4 Model Simulation

In modeling, an important task is calculating the solution of a model. Rarely, we will be able to determine the solution analytically. Therefore, we resort to a numerical calculation performed with a computer. In this chapter, we study various ways of accomplishing this task.

4.1 CONCEPTS OF COMPUTER SIMULATION BASED ON ORDINARY DIFFERENTIAL EQUATIONS

We want to determine the solution $X(t)$ of an ordinary differential equation (ODE) model given by a general function $f(t,p,X(t))$, where p denotes the parameters,

$$\frac{dX(t)}{dt} = f(t,p,X(t)) \tag{4.1}$$

and with a known initial condition, X_0. The generality of this function emphasizes that the rate may depend on the time itself, a set of parameters, and the dependent variable. There are several numerical methods to solve ODEs such as Euler and Runge–Kutta (Swartzman and Kaluzny, 1987).

4.2 EULER METHOD

Because of its simplicity, we will first explain the Euler method. Recall that we can get an approximate value of the derivative dX/dt using the slope as a ratio of small quantities:

$$\frac{dX}{dt} \simeq \frac{X(t+\Delta t)-X(t)}{\Delta t} \tag{4.2}$$

This approximation works better if Δt is very small. Next, substitute this approximation on the left-hand side of the ODE given in Equation 4.1:

$$\frac{X(t+\Delta t)-X(t)}{\Delta t} \simeq f(t,p,X(t)) \tag{4.3}$$

Rewrite this as

$$X(t+\Delta t) \simeq X(t) + \Delta t\, f(t,p,X(t)) \tag{4.4}$$

Now iterate Equation 4.4 with a computer program starting at X_0 with $t = t_0$

$$X_1 = X(\Delta t) = X_0 + \Delta t\, f(t,p,X_0)$$

$$X_2 = X(2\Delta t) = X_1 + \Delta t\, f(t,p,X_1)$$

Or, in general, for the ith time step:

$$X_{i+1} = X((i+1)\Delta t) = X_i + \Delta t\, f(t,p,X_i) \tag{4.5}$$

until we get to the final value at the final time t_f:

$$X_f = X(t_f) = X(t_f - \Delta t) + \Delta t\, f(t, p, X(t_f - \Delta t))$$

It should be noted that the solution to the ODE has been replaced by a sequence of arithmetic operations (sums and products), yielding a set of values of the solution $X(\Delta t)$, $X(2\Delta t)$, …, $X(i\Delta t)$ separated by the small time step Δt.

Since Δt is small, we do not want to save all the values because there will be too much data if Δt is small and t_f is large; therefore, we usually save or write to an **output file** only every n time steps or every $t_w = n\Delta t$ time units. This will generate $N = \frac{t_f}{n\Delta t}$ data values after the initial condition for a total of $N + 1$ values of X saved or written to the output file.

When executing the program, we need to store in memory data that would have been read from an **input file**: values for the simulation control (which includes the time step, Δt, the initial time, t_0, the final time, t_f, and the time to save or write, t_w). The program saves or writes an output file containing the numerical solution. Each record has two columns, the value of time and the corresponding X value. Thus, the output file will contain this information:

```
Time  X
0     X0
ndt   X(ndt)
2ndt  X(2ndt)
3ndt  X(3ndt)
...
```

and so on until

```
...
Nndt  X(Nndt)
```

It is convenient to write this output file as an **ASCII** text file to facilitate **exporting** it to a variety of software applications, for example, to perform statistical analysis or to generate a graph of the **time series** $X(t)$ versus t using spreadsheets or data analysis programs such as R.

The flowchart given in Figure 4.1 illustrates the simulation process.

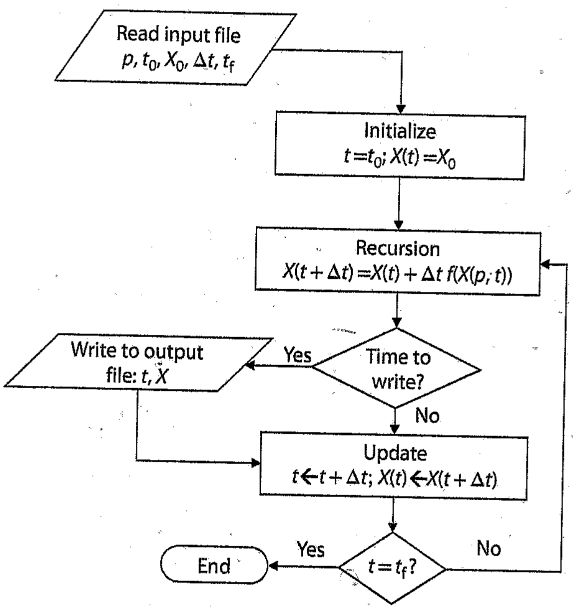

FIGURE 4.1 The simulation flowchart.

Exercise 4.1

What are the files produced by a simulation program? What is the simulation time step? How do you determine how many times the output is written to an output file?

