CBCC-B

Group-B: Numerical Analysis

5. Introduction to Numerical Solution of Differential Equation

Topic: Single Step and Multi Step Methods for Initial Value Problem for ODE (IVP-ODE)

1.1- Introduction:

Calculus has provided various methods for closed form solution of the initial value problem for the first order ordinary differential equation (IVP-ODE):

$$\frac{dy}{dx} = y'(x) = f(x, y), \ y(x_0) = y_0,$$
(1)

as: y(x) = f(x) + c, where c is an arbitrary constant to be determined from the initial condition (IC), $y(x_0) = y_0 : c = y_0 - y(x_0)$.

Based on our experience, we find that although there are many methods available in calculus, still there are many first and higher order ODEs which can NOT be solved by these methods *analytically* and hence we require some other (*Numerical*) methods (may be *computer oriented*!) which can tackle various problems. For example, the IVP-ODE

$$y'(x) = e^{x^2}, y(0) = 1,$$

Can NOT be solved analytically but it can be solved numerically. Computer can also be used for very correct solution.

Our aim here is to know some of these numerical methods.

Those methods are available:

Semi-Numerical methods: Picard's method;

Single Step-methods: Taylor's series method, Euler's method, Runge-Kutta method;

Multi-step methods: Adam-Bashforth method, Adam-Moulton method;

In this discussion, we shall remain interested only in the following numerical methods, namely:

I. Single Step-methods:

(a) Taylor's series method, (b) Runge-Kutta method;

II. Multi-step methods:

(a) Adam-Bashforth method, (b) Adam-Moulton method;

Note 1.1: We first assume that all the conditions which assure that (1) has a unique solution are satisfied.

1.2. Single step methods: In single step methods, the solution at any point $x = x_r$ is obtained using the solution at only the previous point $x = x_{r-1}$.

1.2.1- Taylor's series method:

This is the Mother of all numerical methods for solving IVP-ODE.

Let $y(x_r)$ be the true/exact solution (if available!) of (1) for any particular value of $x = x_r$. Suppose we want to find the approximate numerical solution for y(x), say $y_r \approx y(x_r)$ at $x = x_r$. In this purpose, we divide the interval $[x_0, x_n]$ into n-equal subintervals by the points: $x_0, x_1, ..., x_{r-1}, x_r, x_{r+1}, ..., x_{n-1}, x_n$, where $x_r = x_0 + rh, r = 1, 2, 3, ..., n$, and $h = x_r - x_{r-1}$ is known as the *step length*.

To find y_{r+1} :

Using the Taylor's series in a neighbourhood of x_0 with the Lagrange form of remainder, we can write

$$y_{r+1} \approx y(x_{r+1}) = y(x_r + h) = y_r + hy'(x_r) + \frac{h^2}{2!}y''(x_r) + \frac{h^3}{3!}y'''(x_r) + \dots + \frac{h^n}{n!}y^{(n)}(x_r) + \dots + \frac$$

where $0 < \theta < 1, x_r \in [x_0, x_n]$.

Neglecting the error term, we obtain the n-th order Taylor series method as:

$$y_{r+1} \approx y_r + hy'(x_r) + \frac{h^2}{2!}y''(x_r) + \frac{h^3}{3!}y'''(x_n) + \dots + \frac{h^n}{n!}y^{(n)}(x_r).$$
 (3)

We always need to assume that the step-length h is very small in order to find more accurate numerical solution y_r . So, if h is assumed to be very small, we keep up terms upto $y'''(x_0)$ and neglect the rest terms in (3) yields for r = 0:

$$y_1 \approx y_0 + hy'(x_0) + \frac{h^2}{2!}y''(x_0) + \frac{h^3}{3!}y'''(x_0).$$
 (4)

Now, using the partial derivatives, it is easy to find:

$$y' = f$$
, $y'' = f' = f_x + ff_y$, $y''' = f'' = f_{xx} + 2ff_{xy} + f^2 f_{yy} + f_x f_y + ff_y^2$. (5)

Thus, using (5) at the points (x_0, y_0) (it is the given IC), we can obtain the approximate value of y_1 from (4). To obtain y_2 , we need to just repeat the above steps.

Truncation Error (T.E.):

The n-th order Taylor series method (3) can be written as:

$$y_{r+1} = y_r + hy'(x_r) + \frac{h^2}{2!}y''(x_r) + \dots + \frac{h^n}{n!}y^{(n)}(x_r) + \frac{T_{r+1}(h)}{n!},$$
(6)

where $T_{r+1}(h)$ is called the T.E. for n-th order Taylor series method which is defined as:

T.E. =
$$T_{r+1}(h)$$
 = Exact Solution - Numerical Solution = $y(x_{r+1}) - y_{r+1}$.

It can be shown that:

$$T_{r+1}(h) = \frac{h^{n+1}}{(n+1)!} y^{(n+1)}(\xi), \ x_r < \xi < x_{r+1}.$$

For n=1, we obtain the **first order Taylor series** method as:

$$y_{r+1} = y_r + hy'(x_r) = hf(x_r, y_r).$$

This method is also called the *Euler's method*. The T.E. of the Euler's method is

$$T_{r+1}(h) = \frac{h^2}{2!} y''(\xi), \ x_r < \xi < x_{r+1}.$$

Order of method:

The order of a numerical method for solving IVP-ODE method is the largest integer n for which the T. E. is of order $O(h^{n+1})$.

By the above definition, we can say that an n-th order Taylor's series method is of order n.

Example 1.1: Solve

$$\frac{dy}{dx} = x(y-2), \ y(0) = 3$$

using Taylor series method for x = 0.1. Find the T.E. also.

