INDIAN INSTITUTE OF TECHNOLOGY, BOMBAY

CL 716 - Modelling Chemical and Biological Patterns

Bifurcation analysis of nonlinear reaction-diffusion equations |

https://github.com/akigupta131/the-bifurcation-project

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Abstract
The theoretical expressions are limited to the neighborhood of the marginal stability point. Computer simulations allow not only the verification of their predictions but also the investigation of the behavior of the system for larger deviations from the instability point.

Introduction

The general ideas underlying the theory of dissipative structures have been illustrated on a simple model system involving the following set of coupled chemical reactions:

$$
\begin{aligned}
A &\rightleftharpoons X && \text{(a)} \\
2X + Y &\rightleftharpoons 3X && \text{(b)} \\
B + X &\rightleftharpoons Y + D && \text{(c)} \\
X &\rightleftharpoons E && \text{(d)}
\end{aligned}
\qquad (1.1)
$$

the system is open to the initial and final chemicals A, B, D and E, whose concentrations are imposed throughout the system; nonlinearity is introduced by the auto- and cross-catalytic steps (b) and (c);

We analyze some properties of the dissipative structures arising in nonlinear reaction-diffusion systems, within the framework of this model. Assuming a bounded, one-dimensional medium, the rate equations describing (1.1) are:

$$
\begin{aligned}
\frac{\partial X}{\partial t} &= A + X^2 Y - (B + 1)X + D_X \cdot \frac{\partial^2 X}{\partial r^2} \\
\frac{\partial Y}{\partial t} &= BX - X^2 Y + D_Y \cdot \frac{\partial^2 Y}{\partial r^2} \quad (0 \leqslant r \leqslant L).
\end{aligned}
\qquad (1.2)
$$

where D_x and D_y are the diffusion coefficients of X and Y assuming that Fick's law is valid. Two types of boundary conditions will be considered:

1. Zero flux boundary conditions (Neumann conditions):

$$
\frac{\partial}{\partial r} X(0, t) = \frac{\partial}{\partial r} X(L, t) = \frac{\partial}{\partial r} Y(0, t) = \frac{\partial}{\partial r} Y(L, t) = 0 \quad (t \geqslant 0). \quad (1.3)
$$

2. Fixed boundary conditions (Dirichlet conditions):

$$
\begin{aligned}
X(0, t) &= X(L, t) = A \\
Y(0, t) &= Y(L, t) = B/A \quad (t \geqslant 0).
\end{aligned}
\qquad (1.4)
$$

MATLAB Code

The Matlab code consists of four files:-

The main script file

```
function pdex4

m=0; %slab
r=linspace(0,pi,100);
t=linspace(0,200,100);
sol=pdepe(m,@pdex4pde,@pdex4ic,@bc2fn,r,t);
disp(sol);

u1 = sol(:,:,1);
u2 = sol(:,:,2);

figure
surf(r,t,u1)
title('X(r,t)')
xlabel('Distance r')
ylabel('Time t')

figure
surf(r,t,u2)
title('Y(r,t)')
xlabel('Distance r')
ylabel('Time t')
```

Boundary condition definition file

Note: Two types of boundary conditions will be considered:-

1. Zero Flux Boundary Conditions (Neumann conditions)
2. Fixed Boundary Conditions (Dirichlet conditions)

```
function [pl,ql,pr,qr]=bc2fn(xl,ul,xr,ur,t)

% Constants
A = 2;
B = 0.4; %NOT GIVEN | TO BE CHANGED

% Case 1:- Zero Flux Boundary Conditions (Neumann conditions)
pl= [0;0];
ql=[1;1];
pr =[0;0];
qr =[1;1];

% Case 2:- Fixed Boundary Conditions (Dirichlet conditions)
% pl = [A; B/A];
% ql = [0; 0];
% pr = [A; B/A];
% qr = [0; 0];
```

Initial condition definition file

```
function u0 = pdex4ic(r);

% Constants
A = 2;
B = 3.7; %NOT GIVEN | TO BE CHANGED

c1 = 10;
c2 = 10;
L = 1;

u0 = [A;B/A];
```

