Prof. Mark D Shattuck
Physics 39907 Computational Physics
October 17, 2024

Finite difference Boundary Conditions

1. Dirichlet boundary conditions (Fixed-Fixed)

Consider the special matrix K:

$$K = \begin{bmatrix} 2 & -1 & 0 & 0 & 0 & \dots & 0 \\ -1 & 2 & -1 & 0 & 0 & \dots & 0 \\ 0 & -1 & 2 & -1 & 0 & & \vdots \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & \dots & 0 & -1 & 2 & -1 & 0 \\ 0 & \dots & 0 & 0 & -1 & 2 & -1 \\ 0 & \dots & 0 & 0 & 0 & -1 & 2 \end{bmatrix}$$

We wish to solve the equation $Ku = h^2 f$ on the interval $[0, 1]$, where u and f are $N \times 1$ vectors with the boundary conditions $u(0) = U_0$ and $u(1) = U_N$. For concreteness let $N = 6$, and $h = \frac{1}{5}$ then:

$$Ku = h^2 f$$

$$\begin{bmatrix} 2 & -1 & 0 & 0 \\ -1 & 2 & -1 & 0 \\ 0 & -1 & 2 & -1 \\ 0 & 0 & -1 & 2 \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \end{bmatrix} = h^2 \begin{bmatrix} f_1 \\ f_2 \\ f_3 \\ f_4 \end{bmatrix}$$

with boundary conditions:

$$u_0 = U_0$$
$$u_5 = U_N$$

First create the extended system:

$$\begin{bmatrix} \color{red}{-1} & 2 & -1 & 0 & 0 & \color{red}{0} \\ \color{red}{0} & -1 & 2 & -1 & 0 & \color{red}{0} \\ \color{red}{0} & 0 & -1 & 2 & -1 & \color{red}{0} \\ \color{red}{0} & 0 & 0 & -1 & 2 & \color{red}{-1} \end{bmatrix} \begin{bmatrix} \color{red}{u_0} \\ u_1 \\ u_2 \\ u_3 \\ u_4 \\ \color{red}{u_5} \end{bmatrix} = h^2 \begin{bmatrix} f_1 \\ f_2 \\ f_3 \\ f_4 \end{bmatrix}$$

This gives 2 additional equations:

$$\begin{bmatrix} -1 & 2 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 2 & -1 \end{bmatrix} \begin{bmatrix} u_0 \\ u_1 \\ u_2 \\ u_3 \\ u_4 \\ u_5 \end{bmatrix} = h^2 \begin{bmatrix} f_1 \\ f_4 \end{bmatrix}$$

$$-u_0 + 2u_1 - u_2 = h^2 f_1$$

$$-u_3 + 2u_4 - u_5 = h^2 f_4$$

substituting:

$$u_0 = U_0$$

$$u_5 = U_N$$

gives:

$$-U_0 + 2u_1 - u_2 = h^2 f_1$$

$$2u_1 - u_2 = h^2 \left(f_1 + \frac{U_0}{h^2} \right)$$

$$-u_3 + 2u_4 - U_N = h^2 f_4$$

$$-u_3 + 2u_4 = h^2 \left(f_4 + \frac{U_N}{h^2} \right)$$

These equations can be incorporated into the matrix version:

$$\begin{bmatrix} 2 & -1 & 0 & 0 \\ -1 & 2 & -1 & 0 \\ 0 & -1 & 2 & -1 \\ 0 & 0 & -1 & 2 \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \end{bmatrix} = h^2 \begin{bmatrix} f_1 + \frac{U_0}{h^2} \\ f_2 \\ f_3 \\ f_4 + \frac{U_N}{h^2} \end{bmatrix}$$

