Turing-Hopf Patterns near onset

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Objectives

Our concern in this presentation:

- pattern formation in reaction diffusion systems near a codimension two Turing-Hopf bifurcation point.
- The travelling wave initiation of time-oscillatory patterns.

Plan

- The normal mode approach in the study of Turing instabilities

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- The Hopf bifurcation revisited

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- The Hopf bifurcation revisited
- Turing-Hopf bifurcation: more than the overlap of TI and HB

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- The normal mode approach in the study of Turing instabilities
- The Hopf bifurcation revisited
- Turing-Hopf bifurcation: more than the overlap of TI and HB
- Way of propagation of Turing-Hopf patterns

Turing instability in reaction diffusion systems

$$
\begin{aligned}
u_t &= D_u\,\Delta u + f\left(u, v; a\right) &\quad (1)\\
v_t &= D_v\,\Delta v + g\left(u, v; a\right)
\end{aligned}
$$

$$
\frac{\partial u}{\partial n} = \frac{\partial v}{\partial n} = 0 \text{ on } \partial\Omega \qquad (2)
$$

u, v - the profiles of reactant concentrations under diffusion,
(u_0, v_0) spatially homogeneous steady solution

Normal modes

Let us consider *normal modes* of the type

$$Z(x, t) = \exp(\sigma t) \ U_k(x) \ R \tag{3}$$

as non-trivial solutions to the linearized equation

$$\frac{\partial Z}{\partial t} = D \ \Delta Z + J_a \ Z \tag{4}$$

where

$$
\begin{aligned}
-\Delta U_k(x) &= \lambda_k \ U_k(x) \\
\partial_n U_k &= 0 \text{ on } \partial\Omega
\end{aligned}
$$

spatial eigenfunctions associated to the *spatial eigenvalues* λ_k ($k \in \mathbb{N}$)

Normal modes

Stability analysis by small disturbances with the form

$$Z(x, t) = \sum_{k=1}^{\infty} \exp(\sigma_k \ t) \ U_k(x) \ R_k \tag{5}$$

- $J_a = \left(j_{ij}^a\right)$ be the jacobian matrix
- $\delta_a = \det(J_a) > 0$, and $\tau_a = \text{trace}(J_a)$
- for each k, σ_k is an *eigenvalue*; R_k corresponding *eigenvector* of $E_k = (J_a - \lambda_k \ D)$

conditions for diffusive instability

- linear **stable** steady state (u_0, v_0) in an **activator-inhibitor** (or positive feedback) **system**

$$\tau_a < 0 \; , \; \delta_a > 0$$

- so,

$$\tau_T < 0$$

$$\tau_T = \text{trace}\,(J_a - \lambda_k \, D) = \tau_a - \lambda_k \,(D_u + D_v) \tag{6}$$

- and, follows the **condition** for instability

$$\delta_T < 0$$

$$\delta_T = \det\,(J_a - \lambda_k \, D) = \delta_a - \lambda_k \,(D_u \, j_{22}^a + D_v \, j_{11}^a) + \lambda_k^2 \, D_u D_v \tag{7}$$

- the boundary

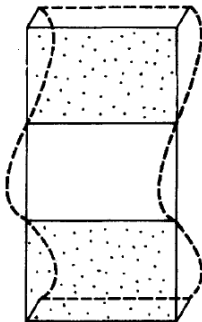$$\delta_T = 0$$

- $d = D_v / D_u$

$$d\, j_{11}^a + j_{22}^a > 0 \qquad (8)$$

so

$$d \neq 1.$$

Remark
Turing patterns might be represented by the set of positiveness of the
dominant unstable spatial eigenfunction.

steady spatially varying profiles in the reactant concentrations

Definition of pattern

Turing showed that dissimilar diffusion coefficients of the participating reactants would destabilize the steady state of the reaction kinetics leading to pattern formation.

