DEPARTMENT OF AEROSPACE ENGINEERING

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UNIT I - FUNDAMENTAL CONCEPTS

Discretization of Partial Differential Equations

To solve the governing equations of the fluid motion, first, their numerical analog must be generated. This is done by a process referred to as discretization. In the discretization process, each term within the partial differential equation describing the flow is written in such a manner that the computer can be programmed to calculate. There are various techniques for numerical discretization. Here we will introduce three of the most commonly used techniques, namely:

(1) The Finite Difference Method,

(2) The Finite Element Method and

(3) The Finite Volume Method.

Spectral methods are also used in CFD, which will be briefly discussed.

The Finite Difference Method

The finite difference method utilizes the Taylor series expansion to write the derivatives of a variable as the differences between values of the variable at various points in space or time. Utilization of the Taylor series to discretize the derivative of the dependent variable, e.g., velocity *u*, concerning the independent variable, e.g., special coordinated *x*, is shown in Figure 1.13. Consider the curve in Figure 1.13 which represents the variation of *u* with *x*, *i.e., u(x).* After discretization, the curve *u(x)* can be represented by a set of discrete points, *ui*'s. These discrete points can be related to each other using a Taylor series expansion.

Consider two points, (*i+1*) and (*i-1*), a small distance Δx from the central point, (*i*). Thus velocity *ui* can be expressed in terms of Taylor series expansion about point (*i*) as:

$$u_{i+1} = u_i + \left(\frac{\partial u}{\partial x}\right)\Delta x + \left(\frac{\partial^2 u}{\partial x^2}\right)\frac{(\Delta x)^2}{2} + \left(\frac{\partial^3 u}{\partial x^3}\right)_i \frac{(\Delta x^3)}{6} + \ldots$$

……Equation 1.58

$$u_{i-1} = u_i - \left(\frac{\partial u}{\partial x}\right)\Delta x + \left(\frac{\partial^2 u}{\partial x^2}\right)\frac{(\Delta x)^2}{2} - \left(\frac{\partial^3 u}{\partial x^3}\right)_i \frac{(\Delta x^3)}{6} + \ldots$$

……Equation 1.59

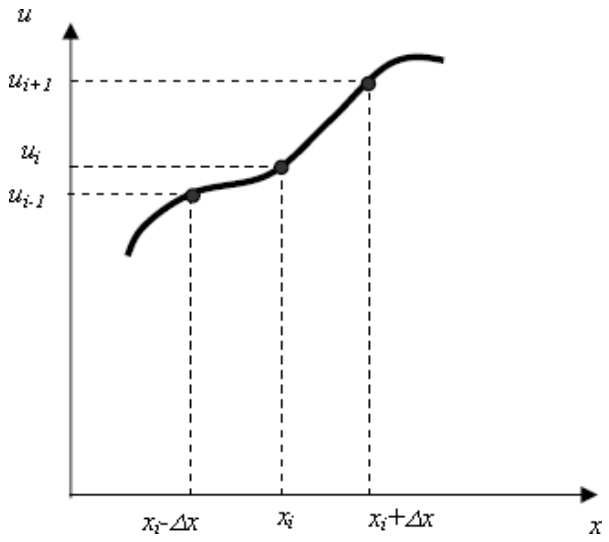

Figure 1.13 Location of points for the Taylor series

These equations are mathematically exact if the numbers of terms are infinite and Δx is small .Note that ignoring these terms leads to a source of error in the numerical calculations as the equation for the derivatives is truncated. This error is referred to as the truncation error. For the second-order accurate expression, the truncation error is:

$$\sum_{n=3}^{\infty}\left(\frac{\partial^n u}{\partial x^n}\right)_i \frac{(\Delta x)^{n-1}}{n!}$$

……Equation 1.60

By subtracting or adding these two equations, new equations can be found for the first and second derivatives at the central position *i*. These derivatives are

$$\left(\frac{\partial u}{\partial x}\right)_i = \frac{u_{i+1} - u_{i-1}}{2\Delta x} - \left(\frac{\partial^3 u}{\partial x^3}\right)_i \frac{(\Delta x)^2}{6}$$

……Equation 1.61

$$\left(\frac{\partial^2 u}{\partial x^2}\right)_i = \frac{u_{i-1} - 2u_i + u_{i+1}}{(\Delta x)^2} + O(\Delta x)^2$$

……Equation 1.62

Equations 1.61 and 1.62 are referred to as the Central Difference Equations for first and second order respectively. The first-order derivative can be formed as

$$\left(\frac{\partial u}{\partial x}\right)_i = \frac{u_{i+1} - u_i}{\Delta x} - \left(\frac{\partial^2 u}{\partial x^2}\right)_i \frac{(\Delta x)}{2}$$

……Equation 1.63

This is referred to as the Forward difference. Similarly, another first-order derivative can be formed as

$$\left(\frac{\partial u}{\partial x}\right)_i = \frac{u_i - u_{i-1}}{\Delta x} - \left(\frac{\partial^2 u}{\partial x^2}\right)_i \frac{(\Delta x)}{2}$$

……Equation 1.64

This is referred to as the Backward difference. As noted by the expressions, different formulae are classified in two ways:

(1) By the geometrical relationship of the points, namely, central, forward, and backward differencing

(2) By the accuracy of the expressions, for instance, the central difference is second-order accurate, whereas, both forward and backward differences are first-order accurate, as the higher-order terms are neglected.

