (second order accurate)}$$

Difference Approximation = Derivative + Truncation Error

The error introduced by the central difference approximation is of the order of Δx^2 and is said to be of second order accuracy.

Similarly, for the forward difference approximation

$$\frac{\phi_{i+1}-\phi_{i}}{\Delta x}=\left.\frac{\partial\phi}{\partial x}\right|_i+\frac{\Delta x}{2}\left.\frac{\partial^2\phi}{\partial x^2}\right|_i+\cdots\text{, (first order accurate)}$$

For the backward difference approximation

$$\frac{\phi_{i}-\phi_{i-1}}{\Delta x}=\left.\frac{\partial\phi}{\partial x}\right|_i-\frac{\Delta x}{2}\left.\frac{\partial^2\phi}{\partial x^2}\right|_i+\cdots\text{, (first order accurate)}$$

(ii) Spatial second derivatives
The following difference quotients represent central and backward approximations for a second derivative.

$$\frac{\partial^2\phi}{\partial x^2}\simeq\begin{cases}\dfrac{\phi_{i+1}-2\phi_i+\phi_{i-1}}{\Delta x^2}=\left.\dfrac{\partial^2\phi}{\partial x^2}\right|_i+\dfrac{2\Delta x^2}{4!}\left.\dfrac{\partial^4\phi}{\partial x^4}\right|_i+\cdots, & \text{second order accurate}\\[2ex] \dfrac{\phi_{i}-2\phi_{i-1}+\phi_{i-2}}{\Delta x^2}=\left.\dfrac{\partial^2\phi}{\partial x^2}\right|_i-\Delta x\left.\dfrac{\partial^3\phi}{\partial x^3}\right|_i+\cdots, & \text{first order accurate}\end{cases}$$

<u>3.3 Numerical Approximation on an Non- Equally Spaced Mesh</u>

Using central difference approximations for first and second derivatives on a stretched mesh, we obtain the following formulas.

$$\frac{\partial\phi}{\partial x}\simeq\frac{\phi_{i+1}-\phi_{i-1}}{x_{i+1}-x_{i-1}}$$

$$\frac{\partial^2\phi}{\partial x^2}\simeq\frac{\dfrac{\phi_{i+1}-\phi_i}{x_{i+1}-x_i}-\dfrac{\phi_i-\phi_{i-1}}{x_i-x_{i-1}}}{(x_{i+1}-x_{i-1})/2}$$

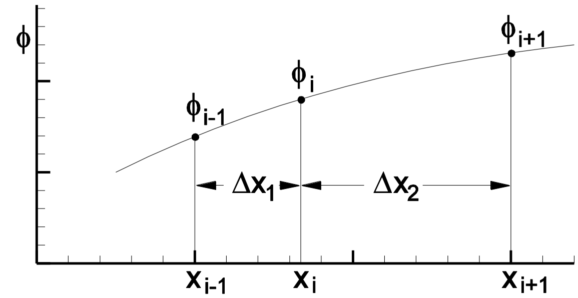

Figure 3.2 Equally spaced mesh

If the difference approximation is of second order on an equally spaced mesh, it is also second order on a stretched mesh if the stretching function is smooth. For example, we obtain for the above central difference approximation for a first derivative by Taylor series expansion

$$\frac{\phi_{i+1}-\phi_{i-1}}{x_{i+1}-x_{i-1}} = \left.\frac{\partial\phi}{\partial x}\right|_i + \frac{\Delta x_2^2-\Delta x_1^2}{\Delta x_1+\Delta x_2}\frac{1}{2}\left.\frac{\partial^2\phi}{\partial x^2}\right|_i + \cdots$$

$$= \left.\frac{\partial\phi}{\partial x}\right|_i + \frac{\Delta x_2-\Delta x_1}{2}\left.\frac{\partial^2\phi}{\partial x^2}\right|_i + \cdots$$

where $\Delta x_1 = x_i - x_{i-1}$ and $\Delta x_2 = x_{i+1} - x_i$.

Although it appears that the leading term of the truncation error is of first order, it is actually of second order, as we will demonstrate. Let $\xi(x)$ and its inverse $f(\xi)$ represent the stretching functions, with continuous derivatives at least up to second degree, between the physical and computational spaces, as shown below.

