PROBLEM SET 21.3

1–6 EULER FOR SYSTEMS AND SECOND-ORDER ODEs

Solve by the Euler's method. Graph the solution in the y_1y_2-plane. Calculate the errors.

1. $y_1' = 2y_1 - 4y_2$, $y_2' = y_1 - 3y_2$, $y_1(0) = 3$, $y_2(0) = 0$, $h = 0.1$, 10 steps
2. **Spiral.** $y_1' = -y_1 + y_2$, $y_2' = -y_1 - y_2$, $y_1(0) = 0$, $y_2(0) = 4$, $h = 0.2$, 5 steps
3. $y'' + \frac{1}{4}y = 0$, $y(0) = 1$, $y'(0) = 0$, $h = 0.2$, 5 steps
4. $y_1' = -3y_1 + y_2$, $y_2' = y_1 - 3y_2$, $y_1(0) = 2$, $y_2(0) = 0$, $h = 0.1$, 5 steps
5. $y'' - y = x$, $y(0) = 1$, $y'(0) = -2$, $h = 0.1$, 5 steps
6. $y_1' = y_1$, $y_2' = -y_2$, $y_1(0) = 2$, $y_2(0) = 2$, $h = 0.1$, 10 steps

7–10 RK FOR SYSTEMS

Solve by the classical RK.

7. The ODE in Prob. 5. By what factor did the error decrease?
8. The system in Prob. 2
9. The system in Prob. 1
10. The system in Prob. 4
11. **Pendulum equation** $y'' + \sin y = 0$, $y(\pi) = 0$, $y'(\pi) = 1$, as a system, $h = 0.2$, 20 steps. How does your result fit into Fig. 93 in Sec. 4.5?
12. **Bessel Function J_0.** $xy'' + y' + xy = 0$, $y(1) = 0.765198$, $y'(1) = -0.440051$, $h = 0.5$, 5 steps. (This gives the standard solution $J_0(x)$ in Fig. 110 in Sec. 5.4.)
13. Verify the formulas and calculations for the Airy equation in Example 2 of the text.
14. **RKN.** The classical RK for a first-order ODE extends to second-order ODEs (E. J. Nyström, *Acta fenn.* No 13, 1925). If the ODE is $y'' = f(x, y)$, not containing y', then

$$k_1 = \tfrac{1}{2}hf(x_n, y_n)$$

$$k_2 = \tfrac{1}{2}hf(x_n + \tfrac{1}{2}h, y_n + \tfrac{1}{2}h(y_n' + \tfrac{1}{2}k_1)) = k_3$$

$$k_4 = \tfrac{1}{2}hf(x_n + h, y_n + h(y_n' + k_2))$$

$$y_{n+1} = y_n + h(y_n' + \tfrac{1}{3}(k_1 + 2k_2))$$

$$y_{n+1}' = y_n' + \tfrac{1}{8}(k_1 + 4k_2 + k_4).$$

Apply this RKN (Runge–Kutta–Nyström) method to the Airy ODE in Example 2 with $h = 0.2$ as before, to obtain approximate values of $\mathrm{Ai}(x)$.

15. **CAS EXPERIMENT. Backward Euler and Stiffness.** Extend Example 3 as follows.

(a) Verify the values in Table 21.13 and show them graphically as in Fig. 452.

(b) Compute and graph Euler values for h near the "critical" $h = 0.18$ to determine more exactly when instability starts.

(c) Compute and graph RK values for values of h between 0.2 and 0.3 to find h for which the RK approximation begins to increase away from the exact solution.

(d) Compute and graph backward Euler values for large h; confirm stability and investigate the error increase for growing h.

21.4 Methods for Elliptic PDEs

We have arrived at the second half of this chapter, which is devoted to numerics for partial differential equations (PDEs). As we have seen in Chap.12, there are many applications to PDEs, such as in dynamics, elasticity, heat transfer, electromagnetic theory, quantum mechanics, and others. Selected because of their importance in applications, the PDEs covered here include the Laplace equation, the Poisson equation, the heat equation, and the wave equation. By covering these equations based on their importance in applications we also selected equations that are important for theoretical considerations. Indeed, these equations serve as models for elliptic, parabolic, and hyperbolic PDEs. For example, the Laplace equation is a representative example of an elliptic type of PDE, and so forth.

Recall, from Sec. 12.4, that a PDE is called **quasilinear** if it is linear in the highest derivatives. Hence a second-order quasilinear PDE in two independent variables x, y is of the form

$$au_{xx} + 2bu_{xy} + cu_{yy} = F(x, y, u, u_x, u_y). \tag{1}$$

u is an unknown function of x and y (a solution sought). F is a given function of the indicated variables.

Depending on the discriminant $ac - b^2$, the PDE (1) is said to be of

elliptic type	if	$ac - b^2 > 0$	(example: *Laplace equation*)
parabolic type	if	$ac - b^2 = 0$	(example: *heat equation*)
hyperbolic type	if	$ac - b^2 < 0$	(example: *wave equation*).

Here, in the heat and wave equations, y is time t. The *coefficients* a, b, c may be functions of x, y, so that the type of (1) may be different in different regions of the xy-plane. This classification is not merely a formal matter but is of great practical importance because the general behavior of solutions differs from type to type and so do the additional conditions (boundary and initial conditions) that must be taken into account.

Applications involving ***elliptic equations*** usually lead to boundary value problems in a region R, called a *first boundary value problem* or **Dirichlet problem** if u is prescribed on the boundary curve C of R, a *second boundary value problem* or **Neumann problem** if $u_n = \partial u/\partial n$ (normal derivative of u) is prescribed on C, and a *third* or **mixed problem** if u is prescribed on a part of C and u_n on the remaining part. C usually is a closed curve (or sometimes consists of two or more such curves).

Difference Equations for the Laplace and Poisson Equations

In this section we develop numeric methods for the two most important elliptic PDEs that appear in applications. The two PDEs are the **Laplace equation**

$$\nabla^2 u = u_{xx} + u_{yy} = 0 \tag{2}$$

and the **Poisson equation**

$$\nabla^2 u = u_{xx} + u_{yy} = f(x, y). \tag{3}$$

The starting point for developing our numeric methods is the idea that we can replace the partial derivatives of these PDEs by corresponding **difference quotients**. Details are as follows:

To develop this idea, we start with the Taylor formula and obtain

$$\begin{aligned} &\text{(a)} \quad u(x + h, y) = u(x, y) + hu_x(x, y) + \tfrac{1}{2}h^2u_{xx}(x, y) + \tfrac{1}{6}h^3u_{xxx}(x, y) + \cdots \\ &\text{(b)} \quad u(x - h, y) = u(x, y) - hu_x(x, y) + \tfrac{1}{2}h^2u_{xx}(x, y) - \tfrac{1}{6}h^3u_{xxx}(x, y) + \cdots. \end{aligned} \tag{4}$$

We subtract (4b) from (4a), neglect terms in $h^3, h^4, \cdots$, and solve for u_x. Then

$$u_x(x, y) \approx \frac{1}{2h}\left[u(x + h, y) - u(x - h, y)\right]. \tag{5a}$$

Similarly,

$$u(x, y + k) = u(x, y) + ku_y(x, y) + \tfrac{1}{2}k^2u_{yy}(x, y) + \cdots$$

and

$$u(x, y - k) = u(x, y) - ku_y(x, y) + \tfrac{1}{2}k^2u_{yy}(x, y) + \cdots.$$

By subtracting, neglecting terms in $k^3, k^4, \cdots$, and solving for u_y we obtain

$$u_y(x, y) \approx \frac{1}{2k}\left[u(x, y + k) - u(x, y - k)\right]. \tag{5b}$$

We now turn to second derivatives. Adding (4a) and (4b) and neglecting terms in $h^4, h^5, \cdots$, we obtain $u(x + h, y) + u(x - h, y) \approx 2u(x, y) + h^2u_{xx}(x, y)$. Solving for u_{xx} we have

$$u_{xx}(x, y) \approx \frac{1}{h^2}\left[u(x + h, y) - 2u(x, y) + u(x - h, y)\right]. \tag{6a}$$

Similarly,

$$u_{yy}(x, y) \approx \frac{1}{k^2}\left[u(x, y + k) - 2u(x, y) + u(x, y - k)\right]. \tag{6b}$$

We shall not need (see Prob. 1)

$$u_{xy}(x, y) \approx \frac{1}{4hk}\left[u(x + h, y + k) - u(x - h, y + k) - u(x + h, y - k) + u(x - h, y - k)\right]. \tag{6c}$$

Figure 453a shows the points $(x + h, y), (x - h, y), \cdots$ in (5) and (6).

We now substitute (6a) and (6b) into the ***Poisson equation*** (3), choosing $k = h$ to obtain a simple formula:

$$\textbf{(7)} \qquad u(x + h, y) + u(x, y + h) + u(x - h, y) + u(x, y - h) - 4u(x, y) = h^2f(x, y).$$

This is a **difference equation** corresponding to (3). Hence for the ***Laplace equation*** (2) the corresponding difference equation is

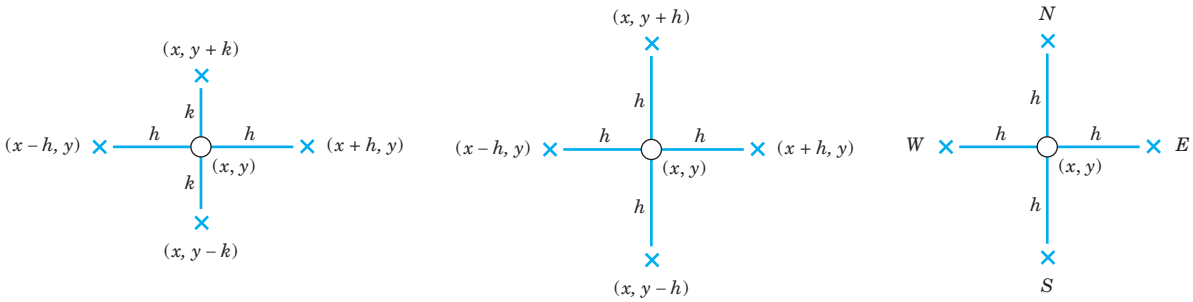
$$\textbf{(8)} \qquad u(x + h, y) + u(x, y + h) + u(x - h, y) + u(x, y - h) - 4u(x, y) = 0.$$

h is called the **mesh size**. Equation (8) relates u at (x, y) to u at the four neighboring points shown in Fig. 453b. It has a remarkable interpretation: u at (x, y) equals the mean of the

values of u at the four neighboring points. This is an analog of the mean value property of harmonic functions (Sec. 18.6).