Solution:

Here, we find

$$y'(x) = xy - 2x$$
, $y''(x) = xy' + y - 2$, $y'''(x) = xy'' + 2y'$.

To find y(0.1), we take h = 0.1, $x_0 = 0$, $y_0 = 3$. Using the formula (4), we get

$$y_1 \approx y(x_1) = y_0 + hy'(x_0) + \frac{h^2}{2!}y''(x_0) + \frac{h^3}{3!}y'''(x_0)$$

$$= y_0 + hy'(0) + \frac{h^2}{2!}y''(0) + \frac{h^3}{3!}y'''(0)$$

$$= 3 + 0 + \frac{(0.1)^2}{2!} \times 1 + 0 = 3.005.$$

Thus, we find: $y(0.1) \approx 3.005$, correct to 4 decimal places.

T.E.:

Exact solution of the given IVP-ODE is: $y(x) = 2 + e^{\frac{x^2}{2}}$.

Therefore,

T.E. =
$$y(0.1)|_{\text{Exact}} - y(0.1) = 3.005 - 3.005 = 0.$$

Assignment 1.1:

Solve

$$\frac{dy}{dx} = xy, \ y(1) = 2$$

using Taylor series method for x = 1.2. Find the T.E. also.

1.2.2- Runge-Kutta (RK) method:

The RK method for solving IVP-ODE (1) gives us greater accuracy and also avoid disadvantage of Taylor series method which demands the higher order total derivatives of y(x).

First order RK method:

Taking terms upto order of h in the Taylor series (3), we obtain

$$y_{r+1} = y_r + hy'(x_r).$$

This method is also called the First order RK method.

The T.E. error of this method is of order h^2 and hence it is an first order method.

Second order RK method:

Taking terms upto order of h^2 in the Taylor series (3), Runge and Kutta deduced the second order RK method as:

$$y_1 = y_0 + \frac{1}{2}(k_1 + k_2),$$

 $k_1 = hf(x_0, y_0), k_2 = hf(x_0 + h, y_0 + k_1)$

The T.E. error of this method is of $O(h^3)$, and hence it is an second order method.

Third order RK method:

Taking terms upto order of h^3 in the Taylor series (3), Runge and Kutta deduced the third order RK method as:

$$y_1 = y_0 + \frac{1}{6}(k_1 + 4k_2 + k_3),$$

$$k_1 = hf(x_0, y_0), \ k_2 = hf\left(x_0 + \frac{h}{2}, y_0 + \frac{k_1}{2}\right), k_3 = hf(x_0 + h, y_0 - k_1 + 2k_2).$$

The T.E. error of this method is of $O(h^4)$, and hence it is an third order method.

Fourth order RK method:

Taking terms upto order of h^4 in the Taylor series (3), Runge and Kutta deduced the Fourth order RK method as:

$$y_1 = y_0 + \frac{1}{6} [k_1 + 2(k_2 + k_3) + k_4],$$

$$k_1 = hf(x_0, y_0), \quad k_2 = hf(x_0 + \frac{h}{2}, y_0 + \frac{k_1}{2}),$$

$$k_3 = hf(x_0 + \frac{h}{2}, y_0 + \frac{k_2}{2}), k_4 = hf(x_0 + h, y_0 + k_3).$$

The T.E. error of this method is of $O(h^5)$, and hence it is an fourth order method.

Note 1.2: Since h is very small, h^5 is pretty small and the fourth order RK method gives the more accurate results. That is why the forth order RK method is mostly used in solving IVP-ODE.

Example 1.2: *Solve the IVP-ODE:*

$$y' = 2x + y$$
, $y(1) = 2$

using RK methods for y(1.2).

Solution:

Here,
$$x_0 = 1$$
, $y_0 = 2$, $h = 0.2$, $f(x, y) = 2x + y$.

(i) First order RK method:

$$y_1 = y_0 + hf(x_0, y_0)$$

$$\therefore y(1.2) = 2 + 0.2(2 \times 1 + 2) = 2.8.$$

(ii) Second order RK method:

$$k_1 = hf(x_0, y_0) = 0.2 \times f(1, 2) = 0.8,$$

 $k_2 = hf(x_0 + h, y_0 + k_1) = 0.2 \times f(1.2, 2.8) = 1.04.$

Therefore,

$$y_1 = y_0 + \frac{1}{2}(k_1 + k_2) \Rightarrow y(1.2) = 2 + \frac{1}{2}(0.8 + 1.04) = 2.92$$

(iii) Third order RK method:

$$k_1 = hf(x_0, y_0) = 0.2 \times f(1, 2) = 0.8,$$

$$k_2 = hf\left(x_0 + \frac{h}{2}, y_0 + \frac{k_1}{2}\right) = 0.2 \times f(1.1, 2.4) = 0.92$$

$$k_3 = hf(x_0 + h, y_0 - k_1 + 2k_2) = 0.2 \times f(1.2, 3.04) = 1.088$$

$$\therefore y(1.2) = y_0 + \frac{1}{6}(k_1 + 4k_2 + k_3) = 2.928$$

Therefore,

$$y_1 = y_0 + \frac{1}{2}(k_1 + k_2) \Rightarrow y(1.2) = 2 + \frac{1}{2}(0.8 + 1.04) = 2.92$$

(iv) Fourth order RK method

$$k_1 = hf(x_0, y_0) = 0.8, \ k_2 = hf(x_0 + \frac{h}{2}, y_0 + \frac{k_1}{2}) = 0.92$$

 $k_3 = hf(x_0 + \frac{h}{2}, y_0 + \frac{k_2}{2}) = 0.932, k_4 = hf(x_0 + h, y_0 + k_3) = 1.0664.$
 $\therefore y(1.2) = y_0 + \frac{1}{6}[k_1 + 2(k_2 + k_3) + k_4] = 2.928$, correct to 3 decimal places.

