is possible to find only finite, but very long escape times. These periodic trajectories form closed curves, and the regions enclosed by them are called KAM surfaces. ■

Project 6.29 Chemical reactions

In Project 4.17 we discussed how chemical oscillations can occur when the reactants are continuously replenished. In this project we introduce a set of chemical reactions that exhibits the period doubling route to chaos. Consider the following reactions (see Peng et al.):

$$P \to A \tag{6.65a}$$
$$P + C \to A + C \tag{6.65b}$$
$$A \to B \tag{6.65c}$$
$$A + 2B \to 3B \tag{6.65d}$$
$$B \to C \tag{6.65e}$$
$$C \to D. \tag{6.65f}$$

Each of the above reactions has an associated rate constant. The time dependence of the concentrations of A, B, and C is given by

$$\frac{dA}{dt} = k_1 P + k_2 PC - k_3 A - k_4 AB^2 \tag{6.66a}$$
$$\frac{dB}{dt} = k_3 A + k_4 AB^2 - k_5 B \tag{6.66b}$$
$$\frac{dC}{dt} = k_4 B - k_5 C. \tag{6.66c}$$

We assume that P is held constant by replenishment from an external source. We also assume the chemicals are well mixed so that there is no spatial dependence. In Section 7.8 we discuss the effects of spatial inhomogeneities due to molecular diffusion. Equations (6.65) can be written in a dimensionless form as

$$\frac{dX}{d\tau} = c_1 + c_2 Z - X - XY^2 \tag{6.67a}$$
$$c_3 \frac{dY}{d\tau} = X + XY^2 - Y \tag{6.67b}$$
$$c_4 \frac{dZ}{d\tau} = Y - Z, \tag{6.67c}$$

where the c_i are constants, $\tau = k_3 t$, and X, Y, and Z are proportional to A, B, and C, respectively.

(a) Write a program to solve the coupled differential equations in (6.67). Use a fourth-order Runge–Kutta algorithm with an adaptive step size. Plot $\ln Y$ versus the time τ.

(b) Set $c_1 = 10$, $c_3 = 0.005$, and $c_4 = 0.02$. The constant c_2 is the control parameter. Consider $c_2 = 0.10$ to 0.16 in steps of 0.005. What is the period of $\ln Y$ for each value of c_2?

(c) Determine the values of c_2 at which the period doublings occur for as many period doublings as you can determine. Compute the constant δ (see (6.9)) and compare its value to the value of δ for the logistic map.

(d) Make a bifurcation diagram by taking the values of $\ln Y$ from the Poincaré plot at $X = Z$ and plotting them versus the control parameter c_2. Do you see a sequence of period doublings?

(e) Use three-dimensional graphics to plot the trajectory of (6.67) with $\ln X$, $\ln Y$, and $\ln Z$ as the three axes. Describe the attractors for some of the cases considered in part (a). ■

APPENDIX 6A: STABILITY OF THE FIXED POINTS OF THE LOGISTIC MAP

In the following, we derive analytical expressions for the fixed points of the logistic map. The fixed-point condition is given by

$$x^* = f(x^*). \tag{6.68}$$

From (6.5) this condition yields the two fixed points

$$x^* = 0 \quad \text{and} \quad x^* = 1 - \frac{1}{4r}. \tag{6.69}$$

Because x is restricted to be positive, the only fixed point for $r < 1/4$ is $x = 0$. To determine the stability of x^*, we let

$$x_n = x^* + \epsilon_n, \tag{6.70a}$$

and

$$x_{n+1} = x^* + \epsilon_{n+1}. \tag{6.70b}$$

Because $|\epsilon_n| \ll 1$, we have

$$x_{n+1} = f(x^* + \epsilon_n) \approx f(x^*) + \epsilon_n f'(x^*) = x^* + \epsilon_n f'(x^*). \tag{6.71}$$

If we compare (6.70b) and (6.71), we obtain

$$\epsilon_{n+1}/\epsilon_n = f'(x^*). \tag{6.72}$$

If $|f'(x^*)| > 1$, the trajectory will diverge from x^* because $|\epsilon_{n+1}| > |\epsilon_n|$. The opposite is true for $|f'(x^*)| < 1$. Hence, the local stability criteria for a fixed point x^* are

1. $|f'(x^*)| < 1$, x^* is stable;
2. $|f'(x^*)| = 1$, x^* is marginally stable;
3. $|f'(x^*)| > 1$, x^* is unstable.