Reaction-Diffusion System in 1D

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1 Introduction

Pattern formation defines the complex structures of living organisms that develop from equivalent cells. Reaction-diffusion systems can model these dynamics. This is a simple system with two or more chemicals diffusing with different diffusion constants and reacting with each other. This system is used to model pattern formations in living systems. The system that is explored in this term paper is the Brusselator Model.

2 Reaction-Diffusion System

For instance, let us consider a simple activator-inhibitor system. Only for a reaction system, at a particular lattice point, the activator increases the concentration of the inhibitor and the inhibitor decreases the concentration of the activator. After a certain time, there wouldn't be any activator to increase the inhibitor's concentration. Now for a diffusion system, the concentration of each chemical will decrease in time. The collective behavior of both reaction and diffusion in a single system will end in a final non-equilibrium steady state. This steady state is equivalent to the pattern formation in living systems.

In this term paper, we are considering a two-chemical reaction-diffusion system in one dimension. Thus the dynamical equation of the concentration of the chemicals will look like the following.

$$\partial_t u = D_u \partial_x^2 u + R_u(u, v) \tag{1}$$

$$\partial_t v = D_v \partial_x^2 v + R_v(u, v) \tag{2}$$

Where D_u and D_v are the diffusion constants of chemical u and chemical v respectively. R_u and R_v are reaction rates of chemical u and chemical v respectively.

3 Brusselator Model

The brusselator model is a reaction system comprising the following set of reactions:

$$\begin{aligned} A &\to u \\ B + u &\to v \\ 2u + v &\to 3u \\ u &\to E \end{aligned}$$

Here u and v are the chemicals of interest. The chemicals A, B, and E are reagents. The concentration of these reagents is kept constant. We will write the reaction rate for u and v.

$$R_u(u,v) = A - (B+1)u + u^2 v \tag{3}$$
$$R_v(u,v) = Bu - u^2 v \tag{4}$$

Where the terms on the right-hand sides of equation (3) and (4) are concentrations of the chemicals.

Substituting equation (3) and (4) in (1) and (2) respectively, we will get our final dynamical equations.

$$\partial_t u = D_u \partial_x^2 u + A - (B+1)u + u^2 v \tag{5}$$
$$\partial_t v = D_v \partial_x^2 v + Bu - u^2 v \tag{6}$$

4 Methodology

We are solving for the Reaction-Diffusion system in a 1D ring. We are solving for a periodic domain of 10π. We will discretize the domain into n spatial grids. The Partial Differential Equations (PDEs) can be made into n Ordinary Differential Equations (ODEs) using the Finite Differencing Method (FDM). We are solving for the time evolution of each of the grids. Thus we should solve $2n$ ODEs.

Let us write the second derivative of the function at each grid in terms of the value of the function at the grids using FDM.

$$\partial_x^2 u_i \approx \frac{u_{i+1} + u_{i-1} - 2u_i}{(\Delta x)^2} \tag{7}$$

Here u_i represents the value of the function u at position x_i.

We can represent equation (7) in matrix representation using the Toeplitz matrix as we impose Periodic Boundary Condition (PBC).

$$\partial_x^2 \begin{pmatrix} u_1 \\ u_2 \\ u_3 \\ \cdot \\ \cdot \\ \cdot \\ u_n \end{pmatrix} = \frac{1}{(\Delta x)^2} \begin{bmatrix} -2 & 1 & 0 & \cdot & \cdot & \cdot & 1 \\ 1 & -2 & 1 & \cdot & \cdot & \cdot & 0 \\ 0 & 1 & -2 & \cdot & \cdot & \cdot & 0 \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ 1 & 0 & 0 & \cdot & \cdot & \cdot & -2 \end{bmatrix} \begin{pmatrix} u_1 \\ u_2 \\ u_3 \\ \cdot \\ \cdot \\ \cdot \\ u_n \end{pmatrix} \tag{8}$$

Now, we will proceed to solve $2n$ ODEs (n for u and n for v) using the standard RK4 the method from the scipy.integrate.solve_ivp package in python. We will choose a smaller step size to avoid missing out on any information.

