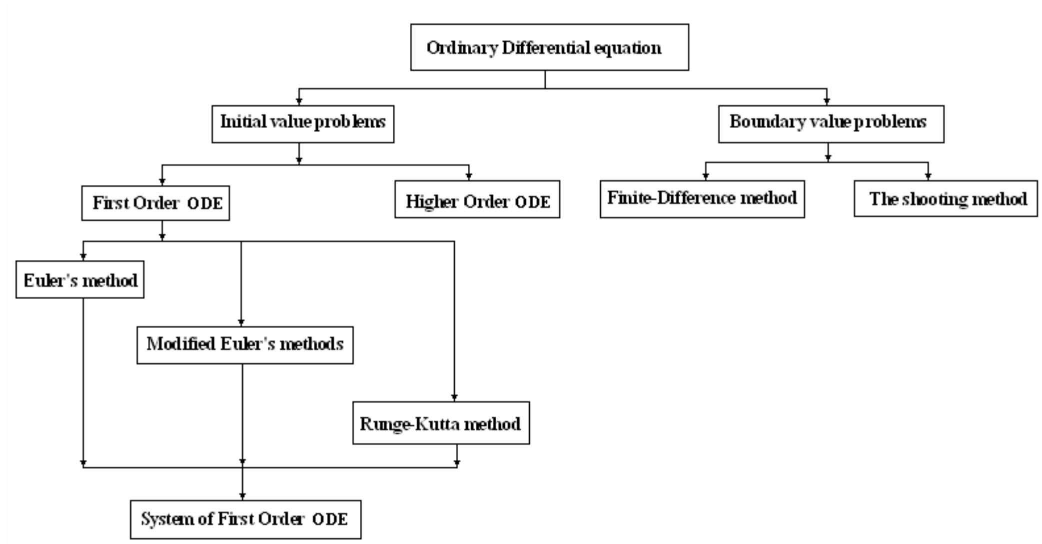
University of Jordan

Faculty of Engineering and Technology
Chemical Engineering Department
0905301 Numerical Methods in Chemical Engineering

Chapter SIX

Ordinary Differential Equations



<u>Initial Value Problems</u>

1) First Order Ordinary Differential Equation

A- Euler's Method

$$y_{i+1} = y_i + f(x_i, y_i)h$$

Where: $f(x_i, y_i)$ is the differential equation evaluated at x_i and y_i.
h is the step size.

B- Heun's Method

The slope at the beginning of an interval

$$y_i' = f(x_i, y_i)$$

is used to extrapolate linearly to y_{i+1}

$$y_{i+1}^P = y_i + f(x_i, y_i)h$$

In Heun's method the y^p_{i+1} calculated is not the final answer but an intermediate prediction.

It provides an estimate of y_{i+1} that allows the calculation of an estimated slope at the end of the interval:

$$y'_{i+1} = f\left(x_{i+1}, y^{p}_{i+1}\right)$$

Thus, the two slopes can be combined to obtain an average slope:

$$y' = \frac{y'_i + y'_{i+1}}{2} = \frac{f(x_i, y_i) + f\left(x_{i+1}, y^{p}_{i+1}\right)}{2}$$

This average slope is then used to extrapolate linearly from y_i to y_{i+1} using Euler's method:

$$y_{i+1} = y_i + \frac{f(x_i, y_i) + f\left(x_{i+1}, y^{p}_{i+1}\right)}{2} h$$

This is called a corrector equation.

