Numerical Methods

Numerical Solution to partial differential Equation

Introduction:

Atmospheric model simulation physical processes described by ordinary and partial differential equations. Gas and aqueous chemistry and gas to partial conversion processes are simulated with ordinary differential equation. In this chapter, ordinary and partial differential equation are defined and numerical methods of solving partial differential equations are discussed. Methods of solving partial differential equations include finite- difference and series expansion methods. In both cases, partial derivatives are approximated with analogs, and analogs are solved numerically. Below, finite-difference analoges and their numerical solutions are given for the advection- diffusion equation, which is a unidirectonal form of the species continuity equation. Solutions that assume constant and variable grid spacing and eddy diffusion cofficients are shown. A special case of finite – difference method is the semi- Lagrangian method. Two series exansion methods, the finite- element and pseudospectral methods are discussed.

1. Ordinary and partial differntial equation

An ordinary differential equation (ODE) is an equation with one independent variable, such as time, and a partial differential equation (PDE) is an equation with more than one independent variable, such as time and space. ODEs and PDEs are classified by their order and degree. The **order** is the highest derivative rank of the equation, and the **degree** is the highest polynomial exponent of the highest derivative. A homogeneous differential equation that does not contain a term involving the independent variable. A liner differential equation is one in which the dependent variable and its derivatives do not appear in second-degree or higher terms and in which the dependent variable is not multiplied by other derivatives of itself.

Table (1) shows ordinary and partial differential equation of varying orders and degrees. In the table (a), (b), (d), (e), and (f) are homogeneous, and the reaming equations are inhomogeneous. Equation b, and e are liner, and the rest are nonlinear. Chemical equation are first-order, first-degree, homogeneous ODEs, such as (a) and (b). these equations are either liner or nonlinear. The species continuity equation and the thermodynamic energy equation are first-order, first degree, homogeneous, nonlinear PDE, such as (f).

Table 1: Examples of the Order and degree of ordinary and Partial Differential Eq.

Order, Degree	Ordinary Differential Equations	Partial Differential Equations
First-order, first-degree	(a) $\frac{dN}{dt} = 16 - 4N^2$	(e) $\frac{\partial N}{\partial t} + \frac{\partial (uN)}{\partial x} = 0$
First-order, first-degree	(b) $\frac{dN}{dt} = 3AB - 4NC$	(f) $\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} + v\frac{\partial u}{\partial y} = 0$
Second-order, first-degree	(c) $\frac{d^2N}{dt^2} + \frac{dN}{dt} + 5t = 0$	(g) $\frac{\partial^2 N}{\partial t^2} + \frac{\partial^2 N}{\partial x^2} = 3t^2 + x$
Second-order, second-degree	(d) $\left(\frac{d^2N}{dt^2}\right)^2 + \frac{dN}{dt} + 4 = 0$	(h) $\left(\frac{\partial^2 N}{\partial t^2}\right)^2 + \frac{\partial N}{\partial x} = t - x$

Boundary conditions for ODEs and PDEs must be specified. When conditions are known at one end of domain but not the other, an initial –value problem arises. If the concentrations (N) are known at time t=0, if time is the independent variable, and if concentration is the dependent variable, the set of ODEs is an initial value problem. When conditions are known at both ends of a domain, a boundary- value problem arises. If time and west - east direction (x) are independent variables if the concentration is the dependent variables and if the concentrations are known everywhere at t=0 and at both ends of spatial domain at all times, the set of PDEs is an initial value problem with respect to time and boundary value problem with respect to space.

2. Operator - Splitting

Each major process in an atmospheric model is generally solved separately from each other process. Suppose a model take account of dynamics, transport, and gas chemistry. Each of these processes may be solved sequentially during a common

time interval, with a unique numerical scheme that takes a unique number of time steps. A time step is as increment in time for a given process. A time interval is the period during which several time steps of process are solved without interference by other processes. Suppose the time step for dynamic is 6 s, the transport time step is 300 s, the chemistry time step is variable, and the time interval common to all processes is 300 s. During the time interval, 50 dynamics time steps are taken, followed by 1 transport time step, followed by a variable number of chemistry time steps. After the dynamic steps, average predicted wind speed is used as inputs into the transport calculations. During the transport step, gases are moved around the grid. Final concentrations from the transport step are used as initial value for the chemistry steps. Final values from the chemistry steps are used as initial values for dynamics steps in the next time interval. Figure 6.1 illustrates this example.