- The appearance of *Turing instabilities* about the stable steady state ($\tau_a < 0$) is a consequence of algebraic inequalities between the (**reaction and diffusion**) parameters. These relations are builded from Fourier normal modes:

$$Z\left(x, t\right) = \exp\left(\sigma t\right) \; U_k\left(x\right) \; R$$

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- The ultimate pattern emerges (see Murray's) due to the boundedness of the unstable modes by the nonlinear reaction terms in Eq.1
- without a nonlinear theory, we have only a presumption about the ultimate pattern towards which the destabilized solution converges, which is connected with the dominant unstable mode.

stationary chemical patterns

P.K. Maini, K.J. Painter and H.N.P. Chau, (1997), Spatial Pattern Formation in chemical and biological systems, J.Chem.Soc., Faraday Trans., 93(20), 3601-3610
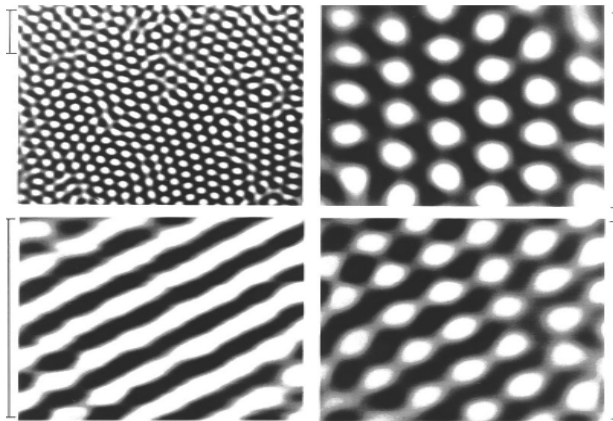

Figure: Stationary patterns in CIMA

patterns in chemical reactions

P.K. Maini, K.J. Painter and H.N.P. Chau, (1997), Spatial Pattern Formation in chemical and biological systems, J.Chem.Soc., Faraday Trans., 93(20), 3601-3610
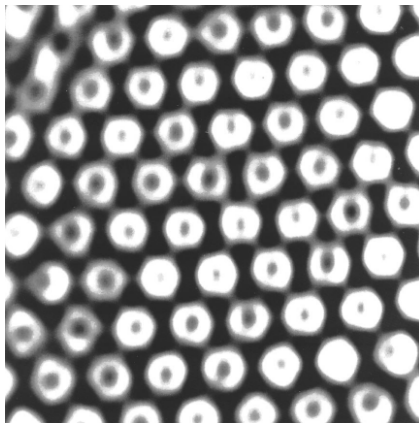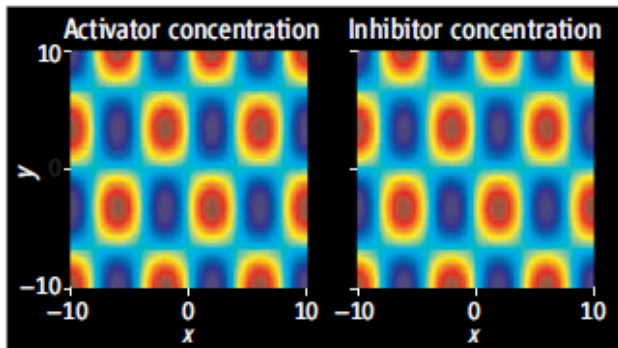

Figure: Black-eye pattern

patterns in morphogenesis

P.K. Maini, R.E. Baker and Cheng-Ming Chuong, (2006), The Turing Model Comes of Molecular Age, Science 314, 1397-1398 (2006); published online 1 December 2006 (10.116/science.1136396)
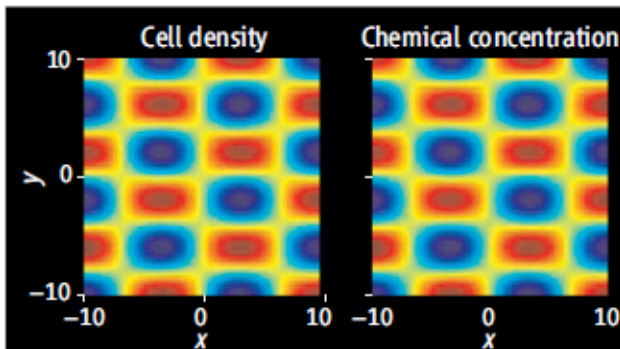
patterns in morphogenesis

