ME 704

Computational Methods in Thermal and Fluids Engineering

(KNI-3 Ordinary Differential Equations)

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Error Analysis of ODE Solvers-I

- Before looking at adaptive methods, let us look at the stability of RK-4 method
- By definition, stability is defined as the propagation of the **Round Off Error**
- Let us first look at the equation that will govern the errors

The exact governing equation is $\frac{d\bar{y}}{dx} = f(x, \bar{y})$ (1)

The Numerical solution is obtained for $\frac{dy_N}{dx} = f(x, y_N)$ (2)

Eq.2 – Eq. 1 implies $\frac{d(y_N - \bar{y})}{dx} = f(x, y_N) - f(x, \bar{y})$ (3)

Error Analysis of ODE Solvers-II

Defining $\varepsilon = y_N - \bar{y}$

Eq. 3 can be written as

$$\frac{d\varepsilon}{dx} = f(x, \bar{y} + \varepsilon) - f(x, \bar{y})$$
$$= f(x, \bar{y}) + \varepsilon \frac{\partial (f(x, \bar{y}))}{\partial y} + O(\varepsilon^2) - f(x, \bar{y})$$

For linear stability analysis, we can write $\frac{d\varepsilon}{dx} = \varepsilon \frac{\partial f(x, \bar{y})}{\partial y}$ (4)

The exact solution for Eq. 4 in the neighbourhood of (x_0, y_0) is

$$\varepsilon = \varepsilon_0 e^{(x - x_0)\left.\frac{\partial f}{\partial y}\right|_{(x_0, y_0)}} \quad (5)$$

Error Analysis of ODE Solvers-III

If we are solving numerically using Euler's Method

$$\varepsilon_{n+1} = \varepsilon_n + h\varepsilon_n \left.\frac{\partial f}{\partial y}\right|_{(x_n, y_n)}$$
$$\Rightarrow \frac{\varepsilon_{n+1}}{\varepsilon_n} = 1 + h\left.\frac{\partial f}{\partial y}\right|_{(x_n, y_n)}$$

This is exactly what we got earlier in a different manner

Thus stability of a differential equation solved by a numerical method is to obtain the solution for the equation

$$\frac{d\varepsilon}{dx} = \varepsilon f_y(x, y)$$

The stability conditions are imposed by $G = \left|\frac{\varepsilon_{n+1}}{\varepsilon_n}\right| \le 1$

Error Analysis of RK-4

- The method gets messy as we attempt the answers for higher order equations

$$\frac{d\varepsilon}{dx} = \varepsilon f_y(x,y) = \lambda\varepsilon \qquad \text{where, } \lambda = f_y(x,y)$$

Applying RK-4

$$\varepsilon^{n+1} = \varepsilon^n + h/6(k_1 + 2k_2 + 2k_3 + k_4)$$

$$k_1 = f(x_n, \varepsilon_n) = \lambda\varepsilon_n$$

$$k_2 = f(x_n + 0.5h, \varepsilon_n + h0.5k_1) = \lambda(\varepsilon_n + h0.5k_1)$$

$$= \lambda(\varepsilon_n + h0.5\lambda\varepsilon_n)$$

$$= \lambda\varepsilon_n(1 + 0.5\lambda h)$$

$$k_3 = f(x_n + 0.5h, \varepsilon_n + h0.5k_2) = \lambda(\varepsilon_n + h0.5k_2)$$

$$= \lambda(\varepsilon_n + h0.5[\lambda\varepsilon_n(1 + 0.5\lambda h)])$$

$$= \lambda(\varepsilon_n + h0.5[\lambda\varepsilon_n + 0.5\lambda^2 h\varepsilon_n])$$

$$= \lambda(\varepsilon_n + h0.5\lambda\varepsilon_n + 0.25\lambda^2 h^2\varepsilon_n)$$

$$= \lambda\varepsilon_n(1 + \lambda h0.5 + 0.25\lambda^2 h^2)$$

$$k_4 = f(x_n + h, \varepsilon_n + hk_3) = \lambda(\varepsilon_n + hk_3)$$

$$= \lambda(\varepsilon_n + h[\lambda\varepsilon_n(1 + 0.5\lambda h + 0.25\lambda^2 h^2)])$$

$$= \lambda(\varepsilon_n + h\lambda\varepsilon_n + 0.5\lambda^2 h^2\varepsilon_n + 0.25\lambda^3 h^3\varepsilon_n)$$

$$= \lambda\varepsilon_n(1 + h\lambda + 0.5\lambda^2 h^2 + 0.25\lambda^3 h^3)$$

Error Analysis of RK-4 (Cont'd)