The isolation of individual processes during a time interval is called time or operators-splitting. Operator-splitting is used because computers today cannot solve

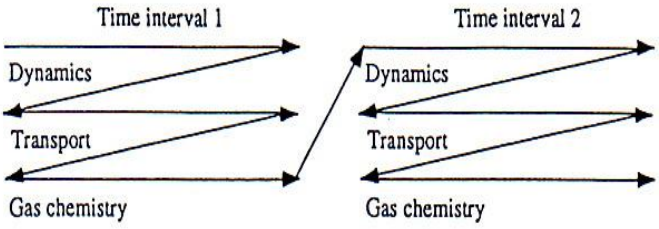

Figure 6.1. Example of operator-splitting scheme. During the first time interval, dynamics, transport, and gas chemistry are solved sequentially. Values determined from the end of a time interval after one processes are used to initialize values at the beginning of the same time interval for another process. Values from the end of the last process in one time interval are used at the beginning of the first process in the next time interval.

All model ODEs and PDEs simultaneously in three dimensions. Yanenko (1971) discusses the theoretical basis behind operator-splitting with respect to certain mathematical equations.

3. Advection – Diffusion Equations

First-order, first-degree, homogenous, linear or nonlinear partial differential equations solved in atmospheric models include the species continuity equation, the

thermodynamic energy equation, and the directional momentum equation. The method of solving these equations together is given. In this chapter methods of solving advection-diffusion equations, which are operator-split forms of the species continuity equation, are discussed advection-diffusion equations are derived by considering that the four-dimensional (t,x,y,z) species continuity equation can be divided into three two-dimensional partial differential equation ([t,x],[t,y], and[t,z]) and single one –dimensional (t) ordinary differential equation. The sequential solution to the four operator-split equations approximates the solution to the original four-dimensional equation. This method of operator- splitting a mathematical equation is called the locally one-dimensional (LOD) procedure or the method of fractional steps, has been used widely in atmospheric models.

From the four-dimensional species continuity equation the west-east, south-north, and vertical unidirectional advection-diffusion equations can be written in number concentration units as:

$$\frac{\partial N}{\partial t}+\frac{\partial (uN)}{\partial x}-\frac{\partial}{\partial x}\left(K_{h,xx}\frac{\partial N}{\partial x}\right)=0 \qquad (6.1)$$

$$\frac{\partial N}{\partial t}+\frac{\partial (vN)}{\partial y}-\frac{\partial}{\partial y}\left(K_{h,yy}\frac{\partial N}{\partial y}\right)=0 \qquad (6.2)$$

$$\frac{\partial N}{\partial t}+\frac{\partial (wN)}{\partial z}-\frac{\partial}{\partial z}\left(K_{h,zz}\frac{\partial N}{\partial z}\right)=0 \qquad (6.3)$$

The solution order of these equations may be reversed each time interval to improve accuracy. Thus, if the equations are solved in the order (6.1), (6.2), (6.3) during one time interval, they may be solved in the order (6.3), (6.2), (6.1) during the next time interval. Fractional – step schemes associated with order reversal are called alternating –direction schemes.

The remaining terms in species continuity equation are external source/sink terms. These terms are operator- split from the advection-diffusion terms as a single ordinary differential equation,

$$\frac{\partial N}{\partial t} = \sum_{n=1}^{N_{e,t}} R_n \quad \text{---------- (6.4)}$$

Or may be split further into several ODEs (6.4) can be solved before or after (6.1)-(6-3) are solved.

In moist- air mass- ratio units, the operator- split west-east advection diffusion equation can be written from (3) as:

$$\frac{\partial q}{\partial t} + u\frac{\partial q}{\partial x} - \frac{1}{\rho_a}\frac{\partial}{\partial x}\left(\rho_a K_{h,xx}\frac{\partial q}{\partial x}\right) = 0 \quad \text{---------- (6.5)}$$

Analogous equations can be written for the south – north and vertical directions and for external source. In the following sections, finite-difference and series expansion methods of approximating derivatives and solving advection- diffusion equations discussed.

