Spatio-temporal Pattern Formation in Reaction-Diffusion Systems

Chiara Mocenni

January 15, 2013
Oscillating Chemical Reactions

Brusselator system: Hopf and Turing bifurcations
The Belousov-Zhabotinsky Reaction

- A paradigm or biological pattern formation, such as embryonic development and complex wave behavior in heart
The Belousov-Zhabotinsky Reaction

- A paradigm or biological pattern formation, such as embryonic development and complex wave behavior in heart
- If maintained out of equilibrium, chemical systems are able to spontaneously self-organize in space
The Belousov-Zhabotinsky Reaction

- A paradigm or biological pattern formation, such as embryonic development and complex wave behavior in heart
- If maintained out of equilibrium, chemical systems are able to spontaneously self-organize in space
- Self-organization follows from kinetic and diffusional characteristics: local activation processes balanced by long-range inhibition
The Belousov-Zhabotinsky Reaction

- A paradigm or biological pattern formation, such as embryonic development and complex wave behavior in heart
- If maintained out of equilibrium, chemical systems are able to spontaneously self-organize in space
- Self-organization follows from kinetic and diffusional characteristics: local activation processes balanced by long-range inhibition
- The concentrations of the different chemical species then form stationary spatial patterns that periodically span the space
The reaction sequence of the Brusselator is:

\[ A \xrightarrow{k_1} X, \ B + X \xrightarrow{k_2} Y + D, \ 2X + Y \xrightarrow{k_3} 3X, \ X \xrightarrow{k_4} E. \]

Applying the Law of Mass Action to this scheme, and including diffusion of \( X \) and \( Y \), we get for concentrations \( x \) and \( y \):

\[
\begin{align*}
\frac{\partial x}{\partial t} &= D_x \nabla^2 x + k_1 A - (k_2 B + k_4)x + k_3 x^2 y \\
\frac{\partial y}{\partial t} &= D_y \nabla^2 y + k_2 B x - k_3 x^2 y
\end{align*}
\]

(1)
Brusselator without diffusion

By nondimensionalization and discarding diffusion, we have the following system of equations

\[
\begin{align*}
\dot{u} &= 1 - (\beta + 1)u + \alpha u^2 v \\
\dot{v} &= \beta u - \alpha u^2 v,
\end{align*}
\]

where \( \alpha = \frac{k_3(k_1A)^2}{k_4^3} \) and \( \beta = \frac{k_2B}{k_4} \).

One steady state \((u^*, v^*) = (1, \beta/\alpha)\) undergoing a Hopf bifurcation at \( \beta = \alpha + 1 \).
Reaction-Diffusion Equation

\[
\frac{\partial c}{\partial t} = f(c) + D \nabla^2 c
\]

- \( c = [c_1, \ldots, c_n]^T \) concentration of species \( c_1, \ldots, c_n \)
Reaction-Diffusion Equation

\[ \frac{\partial c}{\partial t} = f(c) + D \nabla^2 c \]

- \( c = [c_1, \ldots, c_n]^T \) concentration of species \( c_1, \ldots, c_n \)
- \( f : \mathbb{R}^n \rightarrow \mathbb{R}^n \) vector field of reaction rates
Reaction-Diffusion Equation

\[ \frac{\partial c}{\partial t} = f(c) + D \nabla^2 c \]

- \( c = [c_1, \ldots, c_n]^T \) concentration of species \( c_1, \ldots, c_n \)
- \( f : \mathbb{R}^n \to \mathbb{R}^n \) vector field of reaction rates
- \( D(n \times n) \) diagonal matrix of diffusion coefficients of the species

Neumann boundary conditions: zero-flux of species through the boundary \( \Omega \)
Reaction-Diffusion Equation

\[ \frac{\partial c}{\partial t} = f(c) + D \nabla^2 c \]

- \( c = [c_1, \ldots, c_n]^T \) concentration of species \( c_1, \ldots, c_n \)
- \( f : \mathbb{R}^n \to \mathbb{R}^n \) vector field of reaction rates
- \( D(n \times n) \) diagonal matrix of diffusion coefficients of the species
- \( \nabla^2 c = [\nabla^2 c_1, \ldots, \nabla^2 c_n]^T \) Laplacians of the species
Reaction-Diffusion Equation

\[ \frac{\partial c}{\partial t} = f(c) + D \nabla^2 c \]

- \( c = [c_1, \ldots, c_n]^T \) concentration of species \( c_1, \ldots, c_n \)
- \( f : R^n \rightarrow R^n \) vector field of reaction rates
- \( D(n \times n) \) diagonal matrix of diffusion coefficients of the species
- \( \nabla^2 c = [\nabla^2 c_1, \ldots, \nabla^2 c_n]^T \) Laplacians of the species
- Neumann boundary conditions: zero-flux of species through the boundary \( \Omega \)
Eigenfunctions of the Laplacian Operator

