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Research Paper

Pattern Formations Dynamics in a Reaction-Diffusion Model

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Abstract: *We study a reaction diffusion system that models the dynamics of pattern formation. We find the traveling wave solutions and pattern formation using numerical method and Consul finite element package in one and two dimensions. After examining the travelling waves that are generated, we have shown that how diffusion driven instability in this model.*

Keywords: Reaction-diffusion, Traveling wave solutions, pattern formation.

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1. Introduction:

Pattern formation is a topic in mathematical biology that studies how structures and pattern in nature evolve over time (see [1, 8, 9 and 11]). One of the mainstream topics in pattern formation involves the reaction-diffusion mechanisms of two chemicals, originally proposed by Alan Turing in 1952 (see [10]).

Several mathematical models has been proposed, relying on different biological and chemical processes. One of the first models is an activator-inhibitor model due to Murray (see [4]).

In this paper, we study the dynamics of pattern formation for a system of reaction diffusion equations. We show the conditions of diffusion driven instability. We use the numerical method namely finite difference method for the one dimensional problem. We use COMSOL software (see [3]), as a finite element package for solving the two dimensional problem. The model that we study is

$$\frac{\partial U}{\partial t} = D_u \frac{\partial^2 U}{\partial x^2} + k_u U(U - W),$$

$$\frac{\partial W}{\partial t} = D_w \frac{\partial^2 W}{\partial x^2} + k_w W(U^2 - W^2), \qquad \ldots.(1)$$

Where$D_U$and D_w are diffusion coefficients, $k_u U(U-W)$ and $k_w W(U^2-W^2)$ are the interaction of the species U and W. We define dimensionless variables

$$U=u, W=w, x=(\frac{D_u}{k_u})^{0.5}\bar{x},\ \ t=\frac{\bar{t}}{k_u},$$

In terms of which (1) becomes

$$\frac{\partial u}{\partial \bar{t}}=\frac{\partial^2 u}{\partial \bar{x}^2}+u(u-w),$$

$$\frac{\partial \mathrm{w}}{\partial \bar{\mathrm{t}}}=\mathrm{D}\frac{\partial^2 \mathrm{w}}{\partial \bar{\mathrm{x}}^2}+\mathrm{kw}(\mathrm{u}^2-\mathrm{w}^2), \qquad \ldots.(2)$$

The dimensionless parameters are k=$\frac{k_w}{k_u}$, $D=\frac{D_u}{k_u}$, where $k>0$.

For notational convenience we will omit the over bars in what follows.

2. Conditions for Diffusion Driven Instability:

We begin by discussing the conditions of diffusion driven instability in a homogeneous case, a detailed can be found, for example in Murray book [2002] (see for example [1, 2, 4]). The dynamics of pattern formation occur when the stability of steady state changes after we add diffusion. We consider a two species reaction diffusion system

$$\frac{\partial u}{\partial t}=\frac{\partial^2 u}{\partial x^2}+f(u,w),$$

$$\frac{\partial w}{\partial t}=D\frac{\partial^2 w}{\partial x^2}+g(u,w), \qquad \ldots.(3)$$

Assume that the reaction terms $f(u,w)$ and $g(u,w)$hasa non-zero homogeneous steady state(u_0,w_0). This system exhibits diffusion driven instability if the homogeneous steady state (u_0,w_0) is a stable to spatially homogeneous perturbations, but unstable to some non-homogeneous perturbations. The conditions for diffusion driven instability are

$$a+d<0, \qquad ad>bc,$$

$$Da+d>0, (Da+d)^2>4D(ad-bc),$$

Where

$$a=\frac{\partial f(u_0,w_0)}{\partial u}, \qquad b=\frac{\partial f(u_0,w_0)}{\partial w}, \quad c=\frac{\partial g(u_0,w_0)}{\partial u}, \quad d=\frac{\partial g(u_0,w_0)}{\partial w}.$$

