Chapter 3

Discretization of partial differential equations

The mathematical formulation of most problems involving rates of change with respect to two or more independent variables, usually representing time, length, or angle, leads either to a partial differential equation (PDE) or to a system of such equations. Special cases of the two-dimensional second-order partial differential equation

$$A\frac{\partial^2\phi}{\partial x^2} + B\frac{\partial^2\phi}{\partial x\partial y} + C\frac{\partial^2\phi}{\partial y^2} + D\frac{\partial\phi}{\partial x} + E\frac{\partial\phi}{\partial y} + F\phi + G = 0, \tag{3.1}$$

where A, B, C, D, E, F, and G may be functions of independent variables x and y and a dependent variable ϕ, occur more frequently than any others, because they are often the mathematical form of one of the conservation principles of physics.

Equation (3.1), frequently written in the equivalent form

$$A\phi_{xx} + B\phi_{xy} + C\phi_{yy} + D\phi_x + E\phi_y + F\phi + G = 0,$$

is said to be *elliptic* when $B^2 - 4AC < 0$, *parabolic* when $B^2 - 4AC = 0$, and *hyperbolic* when $B^2 - 4AC > 0$.

A comprehensive treatment of partial differential equations can be found in the books of Ames [3], Birkhoff-Lynch [10], and Smith [51]. In this book we restrict our attention to elliptic partial differential equations, arising usually from steady-state diffusion, diffusion-convection, and some fluid flow problems.

The best-known elliptic equations are the *Poisson equation* and the *Laplace equation*. The Poisson equation

$$\frac{\partial^2\phi}{\partial x^2} + \frac{\partial^2\phi}{\partial y^2} + G = 0, \tag{3.2}$$

often written as $\nabla^2\phi + G \equiv \triangle\phi + G = 0$, represents problems of steady-state heat or mass transfer involving diffusion and convection. The Laplace equation is written

$$\frac{\partial^2\phi}{\partial x^2} + \frac{\partial^2\phi}{\partial y^2} \equiv \nabla^2\phi \equiv \triangle\phi = 0, \tag{3.3}$$

where the operator

$$\nabla^2 \equiv \triangle = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \tag{3.4}$$

is called the *Laplace operator* or *Laplacian*.

The domain of integration of a two-dimensional elliptic equation is always an area Ω bounded by a closed curve $\partial\Omega$. The boundary conditions usually specify either the value of the function or the value of its normal derivative at each point of $\partial\Omega$, or a mixture of both. There are three common types:

$$\left.\begin{array}{llcl} \textit{Dirichlet condition} & \phi(x,y) & = & c(x,y), \\ \textit{Neumann condition} & \dfrac{\partial\phi(x,y)}{\partial\vec{n}} & = & 0, \\ \textit{Cauchy condition} & \dfrac{\partial\phi(x,y)}{\partial\vec{n}} + \alpha(x,y)\phi(x,y) & = & \gamma(x,y), \end{array}\right\} \tag{3.5}$$

where the vector $\vec{n}$ usually refers to a unit vector that is normal to $\partial\Omega$ and directed outwards. Note that the Neumann condition is a special case of the Cauchy condition with $\alpha = \gamma = 0$.

A limited number of elliptic partial differential equations can be solved analytically. The typical way to solve such equations is to discretize them, i.e., to approximate them by equations that involve a finite number of unknowns. In the matrix problems that arise from these discretizations, the matrices are generally large and sparse: they have very few nonzero entries. Moreover, those entries are usually located in a regular pattern on a few diagonals.

There are different ways to discretize partial differential equations. The best are *finite-difference* or *finite-element* methods, which are well suited to computer program implementation.

In the simplest method of finite differences, derivatives at a point (x, y) are approximated by difference quotients over a small interval, i.e., $\partial\phi/\partial x$ is replaced by $\delta\phi/\delta x$, where δx is small and y is constant, and $\partial\phi/\partial y$ is replaced by $\delta\phi/\delta y$, where δy is small and x is constant. Finite-difference solutions are usually satisfactory for practical applications.

The finite-element method replaces the original function by a function that has some degree of smoothness over the global domain, but is a piecewise polynomial on simple nodes such as small triangles or rectangles. Finite-element methods are not considered in this book; interested readers are referred to the books of Ames [3] and Reddy [44].

3.1 Finite-difference approximations

The main goal of this chapter is to derive finite-difference approximations for some elliptic differential equations and to study the properties of the associated matrix equations. Three different methods of deriving finite difference approximations are used in practice; they are based on the variational formulation, integration, and Taylor series.

The variational method is based on the self-adjoint property of a given differential equation; therefore, it is not applicable to general differential equations. The integration technique gives particularly simple discretizations in problems with internal interfaces and nonuniform meshes; it is applicable in the general case. The Taylor series method seems to be most popular because it allows us to deduce the order of approximation of the discrete methods and is applicable to differential equations in general; it will be discussed below.