The PDE solver file

```
function [c,f,s] = pdex4pde(r,t,u,DuDr)

% Diffusion Coefficients
Dy = 1.6*10^(-3);
Dx = 8.0*10^(-3);

% Constants
A = 2;
L = 1;
u1 = u(1);
u2 = u(2);

B = 3.7; %NOT GIVEN | TO BE CHANGED

c = [1; 1];
f = [Dx; Dy] .* DuDr;

% Rate equations describing the phenomenon
s1 = A + u1^2*u2 - (B+1)*u1;
s2 = B*u1 - u1^2*u2;

% Linearized equations for the perturbation x and y
% s1 = (B-1)*u1 + A^2*u2;
% s2 = -B*u1 - A^2*u2;

s = [s1; s2];
```

Numerical Analysis

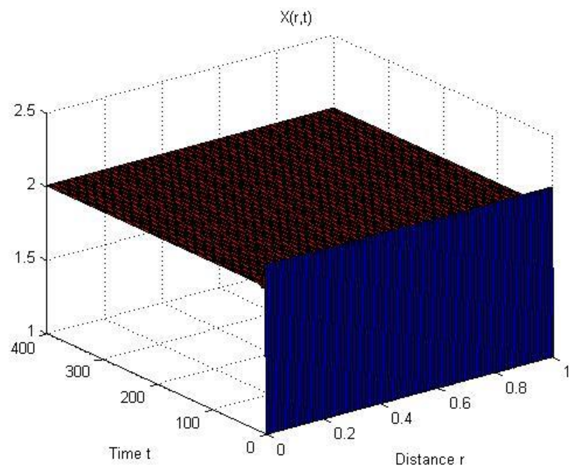
We use the simulation using MATLAB to verify the numerical results with the analytical ones. Following are the major numerical simulations:-

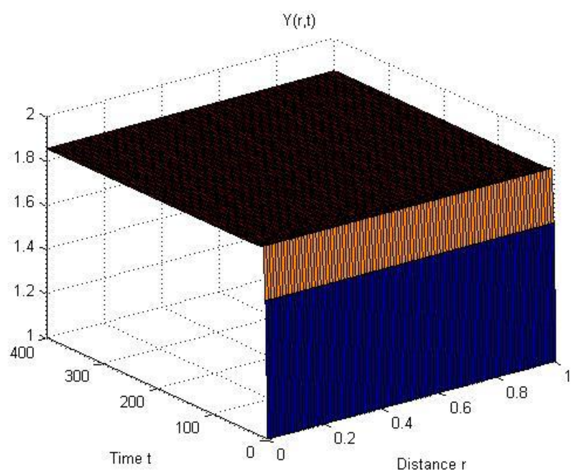
Case 1

All the equations are restricted to the constraint $0 \le r \le L$ and L is taken to be 1.
Also diffusion coefficients are taken to be:-

1. $D_x = 1.6 \times 10^{-3}$
2. $D_y = 8.0 \times 10^{-3}$

A = 2 and B = 3.7 for zero flux boundary condition





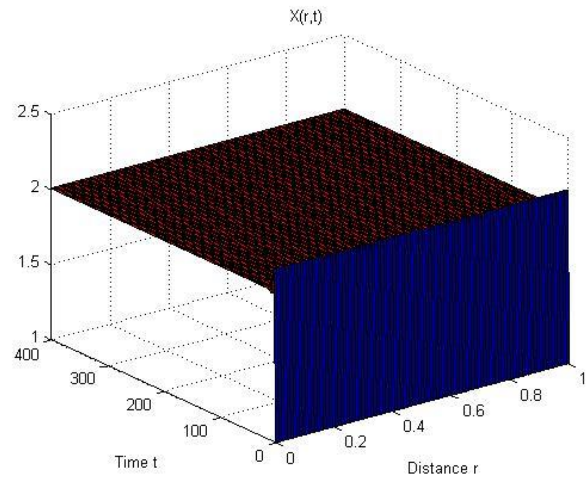
A spatio-temporal curve is plotted between X and Y vs distance ‘r’ and time ‘t’ resulting from solving the system numerically by simulating on MATLAB. Figure 1A: X vs distance ‘r’ and time ‘t’ for A=2, B=3.7, L=1, $D_x = 1.6 \times 10^{-3}$, $D_y = 8.0 \times 10^{-3}$. Figure 1B: Y vs distance ‘r’ and time ‘t’ for A=2, B=3.7, L=1, $D_x = 1.6 \times 10^{-3}$, $D_y = 8.0 \times 10^{-3}$.

