Environmental transport phenomena: Lecture VI

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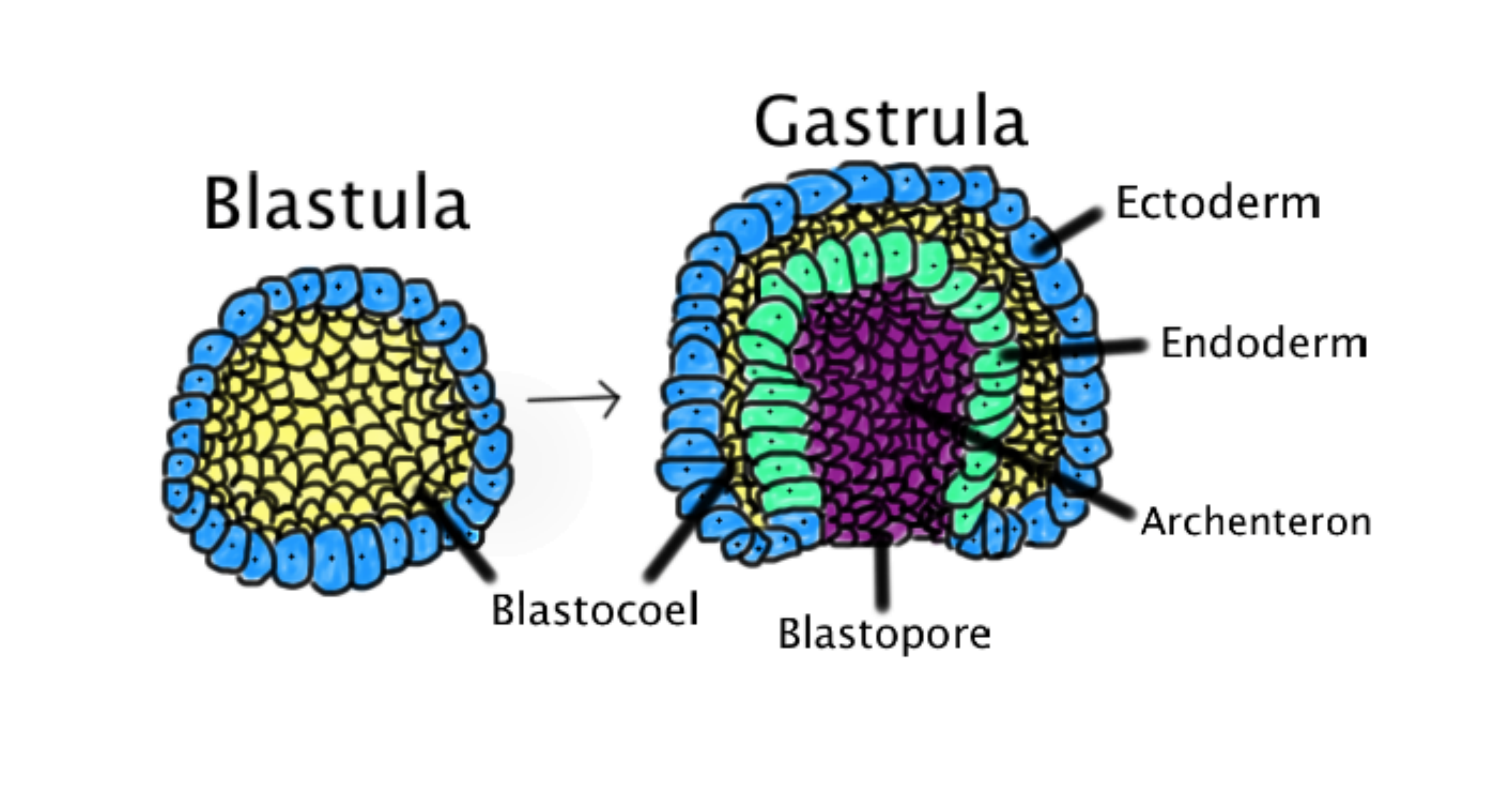
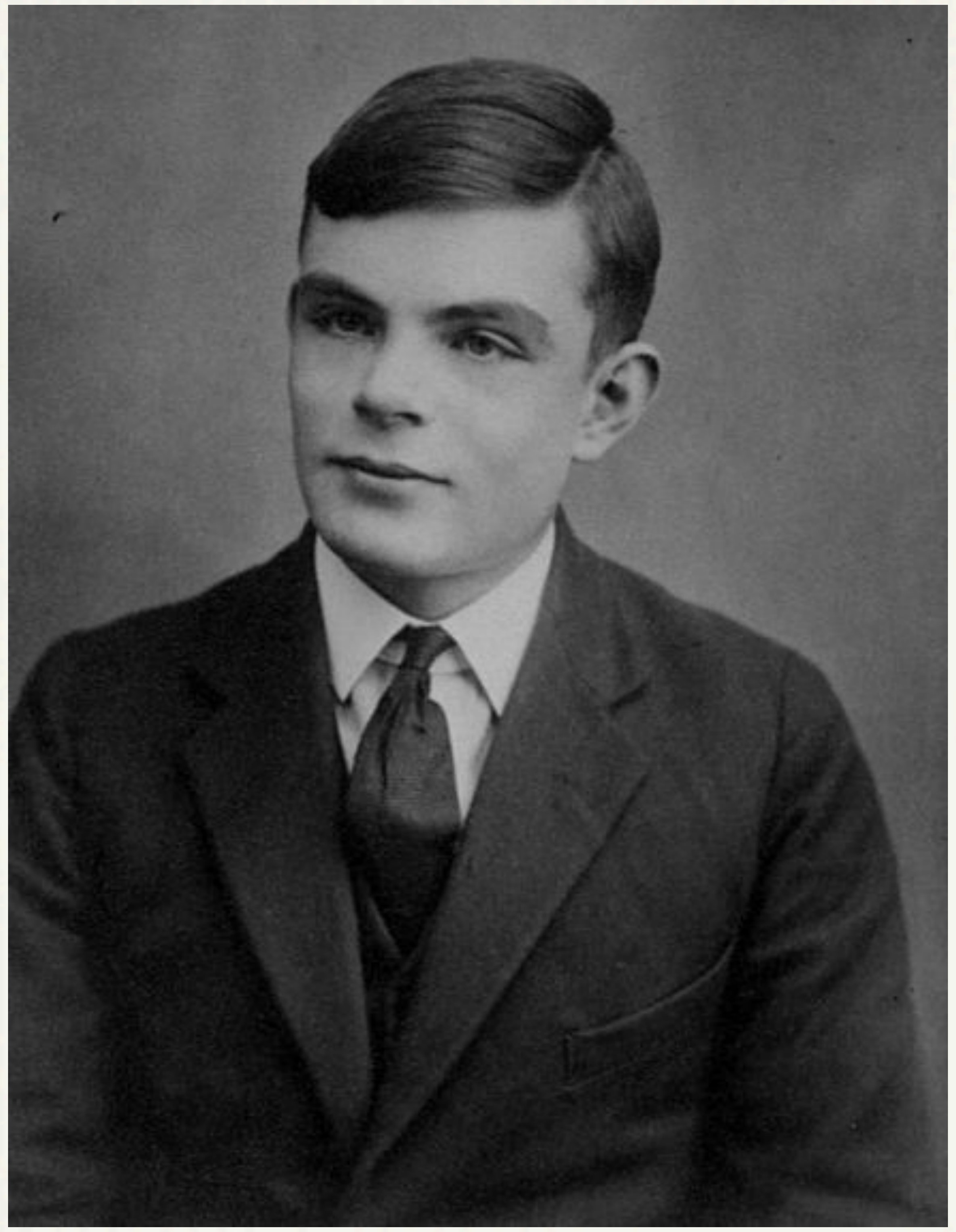
I) Diffusion-reaction equation and patterns

