5

Partial Differential Equations in Two Space Variables

INTRODUCTION

In Chapter 4 we discussed the various classifications of PDEs and described finite difference (FD) and finite element (FE) methods for solving parabolic PDEs in one space variable. This chapter begins by outlining the solution of elliptic PDEs using FD and FE methods. Next, parabolic PDEs in two space variables are treated. The chapter is then concluded with a section on mathematical software, which includes two examples.

ELLIPTIC PDES—FINITE DIFFERENCES

Background

Let R be a bounded region in the $x - y$ plane with boundary ∂R. The equation

$$\frac{\partial}{\partial x}\left[a_1(x, y)\,\frac{\partial w}{\partial x} \right] + \frac{\partial}{\partial y}\left[a_2(x, y)\,\frac{\partial w}{\partial y} \right] = d\left(x, y, w, \frac{\partial w}{\partial x}, \frac{\partial w}{\partial y} \right)$$

$$a_1 a_2 > 0 \qquad\qquad (5.1)$$

is elliptic in R (see Chapter 4 for the definition of elliptic equations), and three problems involving (5.1) arise depending upon the subsidiary conditions prescribed on ∂R:

1. Dirichlet problem:

$$w = f(x, y) \quad \text{on} \quad \partial R \qquad\qquad (5.2)$$

2. Neumann problem:

$$\frac{\partial w}{\partial n} = g(x, y) \quad \text{on} \quad \partial R \tag{5.3}$$

where $\partial/\partial n$ refers to differentiation along the outward normal to ∂R

3. Robin problem:

$$\alpha(x, y)w + \beta(x, y)\frac{\partial w}{\partial n} = \gamma(x, y) \quad \text{on} \quad \partial R \tag{5.4}$$

We illustrate these three problems on Laplace's equation in a square.

Laplace's Equation in a Square

Laplace's equation is

$$\frac{\partial^2 w}{\partial x^2} + \frac{\partial^2 w}{\partial y^2} = 0, \quad 0 \leq x \leq 1, \quad 0 \leq y \leq 1 \tag{5.5}$$

Let the square region R, $0 \leq x \leq 1$, $0 \leq y \leq 1$, be covered by a grid with sides parallel to the coordinate axis and grid spacings such that $\Delta x = \Delta y = h$. If $Nh = 1$, then the number of internal grid points is $(N - 1)^2$. A second-order finite difference discretization of (5.5) at any interior node is:

$$\frac{1}{(\Delta x)^2}[u_{i+1,j} - 2u_{i,j} + u_{i-1,j}] + \frac{1}{(\Delta y)^2}[u_{i,j+1} - 2u_{i,j} + u_{i,j-1}] = 0 \tag{5.6}$$

where

$$u_{i,j} \simeq w(x_i, y_j)$$
$$x_i = ih$$
$$y_j = jh$$

Since $\Delta x = \Delta y$, (5.6) can be written as:

$$u_{i,j-1} + u_{i+1,j} - 4u_{i,j} + u_{i-1,j} + u_{i,j+1} = 0 \tag{5.7}$$

with an error of $0(h^2)$.

Dirichlet Problem   If $w = f(x, y)$ on ∂R, then

$$u_{i,j} = f(x_i, y_j) \tag{5.8}$$

for (x_i, y_j) on ∂R. Equations (5.7) and (5.8) completely specify the discretization, and the ensuing matrix problem is

$$\mathbf{Au} = \mathbf{f} \tag{5.9}$$

where

$$
A = \begin{bmatrix}
J & -I & & & & 0 \\
-I & \cdot & \cdot & & & \\
& \cdot & \cdot & \cdot & & \\
& & \cdot & \cdot & \cdot & \\
& & & \cdot & \cdot & -I \\
0 & & & & -I & J
\end{bmatrix}, \qquad (N-1)^2 \times (N-1)^2
$$

I = identity matrix, $\qquad (N-1) \times (N-1)$

$$
J = \begin{bmatrix}
4 & -1 & & & \\
-1 & \cdot & \cdot & & \\
& \cdot & \cdot & \cdot & \\
& & \cdot & \cdot & -1 \\
& & & -1 & 4
\end{bmatrix}, \qquad (N-1) \times (N-1)
$$

$$\mathbf{u} = [u_{1,1}, \ldots, u_{N-1,1}, u_{1,2}, \ldots, u_{N-1,2}, \ldots, u_{1,N-1}, \ldots, u_{N-1,N-1}]^T$$

$$\mathbf{f} = [f(0, y_1) + f(x_1, 0), f(x_2, 0), \ldots, f(x_{N-1}, 0)$$

$$+ f(1, y_1), f(0, y_2), 0, \ldots, 0, f(1, y_2), \ldots, f(0, y_{N-1})$$

$$+ f(x_1, 1), f(x_1, 1), f(x_2, 1), \ldots, f(x_{N-1}, 1) + f(1, y_{N-1})]^T$$

Notice that the matrix A is block tridiagonal and that most of its elements are zero. Therefore, when solving problems of this type, a matrix-solving technique that takes into account the sparseness and the structure of the matrix should be used. A few of these techniques are outlined in Appendix E.

Neumann Problem   Discretize (5.3) using the method of false boundaries to give:

$$\frac{1}{2h}\, [u_{-1,j} - u_{1,j}] = g_{0,j}$$

or   **(5.10)**

$$\frac{1}{2h}\, [u_{i,-1} - u_{i,1}] = g_{i,0}$$

where

$$g_{0,j} = g(0, jh)$$

Combine (5.10) and (5.7) with the result

$$Au = 2h\mathbf{g} \tag{5.11}$$

where

$$A = \begin{bmatrix} K & -2I & & & \\ -I & \cdot & & \cdot & \\ & \cdot & \cdot & & \cdot \\ & & \cdot & \cdot & -I \\ & & & -2I & K \end{bmatrix}, \qquad (N+1)^2 \times (N+1)^2$$

$$K = \begin{bmatrix} 4 & -2 & & & \\ -1 & 4 & -1 & & \\ -1 & \cdot & & \cdot & \\ & \cdot & \cdot & & \cdot \\ & & \cdot & -1 & 4 & -1 \\ & & & -2 & 4 \end{bmatrix}, \qquad (N+1) \times (N+1)$$

I = identity matrix, $(N+1) \times (N+1)$

$\mathbf{u} = [u_{0,0}, \ldots, u_{N,0}, u_{0,1}, \ldots, u_{N,1}, \ldots, u_{0,N}, \ldots, u_{N,N}]^T$

$\mathbf{g} = [2g_{0,0}, g_{1,0}, \ldots, 2g_{N,0}, g_{0,1}, 0, \ldots, 0, g_{N,1}, \ldots,$

$\qquad 2g_{0,N}, g_{1,N}, \ldots, g_{N-1,N}, 2g_{N,N}]^T$

In contrast to the Dirichlet problem, the matrix A is now singular. Thus A has only $(N+1)^2 - 1$ rows or columns that are linearly independent. The solution of (5.11) therefore involves an arbitrary constant. This is a characteristic of the solution of a Neumann problem.

Robin Problem.   Consider the boundary conditions of form

$$\left. \begin{aligned} \frac{\partial w}{\partial x} - \phi_1 w &= f_0(y), & x = 0 \\[2mm] \frac{\partial w}{\partial x} + \eta_1 w &= f_1(y), & x = 1 \end{aligned} \right\} \quad \text{for } 0 \leqslant y \leqslant 1$$

$$\left. \begin{aligned} \frac{\partial w}{\partial y} - \phi_2 w &= g_0(x), & y = 0 \\[2mm] \frac{\partial w}{\partial y} + \eta_2 w &= g_1(x), & y = 1 \end{aligned} \right\} \quad \text{for } 0 \leqslant x \leqslant 1$$

$$(5.12)$$

where ϕ and η are constants and f and g are known functions. Equations (5.12) can be discretized, say by the method of false boundaries, and then included in the discretization of (5.5). During these discretizations, it is important to maintain the same order of accuracy in the boundary discretization as with the PDE discretization. The resulting matrix problem will be $(N + 1)^2 \times (N + 1)^2$, and its form will depend upon (5.12).

Usually, a practical problem contains a combination of the different types of boundary conditions, and their incorporation into the discretization of the PDE can be performed as stated above for the three cases.

EXAMPLE 1

Consider a square plate $R = \{(x, y): 0 \leqslant x \leqslant 1, 0 \leqslant y \leqslant 1\}$ with the heat conduction equation

$$\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} = 0$$

Set up the finite difference matrix problem for this equation with the following boundary conditions:

$$T(x, y) = T(0, y) = T_1 \qquad \text{(fixed temperature)}$$

$$T(1, y) = T_2 \qquad \text{(fixed temperature)}$$

$$\frac{\partial T}{\partial y}(x, 0) = 0 \qquad \text{(insulated surface)}$$

$$\frac{\partial T}{\partial y}(x, 1) = k[T(x, 1) - T_2] \qquad \text{(heat convected away at } y = 1)$$

where T_1, T_2, and k are constants and $T_1 \geqslant T(x, y) \geqslant T_2$.

SOLUTION

Impose a grid on the square region R such that $x_i = ih$, $y_j = jh$ ($\Delta x = \Delta y$) and $Nh = 1$. For any interior grid point

$$u_{i,j-1} + u_{i+1,j} - 4u_{i,j} + u_{i-1,j} + u_{i,j+1} = 0$$
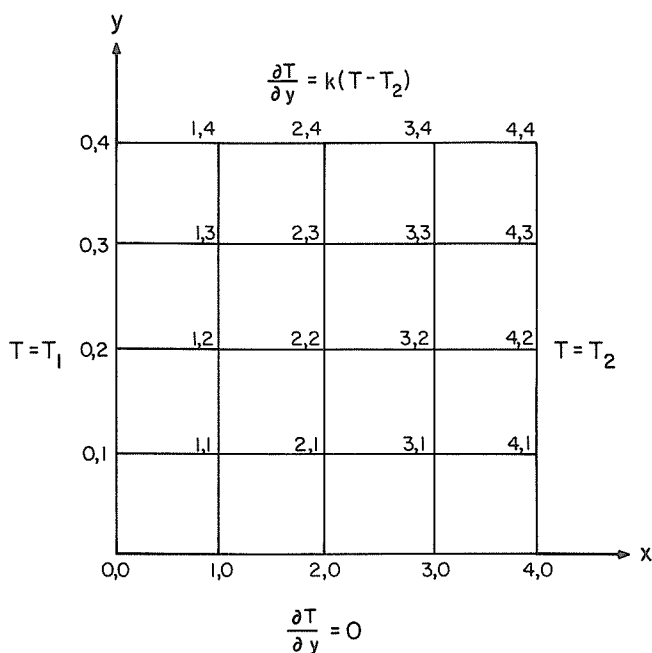
where

$$u_{i,j} \simeq T(x_i, y_j)$$

FIGURE 5.1   Grid for Example 1.

At the boundaries $x = 0$ and $x = 1$ the boundary conditions are Dirichlet. Therefore

$$u_{0,j} = T_1, \qquad \text{for } j = 0, \ldots, N$$

$$u_{N,j} = T_2, \qquad \text{for } j = 0, \ldots, N$$

At $y = 0$ the insulated surface gives rise to a Neumann condition that can be discretized as

$$u_{i,-1} - u_{i,1} = 0, \qquad \text{for } i = 1, \ldots, N - 1$$

and at $y = 1$ the Robin condition is

$$\frac{u_{i,N-1} - u_{i,N+1}}{2h} = k[u_{i,N} - T_2], \qquad \text{for } i = 1, \ldots, N - 1$$

If $N = 4$, then the grid is as shown in Figure 5.1 and the resulting matrix problem is:

$$
\begin{bmatrix}
-4 & 1 & & 2 & & & & & & & & & & & \\
1 & -4 & 1 & & 2 & & & & & & & & & & \\
 & 1 & -4 & & & 2 & & & & & & & & & \\
1 & & & -4 & 1 & & 1 & & & & & & & & \\
 & 1 & & 1 & -4 & 1 & & 1 & & & & & & & \\
 & & 1 & & 1 & -4 & & & 1 & & & & & & \\
 & & & 1 & & & -4 & 1 & & 1 & & & & & \\
 & & & & 1 & & 1 & -4 & 1 & & 1 & & & & \\
 & & & & & 1 & & 1 & -4 & & & 1 & & & \\
 & & & & & & 1 & & & -4 & 1 & & 1 & & \\
 & & & & & & & 1 & & 1 & -4 & 1 & & 1 & \\
 & & & & & & & & 1 & & 1 & -4 & & & 1 \\
 & & & & & & & & & 2 & & & (4+2hk) & 1 & \\
 & & & & & & & & & & 2 & & 1 & -(4+2hk) & 1 \\
 & & & & & & & & & & & 2 & & 1 & -(4+2hk)
\end{bmatrix}
\begin{bmatrix}
u_{1,0} \\ u_{2,0} \\ u_{3,0} \\ u_{1,1} \\ u_{2,1} \\ u_{3,1} \\ u_{1,2} \\ u_{2,2} \\ u_{3,2} \\ u_{1,3} \\ u_{2,3} \\ u_{3,3} \\ u_{1,4} \\ u_{2,4} \\ u_{3,4}
\end{bmatrix}
=
\begin{bmatrix}
-T_1 \\ 0 \\ -T_2 \\ -T_1 \\ 0 \\ -T_2 \\ -T_1 \\ 0 \\ -T_2 \\ -T_1 \\ 0 \\ -T_2 \\ -(T_1+2hkT_2) \\ -2hkT_2 \\ -(T_2+2hkT_2)
\end{bmatrix}
$$

Notice how the boundary conditions are incorporated into the matrix problem. The matrix generated by the finite difference discretization is sparse, and an appropriate linear equation solver should be employed to determine the solution. Since the error is $O(h^2)$, the error in the solution with $N = 4$ is $O(0.0625)$. To obtain a smaller error, one must increase the value of N, which in turn increases the size of the matrix problem.