Those neighbors are often called E (East), N (North), W (West), S (South). Then Fig. 453b becomes Fig. 453c and (7) is

$$\textbf{(7*)} \qquad u(E) + u(N) + u(W) + u(S) - 4u(x, y) = h^2 f(x, y).$$



(a) Points in (5) and (6) (b) Points in (7) and (8) (c) Notation in (7*)

Fig. 453. Points and notation in (5)–(8) and (7*)

Our approximation of $h^2\nabla^2 u$ in (7) and (8) is a 5-point approximation with the coefficient scheme or **stencil** (also called *pattern, molecule,* or *star*)

$$(9) \quad \begin{Bmatrix} & 1 & \\ 1 & -4 & 1 \\ & 1 & \end{Bmatrix}. \quad \text{We may now write (7) as} \quad \begin{Bmatrix} & 1 & \\ 1 & -4 & 1 \\ & 1 & \end{Bmatrix} u = h^2 f(x, y).$$

Dirichlet Problem

In numerics for the Dirichlet problem in a region R we choose an h and introduce a square grid of horizontal and vertical straight lines of distance h. Their intersections are called **mesh points** (or *lattice points* or *nodes*). See Fig. 454.

Then we approximate the given PDE by a difference equation [(8) for the Laplace equation], which relates the unknown values of u at the mesh points in R to each other and to the given boundary values (details in Example 1). This gives a linear system of *algebraic* equations. By solving it we get approximations of the unknown values of u at the mesh points in R.

We shall see that the number of equations equals the number of unknowns. Now comes an important point. If the number of internal mesh points, call it p, is small, say, $p < 100$, then a direct solution method may be applied to that linear system of $p < 100$ equations in p unknowns. However, if p is large, a storage problem will arise. Now since each unknown u is related to only 4 of its neighbors, the coefficient matrix of the system is a **sparse matrix**, that is, a matrix with relatively few nonzero entries (for instance, 500 of 10,000 when $p = 100$). Hence for large p we may avoid storage difficulties by using an iteration method, notably the Gauss–Seidel method (Sec. 20.3), which in PDEs is also

called **Liebmann's method** (note the strict diagonal dominance). Remember that in this method we have the storage convenience that we can overwrite any solution component (value of u) as soon as a "new" value is available.

Both cases, large p and small p, are of interest to the engineer, large p if a fine grid is used to achieve high accuracy, and small p if the boundary values are known only rather inaccurately, so that a coarse grid will do it because in this case it would be meaningless to try for great accuracy in the interior of the region R.

We illustrate this approach with an example, keeping the number of equations small, for simplicity. As convenient ***notations for mesh points and corresponding values of the solution*** (and of approximate solutions) we use (see also Fig. 454)

$$P_{ij} = (ih, jh), \qquad u_{ij} = u(ih, jh). \tag{10}$$

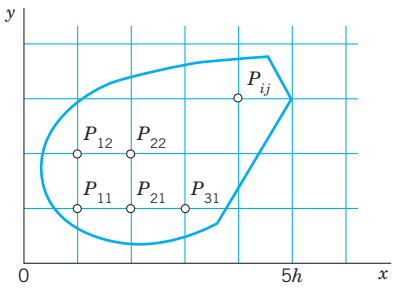


Fig. 454. Region in the xy-plane covered by a grid of mesh h, also showing mesh points $P_{11} = (h, h), \cdots, P_{ij} = (ih, jh), \cdots$

With this notation we can write (8) for any mesh point P_{ij} in the form

$$u_{i+1,j} + u_{i,j+1} + u_{i-1,j} + u_{i,j-1} - 4u_{ij} = 0. \tag{11}$$

Remark. Our current discussion and the example that follows illustrate what we may call the ***reuseability of mathematical ideas and methods***. Recall that we applied the Gauss–Seidel method to a system of ODEs in Sec. 20.3 and that we can now apply it again to elliptic PDEs. This shows that engineering mathematics has a structure and important mathematical ideas and methods will appear again and again in different situations. The student should find this attractive in that previous knowledge can be reapplied.

EXAMPLE 1 **Laplace Equation. Liebmann's Method**

The four sides of a square plate of side 12 cm, made of homogeneous material, are kept at constant temperature 0°C and 100°C as shown in Fig. 455a. Using a (very wide) grid of mesh 4 cm and applying Liebmann's method (that is, Gauss–Seidel iteration), find the (steady-state) temperature at the mesh points.

Solution. In the case of independence of time, the heat equation (see Sec. 10.8)

$$u_t = c^2(u_{xx} + u_{yy})$$

reduces to the Laplace equation. Hence our problem is a Dirichlet problem for the latter. We choose the grid shown in Fig. 455b and consider the mesh points in the order P_{11}, P_{21}, P_{12}, P_{22}. We use (11) and, in each equation, take to the right all the terms resulting from the given boundary values. Then we obtain the system

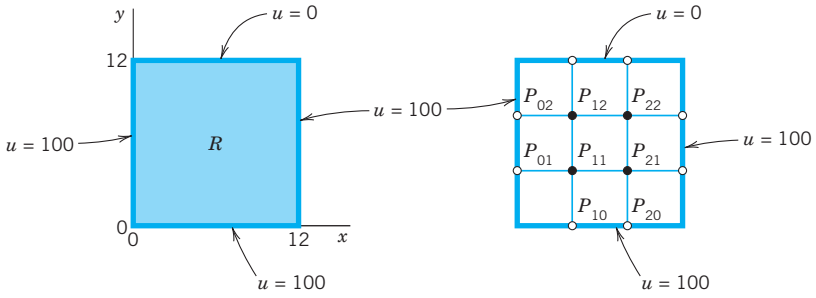
$$
(12)\qquad
\begin{aligned}
-4u_{11} + u_{21} + u_{12} &= -200\\
-u_{11} - 4u_{21} + u_{22} &= -200\\
u_{11} - 4u_{12} + u_{22} &= -100\\
u_{21} + u_{12} - 4u_{22} &= -100.
\end{aligned}
$$

In practice, one would solve such a small system by the Gauss elimination, finding $u_{11} = u_{21} = 87.5$, $u_{12} = u_{22} = 62.5$.

More exact values (exact to 3S) of the solution of the actual problem [as opposed to its model (12)] are 88.1 and 61.9, respectively. (These were obtained by using Fourier series.) Hence the error is about 1%, which is surprisingly accurate for a grid of such a large mesh size h. If the system of equations were large, one would solve it by an indirect method, such as Liebmann's method. For (12) this is as follows. We write (12) in the form (divide by -4 and take terms to the right)

$$
\begin{aligned}
u_{11} &= 0.25u_{21} + 0.25u_{12} + 50\\
u_{21} &= 0.25u_{11} + 0.25u_{22} + 50\\
u_{12} &= 0.25u_{11} + 0.25u_{22} + 25\\
u_{22} &= 0.25u_{21} + 0.25u_{12} + 25.
\end{aligned}
$$

These equations are now used for the Gauss–Seidel iteration. They are identical with (2) in Sec. 20.3, where $u_{11} = x_1$, $u_{21} = x_2$, $u_{12} = x_3$, $u_{22} = x_4$, and the iteration is explained there, with 100, 100, 100, 100 chosen as starting values. Some work can be saved by better starting values, usually by taking the average of the boundary values that enter into the linear system. The exact solution of the system is $u_{11} = u_{21} = 87.5$, $u_{12} = u_{22} = 62.5$, as you may verify.



(a) Given problem (b) Grid and mesh points

Fig. 455. Example 1

Remark. It is interesting to note that, if we choose mesh $h = L/n$ (L = side of R) and consider the $(n-1)^2$ internal mesh points (i.e., mesh points not on the boundary) row by row in the order

$$P_{11}, P_{21}, \cdots, P_{n-1,1}, P_{12}, P_{22}, \cdots, P_{n-2,2}, \cdots,$$

then the system of equations has the $(n-1)^2 \times (n-1)^2$ coefficient matrix

$$
(13)\qquad \mathbf{A} = \begin{bmatrix}
\mathbf{B} & \mathbf{I} & & & & & \\
\mathbf{I} & \mathbf{B} & \mathbf{I} & & & & \\
 & \cdot & \cdot & \cdot & & & \\
 & & \cdot & \cdot & \cdot & & \\
 & & & \mathbf{I} & \mathbf{B} & \mathbf{I} & \\
 & & & & \mathbf{I} & \mathbf{B} &
\end{bmatrix}.
\qquad \text{Here} \qquad
\mathbf{B} = \begin{bmatrix}
-4 & 1 & & & & & \\
1 & -4 & 1 & & & & \\
 & \cdot & \cdot & \cdot & & & \\
 & & \cdot & \cdot & \cdot & & \\
 & & & 1 & -4 & 1 & \\
 & & & & 1 & -4 &
\end{bmatrix}.
$$

is an $(n-1) \times (n-1)$ matrix. (In (12) we have $n = 3$, $(n-1)^2 = 4$ internal mesh points, two submatrices **B**, and two submatrices **I**.) The matrix **A** is nonsingular. This follows by noting that the off-diagonal entries in each row of **A** have the sum 3 (or 2), whereas each diagonal entry of **A** equals -4, so that nonsingularity is implied by Gerschgorin's theorem in Sec. 20.7 because no Gerschgorin disk can include 0. ■

A matrix is called a **band matrix** if it has all its nonzero entries on the main diagonal and on sloping lines parallel to it (separated by sloping lines of zeros or not). For example, **A** in (13) is a band matrix. Although the Gauss elimination does not preserve zeros between bands, it does not introduce nonzero entries outside the limits defined by the original bands. Hence a band structure is advantageous. In (13) it has been achieved by carefully ordering the mesh points.

ADI Method

A matrix is called a **tridiagonal matrix** if it has all its nonzero entries on the main diagonal and on the two sloping parallels immediately above or below the diagonal. (See also Sec. 20.9.) In this case the Gauss elimination is particularly simple.