C- *The improved polygon method*

This technique uses Euler's method to predict a value of y at the midpoint of the interval:

$$y_{i+\frac{1}{2}} = y_i + y'_i \frac{h}{2}$$

Then this predicted value is used to estimate a slope at the midpoint:

$$y'_{i+\frac{1}{2}} = y'\left(x_{i+\frac{1}{2}}, y_{i+\frac{1}{2}}\right)$$

Then

$$y_{i+1} = y_i + y'_{i+\frac{1}{2}} h$$

D- *Runge-Kutta Methods*

Many variations exist but all can be cast in the form:

$$y_{i+1} = y_i + \phi(x_i, y_i, h).h$$

where $\phi(x_i, y_i, h)$ is called an increment function.
The increment can be written in general form:

$$\phi = a_1 k_1 + a_2 k_2 + a_3 k_3 + \dots\dots\dots\dots\dots + a_n k_n$$

where the *a's* are constants and the *k's* are:

$$k_1 = f(x_i, y_i) = y'_i$$
$$k_2 = f(x_i + p_1 h, y_i + q_{11} k_1 h)$$
$$k_3 = f(x_i + p_2 h, y_i + q_{21} k_1 h + q_{22} k_2 h)$$

•

•

$$k_n = f(x_i + p_{n-1} h, y_i + q_{n-1,1} k_1 h + q_{n-1,2} k_2 h + \dots\dots\dots\dots + q_{n-1,n-1} k_{n-1} h)$$

- ***First Order Runge-Kutta Method***

If ***n = 1***

$$\phi = a_1 k_1$$
$$y_{i+1} = y_i + a_1 k_1 h$$
$$y_{i+1} = y_i + a_1 y_i' h$$

This is Euler's method.

- ***Second Order Runge-Kutta Method***

If ***n = 2***

$$y_{i+1} = y_i + (a_1 k_1 + a_2 k_2)h$$
$$where$$
$$k_1 = f(x_i, y_i) = y_i'$$
$$k_2 = f(x_i + p_1 h, y_i + q_{11} k_1 h)$$

a_1, a_2, p_1, q_{11} are evaluated by setting $y_{i+1} = y_i (a_1 k_1 + a_2 k_2)h$ equal to a Taylor series expansion to the second-order term.

$$a_1 + a_2 = 1$$
$$a_2 p_1 = \frac{1}{2}$$
$$a_2 q_{11} = \frac{1}{2}$$

There are 3 equations with 4 unknowns.
We must assume a value of one of the unknowns in order to determine the other three.

If <u>a_2 = 1/2</u>

$$a_2 = \frac{1}{2}$$
$$a_1 = 1 - \frac{1}{2} = \frac{1}{2}$$
$$p_1 = \frac{\frac{1}{2}}{\frac{1}{2}} = 1$$
$$q_{11} = \frac{\frac{1}{2}}{\frac{1}{2}} = 1$$
$$k_1 = f(x_i, y_i)$$
$$k_2 = f(x_i + h, y_i + k_1 h)$$
$$y_{i+1} = y_i + \left(\frac{1}{2}k_1 + \frac{1}{2}k_2\right)h = y_i + \left(\frac{k_1 + k_2}{2}\right)h = y_i + \frac{f(x_i, y_i) + f(x_i + h, y_i + k_1 h)}{2}h$$

This is similar to Heun's method.

<u>If $a_2 = 1$</u>

$$a_2 = 1$$
$$a_1 = 0$$
$$p_1 = \frac{1}{2}$$
$$q_{11} = \frac{1}{2}$$
$$k_1 = f(x_i, y_i)$$
$$k_2 = f\left(x_i + \frac{1}{2}h, y_i + \frac{1}{2}k_1 h\right)$$
$$y_{i+1} = y_i + k_2 h$$

This is the improved polygon method.

<u>If $a_2 = 2/3$</u> (Raltson's Method)

$$a_2 = \frac{2}{3}$$
$$a_1 = \frac{1}{3}$$
$$p_1 = q_{11} = \frac{3}{4}$$
$$k_1 = f(x_i, y_i)$$
$$k_2 = f\left(x_i + \frac{3}{4}h, y_i + \frac{3}{4}k_1 h\right)$$
$$y_{i+1} = y_i + \left(\frac{1}{3}k_1 + \frac{2}{3}k_2\right)h$$

