MAT3005 - Applied Numerical Methods

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Introduction

- Recall that A *partial differential equation* is a differential equation involving more than one independent variable, so that the derivatives occurring in it are partial derivatives.
- Partial differential equations has many applications in physics, chemistry and biology.
- These equations are used to describe physical/biological phenomena such as sound, heat, electrostatics, electrodynamics, fluid/blood flow or elasticity.
- Most of these problems can be formulated as second-order partial differential equations.
- Only some of the partial differential equations can be solved analytically and in most cases, we depend on the numerical solution of PDEs.

Introduction

- Most of the numerical schemes used to solve the PDEs are based on finite differences.
- In this method, the derivatives appearing in the equation and the boundary conditions are replaced by their finite-difference approximations.
- Then the given equation is changed to a difference equation which is solved by iterative procedures.

Classification of second order PDEs

- The general linear PDE of the second order in two independent variables is of the form:

$$A\frac{\partial^2 u}{\partial x^2} + B\frac{\partial^2 u}{\partial x \partial y} + C\frac{\partial^2 u}{\partial y^2} + D\frac{\partial u}{\partial x} + E\frac{\partial u}{\partial y} + Fu = G$$

  where A, B, C, D, E, F and G are functions of x and y.
- The above equation can also be written as

$$Au_{xx} + Bu_{xy} + Cu_{yy} + Du_x + Eu_y + Fu = G \tag{1}$$

- Depending on the values of these coefficients the above equation is classified into one of the three following types:
  - **Elliptic:** if $B^2 - 4AC < 0$,
  - **Hyperbolic:** if $B^2 - 4AC > 0$,
  - **Parabolic:** if $B^2 - 4AC = 0$.

PDE Classification

The partial differential equation

$$xu_{xx} + u_{yy} = 0$$

is

- elliptic if $x > 0$,
- hyperbolic if $x < 0$,
- parabolic if $x = 0$.

Numerical Methods for Solving PDE

In the present analysis we restrict ourselves to three simple particular cases of Eq. (1), namely

Laplace Equation:

$$u_{xx} + u_{yy} = 0$$

Wave Equation:

$$c^2 u_{xx} - u_{tt} = 0$$

Heat Conduction Equation:

$$u_{xx} - u_t = 0$$

Well-posed and ill-posed problems

The region on which the PDE defined plays an important role in the classification of PDEs. In the study of PDEs, usually three types of problems arise:

- ***Dirchlet's problem:*** Given a continuous function f on the boundary C of a region R, to find a function u satisfying the Laplace equation in R i.e., to find u such that

$$\left.\begin{aligned} u_{xx} + u_{yy} &= 0 \text{ in } R \\ u &= f \text{ on } C \end{aligned}\right\} \tag{2}$$

Well-posed and ill-posed problems

- ***Cauchy's problem:***

$$\left.\begin{aligned} u_{tt} - u_{xx} &= 0 \text{ for } t > 0 \\ u(x,0) &= f(x) \\ u_t(x,0) &= g(x) \end{aligned}\right\} \tag{3}$$

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$$\left.\begin{aligned} u_t - u_{xx} &= 0 \text{ for } t > 0 \\ u(x,0) &= f(x) \end{aligned}\right\} \tag{4}$$

The above problems are all *well-posed* i.e., posses unique solutions.

Well-posed and ill-posed problems

- The problems which are not well-posed are called ill-posed problems.
- In contrast to ODE, the form of a PDE is always connected with a particular type of associated conditions. Thus, the problem of Laplace's equation with Cauchy boundary conditions defined by

$$\left.\begin{aligned} u_{xx} + u_{yy} &= 0 \text{ in } R \\ u(x,0) &= f(x) \\ u_y(x,0) &= g(x) \end{aligned}\right\} \tag{5}$$

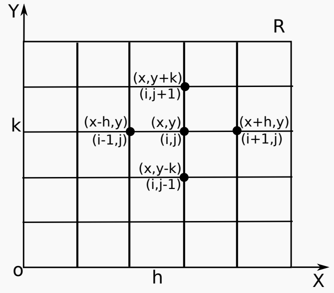
is an ill-posed problem.