4. Finite-Difference Approximation

Approximate solutions to partial differential equations, such as advection-diffusion equation can be found with finite –difference or series expansion methods. The purpose of using an approximation is to reduce the solution space for each continuous differential function from as infinite to a finite number of spatial or temporal nodes in order to speed up computation of the differential equation.

A finite – difference approximation involves the replacement of each continuous differential operator (d) with a discrete difference analog (Δ). This analog is an approximation written in terms of finite number of values of the variable being operated on at each temporal or spatial node. If the west- east scalar velocity is a continuous function in space at given time, vales of the velocity can be mapped from the function to a discretized west –east grid, as shown in Fig. 6.2. The grid consists of several grid cells (also called grid boxes, grid points, or nodes) placed any distance part.

Finite – difference Approximations of a variable are often made with respect to time or space. Table 6.1 (e) and (f) are partial differential equations commonly simulated in atmospheric models. In (e) finite –difference analogs are required for

($\partial N / \partial t$) and $\partial(uN)/\partial x$. In (f), finite-difference analogs are required for ($\partial u / \partial t, \partial u / \partial x$) and $\partial u / \partial y$.

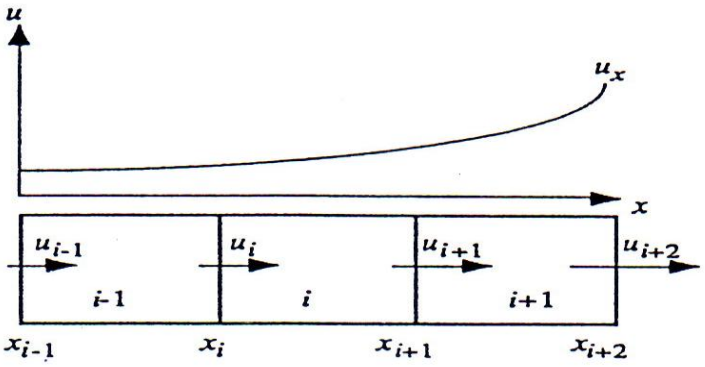

Figure 6.2. Discretization of a continuous west–east scalar velocity u_x. The west–east grid is broken into discrete cells, and u-values are mapped from the continuous function to the edge of each cell. The arrows in the cells represent magnitudes of the wind speed. Distances along the x-axis are also mapped to the cells.

4.1 Consistency, Convergence, and Stability

The ability of numerical solution to replicate the exact solution to partial differential equation depends on several factors. A finite – difference analog in space or time must converge to its differential expression when the analog is reduced towards zero. If $\Delta N / \Delta x$ is a finite –difference analog $\partial N / \partial x$, the condition

$$\frac{\partial N}{\partial x} = \lim_{\Delta x \to 0} \left\| \frac{\Delta N}{\Delta x} \right\| \quad \text{---------- ---------- (6.6)}$$

must be satisfied for the approximation to be useful.

The finite – difference analog $\Delta N / \Delta x$ in Equation (6.6) is obtained from a Taylor series expansion. In the expansion, high- order term are neglected to reduce the computational burden of the approximation. The difference between the full Taylor series expansion and truncated approximation is the truncation error> A finite-approximation approaches zero a Δx or (Δt) approaches zero. Consistency occurs when :

$$\frac{\partial N}{\partial x} = \lim_{\Delta x \to 0} \left\| \frac{\Delta N}{\Delta x} \right\| = 0 \text{ ---------- ---------- (6.7)}$$

Where T.E. is the truncation error of the approximation $\Delta N / \Delta x$.

If a finite- difference approximation is consistent, the rate at which its truncation error approaches zero depends on the order of approximation. The order of approximation is the lowest- order term in the Taylor series expansion neglected in the approximation. The higher the order of approximation, the faster the truncation error converges towards zero upon an increase in spatial (or temporal) resolution thus, with the same Δx, a high-order approximation is more accurate than a low-order approximation. For the same truncation error, a low- order approximation requires a smaller Δx than does a high- order approximation. In sum, a high – order with a large Δx. Because a high – order approximation includes more terms, it requires more computation than does a low – order approximation with the same Δx.

Obtaining high order with respect one variable, such as space, is useful only if the order of the other variable, such as time, is also high. Otherwise, low accuracy in the time derivative swamps the high accuracy in the space derivative. An optimal finite – difference solution has similar order in space and time.

