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ME 704

Computational Methods in Thermal and Fluids Engineering

(Ordinary Differential Equations-2)

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Runge-Kutta Methods

- From two function evaluations, we can go to several functional evaluation methods which improve accuracy.

$$y_{n+1} = y_n + h\sum_{i=1}^{r}\gamma_i k_i, \quad with \quad \sum_{i=1}^{r}\gamma_i = 1$$

Note that k_is are the slopes or $f(x_i,y_i)$ evaluated at several is

- The values of (x_i,y_i) are chosen appropriately

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Runge-Kutta Methods (cont'd)

- In general

$$k_1 = f(x_n, y_n)$$

$$k_i = f\left((x_n + h\alpha_i),(y_n + h\sum_{j=1}^{i-1}\beta_{i,j}k_{j-1})\right)$$

$$y_{n+1} = y_n + h\sum_{i=1}^{r}\gamma_i k_i, \quad with \quad \sum_{i=1}^{r}\gamma_i = 1$$

- The coefficients α, β and γ are obtained using Taylor Series

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Runge-Kutta Fourth Order Method

α_i	$\beta_{i,j}$		
$\frac{1}{2}$	$\frac{1}{2}$		
$\frac{1}{2}$	0	$\frac{1}{2}$	
1	0	0	1
γ_i: $\frac{1}{6}$	$\frac{2}{6}$	$\frac{2}{6}$	$\frac{1}{6}$

$$k_1 = f(x_n, y_n)$$
$$k_2 = f\left(x_n + 0.5h, y_n + h(0.5k_1)\right)$$
$$k_3 = f\left(x_n + 0.5h, y_n + h(0.5k_2)\right)$$
$$k_4 = f\left(x_n + h, y_n + hk_3\right)$$
$$y^{n+1} = y^n + h/6\left(k_1 + 2k_2 + 2k_3 + k_4\right)$$

- A large variety of methods upto sixth order global accuracy are available (Refer Numerical Solution of ODE by M.K. Jain, Wiley Eastern, 1987)

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Multi-step Methods

- Till now we have marched one-step at a time which involves typically n functional evaluations for the n^{th} order method
  - The question is whether we can have the same order of accuracy using fewer functional evaluations?
  - Multi-step methods precisely accomplish this

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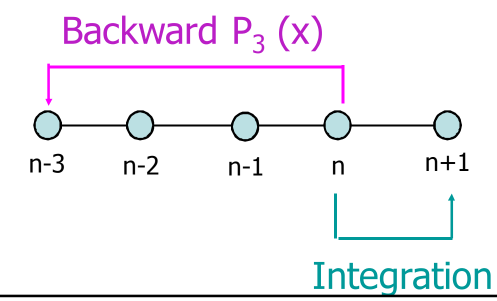
Adams Method

$$\frac{dy}{dx} = f(x, y) \quad \Rightarrow \int_{y_n}^{y_{n+1}} dy = \int_{x_n}^{x_{n+1}} f(x, y)dx$$



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Adams Method (Cont'd)

$$P_3(x) = f(x_n) + s\nabla f(x_n) + \frac{(s)(s+1)}{2!}\nabla^2 f(x_n) + \frac{(s)(s+1)(s+2)}{3!}\nabla^3 f(x_n) + sC4h^4 f^{IV}(\xi)$$

$$y_{n+1} - y_n = \int_0^1 h\left(\begin{array}{l} f(x_n) + s\nabla f(x_n) + \frac{(s)(s+1)}{2!}\nabla^2 f(x_n) \\ + \frac{(s)(s+1)(s+2)}{3!}\nabla^3 f(x_n) + sC4h^4 f^{IV}(\xi) \end{array} \right) ds$$