T.E.:

Exact solution of the given IVP-ODE is: $y(x) = 6e^{x-1} - 2(x+1)$.

So, T.E. =
$$y(1.2)|_{Exact} - y(1.2) = 2.928 - 2.928 = 0$$
.

Note 1.3: In case, we want to find y(1.4), we need to evaluate k_1, k_2, k_3, k_4 for $x_0 = 1 + h = 1.2, y_0 = 2.9284$.

Assignment 1.2:

(i) Find
$$y(0.2)$$
: $y' = x - y$, $y(0) = 1$, $h = 0.1$;

Answer:

$$y(0.1) = 0.9097, y(0.2) = 0.8375$$

(ii) Find
$$y(0.4)$$
: $y' = xy$, $y(0) = 2$, $h = 0.2$;

Answer:
$$y(0.2) = 2.0404, y(0.4) = 2.167$$

Extra credit: Find the T.E. in the above solutions.

1.3. Multi step methods: In multi step methods, the solution at any point $x = x_{i+1}$ is obtained using the solution at a number of previous points. A k-step multi step method requires the k previous values of y(x) to determine the approximation to y(x) at any particular point x.

1.3.1- Adams-Bashforth method:

The 4th order Adams-Bashforth method for solving the IVP-ODE (1) is:

$$y_{i+1} = y_i + \frac{h}{24} [55f_i - 59f_{i-1} + 37f_{i-2} - 9f_{i-3}], \quad f_i = f(x_i, y_i).$$

For using the method, we require the **four** starting (previous) values $y_i, y_{i-1}, y_{i-2}, y_{i-3}$ to find the numerical value y_{i+1} .

The **T.E.** is:

$$T_4(h) = \frac{251}{720} h^5 y^{(5)}(\xi), \ 0 < \xi < 1.$$

Therefore, the method is of *fourth order*.

Remark 1.1: The required starting values for the application of the 4th Adams-Bashforth methods are obtained by using any single step method like Taylor series method, Euler's method, or Runge-Kutta method.

1.3.2- Adams-Moulton method:

The 4th order Adams-Moulton method for solving the IVP-ODE (1) is:

$$y_{i+1} = y_i + \frac{h}{24} [9f_{i+1} + 19f_i - 5f_{i-1} + f_{i-2}].$$

For using the method, we require the *three* starting (previous) values y_i, y_{i-1}, y_{i-2} to find the numerical value y_{i+1} .

The **T.E.** is:

$$T_4(h) = -\frac{19}{720}h^5 y^{(5)}(\xi), \ 0 < \xi < 1.$$

Therefore, the method is of *fourth order*.

Example 1.3: Find the approximate value of y(0.4) using the Adams-Bashforth and Adams-Moulton methods of fourth order for the initial value problem

$$y' = x + y^2, y(0) = 1$$

with h = 0.1. Calculate the starting values using the Euler's method (First order Taylor Series Method) with the same step length.

Solution:

Given:

$$f(x, y) = x + y^2, x_0 = 0, y_0 = 1.$$

The 4th order Adams-Bashforth method is:

$$y_{i+1} = y_i + \frac{h}{24} [55f_i - 59f_{i-1} + 37f_{i-2} - 9f_{i-3}], \quad f_i = f(x_i, y_i).$$

Since
$$h = 0.1$$
, so $x_0 = 0$, $x_1 = 0.1$, $x_2 = 0.2$, $x_3 = 0.3$, $x_4 = 0.4$.

Therefore, to find the numerical value $y_4 \approx y(x_4) = y(0.4)$, we need the starting values y_3, y_2, y_1, y_0 .

The IC gives: $y_0 = 1$.

We find y_3, y_2, y_1 by Euler's method as follows:

Euler's method: $y_{i+1} = y_i + hf_i$.

$$i = 0$$
: $x_0 = 0$, $y_0 = 1$, $f_0 = x_0 + y_0^2 = 1$.
∴ $y(0.1) \approx y_1 = y_0 + hf_0 = 1 + 0.1 \times 1 = 1.1$;
 $i = 1$: $x_1 = 0.1$, $y_1 = 1.1$, $f_1 = x_1 + y_1^2 = 1.31$.
∴ $y(0.2) \approx y_2 = y_1 + hf_1 = 1.231$;
 $i = 2$: $x_2 = 0.2$, $y_1 = 1.231$, $f_2 = x_2 + y_2^2 = 1.715361$.
∴ $y(0.3) \approx y_3 = 1.402536$;

Now, we apply the given Adams-Bashforth method:

i = 3:

$$y_{3+1} = y_3 + \frac{h}{24} \left[55f_3 - 59f_{3-1} + 37f_{3-2} - 9f_{3-3} \right]$$

$$\Rightarrow y_4 = 1.402536 + \frac{0.1}{24} \left[55 \times 2.267107 - 59 \times 1.715361 + 37 \times 1.31 - 9 \times 1 \right], \quad (\because f_3 = x_3 + y_3^2 = 2.267107)$$

$$\therefore y(0.4) \approx 1.664847 \text{ (correct to 6 decimal places)}.$$

The 4th order Adams-Moulton method gives:

$$i = 3: y_4 = y_3 + \frac{h}{24} [9f_4 + 19f_3 - 5f_2 + f_1].$$

Note that:

$$f_4 = x_4 + y_4^2 = 0.4 + y_4^2$$

Here, we use the value of y_4 obtained by <u>Adams-Bashforth method</u> to find f_4 :

$$f_4 = 0.4 + (1.664847)^2 = 3.171716.$$

Hence, the more accurate value of y_4 is

$$y_4 = 1.402536 + \frac{0.1}{24} [9 \times 3.171716 + 19 \times 2.267107 - 5 \times 1.715361 + 1.31]$$

$$\therefore y(0.4) \approx 1.670676.$$

Note 1.4:

Adams-Moulton method always modifies the value of y_i obtained by Adams-Bashforth method. For this reason, in order to use Adams-Moulton method, we always need the Adams-Bashforth method first as shown in the above example.

