Lecture 3: Emergence of Order from Disorder: Turing Patterns

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1. Emergence of order from disorder

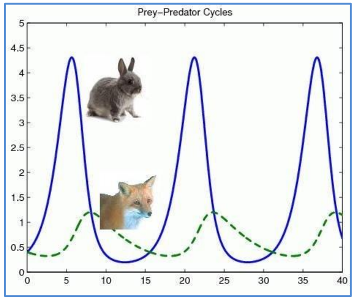
■ Nonlinear dynamical systems can shape complex spatiotemporal structures.

▫ Their sensitivity to initial conditions make possible the exponential **growth of small fluctuations**, switching from a stable to an unstable regime.

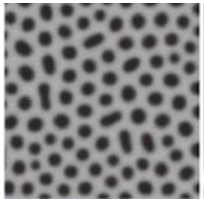
▫ Limit cycles, attractors, … maintain the instability along time.

■ Generally, one can consider the following scenarios:

A) Stable configuration ➡ Oscillatory behavior [classic predator-prey].



B) Stable configuration ➡ Emergence of spatial patterns [Turing instability].

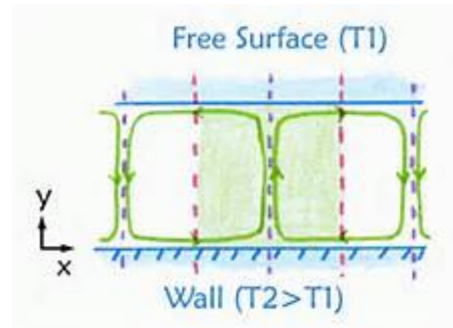


C) Stable configuration ➡ Spatiotemporal, evolving patterns [traveling waves].

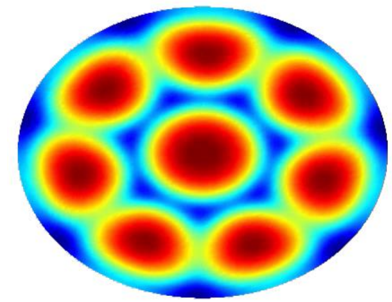
2. Patterns in Nature

■ Convection, chemical reactions,… may generate regular patterns. They have challenged or understanding of Nature for millennia!

Convection on a free surface
(silicone oil + aluminum powder at 300 ºC)
Can be carried out – carefully-- at home



numerical simulation

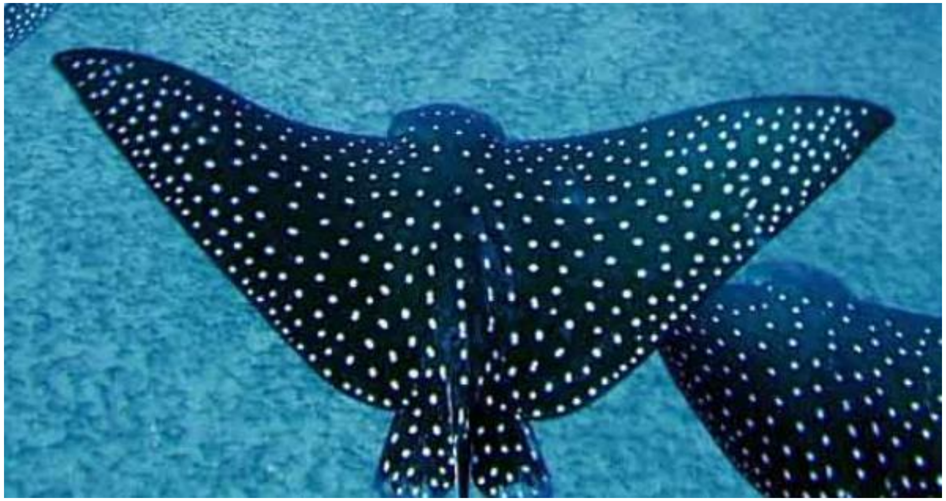


Petrified convection (hexagons) in a volcano

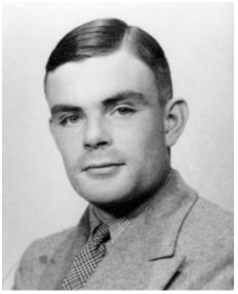
2. Patterns in Nature

- All kind of animals show patterning in their shells / wings / skin:



3. Alan Turing's brightest idea



■ Alan Turing showed in 1952 that a system that **is stable without diffusion** can become **unstable with diffusion** (and generate patterns).

Challenges intuition! Diffusion has been classically seen as stabilizing force. Watch out: **nonlinear systems challenge intuition**!

■ In 1980 the first experimental (laboratory) evidence for Turing patterns was observed. It is knows as **Belousov-Zhabotinsky reaction**.

$$\begin{cases} \dfrac{dX}{dt} = k_1 AY - k_2 XY - 2k_4 X^2 \\[2ex] \dfrac{dY}{dt} = -k_1 AY - k_2 XY + \dfrac{1}{2} k_c f BZ \\[2ex] \dfrac{dZ}{dt} = 2k_3 AX - k_c BZ \end{cases}$$

(+ diffusion over space)

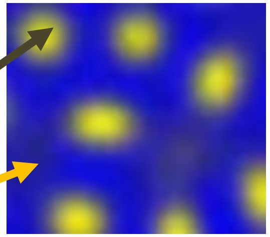
(Each specie, a color spot in the experiment)

■ From 1990 onwards, several new lab-made patterns have been achieved!