Variable Coefficients and Nonlinear Problems

Consider the following elliptic PDE:

$$-(P(x, y)w_x)_x - (P(x, y)w_y)_y + \eta(x, y)w^\sigma = f(x, y) \tag{5.13}$$

defined on a region R with boundary ∂R and

$$a(x, y)w + b(x, y)\frac{\partial w}{\partial n} = c(x, y), \qquad \text{for } (x, y) \text{ on } \partial R \tag{5.14}$$

Assume that P, P_x, P_y, η, and f are continuous in R and

$$P(x, y) > 0$$

$$\eta(x, y) > 0 \tag{5.15}$$

Also, assume a, b, and c are piecewise continuous and

$$\left.\begin{array}{l} a(x, y) \geq 0 \\ b(x, y) \geq 0 \\ a + b > 0 \end{array}\right\} \qquad \text{for } (x, y) \text{ on } \partial R \tag{5.16}$$

If $\sigma = 1$, then (5.13) is called a self-adjoint elliptic PDE because of the form of the derivative terms. A finite difference discretization of (5.13) for any interior node is

$$-\delta_x(P(x_i, y_j)\delta_x u_{i,j}) - \delta_y(P(x_i, y_j)\delta_y u_{i,j}) + \eta(x_i, y_j)u_{i,j}^\sigma = f(x_i, y_j) \tag{5.17}$$

where

$$\delta_x u_{i,j} = \frac{u_{i+1/2,j} - u_{i-1/2,j}}{\Delta x}$$

$$\delta_y u_{i,j} = \frac{u_{i,j+1/2} - u_{i,j-1/2}}{\Delta y}$$

The resulting matrix problem will still remain in block-tridiagonal form, but if $\sigma \neq 0$ or 1, then the system is nonlinear. Therefore, a Newton iteration must be performed. Since the matrix problem is of considerable magnitude, one would like to minimize the number of Newton iterations to obtain solution. This is the rationale behind the Newton-like methods of Bank and Rose [1]. Their methods try to accelerate the convergence of the Newton method so as to minimize the amount of computational effort in obtaining solutions from large systems of

nonlinear algebraic equations. A problem of practical interest, the simulation of a two-phase, cross-flow reactor (three nonlinear coupled elliptic PDEs), was solved in [2] using the methods of Bank and Rose, and it was shown that these methods significantly reduced the number of iterations required for solution [3].

Nonuniform Grids

Up to this point we have limited our discussions to uniform grids, i.e., $\Delta x = \Delta y$. Now let $k_j = y_{j+1} - y_j$ and $h_i = x_{i+1} - x_i$. Following the arguments of Varga [4], at each interior mesh point (x_i, y_j) for which $u_{i,j} \simeq w(x_i, y_j)$, integrate (5.17) over a corresponding mesh region $\bar{r}_{i,j}$ ($\sigma = 1$):

$$- \iint_{\bar{r}_{i,j}} \left\{ (Pw_x)_x + (Pw_y)_y \right\} dx\, dy + \iint_{\bar{r}_{i,j}} \eta w\, dx\, dy = \iint_{\bar{r}_{i,j}} f\, dx\, dy \qquad (5.18)$$

By Green's theorem, any two differentiable functions $s(x, y)$ and $t(x, y)$ defined in $\bar{r}_{i,j}$ obey

$$\iint_{\bar{r}_{i,j}} (s_x - t_y) \, dx\, dy = \int_{\partial \bar{r}_{i,j}} (t\, dx + s\, dy) \qquad (5.19)$$

where $\partial \bar{r}_{i,j}$ is the boundary of $\bar{r}_{i,j}$ (refer to Figure 5.2). Therefore, (5.18) can be written as

$$- \int_{\partial \bar{r}_{i,j}} \left\{ Pw_x\, dy - Pw_y\, dx \right\} + \iint_{\bar{r}_{i,j}} \eta w\, dx\, dy = \iint_{\bar{r}_{i,j}} f\, dx\, dy \qquad (5.20)$$
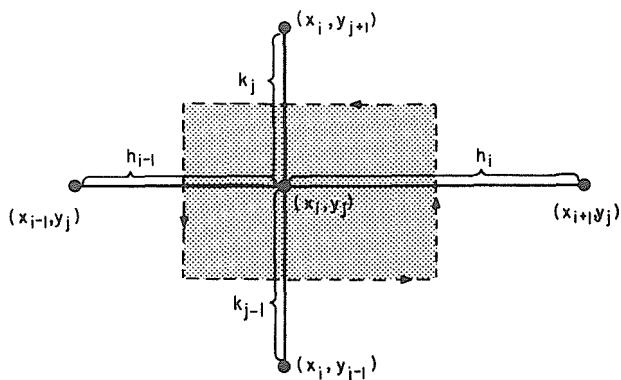

FIGURE 5.2 Nonuniform grid spacing (shaded area is the integration area). Adapted from Richard S. Varga, *Matrix Iterative Analysis*, copyright © 1962, p. 184. Reprinted by permission of Prentice-Hall, Inc., Englewood Cliffs, N. J.

The double integrals above can be approximated by

$$\iint_{r_{i,j}} z \, dx \, dy \simeq A_{i,j} \, z_{i,j} \tag{5.21}$$

for any function $z(x, y)$ such that $z(x_i, y_j) = z_{i,j}$ and

$$A_{i,j} = \frac{(h_{i-1} + h_i)(k_{j-1} + k_j)}{4}$$

The line integral in (5.20) is approximated by central differences (integration follows arrows on Figure 5.2). For example, consider the portion of the line integral from $(x_{i+1/2}, y_{j-1/2})$ to $(x_{i+1/2}, y_{j+1/2})$:

$$-\int_{(x_{i+\frac{1}{2}},y_{j-\frac{1}{2}})}^{(x_{i+\frac{1}{2}},y_{j+\frac{1}{2}})}(Pw_x dy - Pw_y dx)$$

$$= \left(\frac{k_{j-1}}{2}P_{i+\frac{1}{2},j-\frac{1}{2}} + \frac{k_j}{2}P_{i+\frac{1}{2},j+\frac{1}{2}}\right)\left(\frac{u_{i,j} - u_{i+1,j}}{h_i}\right) \tag{5.22}$$

where

$$P_{i+\frac{1}{2},j-\frac{1}{2}} = P(x_{i+\frac{1}{2}}, y_{j-\frac{1}{2}})$$

Therefore, the complete line integral is approximated by

$$\left(\frac{k_{j-1}}{2}P_{i+\frac{1}{2},j-\frac{1}{2}} + \frac{k_j}{2}P_{i+\frac{1}{2},j+\frac{1}{2}}\right)\left(\frac{u_{i,j} - u_{i+1,j}}{h_i}\right)$$

$$+ \left(\frac{k_{j-1}}{2}P_{i-\frac{1}{2},j-\frac{1}{2}} + \frac{k_j}{2}P_{i-\frac{1}{2},j+\frac{1}{2}}\right)\left(\frac{u_{i,j} - u_{i-1,j}}{h_{i-1}}\right)$$

$$+ \left(\frac{h_{i-1}}{2}P_{i-\frac{1}{2},j+\frac{1}{2}} + \frac{h_i}{2}P_{i+\frac{1}{2},j+\frac{1}{2}}\right)\left(\frac{u_{i,j} - u_{i,j+1}}{k_j}\right)$$

$$+ \left(\frac{h_{i-1}}{2}P_{i-\frac{1}{2},j-\frac{1}{2}} + \frac{h_i}{2}P_{i+\frac{1}{2},j-\frac{1}{2}}\right)\left(\frac{u_{i,j} - u_{i,j-1}}{k_{j-1}}\right) \tag{5.23}$$

Using (5.23) and (5.21) on (5.20) gives

$$D_{i,j}u_{i,j} - L_{i,j}u_{i-1,j} - M_{i,j}u_{i+1,j} - T_{i,j}u_{i,j+1} - B_{i,j}u_{i,j-1} = S_{i,j} \tag{5.24}$$

where

$$D_{i,j} = L_{i,j} + M_{i,j} + T_{i,j} + B_{i,j} + \eta_{i,j} \frac{(h_{i-1} + h_i)(k_{j-1} + k_j)}{4}$$

$$h_{i-1}L_{i,j} = \frac{k_{j-1}}{2} P_{i-\frac{1}{2},j-\frac{1}{2}} + \frac{k_j}{2} P_{i-\frac{1}{2},j+\frac{1}{2}}$$

$$h_i M_{i,j} = \frac{k_{j-1}}{2} P_{i+\frac{1}{2},j-\frac{1}{2}} + \frac{k_j}{2} P_{i+\frac{1}{2},j+\frac{1}{2}}$$

$$k_j T_{i,j} = \frac{h_{i-1}}{2} P_{i-\frac{1}{2},j+\frac{1}{2}} + \frac{h_i}{2} P_{i+\frac{1}{2},j+\frac{1}{2}}$$

$$k_{j-1}B_{i,j} = \frac{h_{i-1}}{2} P_{i-\frac{1}{2},j-\frac{1}{2}} + \frac{h_i}{2} P_{i+\frac{1}{2},j-\frac{1}{2}}$$

$$S_{i,j} = f_{i,j} \frac{(h_{i-1} + h_i)(k_{j-1} + k_j)}{4}$$

Notice that if $h_i = h_{i-1} = k_j = k_{j-1}$ and $P(x, y) = $ constant, (5.24) becomes the standard second-order accurate difference formula for (5.17). Also, notice that if $P(x, y)$ is discontinuous at x_i and/or y_j as in the case of inhomogeneous media, (5.24) is still applicable since P is not evaluated at either the horizontal (y_j) or the vertical (x_i) plane. Therefore, the discretization of (5.18) at any interior node is given by (5.24). To complete the discretization of (5.18) requires knowledge of the boundary discretization. This is discussed in the next section.

EXAMPLE 2

In Chapter 4 we discussed the annular bed reactor (see Figure 4.5) with its mass continuity equation given by (4.46). If one now allows for axial dispersion of mass, the mass balance for the annular bed reactor becomes

$$\delta_1 \frac{\partial f}{\partial z} = \left[\frac{Am\,An}{Re\,Sc} \right] \frac{1}{r} \frac{\partial}{\partial r} \left(rD^r \frac{\partial f}{\partial r} \right) + \left[\frac{An/Am}{Re\,Sc} \right] \frac{\partial}{\partial z} \left(D^z \frac{\partial f}{\partial z} \right) + \left[\frac{Am\,An}{Re\,Sc} \right] \delta_2 \phi^2 R(f)$$

where the notation is as in (4.46) except for

$D^r = $ dimensionless radial dispersion coefficient
$D^z = $ dimensionless axial dispersion coefficient

At $r = r_{sc}$, the core-screen interface, we assume that the convection term is equal to zero (zero velocity), thus reducing the continuity equation to

$$\frac{1}{r} \frac{\partial}{\partial r} \left(rD^r \frac{\partial f}{\partial r} \right) + \frac{\partial}{\partial z} \left(D^z \frac{\partial f}{\partial z} \right) = 0$$

Also, since the plane $r = r_{sc}$ is an interface between two media, D^r and D^z are discontinuous at this position. Set up the difference equation at the interface $r = r_{sc}$ using the notation of Figure 5.3. If we now consider D^r and D^z to be constants, and let $h_{i-1} = h_i$, and $k_{j-1} = k_j$, show that the interface discretization simplifies to the standard second-order correct discretization.

SOLUTION

Using (5.18) to discretize the PDE at $r = r_{sc}$ gives

$$-\iint\limits_{\overline{r}_{i,j}} \left[\frac{1}{r}\frac{\partial}{\partial r}\left(rD^r \frac{\partial f}{\partial r} \right) + \frac{\partial}{\partial z}\left(D^z \frac{\partial f}{\partial z} \right) \right] r\, dr\, dz = 0$$

Upon applying Green's theorem to this equation, we have

$$-\int\limits_{\partial \overline{r}_{i,j}} \left[rD^r \frac{\partial f}{\partial r}\, dz - D^z \frac{\partial f}{\partial z} r\, dr \right] = 0$$

If the line integral is approximated by central differences, then

$$r_{i+\frac{1}{2}}\left(\frac{k_{j-1}}{2}D^r_{i+\frac{1}{2},j-\frac{1}{2}} + \frac{k_j}{2}D^r_{i+\frac{1}{2},j+\frac{1}{2}} \right)\left(\frac{u_{i,j} - u_{i+1,j}}{h_i} \right)$$

$$+ r_{i-\frac{1}{2}}\left(\frac{k_{j-1}}{2}D^r_{i-\frac{1}{2},j-\frac{1}{2}} + \frac{k_j}{2}D^r_{i-\frac{1}{2},j+\frac{1}{2}} \right)\left(\frac{u_{i,j} - u_{i-1,j}}{h_{i-1}} \right)$$

$$+ \left(\frac{h_{i-1}}{2}D^z_{i-\frac{1}{2},j+\frac{1}{2}} + \frac{h_i}{2}D^z_{i+\frac{1}{2},j+\frac{1}{2}} \right)r_i\left(\frac{u_{i,j} - u_{i,j+1}}{k_{j+1}} \right)$$

$$+ \left(\frac{h_{i-1}}{2}D^z_{i-\frac{1}{2},j-\frac{1}{2}} + \frac{h_i}{2}D^z_{i+\frac{1}{2},j-\frac{1}{2}} \right)r_i\left(\frac{u_{i,j} - u_{i,j-1}}{k_{j-1}} \right) = 0$$

where

$$D^r_{i-\frac{1}{2},j+\frac{1}{2}} = D^r_{i-\frac{1}{2},j-\frac{1}{2}} = D^r_c$$

$$D^r_{i+\frac{1}{2},j+\frac{1}{2}} = D^r_{i+\frac{1}{2},j-\frac{1}{2}} = D^r_s$$

$$D^z_{i+\frac{1}{2},j+\frac{1}{2}} = D^z_{i+\frac{1}{2},j-\frac{1}{2}} = D^z_s$$

$$D^z_{i-\frac{1}{2},j+\frac{1}{2}} = D^z_{i-\frac{1}{2},j-\frac{1}{2}} = D^z_c$$

Now if D^r and D^z are constants, $h_{i-1} = h_i = h$, and $k_{j-1} = k_j = k$, a second-order correct discretization of the continuity equation at $r = r_{sc}$ is
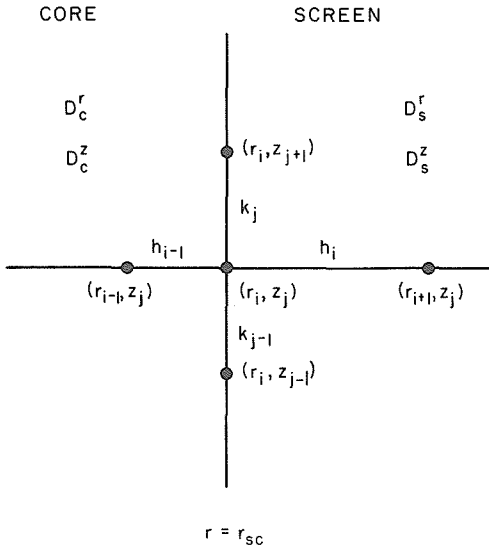
CORE   SCREEN

D_c^r D_s^r

D_c^z (r_i, z_{j+1}) D_s^z

                    k_j

            h_{i-1} h_i

(r_{i-1}, z_j) (r_i, z_j) (r_{i+1}, z_j)

                    k_{j-1}

                 (r_i, z_{j-1})

$r = r_{sc}$

FIGURE 5.3   Grid spacing at core-screen interface of annular bed reactor.

