ME 704

Computational Methods in Thermal and Fluids Engineering

(KNI-4 Ordinary Differential Equations)

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Comments on Shooting Method

- Shooting methods need iterative solutions
- This may create convergence problems but usually it can be circumvented by judicial under relaxation
- The advantage is that we can easily get 4^{th} order solutions
- Non-linearity does not require any special treatment

Direct Solutions of BVP

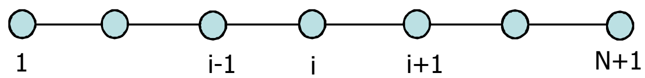
- Finite difference methods can be used to obtain solutions that will satisfy boundary conditions automatically
- For a non-linear system the equations have to be linearized, as otherwise solutions become messy
- Step size sensitivity studies have to be performed before accepting the solutions as satisfactory

Finite difference principles

- In this method, the derivatives are replaced by finite differences
- The domain is discretised into finite number of regions (say N)
- A system of linear equations is formed for the N unknown values of the functions
- Several approaches with varying accuracy are possible
- Popular approaches restrict the order of method upto second order

Finite differences-I

- The finite differences for derivatives can be obtained very easily by Newton interpolating polynomials derived earlier
- The same can also be obtained by Taylor series
- Since Taylor series derivation is easy for first and second derivatives upto second order it is illustrated first.



Finite differences -II

$$f(x+h)=f(x)+hf'(x)+\tfrac{h^2}{2!}f''(x)+\tfrac{h^3}{3!}f'''(x)+O(h^4)$$

$$f(x-h)=f(x)-hf'(x)+\tfrac{h^2}{2!}f''(x)-\tfrac{h^3}{3!}f'''(x)+O(h^4)$$

$$\Rightarrow f(x+h)-f(x-h)=2hf'(x)+2\tfrac{h^3}{3!}f'''(x)+O(h^4)$$

$$\Rightarrow f(x+h)+f(x-h)=2f(x)+h^2f''(x)+O(h^4)$$

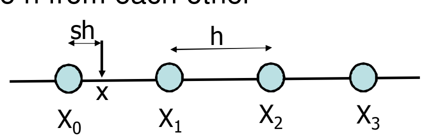
$$\Rightarrow f'(x)=\frac{f(x+h)-f(x-h)}{2h}+O(h^2)$$

$$\Rightarrow f''(x)=\frac{f(x+h)+f(x-h)-2f(x)}{h^2}+O(h^2)$$

The above two relations are called the centered approximations

Finite differences-III

- To get consistent accuracies near boundaries, often we need to get forward and backward differences
- This is easily obtained by using Newton's forward interpolating polynomial
- A system of linear equations is formed for the N unknown values of the functions
- Consider four points in the neighbourhood that are a distance h from each other



Finite differences-IV

- With four points we can fit a polynomial of third order which will be fourth order accurate
- When the first derivative is taken, then this approximation will drop to third order accuracy
- The same will become second order accurate, when second derivative is expressed
- First we shall derive second order accurate formulas by dropping one of the term and compare the results with the previously obtained ones.

Finite differences -V

- Third Order Polynomial

$$P_3(x_0+sh)=f(0)+s\Delta f(0)+\frac{s(s-1)}{2}\Delta^2 f(0)$$
$$+\frac{s(s-1)(s-2)}{6}\Delta^3 f(0)+O(h^4)$$
$$=f_0+s(f_1-f_0)+\frac{s^2-s}{2}(f_2-2f_1+f_0)$$
$$+\frac{s^3-3s^2+2s}{6}(f_3-3f_2+3f_1-f_0)+O(h^4)$$

Finite differences -VI

- The first derivative

$$P_3'(x_0+sh)=\left\{(f_1-f_0)+\frac{2s-1}{2}(f_2-2f_1+f_0)\right.$$
$$\left.+\frac{3s^2-6s+2}{6}(f_3-3f_2+3f_1-f_0)+O(h^4)\right\}\frac{1}{h}$$

- The second derivative

$$P_3''(x_0+sh)=\{(f_2-2f_1+f_0)+$$
$$\left.\frac{6s-6}{6}(f_3-3f_2+3f_1-f_0)+O(h^4)\right\}\frac{1}{h^2}$$