This raises the question of whether, in the solution of the Dirichlet problem for the Laplace or Poisson equations, one could obtain a system of equations whose coefficient matrix is tridiagonal. The answer is yes, and a popular method of that kind, called the **ADI method** (*alternating direction implicit method*) was developed by Peaceman and Rachford. The idea is as follows. The stencil in (9) shows that we could obtain a tridiagonal matrix if there were only the three points in a row (or only the three points in a column). This suggests that we write (11) in the form

$$u_{i-1,j} - 4u_{ij} + u_{i+1,j} = -u_{i,j-1} - u_{i,j+1} \tag{14a}$$

so that the left side belongs to y-Row j only and the right side to x-Column i. Of course, we can also write (11) in the form

$$u_{i,j-1} - 4u_{ij} + u_{i,j+1} = -u_{i-1,j} - u_{i+1,j} \tag{14b}$$

so that the left side belongs to Column i and the right side to Row j. In the ADI method we proceed by iteration. At every mesh point we choose an arbitrary starting value $u_{ij}^{(0)}$. In each step we compute new values at all mesh points. In one step we use an iteration formula resulting from (14a) and in the next step an iteration formula resulting from (14b), and so on in alternating order.

In detail: suppose approximations $u_{ij}^{(m)}$ have been computed. Then, to obtain the next approximations $u_{ij}^{(m+1)}$, we substitute the $u_{ij}^{(m)}$ ***on the right*** side of (14a) and solve for the $u_{ij}^{(m+1)}$ on the left side; that is, we use

$$\mathbf{(15a)} \qquad u_{i-1,j}^{(m+1)} - 4u_{ij}^{(m+1)} + u_{i+1,j}^{(m+1)} = -u_{i,j-1}^{(m)} - u_{i,j+1}^{(m)}. \tag{15a}$$

We use (15a) for a fixed j, that is, ***for a fixed row*** j, and for all internal mesh points in this row. This gives a linear system of N algebraic equations (N = number of internal mesh points per row) in N unknowns, the new approximations of u at these mesh points. Note that (15a) involves not only approximations computed in the previous step but also given boundary values. We solve the system (15a) (j fixed!) by Gauss elimination. Then we go to the next row, obtain another system of N equations and solve it by Gauss, and so on, until all rows are done. In the next step we ***alternate direction***, that is, we compute

the next approximations $u_{ij}^{(m+2)}$ column by column from the $u_{ij}^{(m+1)}$ and the given boundary values, using a formula obtained from (14b) by substituting the $u_{ij}^{(m+1)}$ ***on the right***:

(15b)
$$u_{i,j-1}^{(m+2)} - 4u_{ij}^{(m+2)} + u_{i,j+1}^{(m+2)} = -u_{i-1,j}^{(m+1)} - u_{i+1,j}^{(m+1)}.$$

For each fixed i, that is, ***for each column,*** this is a system of M equations (M = number of internal mesh points per column) in M unknowns, which we solve by Gauss elimination. Then we go to the next column, and so on, until all columns are done.

Let us consider an example that merely serves to explain the entire method.

EXAMPLE 2 Dirichlet Problem. ADI Method

Explain the procedure and formulas of the ADI method in terms of the problem in Example 1, using the same grid and starting values 100, 100, 100, 100.

Solution. While working, we keep an eye on Fig. 455b and the given boundary values. We obtain first approximations $u_{11}^{(1)}, u_{21}^{(1)}, u_{12}^{(1)}, u_{22}^{(1)}$ from (15a) with $m = 0$. We write boundary values contained in (15a) without an upper index, for better identification and to indicate that these given values remain the same during the iteration. From (15a) with $m = 0$ we have for $j = 1$ (first row) the system

$$(i = 1) \quad u_{01} - 4u_{11}^{(1)} + u_{21}^{(1)} = -u_{10} - u_{12}^{(0)}$$
$$(i = 2) \quad u_{11}^{(1)} - 4u_{21}^{(1)} + u_{31} = -u_{20} - u_{22}^{(0)}.$$

The solution is $u_{11}^{(1)} = u_{21}^{(1)} = 100$. For $j = 2$ (second row) we obtain from (15a) the system

$$(i = 1) \quad u_{02} - 4u_{12}^{(1)} + u_{22}^{(1)} = -u_{11}^{(0)} - u_{13}$$
$$(i = 2) \quad u_{12}^{(1)} - 4u_{22}^{(1)} + u_{32} = -u_{21}^{(0)} - u_{23}.$$

The solution is $u_{12}^{(1)} = u_{22}^{(1)} = 66.667$.

Second approximations $u_{11}^{(2)}, u_{21}^{(2)}, u_{12}^{(2)}, u_{22}^{(2)}$ are now obtained from (15b) with $m = 1$ by using the first approximations just computed and the boundary values. For $i = 1$ (first column) we obtain from (15b) the system

$$(j = 1) \quad u_{10} - 4u_{11}^{(2)} + u_{12}^{(2)} = -u_{01} - u_{21}^{(1)}$$
$$(j = 2) \quad u_{11}^{(2)} - 4u_{12}^{(2)} + u_{13} = -u_{02} - u_{22}^{(1)}.$$

The solution is $u_{11}^{(2)} = 91.11$, $u_{12}^{(2)} = 64.44$, For $i = 2$ (second column) we obtain from (15b) the system

$$(j = 1) \quad u_{20} - 4u_{21}^{(2)} + u_{22}^{(2)} = -u_{11}^{(1)} - u_{31}$$
$$(j = 2) \quad u_{21}^{(2)} - 4u_{22}^{(2)} + u_{23} = -u_{12}^{(1)} - u_{32}.$$

The solution is $u_{21}^{(2)} = 91.11$, $u_{22}^{(2)} = 64.44$.

In this example, which merely serves to explain the practical procedure in the ADI method, the accuracy of the second approximations is about the same as that of two Gauss–Seidel steps in Sec. 20.3 (where $u_{11} = x_1$, $u_{21} = x_2$, $u_{12} = x_3$, $u_{22} = x_4$), as the following table shows.

Method	u_{11}	u_{21}	u_{12}	u_{22}
ADI, 2nd approximations	91.11	91.11	64.44	64.44
Gauss–Seidel, 2nd approximations	93.75	90.62	65.62	64.06
Exact solution of (12)	87.50	87.50	62.50	62.50

■

Improving Convergence. Additional improvement of the convergence of the ADI method results from the following interesting idea. Introducing a parameter p, we can also write (11) in the form

$$(16)\quad \begin{aligned} &\text{(a)}\quad u_{i-1,j} - (2+p)u_{ij} + u_{i+1,j} = -u_{i,j-1} + (2-p)u_{ij} - u_{i,j+1} \\ &\text{(b)}\quad u_{i,j-1} - (2+p)u_{ij} + u_{i,j+1} = -u_{i-1,j} + (2-p)u_{ij} - u_{i+1,j}. \end{aligned}$$

This gives the more general ADI iteration formulas

$$(17)\quad \begin{aligned} &\text{(a)}\quad u_{i-1,j}^{(m+1)} - (2+p)u_{ij}^{(m+1)} + u_{i+1,j}^{(m+1)} = -u_{i,j-1}^{(m)} + (2-p)u_{ij}^{(m)} - u_{i,j+1}^{(m)} \\ &\text{(b)}\quad u_{i,j-1}^{(m+2)} - (2+p)u_{ij}^{(m+2)} + u_{i,j+1}^{(m+2)} = -u_{i-1,j}^{(m+1)} + (2-p)u_{ij}^{(m+1)} - u_{i+1,j}^{(m+1)}. \end{aligned}$$

For $p = 2$, this is (15). The parameter p may be used for improving convergence. Indeed, one can show that the ADI method converges for positive p, and that the optimum value for maximum rate of convergence is

$$(18)\quad p_0 = 2 \sin \frac{\pi}{K}$$

where K is the larger of $M + 1$ and $N + 1$ (see above). Even better results can be achieved by letting p vary from step to step. More details of the ADI method and variants are discussed in Ref. [E25] listed in App. 1.

PROBLEM SET 21.4

1. Derive (5b), (6b), and (6c).

2. Verify the calculations in Example 1 of the text. Find out experimentally how many steps you need to obtain the solution of the linear system with an accuracy of 3S.

3. Use of symmetry. Conclude from the boundary values in Example 1 that $u_{21} = u_{11}$ and $u_{22} = u_{12}$. Show that this leads to a system of two equations and solve it.

4. Finer grid of 3×3 inner points. Solve Example 1, choosing $h = \frac{12}{4} = 3$ (instead of $h = \frac{12}{3} = 4$) and the same starting values.

5–10 GAUSS ELIMINATION, GAUSS–SEIDEL ITERATION

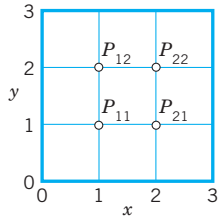


Fig. 456. Problems 5–10

For the grid in Fig. 456 compute the potential at the four internal points by Gauss and by 5 Gauss–Seidel steps with starting values 100, 100, 100, 100 (showing the details of your work) if the boundary values on the edges are:

5. $u(1, 0) = 60$, $u(2, 0) = 300$, $u = 100$ on the other three edges.

6. $u = 0$ on the left, x^3 on the lower edge, $27 - 9y^2$ on the right, $x^3 - 27x$ on the upper edge.

7. U_0 on the upper and lower edges, $-U_0$ on the left and right. Sketch the equipotential lines.

8. $u = 220$ on the upper and lower edges, 110 on the left and right.

9. $u = \sin \frac{1}{3}\pi x$ on the upper edge, 0 on the other edges, 10 steps.

10. $u = x^4$ on the lower edge, $81 - 54y^2 + y^4$ on the right, $x^4 - 54x^2 + 81$ on the upper edge, y^4 on the left. Verify the exact solution $x^4 - 6x^2y^2 + y^4$ and determine the error.

11. Find the potential in Fig. 457 using **(a)** the coarse grid, **(b)** the fine grid 5×3, and Gauss elimination. *Hint.* In (b), use symmetry; take $u = 0$ as boundary value at the two points at which the potential has a jump.