$$\varepsilon^{n+1} = \varepsilon^n + h/6(k_1 + 2k_2 + 2k_3 + k_4)$$

$$\Rightarrow \varepsilon_{n+1} = \varepsilon_n + \frac{h\lambda\varepsilon_n}{6}\begin{pmatrix} 1 + 2(1 + 0.5\lambda h) + 2(1 + 0.5\lambda h + 0.25\lambda^2 h^2) + \\ 1 + \lambda h + 0.5\lambda^2 h^2 + 0.25\lambda^3 h^3 \end{pmatrix}$$

$$\Rightarrow \frac{\varepsilon_{n+1}}{\varepsilon_n} = 1 + \frac{h\lambda}{6}(6 + 3\lambda h + \lambda^2 h^2 + 0.25\lambda^3 h^3)$$

$$= 1 + \lambda h + \frac{\lambda^2 h^2}{2!} + \frac{\lambda^3 h^3}{3!} + \frac{\lambda^3 h^3}{4!}$$

Thus, the stability conditions for RK-4 scheme are:

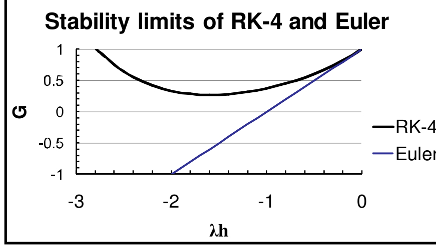
$$-1 \le 1 + \lambda h + \frac{\lambda^2 h^2}{2!} + \frac{\lambda^3 h^3}{3!} + \frac{\lambda^3 h^3}{4!} \le 1$$

Error Analysis of RK-4 (Cont'd)

The condition $1 + \lambda h + \frac{\lambda^2 h^2}{2!} + \frac{\lambda^3 h^3}{3!} + \frac{\lambda^3 h^3}{4!} \le 1$

Implies that for h >0, λ has to be < 0

- Since it is not easy to find the condition of h for a given λ, we shall plot the same and appreciate the condition



- The condition for stability is

$$-2.78 \le \lambda h \le 0$$

- Error propagation is minimum at

$$\lambda h \approx -1.6$$

Error Control

- We have seen that every numerical method has an associated error
- The errors are of two types
- The truncation error is associated with truncating the Taylor series to finite number of terms
- The roundoff error is associated with the limitied digits the computers work with
- The final error is a combination of both the errors.
- Estimation of truncation errors have been presented earlier and we shall visit them again
- The roundoff errors can amplify and have to be controlled by using stable methods
- Arriving at stability criterion can be laborious
- Further, the step size will vary from problem to problem and specifying time steps apriori is difficult

Error Control

- The multistep methods have a problem in adjusting the step size as the formulae are based on constant step sizes
- Though they are inferior, as they cannot adapt without interpolation, they are still used by many for constant step sizes.
- The predictor-corrector methods can estimate the error and this can be exploited.
- We had seen the Adams-Moulton method as

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

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

Error Control (Cont'd)

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

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

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

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

Error Control (Cont'd)

- If the error is too high, then the step size is reduced
- However, once the step is reduced, the method has to be started all over again. Interpolation may be used for generating necessary steps for higher order methods
- The best approach is to use single step method like RK method and adapt accordingly.
- The most popular approach is to use RK-4 and computation is carried out twice
- Once a step of h is taken and then the same is repeated with two steps of h/2 and error is estimated as follows

$$y_{exact} = y_{N\text{-}h} + C\,h^5 \quad (1)$$

$$y_{exact} = y_{N\text{-}0.5h} + 2C\,(h/2)^5 \quad (2)$$

- Eq 1 – Eq 2 gives

$$0 = y_{N\text{-}h} - y_{N\text{-}0.5h} + C\,h^5\,(1\text{-}1/16)$$

Error Control (Cont'd)

$\Rightarrow y_{N-0.5h} - y_{N-h} = (15/16)C\,h^5$

$\Rightarrow (y_{N-0.5h} - y_{N-h})/15 = Ch^5/16$

- Thus the error is estimated and if this is less than tolerance/16, we can double step size
- If error is more than the tolerance, the step size shall be reduced by a factor of two
- Usually a factor of 1.5 to 2 is used as safety to prevent oscillation of the method. Thus the criterion for doubling is error < Tol/(16*safety)

Error Control (Cont'd)

- Often it is better to specify the tolerance on nomalized values of y
- The best way is to divide the error by y and specify a tolerance for this, say 1e-5
- This will have a problem if y crosses zero
- The alternative is to define y_{scale} as

$$y_{scale} = |y| + \left|h\frac{dy}{dx}\right|$$

- Since dy/dx = f(x,y) is the function value that would have been estimated, y_{scale} can be obtained