$(r_i = ih, \; z_j = jk):$

$$\frac{D^r}{h^2}\left[\left(1 + \frac{1}{2i}\right)u_{i+1,j} - 2u_{i,j} + \left(1 - \frac{1}{2i}\right)u_{i-1,j}\right]$$

$$+ \frac{D^z}{k^2}\left[u_{i,j+1} - 2u_{i,j} + u_{i,j-1}\right] = 0$$

Next, we will show that the interface discretization with the conditions stated above simplifies to the previous equation. Since $h_{i-1} = h_i = h$ and $k_{j-1} = k_j = k$, multiply the interface discretization equation by $1/(hkr_i)$ to give

$$\frac{D^r}{h^2 r_i}\left[r_{i+\frac{1}{2}}u_{i+1,j} - \left(r_{i+\frac{1}{2}} + r_{i-\frac{1}{2}}\right)u_{i,j} + r_{i-\frac{1}{2}}u_{i-1,j}\right]$$

$$+ \frac{D^z}{k^2}\left[u_{i,j+1} - 2u_{i,j} + u_{i,j-1}\right] = 0$$

Notice that

$$\frac{r_{i+\frac{1}{2}}}{r_i} = \frac{(i + \frac{1}{2})h}{ih} = 1 + \frac{1}{2i}$$

$$\frac{r_{i+\frac{1}{2}} + r_{i-\frac{1}{2}}}{r_i} = \frac{(i + \frac{1}{2})h + (i - \frac{1}{2})h}{ih} = 2$$

$$\frac{r_{i-\frac{1}{2}}}{r_i} = \frac{(i - \frac{1}{2})h}{ih} = 1 - \frac{1}{2i}$$

and that with these rearrangements, the previous discretization becomes the second-order correct discretion shown above.

Irregular Boundaries

Dirichlet Condition One method of treating the Dirichlet condition with irregular boundaries is to use unequal mesh spacings. For example, in figure 5.4a a vertical mesh spacing from position B of βh and a horizontal mesh spacing of αh would incorporate ∂R into the discretization at the point B.

Another method of treating the boundary condition using a uniform mesh involves selecting a new boundary. Referring to Figure 5.4a, given the curve ∂R, one might select the new boundary to pass through position B, that is, (x_B, y_B). Then, a zeroth-degree interpolation would be to take u_B to be $f(x_B, y_B + \beta h)$ or $f(x_B + \alpha h, y_B)$ where $w = f(x, y)$ on ∂R. The replacement of u_B by $f(x_B, y_B + \beta h)$ can be considered as interpolation at B by a polynomial of degree zero with value $f(x_B, y_B + \beta h)$ at $(x_B, y_B + \beta h)$. Hence the term interpolation of degree zero. A more precise approximation is obtained by an interpolation of degree one. A first-degree interpolation using positions u_B and u_C is:

$$\frac{u_B - f(x_B, y_B + \beta h)}{\beta h} = \frac{u_C - u_b}{h}$$

or

$$u_B = \left(\frac{\beta}{\beta + 1}\right)u_C + \left(\frac{1}{\beta + 1}\right)f(x_B, y_B + \beta h) \qquad (5.25)$$

Alternatively, we could have interpolated in the x-direction to give

$$u_B = \left(\frac{\alpha}{\alpha + 1}\right)u_A + \left(\frac{1}{\alpha + 1}\right)f(x_B + \alpha h, y_B) \qquad (5.26)$$
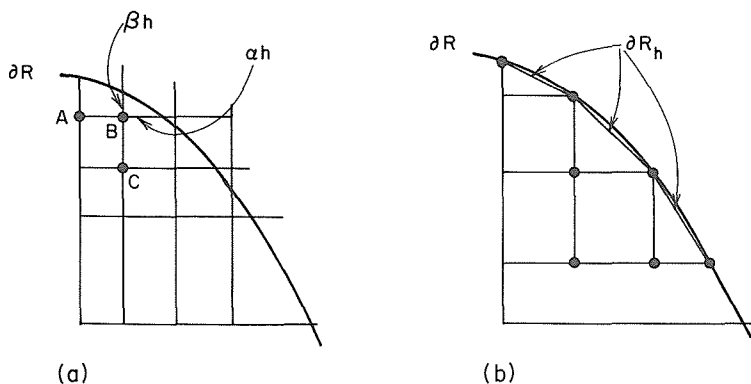

FIGURE 5.4 Irregular boundaries. (*a*) Uniform mesh with interpolation. (*b*) Non-uniform mesh with approximate boundary ∂R_h.

Normal Derivative Conditions.   Fortunately, in many practical applications normal derivative conditions occur only along straight lines, e.g., lines of symmetry, and often these lines are parallel to a coordinate axis. However, in the case where the normal derivative condition exists on an irregular boundary, it is suggested that the boundary ∂R be approximated by straight-line segments denoted ∂R_h in Figure 5.4(b). In this situation the use of nonuniform grids is required. To implement the integration method at the boundary ∂R_h, refer to Figure 5.5 during the following analysis. If $b(x_i, y_j) \neq 0$ in (5.14), then $u_{i,j}$ is unknown. The approximation (5.22) can be used for vertical and horizontal portions of the line integral in Figure 5.5, but not on the portion denoted ∂R_h. On ∂R_h the normal to ∂R_h makes an angle θ with the positive x-axis. Thus, ∂R_h must be parameterized by

$$x = x_{i+1/2} - \lambda \sin \theta$$

$$y = y_{j-1/2} + \lambda \cos \theta \tag{5.27}$$

and on ∂R_h

$$\frac{\partial w}{\partial n} = w_x \cos \theta + w_y \sin \theta \tag{5.28}$$

The portion of the line integral $(x_{i+1/2}, y_{j-1/2})$ to (x_i, y_j) in (5.20) can be written as

$$-\int_0^\ell \{Pw_x \, dy - Pw_y \, dx\}$$

$$= -\int_0^\ell (Pw_x \cos \theta + Pw_y \sin \theta) \, d\lambda = -\int_0^\ell P \frac{\partial w}{\partial n} \, d\lambda$$
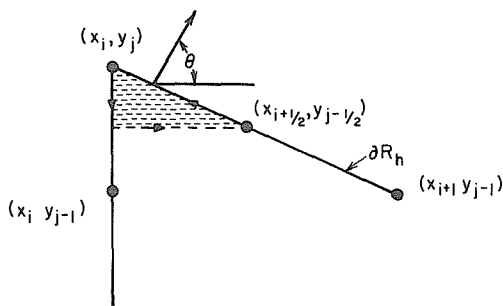

FIGURE 5.5   **Boundary point on ∂R_h. Adapted from Richard S. Varga, *Matrix Iterative Analysis*, © 1962, p. 184. Reprinted by permission of Prentice-Hall, Inc., Englewood Cliffs, N. J.**

or by using (5.14):

$$-\int_0^\ell \{Pw_x \, dy - Pw_y \, dx\} = -\int_0^\ell P\left[\frac{c(\lambda) - a(\lambda)w(\lambda)}{b(\lambda)}\right] d\lambda$$

$$\simeq -P_{i,j}\left[\frac{c_{i,j} - a_{i,j}u_{i,j}}{b_{i,j}}\right]\ell \qquad (5.29)$$

where

$$\ell = \frac{1}{2}\sqrt{h_i^2 + k_{j-1}^2} \qquad \text{(path length of integration)}.$$

Notice that we have used the boundary condition together with the differential equation to obtain a difference equation for the point (x_i, y_j).

ELLIPTIC PDES—FINITE ELEMENTS

Background

Let us begin by illustrating finite element methods with the following elliptic PDE:

$$\frac{\partial^2 w}{\partial x^2} + \frac{\partial^2 w}{\partial y^2} = -f(x, y), \qquad \text{for } (x, y) \text{ in } R \qquad (5.30)$$

and

$$w(x, y) = 0, \qquad \text{for } (x, y) \text{ on } \partial R \qquad (5.31)$$

Let the bounded domain R with boundary ∂R be the unit square, that is, $0 \le x \le 1$, $0 < y \le 1$. Finite element methods find a piecewise polynomial (pp) approximation, $u(x, y)$, to the solution of (5.30). The pp-approximation can be written as

$$u(x, y) = \sum_{j=1}^m \alpha_j \phi_j(x, y) \qquad (5.32)$$

where $\{\phi_j(x, y)|j = 1, \ldots, m\}$ are specified functions that satisfy the boundary conditions and $\{\alpha_j|j = 1, \ldots, m\}$ are as yet unknown constants.

In the collocation method the set $\{\alpha_j|j = 1, \ldots, m\}$ is determined by satisfying the PDE exactly at m points, $\{(x_i, y_i)|i = 1, \ldots, m\}$, the collocation points in the region. The collocation problem for (5.30) using (5.32) as the pp-approximation is given by:

$$A^C\alpha = -\mathbf{f} \qquad (5.33)$$

where

$$A_{ij}^C = \frac{\partial^2 \phi_j}{\partial x^2}(x_i, y_i) + \frac{\partial^2 \phi_j}{\partial y^2}(x_i, y_i)$$

$$\boldsymbol{\alpha} = [\alpha_1, \alpha_2, \ldots, \alpha_m]^T$$

$$\mathbf{f} = [f(x_1, y_1), \ldots, f(x_m, y_m)]^T$$

The solution of (5.33) then yields the vector $\boldsymbol{\alpha}$, which determines the collocation approximation.

To formulate the Galerkin method, first multiply (5.30) by ϕ_i and integrate over the unit square:

$$\iint_R \left(\frac{\partial^2 w}{\partial x^2} + \frac{\partial^2 w}{\partial y^2}\right) \phi_i \, dx \, dy = -\iint_R f(x, y)\phi_i \, dx \, dy$$

$$i = i, \ldots, m \qquad (5.34)$$

Green's first identity for a function t is

$$\iint_R \left(\frac{\partial t}{\partial x}\frac{\partial \phi_i}{\partial x} + \frac{\partial t}{\partial y}\frac{\partial \phi_i}{\partial y}\right) dx \, dy$$

$$= -\iint_R \left(\frac{\partial^2 t}{\partial x^2} + \frac{\partial^2 t}{\partial y^2}\right) \phi_i \, dx \, dy + \int_{\partial R} \frac{\partial t}{\partial n}\phi_i \, d\ell \qquad (5.35)$$

where

$\dfrac{\partial}{\partial n}$ = denotes differentiation in the direction of outward normal

ℓ = path of integration for the line integral

Since the functions ϕ_i satisfy the boundary condition, each ϕ_i is zero on ∂R. Therefore, applying Green's first identity to (5.34) gives

$$\iint_R \left(\frac{\partial w}{\partial x}\frac{\partial \phi_i}{\partial x} + \frac{\partial w}{\partial y}\frac{\partial \phi_i}{\partial y}\right) dx \, dy = \iint_R f(x, y)\, \phi_i \, dx \, dy$$

$$i = 1, \ldots, m \qquad (5.36)$$

For any two piecewise continuous functions η and ψ denote

$$(\eta, \psi) = \iint_R \eta\psi \, dx \, dy \qquad (5.37)$$

Equation (5.36) can then be written as

$$(\nabla w, \nabla \phi_i) = (f, \phi_i), \qquad i = 1, \ldots, m \qquad (5.38)$$

where

$$\nabla = \text{gradient operator.}$$

This formulation of (5.30) is called the weak form. The Galerkin method consists in finding $u(x)$ such that

$$(\nabla u, \nabla \phi_i) = (f, \phi_i), \qquad i = 1, \ldots, m \tag{5.39}$$

or in matrix notation,

$$A^G \alpha = g \tag{5.40}$$

where

$$A_{ij}^G = (\nabla \phi_i, \nabla \phi_j)$$

$$\alpha = [\alpha_1, \ldots, \alpha_m]^T$$

$$g = [g_1, \ldots, g_m]^T$$

$$g_i = (f, \phi_i)$$

Next, we discuss each of these methods in further detail.

Collocation

In Chapter 3 we outlined the collocation procedure for BVPs and found that one of the major considerations in implementing the method was the choice of the approximating space. This consideration is equally important when solving PDEs (with the added complication of another spatial direction). The most straightforward generalization of the basis functions from one to two spatial dimensions is obtained by considering tensor products of the basis functions for the one-dimensional space $\mathcal{L}_k^v(\pi)$ (see Chapter 3). To describe these piecewise polynomial functions let the region R be a rectangle with $a_1 \leq x \leq b_1$, $a_2 \leq y \leq b_2$, where $-\infty < a_i \leq b_i < \infty$ for $i = 1, 2$. Using this region Birkhoff et al. [5] and later Bramble and Hilbert [6,7] established and generalized interpolation results for tensor products of piecewise Hermite polynomials in two space variables. To describe their results, let

$$\pi_1: \quad a_1 = x_1 < x_2 < \ldots < x_{N_x+1} = b_1$$

$$\pi_2: \quad a_2 = y_1 < y_2 < \ldots < y_{N_y+1} = b_2,$$

$$\tag{5.41}$$

$$h = \max_{1 \leq i \leq N_x} h_i = \max_{1 \leq i \leq N_x} (x_{i+1} - x_i)$$

$$k = \max_{1 \leq j \leq N_y} k_j = \max_{1 \leq j \leq N_y} (y_{j+1} - y_j)$$

$$\rho = \max \{h, k\}$$

be the partitions in the x- and y-directions, and set $\pi = \pi_1 \times \pi_2$. Denote by $\mathcal{L}^2(\pi)$ the set of all real valued piecewise polynomial functions ϕ_i defined on π such that on each subrectangle $[x_i, x_{i+1}] \times [y_j, y_{j+1}]$ of R defined by π, ϕ_i is a polynomial of degree at most 3 in each variable (x or y). Also, each ϕ_i,