Finite-difference approximations to derivatives

- Consider a rectangular region R in the $xy-$plane.
- Divide this region into a rectangular mesh of sides $\Delta x = h$ and $\Delta y = k$ by drawing the set of lines

$$x = ih, i = 0, 1, 2, \ldots \text{ and } y = jk, j = 0, 1, 2, \ldots$$

as shown in the figure.



- The points of intersection of the dividing lines are called *mesh points*, *nodal points*, or *grid points*.

Finite-difference approximations to derivatives

- We write $u(x,y) = u(ih, jk)$ as simply $u_{i,j}$.
- Then we have the finite difference approximations for the partial derivatives in $x-$direction are:

$$u_x = \frac{u_{i+1,j} - u_{i,j}}{h} + O(h)$$

$$u_x = \frac{u_{i,j} - u_{i-1,j}}{h} + O(h)$$

$$u_x = \frac{u_{i+1,j} - u_{i-1,j}}{2h} + O(h^2)$$

and

$$u_{xx} = \frac{u_{i-1,j} - 2u_{i,j} + u_{i+1,j}}{h^2} + O(h^2)$$

where $u_{i,j} = u(ih, jk) = u(x,y)$.

Finite-difference approximations to derivatives

- Similarly we have the finite difference approximations for the partial derivatives in $y-$direction are:

$$u_y = \frac{u_{i,j+1} - u_{i,j}}{k} + O(k)$$

$$u_y = \frac{u_{i,j} - u_{i,j-1}}{k} + O(k)$$

$$u_y = \frac{u_{i,j+1} - u_{i,j-1}}{2k} + O(k^2)$$

and

$$u_{yy} = \frac{u_{i,j-1} - 2u_{i,j} + u_{i,j+1}}{k^2} + O(k^2)$$

where $u_{i,j} = u(ih, jk) = u(x,y)$.

Elliptic PDEs

- The Laplace's equation:

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

- and the Poisson's equation:

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = f(x, y)$$

  are examples of elliptic partial differential equations.
- Laplace's equation arises in steady-state flow and potential problems.
- Poisson's equation arises in fluid mechanics, electricity, magnetism and torsion problems.
- Poisson's equation is generalization of Laplace's equation.

Numerical Solution of Laplace's equation

Substituting the finite difference of u_{xx} and u_{yy} in the Laplace equation $u_{xx} + u_{yy} = 0$, we obtain

$$\frac{1}{h^2}\left(u_{i+1,j} - 2u_{i,j} + u_{i-1,j}\right) + \frac{1}{k^2}\left(u_{i,j+1} - 2u_{i,j} + u_{i,j-1}\right) = 0 \qquad (6)$$

If $h = k$, then we have

$$u_{i,j} = \frac{1}{4}\left(u_{i+1,j} + u_{i-1,j} + u_{i,j+1} + u_{i,j-1}\right) \qquad (7)$$

i.e., the value of u at any point is the mean of its values at the four neighbouring points. This is called the *standard five-point formula*.

Numerical Solution of Laplace's equation

The above formula can also be written as

$$u_{i,j} = \frac{1}{4}\left(u_{i-1,j-1} + u_{i+1,j-1} + u_{i+1,j+1} + u_{i-1,j+1}\right) \qquad (8)$$

and called *diagonal five-point formula*.

By applying the above five-point standard formula at each mesh-point, we arrive at linear equations in the pivotal values i, j.

Once all the $u_i (i = 1, 2, 3, \dots)$ are computed, their accuracy can be improved by any of the iterative methods described below.

