Mathematical Methods in Petroleum & Chemical Engineering

PETE/CHE 5355

Numerical Methods to Solve ODE-IVP

Read on this topic in at least two references.

First Order Ordinary Differential Equations

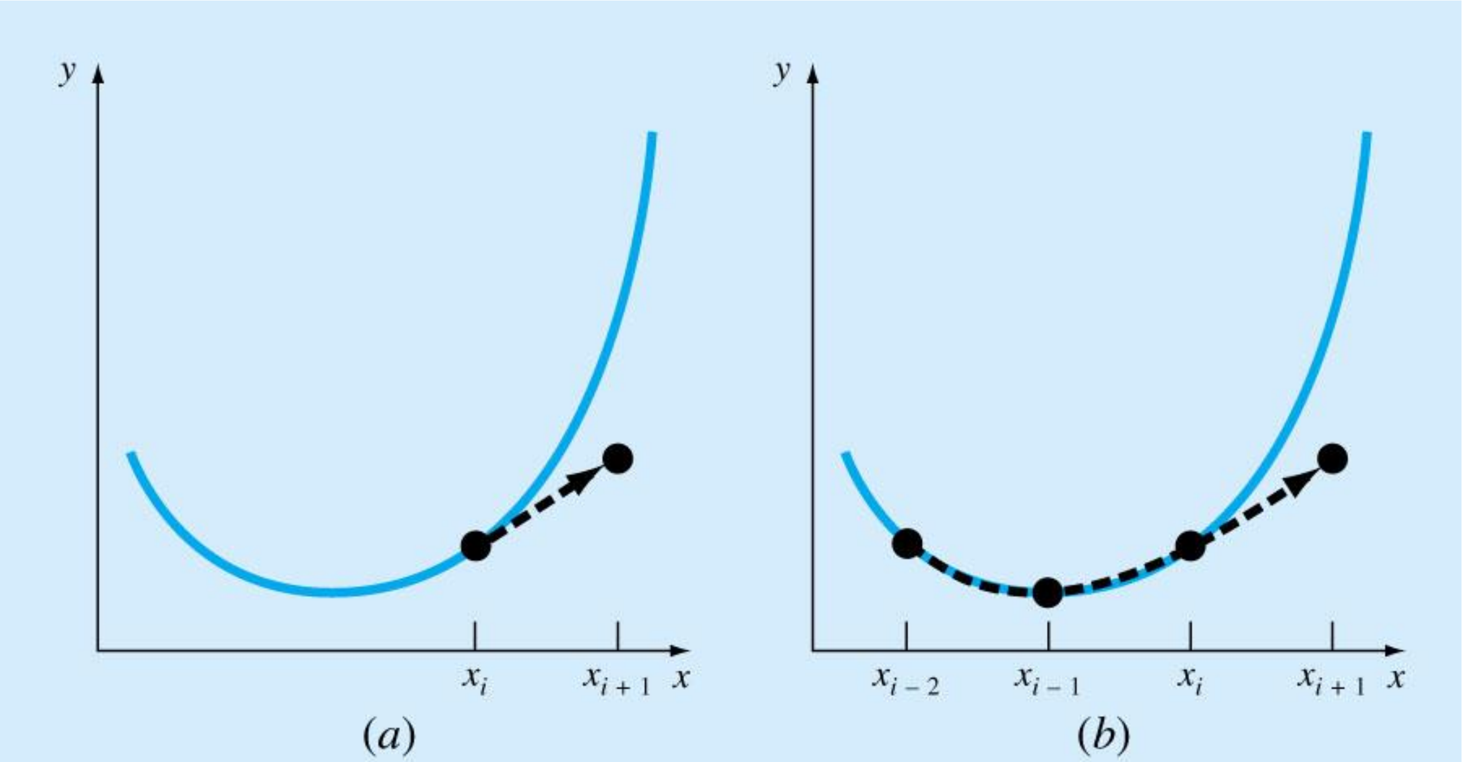
- Our objective is to study methods to solve ordinary differential equations (ODEs) of the general form:

$$\frac{dy}{dx} = f(x, y)$$

$$y(x_0) = y_0$$

- We will consider the following solution methods:
  - ➢One-Step Methods (use information from the previous step only)
    - Euler
    - Runge-Kutta
  - ➢Multi-Step Methods
    - Adams Formulas
    - Predictor-Corrector

One-Step vs Multi-Step Methods



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Euler’s Method

- Euler’s method is a numerical procedure for solving ODEs with a specified initial value.
- It is considered the most basic explicit, first-order one-step method for numerical integration.
- Its local error (error per step) is proportional to the **square** of the step size.
- Its global error (error at a given time) is proportional to the step size.
- The Euler method has been the basis for more accurate methods.

Example 1

The function*

$$y = e^{-t}$$

can be approximated by the following Taylor series expansion

$$y(t) = y_0(0) + \left.\frac{dy}{dx}\right|_{x_0, y_0} \left(t-0\right) + \frac{1}{2!}\left.\frac{d^2y}{dx^2}\right|_{x_i, y_i} \left(t-0\right)^2 + \frac{1}{3!}\left.\frac{d^3y}{dx^3}\right|_{x_i, y_i} \left(t-0\right)^3 + \ldots$$

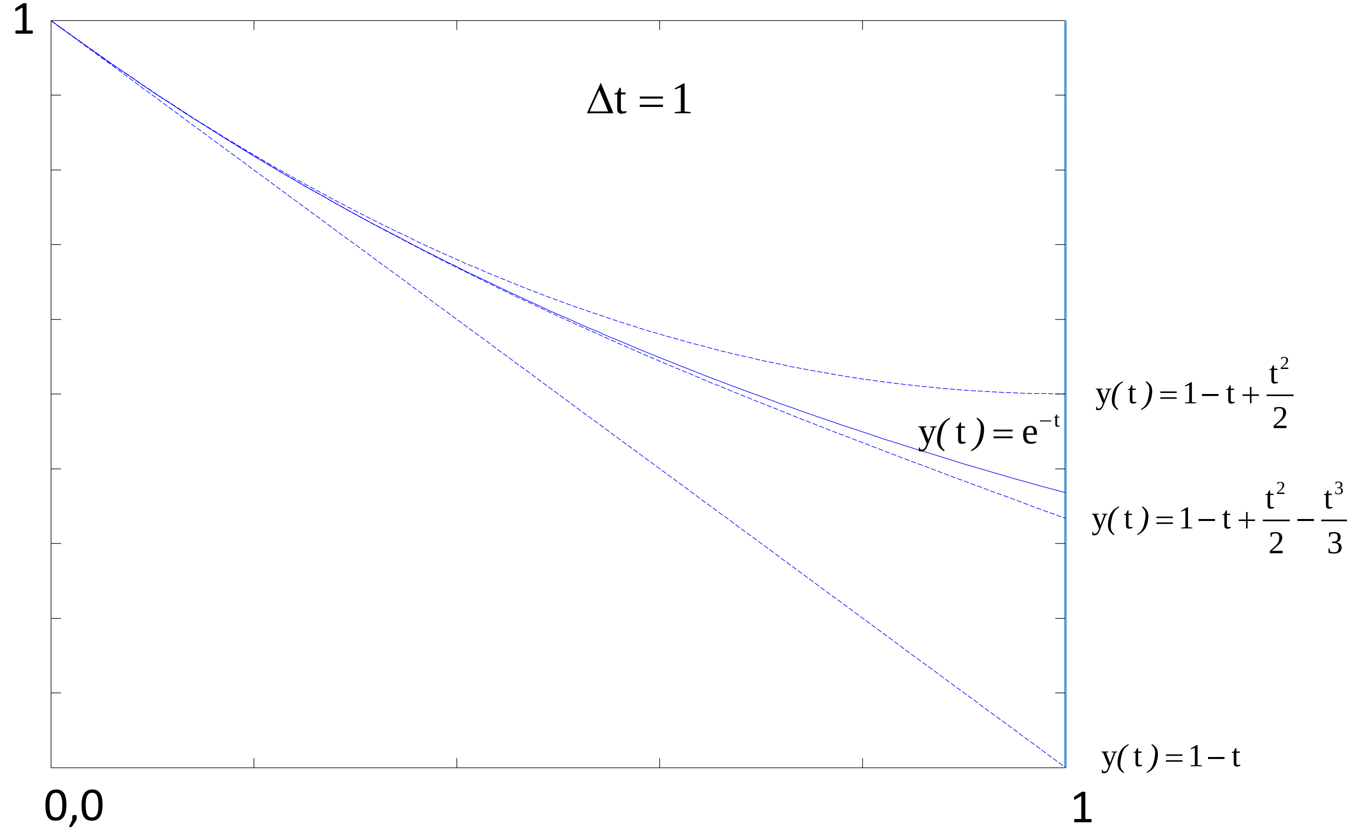
$$y(t) = 1 - t + \frac{t^2}{2} - \frac{t^3}{3} + \ldots(-1)n\frac{t^n}{n!}$$

So, what is the effect of truncation on the quality of our approximation of the original function?