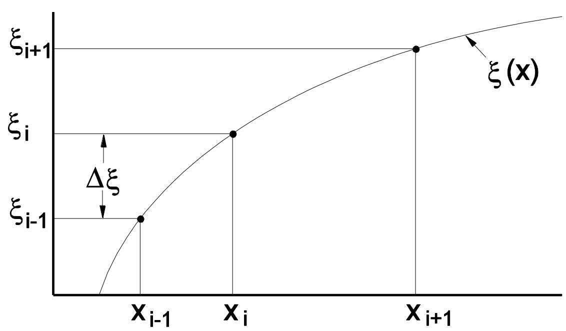

Figure 3.3 Stretching function $\xi(x)$

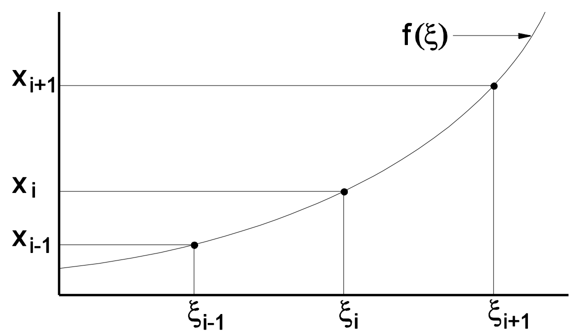

Figure 3.4 Inverse function $f(\xi)$

The stretching function $\xi(x)$ assumes its metric from the mesh index i, i.e. $\xi_i = i$ and $\Delta\xi = 1$. Thus, the computational space is equally spaced while the physical space x is stretched. Therefore

$$\Delta x_i = x_i - x_{i-1} = f(\xi_i) - f(\xi_{i-1}) \approx \Delta\xi\frac{\partial f}{\partial\xi}. \quad \textit{Thus}, \quad \Delta x \propto \Delta\xi$$

and

$$\Delta x_2 - \Delta x_1 = x_{i+1} - 2x_i + x_{i-1} = f(\xi_{i+1}) - 2f(\xi_i) + f(\xi_{i-1}) \approx \Delta\xi^2\frac{\partial^2 f}{\partial\xi^2} \quad \textit{and} \quad \textit{thus} \quad \Delta x_2 - \Delta x_1 \propto \Delta\xi^2 \propto \Delta x^2$$

showing that the truncation error term above is of second order.

For a second argument that the above approximation is second order accurate, we can approximate the derivatives in the equally spaced computational space, instead of approximating them as before directly in the physical space, as shown below.

$$\frac{\partial \phi}{\partial x} = \frac{\partial \phi}{\partial \xi}\frac{\partial \xi}{\partial x} = \frac{\partial \phi}{\partial \xi}\frac{d\xi}{dx} = \frac{\partial \phi}{\partial \xi}\left(\frac{dx}{d\xi}\right)^{-1}$$

Evaluating the derivative $\frac{\partial \phi}{\partial \xi}$ and all metric terms numerically in the equally spaced computational space, using only centered second order accurate difference approximations, we obtain

$$\frac{\partial \phi}{\partial x} = \frac{\partial \phi}{\partial \xi}\left(\frac{dx}{d\xi}\right)^{-1} \simeq \frac{\phi_{i+1}-\phi_{i-1}}{2\Delta\xi}\left(\frac{x_{i+1}-x_{i-1}}{2\Delta\xi}\right)^{-1} = \frac{\phi_{i+1}-\phi_{i-1}}{x_{i+1}-x_{i-1}}$$

which is exactly the same as our second order approximation on a stretched mesh given earlier.

On a given mesh a lower order accurate approximation may agree closer to the derivative being approximated than a higher order one. Order of accuracy only has meaning in the limit as $\Delta x \to 0$. Also, during the mesh refinement process it is understood that the stretching function does not change. During the limiting process as $\Delta x \to 0$ the stretching function appears to be more and linear locally about at any point of the mesh. For example, imagine the refinement about point x_i in figures 3.3 and 4.4 re-plotted, always showing only its two nearest mesh point neighbors. The three points would eventually lie on a straight line, i.e., $\xi = ax + b$, with a and b constant, and $\Delta\xi = a\Delta x$. This, any stretching function becomes locally linear and thus will always preserve order of accuracy.

