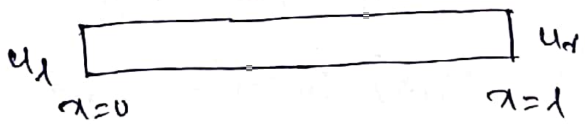
Parabolic PDE - Diffusion equation

Motivation :

Suppose that $u(x,t)$ is the temperature of a metal bar a distance x from one end at time t. For simplicity, let us suppose that the metal bar has length equal to l and that the ends are held at constant temperatures u_l at the left and u_r at the right.



We also suppose that the temperature distribution at the initial time is known to be $f(x)$, with $f(0)=u_l$ and $f(l)=u_r$ so that the initial and boundary conditions do not give rise to a conflict at the ends of the bar at the initial time.
The physical situation may be modelled by

$$\frac{\partial u}{\partial t} = \alpha \frac{\partial^2 u}{\partial x^2} \; ; \quad 0<x<l \text{ and } t>0$$

with $u(0,t)=u_l$; $u(l,t)=u_r$ and $u(x,0)=f(x)$.
in which $\alpha>0$ is a constant called thermal diffusivity or simply the diffusivity of the metal.

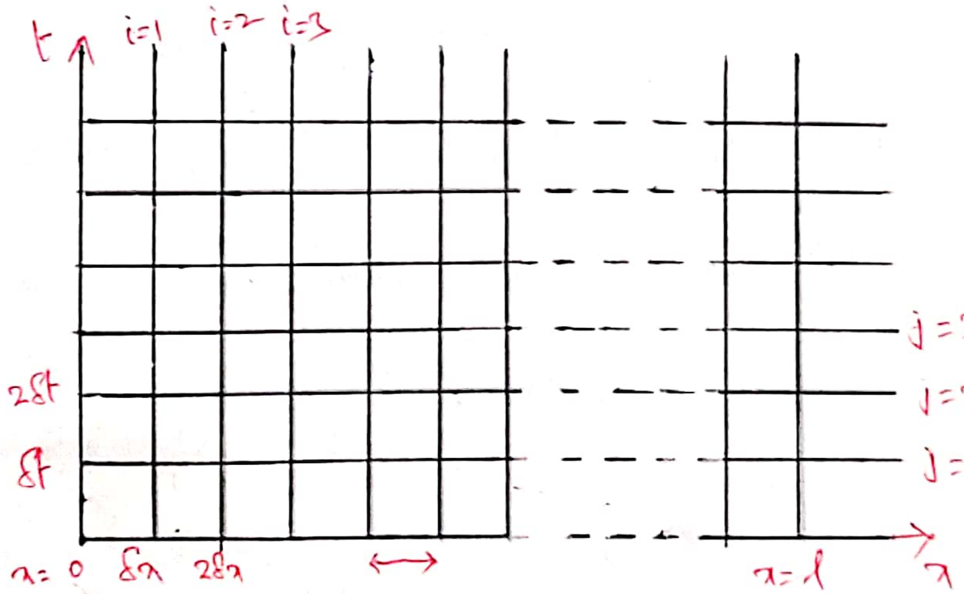
An explicit numerical method for the heat equation:

Consider the 1-D heat equation of the form

$$\frac{\partial u}{\partial t} = \alpha \frac{\partial^2 u}{\partial x^2} \;; \quad 0 < x < l \;; \; t > 0$$

$$u(0,t) = 0 = u(l,t) \text{ and } u(x,0) = f(x).$$

In order to simplify the numerical method, we choose values for δt and δx and use these in in approximations of the two derivatives in the partial differential equation. It is convenient to divide the interval $(0,l)$ into equally spaced sub intervals.



Here, δx = the space step, and δt = the time step.

The numerical solution we shall find is a sequence of numbers which approximate u at a sequence of (x,t) points.

The notation, we use here is

$$u_i^j \approx u(i\,\delta x,\, j\,\delta t)$$

numerical approximation — exact (ie, unknown) solution evaluated at $x = i\,\delta x,\ t = j\,\delta t$.

The idea is that the subscript i counts how many "steps" to the right and the superscript j counts how many time steps we have taken.