Finite differences -VII

- To get derivatives at x_0 the value of s will be 0 and to get the same at x_1, x_2 and x_3, the values of s will be 1, 2 and 3 respectively
- Thus, we can get backward, forward and centered differences from a single expression just by changing the value of s.
- First, let us get relations for first derivatives that are second order accurate at these points
  - The first derivative One sided Difference at x_0 can be expressed as

$$P_2'(x_0+sh)=\left\{(f_1-f_0)+\frac{2s-1}{2}(f_2-2f_1+f_0)\right\}\frac{1}{h}+O(h^2)$$

Finite differences -VIII

- Putting s = 0, we get

$$P_2'(x_0)=\left\{(f_1-f_0)-\frac{1}{2}(f_2-2f_1+f_0)\right\}\frac{1}{h}+O(h^2)$$
$$=\frac{(-f_2+4f_1-3f_0)}{2h}+O(h^2)$$

Forward Difference

- Putting s = 1, we get

$$P_2'(x_1)=\left\{(f_1-f_0)+\frac{1}{2}(f_2-2f_1+f_0)\right\}\frac{1}{h}+O(h^2)$$
$$=\frac{(f_2-f_0)}{2h}+O(h^2)$$

It has become centered Difference

Finite differences -IX

- Putting s = 2, we get

$$P_2'(x_2)=\left\{(f_1-f_0)+\frac{3}{2}(f_2-2f_1+f_0)\right\}\frac{1}{h}+O(h^2)$$

$$=\frac{(3f_2-4f_1+f_0)}{2h}+O(h^2)$$

It has become Backward Difference

- We can get third order accurate one sided differences by using 3 terms and putting s = 0 and 3

$$P_3'(x_0+sh)=\left\{(f_1-f_0)+\frac{2s-1}{2}(f_2-2f_1+f_0)\right.$$

$$\left.+\frac{3s^2-6s+2}{6}(f_3-3f_2+3f_1-f_0)+O(h^4)\right\}\frac{1}{h}$$

Forward Difference

Finite differences -X

$$P_3'(x_0)=\left\{(f_1-f_0)-\frac{1}{2}(f_2-2f_1+f_0)\right.$$

$$\left.+\frac{2}{6}(f_3-3f_2+3f_1-f_0)\right\}\frac{1}{h}+O(h^3)$$

$$=\frac{2f_3-9f_2+18f_1-11f_0)}{6h}+O(h^3)$$

Forward Difference

$$P_3'(x_3)=\left\{(f_1-f_0)+\frac{5}{2}(f_2-2f_1+f_0)\right.$$

$$\left.+\frac{11}{6}(f_3-3f_2+3f_1-f_0)\right\}\frac{1}{h}+O(h^3)$$

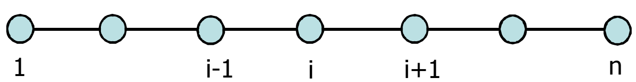
$$=\frac{11f_3-18f_2+9f_1-2f_0)}{6h}+O(h^3)$$

Backward Difference

Simple Application-I

$$\frac{d^2y}{dx^2}+a\frac{dy}{dx}+by=0$$

$$with\quad y(x=0)=y_0,\quad y(x=L)=y_L$$



Simple Application-II

$$\left.\frac{d^2y}{dx^2}\right|_i=\frac{y(i+1)-2y(i)+y(i-1)}{h^2}$$

$$\left.\frac{dy}{dx}\right|_i=\frac{y(i+1)-y(i-1)}{2h}$$

The finite difference equation for node I is

$$\frac{y(i+1)-2y(i)+y(i-1)}{h^2}+a\frac{y(i+1)-y(i-1)}{2h}+by(i)=0$$

Simple Application-III

Multiplying by h^2 and collecting coefficients we get

$$y(i+1)(1+0.5ah)+y(i)(bh^2-2)+y(i-1)(1-0.5ah)=0$$

$$\begin{bmatrix} 1 & 0 & 0 & 0 \\ a_{21} & a_{22} & a_{23} & 0 \\ 0 & a_{32} & a_{33} & a_{34} \\ 0 & 0 & 0 & 1 \end{bmatrix} \begin{Bmatrix} y_1 \\ y_2 \\ y_{n-1} \\ y_n \end{Bmatrix} = \begin{Bmatrix} y_0 \\ b_2 \\ b_{n-1} \\ y_L \end{Bmatrix}$$