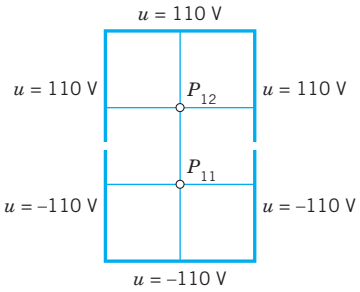


Fig. 457. Region and grids in Problem 11

12. Influence of starting values. Do Prob. 9 by Gauss–Seidel, starting from **0**. Compare and comment.

13. For the square $0 \leqq x \leqq 4$, $0 \leqq y \leqq 4$ let the boundary temperatures be 0°C on the horizontal and 50°C on the vertical edges. Find the temperatures at the interior points of a square grid with $h = 1$.

14. Using the answer to Prob. 13, try to sketch some isotherms.

15. Find the isotherms for the square and grid in Prob. 13 if $u = \sin \frac{1}{4}\pi x$ on the horizontal and $-\sin \frac{1}{4}\pi y$ on the vertical edges. Try to sketch some isotherms.

16. ADI. Apply the ADI method to the Dirichlet problem in Prob. 9, using the grid in Fig. 456, as before and starting values zero.

17. What p_0 in (18) should we choose for Prob. 16? Apply the ADI formulas (17) with that value of p_0 to Prob. 16, performing 1 step. Illustrate the improved convergence by comparing with the corresponding values 0.077, 0.308 after the first step in Prob. 16. (Use the starting values zero.)

18. CAS PROJECT. Laplace Equation. (a) Write a program for Gauss–Seidel with 16 equations in 16 unknowns, composing the matrix (13) from the indicated 4×4 submatrices and including a transformation of the vector of the boundary values into the vector **b** of $\mathbf{Ax} = \mathbf{b}$.

(b) Apply the program to the square grid in $0 \leqq x \leqq 5$, $0 \leqq y \leqq 5$ with $h = 1$ and $u = 220$ on the upper and lower edges, $u = 110$ on the left edge and $u = -10$ on the right edge. Solve the linear system also by Gauss elimination. What accuracy is reached in the 20th Gauss–Seidel step?

21.5 Neumann and Mixed Problems. Irregular Boundary

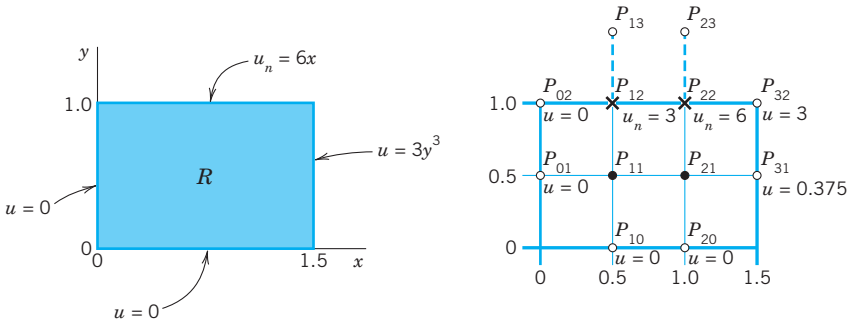
We continue our discussion of boundary value problems for elliptic PDEs in a region R in the xy-plane. The Dirichlet problem was studied in the last section. In solving **Neumann** and **mixed problems** (defined in the last section) we are confronted with a new situation, because there are boundary points at which the (outer) **normal derivative** $u_n = \partial u/\partial n$ of the solution is given, but u itself is unknown since it is not given. To handle such points we need a new idea. This idea is the same for Neumann and mixed problems. Hence we may explain it in connection with one of these two types of problems. We shall do so and consider a typical example as follows.

EXAMPLE 1 Mixed Boundary Value Problem for a Poisson Equation

Solve the mixed boundary value problem for the Poisson equation

$$\nabla^2 u = u_{xx} + u_{yy} = f(x, y) = 12xy$$

shown in Fig. 458a.



(a) Region R and boundary values (b) Grid ($h = 0.5$)

Fig. 458. Mixed boundary value problem in Example 1

Solution. We use the grid shown in Fig. 458b, where $h = 0.5$. We recall that (7) in Sec. 21.4 has the right side $h^2 f(x, y) = 0.5^2 \cdot 12xy = 3xy$. From the formulas $u = 3y^3$ and $u_n = 6x$ given on the boundary we compute the boundary data

$$(1) \qquad u_{31} = 0.375, \qquad u_{32} = 3, \qquad \frac{\partial u_{12}}{\partial n} = \frac{\partial u_{12}}{\partial y} = 6 \cdot 0.5 = 3. \qquad \frac{\partial u_{22}}{\partial n} = \frac{\partial u_{22}}{\partial y} = 6 \cdot 1 = 6.$$

P_{11} and P_{21} are internal mesh points and can be handled as in the last section. Indeed, from (7), Sec. 21.4, with $h^2 = 0.25$ and $h^2 f(x, y) = 3xy$ and from the given boundary values we obtain two equations corresponding to P_{11} and P_{21}, as follows (with -0 resulting from the left boundary).

$$(2a) \qquad \begin{aligned} -4u_{11} + u_{21} + u_{12} &= 12(0.5 \cdot 0.5) \cdot \tfrac{1}{4} - 0 = 0.75 \\ u_{11} - 4u_{21} + u_{22} &= 12(1 \cdot 0.5) \cdot \tfrac{1}{4} - 0.375 = 1.125. \end{aligned}$$

The only difficulty with these equations seems to be that they involve the unknown values u_{12} and u_{22} of u at P_{12} and P_{22} on the boundary, where the normal derivative $u_n = \partial u/\partial n = \partial u/\partial y$ is given, instead of u; but we shall overcome this difficulty as follows.

We consider P_{12} and P_{22}. The idea that will help us here is this. We imagine the region R to be extended above to the first row of external mesh points (corresponding to $y = 1.5$), and we assume that the Poisson equation also holds in the extended region. Then we can write down two more equations as before (Fig. 458b)

$$(2b) \qquad \begin{aligned} u_{11} - 4u_{12} + u_{22} + u_{13} &= 1.5 - 0 = 1.5 \\ u_{21} + u_{12} - 4u_{22} + u_{23} &= 3 - 3 = 0. \end{aligned}$$

On the right, 1.5 is $12xyh^2$ at (0.5, 1) and 3 is $12xyh^2$ at (1, 1) and 0 (at P_{02}) and 3 (at P_{32}) are given boundary values. We remember that we have not yet used the boundary condition on the upper part of the boundary of R, and we also notice that in (2b) we have introduced two more unknowns u_{13}, u_{23}. But we can now use that condition and get rid of u_{13}, u_{23} by applying the central difference formula for du/dy. From (1) we then obtain (see Fig. 458b)

$$3 = \frac{\partial u_{12}}{\partial y} \approx \frac{u_{13} - u_{11}}{2h} = u_{13} - u_{11}, \qquad \text{hence} \qquad u_{13} = u_{11} + 3$$

$$6 = \frac{\partial u_{22}}{\partial y} \approx \frac{u_{23} - u_{21}}{2h} = u_{23} - u_{21}, \qquad \text{hence} \qquad u_{23} = u_{21} + 6.$$

Substituting these results into (2b) and simplifying, we have

$$\begin{aligned} 2u_{11} - 4u_{12} + u_{22} &= 1.5 - 3 = -1.5 \\ 2u_{21} + u_{12} - 4u_{22} &= 3 - 3 - 6 = -6. \end{aligned}$$

Together with (2a) this yields, written in matrix form,

$$(3)\qquad \begin{bmatrix} -4 & 1 & 1 & 0 \\ 1 & -4 & 0 & 1 \\ 2 & 0 & -4 & 1 \\ 0 & 2 & 1 & -4 \end{bmatrix} \begin{bmatrix} u_{11} \\ u_{21} \\ u_{12} \\ u_{22} \end{bmatrix} = \begin{bmatrix} 0.75 \\ 1.125 \\ 1.5 - 3 \\ 0 - 6 \end{bmatrix} = \begin{bmatrix} 0.75 \\ 1.125 \\ -1.5 \\ -6 \end{bmatrix}.$$

(The entries 2 come from u_{13} and u_{23}, and so do -3 and -6 on the right). The solution of (3) (obtained by Gauss elimination) is as follows; the exact values of the problem are given in parentheses.

$$u_{12} = 0.866 \quad \text{(exact 1)} \qquad u_{22} = 1.812 \quad \text{(exact 2)}$$
$$u_{11} = 0.077 \quad \text{(exact 0.125)} \qquad u_{21} = 0.191 \quad \text{(exact 0.25).}$$ ■

Irregular Boundary

We continue our discussion of boundary value problems for elliptic PDEs in a region R in the xy-plane. If R has a simple geometric shape, we can usually arrange for certain mesh points to lie on the boundary C of R, and then we can approximate partial derivatives as explained in the last section. However, if C intersects the grid at points that are not mesh points, then at points close to the boundary we must proceed differently, as follows.

The mesh point O in Fig. 459 is of that kind. For O and its neighbors A and P we obtain from Taylor's theorem

$$(4)\qquad \text{(a)}\quad u_A = u_O + ah\frac{\partial u_O}{\partial x} + \frac{1}{2}(ah)^2\frac{\partial^2 u_O}{\partial x^2} + \cdots$$
$$\text{(b)}\quad u_P = u_O - h\frac{\partial u_O}{\partial x} + \frac{1}{2}h^2\frac{\partial^2 u_O}{\partial x^2} + \cdots.$$

We disregard the terms marked by dots and eliminate $\partial u_O/\partial x$. Equation (4b) times a plus equation (4a) gives

$$u_A + au_P \approx (1 + a)\,u_O + \frac{1}{2}\,a\,(a + 1)\,h^2\frac{\partial^2 u_O}{\partial x^2}.$$

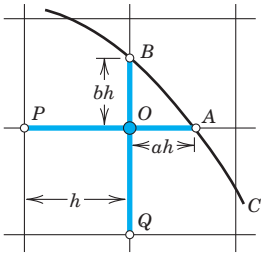


Fig. 459. Curved boundary C of a region R, a mesh point O near C, and neighbors A, B, P, Q

We solve this last equation algebraically for the derivative, obtaining

$$\frac{\partial^2 u_O}{\partial x^2} \approx \frac{2}{h^2}\left[\frac{1}{a(1 + a)}\,u_A + \frac{1}{1 + a}\,u_P - \frac{1}{a}\,u_O\right].$$

Similarly, by considering the points O, B, and Q,

$$\frac{\partial^2 u_O}{\partial y^2} \approx \frac{2}{h^2}\left[\frac{1}{b(1+b)}u_B + \frac{1}{1+b}u_Q - \frac{1}{b}u_O\right].$$

By addition,

$$\text{(5)} \qquad \nabla^2 u_O \approx \frac{2}{h^2}\left[\frac{u_A}{a(1+a)} + \frac{u_B}{b(1+b)} + \frac{u_P}{1+a} + \frac{u_Q}{1+b} - \frac{(a+b)u_O}{ab}\right].$$

For example, if $a = \frac{1}{2}$, $b = \frac{1}{2}$, instead of the stencil (see Sec. 21.4)

$$\begin{Bmatrix} & 1 & \\ 1 & -4 & 1 \\ & 1 & \end{Bmatrix} \qquad \text{we now have} \qquad \begin{Bmatrix} & \frac{4}{3} & \\ \frac{2}{3} & -4 & \frac{4}{3} \\ & \frac{2}{3} & \end{Bmatrix}.$$

because $1/[a(1+a)] = \frac{4}{3}$, etc. The sum of all five terms still being zero (which is useful for checking).