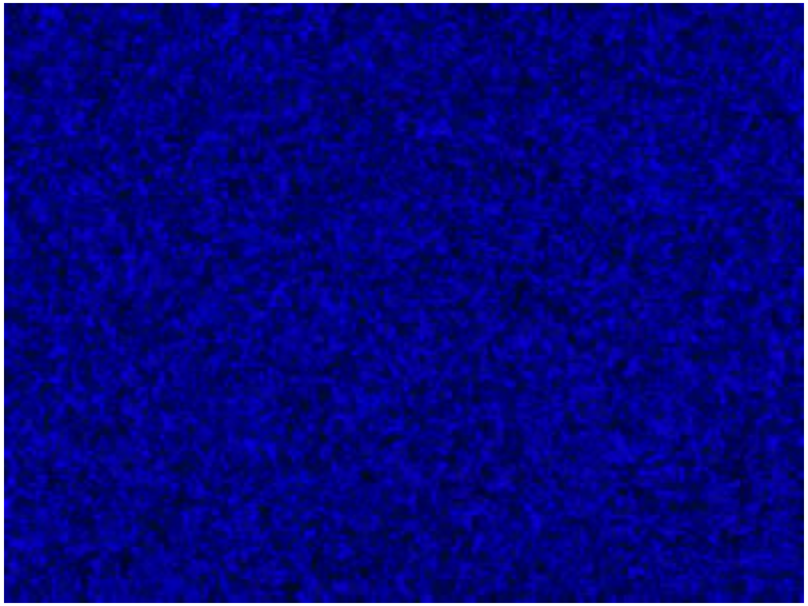
3. Alan Turing's brightest idea

■ Several systems have been explored numerically and analytically, but there are very few experiments.

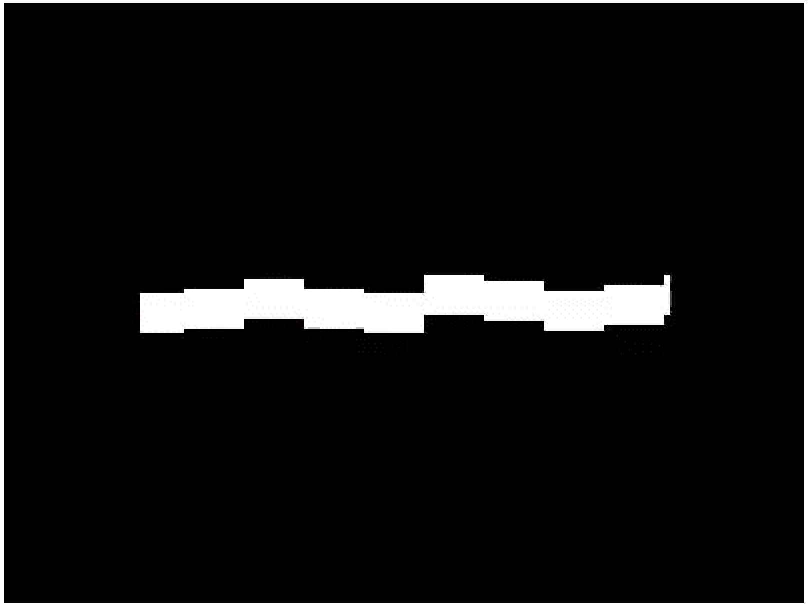
■ Small fluctuations in the environment suffice to amplify the initial concentrations of species {u,v} and trigger a pattern.



Typical Turing pattern: periodic spots.



FitzHugh-Nagumo based system.



4. Analyzing the generation of patterns in a dynamical system

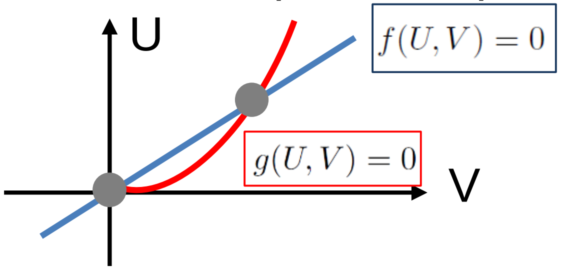
■ Conceptual development:

A) Get the equations.

$$\begin{cases} \dfrac{\partial U}{\partial t} = f(U,V) + D_U \dfrac{\partial^2 U}{\partial x^2} \\ \dfrac{\partial V}{\partial t} = g(U,V) + D_V \dfrac{\partial^2 V}{\partial x^2}. \end{cases}$$

B) Exclude diffusion, analyze nullclines and equilibrium points.

$$\begin{cases} \dfrac{\partial U}{\partial t} = f(U,V) = 0 \\ \dfrac{\partial V}{\partial t} = g(U,V) = 0. \end{cases}$$



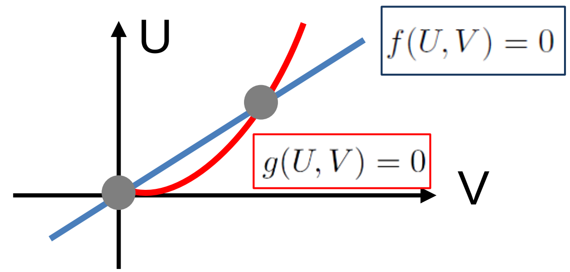
C) Analyze stability of the system. Stable? **Turing condition I**.
Unstable? Other features.

D) Include diffusion. Stable? No pattern.
Unstable? **Turing condition II.** Pattern generated!

5. Stability or instability without diffusion

- Mathematical conditions for stability of the system without **diffusion**:

$$\begin{cases} \frac{\partial U}{\partial t} = f(U,V) = 0 \\ \frac{\partial V}{\partial t} = g(U,V) = 0. \end{cases}$$



  - Consider a linear stability analysis, and compute the linearized matrix:

$$A = \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix} = \begin{pmatrix} \frac{\partial f}{\partial U} & \frac{\partial f}{\partial V} \\ \frac{\partial g}{\partial U} & \frac{\partial g}{\partial V} \end{pmatrix} \equiv \begin{pmatrix} f_U & f_V \\ g_U & g_V \end{pmatrix} \Bigg|_{(U_0,\, V_0)}$$

  - For stability of the system at (U_0, V_0), matrix *A* should obey:

$$\boxed{\begin{cases} \mathrm{tr}(A) = f_U + g_V < 0 \\ \det(A) = f_U \cdot g_V - f_V \cdot g_U > 0. \end{cases}}$$