$(\partial\phi_i)/(\partial x)$, and $(\partial\phi_i)/(\partial y)$ must be piecewise continuous. A basis for $\mathcal{L}^2$ is the tensor products of the Hermite cubic basis given in Chapter 3 and is

$$\left\{ v_i(x)v_j(y), \; s_i(x)v_j(y), \; v_i(x)s_j(y), \; s_i(x)s_j(y) \right\} \Big|_{i=1}^{N_x+1} \Big|_{j=1}^{N_y+1} \tag{5.42}$$

where the v's and s's are listed in Table 3.2. If the basis is to satisfy the homogeneous Dirichlet conditions, then it can be written as:

$$\begin{cases} s_i(x)v_j(y), & s_i(x)s_j(y) & i=1,N_x+1, \quad j=1,\ldots,N_y+1 \\ v_i(x)s_j(y), & s_i(x)s_j(y) & i=1,\ldots,N_x+1, \quad j=1,N_y+1 \\ v_i(x)v_j(y), & s_i(x)v_j(y), \quad v_i(x)s_j(y), s_i(x)s_j(y), & i=2,\ldots,N_x, \quad j=2,\ldots,N_y \end{cases}$$

$$\tag{5.43}$$

Using this basis, Prenter and Russell [8] write the pp-approximation as:

$$u(x, y) = \sum_{i=1}^{N_x+1} \sum_{j=1}^{N_y+1} \left[u(x_i, y_j)v_iv_j + \frac{\partial u}{\partial x}(x_i, y_j)s_iv_j \right.$$

$$\left. + \frac{\partial u}{\partial y}(x_i, y_j)v_is_j + \frac{\partial^2 u}{\partial x \, \partial y}(x_i, y_j)s_is_j \right] \tag{5.44}$$

which involves $4(N_x + 1)(N_y + 1)$ unknown coefficients. On each subrectangle $[x_i, x_{i+1}] \times [y_j, y_{j+1}]$ there are four collocation points that are the combination of the two Gaussian points in the x direction, and the two Gaussian points in the y direction, and are:

$$\tau_{i,j}^1 = \left(x_i + \frac{h_i}{2}\left[1 - \frac{1}{\sqrt{3}}\right], \; y_j + \frac{k_j}{2}\left[1 - \frac{1}{\sqrt{3}}\right] \right)$$

$$\tau_{i,j}^2 = \left(x_i + \frac{h_i}{2}\left[1 + \frac{1}{\sqrt{3}}\right], \; y_j + \frac{k_j}{2}\left[1 - \frac{1}{\sqrt{3}}\right] \right)$$

$$\tau_{i,j}^3 = \left(x_i + \frac{h_i}{2}\left[1 - \frac{1}{\sqrt{3}}\right], \; y_j + \frac{k_j}{2}\left[1 + \frac{1}{\sqrt{3}}\right] \right) \tag{5.45}$$

$$\tau_{i,j}^4 = \left(x_i + \frac{h_i}{2}\left[1 + \frac{1}{\sqrt{3}}\right], \; y_j + \frac{k_j}{2}\left[1 + \frac{1}{\sqrt{3}}\right] \right)$$

Collocating at these points gives $4N_xN_y$ equations. The remaining $4N_x + 4N_y + 4$ equations required to determine the unknown coefficients are supplied by the boundary conditions [37]. To obtain the boundary equations on the sides $x = a_1$ and $x = b_1$ differentiate the boundary conditions with respect to y. For example, if

$$\frac{\partial u}{\partial x} = y^2 \quad \text{at} \quad x = a_1 \text{ and } x = b_1$$

then   **(5.46)**

$$\frac{\partial^2 u}{\partial x \, \partial y} = 2y \quad \text{at} \quad x = a_1 \text{ and } x = b_1$$

Equation (5.46) applied at $N_y - 1$ boundary nodes $(y_j | j = 2, \ldots, N_y)$ gives:

$$\frac{\partial u}{\partial x}(a_1, y_j) \quad = y_j^2$$

$$\frac{\partial^2 u}{\partial x \, \partial y}(a_1, y_j) = 2y_j$$

$$\frac{\partial u}{\partial x}(b_1, y_j) \quad = y_j^2$$

$$\frac{\partial^2 u}{\partial x \, \partial y}(b_1, y_j) = 2y_j \qquad\qquad \textbf{(5.47)}$$

or $4N_y - 4$ equations. A similar procedure at $y = a_2$ and $y = b_2$ is followed to give $4N_x - 4$ equations. At each corner both of the above procedures are applied. For example, if

$$u(a_1, a_2) = g(a_1, a_2) \qquad\qquad \textbf{(5.48)}$$

then

$$\frac{\partial u}{\partial x}(a_1, a_2) = \frac{\partial g}{\partial x}(a_1, a_2)$$

$$\frac{\partial u}{\partial y}(a_1, a_2) = \frac{\partial g}{\partial y}(a_1, a_2)$$

Thus, the four corners supply the final 12 equations necessary to completely specify the unknown coefficients of (5.44).

EXAMPLE 3

Set up the colocation matrix problem for the PDE:

$$\frac{\partial^2 w}{\partial x^2} + \frac{\partial^2 w}{\partial y^2} = \Phi, \qquad 0 \leqslant x \leqslant 1, \quad 0 \leqslant y \leqslant 1$$

with

$$w = 0, \qquad \text{for } x = 1$$

$$w = 0, \qquad \text{for } y = 1$$

$$\frac{\partial w}{\partial x} = 0, \qquad \text{for } x = 0$$

$$\frac{\partial w}{\partial y} = 0, \qquad \text{for } y = 0$$

where Φ is a constant. This PDE could represent the material balance of an isothermal square catalyst pellet with a zero-order reaction or fluid flow in a rectangular duct under the influence of a pressure gradient. Let $N_x = N_y = 2$.

SOLUTION

Using (5.44) as the pp-approximation requires the formulation of 36 equations. Let us begin by constructing the internal boundary node equations (refer to Figure 5.6a for node numberings):

$$\frac{\partial w}{\partial x}(1, 2) = 0, \qquad \frac{\partial^2 w}{\partial x\, \partial y}(1, 2) = 0$$

$$w(3, 2) = 0, \qquad \frac{\partial w}{\partial y}(3, 2) = 0$$

$$\frac{\partial w}{\partial y}(2, 1) = 0, \qquad \frac{\partial^2 w}{\partial x\, \partial y}(2, 1) = 0$$

$$w(2, 3) = 0, \qquad \frac{\partial w}{\partial x}(2, 3) = 0$$

where $w(i, j) = w(x_i, y_j)$. At the corners

$$\frac{\partial w}{\partial x}(1, 1) = \frac{\partial w}{\partial y}(1, 1) = \frac{\partial^2 w}{\partial x\, \partial y}(1, 1) = 0$$
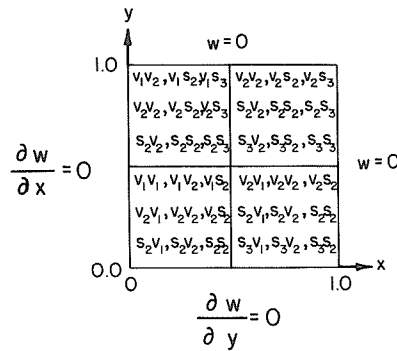
$$w(1, 3) = \frac{\partial w}{\partial x}(1, 3) = \frac{\partial^2 w}{\partial x\, \partial y}(1, 3) = 0$$

$$w(3, 1) = \frac{\partial w}{\partial y}(3, 1) = \frac{\partial^2 w}{\partial x\, \partial y}(3, 1) = 0$$
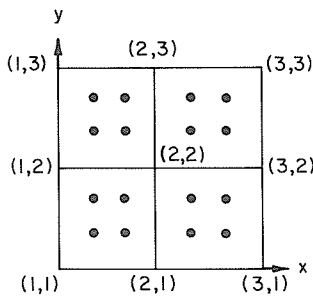
(a)

(b)

FIGURE 5.6 Grid for Example 3. (*a*) Collocation points. (*b*) Nonvanishing basis functions.

and

$$w(3, 3) = \frac{\partial w}{\partial x}(3, 3) = \frac{\partial w}{\partial y}(3, 3) = 0$$

This leaves 16 equations to be specified. The remaining 16 equations are the collocation equations, four per subrectangle (see Figure 5.6a). If the above equations involving the boundary are incorporated in the pp-approximation, then the result is

$$u(x, y) = u_{1,1}v_1v_1 + u_{1,2}v_1v_2 + \frac{\partial u_{1,2}}{\partial y}v_1s_2 + \frac{\partial u_{1,3}}{\partial y}v_1s_3$$

$$+ u_{2,1}v_2v_1 + \frac{\partial u_{2,1}}{\partial x}s_2v_1 + u_{2,2}v_2v_2 + \frac{\partial u_{2,2}}{\partial x}s_2v_2$$

$$+ \frac{\partial u_{2,2}}{\partial y}v_2s_2 + \frac{\partial^2 u_{2,2}}{\partial x\,\partial y}s_2s_2 + \frac{\partial u_{2,3}}{\partial y}v_2s_3 + \frac{\partial^2 u_{2,3}}{\partial x\,\partial y}s_2s_3$$

$$+ \frac{\partial u_{3,1}}{\partial x}s_3v_1 + \frac{\partial u_{3,2}}{\partial x}s_3v_2 + \frac{\partial^2 u_{3,2}}{\partial x\,\partial y}s_3s_2 + \frac{\partial^2 u_{3,3}}{\partial x\,\partial y}s_3s_3$$

where

$$u_{i,j} = u(x_i, y_j)$$

The pp-approximation is then used to collocate at the 16 collocation points. Since the basis is local, various terms of the above pp-approximation can be zero at a given collocation point. The nonvanishing terms of the pp-approximation are given in the appropriate subrectangle in Figure 5.6b. Collocating at the 16 collocation points using the pp-approximation listed above gives the following matrix problem:

$$A^C\mathbf{a} = \Phi\mathbf{1}$$

where

$$\mathbf{1} = [1, \ldots, 1]^T$$

$$\mathbf{a} = \left[u_{1,1},\ u_{1,2},\ \frac{\partial u_{1,2}}{\partial y},\ \frac{\partial u_{1,3}}{\partial y},\ u_{2,1},\ \frac{\partial u_{2,1}}{\partial x},\ u_{2,2} \right.$$

$$\frac{\partial u_{2,2}}{\partial x},\ \frac{\partial u_{2,2}}{\partial y},\ \frac{\partial^2 u_{2,2}}{\partial x\,\partial y},\ \frac{\partial u_{2,3}}{\partial y},\ \frac{\partial^2 u_{2,3}}{\partial x\,\partial y}$$

$$\left. \frac{\partial u_{3,1}}{\partial x},\ \frac{\partial u_{3,2}}{\partial x},\ \frac{\partial^2 u_{3,2}}{\partial x\,\partial y},\ \frac{\partial^2 u_{3,3}}{\partial x\,\partial y} \right]^T$$

$$\nabla^2_{ijs}\psi = \frac{\partial^2}{\partial x^2}\psi\,(\tau^s_{i,j}) + \frac{\partial^2}{\partial y^2}\psi\,(\tau^s_{i,j}) \qquad \text{(for any function } \psi)$$

and for the matrix A^C,

$$A^C = \begin{bmatrix} \nabla^2_{111}v_1v_1 \, \nabla^2_{111}v_1v_2 \, \nabla^2_{111}v_1s_2 & \nabla^2_{111}v_2v_1 \, \nabla^2_{111}s_2v_1 \, \nabla^2_{111}v_2v_2 \, \nabla^2_{111}s_2v_2 \, \nabla^2_{111}v_2s_2 \, \nabla^2_{111}s_2s_2 & \nabla^2_{111}s_3v_1 \\ \vdots & \vdots & \vdots \\ \nabla^2_{114}v_1v_1 \, \nabla^2_{114}v_1v_2 \, \nabla^2_{114}v_1s_2 & \nabla^2_{114}v_2v_1 \, \nabla^2_{114}s_2v_1 \, \nabla^2_{114}v_2v_2 \, \nabla^2_{114}s_2v_2 \, \nabla^2_{114}v_2s_2 \, \nabla^2_{114}s_2s_2 & \nabla^2_{114}s_3v_1 \\ & \vdots & \\ & \nabla^2_{221}v_2v_2 \, \nabla^2_{221}s_2v_2 \, \nabla^2_{221}v_2s_2 \, \nabla^2_{221}s_2s_2 \, \nabla^2_{221}v_2s_3 \, \nabla^2_{221}s_2s_3 & \nabla^2_{221}s_3v_2 \, \nabla^2_{221}s_3s_2 \, \nabla^2_{221}s_3s_3 \\ & \vdots & \vdots \\ & \nabla^2_{224}v_2v_2 \, \nabla^2_{224}s_2v_2 \, \nabla^2_{224}v_2s_2 \, \nabla^2_{224}s_2s_2 \, \nabla^2_{224}v_2s_3 \, \nabla^2_{224}s_2s_3 & \nabla^2_{224}s_3v_2 \, \nabla^2_{224}s_3s_2 \, \nabla^2_{224}s_3s_3 \end{bmatrix}$$

The solution of this matrix problem yields the vector $\mathbf{a}$, which specifies the values of the function and its derivatives at the grid points.

Thus far we have discussed the construction of the collocation matrix problem using the tensor products of the Hermite cubic basis for a linear PDE. If one were to solve a nonlinear PDE using this basis, the procedure would be the same as outlined above, but the ensuing matrix problem would be nonlinear.

In Chapter 3 we saw that the expected error in the pp-approximation when solving BVPs for ODEs was dependent upon the choice of the approximating space, and for the Hermite cubic space, was $0(h^4)$. This analysis can be extended to PDEs in two spatial dimensions with the result that [8]:

$$|u(x, y) - w(x, y)| = 0(\rho^4)$$

Next, consider the tensor product basis for $\mathscr{P}^\nu_{k_x}(\pi_1) \times \mathscr{P}^\nu_{k_y}(\pi_2)$ where π_1 and π_2 are given in (5.41), k_x is the order of the one-dimensional approximating space in the x-direction, and k_y is the order of the one-dimensional approximating space in the y-direction. A basis for this space is given by the tensor products of the B-splines as:

$$B_i^x(x)B_j^y(y) \Big|_{i=1}^{\text{DIMX}} \Big|_{j=1}^{\text{DIMY}} \qquad (5.49)$$

where

$$B_i^x(x) = \text{B-spline in the } x\text{-direction of order } k_x$$

$$B_j^y(y) = \text{B-spline in the } y\text{-direction or order } k_y$$

$$\text{DIMX} = \text{dimension of } \mathscr{P}^\nu_{k_x}$$

$$\text{DIMY} = \text{dimension of } \mathscr{P}^\nu_{k_y}$$

The pp-approximation for this space is given by

$$u(x, y) = \sum_{i=1}^{\text{DIMX}} \sum_{j=1}^{\text{DIMY}} \alpha_{i,j} B_i^x(x) B_j^y(y) \qquad (5.50)$$

where $\alpha_{i,j}$ are constants, with the result that

$$|u(x, y) - w(x, y)| = 0(\rho^\gamma) \qquad (5.51)$$

where

$$\gamma = \min \{k_x, k_y\}$$

Galerkin

The literature on the use of Galerkin-type methods for the solution of elliptic PDEs is rather extensive and is continually expanding. The reason for this growth in use is related to the ease with which the method accommodates complicated

geometries. First, we will discuss the method for rectangles, and then treat the analysis for irregular geometries.