Using the same ideas, you may show that in the case of Fig. 460.

$$\textbf{(6)} \qquad \nabla^2 u_O \approx \frac{2}{h^2}\left[\frac{u_A}{a(a+p)} + \frac{u_B}{b(b+q)} + \frac{u_P}{p(p+a)} + \frac{u_Q}{q(q+b)} - \frac{ap+bq}{abpq}u_O\right],$$

a formula that takes care of all conceivable cases.

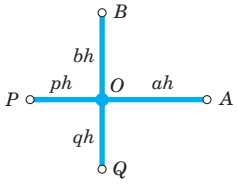


Fig. 460. Neighboring points A, B, P, Q of a mesh point O and notations in formula (6)

EXAMPLE 2 Dirichlet Problem for the Laplace Equation. Curved Boundary

Find the potential u in the region in Fig. 461 that has the boundary values given in that figure; here the curved portion of the boundary is an arc of the circle of radius 10 about (0,0). Use the grid in the figure.

Solution. u is a solution of the Laplace equation. From the given formulas for the boundary values $u = x^3$, $u = 512 - 24y^2, \cdots$ we compute the values at the points where we need them; the result is shown in the figure. For P_{11} and P_{12} we have the usual regular stencil, and for P_{21} and P_{22} we use (6), obtaining

$$\text{(7)} \qquad P_{11}, P_{12}: \begin{Bmatrix} & 1 & \\ 1 & -4 & 1 \\ & 1 & \end{Bmatrix}, \quad P_{21}: \begin{Bmatrix} & 0.5 & \\ 0.6 & -2.5 & 0.9 \\ & 0.5 & \end{Bmatrix}, \quad P_{22}: \begin{Bmatrix} & 0.9 & \\ 0.6 & -3 & 0.9 \\ & 0.6 & \end{Bmatrix}.$$

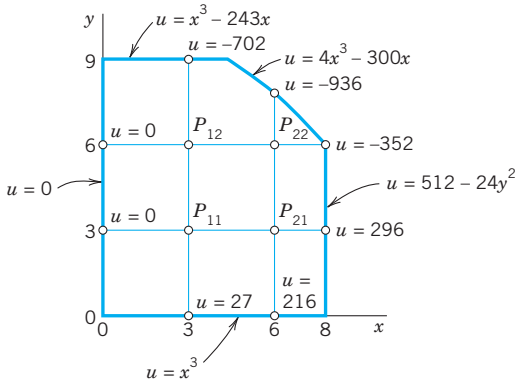


Fig. 461. Region, boundary values of the potential, and grid in Example 2

We use this and the boundary values and take the mesh points in the usual order $P_{11}, P_{21}, P_{12}, P_{22}$. Then we obtain the system

$$\begin{aligned}
-4u_{11} + u_{21} + u_{12} &= 0 - 27 &&= -27\\
0.6u_{11} - 2.5u_{21} + 0.5u_{22} &= -0.9 \cdot 296 - 0.5 \cdot 216 &&= -374.4\\
u_{11} - 4u_{12} + u_{22} &= 702 + 0 &&= 702\\
0.6u_{21} + 0.6u_{12} - 3u_{22} &= 0.9 \cdot 352 + 0.9 \cdot 936 &&= 1159.2
\end{aligned}$$

In matrix form,

$$\text{(8)} \qquad \begin{bmatrix} -4 & 1 & 1 & 0 \\ 0.6 & -2.5 & 0 & 0.5 \\ 1 & 0 & -4 & 1 \\ 0 & 0.6 & 0.6 & -3 \end{bmatrix} \begin{bmatrix} u_{11} \\ u_{21} \\ u_{12} \\ u_{22} \end{bmatrix} = \begin{bmatrix} -27 \\ -374.4 \\ 702 \\ 1159.2 \end{bmatrix}.$$

Gauss elimination yields the (rounded) values

$$u_{11} = -55.6, \quad u_{21} = 49.2, \quad u_{12} = -298.5, \quad u_{22} = -436.3.$$

Clearly, from a grid with so few mesh points we cannot expect great accuracy. The exact solution of the PDE (not of the difference equation) having the given boundary values is $u = x^3 - 3xy^2$ and yields the values

$$u_{11} = -54, \quad u_{21} = 54, \quad u_{12} = -297, \quad u_{22} = -432.$$

In practice one would use a much finer grid and solve the resulting large system by an indirect method. ■

PROBLEM SET 21.5

1–7 MIXED BOUNDARY VALUE PROBLEMS

1. Check the values for the Poisson equation at the end of Example 1 by solving (3) by Gauss elimination.

2. Solve the mixed boundary value problem for the Poisson equation $\nabla^2 u = 2(x^2 + y^2)$ in the region and for the boundary conditions shown in Fig. 462, using the indicated grid.

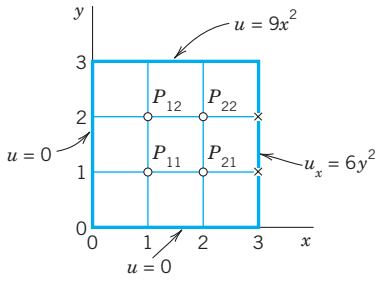


Fig. 462. Problems 2 and 6

3. **CAS EXPERIMENT. Mixed Problem.** Do Example 1 in the text with finer and finer grids of your choice and study the accuracy of the approximate values by comparing with the exact solution $u = 2xy^3$. Verify the latter.

4. Solve the mixed boundary value problem for the Laplace equation $\nabla^2 u = 0$ in the rectangle in Fig. 458a (using the grid in Fig. 458b) and the boundary conditions $u_x = 0$ on the left edge, $u_x = 3$ on the right edge, $u = x^2$ on the lower edge, and $u = x^2 - 1$ on the upper edge.

5. Do Example 1 in the text for the Laplace equation (instead of the Poisson equation) with grid and boundary data as before.

6. Solve $\nabla^2 u = -\pi^2 y \sin \frac{1}{3}\pi x$ for the grid in Fig. 462 and $u_y(1, 3) = u_y(2, 3) = \frac{1}{2}\sqrt{243}$, $u = 0$ on the other three sides of the square.

7. Solve Prob. 4 when $u_n = 110$ on the upper edge and $u = 110$ on the other edges.

8–16 IRREGULAR BOUNDARY

8. Verify the stencil shown after (5).

9. Derive (5) in the general case.

10. Derive the general formula (6) in detail.

11. Derive the linear system in Example 2 of the text.

12. Verify the solution in Example 2.

13. Solve the Laplace equation in the region and for the boundary values shown in Fig. 463, using the indicated grid. (The sloping portion of the boundary is $y = 4.5 - x$.)

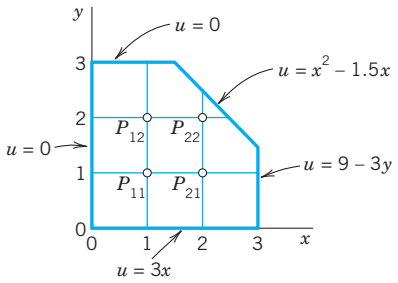


Fig. 463. Problem 13

14. If, in Prob. 13, the axes are grounded ($u = 0$), what constant potential must the other portion of the boundary have in order to produce 220 V at P_{11}?

15. What potential do we have in Prob. 13 if $u = 100$ V on the axes and $u = 0$ on the other portion of the boundary?

16. Solve the Poisson equation $\nabla^2 u = 2$ in the region and for the boundary values shown in Fig. 464, using the grid also shown in the figure.

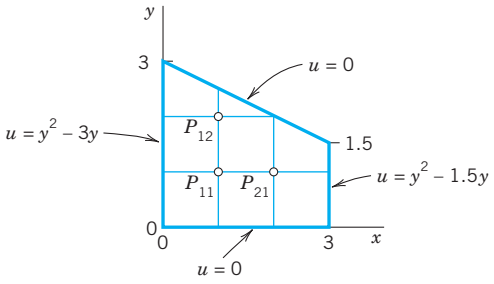


Fig. 464. Problem 16

21.6 Methods for Parabolic PDEs

The last two sections concerned elliptic PDEs, and we now turn to parabolic PDEs. Recall that the definitions of elliptic, parabolic, and hyperbolic PDEs were given in Sec. 21.4. There it was also mentioned that the general behavior of solutions differs from type to type, and so do the problems of practical interest. This reflects on numerics as follows.

For all three types, one replaces the PDE by a corresponding difference equation, but for *parabolic* and *hyperbolic* PDEs this does not automatically guarantee the **convergence** of the approximate solution to the exact solution as the mesh $h \to 0$; in fact, it does not even guarantee convergence at all. For these two types of PDEs one needs additional conditions (inequalities) to assure convergence and **stability**, the latter meaning that small perturbations in the initial data (or small errors at any time) cause only small changes at later times.