Numerical Solution of Laplace's equation

Jacobi's Method: Let $u_{i,j}^{(n)}$ denotes the nth iterative value of $u_{i,j}$. An iterative procedure to solve five-point standard formula is given by

$$u_{i,j}^{(n+1)} = \frac{1}{4}\left(u_{i-1,j}^{(n)} + u_{i+1,j}^{(n)} + u_{i,j-1}^{(n)} + u_{i,j+1}^{(n)}\right) \qquad (9)$$

Gauss-Seidel Method: In this method we use the latest iterative values available and scans the mesh points systematically from left to right along the successive rows. The iterative formula is:

$$u_{i,j}^{(n+1)} = \frac{1}{4}\left(u_{i-1,j}^{(n+1)} + u_{i+1,j}^{(n)} + u_{i,j-1}^{(n+1)} + u_{i,j+1}^{(n)}\right) \qquad (10)$$

Numerical Solution of Poisson's equation

- The Poisson's equation can be solved numerically by using the standard 5− point formula given by

$$u_{i-1,j} + u_{i+1,j} + u_{i,j+1} + u_{i,j-1} - 4u_{i,j} = h^2 f(ih, jh).$$

Exercise Problem

Example

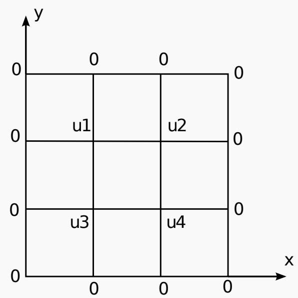
Solve the partial differential equation

$$\nabla^2 u = -10(x^2 + y^2 + 10)$$

over the square with sides $x = 0 = y$, $x = 3 = y$ with $u = 0$ on the boundary and with mesh length $h = k = 1$.

Solution

The mesh formulation by taking $h = 1$ is shown in the below figure:



The standard 5−point formula for the given equation is given by

$$u_{i-1,j} + u_{i+1,j} + u_{i,j+1} + u_{i,j-1} - 4u_{i,j} = -10(i^2 + j^2 + 10) \qquad (*).$$

Solution

For u_1, we have $i = 1, j = 2$ and therefore, $(*)$ gives

$$0 + u_2 + 0 + u_3 - 4u_1 = -10(1 + 4 + 10)$$

Therefore,

$$u_1 = \frac{1}{4}(u_2 + u_3 + 150) \qquad (1)$$

For u_2, we have $i = 2, j = 2$ and therefore, $(*)$ gives

$$u_1 + 0 + 0 + u_4 - 4u_2 = -10(4 + 4 + 10)$$

Therefore,

$$u_2 = \frac{1}{4}(u_1 + u_4 + 180) \qquad (2)$$

Solution

For u_3, we have $i = 1, j = 1$ and therefore, $(*)$ gives

$$0 + u_4 + u_1 + 0 - 4u_3 = -10(1 + 1 + 10)$$

Therefore,

$$u_3 = \frac{1}{4}(u_1 + u_4 + 120) \tag{3}$$

For u_4, we have $i = 2, j = 1$ and therefore, $(*)$ gives

$$u_3 + 0 + u_2 + 0 - 4u_4 = -10(4 + 1 + 10)$$

Therefore,

$$u_4 = \frac{1}{4}(u_2 + u_3 + 150) \tag{4}$$

Solution

Equations (1) and (4) shows that $u_1 = u_4$. Thus, the above equations reduce to

$$u_1 = \frac{1}{4}(u_2 + u_3 + 150)$$
$$u_2 = \frac{1}{2}(u_1 + 90)$$
$$u_3 = \frac{1}{2}(u_1 + 60)$$

Now, solving the above equations by Gauss-Seidel iteration method, we obtain

$$u_1 = 75, u_2 = 82.5, u_3 = 67.5, u_4 = 75.$$

Parabolic Equations

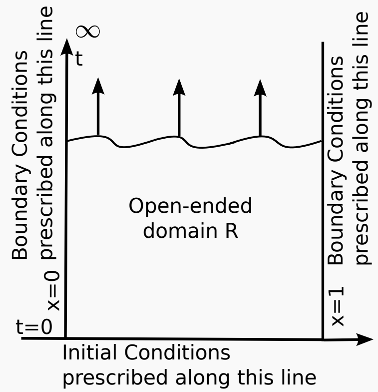
- The one-dimensional heat conduction equation

$$\frac{\partial u}{\partial t} = c^2 \frac{\partial^2 u}{\partial x^2}$$

  (where c^2 is the diffusivity of the substance (cm^2/sec)) is a well-known example of parabolic PDE.
- The solution of this equation is a temperature function $u(x, t)$ which is defined for $x \in [0, 1]$ and for $t \in [0, \infty)$.