- Additionally, quantify the behavior far from equilibrium by solving:

$$\det(A - \lambda \cdot I) = 0.$$

eigenvalues

Identity matrix

$$\lambda = \lambda_R + i\lambda_I \longrightarrow \begin{cases} \lambda_R > 0 & \text{unstable} \\ \lambda_R < 0 & \text{stable} \\ \lambda_I = 0 & \text{non-oscillatory} \\ \lambda_I \neq 0 & \text{oscillatory} \end{cases}$$

5. Stability or instability without diffusion

■ <u>Example 1</u>: Lotka-Volterra (predator-prey) model

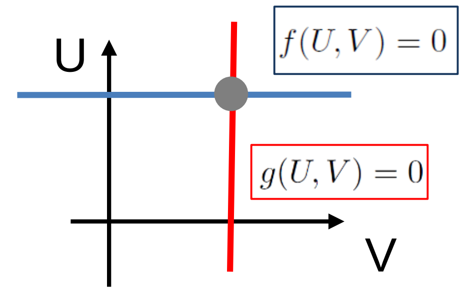
prey
predator

$$\begin{cases} \dfrac{\partial U}{\partial t} = aU - dUV \\ \dfrac{\partial V}{\partial t} = -cV + kdUV. \end{cases}$$

parameters

nullclines

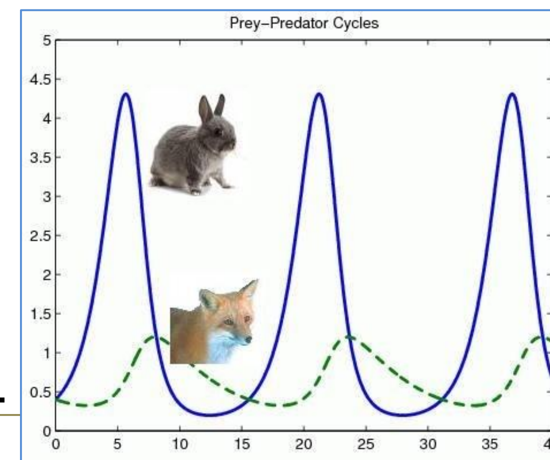
$$\begin{cases} V = \dfrac{a}{d} \quad \forall\, U \\ U = \dfrac{c}{k \cdot d} \quad \forall\, V \end{cases}$$



▫ Matrix A leads to:

$$(U_0, V_0) = \left(\frac{c}{k \cdot d}, \frac{a}{d}\right)$$

$$\begin{cases} A = \begin{pmatrix} a - dV_0 & -dU_0 \\ kdV_0 & -c + kdU_0 \end{pmatrix} = \begin{pmatrix} 0 & -c/k \\ ka & 0 \end{pmatrix} \\ \mathrm{tr}(A) = f_U + g_V = 0 \quad < 0\text{? No} \\ \det(A) = f_U \cdot g_V - f_V \cdot g_U = ca. \quad > 0\text{? Yes} \end{cases}$$



Both conditions are required ⟹ Unstable w/o diffusion.

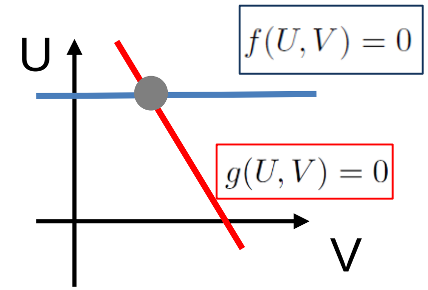
$$\det(A - \lambda \cdot I) = \begin{pmatrix} -\lambda & -c/k \\ ka & -\lambda \end{pmatrix} = \lambda^2 + ca \rightarrow \lambda = \pm i\sqrt{ca}.$$

OSCILLATORY!

5. Stability or instability without diffusion

■ <u>Example 2</u>: Modified Lotka-Volterra with logistic growth:

$$\begin{cases} \dfrac{\partial U}{\partial t} = aU\left(1-\dfrac{U}{b}\right) - dUV \\ \dfrac{\partial V}{\partial t} = -cV + kdUV. \end{cases} \xrightarrow{\text{nullclines}} \begin{cases} U = b\left(1-\dfrac{d}{a}\right)V \\ U = \dfrac{c}{k \cdot d} \quad \forall\, V \end{cases}$$



▫ Logistic growth adds realism to the model, so that the prey do not grow exponential in the absence of predators.

▫ The model leads to:

$$\begin{cases} \mathrm{tr}(A) = -\dfrac{ca}{bkd} < 0 \\ \det(A) = 0 + c\left(1-\dfrac{c}{bkd}\right) > 0. \end{cases}$$

stable without diffusion!

▫ Linear stability analysis shows that depending on parameters the stable point can lead to oscillations:

$$\boxed{\lambda^2 + aA\lambda + ca\,(1-A) = 0\;;\; A = \frac{c}{bkd}.}$$

5. Stability or instability **with diffusion**.

- For the system that verifies…

$$\begin{cases} \dfrac{\partial U}{\partial t} = f(U,V) + D_U \dfrac{\partial^2 U}{\partial x^2} \\ \dfrac{\partial V}{\partial t} = g(U,V) + D_V \dfrac{\partial^2 V}{\partial x^2}. \end{cases}$$

$$\boxed{\begin{cases} \mathrm{tr}(A) = f_U + g_V < 0 \\ \det(A) = f_U \cdot g_V - f_V \cdot g_U > 0. \end{cases}}$$

... then a Turing pattern will emerge if:

$$\boxed{\begin{cases} D_U \cdot g_V + D_V \cdot f_U > 0 \\ D_U \cdot g_V + D_V \cdot f_U > 2\sqrt{D_U \cdot D_V} \cdot \sqrt{f_U \cdot g_V - f_V \cdot g_U}. \end{cases}}$$

▫ These conditions are sufficient to generate a pattern, but the structure of the pattern will depend on the model parameters.