* *See NUMERICAL METHODS FOR DIFFERENTIAL EQUATIONS*

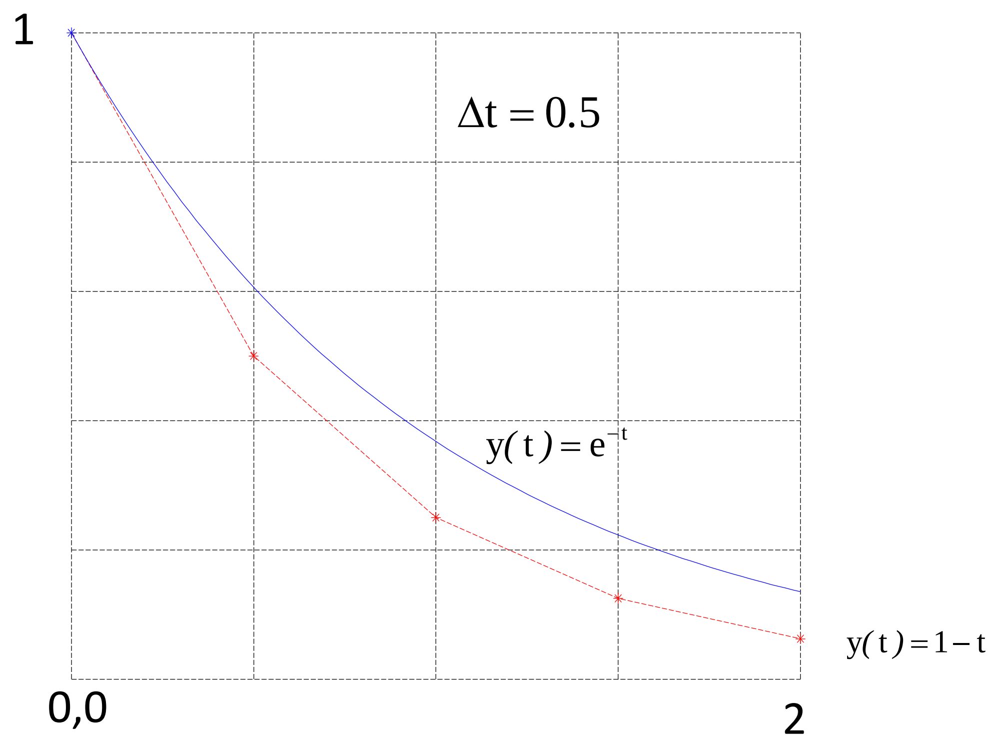
Example 1 (cont.)

Here is what we get. For small increment in t (t<0.1) all looks good; however, for the full step of $\Delta t = 1$, the more terms we have the better the approximation.



Example 1 (cont.)

- Now, what would happen if use the first term approximation repeatedly but with smaller step size? Clearly, we get better results.



Euler's Method

$$\frac{dy}{dx} = f(x, y), \;\; y(0) = y_0$$

$$Slope = \frac{Rise}{Run}$$

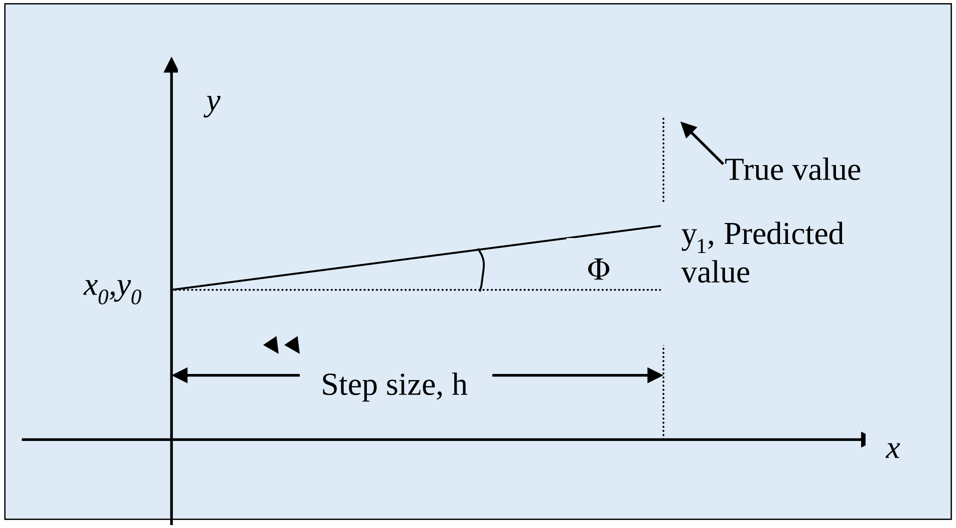
.

$$= \frac{y_1 - y_0}{x_1 - x_0}$$

$$= f(x_0, y_0)$$

$$y_1 = y_0 + f(x_0, y_0)(x_1 - x_0)$$

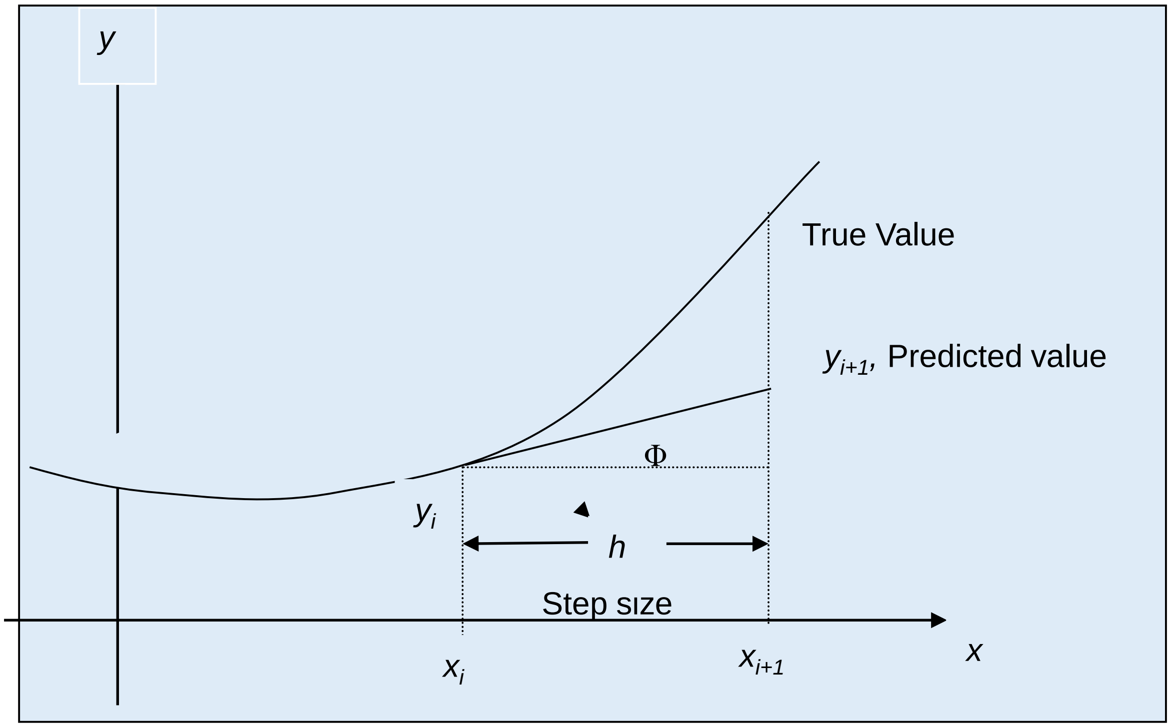
$$= y_0 + f(x_0, y_0)h$$



Graphical interpretation of the first step of Euler's method

Euler's Method

$$\boxed{y_{i+1} = y_i + f\left(x_i, y_i\right)h}$$



General graphical interpretation of Euler's method

How to Write Ordinary Differential Equation

How does one write a first order differential equation in the form of

$$\frac{dy}{dx} = f(x, y)$$

Example

$$\frac{\mathrm{dy}}{\mathrm{dx}} + 2\mathrm{y} = 1.3\mathrm{e}^{-\mathrm{x}}, \quad \mathrm{y}(0) = 5$$

is rewritten as

$$\frac{\mathrm{dy}}{\mathrm{dx}} = 1.3\mathrm{e}^{-\mathrm{x}} - 2\mathrm{y}, \quad \mathrm{y}(0) = 5$$

In this case

$$f(x, y) = 1.3e^{-x} - 2y$$

Example 2

- A ball at 1200K is allowed to cool down in air at an ambient temperature of 300K. Assuming heat is lost only due to radiation, the differential equation for the temperature of the ball is given by

$$\frac{d\theta}{dt} = -2.2067\times10^{-12}\left(\theta^4 - 81\times10^8\right), \theta(0) = 1200K$$

- Find the temperature at t=480 seconds using Euler's method.
- Assume a step size of h=240 seconds.

$$\frac{d\theta}{dt} = -2.2067\times10^{-12}\left(\theta^4 - 81\times10^8\right)$$

$$f(t,\theta) = -2.2067\times10^{-12}\left(\theta^4 - 81\times10^8\right)$$

$$\theta_{i+1} = \theta_i + f(t_i, \theta_i)h$$

Example 2 (cont.)

Solution:

- The ODE: $$\frac{\mathrm{d}\theta}{\mathrm{dt}} = -2.2067 \times 10^{-12}\left(\theta^4 - 81 \times 10^8\right)$$
- The initial condition: $\theta(0) = 1200\mathrm{K}$
- Assume a step size of *h*=240 seconds

We have

$$\frac{d\theta}{dt} = -2.2067 \times 10^{-12}\left(\theta^4 - 81 \times 10^8\right)$$

This means

$$f(t, \theta) = -2.2067 \times 10^{-12}\left(\theta^4 - 81 \times 10^8\right)$$

Now we apply Euler formula:

$$\theta_{i+1} = \theta_i + f(t_i, \theta_i)h$$

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Example 2 (cont.)

