CHAPTER 13A
NUMERICAL METHODS-FUNDAMENTALS

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ABSTRACT

The classification of second-order partial differential equations is given. The solution of partial differential equations by the finite difference method is outlined. Some important considerations in the development of finite differnce approximation solutions to partial differential equations are discussed: various finite difference forms to derivatives; convergence, consistency and stability; explicit and implicit forms; accuracy and conservative formulations. Finally, we consider a few numerical methods that have been used in various reactor thermalhydraulics computer codes.

13.1 Introduction

In Chapter 10, the conservation equations governing the transport of mass, momentum and energy for single- and two-phase flow are given. Analytical solutions to these equations are possible only under extremely simplified conditions. In general, these equations are solved by numerical methods. There are three classes of numerical methods: the finite difference method, the finite element method and the Monte Carlo method. Since most of the computer codes used to date in the thermalhydraulic analysis of nuclear reactors utilize the finite difference method, we shall concentrate on this method to lay the foundation for subsequent understanding of the inner workings of these codes.

13.2 Classification of Partial Difference Equations

Partial differential equations (PDEs) are frequently classified in terms of their mathematical forms as being of the elliptic, hyperbolic or parabolic type. Consider the quasilinear second-order PDE in two independent variables:

$$A\frac{\partial^2 v}{\partial x^2} + B\frac{\partial^2 v}{\partial x \partial y} + C\frac{\partial^2 v}{\partial y^2} + E = 0$$

where A, B, C and E are functions of x, y, v, $\partial v/\partial x$, $\partial v/\partial y$. If $B^2 - 4AC < 0$, the PDE is elliptic. If $B^2 - 4AC = 0$, the PDE is parabolic. If $B^2-4AC > 0$, the PDE is hyperbolic. Since the values of A, B and C depend on the independent variables (x,y), it is possible for a PDE to change class within the different regions of the domain for which the problem is defined.

Physically, elliptic PDEs correspond to the governing equations of equilibrium problems. These are problems of steady state in which the equilibrium configuration v in a domain D is found by solving the PDE within D subject to certain boundary conditions on the boundary of D. Very often, the domain D is closed and bounded. Such problems are known as boundary value problems. Laplace's equation $\partial^2 v/\partial x^2 + \partial^2 v/\partial y^2 = 0$, is a familiar example of

an elliptic PDE. Parabolic and hyperbolic PDEs correspond to the governing equations of propagation problems. One is given the initial state of the system and would like to solve for the unsteady state or transient behaviour of the system for subsequent times subject to certain boundary conditions. These problems are known as initial boundary value problems. A simple example of a parabolic PDE is the diffusion equation, $\partial v/\partial t = D\ \partial^2 v/\partial x^2$. A simple example of a hyperbolic PDE is the one-dimensional wave equation, $\partial^2 v/\partial t^2 = c^2\ \partial^2 v/\partial x^2$.

13.3 Numerical Solution of PDEs by Finite Difference

The finite difference method for the solution of PDE problems is based on the use of finite difference approximations (FDAs) for derivatives. First, the solution domain is divided into a grid of nodal points. This grid is normally uniformly shaped and its shape reflects on the nature of the problem and its boundary conditions. Second, the governing PDE is written in terms of some convenient coordinate system and transformed into a partial difference equation by approximating the continuous derivatives by finite differences involving neighboring grid points. The finite difference equation is written for every point in the grid, and the result is a set of n equations in n unknowns. Finally, the system of n equations and n unknowns is solved by a numerical technique. Although the above description may appear to be simple and straightforward, there is considerable variation in grid types, grid sizes, partial differential equations, finite difference approximations to these equations, and solution techniques for the resulting equation system. The reader is referred to the references cited at the end of the chapter for more details. In the following sections, we shall discuss some important considerations in developing FDA solutions to PDEs.