Note: these conditions are derived by analyzing a solution for a spatial wave of the form:

$$\mathrm{R}\ (\mathbf{r}, t) = \underset{\text{steady state}}{\underset{\uparrow}{\mathbf{u}^*}} + \mathbf{e} \sum_{j=1}^{N} \left(Z_j e^{i\mathbf{k}_j \cdot \mathbf{r}} + \mathrm{c.c.} \right)$$

and on the equation:
(with proper boundary conditions)

$$\frac{\partial \mathrm{R}}{\partial t} = \mathrm{AR} + \mathrm{D}\nabla^2 \mathrm{R}, \qquad \mathrm{D} = \begin{pmatrix} 1 & 0 \\ 0 & d \end{pmatrix}$$

Not easy at all!

5. Stability or instability **with diffusion**.

■ Example 3: It is not easy to find simple models that verify these conditions.

▫ For the Lotka-Volterra with logistic growth, already the first one fails!

$$D_U \cdot g_V + D_V \cdot f_U = D_U \cdot 0 + D_V \left(-\frac{ca}{bkd}\right) < 0.$$

Hence, this model can exhibit instabilities and oscillations, but not Turing patterns!

■ Given the difficulty, it took years to develop experiments that exhibited Turing patterns, but scientists quickly guessed that Turing mechanisms could naturally emerge in biological systems. Their **intrinsic stochasticity** and quick switching of equations' parameters could provide the environment for pattern generation.

↳ Gierer-Meinhardt model in 1972 (foot-head polarity in metazoans)

5. Stability or instability **with diffusion**.

■ <u>Example 4</u>: Gierer-Meihardt model for animal development.

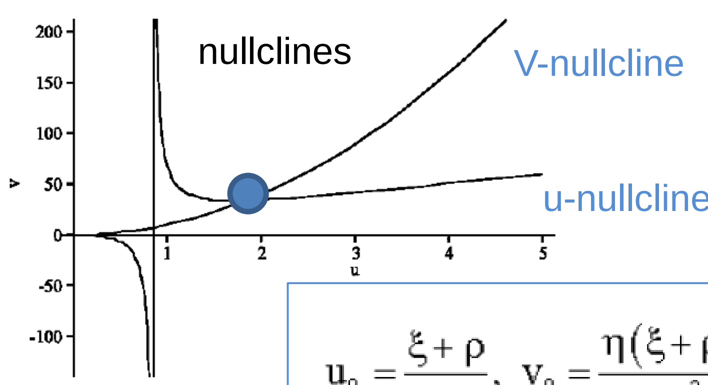
Animals at the embryonic stage use signaling molecules to direct development. A crucial aspect to comprehend development is deriving a model that leads to stable patterns (spinal cord, fingers, foot-head polarity…)

Biological context: Lecture 8

$$\begin{cases} \dfrac{\partial u}{\partial t} = \dfrac{k_3 u^2}{v} - k_2 u + k_1 + D_u \nabla^2 u & \text{(activator)} \\[2ex] \dfrac{\partial v}{\partial t} = k_3 u^2 - k_4 v + + D_v \nabla^2 v & \text{(inhibitor)} \end{cases}$$

▫ Equations can be made more compact by writing dimensionless versions, and in turn considering the ratio of diffusion coefficients rather than their value.

$$\begin{cases} \dfrac{\partial u}{\partial \tau} = \eta \dfrac{u^2}{v} - \zeta u + \rho + \nabla^2 u, \\[2ex] \dfrac{\partial v}{\partial \tau} = \eta u^2 - \xi v + d \nabla^2 v, \end{cases} \qquad d = \frac{D_v}{D_u}.$$



$$u_0 = \frac{\xi + \rho}{\zeta}, \quad v_0 = \frac{\eta (\xi + \rho)^2}{\xi \zeta^2}$$

5. Stability or instability **with diffusion**.

- The analysis **without diffusion** provides:

$$A = \begin{pmatrix} \dfrac{\zeta(\xi-\rho)}{(\xi+\rho)} & -\dfrac{\xi^2\zeta^2}{(\xi+\rho)^2} \\ \dfrac{2\eta(\xi+\rho)}{\zeta} & -\xi \end{pmatrix}. \Rightarrow$$

tr(A)<0 and det(A)>0 satisfied if:

$$\left\{ \xi\left(\frac{\xi+\rho}{\xi-\rho}\right) > \zeta, \qquad \zeta > 0. \right.$$

- In the **presence of diffusion**, the conditions for a Turing pattern can be written as:

$$\begin{cases} da_{11} + a_{22} > 0 \\ \dfrac{(da_{11} + a_{22})^2}{4d} > \text{det(A)} \end{cases}$$

- These conditions are satisfied for:

$$\begin{cases} \xi\left(\dfrac{\xi+\rho}{\xi-\rho}\right) < d\zeta, \\ d >> \dfrac{\xi(\xi+\rho)(3\xi+\rho) + 2\sqrt{2}\xi^{\frac{3}{2}}(\xi+\rho)^{\frac{3}{2}}}{\zeta(\xi-\rho)^2}. \end{cases}$$

5. Stability or instability **with diffusion**.

- The analysis **without diffusion** provides:

$$A = \begin{pmatrix} \frac{\zeta(\xi-\rho)}{(\xi+\rho)} & -\frac{\xi^2\zeta^2}{(\xi+\rho)^2} \\ \frac{2\eta(\xi+\rho)}{\zeta} & -\xi \end{pmatrix}.$$

$\Rightarrow$ tr(A)<0 and det(A)>0 satisfied if:

$$\xi\left(\frac{\xi+\rho}{\xi-\rho}\right) > \zeta, \qquad \zeta > 0.$$

(1)

- In the **presence of diffusion**, the conditions for a Turing pattern can be written as:

$$\begin{cases} da_{11} + a_{22} > 0 \\ \frac{(da_{11} + a_{22})^2}{4d} > \det(A) \end{cases}$$

- These conditions are satisfied for:

$$\xi\left(\frac{\xi+\rho}{\xi-\rho}\right) < d\zeta, \quad \textbf{(2)}$$

$$d \gg \frac{\xi(\xi+\rho)(3\xi+\rho) + 2\sqrt{2}\xi^{\frac{3}{2}}(\xi+\rho)^{\frac{3}{2}}}{\zeta(\xi-\rho)^2}. \quad \textbf{(3)}$$

In order for (1) and (2) to be satisfied, *d* has to be very large, i.e. $D_v \gg D_u$.

