1.0   INTRODUCTION

In the modelling of complex physical systems, all the involved physical processes are represented mathematically by a set of equations. Thus, each physical process is replaced by a set of its governing equations. In most of the cases the physics of the processes involve the rate of change with respect to two or more independent variables resulting in a partial differential equation (PDE) or a set of such equations.

A partial differential equation may be given as a function of independent variables $x, y, \ldots$ and all the derivatives of the function u of the independent variable, e.g.,

$$F(x, y, \ldots, u_x, u_y \ldots, u_{xx}, u_{xy} \ldots) = 0 \quad \ldots (1)$$

Here $ux = \dfrac{\partial u}{\partial x}$, $\qquad u_y = \dfrac{\partial u}{\partial y}$

and

$$u_{xx} = \frac{\partial^2 u}{\partial x^2}, \qquad u_{xy} = \frac{\partial^2 u}{\partial x\, \partial y}$$

Such a function $u = u(x, y \ldots)$ is called a solution of the PDE(1) and the highest derivative appearing in the PDE is termed as the order of the equation.

If the number of independent variable is only one then the PDE becomes an ordinary differential equation.

The general form of the frequently encountered two dimensional second order linear PDE is as given below

L   3(a)-1

$$a \frac{\partial^2 u}{\partial x^2} + b \frac{\partial^2 u}{\partial x \partial y} + c \frac{\partial^2 u}{\partial y^2} + d \frac{\partial u}{dx} + e \frac{\partial u}{dy} + fu + g = 0 \quad \dots\dots(2)$$

Where a,b,c,d,e,f are the functions of x and y. The above equation is said to be elliptic, parabolic, or hyperbolic if the value of the expression $b^2 - 4ac$ is negative, zero or positive respectively. The above equation is said to be linear in terms of principle of superposition of differential operation L, which is defined as

$$L \equiv a \frac{\partial^2}{\partial x^2} + b \frac{\partial^2}{\partial x dy} + c \frac{\partial^2}{\partial y^2} + d \frac{\partial}{\partial x} + e \frac{\partial}{\partial y} \quad \dots(3)$$

Rewriting (2) in terms of L, we get

$$Lu + fu = -g \quad \dots\dots(4)$$

The operation L is _linear_ if

$$L(A.u_1 + B.u_2) = A.Lu_1 + B.Lu_2 \quad \dots(5)$$

A linear PDE is said to be homogeneous if in euqation(4) 'g = O. If $u_1, u_2 \dots\dots u_n$ are the independent solution of a _linear_ homogeneous partial differential equation then,

$$a_1 u_1 + a_2 u_2 + \dots\dots\dots a_n u_n$$ (where $a_1, a_2 \dots a_n$ are the arbitrary constants) will also be a solution of the differential equation.

1.1 Boundary Condition and Initial Condition :

While representing a physical process of a particular system, one often encounters a fixed space or region R, over which the solution of partial differential equation is sought, which means that the solution should satisfy the differential equation at every point in region R and certain other conditions at the boundary of the region R, which are

called boundary conditions. When these conditions are specified at initial time (t=0), they are termed as initial conditions. Therefore, the complete mathematical description of any system consists of a single or a system of partial differential equations together with initial conditions and boundary conditions.

2.0 ANALYTICAL AND NUMERICAL SOLUTIONS

In order to solve a particular problem, a set of differential equations discussed above, along with their boundary and initial conditions must be solved for specific data set of that problem. This can be done by using analytical or numerical techniques. In analytical method, appropriate method of solution has to be determined for each particular problem. For example, solving steady flow in two dimension, method of complex variable is the obvious choice. Various other methods include Fourier transformation, Hankel transformation, infinite series of definite integrals etc.

The analytical method gives accurate solution and has the advantage of immediate availability and gives a good insite into the dependence of solution on various physical parameters. But this advantage may partly or completely be lost when the form of solution is very complicated.

The main limitation of the analytical methods of solution is that they are available only for relatively simple problems and requires the boundary of the system to be of regular geometric shape. For most of the problems of practical interest, because of the irregular shape of the boundaries, the spatial variability of the coefficients appearing in the equations and in the boundary conditions, the non uniformity of the initial conditions, the analytical solution is not feasible and virtually impossible except for very simple cases.

With the advent of fast computers the numerical methods have become powerful tool for solving PDE's for complex problems with reasonable degree of accuracy. In practical application we often meet the following approaches of approximate numerical methods :

1. Finite difference method (FDM)
2. Method of characteristics
3. Finite element method (FEM)
4. Monte Carlo method
5. Integral equation method
6. Perturbation method
7. Boundary element method
8. Analytical element method.