Beyond standard diffusion: patterns

Towards the - abrupt - end of his life, **Alan Turing** (helped breaking Enigma in WWII) raised the question of the **origin of complex biological patterns**.





Beyond standard diffusion: patterns

THE CHEMICAL BASIS OF MORPHOGENESIS

By A. M. TURING, F.R.S. *University of Manchester*

(*Received* 9 *November* 1951—*Revised* 15 *March* 1952)

It is suggested that a system of chemical substances, called morphogens, reacting together and diffusing through a tissue, is adequate to account for the main phenomena of morphogenesis. Such a system, although it may originally be quite homogeneous, may later develop a pattern or structure due to an instability of the homogeneous equilibrium, which is triggered off by random disturbances. Such reaction-diffusion systems are considered in some detail in the case of an isolated ring of cells, a mathematically convenient, though biologically unusual system. The investigation is chiefly concerned with the onset of instability. It is found that there are six essentially different forms which this may take. In the most interesting form stationary waves appear on the ring. It is suggested that this might account, for instance, for the tentacle patterns on *Hydra* and for whorled leaves. A system of reactions and diffusion on a sphere is also considered. Such a system appears to account for gastrulation. Another reaction system in two dimensions gives rise to patterns reminiscent of dappling. It is also suggested that stationary waves in two dimensions could account for the phenomena of phyllotaxis.