While individual finite – difference analogs must converge towards exact differentials, the overall numerical solution to a PDE must converge to an exact solution when spatial and temporal differences decrease towards zero. If $N_{e,x,t}$ is an exact solution and $N_{f,x,t}$ is a finite – difference approximation of a PDE, overall convergence occurs when

$$\lim_{\Delta x, \Delta t \to 0} \left\| N_{e,xt} - N_{f,x,t} \right\| = 0 \quad \text{- --------- ---------- (6.8)}$$

If a numerical solution is non-convergent, it is not useful.

For a numerical method to be successful, it must be stable. Stability occurs if the absolute-value difference between the numerical and exact solutions does not grow over time. Thus,

$$\lim_{t \to \infty} \left\| N_{e,xt} - N_{f,x,t} \right\| \leq C \quad \text{---------- ------- (6.9)}$$

Where C is a constant. Stability often depends on the time step size used. If a numerical solution is stable for any time step smaller than a specified value, the solution is conditionally stable. If a solution is table, regardless of the time step, it is

unconditionally stable. If a solution is unstable, regardless of the time step, it is unconditionally unstable.

Other problem arising from finite – difference and other solutions to partial difference are numerical diffusion (artificial spreading of peak values across several grid cells) and numerical dispersion (waves appearing ahead of and behind peak value). These problems can usually be mitigated by increasing the resolution of the spatial grid (e.g. decreasing Δx), decreasing the time step, or increasing the order of approximation of the finite – difference analog.

4.2 Low- Order Approximations of Derivatives

A finite – difference approximation, such as $\partial u / \partial x$, involves the replacement of individual expression, such as $\partial u / \partial x$, with finite – difference analog, such as $\Delta u - or - \Delta x$, respectively. Suppose $\partial u / \partial x$ is discretized over a west-east grid, as shown in Fig. 6.2, where all cells are rectangular. Each cell is denoted by an index number I, and distance from the western edge of the entire grid to the western edge of cell I is x_i.

On the grid layout just defined, the differential scalar velocity ∂u at point x_i can be estimated as

$\Delta u_i = u_{i+1} - u_{i-1}$, $\Delta u_i = u_{i+1} - u_i$. Or $\Delta u_i = u_i - u_{i-1}$, with are the central, forward, and backward-difference approximations, respectively.

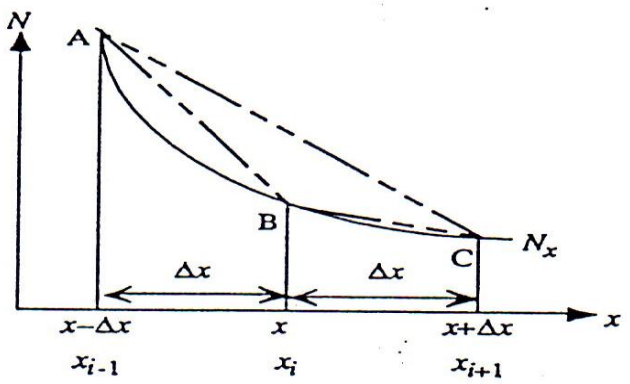

Figure 6.3. Derivative approximations at a point on a continuous function. The derivative at point B is approximated with chords AC, BC, or AB, which give the slope of the tangent at point B for the central-, forward-, and backward-difference approximations, respectively.

The corresponding discretizations of ∂x are $\Delta x_i = x_{i+1} - x_{i-1}$, $\Delta x_i = x_{i+1} - x_i$. and $\Delta x_i = x_i - x_{i-1}$, respectively. In the central – difference case, the slop of the tangent at point xi in Fig. 6.2 is approximately.

$$\frac{\partial u}{\partial x} = \frac{\Delta u}{\Delta x} = \frac{u_{i+1} - u_{i-1}}{x_{i+1} - x_{i-1}} \quad \text{---------- ---------- (6.10)}$$

Similar equation can be written for the forward and backward –difference cases.