In general these numerical methods replace the partial differential eqn. by an algebraic equation or a set of algebraic equations which constitute a system of linear equations. The final solution then requires the solution of this system of equations. The various numerical methods mentioned above differ mainly in approach through which the system of equations is derived and sometimes also in the basic approach to the problem. In this lecture it is not feasible to deal with all the above mentioned methods, hence, we shall be concentrating only on finite difference method which is a widely used method.

3.0 FINITE DIFFERENCE METHOD

The finite difference method is probably the oldest numerical method to be used for systematic numerical solution of partial differential equations. Although, the fundamental ideas behind it have been established and used by mathematicians of 18th century such as Taylor and Lagrange but its application to the solution of engineering problems started by the scientists of the 20th century (Southwell, 1940, Kantorovich and Krylov, 1964).

This method basically consists of an approximation of partial derivative by algebraic expression involving the finite differences of the dependent variable at a limited number of predefined points. Thus, by the virtue of this approximation the partial differential equation defining the problem is replaced by a set of algebraic equations in terms of the values of dependent variables at predefined points and then this set of equations are solved. The linear partial differential equation will result in a set of linear equations.

4.0   APPROXIMATION OF DERIVATIVES BY FINITE DIFFERENCE:

The derivative of a function u(t) is defined as below

$$\frac{du}{dt} = \lim_{\Delta t=0} \frac{u(t+\Delta t)-u(t)}{\Delta t} \qquad \ldots(6)$$

As an approximation the derivatives can be obtained by simply neglecting the limiting process, $\Delta t \longrightarrow 0$. For example consider a function u = u(x,y) which is continuous enough, i.e., possesses a sufficient number of partial derivatives.
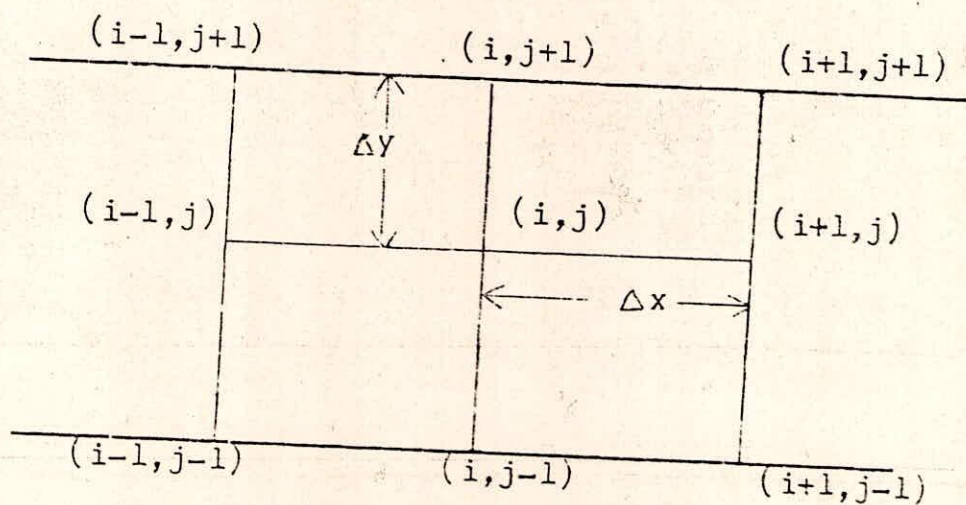
Considering u be continuous, its value at the two points, (i,j) and (i',j') can be expressed by Taylor series expansion. For example

$$u_{i+1,j} = u_{i,j} + \Delta x \frac{\partial u}{\partial x} + \frac{(\Delta x)^2}{2!} \frac{\partial^2 u}{\partial x^2} + \frac{(\Delta x)^3}{3!} \frac{\partial^3 u}{\partial x^3} + \ldots\ldots$$

$$\ldots\ldots(7)$$

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

$$\ldots\ldots(8)$$

Considering the equations (7) and (8) separately, we get

$$\left[\frac{\partial u}{\partial x}\right]_{i,j} = \frac{u_{i+1,j} - u_{i,j}}{\Delta x} + 0(\Delta x) \qquad \ldots\ldots(9)$$

Forward difference

and
$$\left[\frac{\partial u}{\partial x}\right]_{i,j} = \frac{u_{i,j} - u_{i-1,j}}{\Delta x} + 0(\Delta x) \qquad \ldots\ldots(10)$$