Substituting the finite difference approximations, in the given PDE, we get

$$\frac{u_i^{j+1} - u_i^j}{\delta t} = \alpha \cdot \left[\frac{u_{i-1}^j - 2u_i^j + u_{i+1}^j}{(\delta x)^2}\right]$$

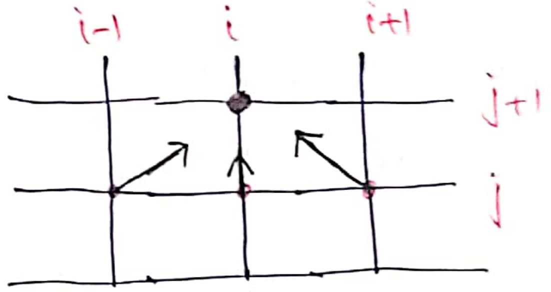
To simplify the numerical method, we define a new quantity $\lambda = \dfrac{\alpha \cdot \delta t}{(\delta x)^2}$ so that our numerical procedure can be written as

$$u_i^{j+1} = u_i^j + \lambda\left(u_{i-1}^j - 2u_i^j + u_{i+1}^j\right)$$

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

Note :

1.



The equation, $u_i^{j+1} = \lambda u_{i-1}^{j} + (1-2\lambda) u_i^{j} + \lambda u_{i+1}^{j}$ allows us to find the value at $j+1$ time level in terms of values at the previous level j.

2. Convergence Condition (Von Neumann stability condition)

This numerical scheme is valid if $0 < \lambda \le \frac{1}{2}$; That is, we should not move too fast in t-direction. To attain sufficient accuracy, we have to choose δx small, which makes δt very small.

3. This explicit method is also known as Bender-Schmidt method.

Example:- The temperature $u(x,t)$ of a metal bar of length 2 at a distance x from one end and at time t is modelled by the partial differential equation,

$$\frac{\partial u}{\partial t} = \alpha \frac{\partial^2 u}{\partial x^2} \quad ; \quad 0 < x < 2 \, ; \quad t > 0$$

It is given that the metal has diffusivity $\alpha = 4$, that the two ends of the bar are kept at the temperature zero, i.e, $u(0,t) = u(2,t) = 0$ and the initial temperature distribution is $u(x,0) = f(x) = x(2-x)$. Use the explicit difference scheme with $\delta x = 0.5$ and $\delta t = 0.01$ to approximate $u(x,t)$ at $t = \delta t$ and $t = 2\delta t$.

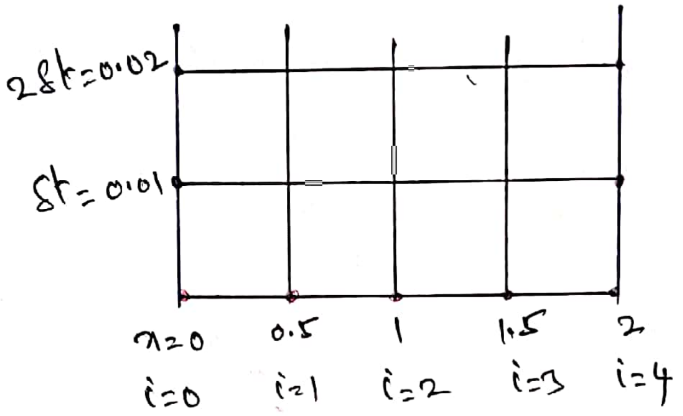
Solution:- In this case,

$$\lambda = \frac{\alpha \cdot \delta t}{(\delta x)^2} = \frac{4 \cdot (0.01)}{(0.5)^2} = 0.16 < \frac{1}{2}$$

The explicit scheme is,

$$u_i^{j+1} = \lambda u_{i-1}^j + (1-2\lambda) u_i^j + \lambda u_{i+1}^j$$

$$u_i^{j+1} = 0.68 u_i^j + 0.16 \left(u_{i-1}^j + u_{i+1}^j \right).$$



From the given initial condition, $u(x,0) = x(2-x)$, we get

$$\underbrace{u_0^0 = 0}_{\text{From B.C}} \; ; \; \underbrace{u_1^0 = 0.75 \; ; \; u_2^0 = 1 \; ; \; u_3^0 = 0.75}_{\text{from initial conditions}} ; \; \underbrace{u_4^0 = 0}_{\text{From B.C}}$$

Note that the symmetry, $u_1^0 = u_3^0$

And $u_0^j = u_4^j$, (from the B.C's)

As a result, it is enough if we calculate the values u_1^j and u_2^j.