The order of accuracy of an approximation does not change on a stretched mesh

3.4 Difference Operator Definitions

3.4.1 First Derivative Approximations for $\frac{\partial \phi}{\partial x}$

	Equally Spaced	Non-equally Spaced	
$\frac{D_+}{\Delta x}\phi_i =$	$\frac{\phi_{i+1}-\phi_i}{\Delta x}$	$\frac{\phi_{i+1}-\phi_i}{x_{i+1}-x_i}$	Forward Difference first order accurate
$\frac{D_-}{\Delta x}\phi_i =$	$\frac{\phi_i-\phi_{i-1}}{\Delta x}$	$\frac{\phi_i-\phi_{i-1}}{x_i-x_{i-1}}$	Backward Difference first order accurate
$\frac{D_0}{\Delta x}\phi_i =$	$\frac{\phi_{i+1}-\phi_{i-1}}{2\Delta x}$	$\frac{\phi_{i+1}-\phi_{i-1}}{x_{i+1}-x_{i-1}}$	Central Difference second order accurate

3.4.2 Second Derivative Approximations for $\frac{\partial^2 \phi}{\partial x^2}$

	Equally Spaced	Non-equally Spaced	
$\frac{D_{xx}}{\Delta x^2}\phi_i =$	$\frac{\phi_{i+1}-2\phi_i+\phi_{i-1}}{\Delta x^2}$	$\frac{\frac{\phi_{i+1}-\phi_i}{x_{i+1}-x_i}-\frac{\phi_i-\phi_{i-1}}{x_i-x_{i-1}}}{(x_{i+1}-x_{i-1})/2}$	Central Difference second order accurate
$\frac{D_{xx}}{\Delta x^2}\phi_{i-1} =$	$\frac{\phi_i-2\phi_{i-1}+\phi_{i-2}}{\Delta x^2}$	$\frac{\frac{\phi_i-\phi_{i-1}}{x_i-x_{i-1}}-\frac{\phi_{i-1}-\phi_{i-2}}{x_{i-1}-x_{i-2}}}{(x_i-x_{i-2})/2}$	Backward Difference first order accurate

3.4.3 Time Derivative Approximation

$\frac{D_+}{\Delta t}\phi_i^n = \frac{\phi_i^{n+1}-\phi_i^n}{\Delta t}$, first order accurate in time, where the superscripts refer to $t^n = n\Delta t$ and $t^{n+1} = (n+1)\Delta t$.

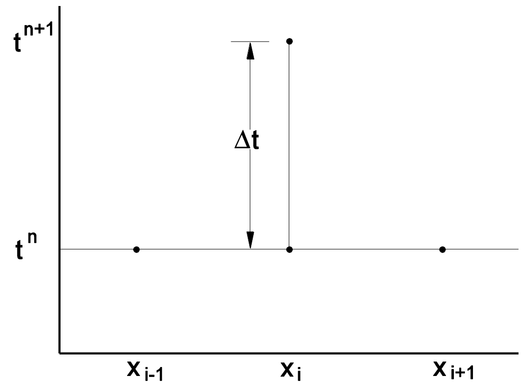

Figure 3.5 Mesh point stencil

3.5 Finite Difference Equations

3.5.1 Explicit Difference Equations

Consider the following model hyperbolic equation.

$$\frac{\partial u}{\partial t} + c\frac{\partial u}{\partial x} = 0\text{, where } c \text{ is constant.} \qquad (3.1)$$

Approximating the above equation using forward in time and centered in space difference quotients we obtain

$$\frac{u_i^{n+1}-u_i^n}{\Delta t} + c\frac{u_{i+1}^n - u_{i-1}^n}{2\Delta x} = 0 \qquad (3.2)$$

This can be written in difference operator notation as follows

$$\frac{D_+}{\Delta t}u_i^n + c\frac{D_0}{\Delta x}u_i^n = \left\{\frac{D_+\cdot}{\Delta t} + c\frac{D_0\cdot}{\Delta x}\right\}u_i^n = Lu_i^n = 0$$