Parabolic Equations

- The solution is not defined in a closed domain but advances in an open-ended region from initial values, satisfying the prescribed boundary conditions.



Explicit Numerical Scheme to Solve Heat Equation

- Consider a recatngular mesh in the $xt-$space with spacing h along $x-$direction and k along $t-$direction.
- Denoting a mesh point $(x, t) = (ih, jk)$ as simply i, j we have

$$\frac{\partial u}{\partial t} = \frac{u_{i,j+1} - u_{i,j}}{k}$$

$$\text{and } \frac{\partial^2 u}{\partial x^2} = \frac{u_{i,j-1} - 2u_{i,j} + u_{i+1,j}}{h^2}$$

- substituting this in the above Heat equation, we obtain

$$u_{i,j+1} = \alpha u_{i-1,j} + (1 - 2\alpha)u_{i,j} + \alpha u_{i+1,j}$$

  where $\alpha = \frac{kc^2}{h^2}$ is the mesh ratio parameter.
- The above formula relates the functions values at two time levels $j + 1$ and j and is therfore, called a *2-level formula*.
- This is also called **Schmidt explicit formula** and is valid only for $0 < \alpha \le \frac{1}{2}$.

Exercise Problems

Example

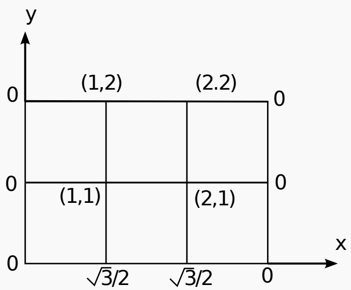
Solve the equation

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2}$$

subject to the conditions $u(x, 0) = \sin \pi x, 0 \le x \le 1; u(0, t) = u(1, t) = 0.$
Carry out computations for two levels taking $h = \frac{1}{3}, k = \frac{1}{36}.$

Solution

Here $c^2 = 1$ and $h = \frac{1}{3}, k = \frac{1}{36}$. Therefore, $\alpha = \frac{kc^2}{h^2} = \frac{1}{4}$.
Given initial condition is $u(x, 0) = \sin \pi x$ for $0 \le x \le 1$. Therefore,
$u_{1,0} = \sin \frac{\pi}{3} = \frac{\sqrt{3}}{2}$ and $u_{2,0} = \sin \frac{2\pi}{3} = \frac{\sqrt{3}}{2}$.
Since, $u(0, t) = u(1, t) = 0$, we have all the boundary values are zero. Thus, the mesh can be pictorially represented as follows:



Solution

Now, Schmidt's formula get reduces to

$$u_{i,j+1} = \frac{1}{4}\left[u_{i-1,j} + 2u_{i,j} + u_{i+1,j}\right].$$

To find $u_{1,1}$: Here $i = 1, j = 0$. So,

$$u_{1,1} = \frac{1}{4}\left[u_{0,0} + 2u_{1,0} + u_{2,0}\right]$$

$$= \frac{1}{4}\left(0 + 2 \times \frac{\sqrt{3}}{2} + \frac{\sqrt{3}}{2}\right) = 0.65$$

Solution

To find $u_{2,1}$: Here $i = 2, j = 0$. So,

$$\begin{aligned} u_{2,1} &= \frac{1}{4}[u_{1,0} + 2u_{2,0} + u_{3,0}] \\ &= \frac{1}{4}\left(\frac{\sqrt{3}}{2} + 2 \times \frac{\sqrt{3}}{2} + 0\right) = 0.65 \end{aligned}$$