The approximations just discussed can be derived from a Taylor series expansion. If gas concentration is a continuous function of west –east distance, as shown in Fig. 6.3 the values, of (N) at points +Δx and -Δx, respectively, are determined from Taylor's theorem as

$$N_{x+\Delta x} = N_x + \Delta x \frac{\partial N_x}{\partial x} + \frac{1}{2}\Delta x^2 \frac{\partial^2 N_x}{\partial x^2} + \frac{1}{6}\Delta x^3 \frac{\partial^3 N_x}{\partial x^3} + \frac{1}{24}\Delta x^4 \frac{\partial^4 N_x}{\partial x^4} + \cdots \quad (6.11)$$

$$N_{x-\Delta x} = N_x - \Delta x \frac{\partial N_x}{\partial x} + \frac{1}{2}\Delta x^2 \frac{\partial^2 N_x}{\partial x^2} - \frac{1}{6}\Delta x^3 \frac{\partial^3 N_x}{\partial x^3} + \frac{1}{24}\Delta x^4 \frac{\partial^4 N_x}{\partial x^4} - \cdots \quad (6.12)$$

If grid spacing is uniform (Δx is constant), the sum of (6.11) and (6.12) is

$$N_{x+\Delta x} + N_{x-\Delta x} = 2N_x + \Delta x^2 \frac{\partial^2 N_x}{\partial x^2} + \frac{1}{12}\Delta x^4 \frac{\partial^4 N_x}{\partial x^4} + \cdots \quad (6.13)$$

Rearranging (6.13) gives

$$\frac{\partial^2 N_x}{\partial x^2} = \frac{N_{x+\Delta x} - 2N_x + N_{x-\Delta x}}{\Delta x^2} + O(\Delta x^2) \quad (6.14)$$

If grid spacing is uniform (Δx is constant), the sum of equation (6.11) and (6.12) is:

$$N_{x+\Delta x} + N_{x-\Delta x} = 2N_x + \Delta x^2 \frac{\partial^2 N_x}{\partial x^2} + \frac{1}{12}\Delta x^4 \frac{\partial^4 N_x}{\partial x^4} + \ldots\ldots \quad \text{---------- (6.13)}$$

Rearranging (6.13) gives:

$$\frac{\partial^2 N_x}{\partial x^2} = \frac{N_{x+\Delta x} - 2N_x + N_{x-\Delta x}}{\Delta x^2} + O(\Delta x^2) \quad \text{---------- ---------- (6.14)}$$

Where

$$O(\Delta x^2) \approx \frac{1}{12}\Delta x^2 \frac{\partial^4 N_x}{\partial x^4} - \ldots\ldots \quad \text{---------- (6.15)}$$

Includes all terms of order Δx^2 and higher. If $O(\Delta x^2)$ is small, equation (6.14) simplifies to :-

$$\frac{\partial^2 N_x}{\partial x^2} = \frac{N_{x+\Delta x} - 2N_x + N_{x-\Delta x}}{\Delta x^2} \quad \text{---------} \quad \text{----------(6.16)}$$

Where $O(\Delta x^2)$ is now the truncation error. Equation (6.16) is a second- order central difference approximation of $\partial^2 N_x / \partial x^2$. The equation is second – order because the lowest –order exponent in the truncation error is two. It is a central –difference approximation because it relies on equally weight of N on each side of node x.

Subtracting equation (6.12) from equation (6.11) gives:

$$N_{x+\Delta x} - N_{x-\Delta x} = 2\Delta x \frac{\partial N_x}{\partial x} + \frac{1}{3}\Delta x^3 \frac{\partial^3 N_x}{\partial x^3} + \ldots\ldots \quad \text{----------(6.17)}$$

Rearranging this equation results in

$$\frac{\partial N_x}{\partial x} = \frac{N_{x+\Delta x} - N_{x-\Delta x}}{2\Delta x} + O(\Delta x^2) \text{ ---------- (6.18)}$$

Where

$$O(\Delta x^2) = -\frac{1}{6}\Delta x^2 \frac{\partial^3 N_x}{\partial x^3} - \ldots\ldots\ldots \quad \text{----------(6.19)}$$

Includes all terms of order Δx^2 and higher. If $O(\Delta x^2)$ is small, equation (6.18) simplifies to:

$$\frac{\partial N_x}{\partial x} \approx \frac{N_{x+\Delta x} + N_{x-\Delta x}}{2\Delta x} = \frac{N_{i+1} - N_{i-1}}{2\Delta x} \quad \text{----------(6.20)}$$

Where (i+1) and (i-1) are surrogates for $x + \Delta x$ and $x - \Delta x$, respectively. This equation is a second-order central- difference approximation of the first order derivative of N_x Equation (6.20) gives the slop of the tangent (represented by chord AC) of N_x at point B in Fig. 6.3.

