Runge-Kutta method. Extra material for *Introduction to Chemical Engineering Computing,* 2nd ed., Bruce A. Finlayson, Wiley (2012).

A popular method for integrating equations in time is the Runge-Kutta-Feldberg method (see p. 359 and Forsythe, Malcolm, and Moler, 1977). This is a fourth-order method but achieves fifth-order accuracy. The RKF45 package is based upon this method. For the problem

$$\frac{dy}{dt} = f(t,y), \quad y(0) = y_0$$

where *y* and *f* can be vectors, the method is:

$$k_1 = \Delta t\, f(t^n, y^n)$$
$$k_2 = \Delta t\, f(t^n + \frac{\Delta t}{4}, y^n + \frac{k_1}{4})$$
$$k_3 = \Delta t\, f(t^n + \frac{3}{8}\Delta t, y^n + \frac{3}{32}k_1 + \frac{9}{32}k_2)$$
$$k_4 = \Delta t\, f(t^n + \frac{12}{13}\Delta t, y^n + \frac{1932}{2197}k_1 - \frac{7200}{2197}k_2 + \frac{7296}{2197}k_3)$$
$$k_5 = \Delta t\, f(t^n + \Delta t, y^n + \frac{439}{216}k_1 - 8k_2 + \frac{3680}{513}k_3 - \frac{845}{4104}k_4)$$
$$k_6 = \Delta t\, f(t^n + \frac{1}{2}\Delta t, y^n - \frac{8}{27}k_1 + 2k_2 - \frac{3544}{2565}k_3 + \frac{1859}{4104}k_4 - \frac{11}{40}k_5)$$
$$y^{n+1} = y^n + \frac{25}{216}k_1 + \frac{1408}{2565}k_3 + \frac{2197}{4104}k_4 - \frac{1}{5}k_5$$
$$z^{n+1} = y^n + \frac{16}{135}k_1 + \frac{6656}{12\,825}k_3 + \frac{28\,561}{56\,430}k_4 - \frac{9}{50}k_5 + \frac{2}{55}k_6$$

The value of $y^{n+1} - z^{n+1}$ is an estimate of the error in y^{n+1} and can be used in step-size control schemes.

Reference

Forsythe, G., Malcolm, M., Moler, C., *Computer Methods for Mathematical Computation*, Prentice-Hall, Englewood Cliffs, N.J. (1977).