Step-1

To obtain the values for u on a three dimensional grid, the differential equation can be replaced by the finite differences:

$$-u_{i+1,j,k} + 2u_{i,j,k} - u_{i-1,j,k} + \left(-u_{i,j+1,k} + 2u_{i,j,k} - u_{i,j-1,k}\right) + \left(-u_{i,j,k+1} + 2u_{i,j,k} - u_{i,j,k-1}\right) = 0$$

Step-2

Note that we are considering the differences along the three directions, x, y, and z. The difference matrix in any one direction is given as follows:

$$A = \begin{bmatrix} 2 & -1 & 0 \\ -1 & 2 & -1 \\ 0 & -1 & 2 \end{bmatrix}$$

At the same time, the identity matrix in any of the other directions is given by,

$$I = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

Step-3

The required matrix is given by the following:

$$A_{3D} = A_{1D} \otimes I \otimes I + I \otimes A_{1D} \otimes I + I \otimes I \otimes A_{1D}$$

Consider the following:

$$\begin{split} A_{\mathrm{1D}} \otimes I \otimes I &= A_{\mathrm{1D}} \otimes \left(I \otimes I \right) \\ &= A_{\mathrm{1D}} \otimes \begin{bmatrix} I & 0 & 0 \\ 0 & I & 0 \\ 0 & 0 & I \end{bmatrix} \\ &= \begin{bmatrix} 2(I \otimes I) & -(I \otimes I) & 0 \\ -(I \otimes I) & 2(I \otimes I) & -(I \otimes I) \\ 0 & -(I \otimes I) & 2(I \otimes I) \end{bmatrix} \end{split}$$

Step-4

Similarly, we get

$$\begin{split} I \otimes A_{\mathrm{1D}} \otimes I &= I \otimes \left(A_{\mathrm{1D}} \otimes I\right) \\ &= I \otimes \begin{bmatrix} 2I & -I & 0 \\ -I & 2I & -I \\ 0 & -I & 2I \end{bmatrix} \\ &= \begin{bmatrix} A_{\mathrm{1D}} \otimes I & 0 & 0 \\ 0 & A_{\mathrm{1D}} \otimes I & 0 \\ 0 & 0 & A_{\mathrm{1D}} \otimes I \end{bmatrix} \end{split}$$

Step-5

Finally, we have

$$\begin{split} I \otimes I \otimes A_{\mathrm{ID}} &= I \otimes \left(I \otimes A_{\mathrm{ID}} \right) \\ &= I \otimes \begin{bmatrix} A & 0 & 0 \\ 0 & A & 0 \\ 0 & 0 & A \end{bmatrix} \\ &= \begin{bmatrix} I \otimes A_{\mathrm{ID}} & 0 & 0 \\ 0 & I \otimes A_{\mathrm{ID}} & 0 \\ 0 & 0 & I \otimes A_{\mathrm{ID}} \end{bmatrix} \end{split}$$

Step-6

Thus, the required matrix is given by,

$$\begin{split} A_{\mathrm{3D}} &= A_{\mathrm{1D}} \otimes I \otimes I + I \otimes A_{\mathrm{1D}} \otimes I + I \otimes I \otimes A_{\mathrm{1D}} \\ &= \begin{bmatrix} 2\left(I \otimes I\right) & -\left(I \otimes I\right) & 0 \\ -\left(I \otimes I\right) & 2\left(I \otimes I\right) & -\left(I \otimes I\right) \\ 0 & -\left(I \otimes I\right) & 2\left(I \otimes I\right) \end{bmatrix} + \begin{bmatrix} A_{\mathrm{1D}} \otimes I & 0 & 0 \\ 0 & A_{\mathrm{1D}} \otimes I & 0 \\ 0 & 0 & A_{\mathrm{1D}} \otimes I \end{bmatrix} + \\ & \begin{bmatrix} I \otimes A_{\mathrm{1D}} & 0 & 0 \\ 0 & I \otimes A_{\mathrm{1D}} & 0 \\ 0 & 0 & I \otimes A_{\mathrm{1D}} \end{bmatrix} \end{split}$$

That is,

$$\begin{bmatrix} 2\big(I\otimes I\big) + A_{\mathsf{ID}}\otimes I + I\otimes A_{\mathsf{ID}} & -\big(I\otimes I\big) & 0 \\ -\big(I\otimes I\big) & 2\big(I\otimes I\big) + A_{\mathsf{ID}}\otimes I + I\otimes A_{\mathsf{ID}} & -\big(I\otimes I\big) \\ 0 & -\big(I\otimes I\big) & 2\big(I\otimes I\big) + A_{\mathsf{ID}}\otimes I + I\otimes A_{\mathsf{ID}} \end{bmatrix}$$