Step 1: For $t = 0, \quad \theta_0 = 1200, \quad h = 240$

$$\theta_1 = \theta_0 + f(t_0, \theta_0)h$$

$$= 1200 + f(0,1200)240$$

$$= 1200 + \left(-2.2067\times10^{-12}\left(1200^4 - 81\times10^8\right)\right)240$$

$$= 1200 + (-4.5579)240$$

$$= 106.09K$$

θ_1 is the approximate temperature at

$$t = t_1 = t_0 + h = 0 + 240 = 240$$

$$\theta_1 = \theta(240) \cong 106.09K$$

Example 2 (cont.)

Step 2: For $i=1$, $t_1=240$, $\theta_1=106.09$

$$\theta_2=\theta_1+f\left(t_1,\theta_1\right)h$$
$$=106.09+f\left(240,106.09\right)240$$
$$=106.09+\left(-2.2067\times10^{-12}\left(106.09^4-81\times10^8\right)\right)240$$
$$=106.09+\left(0.017595\right)240$$
$$=110.32K$$

θ_2 is the approximate temperature at

$$t=t_2=t_1+h=240+240=480$$

$$\theta_2=\theta\left(480\right)\cong110.32K$$

Example 2 (cont.)

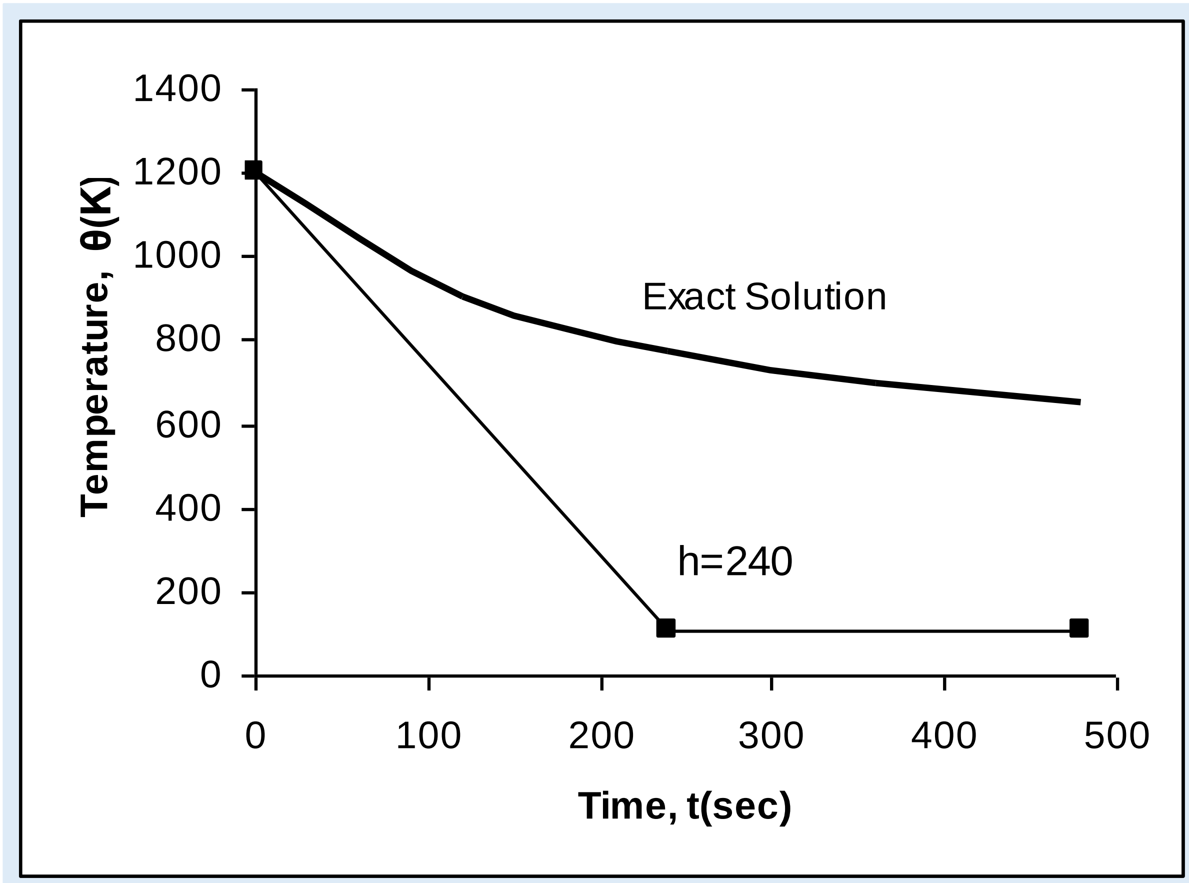
The exact solution of the ordinary differential equation is given by the solution of a non-linear equation as

$$0.92593\ln\frac{\theta-300}{\theta+300}-1.8519\tan^{-1}(0.00333\theta)=-0.22067\times10^{-3}t-2.9282$$