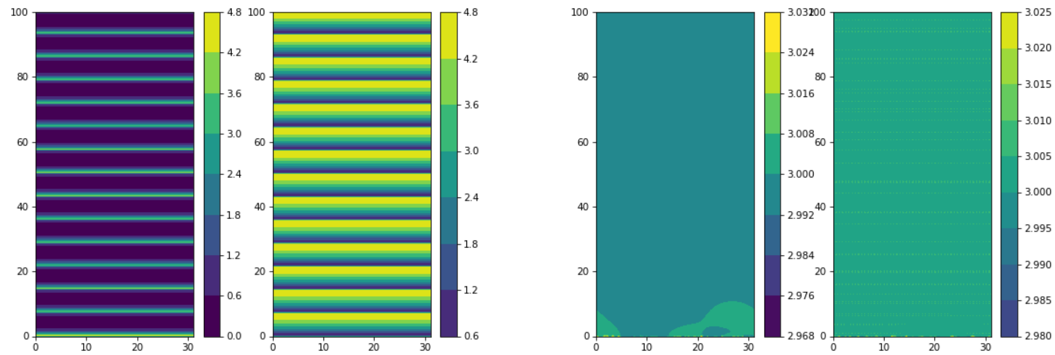
5 Results and Implications

If we begin with equal concentrations of u and v throughout the domain, then the system won't undergo diffusion. We will observe only reactions in the system.

For a non-diffusive system, when there is no reaction, $R_u = R_v = 0$. We will get $u = A$ and $v = \frac{B}{A}$. Thus the Brusselator will have a fixed point at $u = A$, $v = \frac{B}{A}$.

The fixed point becomes unstable when,

$$B > 1 + A^2 \tag{9}$$



(a) Unstable Brusselator reaction system

(b) Stable Brusselator reaction system

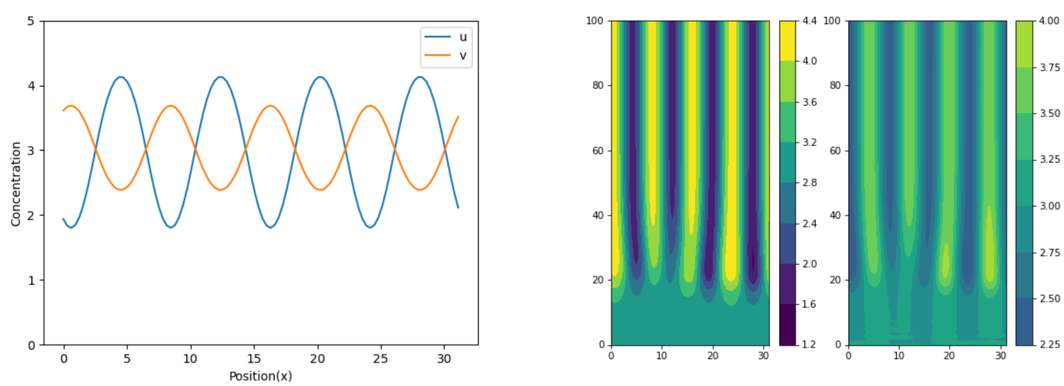
Figure 1: Contour plot of concentration in time

If we initialize the system for $u_0 = v_0 = 3$ with $A = 1$ and $B = 3$, then we observe that the system oscillates as seen in Fig: 1a.

If we initialize the system for $u_0 = v_0 = 3$ with $A = 1$ and $B = 1.7$ (stable fixed point), then we observe that the system comes to equilibrium as seen in Fig: 1b.

For the combined reaction-diffusion system, we should choose the parameters in such a way that the system does not oscillate i.e. A and B should satisfy the stability condition of the reaction system. Also, the value of B should not be so low that the diffusion term dominates and would attain equilibrium. We choose our parameters to be $A = 3$ and $B = 9$.

We are initializing the system with the concentration of u and v with $u_0 = 3+\eta$ and $v_0 = 3+\eta$. Here η is a small thermal noise (of order 10^{-2}). We let the system evolve and we observe that the system attains a non-equilibrium steady state resulting in pattern formation. The final pattern we get is seen in Fig: 2a. The contour plot of concentration of u and v is given in Fig 2b. The full video is given in the reference [1].



(a) Steady-state

(b) Contour plot of concentration in time

Figure 2: Pattern Formation of Brusselator in 1D

References

[1] "Pattern formation(4 peaks)." https://youtu.be/aJ375TY7UBk.