2. Neumann boundary conditions (Free-Free)

If we wish to solve the equation $Ku = h^2 f$ on the interval $[0,1]$, where u and f are $N \times 1$ vectors with the boundary conditions $u'(0) = D_0$ and $u'(1) = D_N$. For concreteness let $N = 6$, and $h = \frac{1}{5}$ then:

$$Ku = h^2 f$$

$$\begin{bmatrix} 2 & -1 & 0 & 0 & 0 & 0 \\ -1 & 2 & -1 & 0 & 0 & 0 \\ 0 & -1 & 2 & -1 & 0 & 0 \\ 0 & 0 & -1 & 2 & -1 & 0 \\ 0 & 0 & 0 & -1 & 2 & -1 \\ 0 & 0 & 0 & 0 & -1 & 2 \end{bmatrix} \begin{bmatrix} u_0 \\ u_1 \\ u_2 \\ u_3 \\ u_4 \\ u_5 \end{bmatrix} = h^2 \begin{bmatrix} f_0 \\ f_1 \\ f_2 \\ f_3 \\ f_4 \\ f_5 \end{bmatrix}$$

with second-order accurate boundary conditions at u_0 and u_5:

$$\frac{u_1 - u_{-1}}{2h} = D_0$$
$$\frac{u_4 - u_6}{2h} = D_N.$$

Notice in this case u_0 and u_{N-1} are not known so they must be included in the system. Now create the extended system:

$$\begin{bmatrix} -1 & 2 & -1 & 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & 2 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 2 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 2 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & -1 & 2 & -1 & 0 \\ 0 & 0 & 0 & 0 & 0 & -1 & 2 & -1 \end{bmatrix} \begin{bmatrix} u_{-1} \\ u_0 \\ u_1 \\ u_2 \\ u_3 \\ u_4 \\ u_5 \\ u_6 \end{bmatrix} = h^2 \begin{bmatrix} f_0 \\ f_1 \\ f_2 \\ f_3 \\ f_4 \\ f_5 \end{bmatrix}$$

This gives 2 additional equations:

$$\begin{bmatrix} -1 & 2 & -1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -1 & 2 & -1 \end{bmatrix} \begin{bmatrix} u_{-1} \\ u_0 \\ u_1 \\ u_2 \\ u_3 \\ u_4 \\ u_5 \\ u_6 \end{bmatrix} = h^2 \begin{bmatrix} f_1 \\ f_4 \end{bmatrix}$$

$$-u_{-1} + 2u_0 - u_1 = h^2 f_1$$
$$-u_4 + 2u_5 - u_6 = h^2 f_4$$

substituting:

$$u_1 - u_{-1} = 2hD_0$$
$$u_4 - u_6 = 2hD_N$$

gives:

$$
\begin{aligned}
-(u_1 - 2hD_0) + 2u_1 - u_2 &= h^2 f_0 \\
u_0 - u_1 &= h^2 \left(\frac{f_0}{2} - \frac{D_0}{h} \right) \\
-u_4 + 2u_5 - (u_4 - 2hD_0) &= h^2 f_5 \\
-u_4 + u_5 &= h^2 \left(\frac{f_5}{2} - \frac{D_N}{h} \right)
\end{aligned}
$$

These equations can be incorporated into the matrix version:

$$
\begin{bmatrix}
1 & -1 & 0 & 0 & 0 & 0 \\
-1 & 2 & -1 & 0 & 0 & 0 \\
0 & -1 & 2 & -1 & 0 & 0 \\
0 & 0 & -1 & 2 & -1 & 0 \\
0 & 0 & 0 & -1 & 2 & -1 \\
0 & 0 & 0 & 0 & -1 & 1
\end{bmatrix}
\begin{bmatrix} u_0 \\ u_1 \\ u_2 \\ u_3 \\ u_4 \\ u_5 \end{bmatrix}
= h^2
\begin{bmatrix} \frac{f_0}{2} - \frac{D_0}{h} \\ f_1 \\ f_2 \\ f_3 \\ f_4 \\ \frac{f_5}{2} - \frac{D_N}{h} \end{bmatrix}
$$

3. Mixed boundary conditions (Fixed-Free or Free-Fixed)

For mixed boundary conditions you can simply combine; for example, $u(0) = U_0$ and $u'(1) = D_N$:

$$
\begin{bmatrix}
2 & -1 & 0 & 0 & 0 \\
-1 & 2 & -1 & 0 & 0 \\
0 & -1 & 2 & -1 & 0 \\
0 & 0 & -1 & 2 & -1 \\
0 & 0 & 0 & -1 & 1
\end{bmatrix}
\begin{bmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \\ u_5 \end{bmatrix}
= h^2
\begin{bmatrix} f_1 + \frac{U_0}{h^2} \\ f_2 \\ f_3 \\ f_4 \\ \frac{f_5}{2} - \frac{D_N}{h} \end{bmatrix}
$$