The exact solution to this nonlinear equation at t=480 seconds is

$$\theta(480)=647.57K$$

Comparison of Exact and Numerical Solutions

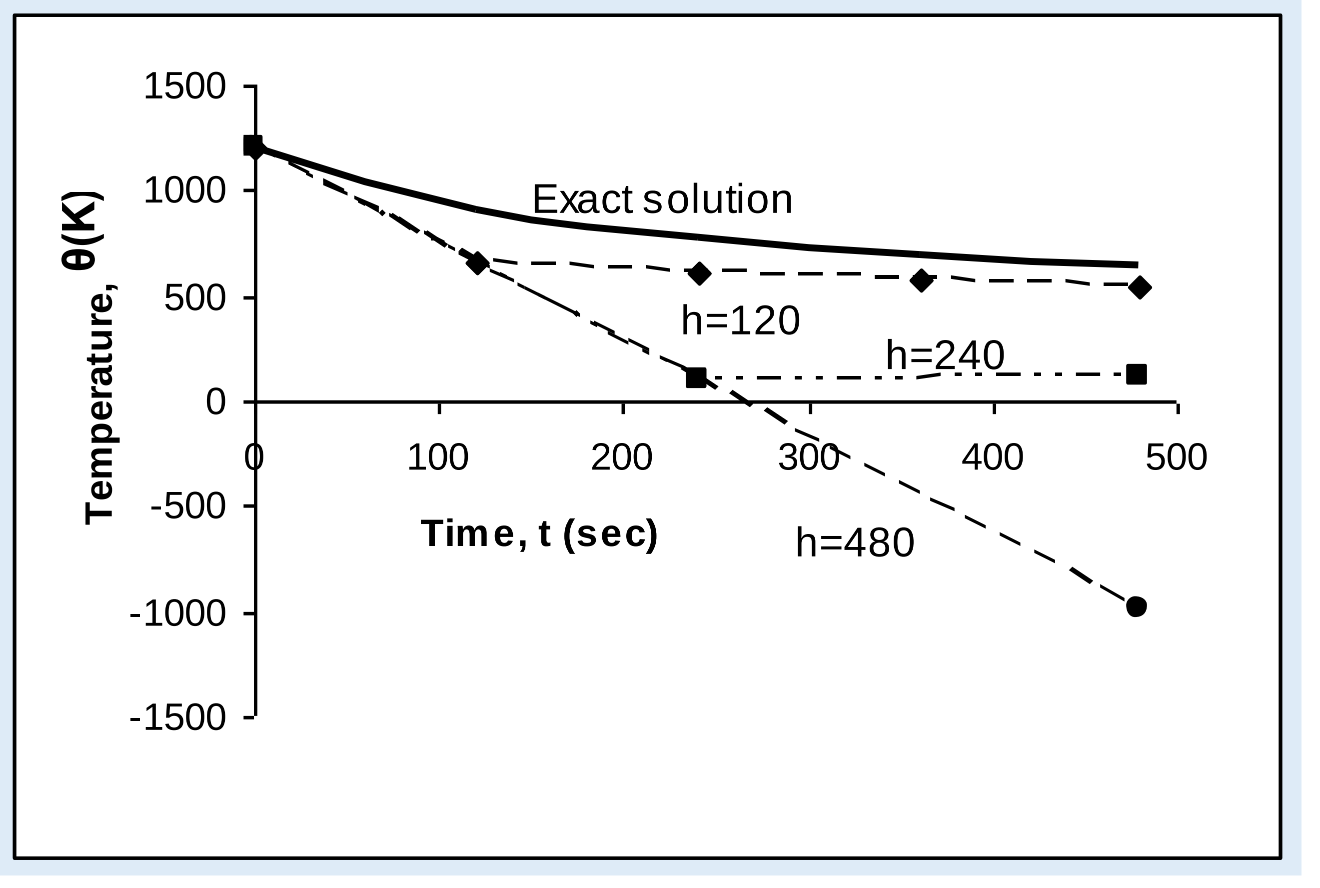


Effect of Step Size

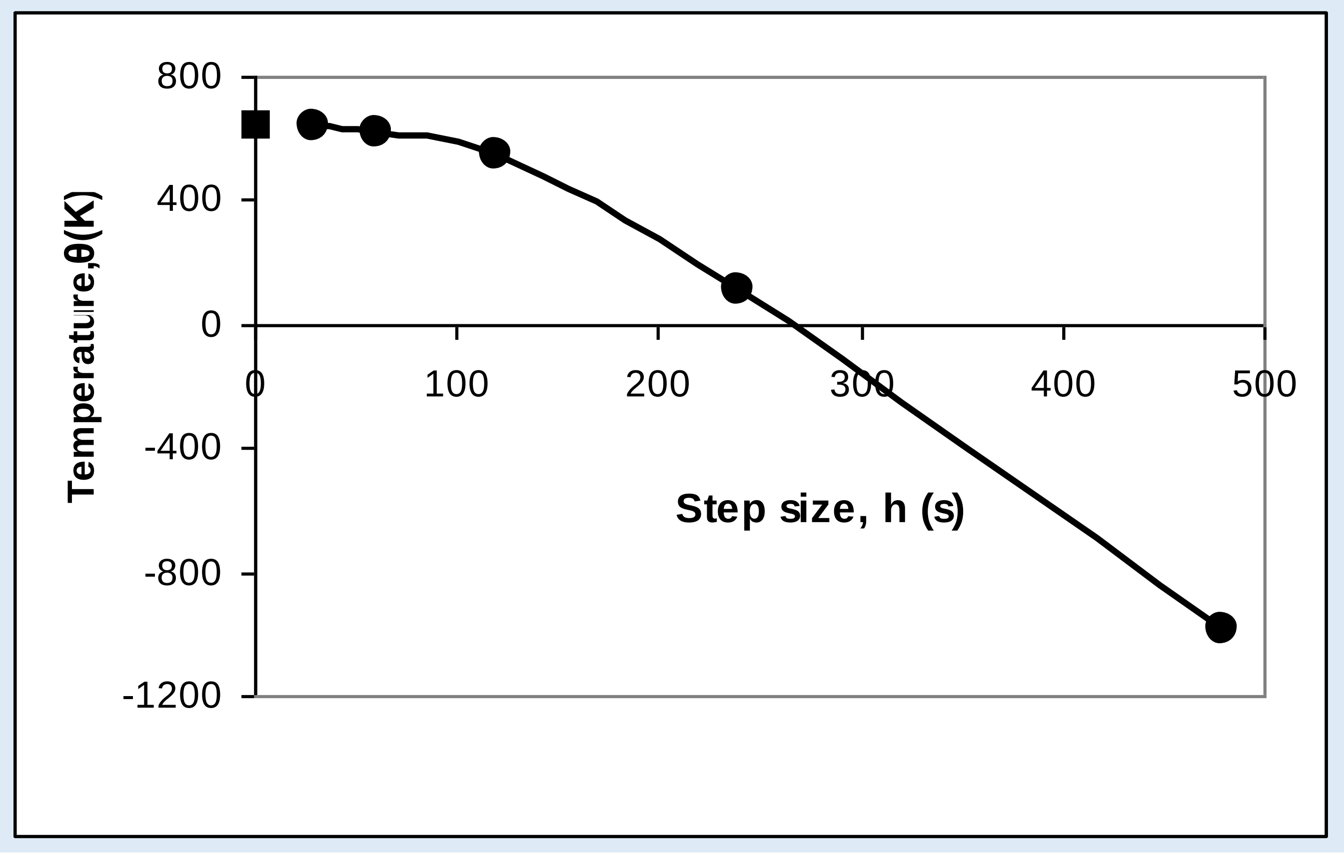
Step h	$\theta(480)$	E_t	$\lvert\in_t\rvert\ \%$
480	-987.81	1635.4	252.54
240	110.32	537.26	82.96
120	546.78	100.8	15.57
60	614.97	32.607	5.03
30	632.77	14.806	2.29

$$\theta(480) = 647.57K \quad \text{(exact)}$$

Comparison with Exact Solution for Different Step Sizes



Effects of Step Size on Euler's Method



Errors in Euler's Method

It can be seen that Euler's method has large errors. This can be illustrated using Taylor series.

$$y_{i+1} = y_i + \left.\frac{dy}{dx}\right|_{x_i, y_i} (x_{i+1} - x_i) + \frac{1}{2!} \left.\frac{d^2 y}{dx^2}\right|_{x_i, y_i} (x_{i+1} - x_i)^2 + \frac{1}{3!} \left.\frac{d^3 y}{dx^3}\right|_{x_i, y_i} (x_{i+1} - x_i)^3 + \ldots$$

$$y_{i+1} = y_i + f(x_i, y_i)(x_{i+1} - x_i) + \frac{1}{2!} f'(x_i, y_i)(x_{i+1} - x_i)^2 + \frac{1}{3!} f''(x_i, y_i)(x_{i+1} - x_i)^3 + \ldots$$

As you can see the first two terms of the Taylor series

$y_{i+1} = y_i + f(x_i, y_i)h$ are the Euler's method.

The true error in the approximation is given by

$$E_t = \frac{f'(x_i, y_i)}{2!} h^2 + \frac{f''(x_i, y_i)}{3!} h^3 + \ldots \qquad E_t \propto h^2$$

Using Higher Order Euler's Method

- Euler's method may have large errors.
- Using smaller step size reduces the error.
- What is the benefit of using higher order Euler?

Runge-Kutta Type Formulas

To over come the deficiencies of Euler's method, other approaches were developed. Among these, the Runge-Kutta finds wide applications.

- Advantages:
  - They are one-step methods, i.e., only x_i information is required.
  - In general, they have good stability characteristics.
  - The step size can be changed as desired without any complications.
  - They are self-starting.
  - They are easy to program.

- Disadvantages:
  - They require significantly more computer time than other methods of comparable accuracy.
  - Local error estimates are somewhat difficult to obtain.

⋮

The Generalized Explicit Runge-Kutta (RK)

- The generalized RK can be written as:

$$y_{n+1} = y_n + h\sum_{i=1}^{s} b_i k_i,$$

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

$$k_2 = f(t_n + c_2 h, y_n + h(a_{21}k_1)),$$

$$k_3 = f(t_n + c_3 h, y_n + h(a_{31}k_1 + a_{32}k_2)),$$

$$k_s = f(t_n + c_s h, y_n + h(a_{s1}k_1 + a_{s2}k_2 + \cdots + a_{s,s-1}k_{s-1})).$$

Where s is the number of stages considered. For example, for fourth-order RK (RK4), we have

$$y_{i+1} = y_i + \frac{1}{6}\left(k_1 + 2k_2 + 2k_3 + k_4\right)h$$

Runge-Kutta 2nd Order (RK2) Method

$$y_{j+1} = y_j + \Delta t f\left(t_{j+1/2}, y^*_{j+1/2}\right)$$

where

$$y^*_{j+1/2} = y_j + \frac{\Delta t}{2} f\left(t_j, y_j\right)$$

and

$$t_{j+1/2} = t_j + \frac{\Delta t}{2}$$

Runge-Kutta 4th Order (RK4) Method

$$y_{j+1} = y_j + \Delta t\left[\frac{1}{6}f\left(t_j, y_j\right) + \frac{1}{3}f\left(t_{j+1/2}, y^{*}_{j+1/2}\right) + \frac{1}{3}f\left(t_{j+1/2}, y^{**}_{j+1/2}\right) + \frac{1}{6}f\left(t_{j+1}, y^{***}_{j+1}\right)\right]$$

where

$$y^{*}_{j+1/2} = y_j + \frac{\Delta t}{2}f\left(t_j, y_j,\right)$$

$$y^{**}_{j+1/2} = y_j + \frac{\Delta t}{2}f\left(t_{j+1/2}, y^{*}_{j+1/2}\right)$$

$$y^{***}_{j+1} = y_j + \Delta t f\left(t_{j+1}, y^{**}_{j+1/2}\right)$$

Runge-Kutta 4th Order Method (RK4)

For $$\frac{dy}{dx} = f(x, y), \quad y(0) = y_0$$

Runge-Kutta 4th order method is given by

$$y_{i+1} = y_i + \frac{1}{6}\left(k_1 + 2k_2 + 2k_3 + k_4\right)h$$

where

$$k_1 = f\left(x_i, y_i\right)$$

$$k_2 = f\left(x_i + \frac{1}{2}h, y_i + \frac{1}{2}k_1 h\right)$$

$$k_3 = f\left(x_i + \frac{1}{2}h, y_i + \frac{1}{2}k_2 h\right)$$

$$k_4 = f\left(x_i + h, y_i + k_3 h\right)$$

Example 3

A ball at 1200K is allowed to cool down in air at an ambient temperature of 300K. Assuming heat is lost only due to radiation, the differential equation for the temperature of the ball is given by

$$\frac{d\theta}{dt} = -2.2067\times10^{-12}\left(\theta^4 - 81\times10^8\right), \theta(0) = 1200K$$

Find the temperature at $t = 480$ seconds using RK4 method.

Assume a step size of h = 240 seconds.

$$\frac{d\theta}{dt} = -2.2067\times10^{-12}\left(\theta^4 - 81\times10^8\right)$$

$$f(t,\theta) = -2.2067\times10^{-12}\left(\theta^4 - 81\times10^8\right)$$

$$\theta_{i+1} = \theta_i + \frac{1}{6}\left(k_1 + 2k_2 + 2k_3 + k_4\right)h$$

Example 3 (cont.)

