Modeling Reaction Diffusion Equations with Cellular Automata

CS 365: Introduction to Scientific Modeling
Assignment 1: Due: Sept. 22, 2014

1 Introduction

In this assignment you will implement a two-dimensional cellular automaton (CA) which simulates *Reaction Diffusion Equations*, and then study the system's dynamics under different parameter regimes.

The assignment is due at the beginning of class on Sept. 22. Please hand in a printed copy of a 2-4 page lab eport, together with the output, and the code you wrote to complete the assignment. I prefer to receive hard copy, but if you submit your assignment electronically, please send the lab report in .pdf format rather than .docx.

2 Reaction Diffusion Equations

2.1 Background

Reaction diffusion equations model a chemical reaction in which two chemicals interact and diffuse across a two-dimensional surface. In this assignment you will implement a specific set of equations known as the *Gray-Scott* equations. Three chemicals, U, V and P, react according to the equation:

$$\mathrm{U} + 2\mathrm{V} \longrightarrow 3\mathrm{V}$$
$$\mathrm{V} \longrightarrow \mathrm{P}$$

Along with the chemical reaction above, the chemicals *diffuse*, i.e. spread throughout the medium on which they are placed. We can directly model the concentrations of U and V in this reaction using partial differential equations as:

$$\frac{\partial u}{\partial t} = r_u \nabla^2 u - uv^2 + f(1-u) \quad (1)$$

$$\frac{\partial v}{\partial t} = r_v \nabla^2 v + uv^2 - (f+k)v \quad (2)$$

where u and v represent the concentration of the chemicals U and V, and r_u, r_v, f, and k are constants.

The lefthand side of the first equation, $\frac{\partial u}{\partial t}$, represents the change in the concentration of chemical u over time, and similarly for the second equation. In the righthand side, the term, $r_u \nabla^2 u$ represents the diffusion of the chemical u across space, where r_u is the diffusion rate of u, and similarly for v. Finally, $uv^2 + f(1 - u)$ and $uv^2 - (f + k)v$ represent the interaction between the two chemicals. Remember f is a constant in this set of equations, NOT a function.

2.2 Cellular Automaton

Rather than try to solve the partial differential equations above, we are going to implement them as a continuous cellular automaton. Each chemical concentration u and v will have its own two-dimensional grid. Each cell in the grid will represent the concentration of that chemical at that location, and will have a value between zero and one. To implement the CA, we separate the equation above into two parts: diffusion and interaction.

Diffusion is calculated based on the 4 nearest neighbors of a cell (von Neumann neighborhood). The value of a cell at $t + 1$ is equal to the sum of it's neighbors minus four times it's value at time t, or:

$$\text{Diff}[u(i,j,t+1)] = u(i+1,j,t) + u(i,j+1,t) + u(i-1,j,t) + u(i,j-1,t) - 4 * u(i,j,t)$$

The interaction of u and v at time $t + 1$ does not depend on the neighborhood, just the concentration of u and v in that cell:

$$\text{Inter}[u(i,j,t+1)] = -u(i,j,t)v(i,j,t)^2 + f(1 - u(i,j,t))$$
$$\text{Inter}[v(i,j,t+1)] = u(i,j,t)v(i,j,t)^2 - (f + k)v(i,j,t)$$

The full transition rule for cells in u and v is just the combination of these two rules

$$u(i,j,t+1) = u(i,j,t) + r_u\text{Diff}[u(i,j,t+1)] + \text{Inter}[u(i,j,t+1)]$$
$$v(i,j,t+1) = v(i,j,t) + r_v\text{Diff}[v(i,j,t+1)] + \text{Inter}[v(i,j,t+1)]$$

3 Assignment

Implement the reaction-diffusion cellular automata for the concentrations of u and v using *periodic* (wrap-around) boundary conditions. Run your cellular automata for at least 10000 time steps. HINT: Only capture the output every 100 time steps.

3.1 Diffusion

First, implement only the diffusion rules for the u and v. Use $r_u = 0.16$ and $r_v = 0.08$ (shown in column 1 of the Table). Once you have the rules defined correctly, try initializing u and v using random initial conditions (real numbers zero and one), and then with with high initial concentrations in the center of the grid. How are the results different? Does the behavior of u differ from that of v? If yes, how?

r_u	0.16	0.16	0.19	0.16
r_v	0.08	0.08	0.05	0.08
f	0.035	0.06	0.06	0.02
k	0.065	0.062	0.062	0.055

Figure 1: Parameter values for Reaction Diffusion CA

3.2 Reaction Diffusion

Next, you will implement both the reaction and diffusion cellular automata with the parameters given in Table 1.

For each set of parameter values, show the steady state value of each CA. Characterized how your results with the parameter sets differ from one another? Try different initial conditions, how do the initial conditions change the end result? How does changing the size of theq grid change the end result? Are u and v fundamentally different? How?

3.3 New Parameters

Finally, try varying the parameters given in 1 to see if you can find new combinations that give interesting results.

3.4 Extra Credit

Make a plot of the distribution of concentrations of u (first plot) and v (second plot). For both plots, the x-axis will be the concentration (ranging from 0 to 1), and the y-axis will be the number of cells with that concentration. Remember to label your axes clearly.

Design a discrete-state CA that exhibits similar dynamics to the continuous-state CA we designed for you.

4 What to hand in

Hand in a short report (not more than 4 pages) that describes your implementation, including some small sample runs that will **convince** me that your simulation works correctly. Think carefully about which runs will **demonstrate** that your CA is working correctly. Document the programming language, any external or built-in libraries that you used, major design decisions, etc.

For each assigned experiment, hand in some sample output and a short discussion of your results. Note: I am not interested in looking at endless printouts of your CA. Think carefully about how to present your results in a convincing but succinct manner. Are there oscillations in concentration or does it converge to a steady state? Please include a listing of your code as an appendix.

5 Late Policy

You are allowed three free “late days” to be used at your discretion throughout the semester. After you have used up your late days, I will deduct 10% per day from the grade you would have received on any late work.