13.4 Finite Difference Approximations to Partial Derivatives

By applying Taylor series expansions about a point (i,j) in a rectangular grid, we obtain the following FDAs to first and second-order derivatives at (i,j):

$$\frac{\partial v}{\partial x} \simeq \frac{v_{i+1,j} - v_{i,j}}{\Delta x} \tag{1}$$

$$\frac{\partial v}{\partial x} \simeq \frac{v_{i,j} - v_{i-1,j}}{\Delta x} \tag{2}$$

$$\frac{\partial v}{\partial x} \simeq \frac{v_{i+1,j} - v_{i-1,j}}{2\Delta x} \tag{3}$$

$$\frac{\partial^2 v}{\partial x^2} \simeq \frac{v_{i+1,j} - 2\,v_{i,j} + v_{i-1,j}}{\Delta x^2} \tag{4}$$

Equations (1), (2) and (3) are known as forward, backward and central difference forms, respectively. Equation (4) is the central difference form for the second derivative.

13.5 Convergence, Consistency and Stability

A solution to an FDA to a given PDE is said to be convergent if, at each point (x,y) in the solution region, the solution to the FDA approaches the solution to the PDE as the grid spacings, Δx and Δy, approaches zero. In general, it is very difficult to show convergence of the solution of an FDA to that of a PDE. Fortunately, we can make use of an equivalence theorem due to Lax which states: Given a properly posed linear initial value problem and an FDA to it that satisfies the consistency condition, stability is the necessary and sufficient condition for convergence. This theorem is of great practical importance because it is relatively easy to show the stability of an FDA and its consistency with a PDE.

A finite difference equation is said to be consistent with a PDE if in the limit as the grid spacings tend to zero, the FDA becomes the same as the PDE at each point in the domain. For example, consider the diffusion equation, $\partial v/\partial t = D\,\partial^2 v/\partial x^2$. Applying forward difference in time and central difference in space (FTCS), we obtain

$$\frac{v_{i+1,j} - v_{i,j}}{\Delta t} = D\,\frac{(v_{i,j+1} - 2\,v_{i,j} + v_{i,j-1})}{\Delta x^2} \tag{5}$$

By Taylor series expansion, Eq. (5) becomes

$$\left.\frac{\partial v}{\partial t}\right|_{i,j} = D\left.\frac{\partial^2 v}{\partial x^2}\right|_{i,j} + E_{i,j} \tag{6}$$

where

$$E_{i,j} = -\frac{\Delta t}{2}\left.\frac{\partial^2 v}{\partial t^2}\right|_{i,j} + \frac{D(\Delta x)^2}{12}\frac{\partial^4 v}{\partial x^4} + 0\,\{(\Delta t)^2, (\Delta x)^4\}$$

This error, $E_{i,j}$, is called the truncation error. Since the truncation error tends to zero as Δt, $\Delta x \rightarrow 0$, the FDA is consistent with the original PDE. Consistency is often taken for granted. Carnathan et al. (1969) gave an example for which consistency may not be guaranteed if we are not careful.

Stability of an FDA is concerned with the behaviour of errors introduced (typically by round-off) in previously calculated values at each grid point. An FDA is stable if the difference between its theoretical and its numerical solution remains bounded at all grid points as the number of time steps increases and Δt remains constant. Any numerical scheme which allows the growth of error is unstable, and the resulting error will soon obliterate the desired solution leading to entirely spurious results. Note that the stability of an FDA has nothing to do with the original PDE. There are many different methods for studying the stability characteristics of an FDA. See, for example, Ames (1977) and Roache (1976). For the diffusion equation, $\partial v/\partial t = D\,\partial^2 v/\partial x^2$, it can be shown that the FTCS FDA scheme is stable for

$$0 < \frac{D\Delta t}{\Delta x^2} \leq \frac{1}{2} \tag{7}$$

For a given D and a fixed space interval Δx, Eq. (7) places a limitation on the time step Δt, namely $\Delta t \leq (\Delta x)^2/2D$. Restrictions on the grid step size in order to ensure stability of the FDA can dictate long computational times.

Finally, it is noted (Noye, 1978) that attempts to find an equivalence theorem for non-linear PDEs have been unsuccessful. According to Roache (1976): The existing mathematical theory for numerical solutions of nonlinear PDEs is still inadequate. There are no rigorous stability analyses, error estimates, or convergence proofs... it is still necessary to rely heavily on rigorous mathematical analysis of simpler, linearized, more or less related problems, and on heuristic reasoning, physical intuition, wind tunnel experience, and trial-and-error procedures.

13.6 Explicit and Implicit FDA

An explicit FDA is one which expresses one unknown value of the function directly in terms of known function values at other grid points. Hence, explicit FDAs are simple to calculate; however, they usually suffer from inefficiency due to restrictions on the grid size from stability considerations.