Another approximation of the first derivative of N_x is obtained the first two terms of equation (6.11). Rearranging these terms gives:

$$\frac{\partial N_x}{\partial x} \approx \frac{N_{x+\Delta x} + N_{x-\Delta x}}{2\Delta x} = \frac{N_{i+1} - N_{i-1}}{2\Delta x} \text{ ----------(6.20)}$$

$$\frac{\partial N_x}{\partial x} \approx \frac{N_{x+\Delta x} + N_x}{\Delta x} = \frac{N_{i+1} - N_i}{\Delta x} \text{ ----------(6.21)}$$

The truncated portion of approximation includes terms first –order and higher $[O(\Delta x)]$; thus, equation(6.21) is a first-order forward-difference approximation of the first derivative of N_x. The slop of this derivative is represented by chord BC in Fig. 6.3. Rearranging the first two terms of equation (6.12) gives:

$$\frac{\partial N_x}{\partial x} \approx \frac{N_x - N_{x-\Delta x}}{\Delta x} = \frac{N_i - N_{i-1}}{\Delta x} \text{ ----------(6.22)}$$

Which is the first – order backward –difference approximation of the first derivative of N_x, represented by chord AB in fig. 6.3.

If time, not space, is the independent variable, the second order central, first order forward and first backward difference approximations of $N_t / \partial t$ are :

$$\frac{\partial N_t}{\partial t} \approx \frac{N_{t+b} - N_{t-b}}{2b} \ldots\ldots \frac{\partial N_t}{\partial t} \approx= \frac{N_{t+b} - N_t}{b} \ldots\ldots \frac{\partial N_t}{\partial t} \approx \frac{N_t - N_{t-b}}{b} \ldots\ldots (6.23)$$

Respectively, where $b = \Delta t$ is the time-step size, t is the current time, $t+b$ is one time step forward, and t-b is one time step backward. These equations are derived in the sane manner as equation (6.20), (6.21), and (6.22), respectively.

4.3 Arbitrary- Order Approximations of Derivatives

Finite difference approximations of arbitrary order can be obtained systematically (e.g., Celia and Gray 1992). The approximation of $\partial^m N / \partial x^m$, which is the m^{th} derivative of *N*, can be obtained by expanding the derivative across q discrete

nodes in the x-direction. If the independent variable is time, the derivative can be expanded along *q* time steps. The minimum number of nodes allowed in the expansion is *m+1*. In general, the maximum order of approximation of a finite difference solution is q-m, although it may be smaller or larger for individual cause. For instance, when *m* is even and the grid spacing is constant, the order of approximation can be increased to (*q-m+1)*.

Figure 6.4 shows the arbitrary grid spacing for the derivation to come. The point at which the derivative is taken does not need to correspond to a node point, although in the figure the derivative is assumed to be taken t node point *x3*. The distance between two nodes is $\Delta x_i = x_{i+1} - x_i$, where i varies from *1* to *q-1*.

The finite difference solution to m^{th} derivative across q nodes is approximately.

$$\frac{\partial^m N}{\partial x^m} \approx \sum_{i=1}^{q} \gamma_i N_i = \gamma_1 N_1 + \gamma_2 N_2 + \ldots\ldots\ldots + \gamma_q N_q \quad \ldots\ldots(6.24)$$

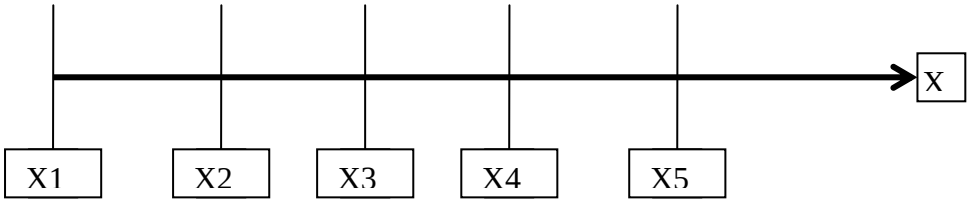

Figure 6.4: Grid spacing of an arbitrary –spaced grid where *q=5*. The derivative is taken at point *x3*, marked.