The Finite Element Method

In the finite element method, the fluid domain under consideration is divided into a finite number of sub-domains, known as elements. A simple function is assumed for the variation of each variable inside each element. The summation of the variation of the variable in each element is used to describe the whole flow field. Consider the two nodded elements shown in Figure 1.14, in which variable *u* varies linearly inside the element. The end points of the element are called the nodes of the element. For a linear variation of *u*, the first derivative of *u* concerning *x* is simply a constant. If *u* is assumed to vary linearly inside an element, we cannot define a second derivative for it. Since most fluid problems include a second derivative, the following technique is designed to overcome this problem. First, the partial differential

equation is multiplied by an unknown function, and then the whole equation can be integrated over the domain in which it applies. Finally, the terms that need to have the order of their derivatives reduced are integrated into parts. This is known as producing a variational formulation.

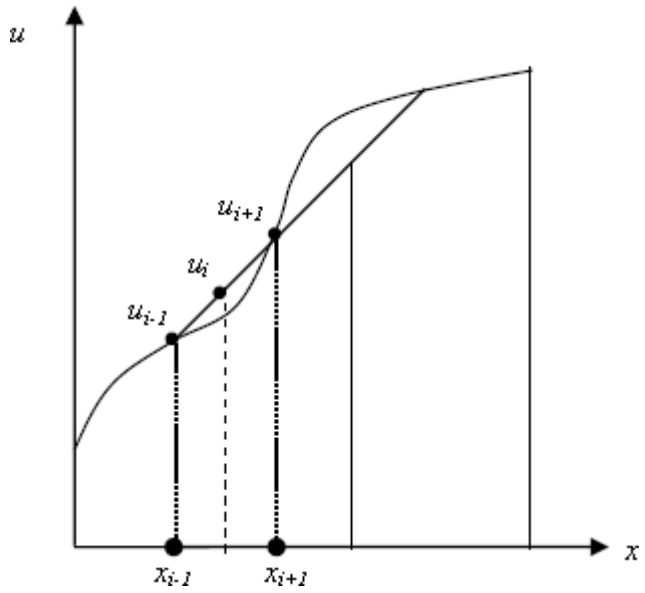

Figure 1.14 A two-noded linear element

As an example, we will develop the finite element formulation of Laplace's Equation in one dimension:

$$\frac{d^2u}{dx^2} = 0$$

……Equation 1.65

where velocity *u* is a function of the spatial coordinates *x*. We multiply equation 1.65 by Some function *W* and integrate it over the domain of interest denoted by Ω:

$$\int W\left[\frac{d^2u}{dx^2}\right] d\Omega = 0$$

…Equation 1.66

The above equation can be integrated into parts as,

$$\int\left[-\frac{dW}{dx}\frac{du}{dx}\right] d\Omega + \int\left[W\frac{du}{dx}n_x\right] d\Gamma = 0$$

……Equation 1.67

where Γ denotes the boundary of the domain Ω and *nx* is the unit outward normal vector to the boundary Γ. We will now divide the domain into several elements and assume a function.

For the variation of the variable *u* in each element. If a two-noded linear element is assumed, the variation of *u* in each element can be represented by

$$u_i = u_{i-1} + (u_{i+1} - u_{i-1})\left[\frac{x_i - x_{i-1}}{x_{i+1} - x_{i-1}}\right]$$

$$u_i = u_{i-1}\left[\frac{x_{i+1} - x_i}{x_{i+1} - x_{i-1}}\right] + u_{i+1}\left[\frac{x_i - x_{i-1}}{x_{i+1} - x_{i-1}}\right]$$

…Equation 1.68

The terms in the brackets are called the shape functions and are denoted as *Ni*'s. *ui-1* and *ui+1* are the nodal values of the variable *u* and are denoted as *u*i's. Therefore, the variable *u* can be written in the following form

$$u_i = N_{i-1}u_{i-1} + N_{i+1}u_{i+1}$$

……Equation 1.69

Thus, the shape functions corresponding to the two-nodal linear element, represented by

$$N_{i-1} = \frac{x_{i+1} - x_i}{x_{i+1} - x_{i-1}}$$

$$N_{i+1} = \frac{x_i - x_{i-1}}{x_{i+1} - x_{i-1}}$$

……Equation 1.70

We can now determine the derivatives of the variable *u*, using the equation

$$\frac{du}{dx} = \sum_{i=1}^{m} \frac{dN_i}{dx} u_i$$

……Equation 1.71

Where *m* is the number of nodes on the element. Note that *UI's* are nodal values of *u* and they are not variables, therefore, they are not differentiated. To solve the equation we still need to describe the function *W*. There are several methods, which are used for the specification of the variable *W*. However, the most common method is the Galerkin method in which *W* is assumed to be the same as the shape function for each element.