Inhibitor v: fast diffusion (long range)
Activator u: slow diffusion (short range)

5. Stability or instability **with diffusion**.

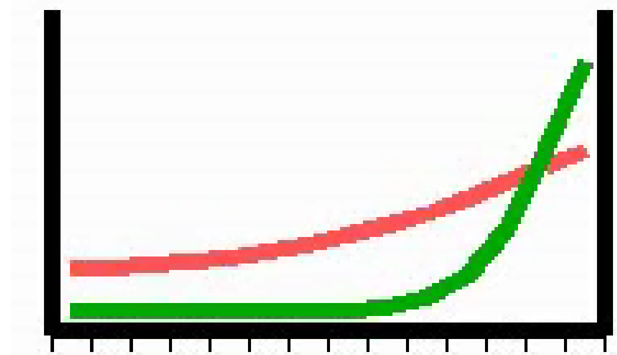
- Gierer-Meinhardt simulations:

  - Zero-flux boundary conditions.

  - A system with a polarity (pattern) stablished is destroy. System’s fluctuations restore it

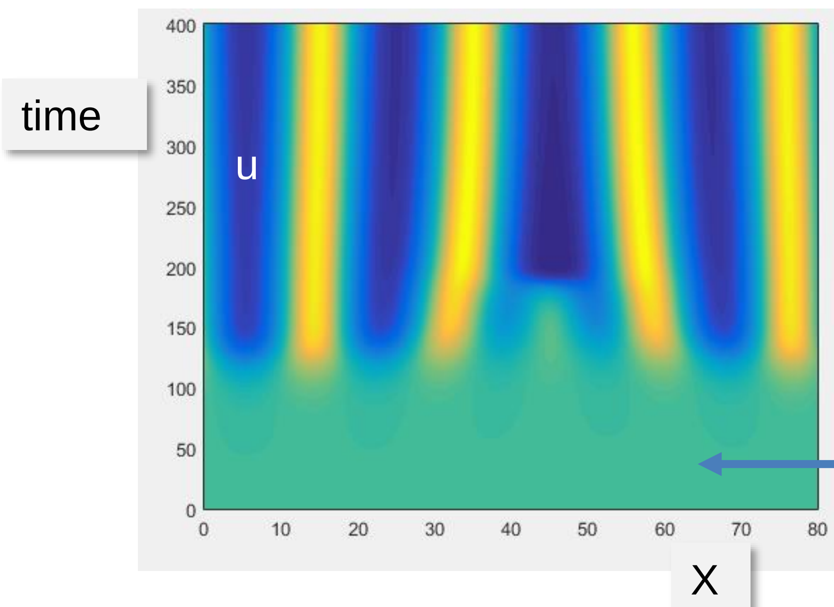
Inhibitor v

activator u



foot-head polarity

Matlab exercise!



Small initial fluctuations grow

5. Stability or instability **with diffusion**.

kinds of pattern

■ <u>Example 5</u>: Predator-prey with Turing instability.

(try to analyze it as exercise)

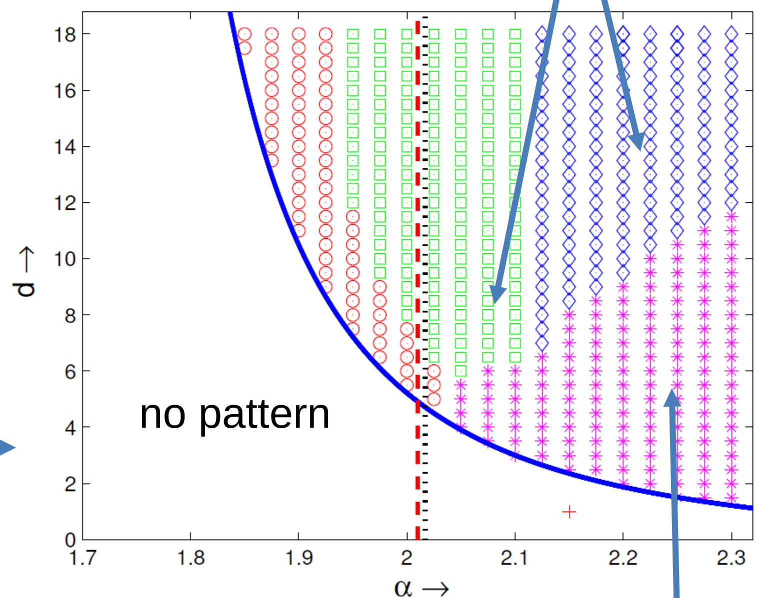
prey

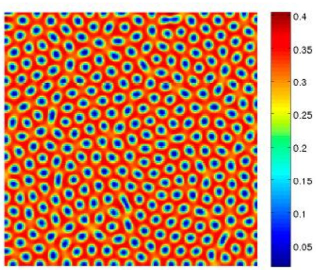
$$\frac{\partial u}{\partial t} = u(1-u) - \frac{\alpha u v}{u+v} + \nabla^2 u$$

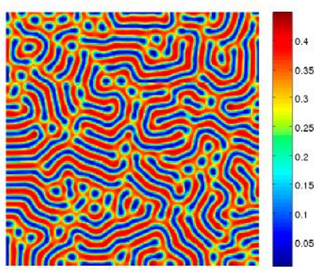
predat.

