Discretization Methods

("Numerical heat transfer and fluid flow" by Suhas V. Patankar)

The physical phenomena we are interested in are usually governed by differential equations. It is our main task to develop the means of solving those equations.

We assume here that the variable θ is a function of only one independent variable x. However, the ideas developed here continue to be applicable when more than one independent variable is active.

The nature of numerical methods

A numerical solution of a differential equation consists of a set of numbers from which the distribution of the dependent variable θ can be constructed. In this sense, a numerical method is akin to a laboratory experiment, in which a set of instrument readings enables us to establish the distribution of the measured quantity in the domain under investigation.

Suppose that we represent the variation of θ by a polynomial in x,

$$\theta = a_0 + a_1 x + a_2 x^2 + \cdots + a_m x^m$$

and employ a numerical method to find the finite number of coefficients $a_0, a_1, a_2, \ldots, a_m$. This will enable us to evaluate θ at any location x by substituting the value of x.

The discretization concept

In focusing attention on the values at the grid points, we have replaced the continuous information contained in the exact solution of the differential equation with discrete values. We have thus discretized the distribution of θ, and it is appropriate to refer to this class of numerical methods as discretization methods.

The algebraic equations involving the unknown values of θ at chosen grid points, which we shall now name the discretization equations, are derived from the differential equation governing θ. In this derivation, we must employ some assumption about how θ varies between the grid points. Although this "profile" of θ could be chosen such that a single algebraic expression suffices for the whole calculation domain, it is often more practical to use piecewise profiles such that a given segment describes the variation of θ over only a small region in terms of the θ values at the grid points and around that region. It is common to subdivide the calculation domain into a number of subdomains or elements such that a separate profile assumption can be associated with each subdomain.

The structure of the discretization equation

A discretization equation is an algebraic relation connecting the values of θ for group of grid points. Such an equation is derived from the differential equation governing θ and expresses the same physical information.

For a given differential equation, the possible discretization equations are by no means unique, although all types of discretization equations are in the limit of a very large number of grid points, expected to give the same solution. The different types arise from the differences in the profile assumptions and in the methods of derivation.

Until now we have deliberately refrained from making reference to finite-difference and finite-element methods. Now it may be stated that these can be thought of as two alternative versions of the discretization method. The distinction between the finite-difference method and the finite-element method results from the ways of choosing the profiles and deriving the discretization equations.

Methods of deriving the discretization equations

For a given differential equation, the required discretization equations can be derived in many ways. Here we shall outline a few common methods and then indicate a preference.

1. *Taylor series formulation*

The usual procedure for deriving finite-difference equations consists of approximating the derivatives in the differential equation via a truncated Taylor series. For example, for grid point 2 located midway between grid point 1 and 3 such that $\Delta x = x_2 - x_1 = x_3 - x_2$, the Taylor-series expansion around 2 gives

$$\theta_1 = \theta_2 - \Delta x \left(\frac{d\theta}{dx}\right)_2 + \frac{1}{2} * (\Delta x)^2 \left(\frac{d^2\theta}{dx^2}\right)_2 - \cdots$$

And

$$\theta_3 = \theta_2 + \Delta x \left(\frac{d\theta}{dx}\right)_2 + \frac{1}{2} * (\Delta x)^2 \left(\frac{d^2\theta}{dx^2}\right)_2 + \cdots$$

Truncating the series just after the third term, and adding and subtracting the two equations, we obtain

$$\left(\frac{\mathrm{d}\theta}{\mathrm{dx}}\right)_2 = (\theta_3 - \theta_1)/(2\Delta x)$$

$$\left(\frac{\mathrm{d}^2\theta}{dx^2}\right)_2 = (\theta_1 + \theta_3 - 2\theta_2)/(\Delta x)^2$$

The substitution of such expressions into the differential equation leads to the finite-difference equation.

2. *Variational formulation*

Another method of obtaining the discretization equations is based on the calculus of variations. The calculus of variations show that solving certain differential equations is equivalent to minimizing a related quantity called the functional. This equivalence is known s a variational principle. If the functional is minimized with respect to the grid-point values of the dependent variable, the resulting

conditions give the required discretization equations. The variational formulation is very commonly employed in finite-element methods for stress analysis, where it can be linked to the virtual-work principle. In additional to its algebraic and conceptual complexity, the main drawback of this formulation is its limited applicability, since a variational principle does not exist for all differential equations of interest.

3. *Method of weighted residuals*

A powerful method for solving differential equations is the method of weighted residuals.

Let the differential equation be represented by

$$\mathrm{L}(\theta) = 0.$$

Further, let's assume that an approximate solution $\bar{\theta}$ that contains a number of undetermined parameters, for example,

$$\bar{\theta} = a_0 + a_1 x + a_2 x^2 + \cdots + a_m x^m$$

the a's being the parameters. The substitution of $\bar{\theta}$ into the differential equation leaves a residual R, defined as

$$\mathrm{R} = \mathrm{L}(\bar{\theta}).$$

We wish to make this residual small in some sense. Let's propose that

$$\int WR\, dx = 0$$

where W is a weighting function and the integration is performed over the domain of interest. By choosing a succession of weighting functions, we can generate as many equations as are required for evaluating the parameters. These algebraic equations containing the parameters as the unknowns are solved to obtain the approximate solution to the differential equation.

The simplest weighting function is W=1. From this, a number of weighted-residual equations can be generated by dividing the calculation domain into subdomain or control volumes, and setting the weighting function to be unity over one subdomain at a time and zero everywhere else. This variant of the method of weighted residuals is called the subdomain method or the control-volume formulation. It implies that the integral of the residual over each control volume must become zero.

4. *Control-volume formulation*

The control-volume formulation can be seen as a special version of the method of weighted residuals. The calculation domain is divided into a number of non-overlapping control-volume such that there is one control-volume surrounding each grid point. The differential equation is integrated over each control-volume. Piecewise profiles expressing the variation of θ between the grid points are used to

evaluate the required integral. The result is the discretization equation containing the values of θ for a group of grid points.

The discretization equation obtained in this manner expresses the conservation principle for θ for the finite control volume, just as the differential equation expresses it for an infinitesimal control volume.

The most attractive feature of the control-volume formulation is that the resulting solution would imply that the integral conservation of quantities such as mass, momentum and energy is exactly satisfied over any group of control volumes and, of course, over the whole calculation domain. Thus, even the coarse-grid solution exhibits exact integral balances.

In the finite element method and in most weighted-residual methods, the assumed variation of θ consisting of the grid-point values and the interpolation functions (or profiles) between the grid points is taken as the approximate solution. In the finite difference method, only the grid-point values of θ are considered to constitute the solution, without any explicit reference as to how θ varies between the grid points. This is akin to a lab experiment where the distribution of a quantity is obtained in terms of the measured values at some discrete locations without any statement about the variation between these locations. In control-volume approach we shall also adopt this view.