Assignment 1.3:

Find the approximate value of y(1.4) using the Adams-Bashforth and Adams-Moulton methods of fourth order for the initial value problem

$$y' + \frac{y}{x} = \frac{1}{x^2},$$

and y(1) = 1, y(1.1) = 0.996, y(1.2) = 0.986, y(1.3) = 0.972. (The starting values are given guestion!)

CBCC-B

Group-B: Numerical Analysis

5. Introduction to Numerical Solution of Differential Equation

Topic: Finite Difference Method (FDM) for two-point BVP in ODE

2.1- Introduction:

Boundary value problems are of great importance in science and engineering. In this discussion, we shall discuss the numerical solution of the following problem:

Boundary Value Problem (BVP) in Ordinary Differential Equation (ODE)

For our discussion in this chapter, we shall consider only the following linear second order ODE

ODE:
$$y''(x) + p(x)y'(x) + q(x)y(x) = r(x), a \le x \le b,$$
 (1)

subject to the following boundary conditions (BCs):

BCs:
$$y(a) = A$$
, $y(b) = B$. (2)

■ *Note-1*: We assume that the functions p(x), q(x), r(x) are all continuous for $a \le x \le b$ so that the BVP (1)-(2) has a *unique solution*.

2.2 Finite Difference Method:

Subdivide the interval [a, b] into n equal sub-intervals with of the sub-interval h. Therefore,

$$h = \frac{b-a}{n}$$
.

The points $a = x_0, x_1 = x_0 + h, ..., x_i = x_0 + ih, ..., x_n = x_0 + nh = b$ are called nodes or nodal points.

We denote the numerical solution at any point x_i by y_i and the exact solution by $y(x_i)$.

Approximation to y'(x) at the point $x = x_i$:

By Taylor series, we have

$$y(x_{i+1}) = y(x_i) + hy'(x_i) + \frac{h^2}{2!}y''(x_i) + O(h^3)$$
(3)

$$y(x_{i-1}) = y(x_i) - hy'(x_i) + \frac{h^2}{2!}y''(x_i) - O(h^3)$$
(4)

(i) Forward difference approximation of first order or O(h) approximation: From (3), we find after truncating terms from $O(h^2)$:

$$\frac{y(x_{i+1}) - y(x_i)}{h} = y'(x_i) + O(h), \text{ Or, } y_i' = \frac{y_{i+1} - y_i}{h} [+O(h)].$$
 (5)

(ii) Backward difference approximation of first order or O(h) approximation:

Similarly, from (4), we find

$$y_i' = \frac{y_i - y_{i-1}}{h} [+O(h)]. \tag{6}$$

(ii) Central difference approximation of second order or $O(h^2)$ approximation: Subtract (4) from (3), we find

$$y_i' = \frac{y_{i+1} - y_{i-1}}{2h} \left[+O(h^2) \right]. \tag{7}$$

Approximation to y''(x) at the point $x = x_i$ or order $O(h^2)$: By Taylor series, we have

$$y(x_{i+1}) = y(x_i) + hy'(x_i) + \frac{h^2}{2!}y''(x_i) + \frac{h^3}{3!}y'''(x_i) + O(h^4)$$
(8)

$$y(x_{i-1}) = y(x_i) - hy'(x_i) + \frac{h^2}{2!}y''(x_i) - \frac{h^3}{3!}y'''(x_i) + O(h^4)$$
(9)

Adding (8) and (9), we find

$$y_i'' = \frac{y_{i+1} - 2y_i + y_{i-1}}{h^2} \left[+ O(h^2) \right]. \tag{10}$$

Approximation to the BVP (1)-(2) at the nodal point:

Applying the BVP (1)-(2) at the nodal point $x = x_i$, we obtain:

ODE:
$$y''(x_i) + p(x_i)y'(x_i) + q(x_i)y(x_i) = r(x_i), a \le x_i \le b,$$
 (11)

BCs:
$$y_0 = A, y_n = B.$$
 (12)

Now, $y'(x_i)$ can be approximated by one of the approximations given in Eqs. (5), (6), (7) and $y''(x_i)$ by the approximation given in Eq. (10). Then, we have:

- > Since the approximations (7) and (10) are both of **second order**, the approximation to the differential Eq. (11) is of **second order**.
- However, if $y'(x_i)$ is approximated by (5) or (6), which are of **first order**, then the approximation to the differential Eq. (11) is only of **first order**. But, in many practical problems, particularly in Fluid Mechanics, approximations (5), (6) give better results (non-oscillatory solutions) than the central difference approximation (9).

So, using the approximations (7) and (10) in Eq. (11), we may easily obtain a system of $(n-1)\times(n-1)$ equations of the form Ay=b for the unknowns $y=[y_1,y_2,...,y_{n-1}]^T$ (since y_0,y_n are **known** by (12)), where A is the coefficient matrix and b is some column matrix. Then, we can solve this system to obtain $y_1,y_2,...,y_{n-1}$ as desired.

Let us consider the following example for better understanding:

Example 2.1: Solve the boundary value problem

$$(1+x^2)y''(x) + 4xy'(x) + 2y(x) = 2, y(0) = 0, y(1) = \frac{1}{2},$$

by finite difference method. Use central difference approximations with $h = \frac{1}{3}$.