<u>At the first time-step</u> ($t = 0.01$) <u>will find u_i^1</u>:

$$u_i^{j+1} = 0.68\, u_i^j + 0.16\left(u_{i-1}^j + u_{i+1}^j\right)$$

$$u_1^1 = 0.68\, u_1^0 + 0.16\left(u_0^0 + u_2^0\right)$$

$$u_1^1 = 0.68\,(0.75) + 0.16\,(0+1) = 0.670$$

$$u_2^1 = 0.68\, u_2^0 + 0.16\left(u_1^0 + u_3^0\right)$$

$$u_2^1 = 0.68\,(1) + 0.16\,(0.75 + 0.75) = 0.920$$

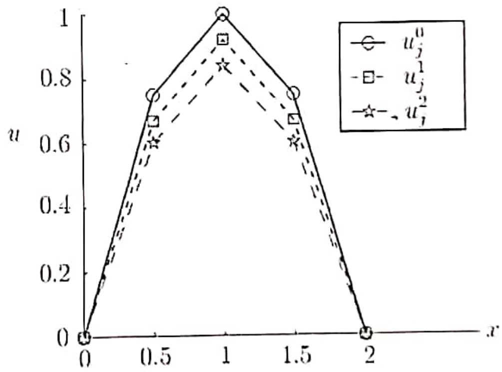
The second time step ($t = 0.02$) will find u_i^2:

$$u_1^2 = 0.68\,u_1^1 + 0.16\,(u_0^1 + u_2^1)$$

$$u_1^2 = 0.68\,(0.67) + 0.16\,(0 + 0.92) = 0.603$$

$$u_2^2 = 0.68\,u_2^1 + 0.16\,(u_1^1 + u_3^1)$$

$$u_2^2 = 0.68\,(0.92) + 0.16\,(0.67 + 0.67) = 0.84.$$



Example: 2

The temperature $u(x,t)$ of a metal bar of length 1 at a distance x from one end and at time t is modelled by the PDE

$$\frac{\partial u}{\partial t} = \alpha \frac{\partial^2 u}{\partial x^2}\,; \quad 0 < x < 1\,; \quad t > 0$$

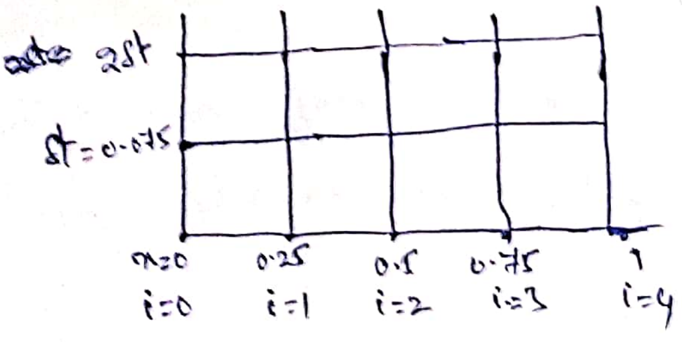
It is given that the metal has diffusivity $\alpha = 1$. That the two ends of the bar are kept at temperature $u = 0$ and that the initial temperature distribution is $u(x,0) = f(x) = x(1-x)$. Use the explicit scheme with $\delta x = 0.25$; and $\delta t = 0.075$ to approximate $u(x,t)$ at $t = \delta t$ and $t = 2\delta t$.

Solution: Here $\lambda = \dfrac{\alpha \cdot \delta t}{(\delta x)^2} = \dfrac{1 \cdot (0.075)}{(0.25)^2} = 1.2 > \dfrac{1}{2}$

The explicit scheme is

$$u_i^{j+1} = \lambda u_{i-1}^{j} + (1-2\lambda) u_i^{j} + \lambda u_{i+1}^{j}$$

$$u_i^{j+1} = 1.2\left(u_{i-1}^{j} + u_{i+1}^{j}\right) - 1.4\, u_i^{j}$$



From the B.C's, we have $u_0^0 = u_4^0 = 0$

From the initial condition, $u(x,0) = f(x) = x(1-x)$, we get

$$u_1^0 = 0.188 \; ; \quad u_2^0 = 0.25 \; ; \quad u_3^0 = 0.188$$

Note that $u_1^0 = u_3^0$. In general $u_1^j = u_3^j$

As a result, it is enough to calculate u_1^j and u_2^j.