Step 1: $i=0,\ t_0=0,\ \theta_0=\theta(0)=1200$

$$k_1 = f\left(t_0,\theta_o\right) \boxed{= f\left(0,1200\right)} = -2.2067\times 10^{-12}\left(1200^4-81\times 10^8\right) = -4.5579$$

$$k_2 = f\left(t_0+\frac{1}{2}h,\theta_0+\frac{1}{2}k_1h\right) = f\left(0+\frac{1}{2}(240),1200+\frac{1}{2}(-4.5579)240\right) \boxed{= f\left(120,\ 653.05\right)}$$

$$= -2.2067\times 10^{-12}\left(653.05^4-81\times 10^8\right) = -0.38347$$

$$k_3 = f\left(t_0+\frac{1}{2}h,\theta_0+\frac{1}{2}k_2h\right) = f\left(0+\frac{1}{2}(240),1200+\frac{1}{2}(-0.38347)240\right) \boxed{= f\left(120,1154.0\right)}$$

$$= 2.2067\times 10^{-12}\left(1154.0^4-81\times 10^8\right) = -3.8954$$

$$k_4 = f\left(t_0+h,\theta_0+k_3h\right) = f\left(0+240,1200+(-3.894)240\right) \boxed{= f\left(240,\ 265.10\right)}$$

$$= 2.2067\times 10^{-12}\left(265.10^4-81\times 10^8\right) = 0.0069750$$

Example 3 (cont.)

$$\theta_1 = \theta_0 + \frac{1}{6}(k_1 + 2k_2 + 2k_3 + k_4)h$$

$$= 1200 + \frac{1}{6}\left(-4.5579 + 2\left(-0.38347\right) + 2\left(-3.8954\right) + \left(0.069750\right)\right)240$$

$$= 1200 + \frac{1}{6}\left(-13.046\right)240$$

$$= 675.65K$$

θ_1 is the approximate temperature at

$$t = t_1 = t_0 + h = 0 + 240 = 240$$

$$\theta_1 = \theta\left(240\right) \approx 675.65K$$

Example 3 (cont.)

Step 2: $i = 1,\ t_1 = 240,\ \theta_1 = 675.65\text{K}$

$$k_1 = f(t_1, \theta_1) \boxed{= f(240, 675.65)} = -2.2067\times10^{-12}\left(675.65^4 - 81\times10^8\right) = -0.44199$$

$$k_2 = f\left(t_1 + \frac{1}{2}h, \theta_1 + \frac{1}{2}k_1 h\right) = f\left(240 + \frac{1}{2}(240), 675.65 + \frac{1}{2}(-0.44199)240\right) \boxed{= \mathrm{f}(360, 622.61)}$$

$$= -2.2067\times10^{-12}\left(622.61^4 - 81\times10^8\right) = -0.31372$$

$$k_3 = f\left(t_1 + \frac{1}{2}h, \theta_1 + \frac{1}{2}k_2 h\right) = f\left(240 + \frac{1}{2}(240), 675.65 + \frac{1}{2}(-0.31372)240\right) \boxed{= \mathrm{f}(360, 638.00)}$$

$$= -2.2067\times10^{-12}\left(638.00^4 - 81\times10^8\right) = -0.34775$$

$$k_4 = f(t_1 + h, \theta_1 + k_3 h) = f\left(240 + 240, 675.65 + (-0.34775)240\right) \boxed{= \mathrm{f}(480, 592.19)}$$

$$= 2.2067\times10^{-12}\left(592.19^4 - 81\times10^8\right) = -0.25351$$

Example 3 (cont.)

$$\theta_2 = \theta_1 + \frac{1}{6}(k_1 + 2k_2 + 2k_3 + k_4)h$$

$$= 675.65 + \frac{1}{6}\left(-0.44199 + 2\left(-0.31372\right) + 2\left(-0.34775\right) + \left(-0.25351\right)\right)240$$

$$= 675.65 + \frac{1}{6}\left(-2.0184\right)240$$

$$= 594.91K$$

θ_2 is the approximate temperature at

$$t_2 = t_1 + h = 240 + 240 = 480$$

$$\theta_2 = \theta\left(480\right) \approx 594.91\mathrm{K}$$

Example 3 (cont.)

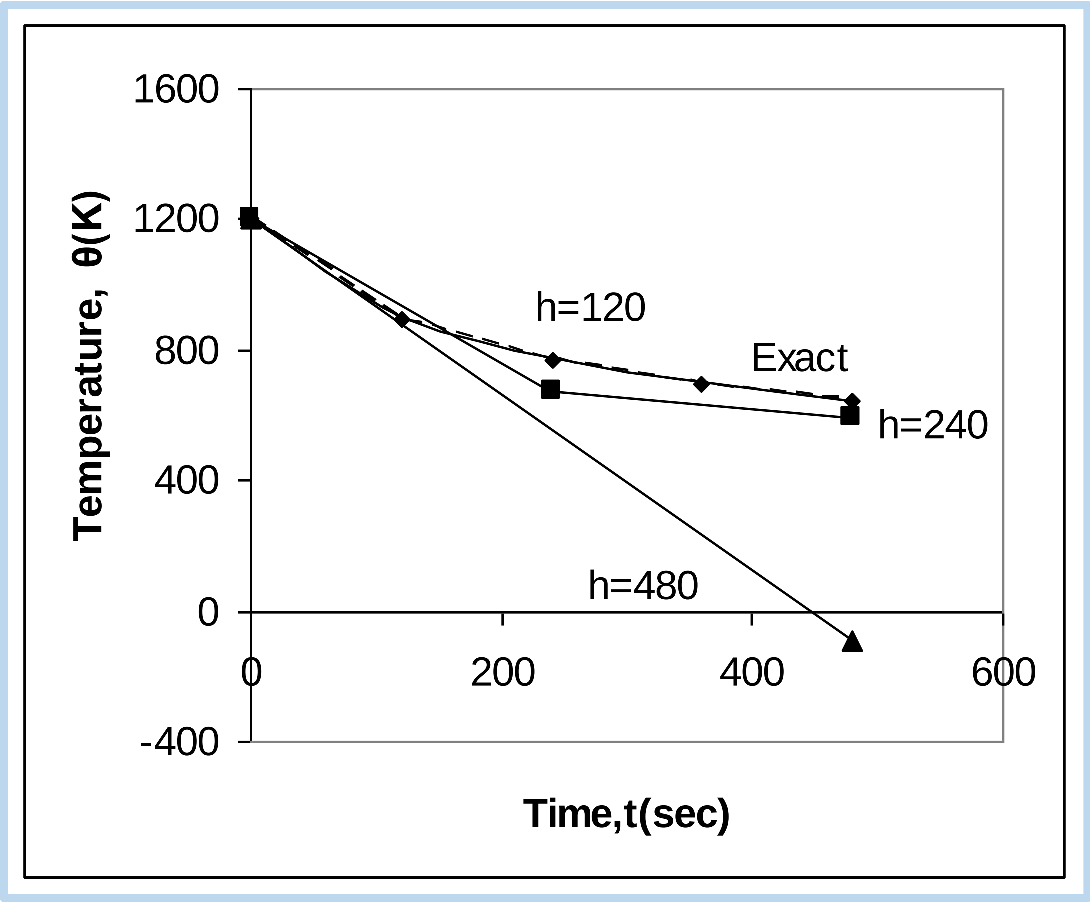
The exact solution of the ordinary differential equation is given by the solution of a non-linear equation as

$$0.92593 \ln \frac{\theta - 300}{\theta + 300} - 1.8519 \tan^{-1}\left(0.00333\theta\right) = -0.22067 \times 10^{-3} t - 2.9282$$

The solution to this nonlinear equation at t=480 seconds is

$$\theta(480) = 647.57K$$

Comparison of Runge-Kutta 4th Order with Exact Solution



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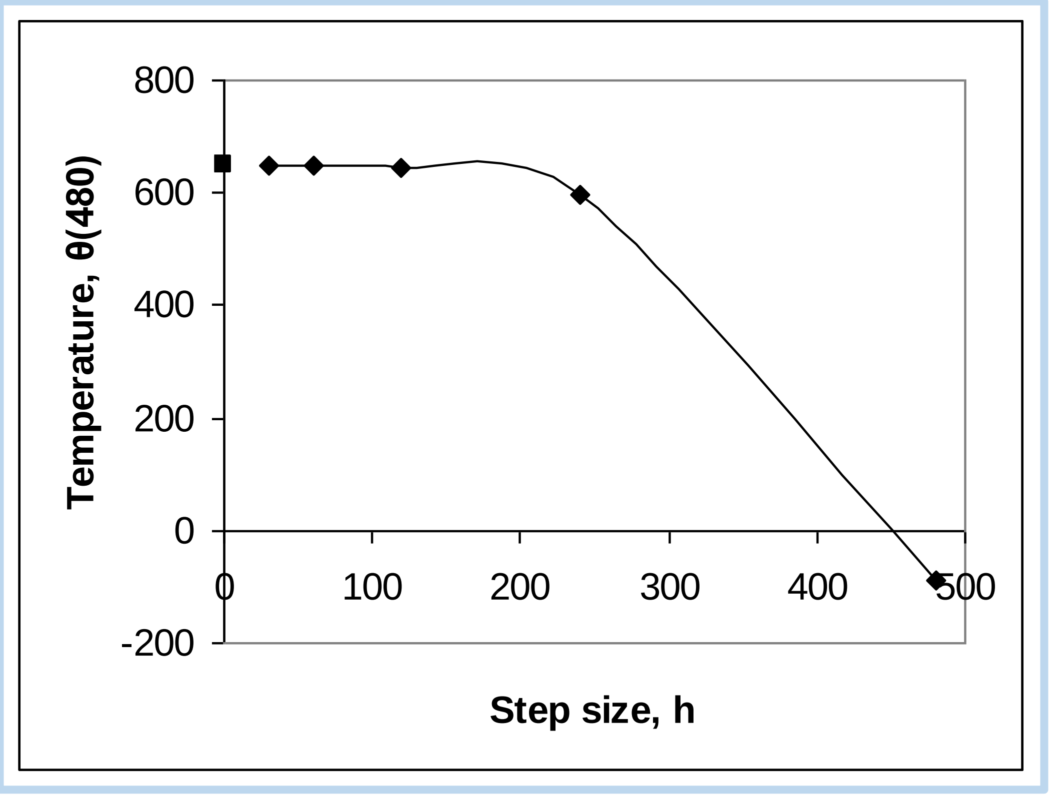
Effect of Step Size