P.K. Maini, R.E. Baker and Cheng-Ming Chuong, (2006), The Turing Model Comes of Molecular Age, Science 314, 1397-1398 (2006); published online 1 December 2006 (10.116/science.1136396)

observed and simulated patterns

R.Erban, H.G. Othmer, (2005), From signal transduction to spatial pattern formation in E. Coli: a paradigm for multiscale modeling in Biology, Multiscale Model Simul., 3(2), 362-394
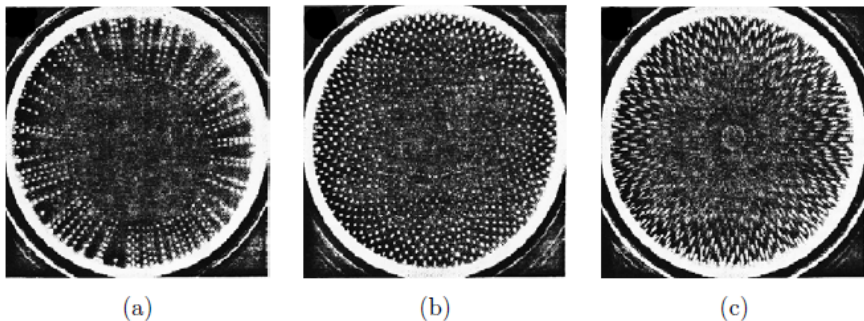

(a)　　　　　　(b)　　　　　　(c)

Figure: Spatial patterns arising in E.Coli

The Hopf bifurcation

$$\begin{cases} \dot{u} = f(u, v; a) \\ \dot{v} = g(u, v; a) \end{cases} \tag{9}$$

-

$$P_a = (u_0(a); v_0(a)) \tag{10}$$

- $J_a = \left(j_{ij}^a\right)$ be the jacobian matrix of Eq.9

-

$$\tau_a^2 - 4\delta_a < 0 \tag{11}$$

- $\delta_a = \det(J_a) > 0$, and $\tau_a = \text{trace}(J_a)$.

reduction to a second order oscillator

[M.R. Ricard, On degenerate planar Hopf bifurcations, J. Phys. A: Math. Theor. 44 (2011) 065202 (15pp)
weakly nonlinear oscillator in *normal form*:

$$\ddot{\varsigma} - \tau_a \dot{\varsigma} + \delta_a \, \varsigma = \, \varepsilon \, G\left(\varsigma, \dot{\varsigma}; \varepsilon\right) \, . \qquad (12)$$

ε- small parameter to be determined later

subsequent reduction via averaging

(Krylov-Bogoliubov technique)

$$\dot{r} = \frac{r}{2} \left\{ \tau_a - p\left(r; \varepsilon\right) \right\} \tag{13}$$

$$\dot{\theta} = q\left(r; \varepsilon\right) \tag{14}$$

considering $\phi = \omega_a t + \theta$.

$$p\left(r; \varepsilon\right) = \frac{\varepsilon}{\pi \omega_a r} \int\limits_0^{2\pi} \sin\phi \; G\left(r\cos\phi, -r\omega_a \sin\phi; \varepsilon\right) \; d\phi \tag{15}$$

$$q\left(r; \varepsilon\right) = -\frac{\varepsilon}{2\pi \omega_a r} \int\limits_0^{2\pi} \cos\phi \; G\left(r\cos\phi, -r\omega_a \sin\phi; \varepsilon\right) \; d\phi \; . \tag{16}$$

properties of the discriminant

- $p(r;\varepsilon)/r^2$ and $q(r;\varepsilon)/r^2$ have a finite limit as $r \to 0$.
- the Taylor expansions of $p(r;\varepsilon)$ and $q(r;\varepsilon)$ must not contain odd powers of r, and

$$p(r;\varepsilon) = p_3 \; \varepsilon^2 r^2 + p_5 \; \varepsilon^4 r^4 + \cdots \qquad (17)$$

in which $p_s = p_s(\tau_a)$.

- The classical perturbation theory gives a uniform $O(\varepsilon)$-estimation for the difference between the corresponding solutions to the given system and to the average systems, but only on the time scale $1/\varepsilon$. In our scenario, we have that the amplitude of any solution to the given system starting in the region of attraction of the limit cycle can be uniformly expanded by the average solution uniformly for $t > 0$.

negligible coefficients

Definition

Let p_{2s+1} be a coefficient in the formal development Eq.17, which is derived from the formal ∞-jet of F. It shall be called *negligible* if satisfying

$$|p_{2s+1}| \leq K_s |\tau_a| \tag{18}$$

for a certain constant $K_s > 0$ as $\tau_a \rightarrow 0$.