Where the γ_i's are constants to be determined. A Taylor series expansion of N at node *i* across the point at which the derivative is taken (*) is:

$$N_i = N_* + (x_i - x_*)\frac{\partial N_*}{\partial x} + \frac{1}{2}(x_i - x_*)^2 \frac{\partial^2 N_*}{\partial x^2} + \frac{1}{6}(x_i - x_*)^3 \frac{\partial^3 N_*}{\partial x^3} + \ldots\ldots\ldots\ldots(6.25)$$

Combining (6.24) with (6.24) and gathering terms gives:

$$\frac{\partial^m N}{\partial x^m} \approx \sum_{i=1}^{q} \gamma_i N_i = \sum_{i=1}^{q} \gamma_i N_* + \sum_{i=1}^{q} \gamma_i (x_i - x_*)\frac{\partial N_*}{\partial x} + \sum_{i=1}^{q} \gamma_i \frac{1}{2}(x_i - x_*)^2 \frac{\partial^2 N_*}{\partial x^2} + \ldots\ldots\ldots\ldots(6.26)$$

This equation can be rewritten:

$$\sum \gamma_i N_i = B_o N_* + B_1 \frac{\partial N_*}{\partial X} + B_2 \frac{\partial^2 N_*}{\partial x^2} + \ldots\ldots \ldots\ldots\ldots (6.27)$$

Where

$$\ldots\ldots\ldots (6.28)\ B_n = \sum_{i=1}^{q} \gamma \frac{1}{n!} (x_i - x_*)^n \ldots\ldots\ldots \quad for \ - - n = 0, \ldots q - 1$$

Equation (6.28) represents a matrix of q equations and unknowns. Multiplying (6.28) by *n!* gives:

$$\begin{bmatrix} 1 & 1 & 1 & .. & 1 \\ (x_1 - x_*) & (x_2 - x_*) & (x_3 - x_*) & .. & (x_q - x_*) \\ (x_1 - x_*)^2 & (x_2 - x_*)^2 & (x_3 - x_*)^2 & .. & (x_q - x_*)^2 \\ . & . & . & .. & . \\ (x_1 - x_*)^q & (x_2 - x_*)^q & (x_3 - x_*) & .. & (x_q - x_*)^q \end{bmatrix} \begin{bmatrix} \gamma_1 \\ \gamma_2 \\ \gamma_3 \\ . \\ \gamma_q \end{bmatrix} = \begin{bmatrix} 0! B_o \\ 1! B_1 \\ 2! B_2 \\ . \\ (q-1)! B_{q-1} \end{bmatrix} \ldots\ldots\ldots (6.29)$$

The highest – order derivative is found when $B_n=1$ for $n=m$ and $B_n=o$
For all other *n*.

The first order backward difference approximation of $\partial N / \partial x (m-1)$ is found from (6.29) by discretizing $\partial N / \partial x$ across two equally spaced grid cells (q=2), setting B_1= -1, and B_1= 0 for all other n. the resulting matrix is :

$$\begin{bmatrix} 1 & 1 \\ -\Delta x & 0 \end{bmatrix} \begin{bmatrix} \gamma_i - 1 \\ \gamma_i \end{bmatrix} = \begin{bmatrix} 0 \\ 1 \end{bmatrix} \ldots\ldots\ldots\ldots\ldots\ldots (6.30)$$

Where the subscript *(i-1)* indicates one node to the left of i. the matrix has solution $\gamma_{i-1} = -1/\Delta x$ and $\gamma_i = 1/\Delta x$. Substituting these coefficients into

$$\frac{\partial N}{\partial x} \approx \gamma_1 N_1 + \gamma_2 N_2 = \gamma_{i-1} N_{i-1} + \gamma_i N_i \ldots\ldots (6.31)$$

From equation (6.24) gives the approximation shown in equation (6.22) and table (6.2) a.