Backward difference

Substracting or adding Eq.(7) and (8), we get the following equations.

$$\left[\frac{\partial u}{\partial x}\right]_{i,j} = \frac{u_{i+1,j} - u_{i-1,j}}{2\Delta x} + 0(\Delta x)^2 \qquad \ldots\ldots(11)$$

Central difference

and
$$\left[\frac{\partial^2 u}{\partial x^2}\right]_{i,j} = \frac{u_{i+1,j} - 2u_{i,j} + u_{i-1,j}}{(\Delta x)^2} + 0(\Delta x)^2 \qquad \ldots\ldots(12)$$

Equation (12) can also be obtained from (9) and (10) considering the fact that the derivative of first order derivative is the second order derivative. Similar formulae can also be obtained for $\partial u/\partial y$ and $\partial^2 u/\partial y^2$. For mixed

derivatives, we have (in same way)

$$\frac{\partial^2 u}{\partial x \partial y} = \frac{u_{i+1,j+1} - u_{i-1,j+1} - u_{i+1,j-1} + u_{i-1,j-1}}{4 \Delta x \Delta y} \quad \ldots\ldots(13)$$

The O['] terms are the estimates of the trumcation error when Δx, $\Delta y \longrightarrow 0$. In other words they group the terms of Taylor expansion composed with the Kth derivative of the function u multiplied by $(\Delta x)^k$, which are called higher order terms.

Example : Let us consider simple differential equation

$$\frac{\partial u}{\partial t} = -u \qquad [E-1].$$

Subjected to the initial conditions u(0)=1.0.

Replacing the above differential equation by finite differences omitting the limit operation, we have

$$\frac{u(t+\Delta t) - u(t)}{\Delta t} = -u(t)$$

or

$$u(t+\Delta t) = u(t) - \Delta t \times u(t) \qquad [E-2]$$

The above equation forms the simple algorithm from which the values of u(t) can be determined in successive steps, starting from the initial value u(0)=1.0. If Δt is taken as 0.1 the series of values obtained upto t = 1.0 is

u(0.0) = 1.0000   u(0.6) = 0.5314
u(0.1) = 0.9000   u(0.7) = 0.4783
u(0.2) = 0.8100   u(0.8) = 0.4305
u(0.4) = 0.6561   u(1.0) = 0.3487
u(0.5) = 0.5905

The exact solution of [E-1] is u(t) = exp(-t). Therefore, at t=1.0. exact result is u(1.0)=0.3679. Thus we see that

the approximation is not very good but may be sufficient for practical purposes. The accuracy can be increased by taking smaller time steps.

For different value of Δt, the value of $u(1.0)$ are given below

$\Delta t = 0.1$

$\Delta t = 0.01$

$\Delta t = 0.001$

$u(1.0) = 0.3487$

$u(1.0) = 0.3660$

$u(1.0) = 0.3677$

This shows that the degree of accuracy depends strongly upon the magnitude of time step taken. The above example shows that the finite difference approximation of the derivatives may lead to a very simple numerical algorithm.

In equation [E-2], Δt was assumed to be positive, in otherwords forward difference scheme was adopted. Let us take the backward difference, then

$$\frac{u(t)-u(t-\Delta t)}{\Delta t} = -u(t)$$

or

$$u(t)-u(t-\Delta t) = -u(t) \times \Delta t$$

or $\quad u(t) = u(t-\Delta t)/(1+\Delta t) \qquad$ [E-3]

Starting from $u(0) = 1.0$ and taking $\Delta t=0.1$, one now obtains $u(1.0) = 0.3855$. This result is as good or bad as in previous case. Again, the accuracy will be much better if smaller ~~sample~~ time steps are taken.

A third alternative algorithm can be obtained when the values of the function u on the right hand side of [E-1] is taken as the average of the values $u(t)$ and $u(t+\Delta t)$. The formulation of this algorithm is as follows.

$$\frac{u(t+\Delta t)-u(t)}{\Delta t} = -\left[\frac{u(t)+u(t+\Delta t)}{2}\right]$$

Or $\quad u(t+\Delta t) - u(t) = -\dfrac{u(t) \times \Delta t}{2} - \dfrac{u(t+\Delta t) \times \Delta t}{2}$

Or $\quad (1 - \dfrac{\Delta t}{2}) u(t) = (1 + \dfrac{\Delta t}{2}) \, u(t+\Delta t)$

Or $\quad u(t+\Delta t) = u(t) \times (1 - \Delta t/2) / (1 + \dfrac{\Delta t}{2})$ ——[c-4]

This algorithm gives $u(1.0) = 0.3676$ when $\Delta t = 0.1$. The result is very close to the exact value. Thus, with a balanced and careful approximation of the various terms, a very good approximation can be obtained.