Definition

The function $p(r; \varepsilon)$ in Eq.17 is said to be *negligible* if for all $s \in \mathbb{N}$ the coefficient p_{2s+1} is negligible.

Theorem on non-negligible discriminant

Theorem

If the function $p(r; \varepsilon)$ is non-negligible, there must exist a positive integer N and a positive real value $r_0 = r_0(\tau_a)$ such that $p(r, \varepsilon)$ has the non-trivial Taylor expansion:

$$p(r; \varepsilon) = \chi \, \varepsilon^{2N} \, r_0^{-2N} \, r^{2N} + O\left(\varepsilon^{2N+2} \, r^{2N+2}\right) \tag{19}$$

where $\chi = +1$ or -1. In addition, the behavior of the factor r_0^{-2N} as $\tau_a \to 0$ obeys the following alternative: **either**

$$\lim_{\tau_a \to 0} r_0^{-2N} = r_*^{-2N} > 0 \tag{20}$$

or, *for a given γ, $0 < \gamma < 1$,*

$$r_0^{-2N} = O_S\left(|\tau_a|^{\gamma}\right) \text{ as } \tau_a \to 0 . \tag{21}$$

Classifying HB

Definition

We shall say that the HB is *first type degenerate* if p is negligible. Let N be given as in Eq.19. The bifurcation shall be called *second type degenerate*, if there exists a number γ, $0 < \gamma < 1$, such that

$$r_0^{-2N} = O_S\left(|\tau_a|^\gamma\right) \text{ as } \tau_a \to 0 .$$

holds. The HB shall be called *non-degenerate*, provided

$$\lim_{\tau_a \to 0} r_0^{-2N} = r_*^{-2N} > 0 .$$

Amplitude of the limit cycle at non-degenerate HB

Let $p(r; \varepsilon)$ be non-negligible and also, that r_0 in Eq.19 has the property in Eq.20 then, there is a positive root ρ to the *discriminant equation*

$$p(r; \varepsilon) - \tau_a = 0 . \tag{22}$$

Furthermore, up to the leading term, the root to Eq.22 has the form

$$\rho = \left(\frac{|\tau_a|}{\varepsilon^{2N}} \right)^{1/2N} (r_* + O(|\tau_a|)) + O(\varepsilon^2) . \tag{23}$$

Taking

$$\varepsilon^{2N} = |\tau_a| . \tag{24}$$

from Eq.24 it follows that Eq.23 can now be written as

$$\rho = r_* + O\left(|\tau_a|^{1/N} \right) . \tag{25}$$

If Eq.21 takes place instead of Eq.20, we may proceed similarly as we do to obtain Eq.24, to get

$$\varepsilon^{2N} = |\tau_a|^{1-\gamma} \ . \tag{26}$$

Moreover, if $r_0^{-2N} = r_L |\tau_a|^{\gamma} + o\left(|\tau_a|^{\gamma}\right)$ as $\tau_a \to 0$ for a certain positive number r_L, then Eq.23 can be rewritten as

$$\rho = r_L + \ O\left(|\tau_a|^{(1-\gamma)/N}\right) \ . \tag{27}$$

The Hopf bifurcation Theorem (N-D)

Theorem (Hopf bifurcation)

*Let us assume that Eq.11 holds. Then, one of the following possibilities arises: (i) **(Non-degeneracy at HB)** If Eq.22 has a root Eq.25 with the property Eq.20 for positive (respectively, negative) values of the bifurcation parameter τ_a but sufficiently close to zero then, a single limit cycle to the former system emerges. Furthermore, the limit cycle is orbitally asymptotically stable (respect., unstable) if and only if the bifurcation is supercritical (respect., subcritical). The amplitude of the emerging cycle is $r = O_S\left(|\tau_a|^{1/2N}\right)$, while the frequency is $\varpi = \omega_a + O\left(|\tau_a|^{1/N}\right)$ as $\tau_a \to 0$.*

Theorem (Hopf bifurcation)

