Ordinary differential equations

Most problems in physics and engineering appear in the form of differential equations. For example, the motion of a classical particle is described by Newton's equation, which is a second-order ordinary differential equation involving at least a second-order derivative in time, and the motion of a quantum particle is described by the Schrödinger equation, which is a partial differential equation involving a first-order partial derivative in time and second-order partial derivatives in coordinates. The dynamics and statics of bulk materials such as fluids and solids are all described by differential equations.

In this chapter, we introduce some basic numerical methods for solving ordinary differential equations. We will discuss the corresponding schemes for partial differential equations in Chapter 7 and some more advanced techniques for the many-particle Newton equation and the many-body Schrödinger equation in Chapters 8 and 10. Hydrodynamics and magnetohydrodynamics are treated in Chapter 9.

In general, we can classify ordinary differential equations into three major categories:

(1) initial-value problems, which involve time-dependent equations with given initial conditions;
(2) boundary-value problems, which involve differential equations with specified boundary conditions;
(3) eigenvalue problems, which involve solutions for selected parameters (eigenvalues) in the equations.

In reality, a problem may involve more than just one of the categories listed above. A common situation is that we have to separate several variables by introducing multipliers so that the initial-value problem is isolated from the boundary-value or eigenvalue problem. We can then solve the boundary-value or eigenvalue problem first to determine the multipliers, which in turn are used to solve the related initial-value problem. We will cover separation of variables in Chapter 7. In this chapter, we concentrate on the basic numerical methods for all the three categories listed above and illustrate how to use these techniques to solve problems encountered in physics and other related fields.

Typically, initial-value problems involve dynamical systems, for example, the motion of the Moon, Earth, and the Sun, the dynamics of a rocket, or the propagation of ocean waves. The behavior of a dynamical system can be described by a set of first-order differential equations,

$$\frac{d\mathbf{y}}{dt} = \mathbf{g}(\mathbf{y}, t), \tag{4.1}$$

where

$$\mathbf{y} = (y_1, y_2, \ldots, y_l) \tag{4.2}$$

is the dynamical variable vector, and

$$\mathbf{g}(\mathbf{y}, t) = [g_1(\mathbf{y}, t), g_2(\mathbf{y}, t), \ldots, g_l(\mathbf{y}, t)] \tag{4.3}$$

is the generalized velocity vector, a term borrowed from the definition of the velocity $\mathbf{v}(\mathbf{r}, t) = d\mathbf{r}/dt$ for a particle at position $\mathbf{r}$ and time t. Here l is the total number of dynamical variables. In principle, we can always obtain the solution of the above equation set if the initial condition $\mathbf{y}(t = 0) = \mathbf{y}_0$ is given and a solution exists. For the case of the particle moving in one dimension under an elastic force discussed in Chapter 1, the dynamics is governed by Newton's equation

$$f = ma, \tag{4.4}$$

where a and m are the acceleration and mass of the particle, respectively, and f is the force exerted on the particle. This equation can be viewed as a special case of Eq. (4.1) with $l = 2$: that is, $y_1 = x$ and $y_2 = v = dx/dt$, and $g_1 = v = y_2$ and $g_2 = f/m = -kx/m = -ky_1/m$. Then we can rewrite Newton's equation in the form of Eq. (4.1):

$$\frac{dy_1}{dt} = y_2, \tag{4.5}$$

$$\frac{dy_2}{dt} = -\frac{k}{m}y_1. \tag{4.6}$$

If the initial position $y_1(0)$ and the initial velocity $y_2(0) = v(0)$ are given, we can solve the problem numerically as demonstrated in Chapter 1.

In fact, most higher-order differential equations can be transformed into a set of coupled first-order differential equations in the form of Eq. (4.1). The higher-order derivatives are usually redefined into new dynamical variables during the transformation. The velocity in Newton's equation discussed above is such an example.

4.4 The Runge–Kutta method

The accuracy of the methods that we have discussed so far can be improved only by including more starting points, which is not always practical, because a problem associated with a dynamical system usually has only the first point, namely, the initial condition, given. A more practical method that requires only the first point in order to start or to improve the algorithm is the *Runge–Kutta method*, which is derived from two different Taylor expansions of the dynamical variables and their derivatives defined in Eq. (4.1).

Formally, we can expand $y(t+\tau)$ in terms of the quantities at t with the Taylor expansion

$$\begin{aligned} y(t+\tau) &= y + \tau y' + \frac{\tau^2}{2} y'' + \frac{\tau^3}{3!} y^{(3)} + \cdots \\ &= y + \tau g + \frac{\tau^2}{2}(g_t + g g_y) + \frac{\tau^3}{6}\left(g_{tt} + 2 g g_{ty} + g^2 g_{yy} + g g_y^2 + g_t g_y\right) + \cdots, \end{aligned} \tag{4.22}$$

where the subscript indices denote partial derivatives for example, $g_{yt} = \partial^2 g / \partial y \partial t$. We can also formally write the solution at $t+\tau$ as