The purpose of this paper is to discuss a possible mechanism by which the genes of a zygote may determine the anatomical structure of the resulting organism. The theory does not make any new hypotheses; it merely suggests that certain well-known physical laws are sufficient to account for many of the facts. The full understanding of the paper requires a good knowledge of mathematics, some biology, and some elementary chemistry. Since readers cannot be expected to be experts in all of these subjects, a number of elementary facts are explained, which can be found in text-books, but whose omission would make the paper difficult reading.

Beyond standard diffusion: patterns

Very simple model where diffusion and reaction between species give rise to patterns.

$$\frac{\partial C_A}{\partial t} = D_A \nabla^2 C_A + f(C_A, C_B)$$

$$\frac{\partial C_B}{\partial t} = D_B \nabla^2 C_B + g(C_A, C_B)$$

Two species diffusion reaction

Possible choice (Gray-Scott model)

reaction

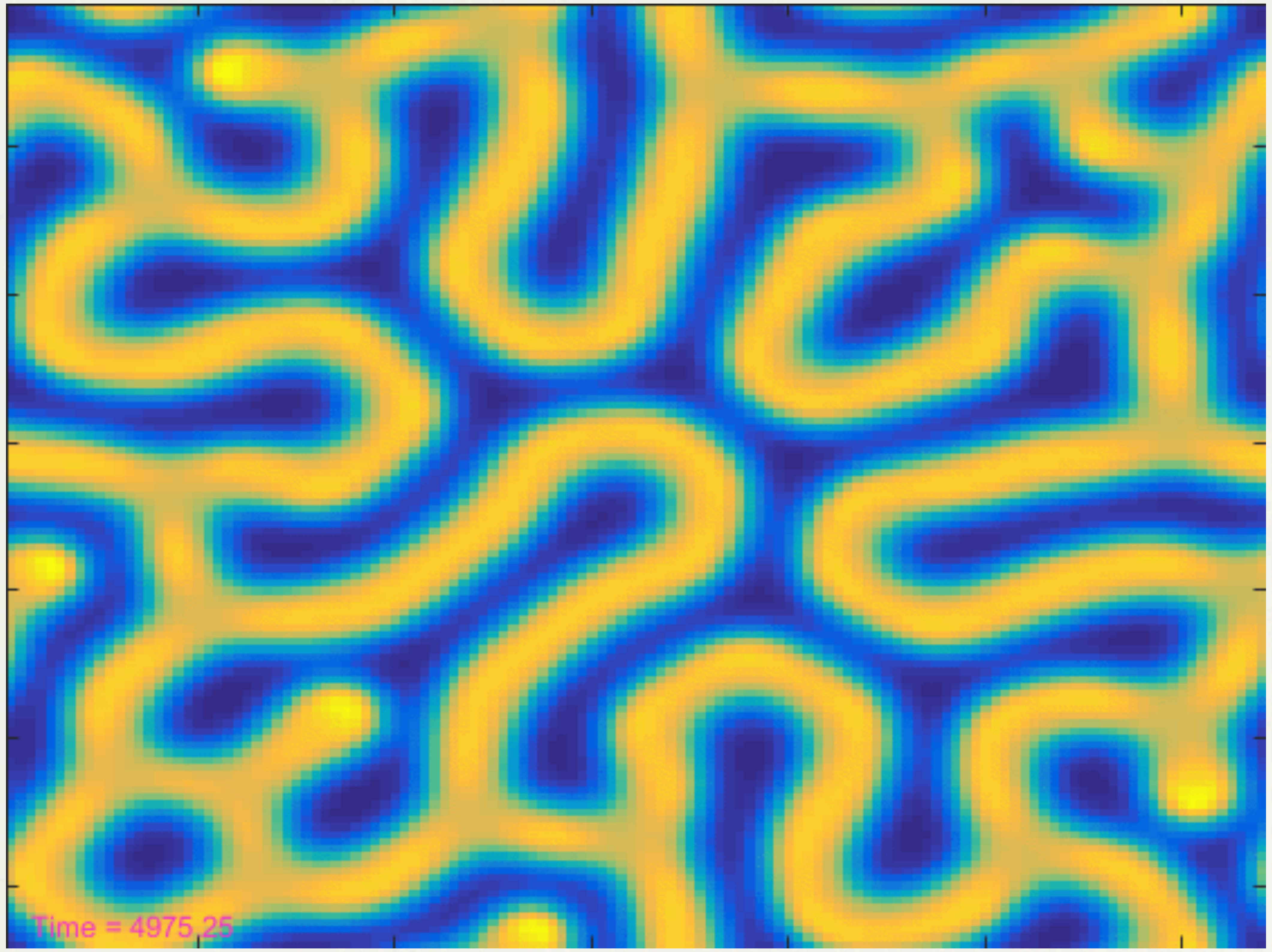
replenishment (up to a limit, here set to one)

$$f(C_A, C_B) = -C_A C_B^2 + F(1 - C_A)$$

depletion (mortality, otherwise no limit to production of B)