(ii) **(First type degenerate HB)** *If p negligible, then none of the cycles surrounding the singular point bifurcate from this point. (iii)* **(Second type degenerate HB)** *If Eq.22 has a root with the property Eq.21 for sufficiently close to zero values of the parameter τ_a, then the emergence can be assured of at least one limit cycle to the former system, the amplitude of which has order $r = O_S\left(|\tau_a|^{(1-\gamma)/2N}\right)$ while the frequency is $\varpi = \omega_a + O\left(|\tau_a|^{(1-\gamma)/N}\right)$ as $\tau_a \rightarrow 0$.*

classification

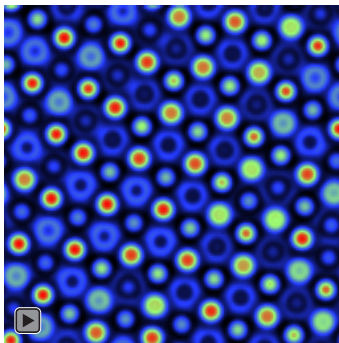the number N corresponds to the considered $(2N+1)$-jet, provided conditions for HB:

behavior at $\tau_a = 0$	standard classification	classification on the basis of C	C
weak focus	non-degenerate	**non-degenerate** $(N = 1)$	**1**
center	degenerate	**non-degenerate** $(N > 1)$	**1**
		first type degenerate	**0**
		second type degenerate	**>1**

oscillatory patterns (hexagonal chemical)

http://hopf.chem.brandeis.edu/yanglingfa/pattern/oscTu/index.html
regular tesselation pattern
hexagonal cells

http://hopf.chem.brandeis.edu/yanglingfa/pattern/oscTu/index.html
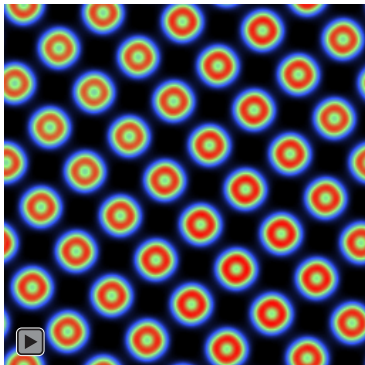regular tesselation pattern
hexagonal cells

Turing-Hopf bifurcation

- use to be considered as the overlap of the corresponding regions for TI and for HB in the parameter space. So, the problem can be considered near a codimension-two bifurcation point.
- we considered the problem starting from the diffusive instabilities generated by the limit cycle emerging at HB

M.R. Ricard, S. Mischler, Turing instabilities at Hopf bifurcation, J. Nonlinear Sci., Vol.19, Issue 5 (2009), 467-496

Turing-Hopf bifurcation

We remark the following differences,

- in Turing-Hopf instabilities, the limit cycle is always unstable. This instability may be weak or strong.
- In the first case slight oscillations superpose over a dominant steady inhomogeneous pattern. In the second, the unstable modes show an intermittent switching between "complementary" spatial patterns, producing the effect known as twinkling patterns.
- Turing-Hopf instabilities may appear even though the diffusion coefficients are equal, while diffusive instabilities may appear provided the diffusion coefficients are different enough.

Definition of oscillatory pattern

Diffusive instabilities generated by the limit cycle are often called **Turing-Hopf** (TH) **instabilities** or **bifurcations**, which eventually result in **time-oscillatory patterns**.

The behavior of such TH instabilities is considered "chaotic" by many authors. The alternative: the system is directed forward **steady patterns**, the system oscillates near the steady pattern, the system shows a **twinkling pattern**.

Now, we may have

$$\tau_T = \tau_a - \lambda_k \left(D_u + D_v \right) > 0 \tag{28}$$

- The sign of τ_T becomes relevant in the study of these instabilitites, because the supercritical HB happens provided $\tau_a > 0$.
- Consequently, if $\tau_T > 0$ then the sign of δ_T is irrelevant, so we would expect the appearance of TH instabilities even if $D_u = D_v$.

For instance, real or even complex roots with positive real part always appear if $\tau_T > 0$, and it would be interesting to study the way in which the oscillations due to the limit cycle are transferred to the resulting diffusive instabilities.

Turing-Hopf instabilities

Let the spatially homogeneous periodic solution

$$\Theta\left(t\right) = \left(\overline{u}\left(t\right), \overline{v}\left(t\right)\right) \tag{29}$$

to Eqs.1 and 2.