Analysis by Taylor series expansion about the point (x_i, t^n) can be obtained using the following general equation

$$u_{i+k}^{n+m} = u_i^n + k\Delta x \frac{\partial u}{\partial x}\bigg|_i^n + m\Delta t \frac{\partial u}{\partial t}\bigg|_i^n +$$
$$\frac{(k\Delta x)^2}{2}\frac{\partial^2 u}{\partial x^2}\bigg|_i^n + \frac{2(k\Delta x)(m\Delta t)}{2}\frac{\partial^2 u}{\partial x \partial t}\bigg|_i^n + \frac{(m\Delta t)^2}{2}\frac{\partial^2 u}{\partial t^2}\bigg|_i^n +$$
$$\frac{(k\Delta x)^3}{3!}\frac{\partial^3 u}{\partial x^3}\bigg|_i^n + \frac{3(k\Delta x)^2(m\Delta t)}{3!}\frac{\partial^3 u}{\partial x^2 \partial t}\bigg|_i^n + \frac{3(k\Delta x)(m\Delta t)^2}{3!}\frac{\partial^3 u}{\partial x \partial t^2}\bigg|_i^n + \frac{(m\Delta t)^3}{3!}\frac{\partial^3 u}{\partial t^3}\bigg|_i^n + \cdots$$

By expansion of Equation (3.2) becomes

$$Lu_i^n = \left\{\frac{\partial u}{\partial t} + c\frac{\partial u}{\partial x}\right\}\bigg|_i^n + \frac{\Delta t}{2}\frac{\partial^2 u}{\partial t^2}\bigg|_i^n + c\frac{\Delta x^2}{3!}\frac{\partial^3 u}{\partial x^3}\bigg|_i^n + \cdots = 0 \qquad (3.3)$$

Difference Equation = Differential Equation + Truncation Error

The approximation is first-order accurate in time and second-order accurate in space. The overall order of accuracy of a difference equation is equal to its least accurate non-vanishing component. It makes little sense to give meaning to the difference in the order of accuracy in time and space because the time derivatives are related to spatial derivatives, for example through the differential equation itself. The above difference equation, is therefore of first-order accuracy. However, the difference equation is equal to the sum of the original differential equation plus the truncation error, a combined differential equation of infinite degree. Equation (3.3) could be used repeatedly by itself to replace all the derivatives with respect to time by spatial derivatives to create the modified equation, as will be discussed below. This is the actual differential equation represented and solved by the difference equations.

Consistency Requirement: Truncation Error must $\to$ 0
as Δx and Δt $\to$ 0 in any manner

The solution of Equation (3.2) for one time step is

$$u_i^{n+1} = u_i^n - \frac{c\Delta t}{2\Delta x}(u_{i+1}^n - u_{i-1}^n) = \left\{I - c\Delta t \frac{D_0 \cdot}{\Delta x}\right\}u_i^n$$

The new solution at (x_i, t^{n+1}) depends *explicitly* on data at time t^n only.

3.5.2 Implicit Difference Equations

Consider the following difference equation for approximating Equation (3.1)

$$\frac{u_i^{n+1} - u_i^n}{\Delta t} + \frac{c}{2}\left\{\frac{u_{i+1}^n - u_{i-1}^n}{2\Delta x} + \frac{u_{i+1}^{n+1} - u_{i-1}^{n+1}}{2\Delta x}\right\} = 0$$

This difference equation is of second order accurate in space and time. Solving for u_i^{n+1}

$$u_i^{n+1} = u_i^n - \frac{c\Delta t}{2}\frac{D_0 \cdot}{\Delta x} u_i^n - \frac{c\Delta t}{2}\frac{D_0 \cdot}{\Delta x} u_i^{n+1}$$

The new solution at (x_i, t^{n+1}) depends *implicitly* on itself at other points at time t^{n+1}. Thus, the new solution must in general be solved for simultaneously at all points (x_i, t^{n+1}), by inverting a matrix.