In (3), the steady states are the solutions of$u=w$, and therefore we assume $u_0=w_0$, we get

$$a=u_0, \qquad b=-u_0, \quad c=-2ku_0, \quad d=-2k{u_0}^2$$

Thus these conditions become

$$a + d = u_0 - 2ku_0{}^2 < 0$$
$$ad > bc$$

The above conditions show the homogeneous steady state $(u_0, w_0)$is a stable. Now, when the diffusion is added to the problem, the stability of the steady state (u_0, w_0) should change from stable to unstable in order to have the dynamics of pattern formation. In other words, when the following conditions are satisfied, we get pattern formation,

$$Dka + d = Dku_0 - 2ku_0{}^2 > 0,$$

Which can be true when $D \gg 1$. The following condition also satisfied

$$(Dku_0 - 2ku_0{}^2)^2 > 0.$$

In conclusion, it is clear that the dynamics of pattern formation can be found in(3).

3. Numerical Study of Pattern Formation In (3):

In this section we solve (3) numerically and try to find the traveling wave solutions that are generated by the initial condition. A semi-implicit finite difference method, the unconditionally stable method is applied. An implicit method is used to discretize the diffusion operator. For the non-linear reaction part we use an explicit method. Finite difference method can be derived using Taylor series expansion $u(x_0 + \Delta x)$and$u(x_0 - \Delta x)$, where Δx is the step size of x. The discretization equation of (1) is

$$\frac{u_n^{t+\Delta t} - u_n^t}{\Delta t} = \frac{u_{n+\Delta x}^{t+\Delta t} - 2u_n^{t+\Delta t} + u_{n-\Delta x}^{t+\Delta t}}{(\Delta x)^2} + F(u_n^t, w_n^t)$$

$$\frac{w_n^{t+\Delta t} - w_n^t}{\Delta t} = \frac{D}{\lambda}\frac{w_{n+\Delta x}^{t+\Delta t} - 2w_n^{t+\Delta t} + w_{n-\Delta x}^{t+\Delta t}}{(\Delta x)^2} + G(u_n^t, w_n^t)$$

or

$$ru_{n+\Delta x}^{t+\Delta t} - (1 + 2r)u_n^{t+\Delta t} + ru_{n-\Delta x}^{t+\Delta t} = -u_n^t + (\Delta t)F(u_n^t, w_n^t)$$

$$rDw_{n+\Delta x}^{t+\Delta t} - (1 + 2rD)w_n^{t+\Delta t} + rDw_{n-\Delta x}^{t+\Delta t} = -w_n^t - (\Delta t)G(u_n^t, w_n^t)$$

where$r = \frac{\Delta t}{(\Delta x)^2}$. The domain of solution $0 < x < l$ is divided into N discrete equally spaced points$x = x_i = (i - 1)\Delta x$, where $i = 1,2, \ldots, N$and$\Delta x = l/(N - 1)$. The initial conditions are $u(x, 0) = u_0(x)$and$w(x, 0) = w_0(x)$. The boundary conditions are no flux Neumann boundary conditions, $u_x = w_x = 0$at$x = 0, l$, which are imposed using three point formula (this is a second order accuracy stable).

$$u'(x) = \frac{-3u_n^{t+\Delta t} + 4u_{n+\Delta x}^{t+\Delta t} - u_{n+2\Delta x}^{t+\Delta t}}{2\Delta x} = 0$$

$$w'(x) = \frac{-3w_n^{t+\Delta t} + 4w_{n+\Delta x}^{t+\Delta t} - w_{n+2\Delta x}^{t+\Delta t}}{2\Delta x} = 0$$