Denoting the corresponding perturbations by capital letters we get,

$$
\begin{aligned}
u\left(t,x\right) &= \overline{u}\left(t\right) + U\left(t,x\right) \\
v\left(t,x\right) &= \overline{v}\left(t\right) + V\left(t,x\right)
\end{aligned}
$$

The linear stability problem leads to the system with periodic coefficients for the perturbations

$$\frac{\partial Z}{\partial t} = D \; \Delta Z + J_{\Theta}\left(t\right) \; Z \tag{30}$$

where $Z\left(x,t\right) = \left(U\left(t,x\right), V\left(t,x\right)\right)^{T}$.

Substituting the development of Θ we get

$$J_{\Theta}(t) = J_a + \tau_a^{\frac{1}{2N}} \; J_{1/2N}(t) + O\left(\tau_a^{\frac{1}{N}}\right)$$

where

$$J_{1/2N}(t) = (\kappa_{ij}) \qquad (31)$$

Let us assume that the solutions to Eq.30

$$Z = Z_0(t, x) + \tau_a^{\frac{1}{2N}} \; Z_1(t, x) + O\left(\tau_a^{\frac{1}{N}}\right) \; . \qquad (32)$$

Proposition. Let us assume the existence of a supercritical non-degenerate HB, and let $0 < \tau_a \ll 1$. Then, the *extended normal modes*:

$$Z\left(x, t\right) = \exp\left(\sigma t\right) U_k\left(x\right) \left\{ I + \tau_a^{\frac{1}{2N}} \ \overline{W_k}\left(t\right) + O\left(\tau_a^{\frac{1}{N}}\right) \right\} \ R \qquad (33)$$

are asymptotic expansions of solutions to Eq.30, or more exactly, they are normal modes disturbances corresponding to the spatial eigenvalue λ_k in the stability analysis of $\Theta\left(t\right)$ as a spatially homogeneous solution to Eqs.1 and 2.

The expansion between brackets in Eq.33 is **uniform** up to the leading term or can be easily transformed into a uniform one.

Weak or strong Turing-Hopf instabilities

Definition

Let us assume that the reaction part in Eq.1 admits a supercritical HB and let $0 < \tau_a \ll 1$. Then, TH instabilities generated by the limit cycle arise if $\Re e\,(\sigma) > 0$. We shall call this **weak TH instability** if there is at least one real root $\sigma > 0$. If the roots are complex conjugated $\sigma = \sigma_r \pm i\,\sigma_i$ with $\sigma_r > 0$, then we shall call it **strong TH instability.**

Turing-Hopf instabilities

Theorem

Let λ_k be a given positive spatial eigenvalue. Assume further that the reaction system has a limit cycle via an HB. If $\tau_T \leq 0$, $\delta_T < 0$ then, TH instabilities appear and they are weak. If $\tau_T > 0$ instabilities appear and they are weak provided $\tau_T^2 - 4\delta_T \geq 0$, while they are strong if $\tau_T^2 - 4\delta_T < 0$. **If the diffusion coefficients are equal ($d = 1$), or close enough each other, only strong TH instabilities could appear.**

Turing-Hopf instabilities

So, if instabilities are **weak** ($\sigma \in \mathbb{R}_+$)

$$Z(x, t) = \exp(\sigma t) \left\{ I + \tau_a^{\frac{1}{2N}} \overline{W_k}(t) + O\left(\tau_a^{\frac{1}{N}}\right) \right\} U_k(x) \; R$$

If the TH instabilities are **strong** we have

$$Z(x, t) = \exp(\sigma_r t) \left\{ \cos(\sigma_i t) \; U_k(x) + O\left(\tau_a^{\frac{1}{2N}}\right) \right\} \; R \; . \qquad (34)$$

For strong TH instabilities we would depict the oscillatory pattern by the set of positiveness of

$$\cos(\sigma_i t) \; U_k(x) \qquad (35)$$

oscillating with the frequency $\sigma_i = \sqrt{\delta_T - \tau_T^2/4}$, which is different from the frequency of the limit cycle.

While strong instabilities are featured by an intermittent switching between the inhomogeneous pattern, represented by the set of positiveness of the spatial eigenfunction, with its "complementary pattern", represented by the set of negativeness of the eigenfunction. The frequency of these oscillations are different from the frequency of the cycle.

