V. Choose $R = 2000\,\Omega$, $C = 10^{-6}$ farads, and $V = 10$ volts. Do you expect $Q(t)$ to increase with t? Does $Q(t)$ increase indefinitely, or does it reach a steady-state value? Use a program to solve (4.23) numerically using the Euler algorithm. What value of Δt is necessary to obtain three decimal accuracy at $t = 0.005$?

(b) What is the nature of your numerical solution to (4.23) at $t = 0.05$ for $\Delta t = 0.005$, 0.0025, and 0.001? Does a small change in Δt lead to a large change in the computed value of Q? Is the Euler algorithm stable for reasonable values of Δt? ■

4.7 ■ PROJECTS

Project 4.17 Chemical oscillations

The kinetics of chemical reactions can be modeled by a system of coupled first-order differential equations. As an example, consider the following reaction:

$$A + 2B \to 3B + C, \tag{4.26}$$

where A, B, and C represent the concentrations of three different types of molecules. The corresponding rate equations for this reaction are

$$\frac{dA}{dt} = -kAB^2 \tag{4.27a}$$

$$\frac{dB}{dt} = kAB^2 \tag{4.27b}$$

$$\frac{dC}{dt} = kAB^2. \tag{4.27c}$$

The rate at which the reaction proceeds is determined by the reaction constant k. The terms on the right-hand side of (4.27) are positive if the concentration of the molecule increases in (4.26) as it does for B and C, and negative if the concentration decreases as it does for A. Note that the term $2B$ in the reaction (4.26) appears as B^2 in the rate equation (4.27). In (4.27) we have assumed that the reactants are well stirred so that there are no spatial inhomogeneities. In Section 7.8 we will discuss the effects of spatial inhomogeneities due to molecular diffusion.

Most chemical reactions proceed to equilibrium, where the mean concentrations of all molecules are constant. However, if the concentrations of some molecules are replenished, it is possible to observe oscillations and chaotic behavior (see Chapter 6). To obtain oscillations, it is essential to have a series of chemical reactions such that the products of some reactions are the reactants of others. In the following, we consider a simple set of reactions that can lead to oscillations under certain conditions (see Lefever and Nicolis):

$$A \to X \tag{4.28a}$$

$$B + X \to Y + D \tag{4.28b}$$

$$2X + Y \to 3X \tag{4.28c}$$

$$X \to C. \tag{4.28d}$$

If we assume that the reverse reactions are negligible and A and B are held constant by an external source, the corresponding rate equations are

$$\frac{dX}{dt} = A - (B+1)X + X^2Y \tag{4.29a}$$

$$\frac{dY}{dt} = BX - X^2Y. \tag{4.29b}$$

For simplicity, we have chosen the rate constants to be unity.

(a) The steady state solution of (4.29) can be found by setting dX/dt and dY/dt equal to zero. Show that the steady state values for (X, Y) are $(A, B/A)$.

(b) Write a program to solve numerically the rate equations given by (4.29). Your program should input the initial values of X and Y and the fixed concentrations A and B, and plot X versus Y as the reactions evolve.

(c) Systematically vary the initial values of X and Y for given values of A and B. Are their steady state behaviors independent of the initial conditions?

(d) Let the initial value of (X, Y) equal $(A + 0.001, B/A)$ for several different values of A and B, that is, choose initial values close to the steady state values. Classify which initial values result in steady state behavior (stable) and which ones show periodic behavior (unstable). Find the relation between A and B that separates the two types of behavior. ■

Project 4.18 Nerve impulses

In 1952 Hodgkin and Huxley developed a model of nerve impulses to understand the nerve membrane potential of a giant squid nerve cell. The equations they developed are known as the Hodgkin–Huxley equations. The idea is that a membrane can be treated as a capacitor where $CV = q$, and thus the time rate of change of the membrane potential V is proportional to the current dq/dt flowing through the membrane. This current is due to the pumping of sodium and potassium ions through the membrane, a leakage current, and an external current stimulus. The model is capable of producing single nerve impulses, trains of nerve impulses, and other effects. The model is described by the following first-order differential equations:

$$C\frac{dV}{dt} = -g_K n^4(V - V_K) - g_{Na}m^3h(V - V_{Na}) - g_L(V - V_L) + I_{\text{ext}}(t) \tag{4.30a}$$