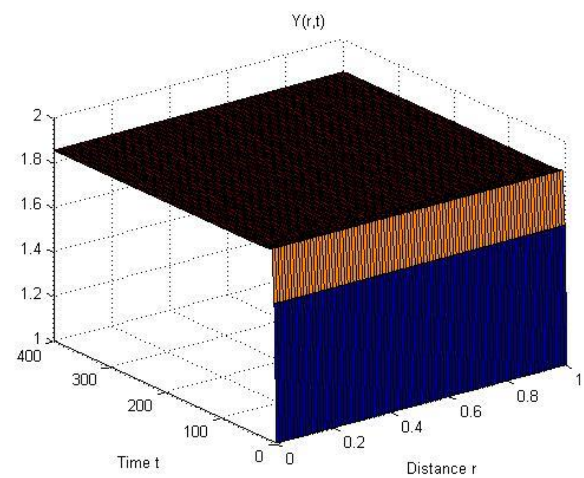
Case 2

All the equations are restricted to the constraint $0 \le r \le L$ and L is taken to be 1.
Also diffusion coefficients are taken to be:-

1. $D_x = 8.0 \times 10^{-3}$
2. $D_y = 1.6 \times 10^{-3}$

A = 2 and B = 3.7 for zero flux boundary condition





A spatio-temporal curve is plotted between X and Y vs distance ‘r’ and time ‘t’ resulting from solving the system numerically by simulating on MATLAB. Figure 2A: X vs distance ‘r’ and time ‘t’ for A=2, B=3.7, L=1, $D_x = 8.0 \times 10^{-3}$, $D_y = 1.6 \times 10^{-3}$. Figure 2B: Y vs distance ‘r’ and time ‘t’ for A=2, B=3.7, L=1, $D_x = 8.0 \times 10^{-3}$, $D_y = 1.6 \times 10^{-3}$.

Analytical Solution

For zero – flux boundary conditions,

$$\begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} c_1 \\ c_2 \end{pmatrix} e^{w_n t} \cos \frac{n\pi r}{L} \quad (n = 0, 1, 2, 3 \ldots). \tag{2.5b}$$

Inserting this into the rate equations, we get secular equation relating w_n to the wavenumber n and the system's parameters:

$$w_n^2 - \mathrm{Tr}\, w_n + \Delta = 0 \tag{2.6}$$

where

$$\mathrm{Tr} = B - (A^2 + 1) - \beta(D_X + D_Y)$$
$$\Delta = A^2 + \beta[A^2 D_X + (1 - B)D_Y] + \beta^2 D_X D_Y$$

and

$$\beta = \left(\frac{n\pi}{L}\right)^2.$$

Instability of the thermodynamic branch will occur for some value of n, if at least one of the roots of (2.6) has a positive Re w_n part. The main point is thus to establish the conditions for marginal stability, Re $w_n = 0$, corresponding either to 'exchange of stability', Im $w_n = 0$, or to 'overstability' Im $w_n \neq 0$. A close analysis of (2.6) shows that:

(a) *the values of w_n are complex if:*

$$(A - \delta^{1/2})^2 < B < (A + \delta^{1/2})^2 \tag{2.7}$$

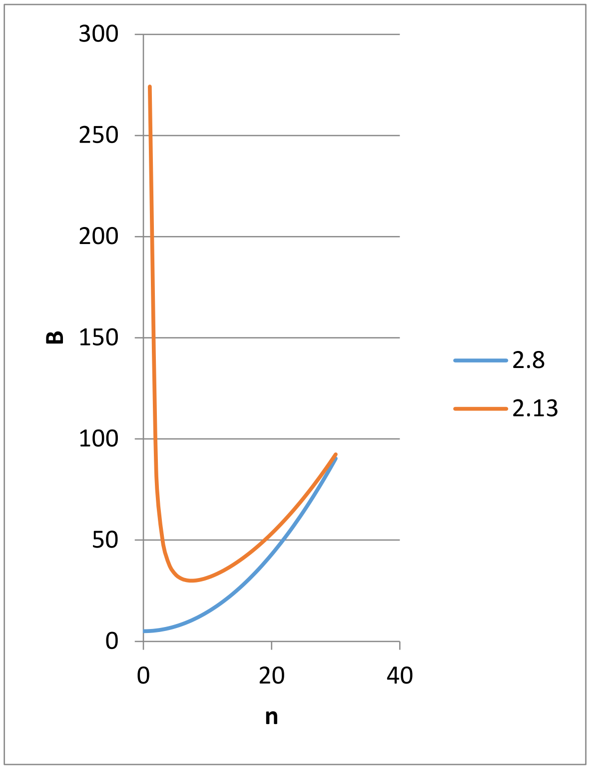
where $\delta = 1 - \beta(D_X - D_Y)$ must be a positive quantity. In this case marginal stability occurs at the critical point:

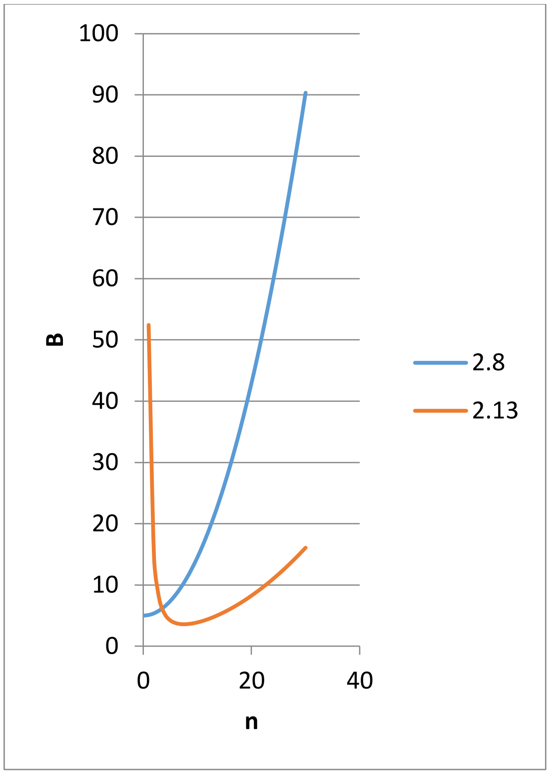
$$B = B_{1c}(n) = 1 + A^2 + \beta(D_X + D_Y). \tag{2.8}$$

For real w_n's the instability conditions reads:-

$$B \geqslant B(n_c) = \min_{\substack{n \geq 1 \\ \text{integer}}} \left\{1 + \frac{D_X}{D_Y} A^2 + \frac{A^2}{D_Y \beta} + \beta D_X\right\} \tag{2.13}$$

Graphs are plotted for these in Microsoft Excel match with the ones shown in the paper:-





Linear stability diagrams resulting from above equations. Figure 3A: A=2, B=3.7, L=1, Dx = 8.0 x 10^{-3}, Dy = 1.6 x 10^{-3}. Figure 3B: A=2, B=3.7, L=1, Dx = 1.6 X 10^{-3}, Dy = 8.0 X 10^{-3}.

Critical Wave Number

The critical wave number corresponding to the onset of stability is given by n_{min} if it is an integer or by one of the two closest integers.

$$n_{\min} = \frac{L}{\pi} \cdot \frac{A^{1/2}}{(D_X D_Y)^{1/4}} \tag{2.11}$$

Case I: A=2, B=3.7, L=1, Dx = 8.0 x 10^{-3}, Dy = 1.6 x 10^{-3}

Critical Wave number = [1/∏ * $2^{1/2}$/(8*10^{-3}*1.6*10^{-3})$^{1/4}$]= 8

Case II: A=2, B=3.7, L=1, Dx = 1.6 x 10^{-3}, Dy = 8.0 x 10^{-3}

Critical Wave number = [1/∏ * $2^{1/2}$/(1.6*10^{-3}*8*10^{-3})$^{1/4}$]= 8 (same)