Consider a region R that is a rectangle with $a_1 \leqslant x \leqslant b_1$, $a_2 \leqslant y \leqslant b_2$, with $-\infty < a_i \leqslant b_i < \infty$ for $i = 1, 2$. A basis for the simplest approximating space is obtained from the tensor products of the one-dimensional basis of the space $\mathscr{L}_2^1(\pi)$, i.e., the piecewise linears. If the mesh spacings in x and y are given by π_1 and π_2 of (5.41), then the tensor product basis functions $\omega_{i,j}(x, y)$ are given by

$$\omega_{i,j} = \begin{cases} \left[\dfrac{x - x_{i-1}}{h_{i-1}} \right] \left[\dfrac{y - y_{j-1}}{k_{j-1}} \right], & x_{i-1} \leqslant x \leqslant x_i, \quad y_{j-1} \leqslant y \leqslant y_j \\[2ex] \left[\dfrac{x - x_{i-1}}{h_{i-1}} \right] \left[\dfrac{y_{j+1} - y}{k_j} \right], & x_{i-1} \leqslant x \leqslant x_i, \quad y_j \leqslant y \leqslant y_{j+1} \\[2ex] \left[\dfrac{x_{i+1} - x}{h_i} \right] \left[\dfrac{y - y_{j-1}}{k_{j-1}} \right], & x_i \leqslant x \leqslant x_{i+1}, \quad y_{j-1} \leqslant y \leqslant y_j \\[2ex] \left[\dfrac{x_{i+1} - x}{h_i} \right] \left[\dfrac{y_{j+1} - y}{k_j} \right], & x_i \leqslant x \leqslant x_{i+1}, \quad y_j \leqslant y \leqslant y_{j+1} \end{cases} \tag{5.52}$$

with a pp-approximation of

$$u(x, y) = \sum_{i=1}^{N_x+1} \sum_{j=1}^{N_y+1} u(x_i, y_j)\omega_{i,j} \tag{5.53}$$

Therefore, there are $(N_x + 1)(N_y + 1)$ unknown constants $u(x_i, y_j)$, each associated with a given basis function $\omega_{i,j}$. Figure 5.7 illustrates the basis function $\omega_{i,j}$, from now on called a bilinear basis function.

EXAMPLE 4

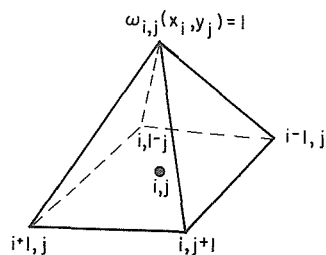Solve (5.30) with $f(x, y) = 1$ using the bilinear basis with $N_x = N_y = 2$.

FIGURE 5.7 Bilinear basis function.

SOLUTION

The PDE is

$$\frac{\partial^2 w}{\partial x^2} + \frac{\partial^2 w}{\partial y^2} = -1, \qquad 0 \le x \le 1, \quad 0 \le y \le 1$$

with

$$w(x, y) = 0 \qquad \text{on the boundary}$$

The weak form of the PDE is

$$\iint_R \left(\frac{\partial w}{\partial x} \frac{\partial \phi_i}{\partial x} + \frac{\partial w}{\partial y} \frac{\partial \phi_i}{\partial y} \right) dx \, dy = \iint_R \phi_i \, dx \, dy$$

where each ϕ_i satisfies the boundary conditions. Using (5.53) as the pp-approximation gives

$$u(x, y) = \sum_{i=1}^{3} \sum_{j=1}^{3} u(x_i, y_j) \omega_{i,j}$$

Let $h_i = k_j = h = 0.5$ as shown in Figure 5.8, and number each of the sub-rectangles, which from now on will be called elements. Since each $\omega_{i,j}$ must satisfy the boundary conditions,

$$\omega_{1,1} = \omega_{1,2} = \omega_{1,3} = \omega_{2,1} = \omega_{3,1} = \omega_{2,3} = \omega_{3,2} = \omega_{3,3} = 0$$

leaving the pp-approximation to be
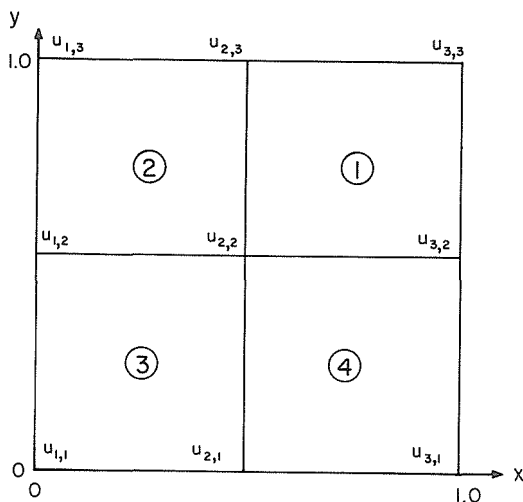
$$u(x, y) = u(x_2, y_2) \omega_{2,2} = u_2 \omega_2$$

FIGURE 5.8 Grid for Example 4. (i) = element *i.*

Therefore, upon substituting $u(x, y)$ for $w(x, y)$, the weak form of the PDE becomes

$$\iint_R \left(u_2 \frac{\partial \omega_2}{\partial x} \frac{\partial \omega_2}{\partial x} + u_2 \frac{\partial \omega_2}{\partial y} \frac{\partial \omega_2}{\partial y} \right) dx \, dy = \iint_R \omega_2 \, dx \, dy$$

or

$$A_{22} u_2 = g_2$$

where

$$A_{22} = \iint_R \left(\frac{\partial \omega_2}{\partial x} \frac{\partial \omega_2}{\partial x} + \frac{\partial \omega_2}{\partial y} \frac{\partial \omega_2}{\partial y} \right) dx \, dy$$

$$g_2 = \iint_R \omega_2 \, dx \, dy$$

This equation can be solved on a single element e_i as

$$A_{22}^{e_i} u_2 = g_2^{e_i}, \qquad e_i = 1, \ldots, 4$$

and then summed over all the elements to give

$$A_{22} u_2 = \sum_{e_i=1}^{4} A_{22}^{e_i} u_2 = \sum_{e_i=1}^{4} g_2^{e_i} = g_2$$

In element 1:

$$u(x, y) = \frac{u_2}{h^2} (1 - x)(1 - y), \qquad 0.5 \leqslant x \leqslant 1, \quad 0.5 \leqslant y \leqslant 1$$

and

$$\omega_2 = \frac{1}{h^2} (1 - x)(1 - y)$$

Thus

$$A_{22}^1 = \frac{1}{h^4} \int_{0.5}^{1} \int_{0.5}^{1} [(1 - y)^2 + (1 - x)^2] \, dx \, dy = \frac{2}{3} \qquad (h = 0.5)$$

and

$$g_2^1 = \frac{1}{h^2} \int_{0.5}^{1} \int_{0.5}^{1} (1 - x)(1 - y) \, dx \, dy = \frac{h^2}{4}$$

For element 2:

$$u(x, y) = \frac{u_2}{h^2} (1 - y)x, \qquad 0 \leqslant x \leqslant 0.5, \quad 0.5 \leqslant y \leqslant 1.0$$

and

$$\omega_2 = \frac{1}{h^2} x(1 - y)$$

giving

$$A_{22}^2 = \tfrac{2}{3}$$

and

$$g_2^2 = \frac{h^2}{4}$$

The results for each element are

Element	$A_{22}^{e_i}$	$g_2^{e_i}$
1	$\tfrac{2}{3}$	$\dfrac{h^2}{4}$
2	$\tfrac{2}{3}$	$\dfrac{h^2}{4}$
3	$\tfrac{2}{3}$	$\dfrac{h^2}{4}$
4	$\tfrac{2}{3}$	$\dfrac{h^2}{4}$

Thus, the solution is given by the sum of these results and is

$$u_2 = \tfrac{3}{8} h^2 = 0.09375$$

In the previous example we saw how the weak form of the PDE could be solved element by element. When using the bilinear basis the expected error in the pp-approximation is

$$|u(x, y) - w(x, y)| = 0(\rho^2) \tag{5.54}$$

where ρ is given in (5.41). As with ODEs, to increase the order of accuracy, the order of the tensor product basis functions must be increased, for example, the tensor product basis using Hermite cubics given an error of $0(\rho^4)$. To illustrate the formulation of the Galerkin method using higher-order basis functions, let the pp-approximation be given by (5.50) and reconsider (5.30) as the elliptic PDE. Equation (5.39) becomes

$$\left(\nabla \sum_{i=1}^{\text{DIMX}} \sum_{j=1}^{\text{DIMY}} \alpha_{i,j} B_i^x(x) B_j^y(y), \ \nabla B_m^x(x) B_n^y(y) \right) = \left(f, \ B_m^x(x) B_n^y(y) \right) \tag{5.55}$$

$$m = 1, \ldots, \text{DIMX}, \quad n = 1, \ldots, \text{DIMY}$$

In matrix notation (5.55) is

$$A\alpha = g \tag{5.56}$$

where

$$\alpha = [\tilde{\alpha}_1, \ldots, \tilde{\alpha}_{\text{DIMX}}]^T$$

$$\tilde{\alpha}_i = [\alpha_{i,1}, \ldots, \alpha_{i,\text{DIMY}}]^T$$

$$g = [\tilde{g}_1, \ldots, \tilde{g}_2]^T$$

$$\tilde{g}_i = [(f, B_i^x(x)B_1^y(y)), \ldots, (f, B_i^x(x)B_{\text{DIMY}}^y(y))]^T$$

$$A_{p,q} = (\nabla B_i^x(x)B_j^y(y), \nabla B_m^x(x)B_n^y(y))$$

$$p = \text{DIMY}(m - 1) + n \quad (1 \leq p \leq \text{DIMX} \times \text{DIMY})$$

$$q = \text{DIMY}(i - 1) + j \quad (1 \leq q \leq \text{DIMX} \times \text{DIMY})$$

Equation (5.56) can be solved element by element as

$$\sum_{e_i=1}^{\text{No. of elements}} A_{pq}^{e_i} \alpha_q = \sum_{e_i=1}^{\text{No. of elements}} g_p^{e_i} \tag{5.57}$$

The solution of (5.56) or (5.57) gives the vector α, which specifies the pp-approximation $u(x, y)$ with an error given by (5.51).

Another way of formulating the Galerkin solution to elliptic problems is that first proposed by Courant [9]. consider a general plane polygonal region R with boundary ∂R. When the region R is not a rectangular parallelepiped, a rectangular grid does not approximate R and especially ∂R as well as a triangular grid, i.e., covering the region R with a finite number of arbitrary triangles. This point is illustrated in Figure 5.9. Therefore, if the Galerkin method can be formulated with triangular elements, irregular regions can be handled through the use of triangulation. Courant developed the method for Dirichlet-type boundary conditions and used the space of continuous functions that are linear polynomials on each triangle. To illustrate this method consider (5.30) with the pp-approximation (5.32). If there are TN vertices not on ∂R in the triangulation, then (5.32) becomes

$$u(x, y) = \sum_{s=1}^{TN} \alpha_s \phi_s(x, y) \tag{5.58}$$

Given a specific vertex $s = \ell$, $\alpha_\ell = u(x_\ell, y_\ell)$ with an associated basis function $\phi_\ell(x, y)$. Figure 5.10a shows the vertex (x_ℓ, y_ℓ) and the triangular elements that contain it, while Figure 5.10b illustrates the associated basis function. The weak form of (5.30) is

$$\iint_R \left(\frac{\partial u}{\partial x}\frac{\partial \phi_s}{\partial x} + \frac{\partial u}{\partial y}\frac{\partial \phi_s}{\partial y} \right) dx\, dy = \iint_R f(x, y)\phi_s\, dx\, dy$$

$$s = 1, \ldots, TN \tag{5.59}$$

(a)   (b)
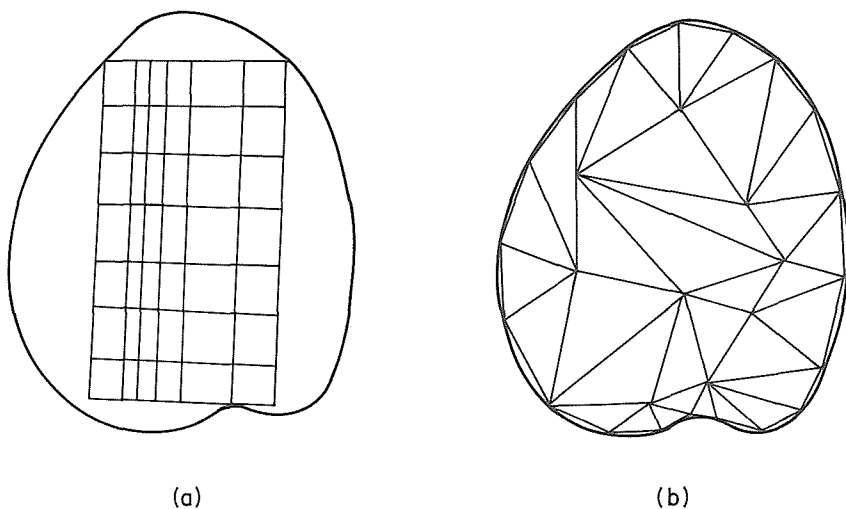
FIGURE 5.9   Grids on a polygonal region. (*a*) Rectangular grid. (*b*) Triangular grid.

or in matrix notation

$$A\alpha = g \tag{5.60}$$

where

$$A_{sq} = \iint\limits_{R} \left[\frac{\partial\phi_s}{\partial x} \frac{\partial\phi_q}{\partial x} + \frac{\partial\phi_s}{\partial y} \frac{\partial\phi_q}{\partial y} \right] dx\, dy$$

$$\alpha = [\alpha_1, \dots, \alpha_{TN}]^T$$

$$g = \left[\iint\limits_{R} f(x, y)\phi_1\, dx\, dy, \dots, \iint\limits_{R} f(x, y)\phi_{TN}\, dx\, dy \right]^T$$

(a)   (b)
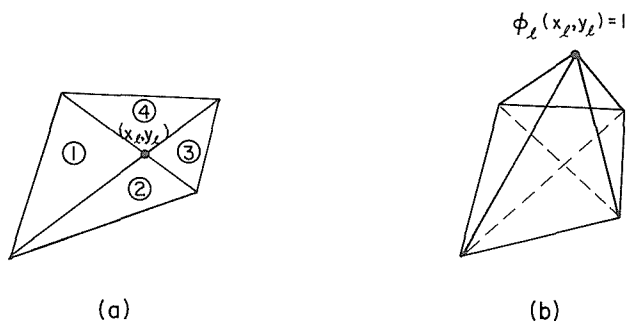
FIGURE 5.10   Linear basis function for triangular elements. (*a*) Vertex (x_ℓ, y_ℓ). (*b*) Basis function ϕ_ℓ.