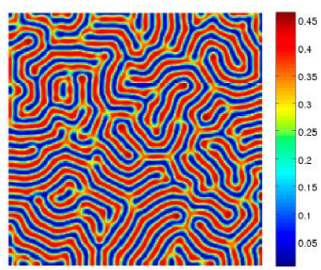
$$\frac{\partial v}{\partial t} = \frac{\beta u v}{u+v} - \gamma v - \delta v^2 + d\nabla^2 v$$

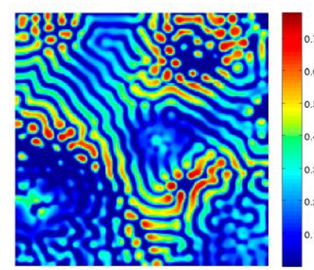
▫ Turing patterns are particularly sensitive to α and d.
(logistic growth is very important!)

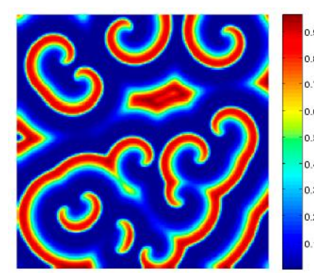












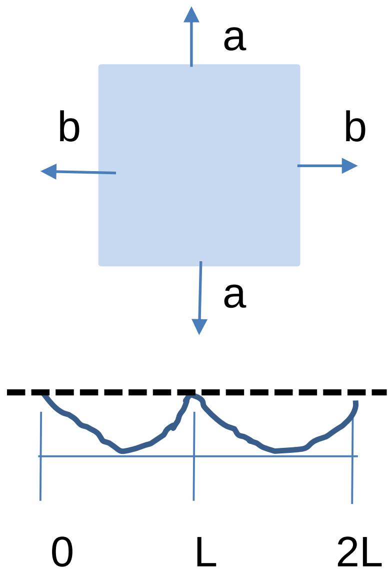
6. On the boundary conditions

■ In general, the evolution of Turing patterns and their structure may depend on the boundary conditions of the system.

■ One may consider the following cases:

▫ A) PERIODIC

(surface of a sphere, shells…)

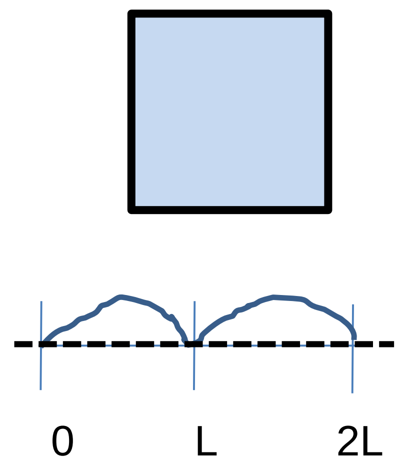


$$u\,(t,\,0) = u\,(t,\,L)$$

▫ B) DIRICHLET

(no substances

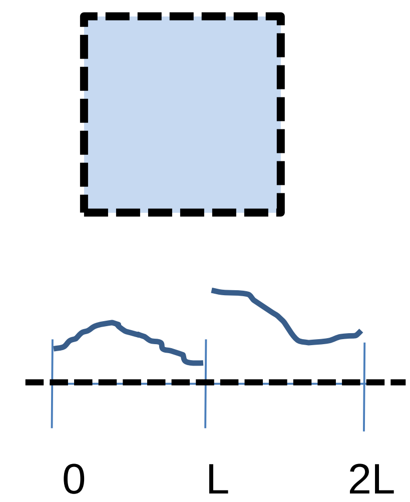
at the borders)



$$u\,(t,\,0) = u\,(t,\,L) = 0$$

▫ B) NEWMAN

(zero flux)



