

Partial Differential Equations

Three types of PDEs: elliptic, parabolic, and hyperbolic

Examples:

Poisson equation $\nabla^2 \phi(\mathbf{r}) = -\rho(\mathbf{r})/\epsilon_0$ elliptic

Diffusion equation $\frac{\partial n(\mathbf{r}, t)}{\partial t} - \nabla \cdot D(\mathbf{r}) \nabla n(\mathbf{r}, t) = S(\mathbf{r}, t)$ parabolic

Time-dependent Schrodinger equation

$$-\frac{\hbar}{i} \frac{\partial \Psi(\mathbf{r}, t)}{\partial t} = \mathcal{H} \Psi(\mathbf{r}, t)$$

Wave equation $\frac{1}{c^2} \frac{\partial^2 u(\mathbf{r}, t)}{\partial t^2} - \nabla^2 u(\mathbf{r}, t) = R(\mathbf{r}, t)$ hyperbolic

Solution of the PDE

Separation of Variables

Basic idea: transform the PDE to a set of equations with fewer variables

Consider a simple wave equation

$$\frac{\partial^2 u(x, t)}{\partial t^2} - c^2 \frac{\partial^2 u(x, t)}{\partial x^2} = 0.$$

Assume the solution is of the form $u(x, t) = X(x)\Theta(t)$

The wave equation becomes $\frac{\Theta''(t)}{\Theta(t)} = c^2 \frac{X''(x)}{X(x)} = -\omega^2$

Thus $X''(x) = -\frac{\omega^2}{c^2} X(x) = -k^2 X(x)$

and the solution is $X(x) = A \sin kx + B \cos kx$.

Similarly, one can obtain the solution for $\Theta(t)$

Solution of the PDE

Discretization of the PDE

Basic scheme:

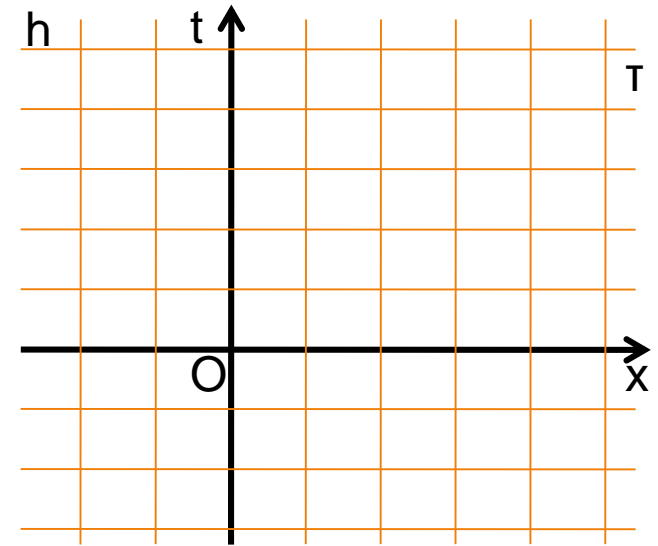
- Construct the lattice
- Use finite difference to replace derivatives
- Find solution at lattice points

$$f'(x_i) = \lim_{\Delta x \rightarrow 0} \frac{f(x_i + \Delta x) - f(x_i)}{\Delta x}$$

$$f'_i = \frac{f_{i+1} - f_i}{h} + O(h)$$

$$f'_i = \frac{f_{i+1} - f_{i-1}}{2h} + O(h^2)$$

$$f''_i = \frac{f_{i+1} - 2f_i + f_{i-1}}{h^2} + O(h^2)$$



Solution of the PDE

The matrix method i.e, $u_0 = u_{n+1} = 0$

Example: Consider a person sitting at the middle of a bench supported at both ends

Newton's equation: $YI \frac{d^2 u(x)}{dx^2} = f(x)$

Discretize the equation with evenly spaced intervals, $x_0 = 0, x_1 = h, \dots, x_{n+1} = L$

and use the three-point formula for the second-order derivative,

$$\Delta_2 = \frac{u_{i+1} - 2u_i + u_{i-1}}{h^2} = u_i'' + \frac{h^2 u_i^{(4)}}{12} + O(h^4).$$