Equation (5.60) can be solved element by element (triangle by triangle) and summed to give

$$\sum_{e_i} A^{e_i}_{sq} \alpha_q = \sum_{e_i} g^{e_i}_s$$

$$s = 1, \ldots, TN, \quad q = 1, \ldots, TN \tag{5.61}$$

Since the PDE can be solved element by element, we need only discuss the formulation of the basis functions on a single triangle. To illustrate this formulation, first consider a general triangle with vertices (x_i, y_i), $i = 1, 2, 3$. A linear interpolation $P_1(x, y)$ of a function $C(x, y)$ over the triangle is given by [10]:

$$P_1(x, y) = \sum_{i=1}^{3} a_i(x, y) C(x_i, y_i) \tag{5.62}$$

where

$$a_1(x, y) = \psi(\tau_{23} + \eta_{23}x - \xi_{23}y)$$

$$a_2(x, y) = \psi(\tau_{31} + \eta_{31}x - \xi_{31}y)$$

$$a_3(x, y) = \psi(\tau_{12} + \eta_{12}x - \xi_{12}y)$$

$$\psi = (\text{twice the area of the triangle})^{-1}$$

$$\tau_{ij} = x_i y_j - x_j y_i$$

$$\xi_{ij} = x_i - x_j$$

$$\eta_{ij} = y_i - y_j$$

To construct the basis function ϕ_ℓ associated with the vertex (x_ℓ, y_ℓ) on a single triangle set $(x_\ell, y_\ell) = (x_1, y_1)$ in (5.62). Also, since $\phi_\ell(x_\ell, y_\ell) = 1$ and ϕ_ℓ is zero at all other vertices set $C(x_1, y_1) = 1$, $C(x_2, y_2) = 0$ and $C(x_3, y_3) = 0$ in (5.62). With these substitutions, $\phi_\ell = P_1(x, y) = a_1(x, y)$. We illustrate this procedure in the following example.

EXAMPLE 5

Solve the problem given in Example 3 with the triangulation shown in Figure 5.11.

SOLUTION

From the boundary conditions

$$u_{1,1} = u_{2,1} = u_{3,1} = u_{3,2} = u_{3,3} = u_{2,3} = u_{1,3} = u_{1,2} = 0$$
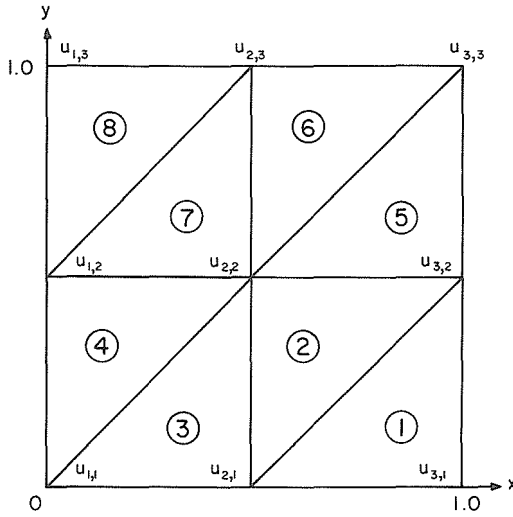
FIGURE 5.11 Triangulation for Example 5. ⓘ = element *i*

Therefore, the only nonzero vertex is $u_{2,2}$, which is common to elements 2, 3, 4, 5, 6, and 7, and the pp-approximation is given by

$$u(x, y) = u_{2,2}\phi_2(x, y) = u_2\phi_2$$

Equation (5.61) becomes

$$\sum_{e_i=2}^{7} A_{22}^{e_i} u_2 = \sum_{e_i=2}^{7} g_2^{e_i}$$

where

$$A_{22}^{e_i} = \iint\limits_{\substack{\text{Triangle} \\ e_i}} \left(\frac{\partial\phi_2}{\partial x}\frac{\partial\phi_2}{\partial x} + \frac{\partial\phi_2}{\partial y}\frac{\partial\phi_2}{\partial y} \right) dx\,dy$$

$$g_2^{e_i} = \iint\limits_{\substack{\text{Triangle} \\ e_i}} \phi_2 \, dx\,dy$$

The basis function $\phi_2^{e_i}$ can be constructed using (5.62) with $(x_1, y_1) = (0.5, 0.5)$ giving

$$\phi_2^{e_i} = \psi(\tau_{23}^{e_i} + \eta_{23}^{e_i}x - \xi_{23}^{e_i}y)$$

Thus,

$$\frac{\partial\phi_2^{e_i}}{\partial x} = \psi\eta_{23}^{e_i}$$

$$\frac{\partial\phi_2^{e_i}}{\partial y} = -\psi\xi_{23}^{e_i}$$

$$A_{22}^{e_i} = \iint\limits_{e_i} \psi^2[(\eta_{23}^{e_i})^2 + (\xi_{23}^{e_i})^2] \, dx\,dy$$

and

$$g_2^{e_i} = \iint\limits_{e_i} \psi(\tau_{23}^{e_i} + \eta_{23}^{e_i}x - \xi_{23}^{e_i}y) \, dx \, dy$$

For element 2 we have the vertices

$$(x_1, y_1) = (0.5, 0.5)$$
$$(x_2, y_2) = (1, 0.5)$$
$$(x_3, y_3) = (0.5, 0)$$

and

$$\psi = \frac{1}{0.25}$$

$$\tau_{23} = (1)(0) - (0.5)(0.5) = -0.25$$

$$\xi_{23} = 1 - 0.5 = 0.5$$

$$\eta_{23} = 0.5$$

$$A_{22}^2 = \iint (0.25)^{-2}[(0.5)^2 + (0.5)^2] \, dx \, dy = 1$$

$$g_2^2 = \iint \frac{1}{(0.25)}[-0.25 + 0.5x - 0.5y] \, dx \, dy = \frac{0.25}{6}$$

Likewise, the results for other elements are

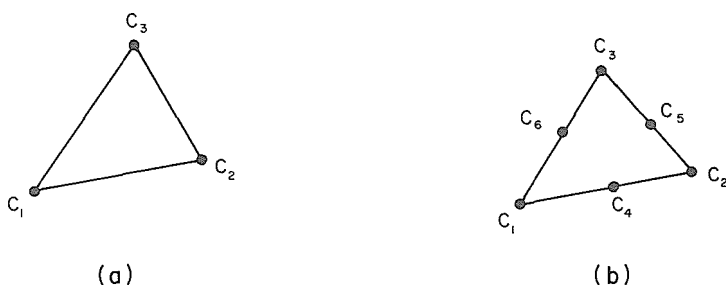| Element	$A_{22}^{e_i}$	$g_2^{e_i}$
2	1.0	$\frac{0.25}{6}$
3	0.5	$\frac{0.25}{6}$
4	0.5	$\frac{0.25}{6}$
5	0.5	$\frac{0.25}{6}$
6	0.5	$\frac{0.25}{6}$
7	1.0	$\frac{0.25}{6}$
Total	4.0	0.25

which gives

$$u_2 = 0.0625$$

FIGURE 5.12 Node positions for triangular elements. (*a*) Linear basis. (*b*) Quadratic basis: $C_i = C(x_i, y_i)$.

The expected error in the pp-approximation using triangular elements with linear basis functions is $0(h^2)$ [11], where h denotes the length of the largest side of any triangle. As with rectangular elements, to obtain higher-order accuracy, higher-order basis functions must be used. If quadratic functions are used to interpolate a function, $C(x, y)$, over a triangular element, then the interpolation is given by [10]:

$$P_2(x, y) = \sum_{i=1}^{6} b_i(x, y) C(x, y) \tag{5.63}$$

where

$$b_j(x, y) = a_j(x, y)[2a_j(x, y) - 1], \qquad j = 1, 2, 3$$

$$b_4(x, y) = 4a_1(x, y)a_2(x, y)$$

$$b_5(x, y) = 4a_1(x, y)a_3(x, y)$$

$$b_6(x, y) = 4a_2(x, y)a_3(x, y)$$

and the $a_i(x, y)$'s are given in (5.62). Notice that the linear interpolation (5.62) requires three values of $C(x, y)$ while the quadratic interpolation (5.63) requires six. The positions of these values for the appropriate interpolations are shown in Figure 5.12. Interpolations of higher order have also been derived, and good presentations of these bases are given in [10] and [12].

Now, consider the problem of constructing a set of basis functions for an irregular region with a curved boundary. The simplest way to approximate the curved boundary is to construct the triangulation such that the boundary is approximated by the straight-line segements of the triangles adjacent to the boundary. This approximation is illustrated in Figure 5.9*b*. An alternative procedure is to allow the triangles adjacent to the boundary to have a curved side that is part of the boundary. A transformation of the coordinate system can then restore the elements to the standard triangular shape, and the PDE solved as previously outlined. If the same order polynomial is chosen for the coordinate change as for the basis functions, then this method of incorporating the curved

boundary is called the isoparametric method [10–12]. To outline the procedure, consider a triangle with one curved edge that arises at a boundary as shown in Figure 5.13*a*. The simplest polynomial able to describe the curved side of the triangular element is a quadratic. Therefore, specify the basis functions for the triangle in the λ_1-λ_2 plane to be quadratics. These basis functions are completely specified by their values at the six nodes shown in Figure 5.13*b*. Thus the isoparametric method maps the six nodes in the *x-y* plane onto the λ_1-λ_2 plane. The PDE is solved in this coordinate system, giving $u(\lambda_1, \lambda_2)$, which can be transformed to $u(x, y)$.

PARABOLIC PDES IN TWO SPACE VARIABLES

In Chapter 4 we treated finite difference and finite element methods for solving parabolic PDEs that involved one space variable and time. Next, we extend the discussion to include two spatial dimensions.

Method of Lines

Consider the parabolic PDE

$$\frac{\partial w}{\partial t} = D\left[\frac{\partial^2 w}{\partial x^2} + \frac{\partial^2 w}{\partial y^2}\right]$$

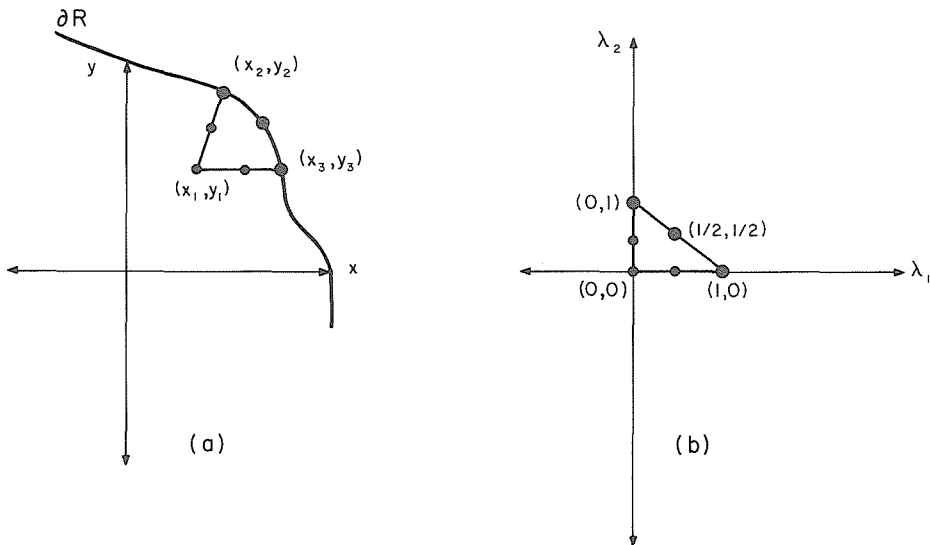$$0 \leqslant t, \qquad 0 \leqslant x \leqslant 1, \qquad 0 \leqslant y \leqslant 1 \qquad\qquad (5.64)$$

FIGURE 5.13   Coordinate transformation. (*a*) *xy*-plane. (*b*) $\lambda_1\lambda_2$-plane.

with D = constant. Discretize the spatial derivatives in (5.64) using finite differences to obtain the following system of ordinary differential equations:

$$\frac{\partial u_{i,j}}{\partial t} = \frac{D}{(\Delta x)^2}[u_{i+1,j} - 2u_{i,j} + u_{i-1,j}] + \frac{D}{(\Delta y)^2}[u_{i,j+1} - 2u_{i,j} + u_{i,j-1}] \qquad (5.65)$$

where

$$u_{i,j} \simeq w(x_i, y_j)$$

$$x_i = i\,\Delta x$$

$$y_j = j\,\Delta y$$

Equation (5.65) is the two-dimensional analog of (4.6) and can be solved in a similar manner. To complete the formulation requires knowledge of the subsidiary conditions. The parabolic PDE (5.64) requires boundary conditions at $x = 0$, $x = 1$, $y = 0$, and $y = 1$, and an initial condition at $t = 0$. As with the MOL in one spatial dimension, the two-dimensional problem incorporates the boundary conditions into the spatial discretizations while the initial condition is used to start the IVP.

Alternatively, (5.64) could be discretized using Galerkin's method or by collocation. For example, if (5.32) is used as the pp-approximation, then the collocation MOL discretization is

$$\sum_{j=1}^{m} \frac{\partial \alpha_j}{\partial t} \phi_j(x_i, y_i) = D \sum_{j=1}^{m} \alpha_j \left[\frac{\partial^2}{\partial x^2} \phi_j(x_i, y_i) + \frac{\partial^2}{\partial y^2} \phi_j(x_i, y_i) \right], \qquad (5.66)$$

$$i = 1, \ldots, m$$

where (x_i, y_i) designates the position of the ith collocation point. Since the MOL was discussed in detail in Chapter 4 and since the multidimensional analogs are straightforward extensions of the one-dimensional cases, no rigorous presentation of this technique will be given.