3.5.3 The Modified Equation

It was pointed out above that the difference equation is equal to an infinite order partial differential equation. For example, using forward in time and backward in space difference quotients to approximation Equation 3.1 we obtain by Taylor series expansion

$$\frac{u_i^{n+1} - u_i^n}{\Delta t} + c\frac{u_i^n - u_{i-1}^n}{\Delta x} = 0 = \frac{\partial u}{\partial t} + c\frac{\partial u}{\partial x} + \frac{\Delta t}{2}\frac{\partial^2 u}{\partial t^2} - c\frac{\Delta x}{2}\frac{\partial^2 u}{\partial x^2} + \frac{\Delta t^2}{3!}\frac{\partial^3 u}{\partial t^3} + c\frac{\Delta x^2}{3!}\frac{\partial^3 u}{\partial x^3} \cdots = 0$$

Attempts were made to remove the derivatives with respect to time higher than first order to analyze this differential equation for its stability, dissipation and wave dispersion error. The initial and simplest procedure used the original differential equation itself to eliminate the higher order time derivative terms, as follows.

$$\frac{\partial u}{\partial t} = -c\frac{\partial u}{\partial x} \Rightarrow \frac{\partial^2 u}{\partial t^2} = -c\frac{\partial \frac{\partial u}{\partial x}}{\partial t} = -c\frac{\partial \frac{\partial u}{\partial t}}{\partial x} = c^2\frac{\partial^2 u}{\partial x^2} \quad \text{and in general} \quad \frac{\partial^m u}{\partial t^m} = (-c)^m \frac{\partial^m u}{\partial x^m}$$

Therefore

$$\frac{u_i^{n+1} - u_i^n}{\Delta t} + c\frac{u_i^n - u_{i-1}^n}{\Delta x} = \frac{\partial u}{\partial t} + c\frac{\partial u}{\partial x} +$$

$$\frac{\Delta t}{2}c^2\frac{\partial^2 u}{\partial x^2} - c\frac{\Delta x}{2}\frac{\partial^2 u}{\partial x^2} - \frac{\Delta t^2}{3!}c^3\frac{\partial^3 u}{\partial x^3} + c\frac{\Delta x^2}{3!}\frac{\partial^3 u}{\partial x^3} + \cdots \frac{\Delta t^{m-1}}{m!}(-c)^m\frac{\partial^m u}{\partial x^m} - (-1)^m c\frac{\Delta x^{m-1}}{m!}\frac{\partial^m u}{\partial x^m} + \cdots = 0$$

Note that if Δt is chosen so that $\Delta t = \frac{\Delta x}{c}$ all the truncation error terms vanish, which indicates that the finite difference approximation is exact, with no dissipation error (the even order special derivative truncation error terms) or wave dispersion error (the odd order spacial derivative truncation error terms). Dissipation rounds out sharp features of the flow and wave dispersion will cause Fourier wave components of the solution to spread out from each other.

However, Warming and Hyatt showed that this procedure sometimes led to incorrect analyses and that one needed to use the entire infinite order differential equation, Equation (3.3), itself to *boot strap* its own removal of the higher order time derivative terms. The infinite order differential equation is the actual equation solved via the difference equation. This procedure is much more difficult to carry out analytically, but can be done by symbolic manipulation by computer. The resulting equation is called *the modified equation*. The simpler original differential equation can be used, however, for only the removal of the lowest order time derivative truncation error term, which may be sufficient to determine the order of accuracy of the approximation if truncation error cancellation occurs between the spacial and time derivative lowest order terms.

3.6 Time Accurate and Steady State Solutions

a) Model Hyperbolic Initial Value Problem

$$\frac{\partial u}{\partial t} + c\frac{\partial u}{\partial x} = 0$$

at $t = t_0, \quad u(x,t_0) = g(x)$,

at $x = x_0, \quad u(x_0,t) = u_0$,

$$\frac{u_i^{n+1} - u_i^n}{\Delta t} + c\frac{u_i^n - u_{i-1}^n}{\Delta x} = 0$$

The explicit solution algorithm

$$u_i^{n+1} = u_i^n - \frac{c\Delta t}{\Delta x}(u_i^n - u_{i-1}^n),$$

First-order accurate difference equation

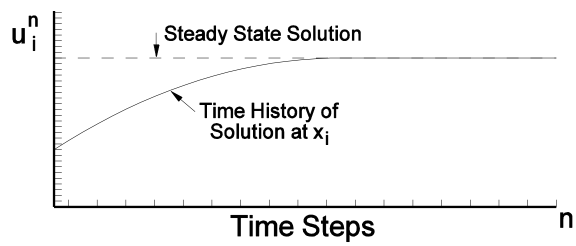

Figure 3.6 Time history

b) Model Elliptic Boundary Value Problem

$A\phi_{xx} + \phi_{yy} = 0$, on domain interior.