One way to learn a numerical method is to iterate it by hand a few times. So, let us work on the following exercise. We do not need simulation to study the exponential growth or decline because we know the exact mathematical solution of this simple ODE. However, we will use it here because it facilitates the calculations and thus helps explain the main concepts involved in the simulation. Therefore, we will **numerically** solve the exponential model by calculator. The basic relation of Equation 4.4 is simply

$$X(t+\Delta t) = X(t) + \Delta t\, rX(t)$$

where the parameter set p consists of the coefficient r and there is no explicit dependence on t. Thus, the recursive expression Equation 4.5 for any i reduces to

$$X_{i+1} = X((i+1)\Delta t) = X_i + \Delta t\, rX_i \tag{4.6}$$

Exercise 4.2

Use your calculator to simulate the exponential growth using the Euler technique from $X_0 = 1$ ind at $t_0 = 0$ days at the rate of $r = 0.1$ day^{-1}. Use $\Delta t = 0.1$ and $t_f = 1$ day. Write the result for every two time steps and use four significant figures.

Hint:
$X(0) = X_0 = 1$, write to file
$X(0.1) = 1. + 0.01 = 1.01$, skip writing to file
$X(0.2) = 1.01 + 0.01 \times 1.01 = 1.02$, write to file
$X(0.3) = 1.02 + 0.01 \times 1.02 = 1.030$, skip writing to file
$X(0.4) = ?$, write to file
......
$X(1) = ?$, write to file

Complete the calculations. Write (handwrite) the output file as two columns: t and $X(t)$. Plot (just sketch) X(t) versus t using the values in the output file.

In essence, the Euler method is based on including the first-order terms of a Taylor series expansion of function $f(\,)$, that is to say, ignoring terms of second order and above. Thus, the error in each step is proportional to $(\Delta t)^2$. Also, the number of steps is proportional to $1/\Delta t$, and therefore, the accumulated error is proportional to $(\Delta t)^2 \times \frac{1}{\Delta t} = \Delta t$. This is why the Euler method is a first-order method.

4.3 FOURTH-ORDER RUNGE–KUTTA METHOD

The Runge–Kutta methods use values in between each time step and are more precise for the same time step. We will focus on the fourth-order method (RK4). We rewrite Equation 4.1 to explicitly show the dependence on time t in the function $f(\,)$:

$$\frac{dX(t)}{dt} = f(t, p, X(t)) \tag{4.7}$$

The recursive relation is

$$X_{i+1} = X((i+1)\Delta t) = X_i + \frac{\Delta t}{6}(k_1 + 2k_2 + 2k_3 + k_4) \tag{4.8}$$

where

$$\begin{aligned} k_1 &= f(t_i, p, X_i) \\ k_2 &= f\left(t_i + \frac{\Delta t}{2}, p, X_i + \frac{\Delta t}{2}k_1\right) \\ k_3 &= f\left(t_i + \frac{\Delta t}{2}, p, X_i + \frac{\Delta t}{2}k_2\right) \\ k_4 &= f(t_i + \Delta t, p, X_i + \Delta t k_3) \end{aligned} \tag{4.9}$$

Here, note the following:

- k_1 is the slope at the beginning of the time step as in the Euler method.
- k_2 is the slope at the middle of the time step $t_i + \frac{\Delta t}{2}$ with X calculated from k_1 using Euler.
- k_3 is the slope at the middle of the time step $t_i + \frac{\Delta t}{2}$ with X calculated from k_2 using Euler.
- k_4 is the slope at the end of the time step $t_i + \Delta t$ with X calculated from k_3 using Euler.

Compared to Euler's method, we have substituted the slope $\Delta t f(p, X_i)$ in Equation 4.5 for a weighted average of four slopes where more weight is given to the two slopes k_2 and k_3 at the mid-point of the time step. The method is equivalent to dropping the terms of the fifth order and above in a Taylor series; therefore, the error in each time step is proportional to $(\Delta t)^5$. As in the Euler method, the number of steps is proportional to $1/\Delta t$; therefore, the accumulated error is proportional to $(\Delta t)^5 \times \frac{1}{\Delta t} = (\Delta t)^4$. This is why the RK4 method is a fourth-order method.

Exercise 4.3

Use your calculator to simulate one time step of exponential growth using the RK4 method from $X_0 = 1$ ind at $t_0 = 0$ days, at the rate of $r = 0.1$ day^{-1}. Use $\Delta t = 0.1$ and use four significant figures.

Hint:
$X_0 = 1.$
Calculate $k_1 = rX_0 = 0.1 \times 1. = 0.1$
Calculate $k_2 = r(X_0 + (\Delta t/2)k_1) = 0.1 \times (1. + 0.05 \times 0.1) = 0.1 \times 1.005 = 0.1005$
Calculate $k_3 = r(X_0 + (\Delta t/2)k_2) = 0.1 \times (1. + 0.05 \times 0.1005) = 0.1 \times 1.05 = 0.105$
Calculate $k_4 = r(X_0 + (\Delta t)k_3) = 0.1 \times (1.000 + 0.1 \times 0.105) = 0.1 \times 1.010 = 0.101$
Calculate the slope weighted average $(0.1/6) \times (0.1 + 2 \times 0.1005 + 2 \times 0.105 + 0.101) = 0.0102$
Now $X_1 = 1. + 0.0102 = 1.0102$
Compared to $X_1 = 1.01$ of Exercise 4.2, we can appreciate the potential decrease in error.

4.4 RANDOM NUMBER GENERATION

Random variables (RV) are used in modeling to simulate natural processes that include variability or uncertainty. A sequence of samples from a random variable behave as a **realization** of a **stochastic** process. Choosing numbers at random consists of generating a pseudorandom number sequence for the values of the RV.