Step *h*	$\theta(480)$	E_t	$\lvert\in_t\rvert$ %
480	-90.278	737.85	113.94
240	594.91	52.660	8.13
120	646.16	1.4122	0.218
60	647.54	0.0336	0.0052
30	647.57	0.000869	0.00013

$$\theta(480) = 647.57K \quad \text{(exact)}$$

Effects of step Size on Runge-Kutta 4th Order Method



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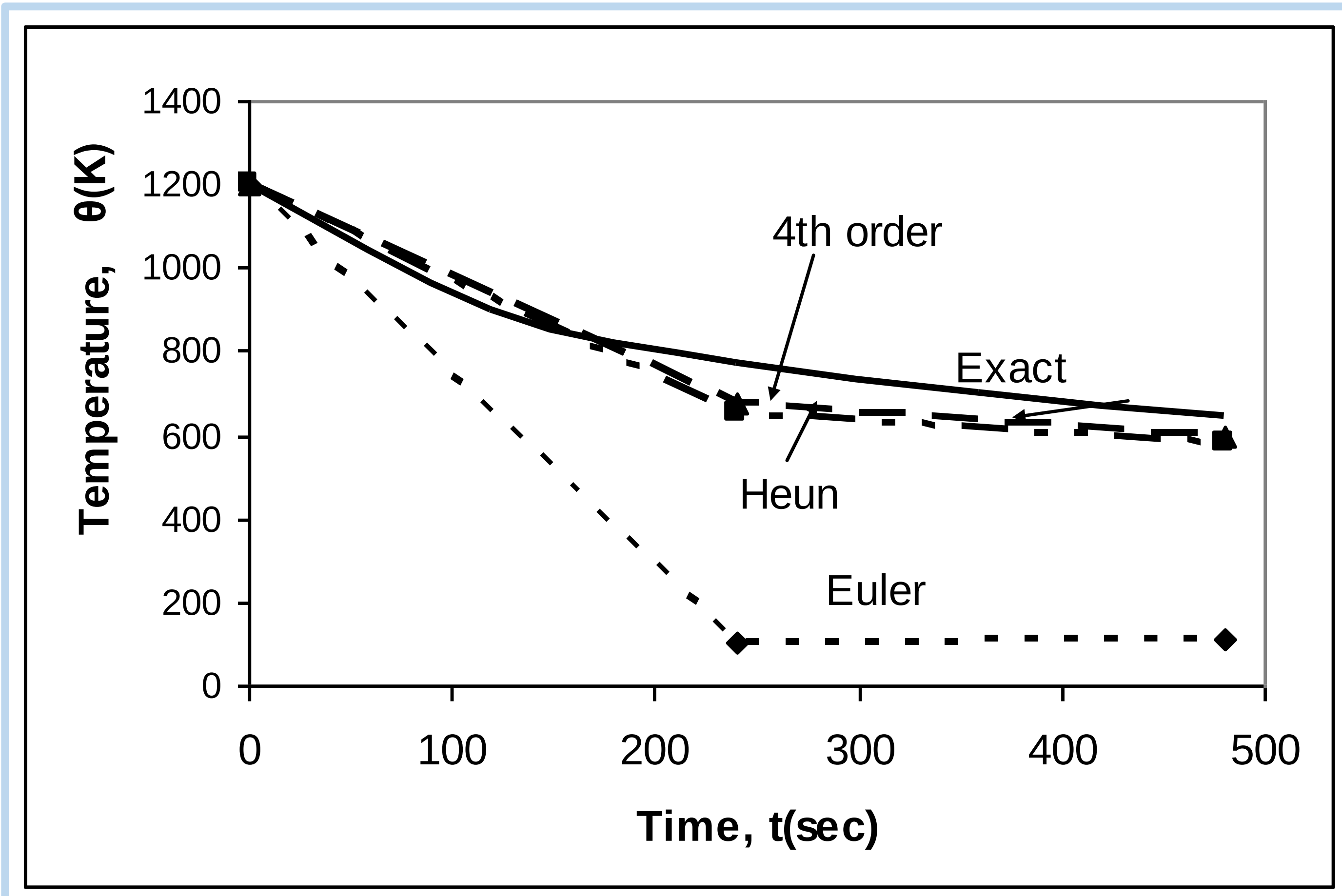
Comparison of Euler and Runge-Kutta Methods



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The Implicit Runge-Kutta

- Explicit RK methods often fail to provide accurate solutions for **stiff** ODEs, for which unstable solutions are generated with typical step sizes.
- This has promoted the development of implicit RK methods, which are given as

$$y_{n+1} = y_n + h \sum_{i=1}^{s} b_i k_i,$$

$$k_i = f\left(t_n + c_i h, y_n + h \sum_{j=1}^{s} a_{ij} k_j\right), \quad i = 1, \ldots, s.$$

where the summation over j is complete in the coefficients a_{ij} and k_j.

The Solution of Sets of Simultaneous First Order ODEs

$$\frac{dy_1}{dt} = f_1(y_1, y_2, y_3, \ldots, y_n, t)$$

$$\frac{dy_2}{dt} = f_2(y_1, y_2, y_3, \ldots, y_n, t)$$

$$\frac{dy_3}{dt} = f_3(y_1, y_2, y_3, \ldots, y_n, t)$$

$$\vdots$$

$$\frac{dy_n}{dt} = f_n(y_1, y_2, y_3, \ldots, y_n, t)$$

$$\frac{d\bar{y}}{dt} = \bar{f}(\bar{y}, t)$$

The Solution of Sets of Simultaneous First Order ODEs

- For a coupled set of equations, f and y become the vectors $\bar{f}$ and $\bar{y}$.
- The complete vectors $\bar{y}$ and then $\bar{f}$ must be calculated at each intermediate point before moving to the next intermediate calculation.

Example 4

Let us look at two coupled equations:

$$\frac{dy_1}{dt} = f_1\left(t, y_1, y_2\right)$$

$$\frac{dy_2}{dt} = f_2\left(t, y_1, y_2\right)$$

Calculation nesting:

For step i [i=0, i_{max}]

Do m=1,4 (RK4 terms)

Do J=1,n (n # equations)

RK4 terms and sequence is as follows:

$$y_{1i+1} = y_{1i} + \frac{1}{6}\left(k_{11} + 2k_{12} + 2k_{13} + k_{14}\right)h; \quad y_{2i+1} = y_{2i} + \frac{1}{6}\left(k_{21} + 2k_{22} + 2k_{23} + k_{24}\right)h$$

$$k_{11} = f_1\left(t_i, y_{1i}, y_{2i}\right) \rightarrow k_{21} = f_2\left(t_i, y_{1i}, y_{2i}\right)$$

$$k_{12} = f_1\left(t_i + \frac{1}{2}h, y_{1i} + \frac{1}{2}k_{11}h, y_{2i} + \frac{1}{2}k_{21}h\right) \rightarrow k_{22} = f_2\left(t_i + \frac{1}{2}h, y_{1i} + \frac{1}{2}k_{11}h, y_{2i} + \frac{1}{2}k_{21}h\right)$$

$$k_{13} = f_1\left(t_i + \frac{1}{2}h, y_{1i} + \frac{1}{2}k_{12}h, y_{2i} + \frac{1}{2}k_{22}h\right) \rightarrow k_{23} = f_2\left(t_i + \frac{1}{2}h, y_{1i} + \frac{1}{2}k_{12}h, y_{2i} + \frac{1}{2}k_{22}h\right)$$

$$k_{14} = f_1\left(t_i + h, y_{1i} + k_{13}h, y_{2i} + k_{23}h\right) \rightarrow k_{24} = f_2\left(t_i + h, y_{1i} + k_{13}h, y_{2i} + k_{23}h\right)$$

Example 4-Cont'd

Let us look at two coupled equations:

$$\frac{dx}{dt} = f\left(t, x, y\right)$$
$$\frac{dy}{dt} = g\left(t, x, y\right)$$

RK4 terms and sequence is as follows:

$$x_{i+1} = x_i + \frac{1}{6}\left(k_1 + 2k_2 + 2k_3 + k_4\right)h; \quad y_{i+1} = y_i + \frac{1}{6}\left(l_1 + 2l_2 + 2l_3 + l_4\right)h$$

$$k_1 = f\left(t_i, x_i, y_i\right) \rightarrow l_1 = g\left(t_i, x_i, y_i\right)$$

$$k_2 = f\left(t_i + \frac{1}{2}h,\, x_i + \frac{1}{2}k_1 h,\, y_i + \frac{1}{2}l_1 h\right) \rightarrow l_2 = g\left(t_i + \frac{1}{2}h,\, x_i + \frac{1}{2}k_1 h,\, y_i + \frac{1}{2}l_1 h\right)$$

$$k_3 = f\left(t_i + \frac{1}{2}h,\, x_i + \frac{1}{2}k_2 h,\, y_i + \frac{1}{2}l_2 h\right) \rightarrow l_3 = g\left(t_i + \frac{1}{2}h,\, x_i + \frac{1}{2}k_2 h,\, y_i + \frac{1}{2}l_2 h\right)$$

$$k_4 = f\left(t_i + h,\, x_i + k_3 h,\, y_i + l_3 h\right) \rightarrow l_4 = g\left(t_i + h,\, x_i + k_3 h,\, y_i + l_3 h\right)$$