The result of discretization is a system of algebraic equations in the form,

$$AU^{t+1} = bU^t$$

$$BW^{t+1} = cW^t \dots .(4)$$

or

$$\begin{bmatrix} 3 & -4 & 1 & & \\ -r & (1+2r) & -r & & \\ \ddots & \ddots & \ddots & & \\ & -r & (1+2r) & -r & \\ & 1 & -4 & 3 & \end{bmatrix} \begin{bmatrix} u_1^{t+1} \\ u_2^{t+1} \\ \vdots \\ u_{N-1}^{t+1} \\ u_N^{t+1} \end{bmatrix} = \begin{bmatrix} 0 \\ u_2^t + (\Delta t)F(u_2^t, w_2^t) \\ \vdots \\ u_{N-1}^t + (\Delta t)F(u_{N-1}^t, w_{N-1}^t) \\ 0 \end{bmatrix},$$

in the case of w

$$B = \begin{pmatrix} 3 & -4 & 1 & & \\ -Dr & (1+2Dr) & -Dr & & \\ \ddots & \ddots & \ddots & & \\ & -Dr & (1+2Dr) & -Dr & \\ & 1 & -4 & 3 & \end{pmatrix}$$

$$cW^t = \begin{bmatrix} 0 \\ w_2^t + (\Delta t)G(u_2^t, w_2^t) \\ \vdots \\ w_{N-1}^t + (\Delta t)G(u_{N-1}^t, w_{N-1}^t) \\ 0 \end{bmatrix}, \qquad W^{t+1} = \begin{bmatrix} w_1^{t+1} \\ w_2^{t+1} \\ \vdots \\ w_{N-1}^{t+1} \\ w_N^{t+1} \end{bmatrix}.$$

The initial condition that we use, $u_0(x)$ and $w_0(x)$ are step functions and we consider for the numerical problem, the stable steady state(1,1). The traveling wave that are generated connects a stable steady state to other steady state. A simple traveling wave can be generated numerically as shown in Figure 1, and connects the steady state $(1,1)$ to the state $(0,0)$. The diffusion coefficient here$D = 1$, and if we change it to $D = 8$ we see how the dynamics of the solution changes as shown in Figure 2. This is because the diffusion driven instability as we increase the diffusion coefficient.