To find $u_{1,2}$: Here $i = 1, j = 1$. So,

$$\begin{aligned} u_{1,2} &= \frac{1}{4}[u_{0,1} + 2u_{1,1} + u_{2,1}] \\ &= \frac{1}{4}(0 + 2 \times 0.65 + 0.65) = 0.49 \end{aligned}$$

Solution

To find $u_{2,2}$: Here $i = 2, j = 1$. So,

$$\begin{aligned} u_{2,2} &= \frac{1}{4}[u_{1,1} + 2u_{2,1} + u_{3,1}] \\ &= \frac{1}{4}(0.65 + 2 \times 0.65 + 0) = 0.49 \end{aligned}$$

Crank-Nicolson Implicit Scheme to Solve Parabolic Equations

Consider the heat conduction equation

$$\frac{\partial u}{\partial t} = c^2 \frac{\partial^2 u}{\partial x^2}$$

Using the approximations

$$\frac{\partial u}{\partial t} = \frac{u_{i,j+1} - u_{i,j}}{k}$$

(as in the previous case). We replace $\frac{\partial^2 u}{\partial x^2}$ by average of its finite-difference approximations on the j^{th} and $(j+1)^{\text{th}}$ rows. Thus,

$$\frac{\partial^2 u}{\partial x^2} = \frac{1}{2}\left(\frac{u_{i-1,j} - 2u_{i,j} + u_{i+1,j}}{h^2} + \frac{u_{i-1,j+1} - 2u_{i,j} + u_{i+1,j+1}}{h^2}\right)$$

Crank-Nicolson Implicit Scheme to Solve Parabolic Equations

Substituting these in the heat equation and rearranging the terms, we obtain

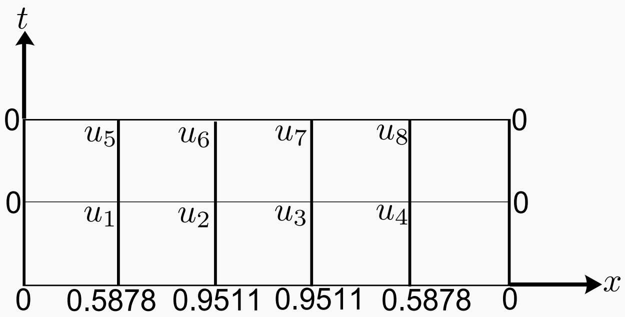
$$-\alpha u_{i-1,j+1} + (2 + 2\alpha)u_{i,j+1} - \alpha u_{i+1,j+1} = \alpha u_{i-1,j} + (2 - 2\alpha)u_{i,j} + \alpha u_{i+1,j},$$

where $\alpha = \frac{kc^2}{h^2}$. This is called *Crank-Nicolson implicit scheme* and is convergent for all values of α.

Crank-Nicolson Implicit Scheme to Solve Parabolic Equations

Example

Solve $u_t = u_{xx}$ subsect to the initial condition $u = \sin \pi x$, at $t = 0$ for $0 \leq x \leq 1$ and the boundary conditions $u = 0$ at $x = 0$ and $x = 1$ for $t > 0$. Taking $h = 0.2$ and $k = 0.04$ compute the values of u at the internal mesh points up to two time steps using Crank-Nicolson implicit scheme.



Solution

We have $c^2 = 1$, $h = 0.2$ and $k = 0.04$, So, $\alpha = \frac{kc^2}{h^2} = 1$. The Crank-Nicolson implicit scheme for $\alpha = 1$ is:

$$u_{i-1,j+1} - 4u_{i,j+1} + u_{i+1,j+1} = -u_{i-1,j} - u_{i+1,j} \qquad (i)$$

Applying (i) at the mesh point u_1, (we have $i = 1, j = 0$) we obtain

$$0 - 4u_1 + u_2 = -0.9511 \qquad (ii)$$

Applying (i) at the mesh point u_2, (we have $i = 2, j = 0$) we obtain

$$u_1 - 4u_2 + u_3 = -0.5878 - 0.9511 = -1.5389 \qquad (iii)$$

Applying (i) at the mesh point u_3, (we have $i = 3, j = 0$) we obtain

$$u_2 - 4u_3 + u_4 = -0.9511 - 0.5878 = -1.5389 \qquad (iv)$$

Applying (i) at the mesh point u_4, (we have $i = 4, j = 0$) we obtain

$$u_3 - 4u_4 + 0 = 0.9511 \qquad (v)$$

Solution

By symmetry, we have $u_1 = u_4$, and $u_2 = u_3$. Hence, Eqs. (ii) to (v) reduce to the two equations:

$$4u_1 - u_2 = 0.9511, \quad u_1 - 3u_2 = -1.5389.$$

Solving, the above two equations we obtain $u_1 = u_4 = 0.3993, u_2 = u_3 = 0.6461$.

For the second time step, applying the formula (i) at the grid points u_5, u_6, u_7 and u_8, we obtain

$$\begin{aligned} -4u_5 + u_6 &= -0.6461 \\ u_5 - 4u_6 + u_7 &= -0.3993 - 0.6461 = -1.0454 \\ u_6 - 4u_7 + u_8 &= -0.6461 - 0.3993 = -1.0454 \\ u_7 - 4u_8 &= -0.6461. \end{aligned}$$

By symmetry, we have $u_5 = u_8$ and $u_6 = u_7$. Hence the above system of equations reduces to the following two equations:

$$-4u_5 + u_6 = -0.6461 \quad u_5 - 3u_6 = -1.0454$$

Solving we obtain $u_5 = u_8 = 0.2712, u_6 = u_7 = 0.4387$.

Crank-Nicolson Implicit Scheme to Solve Parabolic Equations

Example

Solve the heat equation

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2}$$

subject to the conditions

$$u(x, 0) = 0, \quad u(0, t) = 0, \quad u(1, t) = t$$

by taking $k = \frac{1}{8}$ and $h = \frac{1}{2}$.

Hint: The Crank-Nicolson scheme becomes

$$-u_{i-1,j+1} + 6u_{i,j+1} - u_{i+1,j+1} = u_{i-1,j} + 2u_{i,j} + u_{i+1,j}$$

Hyperbolic Equations

We consider the boundary-value problem defined by

$$\frac{\partial^2 u}{\partial t^2} = c^2 \frac{\partial^2 u}{\partial x^2} \tag{11}$$

$$u(x, 0) = f(x) \tag{12}$$

$$u_t(x, 0) = \phi(x) \tag{13}$$

$$u(0, t) = \psi_1(t) \tag{14}$$

$$u(1, t) = \psi_2(t) \tag{15}$$

for $0 \leq t \leq T$, which models the transverse vibrations of a stretched string.

Numerical Scheme to Solve Hyperbolic Equation

Using the finite difference approximations

$$u_{xx} = \frac{1}{h^2}\left(u_{i-1,j} - 2u_{i,j} + u_{i+1,j}\right)$$

and

$$u_{tt} = \frac{1}{k^2}\left(i_{i,j-1} - 2u_{i,j} + u_{i,j+1}\right),$$

where $x = ih, i = 0, 1, 2, \ldots,$ and $t = jk, j = 0, 1, 2, \ldots$

Further, $u_t(x, t)$ is approximated as

$$u_t(x, t) = \frac{u_{i,j+1} - u_{i,j-1}}{2k}$$

in particular, for $u_t(x, 0)$ we have $j = 0$ and that

$$u_t(x, 0) = \frac{u_{i,1} - u_{i,-1}}{2k}.$$

Numerical Scheme to Solve Hyperbolic Equation

Substituting, u_{xx} and u_{tt} in the equation (1) and rearranging the terms, we obtain

$$u_{i,j+1} = -u_{i,j-1} + \alpha^2(u_{i-1,j} + u_{i+1,j}) + 2(1 - \alpha^2)u_{i,j}$$