$\phi = \phi_\infty$, on domain boundary.

$\frac{\partial \phi}{\partial n} = 0$, on body surfaces.

Second-order accurate difference equation

$$A\frac{\phi_{i+1,j} - 2\phi_{i,j} + \phi_{i-1,j}}{\Delta x^2} + \frac{\phi_{i,j+1} - 2\phi_{i,j} + \phi_{i,j-1}}{\Delta y^2} = 0$$

The Point Jacoby solution algorithm,
using the notation $\phi_{i,j \leftarrow spacial\ indices\ for\ (x_i,y_j)}^{n \leftarrow iteration\ index}$, is

$$\phi_{i,j}^{n+1} = \frac{1}{2\left(\frac{A}{\Delta x^2} + \frac{1}{\Delta y^2}\right)}\left\{A\frac{\phi_{i+1,j}^n + \phi_{i-1,j}^n}{\Delta x^2} + \frac{\phi_{i,j+1}^n + \phi_{i,j-1}^n}{\Delta y^2}\right\}$$

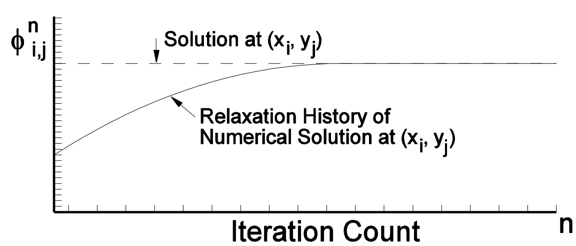

Figure 3.7 Relaxation history

3.7 Conservation Form of the Difference Equations

Using an explicit in time and backward in space finite difference method, as an example, applied to a one dimensional system of equations in conservation form (see Section 2.2), we obtain

$$U_i^{n+1} = U_i^n - \frac{\Delta t}{\Delta x}(F_i^n - F_{i-1}^n)$$

The total U (i.e., mass, momentum, and energy per unit volume) in the flow field at time t^n is $\sum_{i=1}^{I} U_i^n \Delta x$. At time t^{n+1} it is

$$\sum_{i=1}^{I} U_i^{n+1} \Delta x = \sum_{i=1}^{I} U_i^n \Delta x - \Delta t \underbrace{\sum_{i=1}^{I} (F_i^n - F_{i-1}^n)}_{\substack{A\ telescoping\ sum - each\ term \\ appears\ twice, with\ opposite \\ sign,\ except\ F_0^n\ and\ F_I^n.}}$$

Thus

$$\sum_{i=1}^{I} U_i^{n+1} \Delta x = \sum_{i=1}^{I} U_i^n \Delta x - \Delta t F_I^n + \Delta t F_0^n$$

New Total U = Old Total U - Exit Flux + Entrance Flux

Thus, there are no internal sources or sinks of U within the solution domain.

If, in contrast, the same difference scheme is applied to the nonconservation form of the governing equations,

$$\frac{\partial U}{\partial t} + A \frac{\partial U}{\partial x} = 0$$

where A is in general not constant, then we obtain

$$U_i^{n+1} = U_i^n - \frac{A_i^n \Delta t}{\Delta x}(U_i^n - U_{i-1}^n)$$

and $$\sum_{i=1}^{I} U_i^{n+1} \Delta x = \sum_{i=1}^{I} U_i^n \Delta x - \Delta t \underbrace{\sum_{i=1}^{I} A_i^n (U_i^n - U_{i-1}^n)}_{\substack{This\ term\ is\ not\ necessarily \\ telescopic\ and\ may\ contribute \\ to\ \text{sources}\ and\ \text{sinks}\ of\ U.}}$$

Total mass, momentum, and energy may not be conserved. Shock waves may have the wrong *jumps* and speeds {*Lax, 1954*}.