The value of $x_i^{(k+1)}$ is understood to be that calculated by the iteration formula. This can also be written as:

$$x_i^{(k+1)} = \lambda\, x_i^{(k+1)} + (1 - \lambda)\, x_i^{(k)}$$

Thus the value used is the weighted average between the calculated value and the previous value, such that:

$0 < \lambda < 1$ underrelaxation (damping)
$\lambda = 1$ standard Gauss-Seidel iteration
$1 < \lambda < 2$ overrelaxation (acceleration)

3.8.3 Advantages and Disadvantages of Iterative Methods

Some of the advantages of iterative methods include the following:

- it is self-correcting
- round-off error does not accumulate
- it can be programmed to operate only on non-zero terms
- there is no matrix fill-in
- it is suitable for calculators and small computers

The major disadvantage of iterative methods is that they need fast convergence and good initial guess to be competitive with direct methods.

4. FINITE DIFFERENCES

4.1 Basic Principles

The basic objective of finite difference methods is to approximate the differential terms in the governing differential equations by corresponding different terms. The resulting difference equation is then written at a finite number of points in the domain. This results in a set of algebraic equations which are easier to solve than the original partial differential equation.

The procedure is easily visualized in 1D. If, for example, u=u(x) is a continuous function, then:

$$\frac{du}{dx} = \lim_{\Delta x \to 0} \frac{\Delta u}{\Delta x}$$

or

$$\frac{du}{dx} = \frac{\Delta u}{\Delta x} = \varepsilon$$

where ε is an error term.

The error term can be evaluated by using a Taylor expansion for u(x+Δx) about x, as follows (See Fig. 9):

$$u(x+\Delta x) = u(x) + \Delta x\, u'(x) + \frac{(\Delta x)^2}{2!} u''(x) + \frac{(\Delta x)^3}{3!} u'''(x) + \cdots$$

which can be rearranged to yield:

$$u'(x) = \frac{u(x+\Delta x) - u(x)}{\Delta x} - \frac{\Delta x}{2} u''(x) - \cdots$$

where the terms beyond the first term on the right hand side represent the numerical error ε.

Since the error is dominated by the leading term (Δx/2)u″(x), ε is said to be of the order Δx or O(Δx). The above approximation of Δu/Δx is known as a *forward difference* approximation, which is first-order accurate.

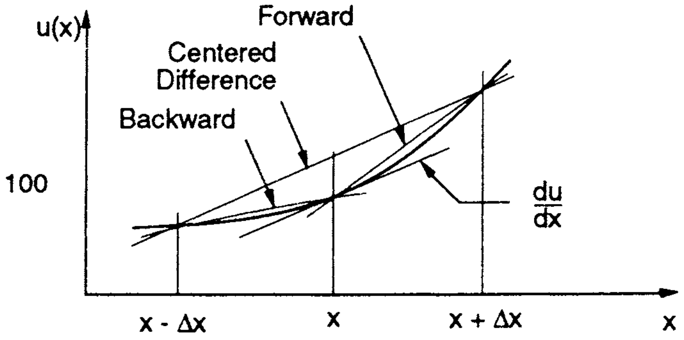

Figure 9: First-derivative approximations

A *backward difference* approximation is obtained by performing a similar expansion for u(x-Δx) about x. This results in:

$$u'(x) = \frac{u(x) - u(x-\Delta x)}{\Delta x} + \frac{\Delta x}{2} u''(x) - \cdots$$

which is also first-order accurate.

An approximation with a higher-order accuracy can be obtained by combining the forward and backward approximations, leading to:

$$u'(x) = \frac{u(x+\Delta x) - u(x-\Delta x)}{2\Delta x} - \frac{(\Delta x)^2}{3} u'''(x) + \cdots$$

where the leading error term is now of second order, or O $(\Delta x)^2$. This is known as a *central difference* approximation.

An approximation for the second derivative can be derived by adding the forward and backward difference approximations to obtain:

$$u''(x) = \frac{u(x+\Delta x) - 2u(x) + u(x-\Delta x)}{(\Delta x)^2} - \frac{(\Delta x)^2}{12} u''''(x) + \cdots$$

which is also second-order accurate.

The above approximations are based on a uniform discretization Δx. Similar approximations can also be developed for non-uniform Δx, but the accuracy in that case will drop by one order.