In this section we explain the numeric solution of the prototype of parabolic PDEs, the one-dimensional heat equation

$$u_t = c^2 u_{xx} \qquad (c \text{ constant}).$$

This PDE is usually considered for x in some fixed interval, say, $0 \leqq x \leqq L$, and time $t \geqq 0$, and one prescribes the initial temperature $u(x, 0) = f(x)$ (f given) and boundary conditions at $x = 0$ and $x = L$ for all $t \geqq 0$, for instance, $u(0, t) = 0$, $u(L, t) = 0$. We may assume $c = 1$ and $L = 1$; this can always be accomplished by a linear transformation of x and t (Prob. 1). Then the **heat equation** and those conditions are

(1) $$u_t = u_{xx} \qquad 0 \leqq x \leqq 1,\ t \geqq 0$$

(2) $$u(x, 0) = f(x) \qquad \text{(Initial condition)}$$

(3) $$u(0, t) = u(1, t) = 0 \qquad \text{(Boundary conditions).}$$

A simple finite difference approximation of (1) is [see (6a) in Sec. 21.4; j is the number of the ***time step***]

(4) $$\frac{1}{k}(u_{i,j+1} - u_{ij}) = \frac{1}{h^2}(u_{i+1,j} - 2u_{ij} + u_{i-1,j}).$$

Figure 465 shows a corresponding grid and mesh points. The mesh size is h in the x-direction and k in the t-direction. Formula (4) involves the four points shown in Fig. 466. On the left in (4) we have used a *forward* difference quotient since we have no information for negative t at the start. From (4) we calculate $u_{i,j+1}$, which corresponds to time row $j + 1$, in terms of the three other u that correspond to time row j. Solving (4) for $u_{i,j+1}$, we have

(5) $$u_{i,j+1} = (1 - 2r)u_{ij} + r(u_{i+1,j} + u_{i-1,j}), \qquad r = \frac{k}{h^2}.$$

Computations by this **explicit method** based on (5) are simple. However, it can be shown that crucial to the convergence of this method is the condition

(6) $$r = \frac{k}{h^2} \leqq \frac{1}{2}.$$

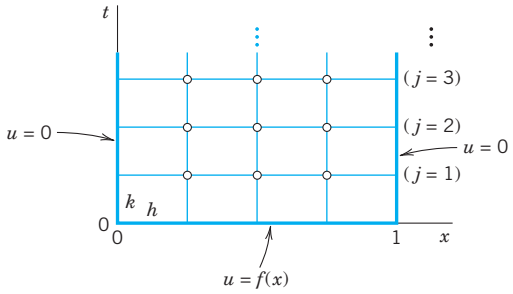


Fig. 465. Grid and mesh points corresponding to (4), (5)

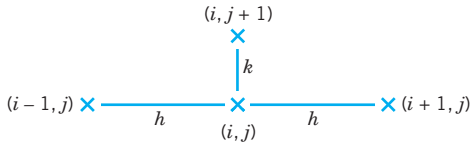


Fig. 466. The four points in (4) and (5)

That is, u_{ij} should have a positive coefficient in (5) or (for $r = \frac{1}{2}$) be absent from (5). Intuitively, (6) means that we should not move too fast in the t-direction. An example is given below.

Crank–Nicolson Method

Condition (6) is a handicap in practice. Indeed, to attain sufficient accuracy, we have to choose h small, which makes k very small by (6). For example, if $h = 0.1$, then $k \leqq 0.005$. Accordingly, we should look for a more satisfactory discretization of the heat equation.

A method that imposes no restriction on $r = k/h^2$ is the **Crank–Nicolson (CN) method**,[5] which uses values of u at the six points in Fig. 467. The idea of the method is the replacement of the difference quotient on the right side of (4) by $\frac{1}{2}$ times the sum of two such difference quotients at two time rows (see Fig. 467). Instead of (4) we then have

$$\frac{1}{k}(u_{i,j+1} - u_{ij}) = \frac{1}{2h^2}(u_{i+1,j} - 2u_{ij} + u_{i-1,j}) + \frac{1}{2h^2}(u_{i+1,j+1} - 2u_{i,j+1} + u_{i-1,j+1}). \tag{7}$$

Multiplying by $2k$ and writing $r = k/h^2$ as before, we collect the terms corresponding to time row $j + 1$ on the left and the terms corresponding to time row j on the right:

$$\textbf{(8)} \quad (2 + 2r)u_{i,j+1} - r(u_{i+1,j+1} + u_{i-1,j+1} = (2 - 2r)u_{ij} + r(u_{i+1,j} + u_{i-1,j}).$$

How do we use (8)? In general, the three values on the left are unknown, whereas the three values on the right are known. If we divide the x-interval $0 \leqq x \leqq 1$ in (1) into n equal intervals, we have $n - 1$ internal mesh points per time row (see Fig. 465, where $n = 4$). Then for $j = 0$ and $i = 1, \cdots, n - 1$, formula (8) gives a linear system of $n - 1$ equations for the $n - 1$ unknown values $u_{11}, u_{21}, \cdots, u_{n-1,1}$ in the first time row in terms of the initial values $u_{00}, u_{10}, \cdots, u_{n0}$ and the boundary values $u_{01}(= 0), u_{n1}(= 0)$. Similarly for $j = 1, j = 2$, and so on; that is, for each time row we have to solve such a linear system of $n - 1$ equations resulting from (8).

Although $r = k/h^2$ is no longer restricted, smaller r will still give better results. In practice, one chooses a k by which one can save a considerable amount of work, without

[5]JOHN CRANK (1916–2006), English mathematician and physicist at Courtaulds Fundamental Research Laboratory, professor at Brunel University, England. Student of Sir WILLIAM LAWRENCE BRAGG (1890–1971), Australian British physicist, who with his father, Sir WILLIAM HENRY BRAGG (1862–1942) won the Nobel Prize in physics in 1915 for their fundamental work in X-ray crystallography. (This is the only case where a father and a son shared the Nobel Prize for the same research. Furthermore, W. L. Bragg is the youngest Nobel laureate ever.) PHYLLIS NICOLSON (1917–1968), English mathematician, professor at the University of Leeds, England.

making r too large. For instance, often a good choice is $r = 1$ (which would be impossible in the previous method). Then (8) becomes simply

(9)
$$4u_{i,j+1} - u_{i+1,j+1} - u_{i-1,j+1} = u_{i+1,j} + u_{i-1,j}.$$

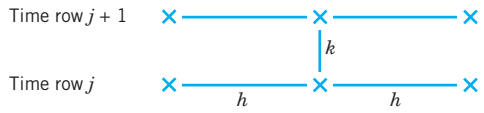


Fig. 467. The six points in the Crank–Nicolson formulas (7) and (8)

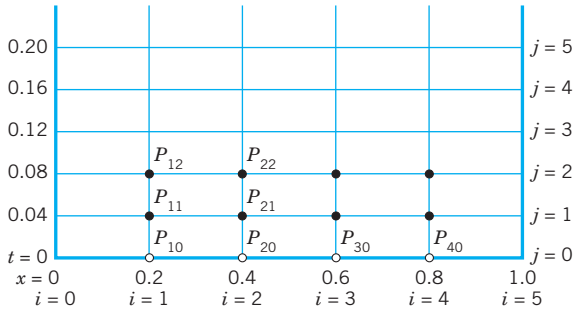


Fig. 468. Grid in Example 1

EXAMPLE 1 **Temperature in a Metal Bar. Crank–Nicolson Method, Explicit Method**

Consider a laterally insulated metal bar of length 1 and such that $c^2 = 1$ in the heat equation. Suppose that the ends of the bar are kept at temperature $u = 0°C$ and the temperature in the bar at some instant—call it $t = 0$—is $f(x) = \sin \pi x$. Applying the Crank–Nicolson method with $h = 0.2$ and $r = 1$, find the temperature $u(x, t)$ in the bar for $0 \leqq t \leqq 0.2$. Compare the results with the exact solution. Also apply (5) with an r satisfying (6), say, $r = 0.25$, and with values not satisfying (6), say, $r = 1$ and $r = 2.5$.

Solution by Crank–Nicolson. Since $r = 1$, formula (8) takes the form (9). Since $h = 0.2$ and $r = k/h^2 = 1$, we have $k = h^2 = 0.04$. Hence we have to do 5 steps. Figure 468 shows the grid. We shall need the initial values

$$u_{10} = \sin 0.2\pi = 0.587785, \qquad u_{20} = \sin 0.4\pi = 0.951057.$$

Also, $u_{30} = u_{20}$ and $u_{40} = u_{10}$. (Recall that u_{10} means u at P_{10} in Fig. 468, etc.) In each time row in Fig. 468 there are 4 internal mesh points. Hence in each time step we would have to solve 4 equations in 4 unknowns. But since the initial temperature distribution is symmetric with respect to $x = 0.5$, and $u = 0$ at both ends for all t, we have $u_{31} = u_{21}$, $u_{41} = u_{11}$ in the first time row and similarly for the other rows. This reduces each system to 2 equations in 2 unknowns. By (9), since $u_{31} = u_{21}$ and $u_{01} = 0$, for $j = 0$ these equations are

$$(i = 1) \qquad 4u_{11} - u_{21} = u_{00} + u_{20} = 0.951057$$
$$(i = 2) \qquad -u_{11} + 4u_{21} - u_{21} = u_{10} + u_{20} = 1.538842.$$

The solution is $u_{11} = 0.399274$, $u_{21} = 0.646039$. Similarly, for time row $j = 1$ we have the system

$$(i = 1) \qquad 4u_{12} - u_{22} = u_{01} + u_{21} = 0.646039$$
$$(i = 2) \qquad -u_{12} + 3u_{22} = u_{11} + u_{21} = 1.045313.$$

The solution is $u_{12} = 0.271221$, $u_{22} = 0.438844$, and so on. This gives the temperature distribution (Fig. 469):

t	$x = 0$	$x = 0.2$	$x = 0.4$	$x = 0.6$	$x = 0.8$	$x = 1$
0.00	0	0.588	0.951	0.951	0.588	0
0.04	0	0.399	0.646	0.646	0.399	0
0.08	0	0.271	0.439	0.439	0.271	0
0.12	0	0.184	0.298	0.298	0.184	0
0.16	0	0.125	0.202	0.202	0.125	0
0.20	0	0.085	0.138	0.138	0.085	0