The first time step will find u_i^1 :-

First we note that the boundary condition implies that $u_0^1 = u_4^1 = 0$.

$$u_1^1 = 1.2\left(u_0^0 + u_2^0\right) - 1.4\,u_1^0 = 1.2\,(0+0.25) - 1.4\,(0.0188) = 0.038$$

$$u_2^1 = 1.2\,(u_1^0 + u_3^0) - 1.4\,u_2^0 = 1.2\,(0.188 + 0.188) - 1.4\,(0.25) = 0.1$$

The second time step $(2\delta t)$ will find u_i^2 :-

Again, from the B.C, $u_0^2 = u_4^2 = 0$.

$$u_1^2 = 1.2\,(u_0^1 + u_2^1) - 1.4\,u_1^1 = 1.2(0+0.1) - 1.4(0.038) = 0.067$$

$$u_2^2 = 1.2\,(u_1^1 + u_3^1) - 1.4\,u_2^1 = 1.2\,(0.038 + 0.038) - 1.4\,(0.1) = -0.05$$

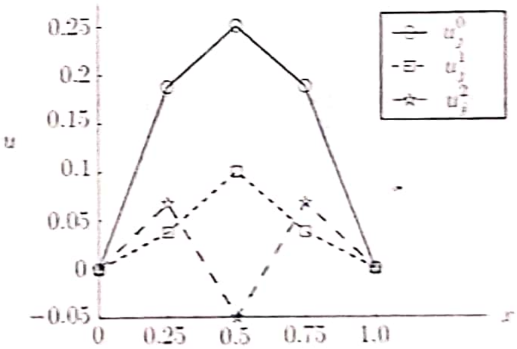
Something has gone wrong here. And it only gets worse in subsequent time-steps.

After 9 time steps the numerical solution approximating $u(x,t)$ at $t = 9\delta t$ is

$$u(0.25, 9\delta t) = u_1^9 = -140.5531$$

$$u(0.5, 9\delta t) = u_2^9 = 198.7722.$$

This is example of instability. A part of the numerical solution wants to keep growing and growing in a way that is not a part of the engineering application being modelled.



Note:- At the point u_i^j, we have

$$\frac{\partial^2 u}{\partial x^2} = \frac{u_{i+1}^j - 2u_i^j + u_{i-1}^j}{(\delta x)^2}$$

Similarly at the point u_i^{j+1}, we have

$$\frac{\partial^2 u}{\partial x^2} = \frac{u_{i+1}^{j+1} - 2u_i^{j+1} + u_{i-1}^{j+1}}{(\delta x)^2}.$$

$$\frac{\partial^2 u}{\partial x^2} = \frac{1}{2.(\delta x)^2}\left[\left(u_{i+1}^j - 2u_i^j + u_{i-1}^j\right) + \left(u_{i+1}^{j+1} - 2u_i^{j+1} + u_{i-1}^{j-1}\right)\right].$$

An implicit numerical method for the heat equation :-

This method is also known as Crank-Nicolson method.

Consider the 1-D heat equation of the form,

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

writing the finite difference approximations, we get

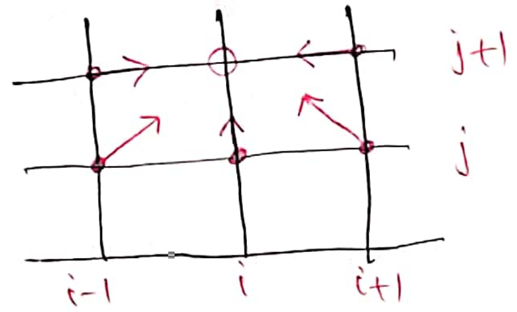
$$\frac{u_i^{j+1} - u_i^j}{\delta t} = \alpha . \frac{1}{2(\delta x)^2}\left[\left(u_{i+1}^j - 2u_i^j + u_{i-1}^j\right) + \left(u_{i+1}^{j+1} - 2u_i^{j+1} + u_{i-1}^{j+1}\right)\right]$$

$$u_i^{j+1} = u_i^j + \frac{\lambda}{2}\left[\left(u_{i+1}^j - 2u_i^j + u_{i-1}^j\right) + \left(u_{i+1}^{j+1} - 2u_i^{j+1} + u_{i-1}^{j+1}\right)\right].$$

where $\lambda = \dfrac{\alpha . \delta t}{(\delta x)^2}$.

Note:-

1.



2. The Crank-Nicolson scheme is implicit.

3. This method is stable for any value of λ. However, the accuracy will be better for small values of λ. This is one of the best method.

Example: The temperature $u(x,t)$ of a metal bar of length $l = 1.2$ at a distance x from one end and at the time t is modelled by the PDE

$$\frac{\partial u}{\partial t} = \alpha \frac{\partial^2 u}{\partial x^2}; \quad 0 < x < l, \quad t > 0$$

It is given that the metal has diffusivity $\alpha = 1$, that two ends of the bar are kept at temperature zero and that the initial temperature distribution is $u(x,0) = f(x) = x\sqrt{(l-x)^3}$

Use the Crank-Nicolson scheme with $\delta x = 0.4$ and $\delta t = 0.1$ to approximate $u(x,t)$ at $t = \delta t$ and $t = 2\delta t$.