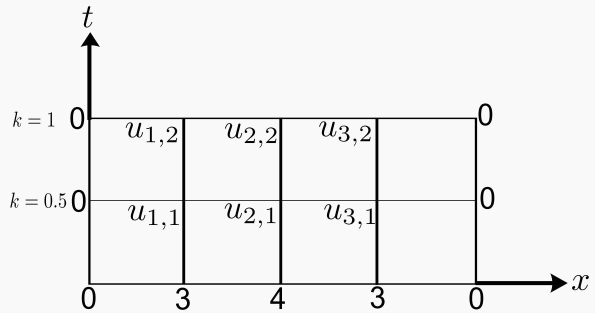
where $\alpha = \frac{ck}{h}$.

The above formula is called *three level* difference scheme as the function values at the j^{th} and $(j-1)^{\text{th}}$ time levels are required in order to determine the values at $(j+1)^{\text{th}}$ time level. This valid for $\alpha < 1$, which is the condition for stability.

Numerical Scheme to Solve Hyperbolic Equation

Example

Solve the BVP $u_{tt} = 4u_{xx}$ subject to the conditions $u(0, t) = 0 = u(4, t), u_t(x, 0) = 0, u(x, 0) = 4x - x^2$, for $0 \leq x \leq 4$, by taking $h = 1$ and $k = 0.5$. Carry out computations for two-levels.



Solution

Given $h = 1$, $k = 0.5$ and we have $c = 2$. So, $\alpha = \frac{ck}{h} = 1$.

Since $u(0, t) = 0 = u(4, t)$ for $0 \leq x \leq 4$, we have $u_{0,j} = u_{4,j} = 0 \forall j$.

Since $u_t(x, 0) = 0$, we have

$$\frac{u_{i,1} - u_{i,-1}}{2k} = 0 \implies u_{i,1} = u_{i,-1} \text{ for } j = 0$$

Finally,

$$u(x, 0) = 4x - x^2 \implies u_{i,0} = 4(ih) - (ih)^2 = 4i - i^2 \text{ (since } h = 1)$$

So,

$$u_{0,0} = 0, u_{1,0} = 3, u_{2,0} = 4, u_{3,0} = 3, u_{4,0} = 0.$$

Solution

For $\alpha = 1$, the explicit scheme for Hyperbolic equations, get reduces to

$$u_{i,j+1} = -u_{i,j-1} + u_{i-1,j} + u_{i+1,j} \qquad (*)$$

At the first time step i.e., $t = 0.5$, we have $j = 0$:

For $j = 0$ we have $u_{i,1} = u_{i,-1}$. So, the above equation $(*)$ reduces to

$$u_{i,1} = -u_{i,-1} + u_{i-1,0} + u_{i+1,0} \implies u_{i,1} = \frac{1}{2}(u_{i-1,0} + u_{i+1,0})$$

So,

$$\begin{aligned} u_{1,1} &= \frac{1}{2}(u_{0,0} + u_{2,0}) = \frac{1}{2}(0 + 4) = 2 \\ u_{2,1} &= \frac{1}{2}(u_{1,0} + u_{3,0}) = \frac{1}{2}(3 + 3) = 3 \\ u_{3,1} &= \frac{1}{2}(u_{2,0} + u_{4,0}) = \frac{1}{2}(4 + 0) = 2 \end{aligned}$$

Solution

At the second time step i.e., $t = 1$, we have $j = 1$:

So, the equation $(*)$ reduces to

$$u_{i,2} = -u_{i,0} + u_{i-1,1} + u_{i+1,1}$$

So,

$$\begin{aligned} u_{1,2} &= -u_{1,0} + u_{0,1} + u_{2,1} = -3 + 0 + 3 = 0 \\ u_{2,2} &= -u_{2,0} + u_{1,1} + u_{3,1} = -4 + 2 + 2 = 0 \\ u_{3,2} &= -u_{3,0} + u_{2,1} + u_{4,1} = -3 + 3 + 0 = 0 \end{aligned}$$