An implicit FDA is one in which an unknown function value is related to a linear combination of other unknown function values at other grid points. Hence, the solution of implicit FDAs will require inversion of large matrices. This imposes severe requirements on the memory capacity and speed of the computer and also calls for skill in efficient inversion of large, sparse matrices (inevitably through some iterative procedure). The advantage of implicit FDAs is that they often possess less stringent stability requirements.

13.7 Accuracy and Conservative Formulations (Cheng, 1975)

The conservation laws of mass, momentum and energy of a fluid can be expressed in differential and integral forms. It is, therefore, desirable to require that the FDAs to PDEs retain the conservative property, at least to the order of accuracy required, locally as well as globally. In practice, since FDAs are derived from the microscopic PDEs, the conservation laws are properly approximated to some order of accuracy by the FDA locally. However, when the FDA of such conservation laws are summed over a large but arbitrary collection of such spatial elements, the conservation laws may not retain the same degree of accuracy globally. This is because the small high-order errors may accumulate when summed over a large number of small discrete elements which make up the domain of computation. Now, for an approximate description of a physical problem of say $0\{\Delta x^2\}$, it is essential that such conservation laws should be accurate to $0\{\Delta x^2\}$ over not only the differential elements, but also finite volumes. If the truncation errors of the conservation laws in finite space are to be $0\{\Delta x^2\}$, the errors must not accumulate when neighboring mesh cells are summed up. If the truncation errors are allowed to so accumulate, the difference formulation used should be higher-order accurate, so that the accumulation of such small higher order truncation errors over arbitrary mesh combinations throughout the field of computation will not exceed $0\{\Delta x^2\}$. For example, consider the equation,

$$\frac{d(\rho u)}{dx} = u\frac{d\rho}{dx} + \rho\frac{du}{dx} \tag{8}$$

Applying forward difference to both sides of Eq. (8), we obtain

$$\text{L.H.S.} = \frac{d(\rho u)}{dx} \approx \frac{\rho_{i+1}u_{i+1} - \rho_i u_i}{\Delta x} \tag{9a}$$

$$\text{R.H.S.} = \rho \frac{du}{dx} + u\frac{d\rho}{dx} \simeq \rho_i \frac{u_{i+1} - u_i}{\Delta x} + u_i \frac{\rho_{i+1} - \rho_i}{\Delta x} \tag{9b}$$

Clearly, the right hand sides of Eq. (9a) and (9b) are not the same. When summed over a finite interval, Eq. (9a) will retain its accuracy to $0\{\Delta x\}$, whereas the errors from Eq. (9b) may accumulate leading to lower order of accuracy.

13.8 A Few Special Methods

Several numerical methods that have been used in various reactor thermalhydraulics computer codes are: the implicit-continuous Eulerian (ICE) method, the Porsching method, and the method of characteristics.

In the ICE method, the standard Navier-Stokes equations with primitive variables of velocity, density, enthalpy and pressure are used. A staggered grid spacing is employed. The PDEs are discretized using advance-time (implicit) treatment of the density in the equation of state and the density and velocity in the mass equation. The ICE method essentially reduces to FDAs corresponding to PDEs of an elliptic flow field. A simultaneous iteration on pressure and velocity components using a Newton-Raphson technique is applied. The ICE method is applicable to one-, two- or three-dimensions. For further details, consult Harlow and Amsden (1968, 1971), Roache (1976), and Browne (1978).

In the Porsching method (Porsching et al., 1971), a hydraulic network is modelled by a series of nodes and links. The mass, momentum and energy conservation equations plus the equation of state are simplified to a system of coupled first-order nonlinear ordinary differential equations involving the flow rates, enthalpy and mass at each node. The use of a convergent, implicit method, together with the help of a block inversion technique, produces an efficient numerical integration procedure for the network equations.

For hyperbolic equations involving only two independent variables, x and t say, the method of characteristics is widely used. This method finds special curves in the x-t plane, called characteristic curves, along which the solution of the partial differential equation is reduced to the integration of an ordinary differential equation. This ordinary equation is generally integrated by numerical methods (Hancox and McDonald, 1980). Carver (1980) proposed the pseudo characteristic method to solve the resulting system of ordinary differential equations using the method of lines approach.

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