- *Third Order Runge-Kutta Method*

$$k_1 = f(x_i, y_i)$$
$$k_2 = f\left(x_i + \frac{1}{2}h, y_i + \frac{1}{2}k_1 h\right)$$
$$k_3 = f(x_i + h, y_i - k_1 h + 2k_2 h)$$
$$y_{i+1} = y_i + \left[\frac{1}{6}(k_1 + 4k_2 + k_3)\right]h$$

- *Fourth Order Runge-Kutta Method*

$$k_1 = f(x_i, y_i)$$
$$k_2 = f\left(x_i + \frac{1}{2}h, y_i + \frac{1}{2}k_1 h\right)$$
$$k_3 = f\left(x_i + \frac{1}{2}h, y_i + \frac{1}{2}k_2 h\right)$$
$$k_4 = f(x_i + h, y_i + k_3 h)$$

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

- *Higher Order Runge-Kutta Methods*

Butcher's fifth order RK method

$$k_1 = f\left(x_i, y_i\right)$$
$$k_2 = f\left(x_i + \frac{1}{4}h, y_i + \frac{1}{4}k_1 h\right)$$
$$k_3 = f\left(x_i + \frac{1}{4}h, y_i + \frac{1}{8}k_1 h + \frac{1}{8}k_2 h\right)$$
$$k_4 = f\left(x_i + \frac{1}{2}h, y_i - \frac{1}{2}k_2 h + k_3 h\right)$$
$$k_5 = f\left(x_i + \frac{3}{4}h, y_i + \frac{3}{16}k_1 h + \frac{9}{16}k_4 h\right)$$
$$k_6 = f\left(x_i + h, y_i - \frac{3}{7}k_1 h + \frac{2}{7}k_2 h + \frac{12}{7}k_3 h - \frac{12}{7}k_4 h + \frac{8}{7}k_5 h\right)$$
$$y_{i+1} = y_i + \left[\frac{1}{90}\left(7k_1 + 32k_3 + 12k_4 + 32k_5 + 7k_6\right)\right]h$$

Fehlberg Runge-Kutta

$$k_1 = f\left(x_i, y_i\right)$$
$$k_2 = f\left(x_i + \frac{1}{4}h, y_i + \frac{1}{4}k_1 h\right)$$
$$k_3 = f\left(x_i + \frac{3}{8}h, y_i + \frac{3}{32}k_1 h + \frac{9}{32}k_2 h\right)$$
$$k_4 = f\left(x_i + \frac{12}{13}h, y_i + \frac{1932}{2197}k_1 h - \frac{7200}{2197}k_2 h + \frac{7296}{2197}k_3 h\right)$$
$$k_5 = f\left(x_i + h, y_i + \frac{439}{216}k_1 h - 8k_2 h + \frac{3860}{513}k_3 h - \frac{845}{4104}k_4 h\right)$$
$$k_6 = f\left(x_i + \frac{h}{2}, y_i - \frac{8}{27}k_1 h + 2k_2 h - \frac{3544}{2565}k_3 h + \frac{1859}{4104}k_4 h - \frac{11}{40}k_5 h\right)$$
$$y_{i+1} = y_i + \left[\frac{25}{216}k_1 + \frac{1408}{2565}k_3 + \frac{2197}{4104}k_4 - \frac{1}{5}k_5\right]h$$

or

$$y_{i+1} = y_i + \left[\frac{16}{135}k_1 + \frac{6656}{12825}k_3 + \frac{28561}{56430}k_4 - \frac{9}{50}k_5 + \frac{2}{55}k_6\right]h$$

2) *Systems of First Ordinary Differential Equations*

$$
\begin{aligned}
y_1' &= f_1(x, y_1, y_2, \ldots\ldots\ldots\ldots\ldots, y_n) \\
y_2' &= f_1(x, y_1, y_2, \ldots\ldots\ldots\ldots\ldots, y_n) \\
y_3' &= f_1(x, y_1, y_2, \ldots\ldots\ldots\ldots\ldots, y_n) \\
&\bullet \\
&\bullet \\
y_n' &= f_1(x, y_1, y_2, \ldots\ldots\ldots\ldots\ldots, y_n)
\end{aligned}
$$

- The system requires that n initial conditions be known at the starting value of x.
- All previous methods can be extended to the system of equations.
- The procedure for solving a system of equations simply involves applying the one-step techniques for every equation at each step before proceeding to the next step.