Consider the eigenvalue problem:

$$\nabla^2 f(\xi) = \lambda f(\xi), \quad \xi \in \Omega,$$

subject to Neumann boundary conditions on domain $\Omega$:

$$\nabla f(\xi) \cdot \hat{n}(\xi) = 0, \quad \xi \in \partial \Omega.$$

Assuming bounded spatial domain $\Omega$ with smooth boundary $\partial \Omega$, then there exist eigenvalues:

$$\lambda_k \leq 0, \quad k = 0, 1, 2, \ldots$$

and orthogonal eigenfunctions $f_k(\xi)$:

$$\int_\Omega f_k(\xi)f_j(\xi)d\xi = 0, \quad j \neq k$$
Modal Decomposition of the Linearized RD Equation

\[ \frac{\partial c}{\partial t} = Ac + D\nabla^2 c, \quad c(\xi, t) : \Omega \times [0, \infty) \to \mathbb{R}^n \]

Look for solutions of the form:

\[ c(\xi, t) = \sum_{k=0}^{\infty} \alpha_k(t)f_k(\xi), \]

where \( \alpha_k \in \mathbb{R}^n \) and \( f_k \) are the eigenfunctions of the Laplacian.

Substitution in the PDE gives:

\[ \sum_{k=0}^{\infty} \dot{\alpha}_k f_k = \sum_{k=0}^{\infty} (A + \lambda_k D)\alpha_k f_k \]

and orthogonality of eigenfunctions implies that

\[ \dot{\alpha}_k = (A + \lambda_k D)\alpha_k, \quad k = 0, 1, 2, \ldots. \]

k is the wave number.
Diffusion-Driven Instability

\[ \dot{c} = f(c) \quad c \in \mathbb{R}^n \]  

If \( c = c^* \) is a fixed point for \( \text{(R)} \), then \( c(\xi) \equiv c^* \) is a steady state for \( \text{(RD)} \)

Alan Turing (1952): stability of \( c^* \) in \( \text{(R)} \) does not imply stability of the homogeneous steady state \( c(\xi) \equiv c^* \) in \( \text{(RD)} \)

Necessary conditions for this phenomenon are:

- Two or more reacting species (\( n \geq 2 \))
- Diffusion coefficients are not identical (\( D \neq dI \))

Interpretation from the Modal Decomposition:

\[ A = \left. \frac{\partial f}{\partial c} \right|_{c = c^*} \]

Hurwitz, but \( A + \lambda k D \) unstable for some eigenvalue of the Laplacian
Diffusion-Driven Instability

\[ \dot{c} = f(c) \quad c \in \mathbb{R}^n \quad \text{(R)} \]
\[ \frac{\partial c}{\partial t} = f(c) + D \nabla^2 c \text{ on domain } \Omega \text{ with Neumann BC} \quad \text{(RD)} \]

- Alan Turing (1952): stability of \( c^* \) in (R) does not imply stability of the homogeneous steady state \( c(\xi) \equiv c^* \) in (RD).

Necessary conditions for this phenomenon are:
- Two or more reacting species (\( n \geq 2 \))
- Diffusion coefficients are not identical (\( D \neq d I \))

Interpretation from the Modal Decomposition:
\[ A = \frac{\partial f}{\partial c} \bigg|_{c = c^*} \] is Hurwitz, but \( A + \lambda_k D \) unstable for some eigenvalue of the Laplacian.
Diffusion-Driven Instability

\[ \dot{c} = f(c) \quad c \in \mathbb{R}^n \quad \text{(R)} \]

\[ \frac{\partial c}{\partial t} = f(c) + D \nabla^2 c \text{ on domain } \Omega \text{ with Neumann BC} \quad \text{(RD)} \]

If \( c = c^* \) is a fixed point for (R), then \( c(\xi) \equiv c^* \) is a steady state for (RD)

Alan Turing (1952): stability of \( c^* \) in (R) does not imply stability of the homogeneous steady state \( c(\xi) \equiv c^* \) in (RD)

Necessary conditions for this phenomenon are:

- Two or more reacting species (\( n \geq 2 \))
- Diffusion coefficients are not identical (\( D \neq d_1 \))

Interpretation from the Modal Decomposition:

\[ A = \frac{\partial f}{\partial c} \bigg|_{c = c^*} \quad \text{Hurwitz, but} \]

\[ A + \lambda_k D \text{ unstable for some eigenvalue of the Laplacian} \]
Diffusion-Driven Instability

\[ \dot{c} = f(c) \quad c \in \mathbb{R}^n \quad (R) \]
\[ \frac{\partial c}{\partial t} = f(c) + D \nabla^2 c \text{ on domain } \Omega \text{ with Neumann BC} \quad (RD) \]