Solution:

Step-1:

Since $h = \frac{1}{3}$ is given and $0 \le x \le 1$, therefore the nodal points are

$$x_0 = 0, x_1 = \frac{1}{3}, x_2 = \frac{2}{3}, x_3 = 1.$$

Step-2:

Using the central difference approximations in the given ODE and BCs, we obtain

$$(1+x_i^2)\frac{y_{i+1}-2y_i+y_{i-1}}{h^2}+4x_i\frac{y_{i+1}-y_{i-1}}{2h}+2y_i=2.$$

Substituting $h = \frac{1}{3}$, we get

$$[9(1+x_i^2)-6x_i]y_{i-1}+[2-18(1+x_i^2)]y_i+[9(1+x_i^2)+6x_i]y_{i+1}=2, i=1,2.$$
(13)

The BCs become:

$$y_0 = 0, y_3 = \frac{1}{2}.$$

Step-3:

Now, we have the following difference equations:

For
$$i = 1$$
: $[9(1 + x_1^2) - 6x_1]y_0 + [2 - 18(1 + x_1^2)]y_1 + [9(1 + x_1^2) + 6x_1]y_2 = 2$.

Substituting $x_1 = \frac{1}{3}$, $y_0 = 0$, we find

$$-18y_1 + 12y_2 = 2 (14)$$

For
$$i = 2: [9(1+x_2^2) - 6x_2]y_1 + [2-18(1+x_2^2)]y_2 + [9(1+x_1^2) + 6x_1]y_3 = 2$$
.

Substituting $x_2 = \frac{2}{3}$, $y_3 = \frac{1}{2}$, we find

$$9y_1 - 24y_2 = -6.5 \tag{15}$$

Step-4:

Finally, solving the Eqs. (14) and (15), we get

$$y_1 = \frac{15}{162} = 0.092592, y_2 = \frac{49.5}{162} = 0.305556.$$

Step-5:

Thus, we find:

$$y\left(\frac{1}{3}\right) \approx y_1 = 0.092592, \quad y\left(\frac{2}{3}\right) \approx 0.305556.$$

Assignment 2.1:

(i) Solve the boundary value problem
$$y''(x) + 3y'(x) + 2y(x) = 1$$
, $y(0) = 1$, $y(1) = 0$,

by finite difference method. Use central difference approximations with $h = \frac{1}{3}$.

(ii) Using the second order finite difference method, find y(0.25), y(0.50), y(0.75) satisfying the differential equation

$$y''-y=x$$

subject to the conditions y(0) = 0, y(1) = 2.

[Answer: $y(0.25) \approx 0.39534$, $y(0.50) \approx 0.83102$, $y(0.75) \approx 1.34989$.]

CBCC-B

Group-B: Numerical Analysis

5. Introduction to Numerical Solution of Differential Equation

Topic: Finite Difference Method (FDM) for IBVP in PDE

3.1- Introduction:

Initial Boundary value problems in partial differential equations are of great importance in science and engineering. In this discussion, we shall discuss the numerical solution of the following problem:

Initial Boundary Value Problem (IBVP) in Partial Differential Equation (PDE).

For our discussion in this chapter, we shall consider only the following initial boundary value problems governed by linear second order partial differential equations. We shall discuss the solution of the *heat equation* $u_t = c^2 u_{xx}$ and the *wave equation* $u_{tt} = c^2 u_{xx}$ under the given initial and boundary conditions.

3.2- FDM for Heat Equation:

The partial differential equation governing the flow of heat in the rod is given by the parabolic equation:

PDE:
$$u_t = c^2 u_{xx}, 0 \le x \le l, t > 0$$
 (1)

where c^2 is a constant and depends on the material properties of the rod. In order that the solution of the problem exists and is unique, we need to prescribe the following conditions:

(i) Boundary Conditions (BCs): As $0 \le x \le l$, BCs at x = 0 and at x = l are to be defined:

$$u(0,t) = g(t), u(l,t) = h(t), t > 0.$$
 (2)

(ii) Initial Condition (IC): At time t = 0, the temperature is prescribed:

$$u(x,0) = f(x), \ 0 \le x \le l.$$
 (3)

3.2.1-Mesh generation:

Superimpose on the domain $0 \le x \le l, t > 0$, a rectangular network of mesh lines. Let the interval [0,l] be divided into M equal parts. Then, the mesh length along the x-axis is $h = \frac{l}{M}$. The points along the x-axis are $x_i = ih, i = 0,1,2,...,M$. Let the mesh length along the t-axis be k and define $t_j = jk$. The mesh points are (x_i, t_j) . We call t_j as the j-th time level (see Fig.3.1). At any point (x_i, t_j) , we denote the numerical solution by $u_{i,j}$ and the exact solution by $u(x_i, t_j)$.

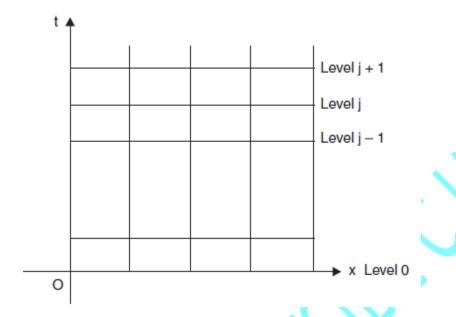


Fig. 3.1 Nodes

3.2.2.-Approximation of the partial derivatives:

Forward approximation to $u_t(x,t)$ at the point $(x,t) = (x_i,t_j)$:

$$(u_t)_{i,j} = \frac{u_{i,j+1} - u_{i,j}}{k} [+O(k)]. \tag{4}$$

Central approximation to $u_{xx}(x,t)$ at the point $(x,t) = (x_i,t_j)$:

$$(u_{xx})_{i,j} = \frac{u_{i+1,j} - 2u_{i,j} + u_{i-1,j}}{h^2} \left[+O(h^2) \right].$$
 (5)