We can solve for y's using TDMA

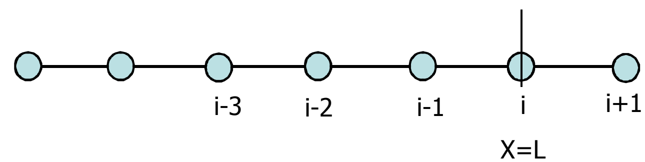
Simple Application-IV

- Treatment of Neumann Boundary Condition

$$\frac{d^2y}{dx^2}+a\frac{dy}{dx}+by=0$$

$$with \quad y(x=0)=y_0, \quad \frac{dy}{dx}(x=L)=y'_L$$

- METHOD-1 Extended Domain Method



Simple Application-V

- Writing FDE at point i

$$\frac{y(i+1)-2y(i)+y(i-1)}{h^2}+a\frac{y(i+1)-y(i-1)}{2h}+by(i)=0 \quad (1)$$

- Boundary Condition at point i

$$\frac{y(i+1)-y(i-1)}{2h}+O(h^2)=y'_L$$

$$\Rightarrow y(i+1)=y(i-1)+2hy'_L+O(h^3) \quad (2)$$

- Substituting Eq. (2) in Eq. (1), we get

$$\frac{y(i-1)+2hy'_L+O(h^3)-2y(i)+y(i-1)}{h^2}+$$

$$a\frac{y(i-1)+2hy'_L+O(h^3)-y(i-1)}{2h}+by(i)=0$$

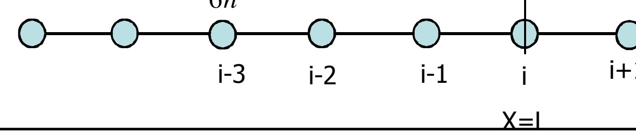
There is degeneration of accuracy

Simple Application-V

- However, the solution can be obtained as for the Dirichlet Boundary Condition as the matrix is tri-diagonal
- The loss of accuracy near the boundary condition may not be acceptable
- This can be overcome by using higher order formulation at the boundary
- METHOD-2 Higher Order Boundary Method

We have shown that a third order accurate derivative can be expressed at the boundary as

$$y'_L=\frac{11y_i-18y_{i-1}+9y_{i-2}-2y_{i-3})}{6h}+O(h^3)$$



Simple Application-VI

The above can be rearranged as

$$6hy'_L = 11y_i - 18y_{i-1} + 9y_{i-2} - 2y_{i-3}$$

This formulation will break the tri-diagonal structure

$$\begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ a_{21} & a_{22} & a_{23} & 0 & 0 & 0 \\ 0 & a_{32} & a_{33} & a_{34} & 0 & 0 \\ 0 & 0 & a_{43} & a_{44} & a_{(i-2)(i-1)} & 0 \\ 0 & 0 & 0 & a_{54} & a_{(i-1)(i-1)} & a_{(i-1)i} \\ 0 & 0 & a_{(i-3)i} & a_{(i-2)i} & a_{(i-1)i} & a_{ii} \end{bmatrix} \begin{Bmatrix} y_1 \\ y_2 \\ y_3 \\ y_4 \\ y_{i-1} \\ y_i \end{Bmatrix} = \begin{Bmatrix} y_0 \\ b_2 \\ b_3 \\ b_4 \\ b_{i-1} \\ 6hy'_L \end{Bmatrix}$$

Simple Application-VII

- A tri-diagonal matrix will be obtained by performing two Gauss operations
- First by performing Gauss Operation between i-2 and i rows, $a_{(i-3),i}$ can be reduced to 0
- Then by performing a Gauss operation between i-1 and I rows, we can reduce $a_{(i-2),i}$ to 0
- Thus, tri-diagonal structure is restored and can be solved by TDMA

Treatment of Non-Linearity-I

- Consider a non-linear Equation

$$y'' + 2y^2y' = 0$$

- When a finite difference equation is written for a node, it will lead to a non-linear equation due to the presence of higher order powers
- In such cases to get a linear form of the equation, we need to resort to iterations
- The procedure is to assume a y distribution
- Linearise and solve for y
- Iterate until convergence is reached
- The underlying principles used in linearisation are discussed in next slide

Treatment of Non-Linearity-II

- The term y^2y' is linearised as

$$(y^2)^k (y')^{k+1}$$

- Thus, while solving, y^2 value is always known and becomes a coefficient in the matrix
- Frequently, the methods tend to diverge
- To facilitate convergence, under-relaxation is employed

$$(y)^{k+1} = \alpha(y)^{k+1} + (1-\alpha)(y)^k$$

- α is assumed to have a value between 0 and 1
- The above suppresses wild variations of y introduced by the iteration method
- Severe non-linearity may force the value of α close to zero
- Convergence criterion is similar to what we normally do by controlling the normalized values between the iterations