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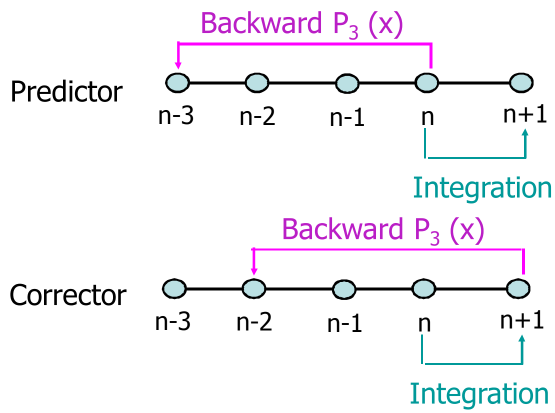
Adams Method (Cont'd)

x	f	∇f	$\nabla^2 f$	$\nabla^3 f$
x_0	f_0	--	--	--
x_1	f_1	(f_1-f_0)	--	--
x_2	f_2	(f_2-f_1)	$(f_2-2f_1+f_0)$	--
x_3	f_3	(f_3-f_2)	$(f_3-2f_2+f_1)$	$(f_3-3f_2+3f_1-f_0)$

$$y_{n+1} = y_n + \frac{h}{24}\left(55 f_n - 59 f_{n-1} + 37 f_{n-2} - 9 f_{n-3}\right) + \frac{251}{720} h^5 y^V(\xi)$$

Adams-Moulton Method



Adams-Moulton Method (Cont'd)

Predictor

$$y_{n+1}^{P} = y_n + \frac{h}{24}\left(55 f_n - 59 f_{n-1} + 37 f_{n-2} - 9 f_{n-3}\right) + \frac{251}{720} h^5 y^V(\xi)$$

Corrector

$$y_{n+1}^{C} = y_n + \frac{h}{24}\left(9 f_{n+1} + 19 f_n - 5 f_{n-1} + f_{n-2}\right) - \frac{19}{720} h^5 y^V(\xi)$$

A-M with Error Correction

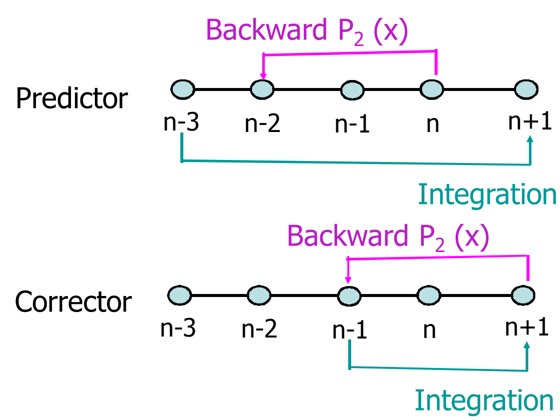
$$\bar{y}_{n+1} = y_{n+1}^{P} + \frac{251}{720} h^5 y^V(\xi)$$

$$\bar{y}_{n+1} = y_{n+1}^{C} - \frac{19}{720} h^5 y^V(\xi)$$

$$\therefore\ y_{n+1}^{C} - y_{n+1}^{P} = h^5 y^V(\xi)\left(\frac{19+251}{720}\right)$$

$$y_{n+1}^{C,Mop} = y_{n+1}^{C} - \left(\frac{19}{19+251}\right)\left(y_{n+1}^{C} - y_{n+1}^{P}\right)$$

Milne's Method



Milne's Method (Cont'd)

Predictor

$$y_{n+1}^{P} = y_{n-3} + \frac{4h}{3}\left(2f_n - f_{n-1} + 2f_{n-2}\right) + \frac{28}{90}h^5 y^V(\xi)$$

Corrector

$$y_{n+1}^{C} = y_{n-1} + \frac{h}{3}\left(f_{n+1} + 4f_n + f_{n-1}\right) - \frac{1}{90}h^5 y^V(\xi)$$

General Comments

- Multi-step methods are efficient as they can give higher order accuracy with just one function evaluation
- Milne's method had simple coefficients, but has stability issues
- Adam's Moulton is the most preferred among multi-step methods
- Error estimated with the method can be used to correct and mop the error
- However, explicit methods like R-K methods can be used to adapt and control errors

Method for Error Control

- We have seen earlier that for stability of the algorithms, step size has to be controlled
- Establishing stability limits for higher order methods is laborious.
- These have been done, but rarely are they applied as many times the accuracy overrides stability
- Usually error control is established by choosing adaptive methods which chooses h automatically.
- R-K methods are most suited for adaptive algorithms as these are one-step methods

Error Control (Cont'd)

- If the magnitude of tolerable error is known, then the step size can be reduced till the estimated error is smaller than the acceptable error.
- If during later part of the computation, the error is too small, then the step size can be doubled.
- We shall look at these in the next lecture
- We shall also look at the methods for higher order ODEs.