Scaling

We recall that in a practical problem a length scale is selected (for instance, $S = (\text{diffusivity} \times \text{time scale})^{1/2}$) and the spatial eigenvalues depend on the nondimensional size of it. It can be noted that the relation $\lambda_k L^2 = \widehat{\lambda}_k \widehat{L}^2$ holds if λ_k and $\widehat{\lambda}_k$ are the spatial eigenvalues for two similar domains with nondimensional characteristic lengths L and $\widehat{L}$ respectively.

conditions for twinkling patterns

If we have an appropriate nondimensional characteristic length in Ω, the lowest positive spatial eigenvalue λ_1 would be so small that $\tau_T > 0$. If in addition $\tau_T^2 - 4\delta_T < 0$ holds, then TH instabilities associated with this eigenvalue induce a "twinkling" pattern.

presumptions from the linear theory

TH spatially inhomogeneous patterns based on the extended modes near a codimension-2 TH point (i.e., laying at the intersection of the manifolds $\tau_a = 0$, and $\delta_T = 0$), and recalling that $\tau_a > 0$.

Case			THI type	expected
				patterns
1	$\tau_T \leq 0$,	$\delta_T < 0$,	weak	SO
2	$\tau_T > 0$,	$\delta_T \leq 0$,	weak	SO
3	$\tau_T > 0$,	$0 < \delta_T < \tau_T^2 /4$,	weak	steady or SO
4	$\tau_T > 0$,	$\delta_T = \tau_T^2 /4$,	weak	SO
5	$\tau_T > 0$,	$\delta_T > \tau_T^2 /4$,	strong	twinkling

(SO- slightly oscillatory)

and phase

$$r_t = \frac{r}{2} \{\tau_a - p(r; \tau_a)\} + \frac{1}{2\omega_a} \{(D_u - D_v) \, j_{11}^a (2\nabla r \cdot \nabla \theta + r\Delta\theta) \quad (36)$$
$$+ \omega_a D_v \left(\Delta r - r \|\nabla\theta\|^2\right)\} \ ,$$

$$\theta_t = q(r; \tau_a) + \frac{1}{2\omega_a r} \left\{(D_u - D_v) \, j_{11}^a \left(-\Delta r + r \|\nabla\theta\|^2\right) \quad (37)\right.$$
$$\left. + \omega_a D_v (2\nabla r \cdot \nabla \theta + r\Delta\theta)\right\} \ .$$

$D_u = D_v$
takes the λ-ω normal form:

$$
\begin{aligned}
r_t &= \frac{r}{2}\left\{\tau_a - p\left(r; \tau_a\right)\right\} + \frac{\widehat{D}}{2}\left(\Delta r - r\left\|\nabla\theta\right\|^2\right) \qquad (38)\\
\theta_t &= q\left(r; \tau_a\right) + \frac{\widehat{D}}{2}\; r^{-2}\;\nabla \cdot \left(r^2\;\nabla\theta\right)\;.
\end{aligned}
$$

equal diffusivities

- $|\theta_x|$ is negligible with respect to the $O(\tau_a)$ terms, because $|\theta_x| = O(\tau_a/c)$ as $\tau_a \to 0$,
- $1/c$ is another small parameter to be considered.

Then, up to main terms, we arrive to the following uncoupled system

$$
\begin{aligned}
r_t &= \frac{\tau_a}{2} r \left\{ 1 - r_0^{-2N} \, r^{2N} \right\} + \frac{\widehat{D}}{2} \, \Delta r \quad (39) \\
\theta_t &= q(r; \tau_a) \, , \quad (40)
\end{aligned}
$$

Conclusions

Many different oscillatory patterns may appear in presence of Turing-Hopf instability. If D_u and D_v are close, we may expect strongly time oscillatory patterns. The way of propagation of such bifurcations is given by a travelling wave
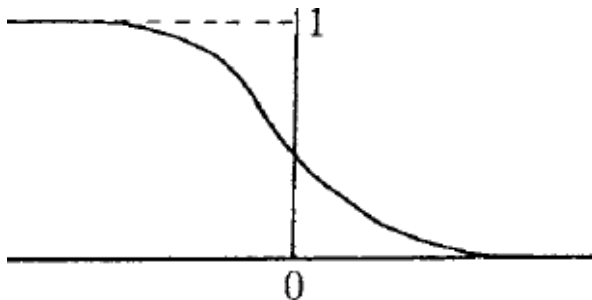
MANY THANKS!

📄 J.D. Murray, *Mathematical Biology II: Spatial Models and Biomedical applications*, Third Edition, Interdisciplinary Applied Mathematics Vol.18, Springer-Verlag, NewYork (2003)

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