Solution: In this case,

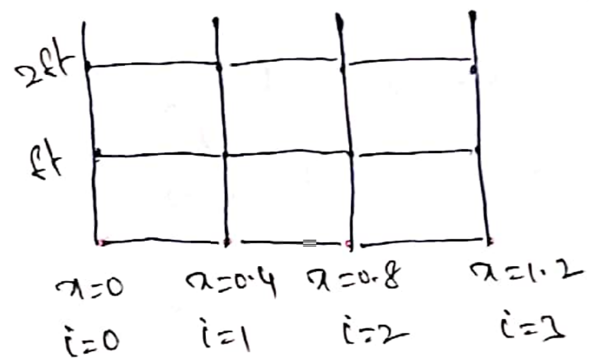
$$\lambda = \frac{\alpha \cdot \delta t}{(\delta x)^2} = \frac{1\cdot(0.1)}{(0.4)^2} = 0.625$$

The Crank-Nicolson scheme can be written as,

$$u_i^{j+1} = u_i^j + \frac{\lambda}{2}\left[u_{i+1}^j - 2u_i^j + u_{i-1}^j + u_{i+1}^{j+1} - 2u_i^{j+1} + u_{i-1}^{j+1}\right]$$

$$u_i^{j+1} = u_i^j + \frac{0.625}{2}\left[u_{i+1}^j - 2u_i^j + u_{i-1}^j + u_{i+1}^{j+1} - 2u_i^{j+1} + u_{i-1}^{j+1}\right]$$

$$-0.3125\, u_{i-1}^{j+1} + 1.625\, u_i^{j+1} - 0.3125\, u_{i+1}^{j+1} = 0.375\, u_i^j + 0.3125\left(u_{i-1}^j + u_{i+1}^j\right)$$



From the B.C's, $u_0^0 = u_3^0 = 0$

From the initial condition, we get,

$$u_1^0 = f(0.4) = 0.2862 \quad ; \quad u_2^0 = f(0.8) = 0.20239.$$

The 1st time step will find u_i^1 :

First we note that, the B.C implies that $u_0^1 = u_3^1 = 0.$

$$-0.3125\,u_0^1 + 1.625\,u_1^1 - 0.3125\,u_2^1 = 0.375\,u_1^0 + 0.3125\left(u_0^0 + u_2^0\right)$$
$$= 0.17058$$

$$-0.3125\,u_1^1 + 1.625\,u_2^1 - 0.3125\,u_3^1 = 0.375\,u_2^0 + 0.3125\left(u_1^0 + u_3^0\right)$$
$$= 0.16534.$$

The simplest equations are:

$$1.625\, u_1^1 - 0.3125\, u_2^1 = 0.17058$$

$$-0.3125\, u_1^1 + 1.625\, u_2^1 = 0.16534$$

The implicit nature of this method means that we have to do some extra work to complete the time step.

Now, we solve the simultaneous equations.

$$\begin{bmatrix} 1.625 & -0.3125 \\ -0.3125 & 1.625 \end{bmatrix} \begin{bmatrix} u_1^1 \\ u_2^1 \end{bmatrix} = \begin{bmatrix} 0.17058 \\ 0.16534 \end{bmatrix}$$

There are only two unknowns and it is a simple matter to solve the pair of equations to give

$$u_1^1 = 0.12932 \quad \text{and} \quad u_2^1 = 0.12662$$

The 2nd time step will find u_i^2:

Note that the B.C implies that $u_0^2 = u_3^2 = 0$.

$$-0.3125\, u_0^2 + 1.625\, u_1^2 - 0.3125\, u_2^2 = 0.375\, u_1^1 + 0.3125\,(u_0^1 + u_2^1)$$

$$= 0.08806$$

$$-0.3125\, u_1^2 + 1.625\, u_2^2 - 0.3125\, u_3^2 = 0.375\, u_2^1 + 0.3125\,(u_1^1 + u_3^1)$$

$$= 0.08789$$

$$\begin{bmatrix} 1.625 & -0.3125 \\ -0.3125 & 1.625 \end{bmatrix} \begin{bmatrix} u_1^2 \\ u_2^2 \end{bmatrix} = \begin{bmatrix} 0.08806 \\ 0.08789 \end{bmatrix}$$

Solving this system, we get

$$u_1^2 = 0.06707 \quad \text{and} \quad u_2^2 = 0.06699$$