Then

$$u_{i+1} - 2u_i + u_{i-1} = \frac{h^2 f_i}{YI}$$

With the boundary conditions

$$u(0) = u(L) = 0$$

for $i = 0, 1, \dots, n + 1$, which is equivalent to

$$\text{i.e, } u_0 = u_{n+1} = 0$$

$$\begin{pmatrix} -2 & 1 & \dots & \dots & 0 \\ 1 & -2 & 1 & \dots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & \dots & 0 & 1 & -2 \end{pmatrix} \begin{pmatrix} u_1 \\ u_2 \\ \vdots \\ u_n \end{pmatrix} = \begin{pmatrix} b_1 \\ b_2 \\ \vdots \\ b_n \end{pmatrix}$$

Solution of the PDE

The matrix method

The force distribution on the bench is given by

$$f(x) = \begin{cases} -f_0[e^{-(x-L/2)^2/x_0^2} - e^{-1}] - \rho g & \text{for } |x - L/2| \leq x_0 \\ -\rho g & \text{otherwise,} \end{cases}$$

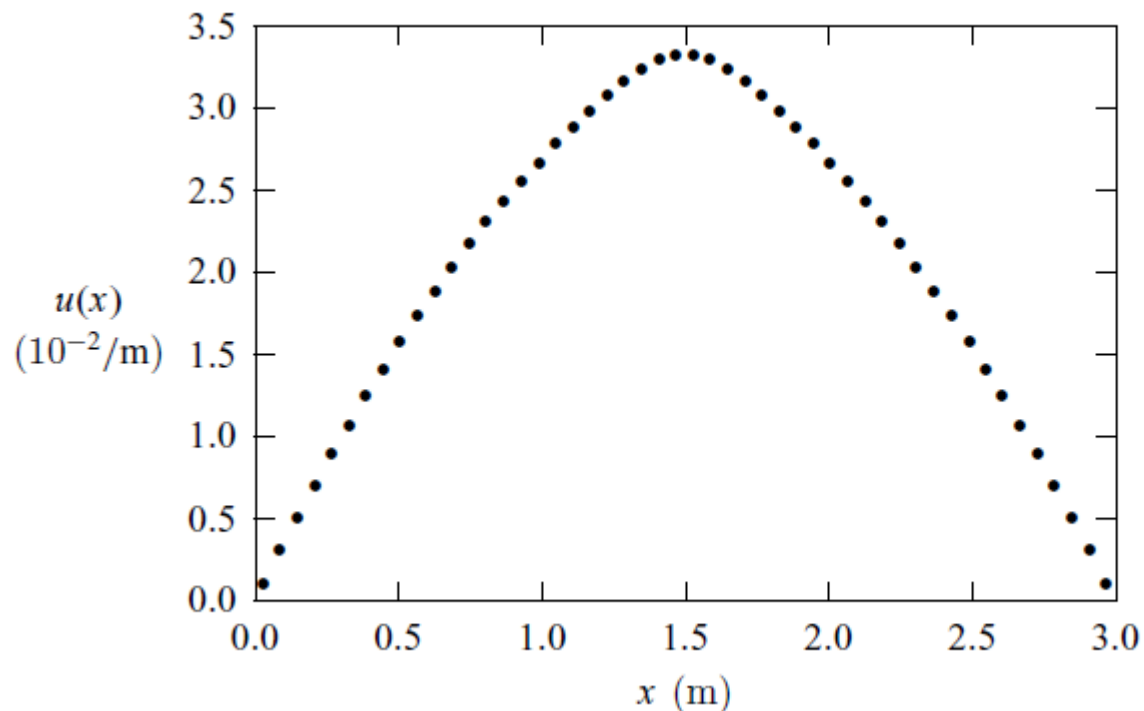


Fig. 7.1 The curvature of the bench, as evaluated with the program given.

