Gear's method. Extra material for *Introduction to Chemical Engineering Computing,* 2nd ed., Bruce A. Finlayson, Wiley (2012).

If the numerical problem has some components that change quickly, but you have to integrate for a long time, the problem is called stiff (see p. 360 and Perry and Green, p. 3-50, 2008). Implicit methods are then needed. The best ones are based upon the work by Gear (1971). For the problem

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

where y and f can be vectors, the methods of different order are:

$$(1): \; y^{n+1} = y^n + \Delta t \; f(y^{n+1})$$

$$(2): \; y^{n+1} = \frac{4}{3}y^n - \frac{1}{3}y^{n-1} + \frac{2}{3}\Delta t \; f(y^{n+1})$$

$$(3): \; y^{n+1} = \frac{18}{11}y^n - \frac{9}{11}y^{n-1} + \frac{2}{11}y^{n-2} + \frac{6}{11}\Delta t \; f(y^{n+1})$$

$$(4): \; y^{n+1} = \frac{48}{25}y^n - \frac{36}{25}y^{n-1} + \frac{16}{25}y^{n-2} - \frac{3}{25}y^{n-3} + \frac{12}{25}\Delta t \; f(y^{n+1})$$

$$(5): \; y^{n+1} = \frac{300}{137}y^n - \frac{300}{137}y^{n-1} + \frac{200}{137}y^{n-2} - \frac{75}{137}y^{n-3} + \frac{12}{137}y^{n-4} + \frac{60}{137}\Delta t \; f(y^{n+1})$$

In Gear's method, the nonlinear equations are solved. If they cannot be solved, then the step size is reduced and you try again. Keep reducing the step size until the implicit equations can be solved. If the step size is extremely small, the computer program will stop. The order can be changed, too, and it is changed in the Gear algorithm to minimize the computational cost for a specified accuracy.

Reference

Gear, G. W., *Numerical Initial Value Problems in Ordinary Differential Equations*, Prentice-Hall, Englewood Cliffs, N. J. (1971).

Perry, R. H. and Green, D. W. (ed.), *Perry's Chemical Engineers' Handbook*, 8th ed., McGraw-Hill: New York, 2008.