Alternating Direction Implicit Methods

Discretize (5.65) in time using Euler's method to give

$$u_{i,j}^n = \left[\frac{D\,\Delta t}{(\Delta x)^2} \right]\left[u_{i+1,j}^n + u_{i-1,j}^n \right] + \left[\frac{D\,\Delta t}{(\Delta y)^2} \right]\left[u_{i,j+1}^n + u_{i,j-1}^n \right]$$

$$+ u_{i,j}^n \left[1 - \frac{2D\,\Delta t}{(\Delta x)^2} - \frac{2D\,\Delta t}{(\Delta y)^2} \right] \qquad (5.67)$$

where

$$u_{i,j}^n \simeq w(x_i, y_j, t_n)$$

$$t_n = n\,\Delta t$$

For stability

$$D \, \Delta t \left[\frac{1}{(\Delta x)^2} + \frac{1}{(\Delta y)^2} \right] < \frac{1}{2} \tag{5.68}$$

If $\Delta x = \Delta y$, then (5.68) becomes

$$\frac{D \, \Delta t}{(\Delta x)^2} \leq \frac{1}{4} \tag{5.69}$$

which says that the restriction on the time step-size is half as large as the one-dimensional analog. Thus the stable time step-size decreases with increasing dimensionality. Because of the poor stability properties common to explicit difference methods, they are rarely used to solve multidimensional problems. Inplicit methods with their superior stability properties could be used instead of explicit formulas, but the resulting matrix problems are not easily solved. Another approach to the solution of multidimensional problems is to use alternating direction implicit (ADI) methods, which are two-step methods involving the solution of tridiagonal sets of equations (using finite difference discretizations) along lines parallel to the x-y axes at the first-second steps, respectively.

Consider (5.64) with $D = 1$ where the region to be examined in (x, y, t) space is covered by a rectilinear grid with sides parallel to the axes, and $h = \Delta x = \Delta y$. The grid points (x_i, y_j, t_n) given by $x = ih$, $y = jh$, and $t = n \, \Delta t$, and $u_{i,j}^n$ is the function satisfying the finite difference equation at the grid points. Define

$$\delta_x u_{i,j}^n = u_{i+1/2,j}^n - u_{i-1/2,j}^n$$

$$\delta_y u_{i,j}^n = u_{i,j+1/2}^n - u_{i,j-1/2}^n$$

$$\tau = \frac{\Delta t}{h^2} \tag{5.70}$$

Essentially, the principle is to employ two difference equations that are used in turn over successive time-steps of $\Delta t/2$. The first equation is implicit in the x-direction, while the second is implicit in the y-direction. Thus, if $\bar{u}_{i,j}$ is an intermediate value at the end of the first time-step, then

$$\bar{u}_{i,j} - u_{i,j}^n = \frac{\tau}{2} [\delta_x^2 \bar{u}_{i,j} + \delta_y^2 u_{i,j}^n]$$

$$u_{i,j}^{n+1} - \bar{u}_{i,j} = \frac{\tau}{2} [\delta_x^2 \bar{u}_{i,j} + \delta_y^2 u_{i,j}^{n+1}] \tag{5.71}$$

or

$$[1 - \tfrac{1}{2} \tau \delta_x^2] \bar{\mathbf{u}} = [1 + \tfrac{1}{2} \tau \delta_y^2] \mathbf{u}^n$$

$$[1 - \tfrac{1}{2} \tau \delta_y^2] \mathbf{u}^{n+1} = [1 + \tfrac{1}{2} \tau \delta_x^2] \bar{\mathbf{u}} \tag{5.72}$$

where

$$\mathbf{u}^n = u_{i,j}^n, \qquad \text{for all } i \text{ and } j$$

These formulas were first introduced by Peaceman and Rachford [13], and produce an approximate solution which has an associated error of $0(\Delta t^2 + h^2)$. A higher-accuracy split formula is due to Fairweather and Mitchell [14] and is

$$[1 - \tfrac{1}{2}(\tau - \tfrac{1}{6}) \delta_x^2]\tilde{u} = [1 + \tfrac{1}{2}(\tau + \tfrac{1}{6}) \delta_y^2]\mathbf{u}^n$$

$$[1 - \tfrac{1}{2}(\tau - \tfrac{1}{6}) \delta_y^2]\mathbf{u}^{n+1} = [1 + \tfrac{1}{2}(\tau + \tfrac{1}{6}) \delta_x^2]\tilde{u} \qquad (5.73)$$

with an error of $0(\Delta t^2 + h^4)$. Both of these methods are unconditionally stable. A general discussion of ADI methods is given by Douglas and Gunn [15].

The intermediate value $\tilde{u}$ introduced in each ADI method is not necessarily an approximation to the solution at any time level. As a result, the boundary values at the intermediate level must be chosen with care. If

$$w(x, y, t) = g(x, y, t) \qquad (5.74)$$

when (x, y, t) is on the bounadry of the region for which (5.64) is specified, then for (5.72)

$$\tilde{u}_{i,j} = \tfrac{1}{2}(1 - \tfrac{1}{2} \tau\delta_y^2)g_{i,j}^{n+1} + \tfrac{1}{2}(1 + \tfrac{1}{2} \tau\delta_y^2) g_{i,j}^n \qquad (5.75)$$

and for (5.73)

$$\tilde{u}_{i,j} = \frac{\tau - \tfrac{1}{6}}{2\tau} [1 - \tfrac{1}{2}(\tau - \tfrac{1}{6}) \delta_y^2]g_{i,j}^{n+1} + \frac{\tau + \tfrac{1}{6}}{2\tau} [1 + \tfrac{1}{2}(\tau + \tfrac{1}{6}) \delta_y^2]g_{i,j}^n \qquad (5.76)$$

If g is not dependent on time, then

$$\tilde{u}_{i,j} = g_{i,j} \qquad \text{(for 5.72)} \qquad (5.77)$$

$$\tilde{u}_{i,j} = (1 + \tfrac{1}{6} \delta_y^2)g_{i,j} \qquad \text{(for 5.73)} \qquad (5.78)$$

A more detailed investigation of intermediate boundary values in ADI methods is given in Fairweather and Mitchell [16].

ADI methods have also been developed for finite element methods. Douglas and Dupont [17] formulated ADI methods for parabolic problems using Galerkin methods, as did Dendy and Fairweather [18]. The discussion of these methods is beyond the scope of this text, and the interested reader is referred to Chapter 6 of [11].

MATHEMATICAL SOFTWARE

As with software for the solution of parabolic PDEs in one space variable and time, the software for solving multidimensional parabolic PDEs uses the method of lines. Thus a computer algorithm for multidimensional parabolic PDEs based

upon the MOL must include a spatial discretization routine and a time integrator. The principal obstacle in the development of multidimensional PDE software is the solution of large, sparse matrices. This same problem exists for the development of elliptic PDE software.

Parabolics

The method of lines is used exclusively in these codes. Table 5.1 lists the parabolic PDE software and outlines the type of spatial discretization and time integration for each code. None of the major libraries—NAG, Harwell, and IMSL—contain multidimensional parabolic PDE software, although 2DEPEP is an IMSL product distributed separately from their main library. As with one-dimensional PDE software, the overwhelming choice of the time integrator for multidimensional parabolic PDE software is the Gear algorithm. Next, we illustrate the use of two codes.

Consider the problem of Newtonian fluid flow in a rectangular duct. Initially, the fluid is at rest, and at time equal to zero, a pressure gradient is imposed upon the fluid that causes it to flow. The momentum balance, assuming a constant density and viscosity, is

$$\rho \, \frac{\partial V}{\partial t} = \frac{P_0 - P_L}{L} + \mu \left[\frac{\partial^2 V}{\partial x^2} + \frac{\partial^2 V}{\partial y^2} \right] \qquad (5.79)$$

TABLE 5.1 Parabolic PDE Codes

Code	Spatial Discretization	Time Integrator	Spatial Dimension	Region	Reference
DSS/2	Finite difference	Options including Runge-Kutta and GEARB [24]	2 or 3	Rectangular	[19]
PDETWO	Finite difference	GEARB [24]	2	Rectangular	[20]
FORSIM VI	Finite difference	Options including Runge-Kutta and GEAR [25]	2 or 3	Rectangular	[21]
DISPL	Finite element; Galerkin with tensor products of B-splines for the basis function	Modified version of GEAR [25]	2	Rectangular	[22]
2DEPEP	Finite element; Galerkin with quadratic basis functions on triangular elements; curved boundaries incorporated by isoparametric method	Crank-Nicolson or an implicit method	2	Irregular	[23]

where

$$\rho = \text{fluid density}$$

$$\frac{P_0 - P_L}{L} = \text{pressure gradient}$$

$$\mu = \text{fluid viscosity}$$

$$V = \text{axial fluid velocity}$$

The situation is pictured in Figure 5.14. Let

$$X = \frac{x}{B}$$

$$Y = \frac{y}{W}$$

$$\eta = \frac{V}{(P_0 - P_L)B^2/(2\mu L)}$$

$$\tau = \frac{\mu t}{\rho B^2} \tag{5.80}$$

Substitution of (5.80) into (5.79) gives

$$\frac{\partial \eta}{\partial \tau} = 2 + \frac{\partial^2 \eta}{\partial^2 X} + \left(\frac{B}{W}\right)^2 \frac{\partial^2 \eta}{\partial^2 Y} \tag{5.81}$$

The subsidiary conditions for (5.81) are

$$\eta = 0 \quad \text{at} \quad \tau = 0 \qquad \text{(fluid initially at rest)}$$

$$\eta = 0 \quad \text{at} \quad Y = 0 \qquad \text{(no slip at the wall)}$$

$$\eta = 0 \quad \text{at} \quad X = 1 \qquad \text{(no slip at the wall)}$$

$$\frac{\partial \eta}{\partial X} = 0 \quad \text{at} \quad X = 0 \qquad \text{(symmetry)}$$

$$\frac{\partial \eta}{\partial Y} = 0 \quad \text{at} \quad Y = 1 \qquad \text{(symmetry)}$$

Equation (5.81) was solved using DISPL (finite element discretization) and PDETWO (finite difference discretization). First let us discuss the numerical results form these codes. Table 5.2 shows the affect of the mesh spacing ($\Delta Y = \Delta X = h$) when solving (5.81) with PDETWO. Since the spatial discretization is accomplished using finite differences, the error associated with this
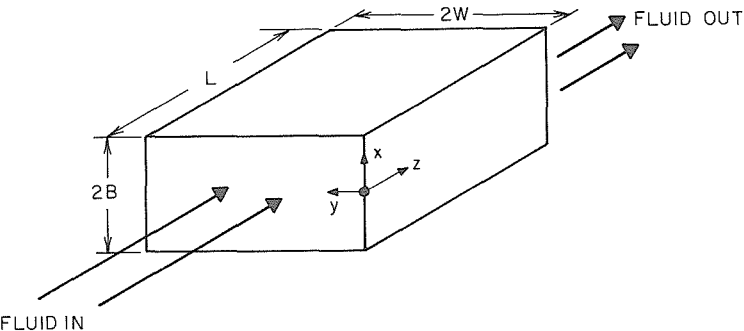
FIGURE 5.14   Flow in a rectangular duct.

discretization is $O(h^2)$. As h is decreased, the values of η shown in Table 5.2 increase slightly. For mesh spacings less than 0.05, the same results were obtained as those shown for $h = 0.05$. Notice that the tolerance on the time integration is 10^{-7}, so the error is dominated by the spatial discretization. When solving (5.81) with DISPL (cubic basis functions), a mesh spacing of $h = 0.25$ produced the same solution as that shown in Table 5.2 ($h = 0.05$). This is an expected result since the finite element discretization is $O(h^4)$.

Figure 5.15 shows the results of (5.81) for various X, Y, and τ. In Figure 5.15a the affect at the Y-position upon the velocity profile in the X-direction is illustrated. Since $Y = 0$ is a wall where no slip occurs, the magnitude of the velocity at a given X-position will increase as one moves away from the wall. Figure 5.15b shows the transient behavior of the velocity profile at $Y = 1.0$. As one would expect, the velocity increases for $0 \leqslant X < 1$ as τ increases. This trend would continue until steady state is reached. An interesting question can now be asked. That is, how large must the magnitude of W be in comparison to the magnitude of B to consider the duct as two infinite parallel plates. If the duct in Figure 5.14 represents two infinite parallel plates at $X = \pm 1$, then the

TABLE 5.2   Results of (5.81) Using PDETWO: $\tau = 0.5$, $\dfrac{B}{W} = 1$, $Y = 1$, TOL $= 10^{-7}$

	η		
X	$h = 0.2$	$h = 0.1$	$h = 0.05$
0.0	0.5284	0.5323	0.5333
0.2	0.5112	0.5149	0.5159
0.4	0.4575	0.4608	0.4617
0.6	0.3614	0.3640	0.3646
0.8	0.2132	0.2146	0.2150
1.0	0	0	0
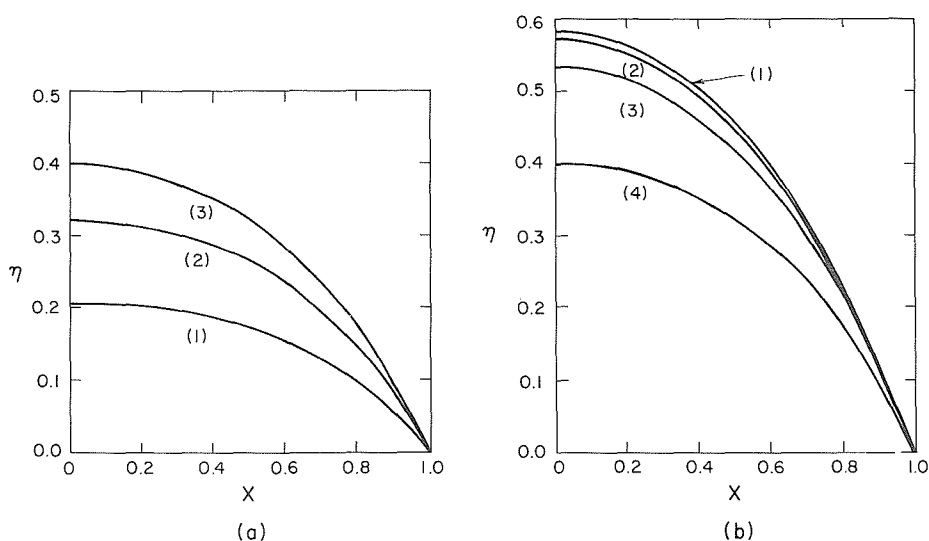
FIGURE 5.15   Results of (5.81).
(a) $\tau = 0.25$, $B/W = 1$. (b) $Y = 1.0$, $B/W = 1$.