Extended Analysis

Analytical steady state dissipative structure

We have,

$$
\begin{aligned}
\frac{\gamma_2}{c_1^2} = & -\frac{3}{4} \cdot \frac{D_X\beta + 1 - B_c}{A^2} + \frac{1}{A^2}[2(D_X\beta + 1) - B_c] \\
& -\frac{2}{9} \cdot \frac{[2(D_X\beta + 1) - B_c][\frac{11}{4}D_X\beta + 2 - B_c]}{A^2 D_X\beta} \\
= & \ \phi(n_c, A, D_X, B_c).
\end{aligned}
\tag{2.39}
$$

The bifurcating non uniform steady state solution near $B = B_c$ is thus approximated by:

$$
\begin{aligned}
x(r) = & \pm\left(\frac{B - B_c}{\phi}\right)^{1/2} \cos\frac{n_c\pi r}{L} \\
& +\frac{2}{9} \cdot \frac{B - B_c}{\phi} \cdot \frac{2(\beta D_X + 1) - B_c}{A D_X\beta} \cos\frac{2n_c\pi r}{L} \\
y(r) = & \pm\left(\frac{B - B_c}{\phi}\right)^{1/2} \cdot \frac{D_X\beta + 1 - B_c}{A^2} \cdot \cos\frac{n_c\pi r}{L} \\
& +\frac{2}{9} \cdot \frac{B - B_c}{\phi} \cdot \frac{[2(\beta D_X + 1) - B_c][\frac{7}{4}D_X\beta + 1 - B_c]}{A^3 D_X\beta} \cos\frac{2n_c\pi r}{L} \\
& -\frac{1}{2} \cdot \frac{B - B_c}{\phi} \cdot \frac{2(\beta D_X + 1) - B_c}{A^3}.
\end{aligned}
\tag{2.41}
$$

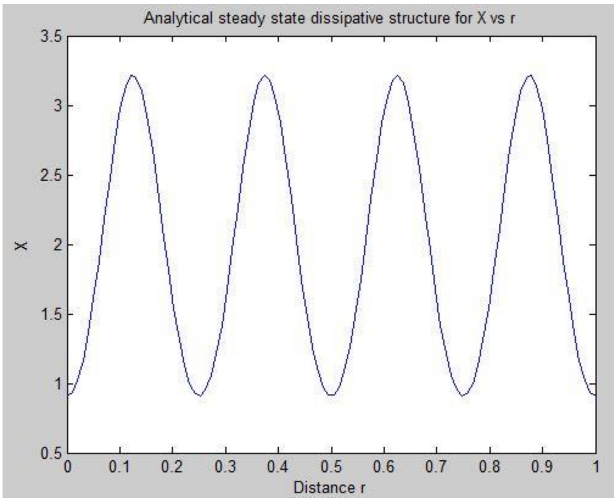
Properties of the Dissipative Structure

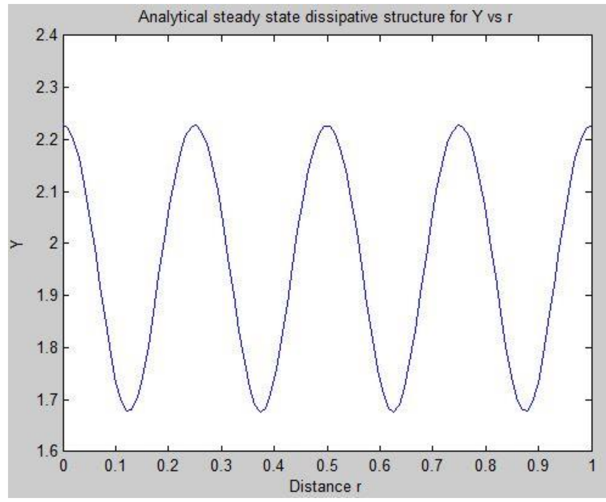
We investigate the properties of the spatial organization emerging beyond instability and compare the theoretical predictions with the results of computer simulation.