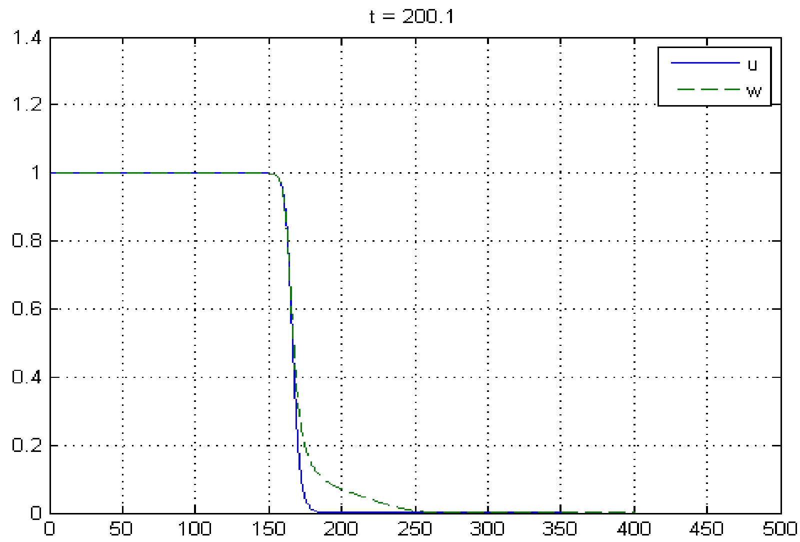

Figure 1: A traveling wave solution is generated when $k = 1, D = 1$

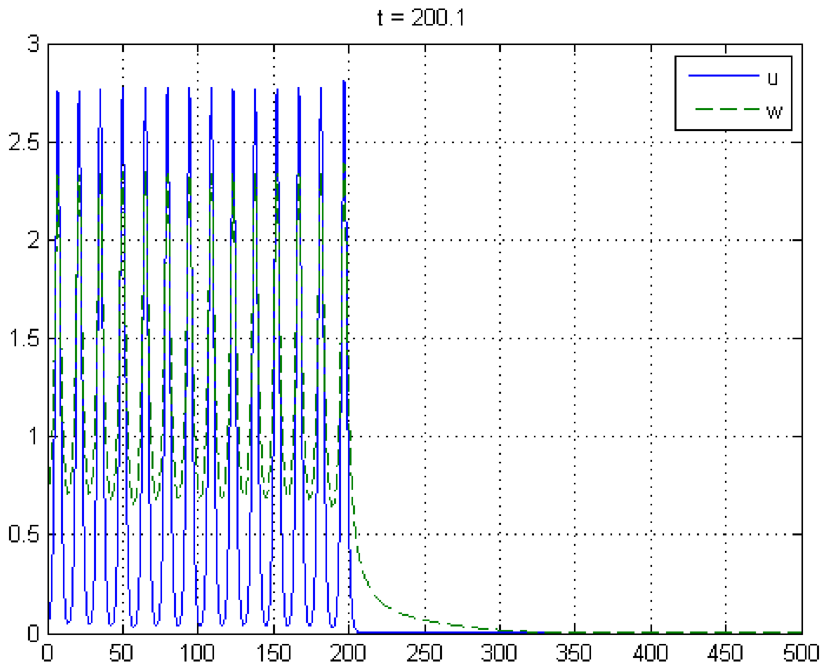

Figure 2: A traveling wave solution is generated when $k = 1, D = 8$

Next, we use COMSOL multiphysics software as a finite element method to solve the system of equations (2)in two dimensions, for more details about COMSOL see [18]. In Figures 3 and 4, we show the pattern formation solutions for both u and w in two dimensions respectively. Also, in Figures 5 and 6, we have shown the pattern formation solutions, and in the last four figures we used the same values of Das in the one dimension and we get the same results.