The Finite Volume Method

The finite volume method is currently the most popular in CFD. The main reason is that it can resolve some of the difficulties that the other two methods have. Generally, the finite volume method is a special case of finite element, when the function *W* is equal to 1 everywhere in the domain. A typical finite volume, or cell, is shown in Figure 1.15. In this figure, the centroid of the volume, point P, is the reference point at which we want to discretize the partial differential equation.

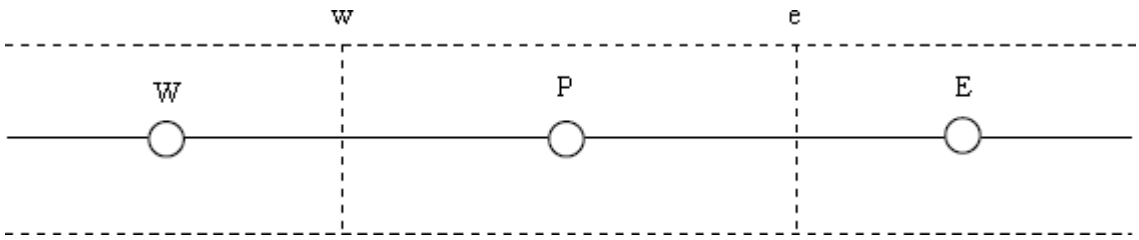

Figure 1.15 A finite volume in one dimension

The neighboring volumes are denoted as, W, the volume to the west side, and E, the volume to the east side of the volume P. For the one-dimensional finite volume shown in Figure 1., the volume with centroid P, has two boundary faces at w and e. The second derivative of a variable at P can be written as the difference between the 1st derivatives of the variable evaluated at the volume faces:

$$\left[\frac{\partial^2 u}{\partial x^2}\right]_p = \frac{\left[\left(\frac{\partial u}{\partial x}\right)_e - \left(\frac{\partial u}{\partial x}\right)_w\right]}{x_e - x_w}$$

Equation 1.72

The first derivatives at the volume faces can be written as the differences in the values of the variable at the neighboring volume centroids:

$$\left[\frac{\partial u}{\partial x}\right]_e = \frac{u_E - u_p}{x_E - x_p} \qquad \left[\frac{\partial u}{\partial x}\right]_w = \frac{u_p - u_W}{x_p - x_W}$$

……Equation 1.73

We can apply this technique to equation 1.73 to obtain its finite volume formulation. The above method is also referred to as the Cell Centered (CC) Method, where the flow variables

are allocated at the center of the computational cell. The CC variable arrangement is the most popular since it leads to considerably simpler implementations than other arrangements. On the other hand, the CC arrangement is more susceptible to truncation errors, when the mesh departs from uniform rectangles. Traditionally the finite volume methods have used regular grids for the efficiency of the computations. However, recently, irregular grids have become more popular for simulating flows in complex geometries. The computational effort is more when irregular grids are used since the algorithm should use a table to look at the geometrical relationships between the volumes or element faces. This involves finding data from a disk store of the computer, which increases the computational time.

Spectral Methods

Another method of generating a numerical analog of a differential equation is by using a Fourier series or series of Chebyshev polynomials to approximate the unknown functions. Such methods are called the Spectral method. Fourier series or series of Chebyshev polynomials are valid throughout the entire computational domain. This is the main difference between the spectral method and the FDM and FEM, in which the approximations are local. Once the unknowns are replaced with the truncated series, certain constraints are used to generate algebraic equations for the coefficients of the Fourier or Chebyshev series. Either a weighted residual technique or a technique based on forcing the approximate function to coincide with the exact solution at several grid points is used as the constraint.

Comparison between Discretization Methods

The main differences between the above three techniques include the followings. The finite difference method and the finite volume method both produce the numerical equations at a given point based on the values at neighboring points, whereas the finite element method produces equations for each element independently of all the other elements. It is only when the finite element equations are collected together and assembled into the global matrices that the interaction between elements is taken into account.

Both FDM and FVM can apply the fixed-value boundary conditions by inserting the values into the solution but must modify the equations to take account of any derivative boundary conditions. However, the finite element method takes care of derivative boundary conditions when the element equations are formed and then the fixed values of variables must be applied to the global matrices. One advantage that the finite element method has is that the programs are written to create matrices for each element, which are then assembled to form the

Global equations before the whole problem is solved. Finite volume and finite difference programs, on the other hand, are written to combine the setting up of the equations and their solution. The decoupling of these two phases, in finite element programs, allows the programmer to keep the organization of the program very clear and the addition of new element types is not a major problem. Adding new cell types to a finite volume program can, however, be a major task involving a rewrite of the program and so some finite volume programs can exhibit problems if they have multiple cell types.