3) *Higher Order Ordinary Differential Equations*

$$y'' = g(x, y, y')$$

Can be converted to a system of two first-order ODE by a simple change of variables:

$$
\begin{aligned}
u &= y \\
v &= y' \\
u' &= y' = v = f(x, u, v) \\
v' &= y'' = g(x, u, v)
\end{aligned}
$$

The initial conditions:

$$y(0) = \alpha_0 \text{ and } y'(0) = \alpha_1$$

These initial conditions become:

$$u(0) = \alpha_0 \text{ and } v(0) = \alpha_1$$

<u>For higher order ODE</u>

$$
\begin{aligned}
& y^{(n)} = f(x, y, y', y'', y''', \ldots\ldots\ldots, y^{n-1}) \\
& y(0) = \alpha_0,\ y'(0) = \alpha_1,\ y''(0) = \alpha_2,\ y'''(0) = \alpha_3, \ldots\ldots\ldots\ldots\ldots, y^{(n-1)}(0) = \alpha_{n-1} \\
& u_1 = y \\
& u_2 = y' \\
& u_3 = y'' \\
& \bullet \\
& u_n = y^{(n-1)}
\end{aligned}
$$

Then

$$
\begin{aligned}
u_1' &= u_2 \\
u_2' &= u_3 \\
u_3' &= u_4
\end{aligned}
$$

$$u_n' = f(x, u_1, u_2, u_3, u_4, \ldots\ldots\ldots, u_n)$$

initial conditions

$$u_1(0) = \alpha_0, u_2(0) = \alpha_1, u_3(0) = \alpha_2, u_4(0) = \alpha_3, \ldots\ldots\ldots\ldots\ldots, u_n(0) = \alpha_{n-1}$$

Boundary Value Problems

$$\frac{d^2T}{dx^2} + h'(T_a - T) = 0$$

h' is a radiative heat loss coefficient (cm^{-2})

$$T(0) = T_1$$
$$T(L) = T_2$$

1) The Shooting Method

It is based on converting the boundary value problem to an equivalent initial value problem.
A trial and error approach is then implemented to solve the initial value version.
For nonlinear boundary value problems, perform three applications of the shooting method and use a quadratic interpolating polynomial to estimate the proper boundary condition.

2) Finite-Difference method

Finite divided differences are substituted for the derivatives in the original equation.
The differential equation is transformed to a set of simultaneous algebraic equations that can be solved as before.

$$\frac{d^2T}{dx^2} + h'(T_a - T) = 0$$
$$T(0) = T_1$$
$$T(L) = T_2$$
$$\frac{d^2T}{dx^2} = \frac{T_{i+1} - 2T_i + T_{i-1}}{\Delta x^2} \qquad \text{(central)}$$
$$\therefore \frac{T_{i+1} - 2T_i + T_{i-1}}{\Delta x^2} - h'(T_i - T_a) = 0$$
$$T_{i+1} - 2T_i + T_{i-1} - h'\Delta x^2 T_i + h'\Delta x^2 T_a = 0$$
$$T_{i+1} - (2 + h'\Delta x^2)T_i + T_{i-1} = -h'\Delta x^2 T_a$$
$$-T_{i-1} + (2 + h'\Delta x^2)T_i - T_{i+1} = h'\Delta x^2 T_a$$

This equation is applies to each of the interior nodes of the rod as an example.
The first and the last interior nodes, T_{i-1} and T_{i+1} are specified by the boundary conditions.
The resulting set of linear equations will be tridiagonal.