$$\frac{dn}{dt} = \alpha_n(1-n) - \beta_n n \tag{4.30b}$$

$$\frac{dm}{dt} = \alpha_m(1-m) - \beta_m m \tag{4.30c}$$

$$\frac{dh}{dt} = \alpha_h(1-h) - \beta_h h, \tag{4.30d}$$

where V is the membrane potential in millivolts (mV), n, m, and h are time dependent functions that describe the gates that pump ions into or out of the cell, C is the membrane capacitance per unit area, the g_i are the conductances per unit area for potassium, sodium, and the leakage current, V_i are the equilibrium potentials for each of the currents, and α_j and β_j are nonlinear functions of V. We use the notation n, m, and h for the gate functions because the notation is universally used in the literature. These gate functions are empirical attempts to describe how the membrane controls the flow of ions into and out of the nerve cell. Hodgkin and Huxley found the following empirical forms for α_j and β_j:

$$\alpha_n = 0.01(V + 10)/[e^{(1+V/10)} - 1] \tag{4.31a}$$

$$\beta_n = 0.125\, e^{V/80} \tag{4.31b}$$

$$\alpha_m = 0.01(V + 25)/[e^{(2.5+V/10)} - 1] \tag{4.31c}$$

$$\beta_m = 4\, e^{V/18} \tag{4.31d}$$

$$\alpha_h = 0.07\, e^{V/20} \tag{4.31e}$$

$$\beta_m = 1/[e^{(3+V/10)} + 1]. \tag{4.31f}$$

The parameter values are $C = 1.0\,\mu\text{F/cm}^2$, $g_K = 36\,\text{mmho/cm}^2$, $g_{Na} = 120\,\text{mmho/cm}^2$, $g_L = 0.3\,\text{mmho/cm}^2$, $V_K = 12\,\text{mV}$, $V_{Na} = -115\,\text{mV}$, and $V_L = 10.6\,\text{mV}$. The unit mho represents ohm^{-1}, and the unit of time is milliseconds (ms). These parameters assume that the resting potential of the nerve cell is zero; however, we now know that the resting potential is about $-70\,\text{mV}$.

We can use the ODE solver to solve (4.30) with the state vector $\{V, n, m, h, t\}$; the rates are given by the right-hand side of (4.30). The following questions ask you to explore the properties of the model.

(a) Write a program to plot n, m, and h as a function of V in the steady state (for which $\dot{n} = \dot{m} = \dot{h} = 0$). Describe how these gates are operating.

(b) Write a program to simulate the nerve cell membrane potential and plot $V(t)$. You can use a simple Euler algorithm with a time step of 0.01 ms. Describe the behavior of the potential when the external current is 0.

(c) Consider a current that is zero except for a one millisecond interval. Try a current spike amplitude of $7\,\mu\text{A}$ (that is, the external current equals 7 in our units). Describe the resulting nerve impulse $V(t)$. Is there a threshold value for the current below which there is no large spike but only a broad peak?

(d) A constant current should produce a train of spikes. Try different amplitudes for the current and determine if there is a threshold current and how the spacing between spikes depends on the amplitude of the external current.

(e) Consider a situation where there is a steady external current I_1 for 20 ms and then the current increases to $I_2 = I_1 + \Delta I$. There are three types of behavior depending on I_2 and ΔI. Describe the behavior for the following four situations: (1) $I_1 = 2.0\,\mu\text{A}$, $\Delta I = 1.5\,\mu\text{A}$; (2) $I_1 = 2.0\,\mu\text{A}$, $\Delta I = 5.0\,\mu\text{A}$; (3) $I_1 = 7.0\,\mu\text{A}$, $\Delta I = 1.0\,\mu\text{A}$; and (4) $I_1 = 7.0\,\mu\text{A}$, $\Delta I = 4.0\,\mu\text{A}$. Try other values of I_1 and ΔI as well. In which cases do you obtain a steady spike train? Which cases produce a single spike? What other behavior do you find?

(f) Once a spike is triggered, it is frequently difficult to trigger another spike. Consider a current pulse at $t = 20$ ms of $7\,\mu\text{A}$ that lasts for one millisecond. Then give a second current pulse of the same amplitude and duration at $t = 25$ ms. What happens? What happens if you add a third pulse at 30 ms? ■

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