Solution of the PDE --- The Relaxation Method

Basic scheme:

- Set up difference equations by discretizing the PDE
- Input an initial guess for the solution
- Perform iteration to obtain converged solution

Example: Consider the bench problem again $YI \frac{d^2 u(x)}{dx^2} = f(x)$

Use the three-point formula to replace the second derivative

$$u_i'' = \frac{u_{i+1} - 2u_i + u_{i-1}}{h^2}$$

$$\longrightarrow u_{i+1} - 2u_i + u_{i-1} = \frac{h^2 f_i}{YI} \longrightarrow u_i = \frac{1}{2} \left(u_{i+1} + u_{i-1} - \frac{h^2 f_i}{YI} \right) \quad (1)$$

Iteration scheme: $u_i^{k+1} = (1-p)u_i^k + pu_i$

where p is an adjustable parameter in the range $[0, 2]$,

u_i^k is the solution of the k th iteration at the i th lattice point, and u_i is calculated from Eq. (1)

with the terms on the right-hand side using the result of k th iteration

```
// A program to solve the problem of a person sitting  
// on a bench with the relaxation scheme.
```

```
// Evaluate the source in the equation  
for (int i=0; i<=n; ++i) {  
    s[i] = rho*g;  
    x = h*i-l2;  
    if (Math.abs(x) < x0)  
        s[i] += f0*(Math.exp(-x*x/x2)-e0);  
    s[i] *= h2/y;  
}  
for (int i=1; i<n; ++i) {  
    x = Math.PI*h*i/l;  
    u[i] = u0*Math.sin(x);  
    d[i] = 1;  
}  
d[0] = d[n] = 1;  
relax(u, d, s, p, del, nmax);
```

$$u_{i+1} - 2u_i + u_{i-1} = \frac{h^2 f_i}{YI}$$

$$u_i = \frac{1}{2} \left(u_{i+1} + u_{i-1} - \frac{h^2 f_i}{YI} \right)$$

Define the initial guessed solution
that satisfies the boundary condition

```
// Method to complete one step of relaxation.
public static void relax(double u[], double d[],
    double s[], double p, double del, int nmax) {
    int n = u.length-1;
    double q = 1-p, fi = 0;
    double du = 2*del;
    int k = 0;

    while ((du>del) && (k<nmax)) {
        du = 0;
        for (int i=1; i<n; ++i) {
            fi = u[i];
            u[i] = p*u[i]
                +q*((d[i+1]+d[i])*u[i+1]
                +(d[i]+d[i-1])*u[i-1]+2*s[i])/(4*d[i]));
            fi = u[i]-fi;
            du += fi*fi;
        }
        du = Math.sqrt(du/n);
        k++;
    }
    if (k==nmax) System.out.println("Convergence not " +
        " found after " + nmax + " iterations");
}
```

$$u_i^{k+1} = (1 - p)u_i^k + pu_i$$

$$u_i = \frac{1}{2} (u_{i+1} + u_{i-1} - \frac{h^2 f_i}{YI})$$

(Ds are constant
p and q are reversed)

Solution of the PDE --- The Relaxation Method

For a 2D case, consider the Poisson equation $\nabla^2 \phi(\mathbf{r}) = -\rho(\mathbf{r})/\epsilon_0 = -s(\mathbf{r})$

Assuming rectangular boundaries, we have

$$\frac{\phi_{i+1j} + \phi_{i-1j} - 2\phi_{ij}}{h_x^2} + \frac{\phi_{ij+1} + \phi_{ij-1} - 2\phi_{ij}}{h_y^2} = -s_{ij}$$

The above equation can be rearranged to

$$\phi_{ij} = \frac{1}{2(1 + \alpha)} [\phi_{i+1j} + \phi_{i-1j} + \alpha(\phi_{ij+1} + \phi_{ij-1}) + h_x^2 s_{ij}], \quad (7.76) \quad \text{with } \alpha = (h_x/h_y)^2$$

A converged solution can be obtained by using the iterative scheme

$$\phi_{ij}^{(k+1)} = (1 - p)\phi_{ij}^{(k)} + p\phi_{ij}$$

where p is an adjustable parameter close to 1. Here $\phi_{ij}^{(k)}$ is the result of the k th iteration, and ϕ_{ij} is obtained from Eq. (7.76) with $\phi_{ij}^{(k)}$ used on the right-hand side.

An example of flow cart