5.0 SCHEMES FOR SOLUTION

In order to deal with the schemes for solution for time discretization, we shall take an example of unsteady flow in an aquifer to have problem oriented idea of them. The governing partial difference equation for unsteady flow in an aquifer is given below.

$$T(\frac{\partial^2 h}{\partial x^2} + \frac{\partial^2 h}{\partial y^2}) + q = S\frac{\partial h}{\partial t} \qquad \ldots\ldots(14)$$

where q is the volumetric flux per unit area and represents sources and/or sinks of water.

T is the transmissivity

S is the storativity

h is the potentiometric head

x,y are the Cartesian coordinates.

The initial condition is assumed to be $t = 0$, $h = h^0$ and some specified boundary condition is assumed.

In the above problem for simplicity T has been considered constant and do not vary with x, y.

5.1 EXPLICIT METHOD

If spacial derivatives are approximated considering all values of the head at the initial value of time, then substituting various approximation in (14), we get.

$$T\left[\frac{h^0_{i+1,j} - 2h^0_{i,j} + h_{i-1,j}}{(\Delta x)^2} + \frac{h^0_{i,j+1} - 2h_{i,j} + h_{i,j-1}}{(\Delta y)^2}\right] + q$$

$$= S\frac{h'_{i,j} - h^0_{i,j}}{\Delta t} \qquad \ldots(15)$$

Here $h'_{i,j}$ is the value of head at (i,j) at the end of the time step, (15) can be rewritten as

$$\frac{T.\Delta t}{S.(\Delta x)^2}[h^0_{i+1,j} - 2h^0_{i,j} + h^0_{i-1,j}] +$$

$$\frac{T.\Delta t}{S.(\Delta y)^2}[h^0_{i,j+1} - 2h^0_{i,j} + h^0_{i,j-1}] + \frac{q\Delta t}{S} = h'_{i,j} - h^0_{i,j}$$

Or $\quad h'_{i,j} = h^0_{i,j} + \frac{q.\Delta t}{S} + \alpha(h^0_{i+1,j} - 2h^0_{i,j} + h^0_{i-1,j})$

$$+ \beta(h^0_{i,j+1} - 2h^0_{i,j} + h^0_{i,j-1}) \qquad \ldots(16)$$

where α and β are the constants defined as

$$\alpha = \frac{T\Delta t}{S.(\Delta x)^2} \quad ; \qquad \beta = \frac{T.\Delta t}{S.(\Delta y)^2}$$

Here, Δx and Δy are the (constant) distances between the grids in x and y direction respectively. Eqn. (16) represents the new value of head at grid point (i,j) in terms of initial values at that node and at its immediate neighbours, all of which are known, hence, the process is called explicit. For all interior nodes, equation (16) specifies how to determine the new values of head. The values of head along the boundary can be determined using the boundary conditions.

5.2   IMPLICIT METHOD :

In the explicit method discussed above, the time steps are restricted by stability criteria (discussed in next section). This shows that in a transient process when the behaviour is very slow, e.g., for large values of time when the process is

L   3(a)-10

approaching the steady state, the magnitude of time step must remain small, Thus, a large number of time steps is required. This can be avoided by employing a more sophisticated procedure, i.e., implicit method.

In the explicit method the spatial derivatives have been approximated at the begining of the time step (15). If we take them at the end of the time step or in general at some intermediate points, as an alternative approach we get

$$h_{i,j} = \epsilon \, h^o_{i,j} + (1-\epsilon) h'_{i,j} \qquad \ldots (16)$$

where ϵ is an interpolation parameter having a value between 0 and 1.

If $\epsilon = 1$, the value of $h_{i,j}$ reduces to initial value which leads to [15], i.e. explicit scheme. For $\epsilon = 0$, the value of $h_{i,j}$ equals the value at the end of the time step, $h'_{i,j}$, i.e., implicit scheme. If ϵ is between 0 and 1 it will result in what is called semi-implicit scheme.