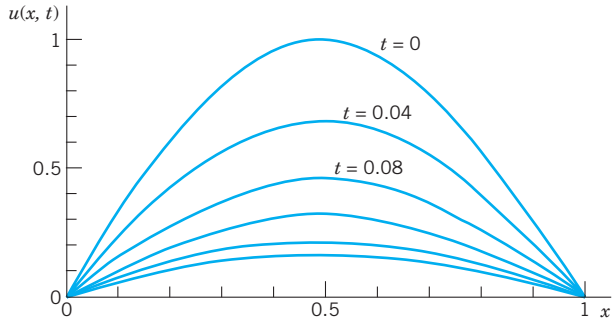


Fig. 469. Temperature distribution in the bar in Example 1

Comparison with the exact solution. The present problem can be solved exactly by separating variables (Sec. 12.5); the result is

$$u(x, t) = \sin \pi x \, e^{-\pi^2 t}. \tag{10}$$

Solution by the explicit method (5) with r = 0.25. For $h = 0.2$ and $r = k/h^2 = 0.25$ we have $k = rh^2 = 0.25 \cdot 0.04 = 0.01$. Hence we have to perform 4 times as many steps as with the Crank–Nicolson method! Formula (5) with $r = 0.25$ is

$$u_{i,j+1} = 0.25(u_{i-1,j} + 2u_{ij} + u_{i+1,j}). \tag{11}$$

We can again make use of the symmetry. For $j = 0$ we need $u_{00} = 0$, $u_{10} = 0.587785$ (see p. 939), $u_{20} = u_{30} = 0.951057$ and compute

$$u_{11} = 0.25(u_{00} + 2u_{10} + u_{20}) = 0.531657$$

$$u_{21} = 0.25(u_{10} + 2u_{20} + u_{30}) = 0.25(u_{10} + 3u_{20}) = 0.860239.$$

Of course we can omit the boundary terms $u_{01} = 0$, $u_{02} = 0, \cdots$ from the formulas. For $j = 1$ we compute

$$u_{12} = 0.25(2u_{11} + u_{21}) = 0.480888$$

$$u_{22} = 0.25(u_{11} + 3u_{21}) = 0.778094$$

and so on. We have to perform 20 steps instead of the 5 CN steps, but the numeric values show that the accuracy is only about the same as that of the Crank–Nicolson values CN. The exact 3D-values follow from (10).

t	$x = 0.2$			$x = 0.4$		
	CN	By (11)	Exact	CN	By (11)	Exact
0.04	0.399	0.393	0.396	0.646	0.637	0.641
0.08	0.271	0.263	0.267	0.439	0.426	0.432
0.12	0.184	0.176	0.180	0.298	0.285	0.291
0.16	0.125	0.118	0.121	0.202	0.191	0.196
0.20	0.085	0.079	0.082	0.138	0.128	0.132

Failure of (5) with r violating (6). Formula (5) with $h = 0.2$ and $r = 1$—which violates (6)—is

$$u_{i,j+1} = u_{i-1,j} - u_{ij} + u_{i+1,j}$$

and gives very poor values; some of these are

t	$x = 0.2$	Exact	$x = 0.4$	Exact
0.04	0.363	0.396	0.588	0.641
0.12	0.139	0.180	0.225	0.291
0.20	0.053	0.082	0.086	0.132

Formula (5) with an even larger $r = 2.5$ (and $h = 0.2$ as before) gives completely nonsensical results; some of these are

t	$x = 0.2$	Exact	$x = 0.4$	Exact
0.1	0.0265	0.2191	0.0429	0.3545
0.3	0.0001	0.0304	0.0001	0.0492.

PROBLEM SET 21.6

1. **Nondimensional form.** Show that the heat equation $\tilde{u}_{\tilde{t}} = c^2 \tilde{u}_{\tilde{x}\tilde{x}}$, $0 \leqq \tilde{x} \leqq L$, can be transformed to the "nondimensional" standard form $u_t = u_{xx}$, $0 \leqq x \leqq 1$, by setting $x = \tilde{x}/L$, $t = c^2\tilde{t}/L^2$, $u = \tilde{u}/u_0$, where u_0 is any constant temperature.
2. **Difference equation.** Derive the difference approximation (4) of the heat equation.
3. **Explicit method.** Derive (5) by solving (4) for $u_{i,j+1}$.
4. **CAS EXPERIMENT. Comparison of Methods.**

   (a) Write programs for the explicit and the Crank—Nicolson methods.

   (b) Apply the programs to the heat problem of a laterally insulated bar of length 1 with $u(x, 0) = \sin \pi x$ and $u(0, t) = u(1, t) = 0$ for all t, using $h = 0.2$, $k = 0.01$ for the explicit method (20 steps), $h = 0.2$ and (9) for the Crank–Nicolson method (5 steps). Obtain exact 6D-values from a suitable series and compare.

   (c) Graph temperature curves in (b) in two figures similar to Fig. 299 in Sec. 12.7.

   (d) Experiment with smaller h (0.1, 0.05, etc.) for both methods to find out to what extent accuracy increases under systematic changes of h and k.

EXPLICIT METHOD

5. Using (5) with $h = 1$ and $k = 0.5$, solve the heat problem (1)–(3) to find the temperature at $t = 2$ in a laterally insulated bar of length 10 ft and initial temperature $f(x) = x(1 - 0.1x)$.
6. Solve the heat problem (1)–(3) by the explicit method with $h = 0.2$ and $k = 0.01$, 8 time steps, when $f(x) = x$ if $0 \leqq x < \frac{1}{2}$, $f(x) = 1 - x$ if $\frac{1}{2} \leqq x \leqq 1$. Compare with the 3S-values 0.108, 0.175 for $t = 0.08$, $x = 0.2, 0.4$ obtained from the series (2 terms) in Sec. 12.5.
7. The accuracy of the explicit method depends on r ($\leqq \frac{1}{2}$). Illustrate this for Prob. 6, choosing $r = \frac{1}{2}$ (and $h = 0.2$ as before). Do 4 steps. Compare the values for $t = 0.04$ and 0.08 with the 3S-values in Prob. 6, which are 0.156, 0.254 ($t = 0.04$), 0.105, 0.170 ($t = 0.08$).

8. In a laterally insulated bar of length 1 let the initial temperature be $f(x) = x$ if $0 \leqq x < 0.5, f(x) = 1 - x$ if $0.5 \leqq x \leqq 1$. Let (1) and (3) hold. Apply the explicit method with $h = 0.2, k = 0.01$, 5 steps. Can you expect the solution to satisfy $u(x, t) = u(1 - x, t)$ for all t?

9. Solve Prob. 8 with $f(x) = x$ if $0 \leqq x \leqq 0.2$, $f(x) = 0.25(1 - x)$ if $0.2 < x \leqq 1$, the other data being as before.

10. Insulated end. If the left end of a laterally insulated bar extending from $x = 0$ to $x = 1$ is insulated, the boundary condition at $x = 0$ is $u_n(0, t) = u_x(0, t) = 0$. Show that, in the application of the explicit method given by (5), we can compute u_{0j+1} by the formula

$$u_{0j+1} = (1 - 2r)u_{0j} + 2ru_{1j}.$$

Apply this with $h = 0.2$ and $r = 0.25$ to determine the temperature $u(x, t)$ in a laterally insulated bar extending from $x = 0$ to 1 if $u(x, 0) = 0$, the left end is insulated and the right end is kept at temperature $g(t) = \sin \frac{50}{3} \pi t$. *Hint.* Use $0 = \partial u_{0j}/\partial x = (u_{1j} - u_{-1j})/2h$.

CRANK–NICOLSON METHOD

11. Solve Prob. 9 by (9) with $h = 0.2$, 2 steps. Compare with exact values obtained from the series in Sec. 12.5 (2 terms) with suitable coefficients.

12. Solve the heat problem (1)–(3) by Crank–Nicolson for $0 \leqq t \leqq 0.20$ with $h = 0.2$ and $k = 0.04$ when $f(x) = x$ if $0 \leqq x < \frac{1}{2}, f(x) = 1 - x$ if $\frac{1}{2} \leqq x \leqq 1$. Compare with the exact values for $t = 0.20$ obtained from the series (2 terms) in Sec. 12.5.

13–15

Solve (1)–(3) by Crank–Nicolson with $r = 1$ (5 steps), where:

13. $f(x) = 5x$ if $0 \leqq x < 0.25$, $f(x) = 1.25(1 - x)$ if $0.25 \leqq x \leqq 1$, $h = 0.2$

14. $f(x) = x(1 - x)$, $h = 0.1$. (Compare with Prob. 15.)

15. $f(x) = x(1 - x)$, $h = 0.2$

21.7 Method for Hyperbolic PDEs

In this section we consider the numeric solution of problems involving hyperbolic PDEs. We explain a standard method in terms of a typical setting for the prototype of a hyperbolic PDE, the **wave equation**:

(1)	$u_{tt} = u_{xx}$	$0 \leqq x \leqq 1, t \geqq 0$
(2)	$u(x, 0) = f(x)$	(Given initial displacement)
(3)	$u_t(x, 0) = g(x)$	(Given initial velocity)
(4)	$u(0, t) = u(1, t) = 0$	(Boundary conditions).

Note that an equation $u_{tt} = c^2 u_{xx}$ and another x-interval can be reduced to the form (1) by a linear transformation of x and t. This is similar to Sec. 21.6, Prob. 1.

For instance, (1)–(4) is the model of a vibrating elastic string with fixed ends at $x = 0$ and $x = 1$ (see Sec. 12.2). Although an analytic solution of the problem is given in (13), Sec. 12.4, we use the problem for explaining basic ideas of the numeric approach that are also relevant for more complicated hyperbolic PDEs.

Replacing the derivatives by difference quotients as before, we obtain from (1) [see (6) in Sec. 21.4 with $y = t$]

$$(5) \qquad \frac{1}{k^2}(u_{i,j+1} - 2u_{ij} + u_{i,j-1}) = \frac{1}{h^2}(u_{i+1,j} - 2u_{ij} + u_{i-1,j})$$

where h is the mesh size in x, and k is the mesh size in t. This difference equation relates 5 points as shown in Fig. 470a. It suggests a rectangular grid similar to the grids for

parabolic equations in the preceding section. We choose $r^* = k^2/h^2 = 1$. Then u_{ij} drops out and we have

(6) $$u_{i,j+1} = u_{i-1,j} + u_{i+1,j} - u_{1,j-1}$$ (Fig. 470b).

It can be shown that for $0 < r^* \leqq 1$ the present **explicit method** is stable, so that from (6) we may expect reasonable results for initial data that have no discontinuities. (For a hyperbolic PDE the latter would propagate into the solution domain—a phenomenon that would be difficult to deal with on our present grid. For unconditionally stable **implicit methods** see [E1] in App. 1.)