3.2.3.-Forward-Time Central-Space (FTCS) approximation to the IBVP (1)-(3):

Applying the IBVP (1)-(3) at the nodal point $(x,t) = (x_i, t_i)$, we obtain:

PDE:
$$u_t(x_i, t_i) = c^2 u_{xx}(x_i, t_i)$$
. (6)

BCs:
$$u(0,t_i) = g(t_i), u(l,t_i) = h(t_i).$$
 (7)

IC:
$$u(x_i, 0) = f(x_i)$$
. (8)

Using (4) and (5) in (6), we get

$$\frac{u_{i,j+1} - u_{i,j}}{k} = c^2 \frac{u_{i+1,j} - 2u_{i,j} + u_{i-1,j}}{h^2}$$
(9)

After simplifying, we get

$$u_{i,j+1} = \alpha u_{i-1,j} + (1 - 2\alpha)u_{i,j} + \alpha u_{i+1,j}, \tag{10}$$

where $\alpha = \frac{c^2 k}{h^2}$.

Equations (7) and (8) gives

$$u_{0,j} = g(t_j), \ u_{M,j} = h(t_j).$$
 (11)

$$u_{i,0} = f(x_i). (12)$$

Note that the value $u_{i,j+1}$ at the node (x_i,t_{j+1}) is being obtained **explicitly** using the values on the previous time level t_j . This is why this method is an **Explicit Method**. The nodes that are used in the computations are given in Fig.3.1. That is why this method is sometime called 'a **two level method**'. This method is called the **Schmidt method**.

3.2.4.-Computational procedure

Step-1: The initial condition u(x,0) = f(x) gives the solution at all the nodal points on the initial line (level 0).

Step-2: The boundary conditions u(0,t) = g(t), u(l,t) = h(t), t > 0 give the solutions at all the nodal points on the boundary lines x = 0 and x = l, (called boundary points), for all time levels.

Step-3: We choose a value for α and h. This gives the value of the time step length k. Alternately, we may choose the values for h and k.

Step-4: The solutions at all nodal points, (called interior points), on level 1 are obtained using the explicit method (10).

Step-5: The computations are repeated for the required number of steps. If we perform m steps of computation, then we have computed the solutions up to time $t_m = mk$.

Let us illustrate the method through the following problem:

Example 3.1: Solve the heat conduction equation

$$u_t = u_{xx}, \ 0 \le x \le 1, t > 0$$

with

$$u(x,0) = \sin(\pi x), \ 0 \le x \le 1; u(0,t) = u(1,t) = 0, t > 0.$$

using the Schmidt method. Assume $h = \frac{1}{3}$. Compute with (i) $\alpha = \frac{1}{2}$ for two time steps, (ii) $\alpha = \frac{1}{4}$

for four time steps. If the exact solution is $u(x,t) = e^{-\pi^2 t} \sin(\pi x)$, compare the solutions at time $t = \frac{1}{9}$.

Solution:

The Schmidt method is given by

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

where
$$\alpha = \frac{c^2 k}{h^2}$$
.

We are given $h = \frac{1}{3}$. Hence, we have four nodes on each mesh line (see the Fig. 3.2). We have to find the solution at the two interior points.

The initial condition gives the values

$$u\left(\frac{1}{3},0\right) = u_{1,0} = \sin\left(\frac{\pi}{3}\right) = \frac{\sqrt{3}}{2};$$

$$u\left(\frac{2}{3},0\right) = u_{2,0} = \sin\left(\frac{2\pi}{3}\right) = \frac{\sqrt{3}}{2};$$

The boundary conditions give the values:

$$u_{0,j} = u_{3,j} = 0$$
 for all j .



Fig. 3.2

(<u>i)</u> Step-1:

Given $\alpha = \frac{1}{2}$, $h = \frac{1}{3}$, $k = \alpha h^2 = \frac{1}{18}$. The computations are to be done for two time steps, that is, upto $t = \frac{1}{9}$. For $\alpha = \frac{1}{2}$, we get the method

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

Step-2:

We have the following values.

$$j = 0$$
:

$$i = 1$$
: $u_{1,1} = \frac{1}{2} (u_{0,0} + u_{2,0}) = 0.5(0 + 0.866025) = 0.433013.$

$$i = 2$$
: $u_{2,1} = \frac{1}{2} (u_{1,0} + u_{3,0}) = 0.5(0.866025 + 0) = 0.433013.$

$$j = 1$$
:

i = 1:
$$u_{1,2} = \frac{1}{2} (u_{0,1} + u_{2,1}) = 0.5(0 + 0.433013) = 0.216507.$$

$$i = 2$$
: $u_{2,2} = \frac{1}{2} (u_{1,1} + u_{3,1}) = 0.5(0.433013 + 0) = 0.216507.$

Step-3:

After two steps $t = 2k = \frac{1}{9}$. Hence,

$$u\left(\frac{1}{3}, \frac{1}{9}\right) = u\left(\frac{2}{3}, \frac{1}{9}\right) \approx 0.216507$$

<u>(ii)</u>

Step-1:

Given $\alpha = \frac{1}{4}$, $h = \frac{1}{3}$, $k = \alpha h^2 = \frac{1}{36}$. The computations are to be done for two time steps, that is, upto $t = \frac{1}{9}$. For $\alpha = \frac{1}{2}$, we get the method

$$u_{i,j+1} = \frac{1}{4} (u_{i-1,j} + 2u_{i,j} + u_{i+1,j}), j = 0,1,2,3; i = 1,2.$$