Taking $\epsilon = 0$ and substituting the approximations into basic equation [24]

$$h'_{i,j} = h^o_{i,j} + \frac{q \cdot \Delta t}{S} + \alpha (h'_{i+1,j} - 2h'_{i,j} + h'_{i-1,j})$$

$$+ \beta(h'_{i,j+1} - 2h'_{i,j} + h'_{i,j-1}) \qquad \ldots (17)$$

The above equation is the basic equation for fully implicit method. In this method, it is obvious that the new values at node points (i,j) is calculated in terms of initial value at that node and new values at the node points surrounding that node. Since these values are also unknown the process no longer remains explicit but all the unknown values must be determined simultaneously from a system of linear equations of the form [17]. Various numerical techniques are available for solving such type of problem and the details can be had from any standard text.

The implicit method is stable for all sizes of time step, and hence said to be unconditionally stable. Thus, larger time steps can be taken when the variation in the process becomes slower, e.g., when steady state is approached.

In [16] if we take $\epsilon = \frac{1}{2}$, it seems to be least biased either towards the initial value or towards the final value in a time step. This will result in a more accurate formulation known as Crank - Nicholson scheme.

5.3 STABILITY

An approximate numerical method can newer yield exact solution of a problem and its accuracy also can not be precisely evaluated because the exact solution is usually unknown. However, some insite into the accuracy of a method can be obtained which are being presented in the following paragraphs with a special attention to the magnitude of time steps in an unsteady process.

The reliability of a numerical method is usually adjudged by certain condition, for example, condition of consistency, convergence and stability.

5.3.1 Consistency :

It is the requirement that when finite intervals approach zero, the numerical equations should reduce to the exact continuum equations. This can be checked from the inspection of the basic algebraic equations by letting the finite differences approach zero.

5.3.2 Convergence :

This condition states that the solution of the numerical equations should approach that of the original partial differential equation if all finite intervals tend to zero.

It is much more difficult to verify the condition of convergence. Therefore, it is usually considered sufficient if the numerical procedure has been verified against a variety of analytical solutions.

5.3.3 Stability :

If the error due to roundoff do not increase in magnitude with time, the process is termed as stable and this condition is called stability condition. It is an imperative condition which restrict the size of time step in an explicit method. A detailed discussion on stability is beyond the scope of this lecture, however, stability of explicit method for unsteady flow problem described at [15] will be considered here which apply to the most important problems of ground water flow. The equation [15] is

$$h'_{i,j} = h^o_{i,j} + \frac{q.\Delta t}{S} + \alpha(h^o_{i+1,j} - 2h^o_{i,j} + h^o_{i-1,j})$$

$$+\beta (h^o_{i,j+1} - 2h^o_{i,j} + h^o_{i,j-1}) \quad \ldots.18)$$

where

$$\alpha = T.\Delta t/[S.(\Delta x)^2] \quad \ldots.(19)$$

$$\beta = T.\Delta t/[S.(\Delta y)^2] \quad \ldots.(20)$$

If this process is stable, any distribution of errors should gradually dissipate in time and should not grow in magnitude. In order to maximize the effect of all terms in the right hand side of [18], it is assumed that at a certain time the errors are

$$h^o_{i-1,j} = h^o_{i+1,j} = h^o_{i,j-1} = h^o_{i,j+1} = -\epsilon; h^o_{i,j} = \epsilon$$

$$\ldots.(21)$$

From equation [18], with q = o we now obtain

$$h'_{i,j} = (1-4\alpha-4\beta)\epsilon$$

$$\ldots.(22)$$

In order that errors will not grow, it must be smaller than ϵ and larger then $-\epsilon$. With equation [19] and [20] this leads to the following condition for the time step Δt.

$$0 < \Delta t < \frac{1}{2} \frac{S}{T} \frac{(\Delta x)^2(\Delta y)^2}{(\Delta x)^2+(\Delta y)^2} \quad \ldots.(23)$$

The above equation gives the criteria for magnitude of the time step- for the problem considered.

SUGGESTED READING

1.   Forsythe,G.E. and Wasow,W.R., 1960, 'Finite Difference Methods for Partial Differential Equations', Wiley, New York.

2.   Fox,L., 1962, 'Numerical Solution of Ordinary and Partial Differential Equations; Pergamon Press, New York.

3.   Kantorovich, L.V. and Krylov,V.I.,1964, 'Approximate Methods of Higher Analysis', Translated by C.D. Benster, Inter Science Publishers, New York.

4.   Ames, W.F., 1977, 'Numerical methods for partial differential equations' Academic Press, New York.

5.   Richtmyen and Norton, K.W., '1967 - Difference method for initial value problems', Wiley, New York.