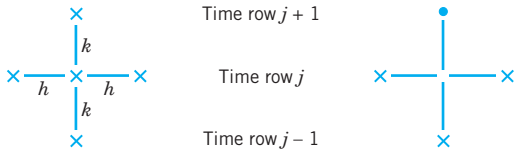


Fig. 470. Mesh points used in (5) and (6)

Equation (6) still involves 3 time steps $j-1, j, j+1$, whereas the formulas in the parabolic case involved only 2 time steps. Furthermore, we now have 2 initial conditions. So we ask how we get started and how we can use the initial condition (3). This can be done as follows.

From $u_t(x, 0) = g(x)$ we derive the difference formula

(7) $$\frac{1}{2k}(u_{i1} - u_{i,-1}) = g_i, \qquad \text{hence} \qquad u_{i,-1} = u_{i1} - 2kg_i$$

where $g_i = g(ih)$. For $t = 0$, that is, $j = 0$, equation (6) is

$$u_{i1} = u_{i-1,0} + u_{i+1,0} - u_{i,-1}.$$

Into this we substitute $u_{i,-1}$ as given in (7). We obtain $u_{i1} = u_{i-1,0} + u_{i+1,0} - u_{i1} + 2kg_i$ and by simplification

(8) $$u_{i1} = \tfrac{1}{2}(u_{i-1,0} + u_{i+1,0}) + kg_i,$$

This expresses u_{i1} in terms of the initial data. It is for the beginning only. Then use (6).

EXAMPLE 1 Vibrating String, Wave Equation

Apply the present method with $h = k = 0.2$ to the problem (1)–(4), where

$$f(x) = \sin \pi x, \qquad g(x) = 0.$$

Solution. The grid is the same as in Fig. 468, Sec. 21.6, except for the values of t, which now are $0.2, 0.4, \cdots$ (instead of $0.04, 0.08, \cdots$). The initial values $u_{00}, u_{10}, \cdots$ are the same as in Example 1, Sec. 21.6. From (8) and $g(x) = 0$ we have

$$u_{i1} = \tfrac{1}{2}(u_{i-1,0} + u_{i+1,0}).$$

From this we compute, using $u_{10} = u_{40} = \sin 0.2\pi = 0.587785$, $u_{20} = u_{30} = 0.951057$,

$$(i = 1) \quad u_{11} = \tfrac{1}{2}(u_{00} + u_{20}) = \tfrac{1}{2} \cdot 0.951057 = 0.475528$$

$$(i = 2) \quad u_{21} = \tfrac{1}{2}(u_{10} + u_{30}) = \tfrac{1}{2} \cdot 1.538842 = 0.769421$$

and $u_{31} = u_{21}$, $u_{41} = u_{11}$ by symmetry as in Sec. 21.6, Example 1. From (6) with $j = 1$ we now compute, using $u_{01} = u_{02} = \cdots = 0$,

$$(i = 1) \quad u_{12} = u_{01} + u_{21} - u_{10} = 0.769421 - 0.587785 = 0.181636$$

$$(i = 2) \quad u_{22} = u_{11} + u_{31} - u_{20} = 0.475528 + 0.769421 - 0.951057 = 0.293892,$$

and $u_{32} = u_{22}$, $u_{42} = u_{12}$ by symmetry; and so on. We thus obtain the following values of the displacement $u(x, t)$ of the string over the first half-cycle:

t	$x = 0$	$x = 0.2$	$x = 0.4$	$x = 0.6$	$x = 0.8$	$x = 1$
0.0	0	0.588	0.951	0.951	0.588	0
0.2	0	0.476	0.769	0.769	0.476	0
0.4	0	0.182	0.294	0.294	0.182	0
0.6	0	−0.182	−0.294	−0.294	−0.182	0
0.8	0	−0.476	−0.769	−0.769	−0.476	0
1.0	0	−0.588	−0.951	−0.951	−0.588	0

These values are exact to 3D (3 decimals), the exact solution of the problem being (see Sec. 12.3)

$$u(x, t) = \sin \pi x \cos \pi t.$$

The reason for the exactness follows from d'Alembert's solution (4), Sec. 12.4. (See Prob. 4, below.) ■

This is the end of Chap. 21 on numerics for ODEs and PDEs, a field that continues to develop rapidly in both applications and theoretical research. Much of the activity in the field is due to the computer serving as an invaluable tool for solving large-scale and complicated practical problems as well as for testing and experimenting with innovative ideas. These ideas could be small or major improvements on existing numeric algorithms or testing new algorithms as well as other ideas.

PROBLEM SET 21.7

VIBRATING STRING

1–3 Using the present method, solve (1)–(4) with $h = k = 0.2$ for the given initial deflection $f(x)$ and initial velocity 0 on the given t-interval.

1. $f(x) = x$ if $0 = x < \frac{1}{5}$, $f(x) = \frac{1}{4}(1 - x)$ if $\frac{1}{5} \leqq x \leqq 1$, $0 \leqq t \leqq 1$
2. $f(x) = x^2 - x^3$, $0 \leqq t \leqq 2$
3. $f(x) = 0.2(x - x^2)$, $0 \leqq t \leqq 2$

4. **Another starting formula.** Show that (12) in Sec. 12.4 gives the starting formula

$$u_{i,1} = \frac{1}{2}(u_{i+1,0} + u_{i-1,0}) + \frac{1}{2}\int_{x_i - k}^{x_i + k} g(s)\, ds$$

(where one can evaluate the integral numerically if necessary). In what case is this identical with (8)?

5. **Nonzero initial displacement and speed.** Illustrate the starting procedure when both f and g are not identically

zero, say, $f(x) = 1 - \cos 2\pi x$, $g(x) = x(1 - x)$, $h = k = 0.1$, 2 time steps.

6. Solve (1)–(3) ($h = k = 0.2$, 5 time steps) subject to $f(x) = x^2$, $g(x) = 2x$, $u_x(0, t) = 2t$, $u(1, t) = (1 + t)^2$.
7. **Zero initial displacement.** If the string governed by the wave equation (1) starts from its equilibrium position with initial velocity $g(x) = \sin \pi x$, what is its displacement at time $t = 0.4$ and $x = 0.2, 0.4, 0.6, 0.8$? (Use the present method with $h = 0.2$, $k = 0.2$. Use (8). Compare with the exact values obtained from (12) in Sec. 12.4.)
8. Compute approximate values in Prob. 7, using a finer grid ($h = 0.1$, $k = 0.1$), and notice the increase in accuracy.
9. Compute u in Prob. 5 for $t = 0.1$ and $x = 0.1, 0.2, \cdots, 0.9$, using the formula in Prob. 8, and compare the values.
10. Show that from d'Alembert's solution (13) in Sec.12.4 with $c = 1$ it follows that (6) in the present section gives the exact value $u_{i,j+1} = u(ih, (j + 1)h)$.

CHAPTER 21 REVIEW QUESTIONS AND PROBLEMS

1. Explain the Euler and improved Euler methods in geometrical terms. Why did we consider these methods?
2. How did we obtain numeric methods from the Taylor series?
3. What are the local and the global orders of a method? Give examples.
4. Why did we compute auxiliary values in each Runge–Kutta step? How many?
5. What is adaptive integration? How does its idea extend to Runge–Kutta?
6. What are one-step methods? Multistep methods? The underlying ideas? Give examples.
7. What does it mean that a method is not self-starting? How do we overcome this problem?
8. What is a predictor–corrector method? Give an important example.
9. What is automatic step size control? When is it needed? How is it done in practice?
10. How do we extend Runge–Kutta to systems of ODEs?
11. Why did we have to treat the main types of PDEs in separate sections? Make a list of types of problems and numeric methods.
12. When and how did we use finite differences? Give as many details as you can remember without looking into the text.
13. How did we approximate the Laplace and Poisson equations?
14. How many initial conditions did we prescribe for the wave equation? For the heat equation?
15. Can we expect a difference equation to give the exact solution of the corresponding PDE?
16. In what method for PDEs did we have convergence problems?
17. Solve $y' = y$, $y(0) = 1$ by Euler's method, 10 steps, $h = 0.1$.
18. Do Prob. 17 with $h = 0.01$, 10 steps. Compute the errors. Compare the error for $x = 0.1$ with that in Prob. 17.
19. Solve $y' = 1 + y^2$, $y(0) = 0$ by the improved Euler method, $h = 0.1$, 10 steps.
20. Solve $y' + y = (x + 1)^2$, $y(0) = 3$ by the improved Euler method, 10 steps with $h = 0.1$. Determine the errors.
21. Solve Prob. 19 by RK with $h = 0.1$, 5 steps. Compute the error. Compare with Prob. 19.
22. **Fair comparison.** Solve $y' = 2x^{-1}\sqrt{y - \ln x} + x^{-1}$, $y(1) = 0$ for $1 \leqq x \leqq 1.8$ **(a)** by the Euler method with $h = 0.1$, **(b)** by the improved Euler method with $h = 0.2$, and **(c)** by RK with $h = 0.4$. Verify that the exact solution is $y = (\ln x)^2 + \ln x$. Compute and compare the errors. Why is the comparison fair?
23. Apply the Adams–Moulton method to $y' = \sqrt{1 - y^2}$, $y(0) = 0$, $h = 0.2$, $x = 0, \cdots, 1$, starting with 0.198668, 0.389416, 0.564637.
24. Apply the A–M method to $y' = (x + y - 4)^2$, $y(0) = 4$, $h = 0.2$, $x = 0, \cdots, 1$, starting with 4.00271, 4.02279, 4.08413.
25. Apply Euler's method for systems to $y'' = x^2 y$, $y(0) = 1$, $y'(0) = 0$, $h = 0.1$, 5 steps.
26. Apply Euler's method for systems to $y_1' = y_2$, $y_2' = -4y_1$, $y_1(0) = 2$, $y_2(0) = 0$, $h = 0.2$, 10 steps. Sketch the solution.
27. Apply Runge–Kutta for systems to $y'' + y = 2e^x$, $y(0) = 0$, $y'(0) = 1$, $h = 0.2$, 5 steps. Determine the errors.
28. Apply Runge–Kutta for systems to $y_1' = 6y_1 + 9y_2$, $y_2' = y_1 + 6y_2$, $y_1(0) = -3$, $y_2(0) = -3$, $h = 0.05$, 3 steps.