Example 4-Cont'd

Let us look at two coupled equations:

$$\frac{dx}{dt} = f\left(t, x, y\right)$$

$$\frac{dy}{dt} = g\left(t, x, y\right)$$

RK4 terms and sequence is as follows:

$$x_{i+1} = x_i + \frac{1}{6}\left(k_1 + 2k_2 + 2k_3 + k_4\right)h; \quad y_{i+1} = y_i + \frac{1}{6}\left(l_1 + 2l_2 + 2l_3 + l_4\right)h$$

$$k_1 = f\left(t_i, x_i, y_i\right) \rightarrow l_1 = g\left(t_i, x_i, y_i\right)$$

$$k_2 = f\left(t_i + \frac{1}{2}h, x_i + \frac{1}{2}k_1h, y_i + \frac{1}{2}l_1h\right) \rightarrow l_2 = g\left(t_i + \frac{1}{2}h, x_i + \frac{1}{2}k_1h, y_i + \frac{1}{2}l_1h\right)$$

$$k_3 = f\left(t_i + \frac{1}{2}h, x_i + \frac{1}{2}k_2h, y_i + \frac{1}{2}l_2h\right) \rightarrow l_3 = g\left(t_i + \frac{1}{2}h, x_i + \frac{1}{2}k_2h, y_i + \frac{1}{2}l_2h\right)$$

$$k_4 = f\left(t_i + h, x_i + k_3h, y_i + l_3h\right) \rightarrow l_4 = g\left(t_i + h, x_i + k_3h, y_i + l_3h\right)$$

Example 4-Cont'd

Consider solving the following second-order ODE equation*:

$$2x\frac{d^2x}{dt^2}+\left(\frac{dx}{dt}\right)^2+1=0$$

with

$$x(1)=1,\ y(1)=0 \quad \text{for} \quad t-\text{range}=[1-1.8] \text{ and } h=0.2$$

We transform this equation into two first-order ODE as follows:

$$\frac{dx}{dt}=y \qquad\Rightarrow\qquad f(t,x,y)=y$$

$$\frac{dy}{dt}=-(1+y^2)/2x \qquad\qquad g(t,x,y)=-(1+y^2)/2x$$

*Adapted from http://nptel.ac.in/courses/111107063/module3/lecture2/lecture2.pdf

Example 4-Cont'd

RK4 terms and sequence is as follows:

$$x_{i+1} = x_i + \frac{1}{6}(k_1 + 2k_2 + 2k_3 + k_4)h; \quad y_{i+1} = y_i + \frac{1}{6}(l_1 + 2l_2 + 2l_3 + l_4)h$$

$$k_1 = f(t_i, x_i, y_i) \rightarrow l_1 = g(t_i, x_i, y_i)$$

$$k_2 = f\left(t_i + \frac{1}{2}h,\ x_i + \frac{1}{2}k_1h,\ y_i + \frac{1}{2}l_1h\right) \rightarrow l_2 = g\left(t_i + \frac{1}{2}h,\ x_i + \frac{1}{2}k_1h,\ y_i + \frac{1}{2}l_1h\right)$$

$$k_3 = f\left(t_i + \frac{1}{2}h,\ x_i + \frac{1}{2}k_2h,\ y_i + \frac{1}{2}l_2h\right) \rightarrow l_3 = g\left(t_i + \frac{1}{2}h,\ x_i + \frac{1}{2}k_2h,\ y_i + \frac{1}{2}l_2h\right)$$

$$k_4 = f(t_i + h,\ x_i + k_3h,\ y_i + l_3h) \rightarrow l_4 = g(t_i + h,\ x_i + k_3h,\ y_i + l_3h)$$

Example 4-Cont'd

i	h	t	x	y	k1	l1
0	0.2	1	1	0	0	-0.5
		t+h/2	**x+h*k1/2**	**y+h*l1/2**	**k2**	**l2**
		1.1	1	-0.0500	-0.0500	-0.5013
		t+h/2	**x+h*k2/2**	**y+h*l2/2**	**k3**	**l3**
		1.1	0.9950	-0.0501	-0.0501	-0.5038
		t+h	**x+h*k3**	**y+h*l3**	**k4**	**l4**
1		1.2	0.9900	-0.1008	-0.1008	-0.5102
			X_{i+1}	**y_{i+1}**		
		1.2	**0.9900**	-0.1007		
1	0.2	1.2	0.9900	-0.1007	-0.1007	-0.5102
		t+h/2	**x+h*k1/2**	**y+h*l1/2**	**k2**	**l2**
		1.3	0.9799	-0.1517	-0.1517	-0.5220
		t+h/2	**x+h*k2/2**	**y+h*l2/2**	**k3**	**l3**
		1.3	0.9748	-0.1529	-0.1529	-0.5249
		t+h	**x+h*k3**	**y+h*l3**	**k4**	**l4**
2		1.4	0.9747	-0.2057	-0.2057	-0.5347
		1.4	0.9595	-0.7284		

x(1)	**x(1.2)**	**x(1.4)**	**x(1.6)**	**x(1.8)**	**x(2)**	
1	**0.9900**	**0.9595**	**0.9071**	**0.8303**	**0.7241**	

The Adams Formulas – Multistep Formulas

Multistep methods improve efficiency by keeping and using the information from previous steps rather than discarding it.

- Adams Open Formulas
  - Uses a Taylor series expansion
  - Can be solved explicitly
  - Second order and higher: Not self-starting – employ a formula which is of the same error order as the formula to be started, i.e. Runge-Kutta type

- Adams Closed Formulas
  - Also, uses a Taylor series expansion
  - Must be solved implicitly – must use an iterative method
  - Third order and higher: Not self-starting

Adams Open Formulas (Explicit Adams)

First Order

$$y_{j+1} = y_j + \Delta t\left[f_j \right] + \vartheta\left(\Delta t\right)^2$$

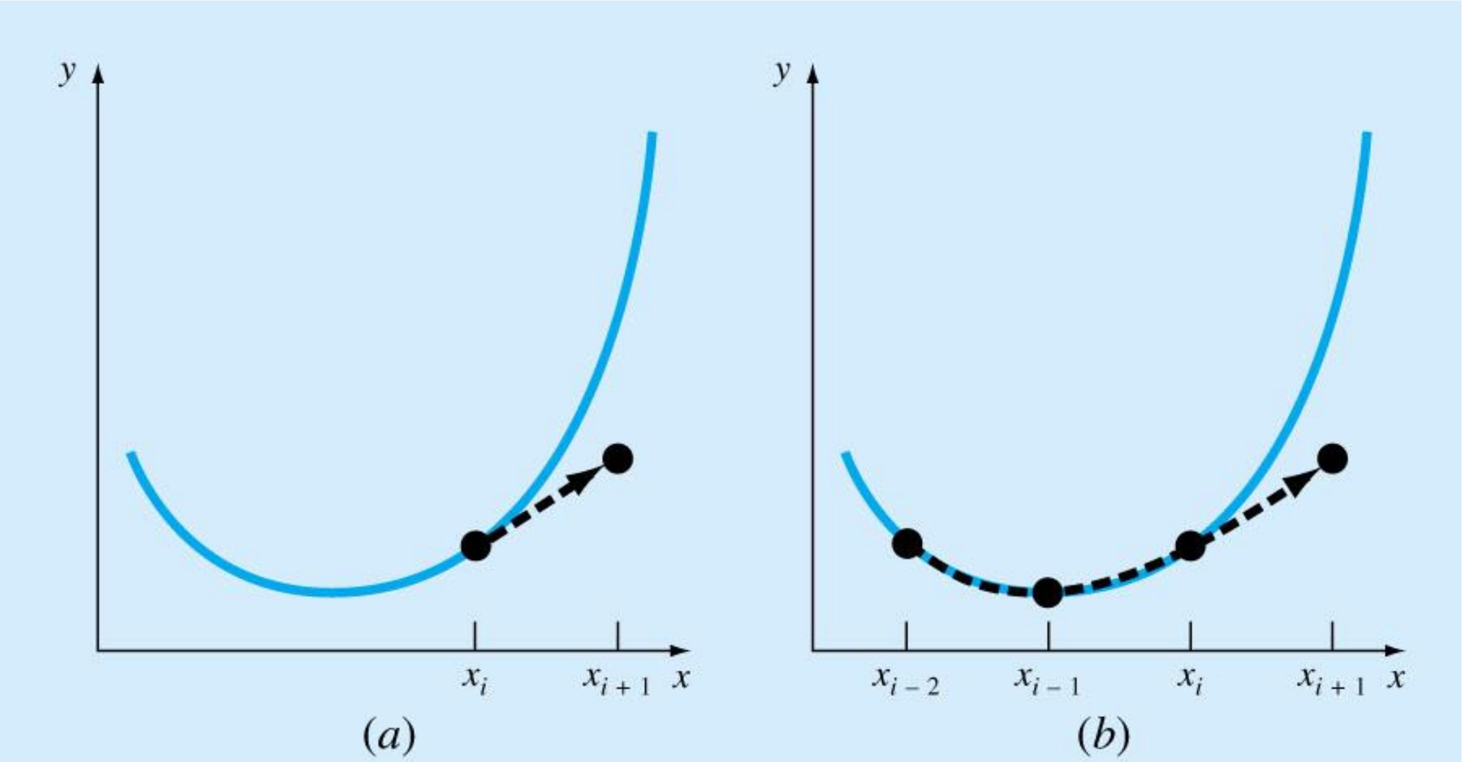
Second Order

$$y_{j+1} = y_j + \Delta t\left[\frac{3}{2} f_j - \frac{1}{2} f_{j-1}\right] + \vartheta\left(\Delta t\right)^3$$

