Reaction-Diffusion Systems and Pattern Formation

For this lab, we will be modeling partial differential equations representing reaction-diffusion systems and observing how different parameters can lead to formation of patterns. We will provide you with functions that simulate these models, and for this lab you will be using these functions to test different system parameters. For your submission, please include answers to all questions, any requested figures, and your MATLAB code. Since we are providing you with code, please be thorough with your analysis of results.

Problem 1: 1D Pattern Formation in the Gierer-Meinhardt Model

The Gierer-Meinhardt model represents reaction and diffusion in a two species activator-inhibitor system. This system is able to account for formation of patterns that are relevant in simulating morphogenesis observed in development. This system is represented by the two partial differential equations below:

$$\frac{\partial a}{\partial t} = \frac{a^2}{h} - a + \rho_a + D_a \frac{\partial^2 a}{\partial x^2}$$

$$\frac{dh}{dt} = \mu(a^2 - h) + \frac{\partial^2 h}{\partial x^2}$$

Where a is a short-range, autocatalytic substance and h is a long-range inhibitor. To simulate this model, we will be using code provided by Hugo Bowne at Yale University. To use this code, download the MATLAB files GM_solve.m, and GMfuns.m on Canvas and ensure that they are in your path you are working in. By default, these functions work by simulating the PDEs under the boundary conditions that flux of each species is zero at the system boundaries and the initial condition that the concentration of inhibitor is at steady state initially (in this case steady state is equal to one) and that the concentration of activator is slightly perturbed away from steady state. For the following problems, use the function GM_solve(P, tmax,n,L,fig_numbers) to simulate the model. The inputs to this function are the vector of parameters $P = [D, \mu, \rho_a]$, the final timepoint in your simulation tmax, the number of timepoints to integrate n, and the length of the one dimensional system L. Additionally, this function generates three figures, so the figure numbers are specified by the vector of three integers fig_numbers. For the following questions, use tmax = 100, n = 100, and L = 10.

A) Simulate the GM model given the the following parameter values:

Run #	D	μ	ρ_a
1	0.1	1.25	0.07
2	0.05	0.05	0.07
3	0.4	0.5	0.07
4	0.05	1.4	0.07

   In your submission, include the two surface plots illustrating the dynamics of a and h and also the final timepoint in the moving plot generated. Compare and contrast the differences between each run. Do any of these parameter combinations lead to pattern formation? If so, describe what occurs.

B) Beginning with the parameters you used in run 1, slowly decrease the value of diffusivity constant D by increments of 0.005 and simulate. At what value of D does the system no longer appear to have a stable, homogenous steady state solution? What happens instead? Why might slow diffusion cause this to happen?

C) Now we will try to modify the initial condition to our system and see how the behavior changes. On Canvas there is a modified version of the function you used previously named

GM_solve_IC.m. This function is identical to the previous function except it now requires a final input IC_func, which is a function that inputs a vector of x positions x = [0 L] and a vector of parameter P (even though it will not be used, it is required for the PDE solver in MATLAB) and outputs a matrix of initial values $y_0 = \begin{bmatrix} a_{x=0} \dots a_{x=L} \\ h_{x=0} \dots h_{x=L} \end{bmatrix}$. Write a function that sets the initial conditions for h to be equal to 1 at all x values and a to be set by the function $a(x) = 1 + \cos\left(\frac{n\pi x}{L}\right)$. Your function should take inputs of position vector x, vector of parameters P, integer n and length L, but to pass it into GM_solve_IC you must modify it to set $n\ and\ L$ and only input x and P. Using your function and the given function GM_solve_IC, simulate the model three times with values of $n = [1\ 2\ 3\ 4]$ and the parameters from run 4. How does the value of n influence the behavior of the system?

Problem 2: 2D Pattern Formation in the Gray-Scott Model

The Gray-Scott system models the reaction-diffusion system with the reaction $V + 2V \rightarrow 3V$. Additionally, there is a first order degradation reaction removing V from the system. This system is represented by the partial differential equations below.

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

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

Here f is the feed rate that replenishes species u and removes species $u\ and\ v$ from the system, and k is the rate of conversion from u to v. To simulate this model, we will be using code provided by nsbalbi on GitHub. Download the files rxn_dfsn_gs.m and laplacian.m on Canvas and add it to the path you are working in. The function rxn_dfsn_gs.m takes four parameter inputs (f, k, D_u, D_v) and a variety of other inputs that can be specified with name value inputs. Additionally, if you wish to only set f and k, you can leave the other inputs blank and they will be set automatically. Running this function will generate an animated figure describing the concentration of u in space and time.

A) Here we will be testing different values of $f\ and\ k$ as well as different initial condition set by the name-value pair ‘InitCondition’. Simulate the model using the following parameter sets. Hint: To use this function to simulate the model with designated values of f and k, default values for diffusivity constants, and a set initial condition write rxn_dfsn_gs(f,k,’InitCondition’,initial condition). Qualitatively describe each of the patterns that arise from these initial conditions. For each run include a screenshot of a long-time point in your simulation.

Run #	f	k	D_u	D_v	Initial Condition
1	0.022	0.051	1	0.5	‘square’
2	0.01	0.041	1	0.5	‘wavefront’
3	0.09	0.059	1	0.5	‘uSpots’
4	0.09	0.059	1	0.5	‘vSpots’

B) Beginning with the parameters and initial condition from Run #1, determine the effects of the diffusivity of species v on the long-term system behavior. To do this, increase the value of D_v in increments of 0.1 until the system no longer forms a pattern and reaches a homogenous steady state. What value of D_v led to a homogenous long-term state? As you approached this value, how did the system behavior change? Why might increasing diffusivity prevent a pattern from being formed? Include a screenshot of the long term behavior of the system after reaching the critical diffusivity and just before.

C) Repeat part B using the parameters and initial conditions from Run 2. Compare your results here to part B.