4.2 Finite Difference Solution of 1D Flow Equation

The governing equation in 1D, with u as the basic unknown, and assuming uniform material, is:

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

We assume that the spatial domain extends between $0 \leq x \leq L$ and that the boundary and initial conditions are specified as:

$u(0,t) = u_0$
$u(L,t) = 0$
$u(x,0) = 0$

These boundary conditions are known as *first-type* or *Dirichlet* boundary conditions. The solution domain is discretized as shown in Fig. 10, where i,j designate the nodal numbers in the spatial and temporal directions, respectively.

A forward difference approximation to the governing equation is:

$$\frac{u_{i-1,j}-2u_{i,j}+u_{i+1,j}}{(\Delta x)^2} = \frac{S}{K}\,\frac{u_{i,j+1}-u_{i,j}}{\Delta t}$$

The equation involves the 4 nodes shown in Fig. 11, of which one is at the new time level j+1 while three are at the old time level j. Letting:

$$\rho = \frac{K}{S}\,\frac{\Delta t}{(\Delta x)^2}$$

the above difference equation can be rearranged to give:

$$u_{i,j+1} = (1-2\rho)u_{i,j} + \rho(u_{i-1,j} + u_{i+1,j})$$

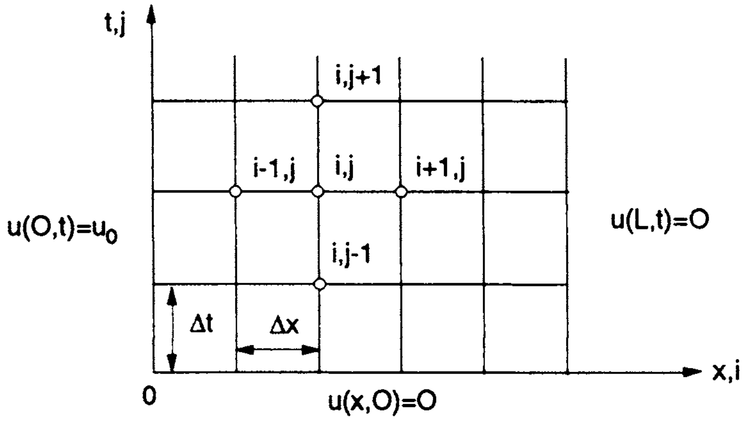

Figure 10: Space-time finite difference grid for 1D flow problem

Thus a value at a new time level j+1 can be calculated directly in terms of values at the old time level j. This is known as an *explicit* finite difference solution. For stability, the explicit solution requires that $\rho \leq 1/2$. The solution is second-order accurate in space (for uniform Δx) and first-order accurate in time.

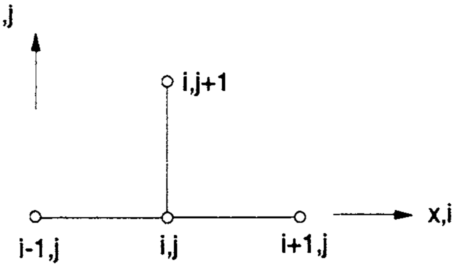

Figure 11: Nodal grouping for explicit difference solution

Alternatively, using a backward difference approximation for the time derivative, the governing equation can be approximated by:

$$\frac{u_{i-1,j}-2u_{i,j}+u_{i+1,j}}{(\Delta x)^2} = \frac{S}{K}\,\frac{u_{i,j}-u_{i,j-1}}{\Delta t}$$

This equation now involves 3 nodes at the new time level j, plus one at the old time level j-1 (Fig. 12). It can be rearranged to give:

$$-u_{i-1,j} + (2+\frac{1}{\rho})u_{i,j} - u_{i+1,j} = \frac{1}{\rho}u_{i,j-1}$$

Since there are 3 unknowns at the new time level j, the equation cannot be solved directly. By writing the equation at all nodes where u is unknown (this excludes the boundary nodes where u is specified), we obtain a set of simultaneous equations which can be solved.

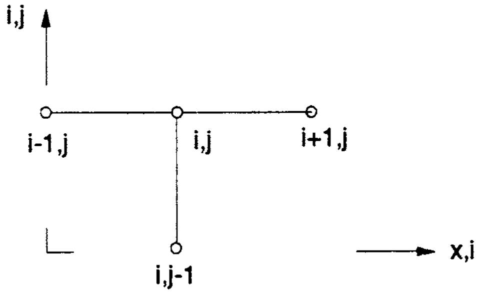

Figure 12: Nodal grouping for implicit difference solution

For example, for the grid shown in Fig. 10, which has 6 nodes in the spatial domain, and where the two boundary nodes carry specified values, we obtain 4 equations in 4 unknowns. These equations can be written in matrix form as follows:

$$\begin{bmatrix} (2+1/\rho) & -1 & & \\ -1 & (2+1/\rho) & -1 & \\ & -1 & (2+1/\rho) & -1 \\ & & -1 & (2+1/\rho) \end{bmatrix} \begin{Bmatrix} u_2 \\ u_3 \\ u_4 \\ u_5 \end{Bmatrix} = \begin{Bmatrix} (1/\rho)u_{2,j-1}+u_{1,j} \\ (1/\rho)u_{3,j-1} \\ 1/\rho)u_{4,j-1} \\ (1/\rho)u_{5,j-1}+u_{6j} \end{Bmatrix}$$

The right-hand side contains the values at the old time level j-1, plus the boundary values. The tridiagonal matrix equation can thus be solved at each time step using the results of the preceding time step. This solution is known as an implicit finite difference solution. The solution is second-order accurate in space and first-order accurate in time, and it is stable for any choice of Δt.

In order to achieve second-order accuracy also with respect to the time derivative, we can write the left-hand side of the finite difference equation as the average between the time levels j and j-1. Thus the entire equation in effect represents the best approximation for a point located midway (centered) between the two time levels (Fig. 13). The algebraic equation then becomes:

$$-u_{i-1,j} + (2+\frac{2}{\rho})u_{ij} - u_{i+1,j} = u_{i-1,j-1} - (2-\frac{2}{\rho})u_{i,j-1} + u_{i+1,j-1}$$

where all the unknowns (the values of u at the new time level j) appear on the left-hand side and all the knowns on the right-hand side. The matrix equation is of the same form as that for the implicit solution. This is known as a *centered* finite difference solution, which has second-order accuracy in both space and time. It is also unconditionally stable.

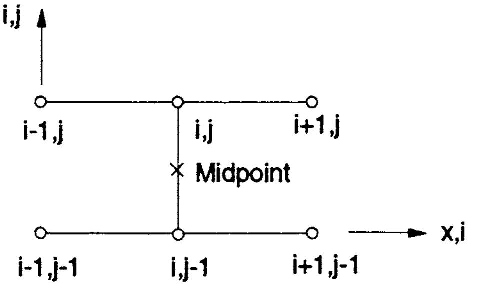

Figure 13: Nodal grouping for centered difference solution

In the above solutions, the boundary has been specified in terms of the unknown u at the boundary (*first-type* boundary condition). If instead a value of the flux q is specified at the boundary we speak of a *second-type* or *Neumann* boundary condition. In that case, we can equate this flux to the gradient of u at the boundary, using the Darcy equation. At the same time, we can approximate the boundary gradient by means of a centered difference approximation, using an extra node (0,j) placed outside the domain (Fig. 14). We obtain:

$$\frac{\partial u}{\partial x} = -\frac{q_n}{K} = \frac{u_{2,j} - u_{0,j}}{2\Delta x}$$

where n refers to the direction normal to the boundary. This yields:

$$u_{o,j} = -2\Delta x\frac{q_n}{K} - u_{2,j}$$

Since the value of u at the boundary is now unknown, we write a difference equation also for the boundary node (1,j), and we use the above equation to substitute for the term u_{0j} occurring in the difference equation. Using the implicit form, the difference equation for the boundary node becomes:

$$(2+\frac{1}{\rho})u_{1,j} - 2u_{2,j} = \frac{1}{\rho}u_{1,j-1} + 2\Delta x\frac{q_n}{K}$$

This equation would be added to the equations previously obtained for the implicit solution. Thus we have one additional equation and one additional unknown for each boundary node where the flux is specified. The above form preserves second-order accuracy in space.

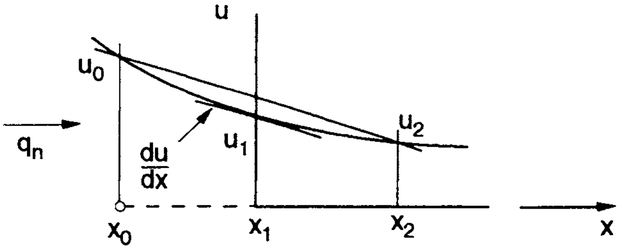

Figure 14: Second-type boundary conditon for 1D flow problem

Each of the above three solution types has its advantages and disadvantages. The explicit form is the easiest to program, but its stability constraint may require rather short time steps. The implicit form overcomes this constraint at the cost of some more elaborate programming. The centered form delivers the best accuracy, again at the cost of additional programming. In implicit or centered solutions of the flow problem, the length of the time step is arbitrary; a shorter time step, however, gives a better resolution of transient behaviour.