- If \( c = c^* \) is a fixed point for \((R)\), then \( c(\xi) \equiv c^* \) is a steady state for \((RD)\)

- **Alan Turing (1952):** *stability of \( c^* \) in \((R)\) does not imply stability of the homogeneous steady state \( c(\xi) \equiv c^* \) in \((RD)\)*
Diffusion-Driven Instability

\[ \dot{c} = f(c) \quad c \in \mathbb{R}^n \quad (R) \]
\[ \frac{\partial c}{\partial t} = f(c) + D \nabla^2 c \text{ on domain } \Omega \text{ with Neumann BC} \quad (RD) \]

If \( c = c^* \) is a fixed point for (R), then \( c(\xi) \equiv c^* \) is a steady state for (RD)

Alan Turing (1952): stability of \( c^* \) in (R) does not imply stability of the homogeneous steady state \( c(\xi) \equiv c^* \) in (RD)

Necessary conditions for this phenomenon are:

- Two or more reacting species \( (n \geq 2) \)
- Diffusion coefficients are not identical \( (D \neq dI) \)
Diffusion-Driven Instability

- \dot{c} = f(c) \quad c \in \mathbb{R}^n \quad (R)
- \frac{\partial c}{\partial t} = f(c) + D \nabla^2 c \text{ on domain } \Omega \text{ with Neumann BC} \quad (RD)
- If \( c = c^* \) is a fixed point for (R), then \( c(\xi) \equiv c^* \) is a steady state for (RD)
- Alan Turing (1952): stability of \( c^* \) in (R) does not imply stability of the homogeneous steady state \( c(\xi) \equiv c^* \) in (RD)
- Necessary conditions for this phenomenon are:
  - Two or more reacting species \((n \geq 2)\)
  - Diffusion coefficients are not identical \((D \neq dl)\)
- Interpretation from the Modal Decomposition: \( A = \frac{\partial f}{\partial c} \big|_{c=c^*} \)
  Hurwitz, but \( A + \lambda_k D \) unstable for some eigenvalue of the Laplacian
Let $\Omega = [0, \pi]$ so that $\lambda_k = -k^2$

We want $A = \begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{bmatrix} = \begin{bmatrix} \beta - 1 & \alpha \\ -\beta & -\alpha \end{bmatrix}$ to be Hurwitz

and $A - \lambda_k D$ to be unstable. Take $k = 1$, then we want $A - D$ unstable ($(a_{11} - D_u)(a_{22} - D_v) - a_{12}a_{21} < 0$)

The above conditions correspond to: $a_{11} = \beta - 1 > 0$ or $a_{22} = -\alpha > 0$ and $D_u \neq D_v$

Condition for diffusion driven instability of Brusselator: If

1. $1 < \beta < \alpha + 1$ (nondim)

then, there exist $D_u, D_v > 0$ such that $A - D$ is unstable.
Figure: $A = 1$, $B = 1$, $k_1 = 2$, $k_2 = 6$, $k_3 = 5$, $k_4 = 2$, $D_u = 0.3$. Top: $D_v = 0.3$. Bottom: $D_v = 1.4$ and $D_v = 3$. 
Figure 3 reports the asymptotic spatial behavior of system (2) for fixed $\alpha$ and $d$ and for different values of parameter $\beta$. The parameter plane $(\beta, d_c)$ shows diffusion-driven instability in the Brusselator.
Figure: Asymptotic spatial behavior of the Brusselator for $\alpha = 7$, $d = 7$ and $\beta$ varying from 3 to 11. The critical value for which the bifurcation curve is crossed vertically is approximately 5.

Note that here $x$ denotes the spatial variable and not a species.
Diffusion-Driven Instability in the Brusselator (5/6)

Figure: Stability and instability of the steady state in the parameter plane $\alpha, \beta$. 

- Unstable steady state
- Limit cycle behavior
- Stable spatial dynamics

- Stable steady state
- Stable spatial dynamics

Turing bifurcation curve
Figure: Spatio-temporal dynamics of the Brusselator. Species $u$ (left) and $v$ (right) for $A = 1$, $B = 1$, $k_1 = 2$, $k_2 = 6$, $k_3 = 5$, $k_4 = 2$, $D_u = 0.3$, $D_v = 2$. $\Omega = [-4\pi, 4\pi]$ with periodic initial conditions $u_0(x) = e^{-x^2}$, $v_0(x) = 2$. 