$$\left.\frac{du}{dx}\right|_0 = \left.\frac{du}{dx}\right|_L = 0$$

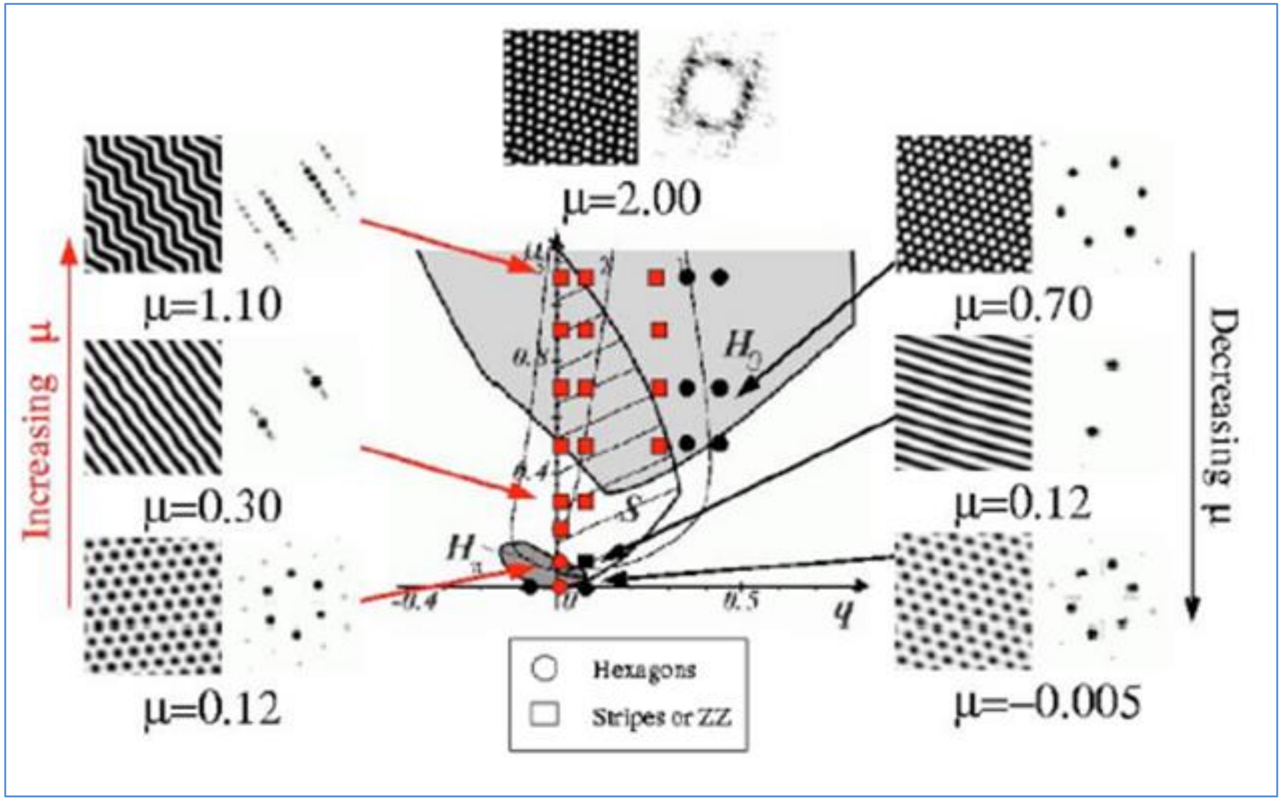
7. Richness of patterns

■ Dependence of the pattern structure on parameters occurs often, and allows for an understanding of natural diversity, e.g. through the Brusselator model.

$$\begin{cases} \dot{x} = 1 - (1+b)x + ax^2y + \nabla^2 x \\ \dot{y} = bx - ax^2y + D\nabla^2 y \end{cases}$$

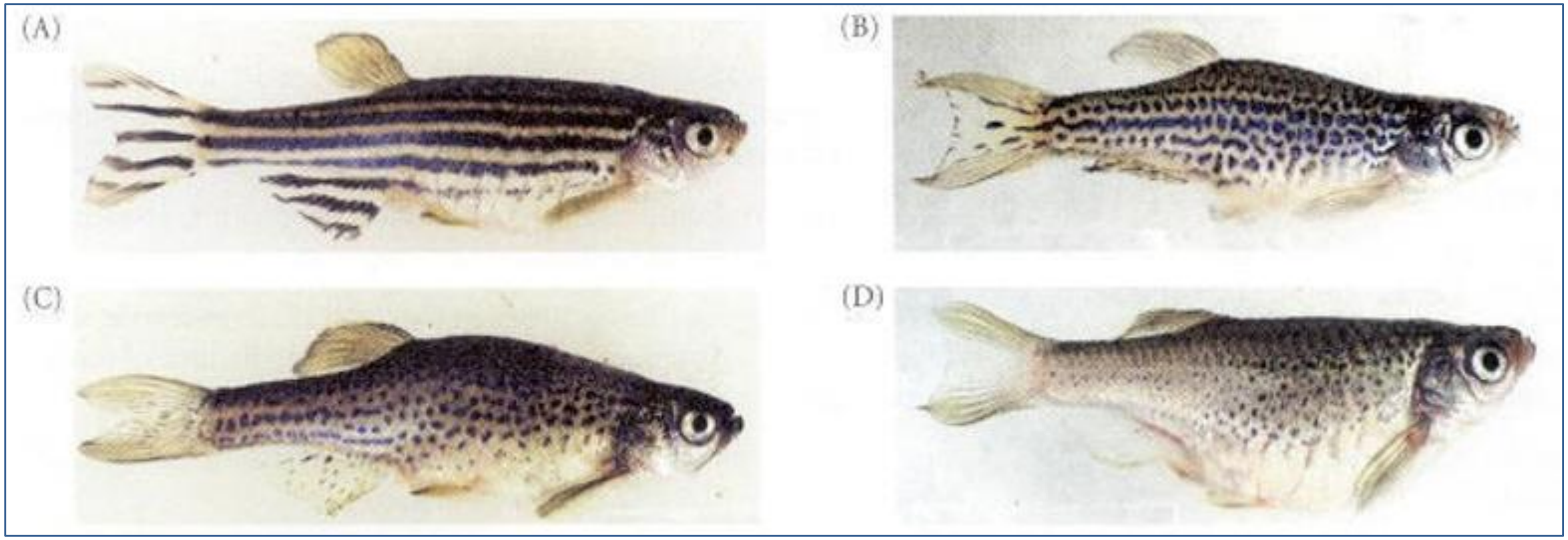
critical value for Turing

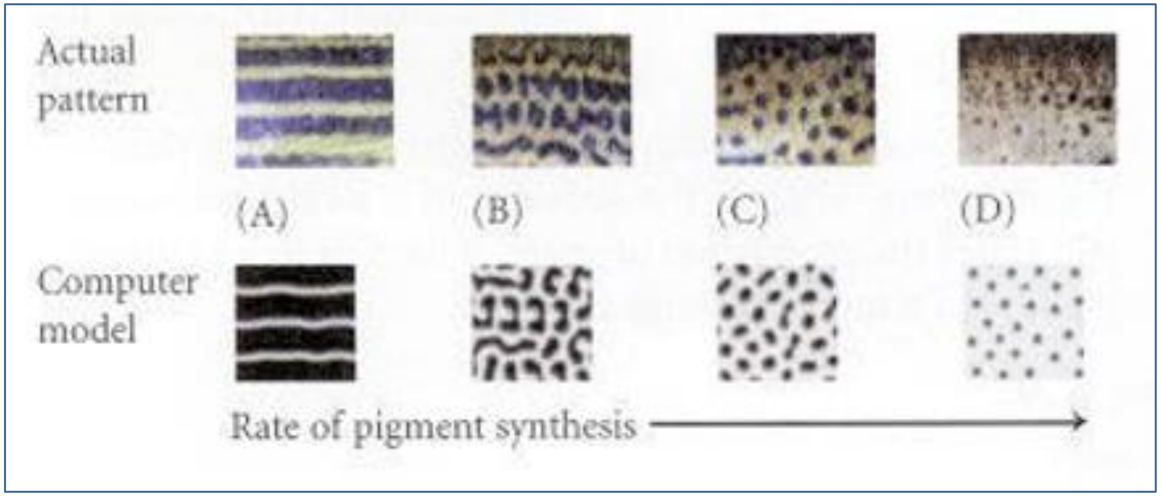
$$\mu = (b - b_c)/b_c.$$



7. Richness of patterns

■ A system may exhibit different patterns depending on changes in the parameters, e.g. the Brusselator model:



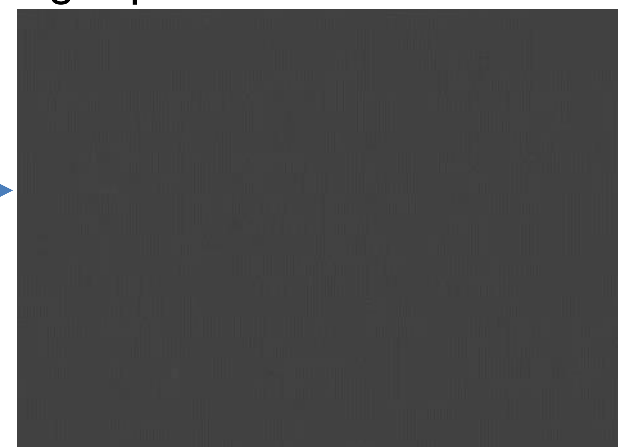


8. Final remarks

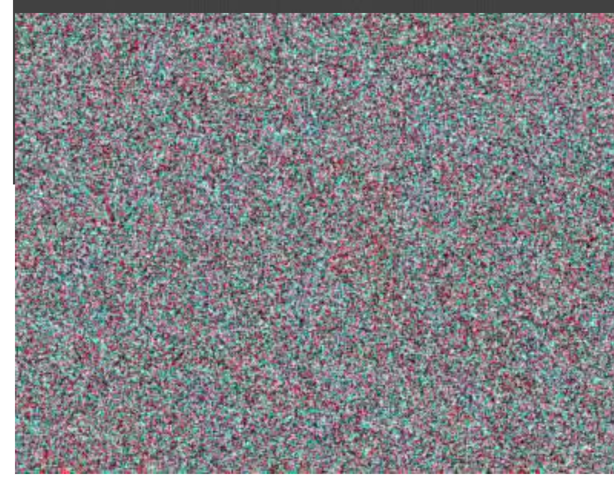
■ Turing patterns are a relatively young research field. For realistic systems, the complete understanding of the patterns that a system may generate is difficult to determine, and may take years of analysis, calculations and simulations.

■ Current research investigates some of the following topics:

▫ Coupled Turing systems, i.e. those in which a reaction occurs within another reaction.



▫ Patterns that evolve in time, e.g. travelling waves or other structures, to simulate heart dynamics.



▫ Systems where the ‘substrate’ over which diffusion occurs is anisotropic or changes in time.

▫ Diffusion across a network, e.g. activity in a neuronal network.

End of lecture 3

TAKE HOME MESSAGE:

- Turing patterns: stable without diffusion; unstable with diffusion.

$$\frac{\partial U}{\partial t} = f(U,V) + D_U \frac{\partial^2 U}{\partial x^2}$$
$$\frac{\partial V}{\partial t} = g(U,V) + D_V \frac{\partial^2 V}{\partial x^2}.$$

$$A = \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix} = \begin{pmatrix} \frac{\partial f}{\partial U} & \frac{\partial f}{\partial V} \\ \frac{\partial g}{\partial U} & \frac{\partial g}{\partial V} \end{pmatrix} \equiv \begin{pmatrix} f_U & f_V \\ g_U & g_V \end{pmatrix}\Bigg|_{(U_0,V_0)}$$

$$\mathrm{tr}(A) = f_U + g_V < 0$$
$$\det(A) = f_U \cdot g_V - f_V \cdot g_U > 0.$$

$$D_U \cdot g_V + D_V \cdot f_U > 0$$
$$D_U \cdot g_V + D_V \cdot f_U > 2\sqrt{D_U \cdot D_V} \cdot \sqrt{f_U \cdot g_V - f_V \cdot g_U}.$$

- Turing patterns are a fundamental tool to understand natural behavior, from predator-prey to skin pigmentation.

Questions and discussion aspects:

- Turing patterns need fluctuations to start, but must be robust against fluctuations. How do you solve this apparent contradiction?

- How do you think Turing patterns can change our understating of ecology and environment?

References

▫ L. Edelstein-Keshet, “Mathematical Models in Biology”, SIAM (2005).
▫ A. M. Turing, Philos. Trans. R. Soc. London, Ser. B (1952).
▫ “Turing at 100: Legacy of a Universal Mind”, Nature (2012).
▫ P. K. Maini et al., “Turing’s model for biological pattern formation and the robustness problem”, Interface Focus (2012).
▫ R. Kapral, “Pattern formation in chemical systems”, Physica D (1995).
▫ Vladimir K. Vanag“Design and control of patterns in reaction-diffusion systems”, Chaos (2008).
▫ Shigeru Kondo, *et al., “*Reaction-Diffusion Model as a Framework for Understanding Biological Pattern Formation”, Science (2010).
▫ L. Narayan Guin, “Spatial patterns through Turing instability in a reaction-diffusion predator-prey model”, Math. Comput. Simul. (2015).
▫ A. Kumar Sirohi et al., “Spatiotemporal pattern formation in a prey-predator model under environmental driving forces”, arXiv:1504.0826 (2015).
▫ P. Gonpot, “Gierer-Meinhardt model: bifurcation analysis and pattern formation”, Trends in Applied Science Research (2008).
▫ B. Peña, “Stability of Turing patterns in the Brusselator model”, Phys. Rev. E (2001).
▫ N. McCullen et al., “Pattern Formation on Networks: from Localised Activity to Turing Patterns”, Scientific Reports (2016).
▫ Karen M. Page et al., “Complex pattern formation in reaction–diffusion systems with spatially varying parameters”, Physica D (2005).