Table 6.2. Finite-Difference Approximations of $\partial N/\partial x$ and $\partial^2 N/\partial x^2$

Order	m	q	Approximation
(a) 1st order backward	1	2	$\frac{\partial N}{\partial x} \approx \frac{N_i - N_{i-1}}{\Delta x}$
(b) 1st order forward	1	2	$\frac{\partial N}{\partial x} \approx \frac{N_{i+1} - N_i}{\Delta x}$
(c) 2nd order central	1	3	$\frac{\partial N}{\partial x} \approx \frac{N_{i+1} - N_{i-1}}{2\Delta x}$
(d) 2nd order backward	1	3	$\frac{\partial N}{\partial x} \approx \frac{N_{i-2} - 4N_{i-1} + 3N_i}{2\Delta x}$
(e) 2nd order forward	1	3	$\frac{\partial N}{\partial x} \approx \frac{-3N_i + 4N_{i+1} - N_{i+2}}{2\Delta x}$
(f) 3rd order backward	1	4	$\frac{\partial N}{\partial x} \approx \frac{N_{i-2} - 6N_{i-1} + 3N_i + 2N_{i+1}}{6\Delta x}$
(g) 3rd order forward	1	4	$\frac{\partial N}{\partial x} \approx \frac{-2N_{i-1} - 3N_i + 6N_{i+1} - N_{i+2}}{6\Delta x}$
(h) 4th order central	1	5	$\frac{\partial N}{\partial x} \approx \frac{N_{i-2} - 8N_{i-1} + 8N_{i+1} - N_{i+2}}{12\Delta x}$
(i) 4th order backward (I)	1	5	$\frac{\partial N}{\partial x} \approx \frac{-N_{i-3} + 6N_{i-2} - 18N_{i-1} + 10N_i + 3N_{i+1}}{12\Delta x}$
(j) 4th order forward (I)	1	5	$\frac{\partial N}{\partial x} \approx \frac{-3N_{i-1} - 10N_i + 18N_{i+1} - 6N_{i+2} + N_{i+3}}{12\Delta x}$
(k) 4th order backward (II)	1	5	$\frac{\partial N}{\partial x} \approx \frac{-3N_{i-4} + 16N_{i-3} - 36N_{i-2} + 48N_{i-1} - 25N_i}{12\Delta x}$
(l) 4th order forward (II)	1	5	$\frac{\partial N}{\partial x} \approx \frac{25N_i - 48N_{i+1} + 36N_{i+2} - 16N_{i+3} + 3N_{i+4}}{12\Delta x}$
(m) 2nd order central	2	3	$\frac{\partial^2 N}{\partial x^2} \approx \frac{N_{i+1} - 2N_i + N_{i-1}}{\Delta x^2}$
(n) 4th order central	2	5	$\frac{\partial^2 N}{\partial x^2} \approx \frac{-N_{i-2} + 16N_{i-1} - 30N_i + 16N_{i+1} - N_{i+2}}{12\Delta x^2}$

Second order central and backward difference approximations of $\partial N / \partial x(m-1)$ are found by discretizing $\partial N / \partial x(m-1)$ across three nodes (q=3). The resulting matrices are:

$$\begin{bmatrix} 1 & 1 & 1 \\ -\Delta x & 0 & +\Delta x \\ (-\Delta x)^2 & 0 & (\Delta x)^2 \end{bmatrix} \begin{bmatrix} \gamma_{i-1} \\ \gamma_i \\ \gamma_{i+1} \end{bmatrix} = \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix}$$

$$\begin{bmatrix} 1 & 1 & 1 \\ -2\Delta x & -\Delta x & 0 \\ (-2\Delta x)^2 & (-\Delta x)^2 & 0 \end{bmatrix} \begin{bmatrix} \gamma_{i-2} \\ \gamma_{i-1} \\ \gamma_i \end{bmatrix} = \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix} \quad \text{..... (6.32)}$$

Respectively substituting solutions to these matrices into (6.24) gives the approximation shown in table 6.2- c and d, respectively. The second order forward difference approximation of $\partial N / \partial x$ is found by discretizing around the first column in

(6.32). The result is shown table 6.2 –e. Foreword and backward difference discretizations are negatively symmetric to each other.

Third order backward and forward difference approximations of $\partial N / \partial x$ are found in similar manner. The results are shown in table 6.2- f and g. respectively where the discretizations are around four cells.