Y	**τ**
(1) 0.25	(1) 1.00
(2) 0.5	(2) 0.75
(3) 1.0	(3) 0.50
	(4) 0.25

momentum balance becomes

$$\frac{\partial \eta}{\partial \tau} = 2 + \frac{\partial^2 \eta}{\partial X^2} \tag{5.82}$$

with

$$\eta = 0 \quad \text{at} \quad \tau = 0$$

$$\eta = 0 \quad \text{at} \quad X = 1$$

$$\frac{\partial \eta}{\partial X} = 0 \quad \text{at} \quad X = 0$$

Equation (5.82) possesses an analytic solution that can be used in answering the posed question. Figure 5.16 shows the affect of the ratio B/W on the velocity profile at various τ. Notice that at low τ, a B/W ratio of $\frac{1}{2}$ approximates the analytical solution of (5.82). At larger τ this behavior is not observed. To match the analytical solution (five significant figures) at all τ, it was found that the value of B/W must be $\frac{1}{4}$ or less.
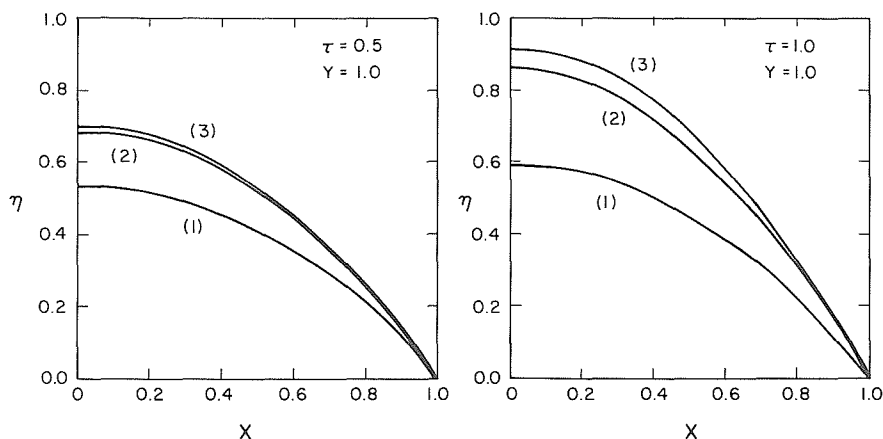
FIGURE 5.16   Further results of (5.81).

$$\underline{\text{B/W}}$$

(1) 1

(2) ½

(3) ¼ and analytical solution of (5.82)

Elliptics

Table 5.3 lists the elliptic PDE software and outlines several features of each code. Notice that the NAG library does contain elliptic PDE software, but this routine is not very robust. Besides the software shown in Table 5.3, DISPL and 2DEPEP contain options to solve elliptic PDEs. Next we consider a practical problem involving elliptic PDEs and illustrate the solution and physical implications through the use of DISPL.

The most common geometry of catalyst pellets is the finite cylinder with length to diameter, L/D, ratios from about 0.5 to 4, since they are produced by either pelleting or by extrusion. The governing transport equations for a finite cylindrical catalyst pellet in which a first-order chemical reaction is occurring are [34]:

$$\text{(Mass)} \qquad \frac{\partial^2 f}{\partial r^2} + \frac{1}{r}\frac{\partial f}{\partial r} + \left(\frac{D}{L}\right)^2 \frac{\partial^2 f}{\partial z^2} = \phi^2 f \exp\left[\frac{\gamma}{t}(t-1)\right]$$

$$\text{(Energy)} \qquad \frac{\partial^2 t}{\partial r^2} + \frac{1}{r}\frac{\partial t}{\partial r} \left(\frac{D}{L}\right)^2 \frac{\partial^2 t}{\partial z^2} = -\beta\phi^2 f \exp\left[\frac{\gamma}{t}(t-1)\right] \qquad \textbf{(5.83)}$$

where

$$r = \text{dimensionless radial coordinate, } 0 \leqslant r \leqslant 1$$
$$z = \text{dimensionless axial coordinate, } 0 \leqslant z \leqslant 1$$

f = dimensionless concentration
t = dimensionless temperature
γ = Arrhenius number (dimensionless)
ϕ = Thiele modulus (dimensionless)
β = Prater number (dimensionless)

with the boundary conditions

$$\frac{\partial f}{\partial r} = \frac{\partial t}{\partial r} = 0 \quad \text{at} \quad r = 0 \qquad \text{(symmetry)}$$

$$\frac{\partial f}{\partial z} = \frac{\partial t}{\partial z} = 0 \quad \text{at} \quad z = 0 \qquad \text{(symmetry)}$$

$f = t = 1$ at $z = 1$ and $r = 1$ (concentration and
                                         temperature specified at
                                         the surface of the pellet)

Using the Prater relationship [35], which is

$$t = 1 + (1 - f)\beta$$

TABLE 5.3 Elliptic PDE Codes

Code	Discretization	Region	Nonlinear Equations	Reference
NAG (D03 chapter)	Finite difference (Laplace's equation in two dimensions)	Rectangular	No	—
FISPACK	Finite difference	Rectangular	No	[26]
EPDE1	Finite difference	Irregular	No	[27]
ITPACK/REGION	Finite difference	Irregular	No	[28]
FFT9	Finite difference	Irregular	No	[29]
HLMHLZ/HEL-MIT/HELSIX/HELSYM	Finite difference	Irregular	No	[30]
PLTMG	Finite element; Galerkin with linear basis functions on triangular elements	Irregular	No	[31]
ELIPTI	ADI with finite differences; integrate to steady state	Irregular	Yes	[32]
ELLPACK	Finite difference; finite element (collocation and Galerkin)	Rectangular	Yes	[33]

TABLE 5.4   Results of (5.84) Using DISPL

$z = 0.25, \beta = 0.1, \gamma = 30, \dfrac{D}{L} = 1$

	$\phi = 1$		$\phi = 2$		
r	$h = 0.5$	$h = 0.25$	$h = 0.5$	$h = 0.25$	$h = 0.125$
0	0.728	0.728	0.724(−3)	0.240(−1)	0.227(−1)
0.25	0.745	0.745	0.384(−1)	0.377(−1)	0.365(−1)
0.50	0.797	0.797	0.109	0.115	0.115
0.75	0.882	0.882	0.414	0.404	0.404
1.0	1.000	1.000	1.000	1.000	1.000

reduces the system (5.83) to the single elliptic PDE:

$$\frac{\partial^2 f}{\partial r^2} + \frac{1}{r}\frac{\partial f}{\partial r} + \left(\frac{D}{L}\right)^2 \frac{\partial^2 f}{\partial z^2} = \phi^2 f \exp\left[\frac{\gamma\beta(1-f)}{1+\beta(1-f)}\right] \qquad (5.84)$$

$$\frac{\partial f}{\partial r} = 0 \quad \text{at} \quad r = 0$$

$$\frac{\partial f}{\partial z} = 0 \quad \text{at} \quad z = 0$$

$$f = 1 \quad \text{at} \quad r = 1 \text{ and } z = 1$$

DISPL (using cubic basis functions) produced the results given in Tables 5.4 and 5.5 and Figure 5.17. In Table 5.4 the affect of the mesh spacing ($h = \Delta r = \Delta z$) is shown. With $\phi = 1$ a coarse mesh spacing ($h = 0.5$) is sufficient to give three-significant-figure accuracy. At larger values of ϕ a finer mesh is required for a similar accuracy. As ϕ increases, the gradient in f becomes larger, especially near the surface of the pellet. This behavior is shown in Figure 5.17. Because of this gradient, a finer mesh is required to obtain an accurate solution over the entire region. Alternatively, one could refine the mesh in the region of the steep gradient. Finally, in Table 5.5 the isothermal results ($\beta = 0$) are compared with those published elsewhere [34]. As shown, DISPL produced accurate results with $h = 0.25$.

TABLE 5.5   Further Results of (5.84) Using DISPL

$\beta = 0.0, \gamma = 30, \phi = 3, \dfrac{L}{D} = 1$

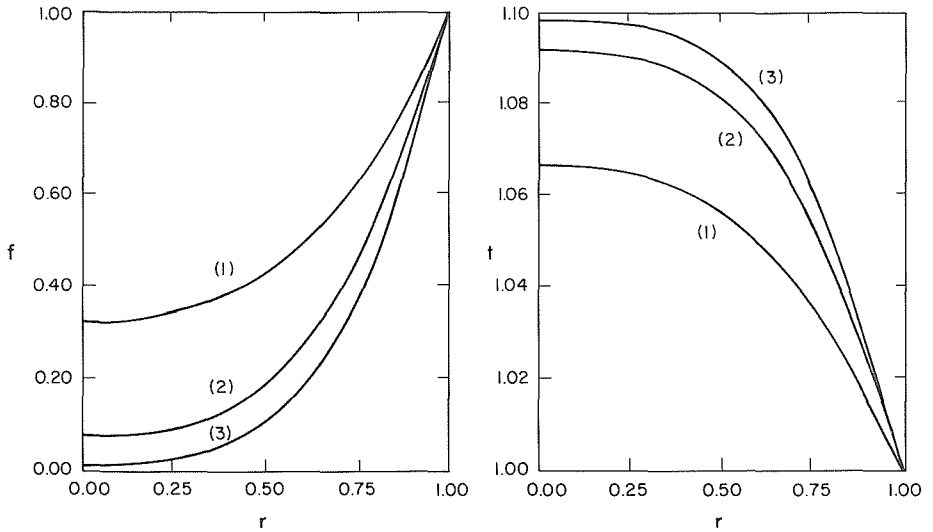| (r, z)	DISPL, $h = 0.25$	From Reference [34]
(0.394, 0.285)	0.337	0.337
(0.394, 0.765)	0.585	0.585
(0.803, 0.285)	0.648	0.648
(0.803, 0.765)	0.756	0.759

FIGURE 5.17 Results of (5.84): $\beta = 0.1$, $\gamma = 30$, $\phi = 2$, $D/L = 1$.

$$\underline{z}$$

(1) 0.75
(2) 0.50
(3) 0.00

PROBLEMS

1. Show that the finite difference discretization of

$$(x + 1)\frac{\partial^2 w}{\partial x^2} + (y^2 + 1)\frac{\partial^2 w}{\partial y^2} - w = 1$$

$$0 \leqslant x \leqslant 1, \qquad 0 \leqslant y \leqslant 1, \qquad \Delta x = \Delta y = \tfrac{1}{3}$$

with

$$w(0, y) = y$$
$$w(1, y) = y^2$$
$$w(x, 0) = 0$$
$$w(x, 1) = 1$$

is given by [36]:

$$\begin{bmatrix} 5 & -\frac{10}{9} & -\frac{4}{3} & 0 \\ -\frac{13}{9} & \frac{17}{3} & 0 & -\frac{4}{3} \\ -\frac{5}{3} & 0 & \frac{17}{3} & -\frac{10}{9} \\ 0 & -\frac{5}{3} & -\frac{13}{9} & \frac{19}{3} \end{bmatrix} \begin{bmatrix} u_{1,1} \\ u_{1,2} \\ u_{2,1} \\ u_{2,2} \end{bmatrix} = \begin{bmatrix} \frac{1}{3} \\ \frac{20}{9} \\ \frac{2}{27} \\ \frac{56}{27} \end{bmatrix}$$

2.* Consider a rectangular plate with an initial temperature distribution of

$$w(x, y, 0) = T - T_0 = 0, \qquad 0 \leqslant x \leqslant 2, \quad 0 \leqslant y \leqslant 1$$

If the edges $x = 2$, $y = 0$, and $y = 1$ are held at $T = T_0$ and on the edge $x = 0$ we impose the following temperature distribution:

$$w(0, y, t) = T - T_0 = \begin{cases} 2ty, & \text{for } 0 \leqslant y \leqslant \frac{1}{2} \\ 2t(1 - y), & \text{for } \frac{1}{2} \leqslant y \leqslant 1 \end{cases}$$

solve the heat conduction equation

$$\frac{\partial w}{\partial t} = \frac{\partial^2 w}{\partial x^2} + \frac{\partial^2 w}{\partial y^2}$$

for the temperature distribution in the plate. The analytical solution to this problem is [22]:

$$w = \frac{4}{\pi} \sum_{m=1}^{\infty} \sum_{n=1}^{\infty} \frac{m}{n^2} \frac{1}{\sigma^2} (e^{-\sigma t} + \sigma t - 1) \sin \left(\frac{n\pi}{2} \right) \sin \left(\frac{m\pi x}{2} \right) \sin (n\pi y)$$

where

$$\sigma = \pi^2 \left(\frac{m^2}{4} + n^2 \right)$$

Calculate the error in the numerical solution at the mesh points.

3.* An axially dispersed isothermal chemical reactor can be described by the following material balance equation:

$$\frac{\partial f}{\partial z} = \frac{1}{\text{Pe}_r} \left[\frac{\partial^2 f}{\partial r^2} + \frac{1}{r} \frac{\partial f}{\partial r} \right] + \frac{1}{\text{Pe}_a} \frac{\partial^2 f}{\partial z^2} + D_a f, \qquad 0 \leqslant r \leqslant 1, \quad 0 \leqslant z \leqslant 1$$

with

$$1 - f = \frac{1}{\text{Pe}_a} \frac{\partial f}{\partial z} \quad \text{at} \quad z = 0, \qquad \frac{\partial f}{\partial r} = 0 \quad \text{at} \quad r = 0 \text{ and } r = 1$$

$$\frac{\partial f}{\partial z} = 0 \quad \text{a.} \quad z = 1$$

where

f = dimensionless concentration

r = dimensionless radial coordinate

z = dimensionless axial coordinate

Pe_r = radial Peclet number

Pe_a = axial Peclet number

D_a = Damkohler number (first-order reaction rate)

The boundary conditions in the axial direction arise from continuity of flux as discussed in Chapter 1 of [34]. Let $D_a = 0.5$ and $Pe_r = 10$. Solve the material balance equation using various values of Pe_a. Compare your results to plug flow ($Pe_a \to \infty$) and discuss the effects of axial dispersion.

4.*   Solve Eq. (5.84) with $D/L = 1$, $\phi = 1$, $\gamma = 30$, and let $-0.2 \leq \beta \leq 0.2$. Comment on the affect of varying β [$\beta < 0$ (endothermic), $\beta > 0$ (exothermic)].

5.*   Consider transient flow in a rectangular duct, which can be described by:

$$\frac{\partial \eta}{\partial \tau} = \bar{\alpha} + \frac{\partial^2 \eta}{\partial X^2} + \left(\frac{B}{W}\right)^2 \frac{\partial^2 \eta}{\partial Y^2}$$

using the same notation as with Eq. (5.81) where $\bar{\alpha}$ is a constant. Solve the above equation with

	$\bar{\alpha}$	Comment
(a)	2	Eq. (5.81)
(b)	4	Twice the pressure gradient as Eq. (5.81)
(c)	1	Half the pressure gradient as Eq. (5.81)

How does the pressure gradient affect the time required to reach steady state?

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