cess. Pearson (see references) modeled these processes by two coupled reaction diffusion equations:

$$\frac{\partial A}{\partial t} = D_A \nabla^2 A - AB^2 + f(1-A) \tag{7.67a}$$

$$\frac{\partial B}{\partial t} = D_B \nabla^2 B + AB^2 - (f+k)B. \tag{7.67b}$$

The AB^2 term represents the reaction $A + 2B \to 3B$. This term is negative in (7.67a) because the reactant A decreases and is positive in (7.67b) because the reactant B increases. The term $+f$ represents the constant addition of A, and the terms $-fA$ and $-fB$ represent the removal process; the term $-kB$ represents the reaction $B \to C$. All the quantities in (7.67) are dimensionless. We assume that the diffusion coefficients are $D_A = 2 \times 10^{-5}$ and $D_B = 10^{-5}$, and the behavior of the system is determined by the values of the rate constant k and the feed rate f.

(a) We first consider the behavior of the reaction kinetics that results when the diffusion terms in (7.67) are neglected. It is clear from (7.67) that there is a trivial steady state solution with $A = 1$, $B = 0$. Are there other solutions, and if so, are they stable? The steady state solutions can be found by solving (7.67) with $\partial A/\partial t = \partial B/\partial t = 0$. To determine the stability, we can add a perturbation and determine whether the perturbation grows or not. However, without the diffusion terms, it is more straightforward to solve (7.67) numerically using a simple Euler algorithm. Choose a time step equal to unity and let $A = 0.1$ and $B = 0.5$ at $t = 0$. Determine the steady state values for $0 < f \leq 0.3$ and $0 < k \leq 0.07$ in increments of $\Delta f = 0.02$ and $\Delta k = 0.005$. Record the steady state values of A and B. Then repeat this exercise for the initial values $A = 0.5$ and $B = 0.1$. You should find that for some values of f and k, only one steady state solution can be obtained for the two initial conditions, and for other initial values of A and B there are two steady state solutions. Try other initial conditions. If you obtain a new solution, change the initial A or B slightly to see if your new solution is stable. On an f versus k plot, indicate where there are two solutions and where there are one. In this way you can determine the approximate phase diagram for this process.

(b) There is a small region in fk-space where one of the steady state solutions becomes unstable and periodic solutions occur (the mechanism is known as a Hopf bifurcation). Try $f = 0.009$, $k = 0.03$, and set $A = 0.1$ and $B = 0.5$ at $t = 0$. Plot the values of A and B versus the time t. Are they periodic? Try other values of f and k and estimate where the periodic solutions occur.

(c) Numerical solutions of the full equation with diffusion (7.67) can be found by making a finite difference approximation to the spatial derivatives as in (3.16) and using a simple Euler algorithm for the time integration. Adopt periodic boundary conditions. Although it is straightforward to write a program to do the numerical integration, an exploration of the dynamics of this system requires much computer resources. However, we can find some preliminary results with a small system and a coarse grid. Consider a 0.5×0.5 system with a spatial mesh of 128×128 grid points on a square lattice. Choose $f = 0.18$, $k = 0.057$, and $\Delta t = 0.1$. Let the entire system be in the initial trivial state ($A = 1$, $B = 0$) except for a 20×20 grid located at the center of the system where the sites are $A = 1/2$, $B = 1/4$ with a $\pm 1\%$ random noise. The effect of the noise is to break the square symmetry. Let the system evolve for approximately 80,000 time steps and look at the patterns that develop. Color code the grid according to the concentration of A, with red representing $A = 1$ and blue representing $A \approx 0.2$ and with several intermediate colors. Very interesting patterns have been found by Pearson. (See Figure 7.15.) ■

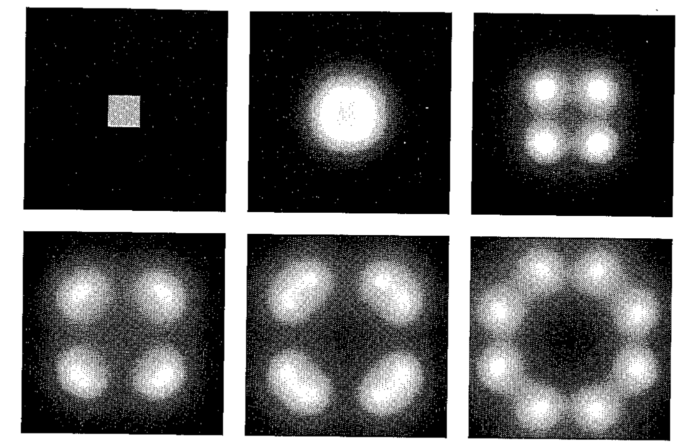

Figure 7.15 Evolution of the pattern starting from the initial conditions suggested in Project 7.42c.

APPENDIX 7A: RANDOM WALKS AND THE DIFFUSION EQUATION

To gain some insight into the relation between random walks and the diffusion equation, we first show that the latter implies that $\langle x(t)\rangle$ is zero and $\langle x^2(t)\rangle$ is proportional to t. We rewrite the diffusion equation (7.27) here for convenience:

$$\frac{\partial P(x,t)}{\partial t} = D\frac{\partial^2 P(x,t)}{\partial x^2}. \tag{7.68}$$

To derive the t-dependence of $\langle x(t)\rangle$ and $\langle x^2(t)\rangle$ from (7.68), we write the average of any function of x as

$$\langle f(x,t)\rangle = \int_{-\infty}^{\infty} f(x)P(x,t)\,dx. \tag{7.69}$$

The average displacement is given by

$$\langle x(t)\rangle = \int_{-\infty}^{\infty} xP(x,t)\,dx. \tag{7.70}$$