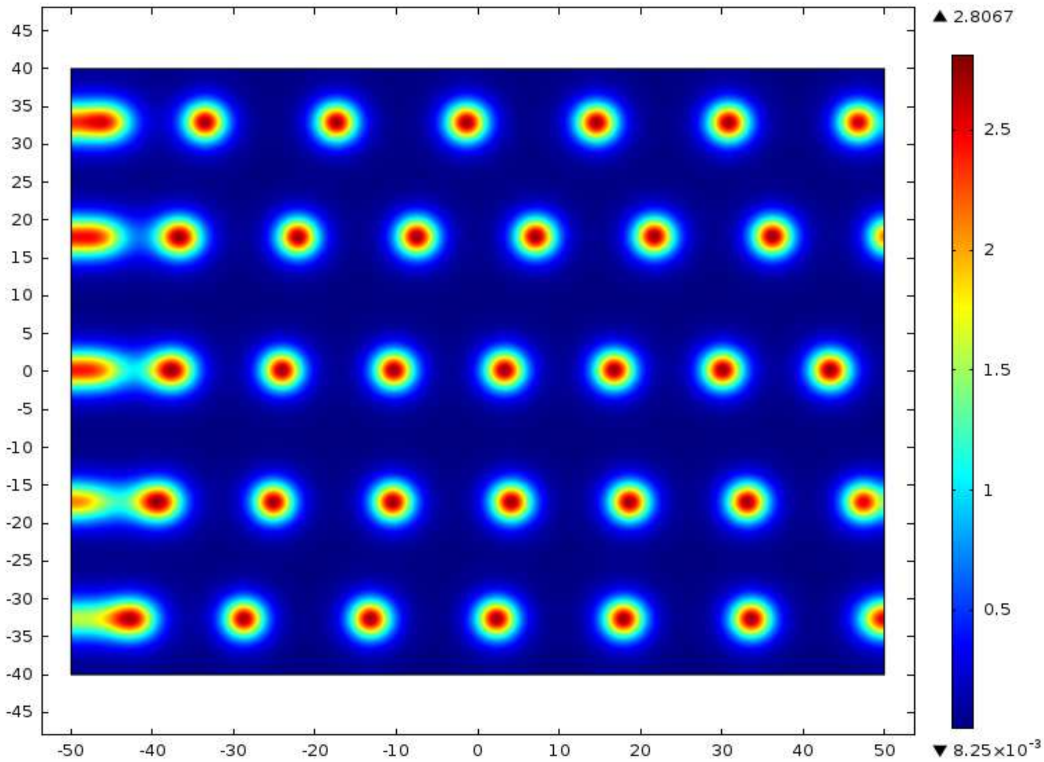

Figure 3: Numerical solution using COMSOL shows pattern formation dynamics in u, when $k = 1$, D $= 8$

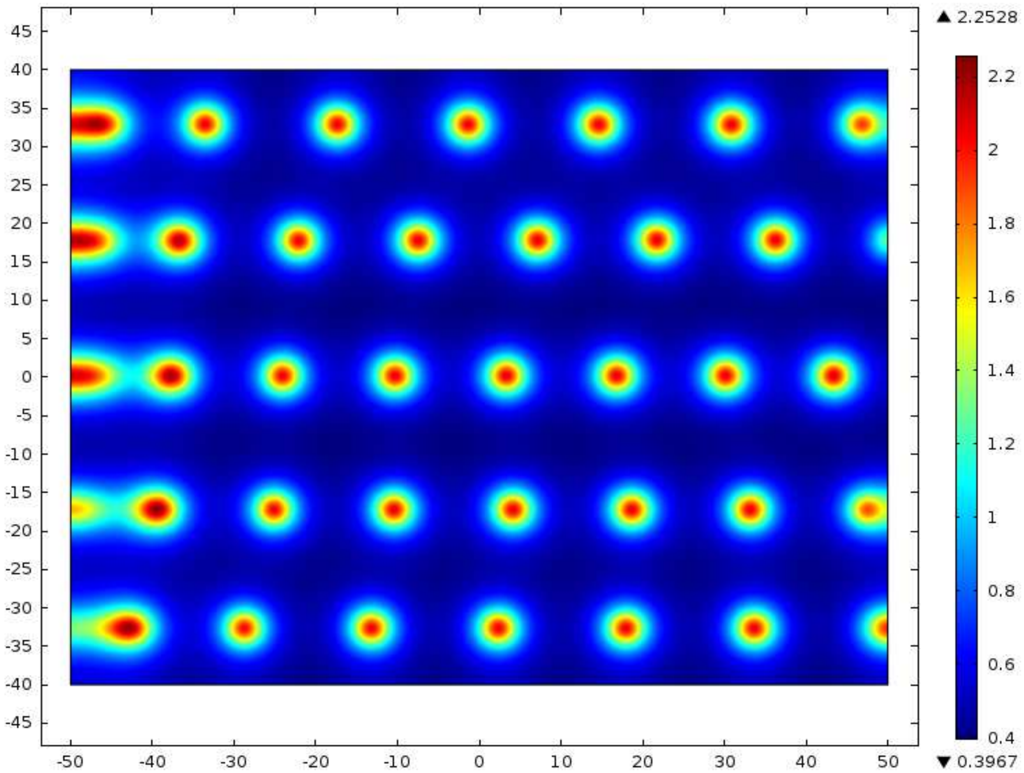

Figure 4: Numerical solutions using COMSOL shows pattern formation dynamics in w, when $k = 1$, D $= 8$