Matlab Code

```
A = 2;
B = 4;
Bc = 3.602;

L = 1;
beta = 631.0144;
Dx = 1.6*10^-3;
nc = 8;
fi = -3/4*(beta*Dx + 1-Bc)/(A^2) + 1/A^2*(2*(beta*Dx + 1)-Bc)/(A^2) -
2/9*(2*(beta*Dx + 1)-Bc)*(11/4*Dx*beta+2-Bc)/(A^2*Dx*beta);
r=linspace(0,1,100);

x = -((B-Bc)/fi)^(1/2)*cos(nc*pi*r/L)+2*L+2/9*(((B-Bc)/fi)*(2*(beta*Dx + 1)-
Bc)/(A*Dx*beta))*cos(2*nc*pi*r/L);

y = ((B-Bc)/fi)^(1/2)*(-0.6)*((Dx*beta+1-Bc)/A^2)*cos(nc*pi*r/L) + 2/9*(((B-
Bc)/fi)*(2*(beta*Dx + 1)-Bc)/(A^3*Dx*beta))*((7/4)*Dx*beta + 1 -
Bc)*cos(2*nc*pi*r/L) - (1/2)*((B-Bc)/fi)*(2*(beta*Dx + 1)-Bc)/A^3+2*L;

figure
plot(r,x)
title('Analytical steady state dissipative structure for X vs r')
xlabel('Distance r')
ylabel('X')

figure
plot(r,y)
title('Analytical steady state dissipative structure for Y vs r')
xlabel('Distance r')
ylabel('Y')
```

Results



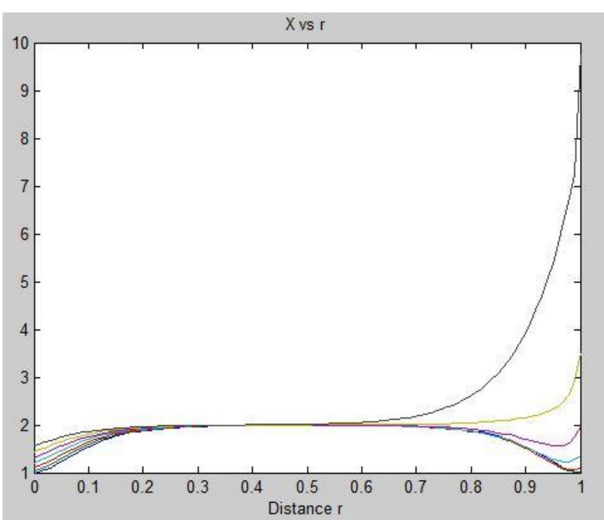


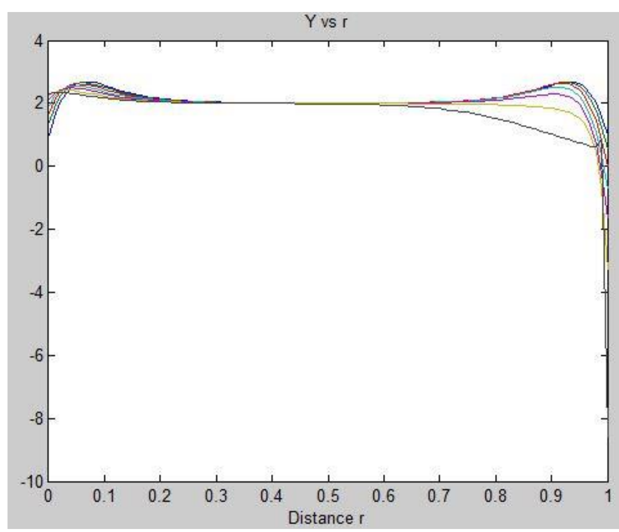
Results obtained from the simulation of the above MATLAB code; Matched with the original solution given in figure 5a and 5b in the paper.

And the pattern obtained from numerical integration of equation 1.2,

$$\begin{aligned}\frac{\partial X}{\partial t} &= A + X^2Y - (B+1)X + D_X \cdot \frac{\partial^2 X}{\partial r^2} \\ \frac{\partial Y}{\partial t} &= BX - X^2Y + D_Y \cdot \frac{\partial^2 Y}{\partial r^2} \quad (0 \leqslant r \leqslant L).\end{aligned} \tag{1.2}$$

comes out to be as follows:-





References

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