Figure 15 shows the transient behaviour of a typical 1D flow system, with u specified at each end, and a change imposed at the left end at the initial time. The solution is formulated in terms of dimensionless time:

$$T^{*} = \frac{Kt}{SL^{2}}$$

The spatial discretization is $\Delta x=0.05$. The exact analytical solution (Carslaw and Jaeger, 1946) is:

$$\frac{u(x,t)}{u_o} = \left\{1-\frac{x}{L}\right\} - \frac{2}{\pi}\sum_{n=1}^{\infty}\frac{1}{n}\sin\left\{\frac{n\pi x}{L}\right\}\exp\left\{\frac{-n^{2}\pi^{2}Kt}{SL^{2}}\right\}$$

where the first term on the right-hand side is the steady-state solution and the summation term represents the transient response.

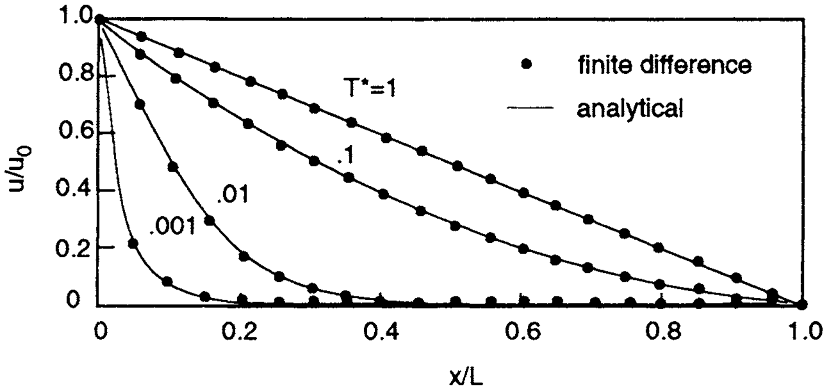

Figure 15: Transient behaviour of 1D flow system: Analytical and numerical solutions

The change imposed consists of setting $u/u_0=1$ at $x=0$. Profiles corresponding to $T^*=0.001$, 0.01, 0.1, and 1.0 are shown in Fig. 15. The response generated by the imposed change gradually penetrates through the system, converging to a linear function at equilibrium. If a larger time step were selected, some of the early-time response, characterized by a steep gradient at the boundary, will be lost, but the solution will still converge to the correct equilibrium condition. It is also possible to go directly to the equilibrium condition in a single step by setting the specific storage to zero.

Finite difference solutions for 2D and 3D problems can also be formulated and numerous models based on this approach are in existence (eg FLOWPATH and MODFLOW). A case study is presented in Appendix 1 to demonstrate how a finite difference model is conceptualized, set up and applied to real situation.

4.3 Cape Cod Study

The case study presented in Appendix 1 was adapted from USGS open file reports 84-475 and 86-481 (de Lima and Olimpio, 1984 and Ragone, 1986 respectively). The study was conducted at Cape Cod, Massachusetts in the United States of America. Treated sewage had been discharged through infiltration beds into underlying sand and gravel aquifer since 1936 at an approximate rate of 0.46 Mgal/day. The contaminant plume that resulted from the discharge was estimated to be 11000 ft long, 3000 ft wide and 75 ft thick. The geology of the area consists of glacial deposits that are underlain by crystalline bedrock. The uppermost 90 to 140 ft consists of stratified sand and gravel which overlies silty sand and till. Average hydraulic conductivity of the aquifer materials was determined to be 380 ft/day and the average linear groundwater velocity was estimated as 1.5 ft/day. A numerical model was developed to provide insight to hydraulic processes at the site and predict the response of the system to different hydraulic stresses. Appendix 1 presents site characterization in cross section and plan view, conceptualization of the problem domain in terms of boundary conditions, discretization of the problem domain, and comparison of results of the calibrated model with the observed data.

5. FINITE ELEMENTS

5.1 Basic Principles

The main advantage of the finite element method is that domains of irregular geometry can be represented naturally. This advantage comes into play with 2D and 3D problems. Thus, although finite element solutions can be developed for any dimensionality, we will focus here on 2D domains. Regardless of the spatial dimensionality, the time dimension always has the same uniformity and is therefore usually handled with finite differences, even when the spatial dimensions are handled with finite elements. Comprehensive discussions of the finite element