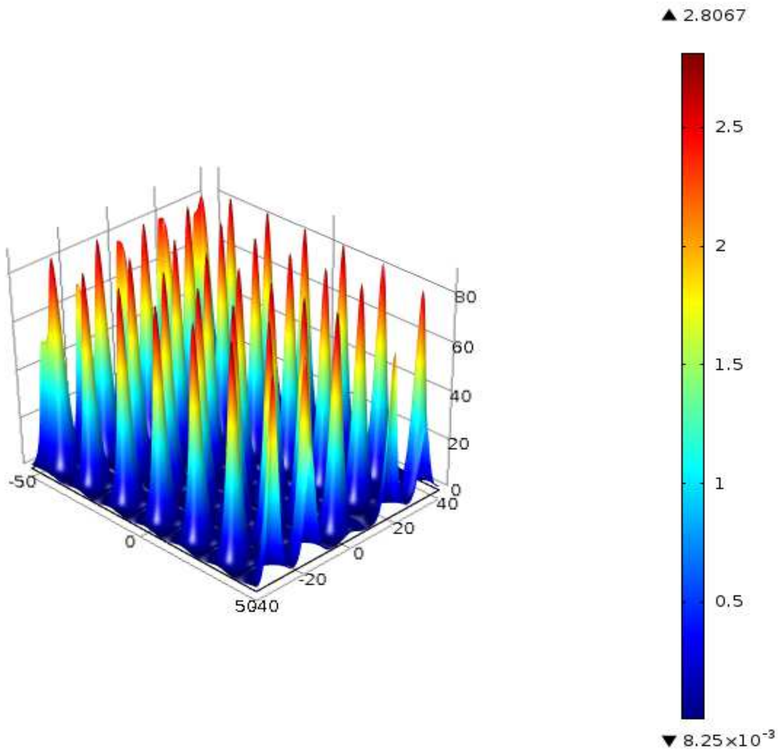

Figure 5: Numerical solutions using COMSOL in two dimensions, shows pattern formation dynamics inu, when $k = 1$, D $= 8$

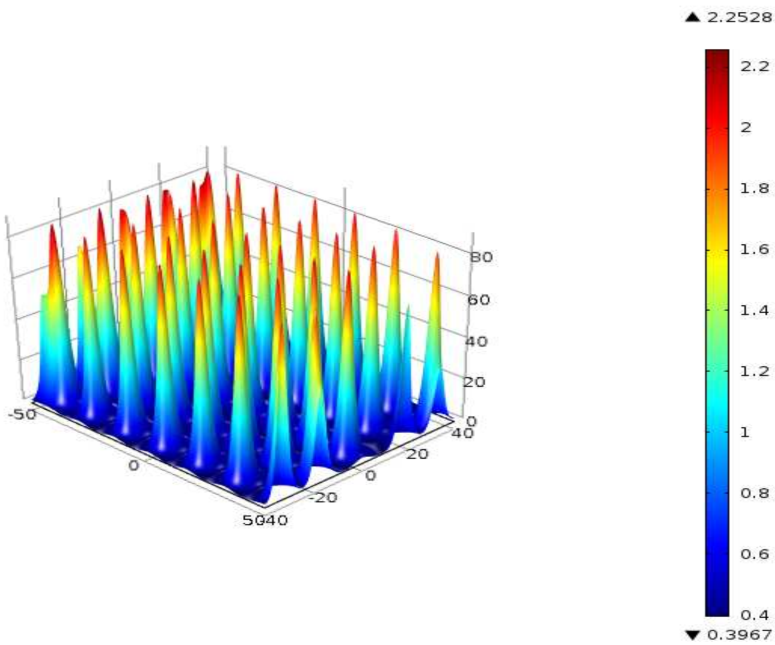

Figure 6: Numerical solution using COMSOL in two dimensions shows pattern formation dynamics in u, when $k = 1$, D $= 8$

4. Results and Discussion:

We study the Reaction-Diffusion system in (2) for pattern formation solutions in one and two dimensions. We use for that finite difference method in the case of one dimension, and the COMSOL finite element method in two dimensions. We have shown that this model satisfies the condition of diffusion driven instability and therefore the pattern formation can be found in this model. The numerical results in one dimension and two dimensions agreed with the conditions of diffusion driven instability and show a nice pattern formations as shown in the figures above.

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