Set of ODE's

- A set of ODEs are solved very similarly

$$\frac{dy}{dx} = f_1(x,y,z) \quad with \quad y = y_o \quad at \quad x = x_o$$

$$\frac{dz}{dx} = f_2(x,y,z) \quad with \quad z = z_o \quad at \quad x = x_o$$

- Modified Euler's method

$$k_{11} = f_1(x_n, y_n, z_n) \qquad k_{21} = f_1\left(x_n + h, y^{n+1}, z^{n+1}\right)$$

$$k_{12} = f_2(x_n, y_n, z_n) \qquad k_{22} = f_2\left(x_n + h, y^{n+1}, z^{n+1}\right)$$

$$y^{n+1} = y^n + h(k_{11}) \qquad y^{n+1} = y^n + h/2(k_{11} + k_{21})$$

$$z^{n+1} = z^n + h(k_{12}) \qquad z^{n+1} = z^n + h/2(k_{12} + k_{22})$$

Higher Order equations

$$\frac{d^2y}{dx^2} + 3.1\frac{dy}{dx} + 0.3y = 0$$

This equation is a stiff equation with Solution $y=e^{-3x}+e^{-0.1x}$

$$with \quad y(x=0) = 2, \quad \frac{dy}{dx}(x=0) = -3.1$$

- We can split the above equation as

$$\frac{dy}{dx} = z \quad with \quad y(x=0) = 2,$$

$$\frac{dz}{dx} = -3.1z - 0.3y \quad with \quad z(x=0) = -3.1$$

Runge-Kutta Fourth Order Method

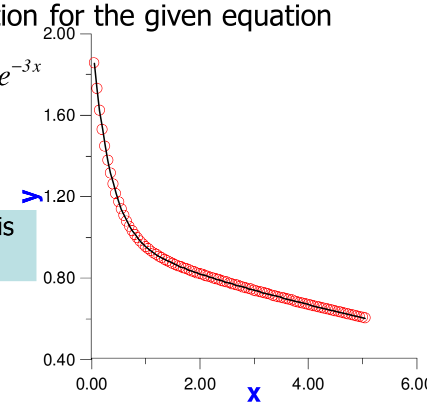
$$k_{11} = f_1(x_n, y_n, z_n)$$
$$k_{12} = f_2(x_n, y_n, z_n)$$
$$k_{21} = f_1\left(x_n + 0.5h, y_n + h(0.5k_{11}), z_n + h(0.5k_{12})\right)$$
$$k_{22} = f_2\left(x_n + 0.5h, y_n + h(0.5k_{11}), z_n + h(0.5k_{12})\right)$$
$$k_{31} = f_1\left(x_n + 0.5h, y_n + h(0.5k_{21}), z_n + h(0.5k_{22})\right)$$
$$k_{32} = f_2\left(x_n + 0.5h, y_n + h(0.5k_{21}), z_n + h(0.5k_{22})\right)$$
$$k_{41} = f_1\left(x_n + h, y_n + hk_{31}, z_n + hk_{32}\right)$$
$$k_{42} = f_2\left(x_n + h, y_n + hk_{31}, z_n + hk_{32}\right)$$
$$y^{n+1} = y^n + h/6\left(k_{11} + 2k_{21} + 2k_{31} + k_{41}\right)$$
$$z^{n+1} = z^n + h/6\left(k_{12} + 2k_{22} + 2k_{32} + k_{42}\right)$$

Sample Problem

- Analytical Solution for the given equation

$$y = e^{-0.1x} + e^{-3x}$$

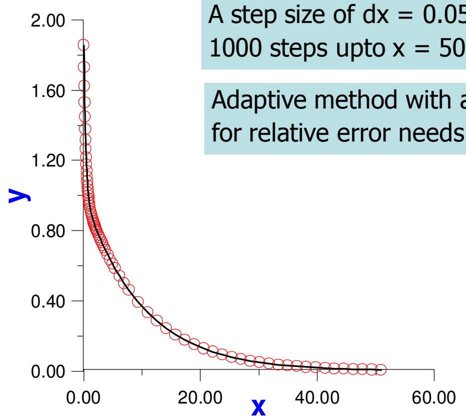
A step sixe of dx = 0.05 is required for accurate sol.



Adaptive method

A step size of dx = 0.05 is would require 1000 steps upto x = 50.

Adaptive method with a tolerance of 10^{-5} for relative error needs only 75 steps



Boundary Value Problem

$$ff'' + 2f''' = 0; \quad f(0) = 0, f'(0) = 0, f'(\infty) = 1.$$

- This equation is the classical Blasius Equation
- It does not have an analytical solution
- Numerical solution obtained suggests x=10 can be considered infinite
- The solution can be found by the IVP approach iteratively
- For this f''(0) is first assumed and adjusted till f'(10) obtained numerically is 0
- This approach is called shooting method

Shooting method

The equation is split into a system of three first order equations

$$\frac{df}{dx} = f_1, \qquad f(0) = 0$$

$$\frac{df_1}{dx} = f_2, \qquad f_1(0) = 0$$

$$\frac{df_2}{dx} = \frac{-ff_2}{2}, \qquad f_2(0) = 0 (assumed)$$