Third Order

$$y_{j+1} = y_j + \Delta t\left[\frac{23}{12} f_j - \frac{16}{12} f_{j-1} + \frac{5}{12} f_{j-2}\right] + \vartheta\left(\Delta t\right)^4$$

One-Step vs Multi-Step Methods



homepages.gac.edu/~hvidsten

Adams Closed Formula (Implicit Adams)

First Order

$$y_j = y_{j-1} + \Delta t\left[f_j \right] + \vartheta\left(\Delta t\right)^2$$

Second Order

$$y_{j+1} = y_j + \Delta t\left[\frac{1}{2} f_{j+1} + \frac{1}{2} f_j \right] + \vartheta\left(\Delta t\right)^3$$

Third Order

$$\mathrm{y}_{\boldsymbol{i+1}} = \mathrm{y}_{\boldsymbol{i}} + \frac{\mathrm{h}}{12}\left[5\mathrm{f}\boldsymbol{(}\mathrm{t}_{\mathrm{i+1}}\boldsymbol{,}\mathrm{y}_{\mathrm{i+1}}\boldsymbol{)} + 8\mathrm{f}\boldsymbol{(}\mathrm{t}_{\mathrm{i}}\boldsymbol{,}\mathrm{y}_{\mathrm{i}}\boldsymbol{)} - \mathrm{f}\boldsymbol{(}\mathrm{t}_{\mathrm{i-1}}\boldsymbol{,}\mathrm{y}_{\mathrm{i-1}}\boldsymbol{)}\right] + +\vartheta\left(\Delta \mathrm{t}\right)^5$$

Higher Order

$$y_{j+1} = y_j + \Delta t \sum_{k=0}^{n} \beta_{nk}^{*} f_{j+1-k} + \vartheta\left(\Delta t\right)^{n+2}$$

Selecting Between a Closed Adams Over Open Adams

- Closed Adams is more time consuming than the Open Adams
- The actual <u>error of a closed formula of a given order is considerably less than that of an open formula</u> of the same order.
- This assumes that the closed formula is iterated an infinite number of times.

Predictor-Corrector Methods

- Implicit multi-step methods (Closed Adams) use the value of y_{i+1} to find the value of y_{i+1}. This is not possible!
- So, we use a combination of Open and Closed formulas.
- We use the Open formula (Predictor) to approximate y_{i+1} "predict" the first estimate of y_{i+1} .
- Then, we use the Closed formula (Corrector) to improve the values of y_{i+1}.

Example 5*

- Use the 3rd order Adams Open Formula (AOF3) explicit method for the initial value.

$$x^*_{i+1} = x_i + \frac{h}{12}\left[23 f_i - 16 f_{i-1} + 5 f_{i-2}\right]$$

- Then use 3rd order Adams Closed Formula (ACF3) implicit method to correct.

$$x_{i+1} = x_i + \frac{h}{12}\left[5 f(t_{i+1}, x^*_{i+1}) + 8 f(t_i, x_i) - f(t_{i-1}, x_{i-1})\right]$$

* Adopted from homepages.gac.edu/~hvidsten

Example 5 (cont.)

- Consider

$$\frac{dx}{dt} = x - t^2;$$

$$\text{Exact Solution}: \; x = 2 + 2t + t^2 - e^{t}$$

- Initial condition: x(0) = 1
- Step size: h = 0.1
- We will use AOF3 and ACF3. Both require 3 points to get started!

Algorithm

1. Use RK4 for initialization to get f_i , f_{i-1}, *and* f_{i-2}
2. Use AOF3 to get x_3^* (predictor)
3. Use ACF3 to get x_3 (corrector)

Example 5 (cont.)

- Initialize using RK4

$$f = f(t,x) = x - t^2$$
$$x(0) = 1;\ h = 0.1$$
Then
$$f_0 = f(t_0, x_0) = f(0,1) = 1.0000$$
and
$$f_1 = f(t_1, x_1) = f(0.1, 1.1048) = 1.0948)$$
$$f_{.2} = f(t_2, x_2) = f(0.2, 1.2186) = 1.1786$$

	Step	t		x	h	
	1	0		1	0.1	
		Coordinates for k				
		t		x	k	
	t	0		1.0000	1.0000	k1
	t+h/2	0.05		1.0500	1.0475	k2
	t+h/2	0.05		1.0524	1.0499	k3
	t+h	0.1		1.1050	1.0950	k4
x(0.1)		1.104829		f(t,x)	1.094829	

For details, see sample RK4 problems.

- OAF3 Predictor Value

$$x^*_{i+1} = x_i + \frac{h}{12}\left[23 f_i - 16 f_{i-1} + 5 f_{i-2}\right]$$

$$x_3^* = x_2 + \frac{0.1}{12}\left[23(1.1786) - 16(1.0948) + 5(1)\right]$$
$$= 1.218597 + 0.121587 = 1.340184$$

Example 5 (cont.)

- To correct, we need $f(t_3 , x_3^*)$

$$f(0.3, 1.340184) = 1.250184$$

- Corrector Value:

$$x_{i+1} = x_i + \frac{h}{12}\left[5f(t_{i+1}, x_{i+1}^*) + 8f(t_i, x_i) - f(t_{i-1}, x_{i-1})\right]$$

$$x_3 = x_2 + \frac{0.1}{12}\left[5(1.250184) + 8(1.178597) - 1(1.094829)\right]$$

$$= 1.218597 + 0.121541$$

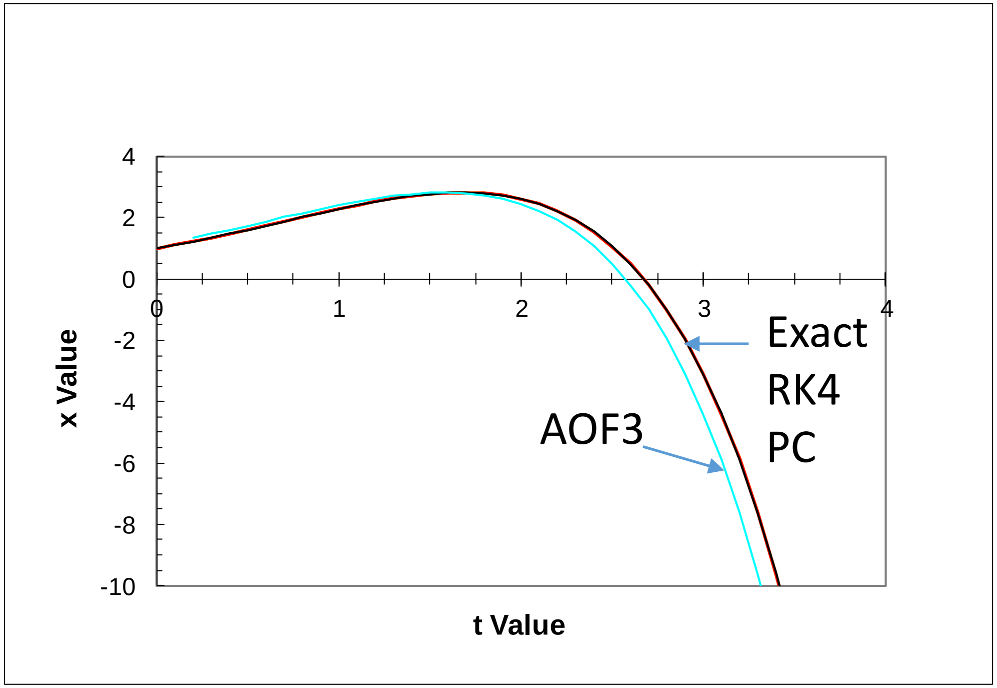
$$= 1.340138$$

Example 5 (cont.)

	Three Point Predictor-Corrector Scheme					
t	x	f	AOF3	x*	f*	ACF3
0	1	1				
0.1	1.104829	1.094829				
0.2	1.218597	1.178597	0.121587	1.340184	1.250184	0.121541
0.3	1.340138	1.250138	0.128081	1.468219	1.308219	0.12803
0.4	1.468168	1.308168	0.133155	1.601323	1.351323	0.133098
0.5	1.601266	1.351266	0.136659	1.737925	1.377925	0.136597
0.6	1.737863	1.377863	0.138429	1.876291	1.386291	0.138359
0.7	1.876222	1.386222	0.13828	2.014502	1.374502	0.138204
0.8	2.014425	1.374425	0.136013	2.150438	1.340438	0.135928
0.9	2.150353	1.340353	0.131404	2.281757	1.281757	0.13131
1	2.281663	1.281663	0.124206	2.405869	1.195869	0.124102

Example 5 (cont.)

The predictor-corrector (PC) method produces a solution with nearly the same accuracy as the RK4 method.



Generally, the n-step method will have truncation error of order at least n.