Step-2:

We have the following values.

$$\begin{aligned} j &= 0: \\ i &= 1: \quad u_{1,1} = 0.25 \left(u_{0,0} + 2u_{1,0} + u_{2,0} \right) = 0.25 [0 + 3(0.866025)] = 0.649519. \\ i &= 2: \quad u_{2,1} = 0.25 \left(u_{1,0} + 2u_{2,0} + u_{3,0} \right) = 0.25 [3(0.866025) + 0] = 0.649519. \\ j &= 1: \\ i &= 1: \quad u_{1,2} = 0.25 \left(u_{0,1} + 2u_{1,1} + u_{2,1} \right) = 0.25 [0 + 3(0.649519)] = 0.487139. \\ i &= 2: \quad u_{2,1} = 0.25 \left(u_{1,1} + 2u_{2,1} + u_{3,1} \right) = 0.25 [3(0.649519) + 0] = 0.487139. \\ j &= 2: \\ i &= 1: \quad u_{1,3} = 0.25 \left(u_{0,2} + 2u_{1,2} + u_{2,2} \right) = 0.25 [0 + 3(0.487139)] = 0.365354. \\ i &= 2: \quad u_{2,3} = 0.25 \left(u_{1,2} + 2u_{2,2} + u_{3,2} \right) = 0.25 [3(0.487139) + 0] = 0.365354. \\ j &= 3: \\ i &= 1: \quad u_{1,4} = 0.25 \left(u_{0,3} + 2u_{1,3} + u_{2,3} \right) = 0.25 [0 + 3(0.365354)] = 0.274016. \\ i &= 2: \quad u_{2,4} = 0.25 \left(u_{1,3} + 2u_{2,3} + u_{3,3} \right) = 0.25 [3(0.365354) + 0] = 0.274016. \end{aligned}$$

Step-3:

After two steps $t = 2k = \frac{1}{9}$. Hence,

$$u\left(\frac{1}{3}, \frac{1}{9}\right) = u\left(\frac{2}{3}, \frac{1}{9}\right) \approx 0.274016$$

Assignment 3.1:

Solve the heat conduction equation

$$u_t = 32u_{xx}, \ 0 \le x \le 1, t > 0$$

with

$$u(x,0) = \sin(\pi x), \ 0 \le x \le 1; u(0,t) = 0, u(1,t) = t, t > 0.$$

Assume h = 0.5. Use an explicit method with $\alpha = \frac{1}{2}$ for four time steps.

[Answer: $u(0.25,4) \approx 0.125$, $u(0.5,4) \approx 0.5$, $u(0.75,4) \approx 1.625$.]

3.3- FDM for Wave Equation:

The vibrations of the elastic string is governed by the one dimensional wave equation

PDE:
$$u_{tt} = c^2 u_{xx}, \ 0 \le x \le l, t > 0$$
 (1)

where c^2 is a constant and depends on the material properties of the string, the tension T in the string and the mass per unit length of the string.. In order that the solution of the problem exists and is unique, we need to prescribe the following conditions:

(i) Boundary Conditions (BCs): We consider the case when the ends of the string are fixed.

Since the ends are fixed, we have the BCs as:

$$u(0,t) = 0, u(l,t) = 0, t > 0.$$
 (2)

(ii) Initial Condition (IC): At time t = 0, the temperature is prescribed:

Initial Displacement:
$$u(x,0) = f(x), \ 0 \le x \le l.$$

Initial Velocity: $u_t(x,0) = g(x), \ 0 \le x \le l.$ (3)

3.3.1.-Explicit Method:

Using central differences, we write the approximations

$$(u_{tt})_{i,j} = \frac{u_{i,j+1} - 2u_{i,j} + u_{i,j-1}}{k^2} \left[+O(k^2) \right].$$

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

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

Applying the IBVP (1)-(3) at the nodal point $(x,t) = (x_i, t_i)$, and using the above central difference approximations, we obtain:

$$\frac{u_{i,j+1} - 2u_{i,j} + u_{i,j-1}}{k^2} = c^2 \frac{u_{i+1,j} - 2u_{i,j} + u_{i-1,j}}{h^2}$$

which may be written as:

$$u_{i,j+1} = (1-r^2)u_{i,j} + r^2[u_{i+1,j} + u_{i-1,j}] - u_{i,j-1},$$
(4)

where $r = \frac{ck}{h}$, is called the mesh ratio parameter.

The nodes that are used in the computations are given in Fig.3.3.

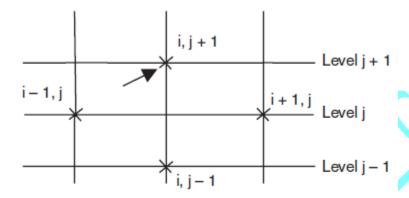


Fig. 3.3: Nodes in explicit method for r = 1.

Remark 3.3.1 We note that the minimum number of levels required for this method is three. Therefore, the method is always a three level method.

Remark 3.3.2 The value $u_{i,j+1}$ at the node (x_i, t_{j+1}) is being obtained explicitly using the values on the previous time level t_j and t_{j-1} . The nodes that are used in the computations are given in Fig.3.3.

Remark 3.3.2

For j = 0, equation (4) gives:

$$u_{i,1} = (1 - r^2)u_{i,0} + r^2[u_{i+1,0} + u_{i-1,0}] - u_{i,-1}.$$
 (5)

Note, that there are external points $u_{i,-1}$ in equation (5). These external points $u_{i,-1}$ will be obtained from the given initial conditions:

The initial condition u(x,0) = f(x) gives the solution at all the nodal points on the initial line (level 0).