$$y(t+\tau) = y(t) + \alpha_1 c_1 + \alpha_2 c_2 + \cdots + \alpha_m c_m, \tag{4.23}$$

with

$$\begin{aligned} c_1 &= \tau g(y, t), \\ c_2 &= \tau g(y + \nu_{21} c_1, t + \nu_{21}\tau), \\ c_3 &= \tau g(y + \nu_{31} c_1 + \nu_{32} c_2, t + \nu_{31}\tau + \nu_{32}\tau), \\ &\vdots \\ c_m &= \tau g\left(y + \sum_{i=1}^{m-1} \nu_{mi} c_i, t + \tau \sum_{i=1}^{m-1} \nu_{mi}\right), \end{aligned} \tag{4.24}$$

where α_i (with $i = 1, 2, \ldots, m$) and ν_{ij} (with $i = 2, 3, \ldots, m$ and $j < i$) are parameters to be determined. We can expand Eq. (4.23) into a power series of τ by carrying out Taylor expansions for all c_i with $i = 1, 2, \ldots, m$. Then we can compare the resulting expression of $y(t+\tau)$ from Eq. (4.23) with the expansion in Eq. (4.22) term by term. A set of equations for α_i and ν_{ij} is obtained by keeping the coefficients for the terms with the same power of τ on both sides equal. By truncating the expansion to the term $O(\tau^m)$, we obtain m equations but with $m + m(m-1)/2$ parameters (α_i and ν_{ij}) to be determined. Thus, there are still options left in choosing these parameters.

Let us illustrate this scheme by working out the case for $m = 2$ in detail. If only the terms up to $O(\tau^2)$ are kept in Eq. (4.22), we have

$$y(t+\tau) = y + \tau g + \frac{\tau^2}{2}(g_t + g g_y). \tag{4.25}$$

We can obtain an expansion up to the same order by truncating Eq. (4.23) at $m = 2$,

$$y(t+\tau) = y(t) + \alpha_1 c_1 + \alpha_2 c_2, \tag{4.26}$$

with

$$c_1 = \tau g(y, t), \tag{4.27}$$

$$c_2 = \tau g(y + \nu_{21} c_1, t + \nu_{21}\tau). \tag{4.28}$$

Now if we perform the Taylor expansion for c_2 up to the term $O(\tau^2)$, we have

$$c_2 = \tau g + \nu_{21}\tau^2(g_t + g g_y). \tag{4.29}$$

Substituting c_1 and the expansion of c_2 above back into Eq. (4.26) yields

$$y(t+\tau) = y(t) + (\alpha_1 + \alpha_2)\tau g + \alpha_2 \tau^2 \nu_{21}(g_t + g g_y). \tag{4.30}$$

If we compare this expression with Eq. (4.25) term by term, we have

$$\alpha_1 + \alpha_2 = 1, \tag{4.31}$$

$$\alpha_2 \nu_{21} = \frac{1}{2}. \tag{4.32}$$

As pointed out earlier, there are only m (2 in this case) equations available but there are $m + m(m-1)/2$ (3 in this case) parameters to be determined. We do not have a unique solution for all the parameters; thus we have flexibility in assigning their values as long as they satisfy the m equations. We could choose $\alpha_1 = \alpha_2 = 1/2$ and $\nu_{21} = 1$, or $\alpha_1 = 1/3$, $\alpha_2 = 2/3$, and $\nu_{21} = 3/4$. The flexibility in choosing the parameters provides one more way to increase the numerical accuracy in practice. We can adjust the parameters according to the specific problems involved.

The most commonly known and widely used Runge–Kutta method is the one with Eqs. (4.22) and (4.23) truncated at the terms of $O(\tau^4)$. We will give the result here and leave the derivation as an exercise to the reader. This well-known fourth-order Runge–Kutta algorithm is given by

$$y(t+\tau) = y(t) + \frac{1}{6}(c_1 + 2c_2 + 2c_3 + c_4), \tag{4.33}$$

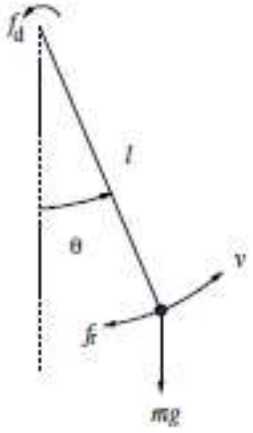

Fig. 4.3 A sketch of a driven pendulum under damping: f_d is the driving force and f_r is the resistive force.

with

$$c_1 = \tau g(y, t), \tag{4.34}$$

$$c_2 = \tau g\left(y + \frac{c_1}{2}, t + \frac{\tau}{2}\right), \tag{4.35}$$

$$c_3 = \tau g\left(y + \frac{c_2}{2}, t + \frac{\tau}{2}\right), \tag{4.36}$$

$$c_4 = \tau g(y + c_3, t + \tau). \tag{4.37}$$

We can easily show that the above selection of parameters does satisfy the required equations. As pointed out earlier, this selection is not unique and can be modified according to the problem under study.