The values required on the level t = k is obtained by writing a suitable approximation to the initial condition:

$$u_{t}(x,0) = g(x).$$

If we write the central difference approximation, we obtain:

$$\left(\frac{\partial u}{\partial t}\right)_{i,0} \approx \frac{u_{i,1} - u_{i,-1}}{2k} = g(x_i).$$

This approximation introduces the external points $u_{i,-1}$. Solving for $u_{i,-1}$, we get

$$u_{i,-1} = u_{i,1} - 2kg(x_i). (6)$$

We then substitute (6) in (5) to eliminate the external points $u_{i,-1}$

Note that, when g(x) = 0, we have: $u_{i,-1} = u_{i,1}$

Let us illustrate the method through the following problem:

Example-2: Solve $u_{tt} = 4u_{xx}$, with boundary conditions u(0, t) = 0 = u(4, t), t > 0 and the initial conditions $u_t(x, 0) = 0$, u(x, 0) = x(4 - x).

Solution We have $c^2 = 4$. The values of the step lengths h and k are not prescribed. The number of time steps up to which the computations are to be performed is not prescribed. Therefore, let us assume that we use an explicit method with h = 1 and k = 0.5. Let the number of time steps up to which the computations are to be performed be 4. Then, we have

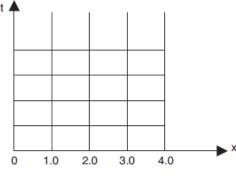


Fig. 3.4

$$r = \frac{ck}{h} = \frac{2(0.5)}{1} = 1.$$

The explicit formula is given by

$$u_{i,j+1} = u_{i+1,j} + u_{i-1,j} - u_{i,j-1}, \quad j = 0, 1, 2, 3 \; ; \; i = 1, 2, 3.$$
 (*)

The boundary conditions give the values $u_{0,j} = 0$, $u_{4,j} = 0$, for all j (see Fig. 3.4). The initial conditions give the following values.

$$\begin{split} u(x,\,0) &= x(4-x), \, \text{gives} \,\, u_{0,0} = 0, \, u_{1,0} = u(1,\,0) = 3, \\ u_{2,0} &= u(2,\,0) = 4, \, u_{3,0} = u(3,\,0) = 3, \, u_{4,0} = u(4,\,0) = 0. \end{split}$$

Central difference approximation to $u_t(x,\ 0)=0$ gives $u_{i,-1}=u_{i,1}.$ We have the following results.

For j = 0: Since, $u_{i-1} = u_{i,1}$, the formula simplifies to $u_{i,1} = 0.5(u_{i+1,0} + u_{i-1,0})$.

$$i = 1$$
: $u_{1.1} = 0.5(u_{2.0} + u_{0.0}) = 0.5(4 + 0) = 2$,

$$i = 2$$
: $u_{2,1} = 0.5(u_{3,0} + u_{1,0}) = 0.5(3 + 3) = 3$,

$$i = 3$$
: $u_{3,1} = 0.5(u_{4,0} + u_{2,0}) = 0.5(0 + 4) = 2$.

These are the solutions at the interior points on the time level t = 0.5.

For j = 1: We use the formula (*) to give $u_{i,2} = u_{i+1,1} + u_{i-1,1} - u_{i,0}$

$$i = 1$$
: $u_{1,2} = u_{2,1} + u_{0,1} - u_{1,0} = 3 + 0 - 3 = 0$,

$$i=2; \hspace{1.5cm} u_{2,2}=u_{3,1}+u_{1,1}-u_{2,0}=2\;+2\;-\;4=0,$$

$$i = 3$$
: $u_{3,2} = u_{4,1} + u_{2,1} - u_{3,0} = 0 + 3 - 3 = 0$.

These are the solutions at the interior points on the time level t = 1.0.

For j = 2: We use the formula (*), to give $u_{i,3} = u_{i+1,2} + u_{i-1,2} - u_{i,1}$.

$$i=1$$
: $u_{1,3} = u_{2,2} + u_{0,2} - u_{1,1} = 0 + 0 - 2 = -2$,

$$i = 2$$
: $u_{2,3} = u_{3,2} + u_{1,2} - u_{2,1} = 0 + 0 - 3 = -3$,

$$i = 3$$
: $u_{3,3} = u_{4,2} + u_{2,2} - u_{3,1} = 0 + 0 - 2 = -2$.

These are the solutions at the interior points on the time level t = 1.5.

For j = 3: We use the formula (*) , to give $u_{i,4} = u_{i+1,3} + u_{i-1,3} - u_{i,2}$.

$$i = 1$$
: $u_{1.4} = u_{2.3} + u_{0.3} - u_{1.2} = -3 + 0 - 0 = -3$,

$$i = 2$$
: $u_{24} = u_{33} + u_{13} - u_{22} = -2 - 2 - 0 = -4$,

$$i = 3$$
: $u_{3,4} = u_{4,3} + u_{2,3} - u_{3,2} = 0 - 3 - 0 = -3$.

These are the solutions at the interior points on the required fourth time level t = 2.0.

Assignment 3.2:

Solve the wave equation

$$u_t = u_{xx}, 0 < x < 1, t > 0$$

with

$$u(x,0) = 0, u_t(x,0) = 0; u(0,t) = 0, u(1,t) = 100\sin(\pi t).$$

Compute for four time steps with h = 0.5.

Answer:

$$\begin{split} &u_{1,1}=u_{2,1}=u_{3,1}=0;\\ &u_{1,2}=u_{2,2}=0, u_{3,2}=50\sqrt{2};\\ &u_{1,3}=0, u_{2,3}=50\sqrt{2}, u_{3,3}=100;\\ &u_{1,4}=50\sqrt{2}, u_{2,4}=100, u_{3,4}=50\sqrt{2}; \end{split}$$