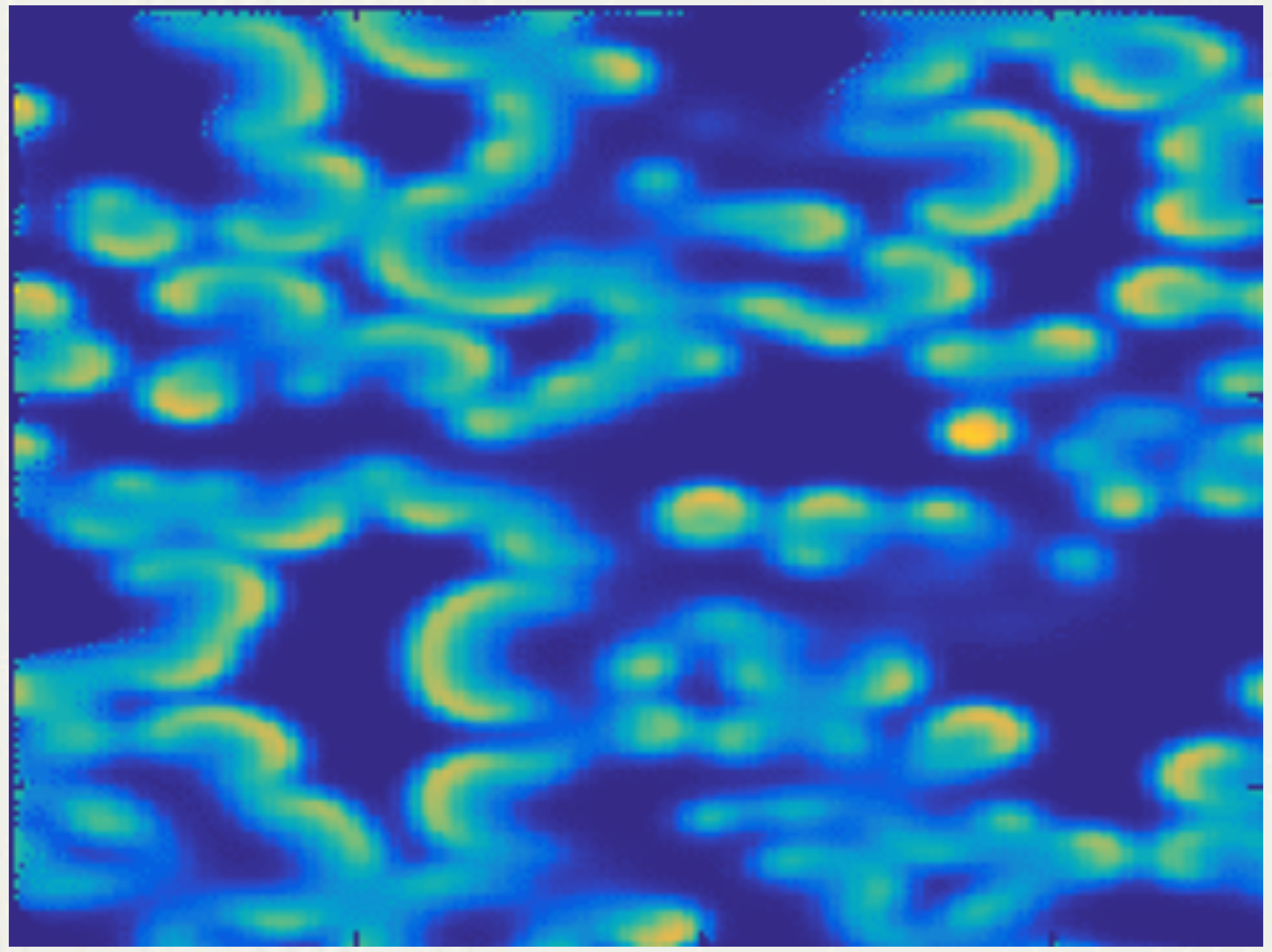
$$g(C_A, C_B) = +C_A C_B^2 - (F + K) C_B$$

Beyond standard diffusion: patterns

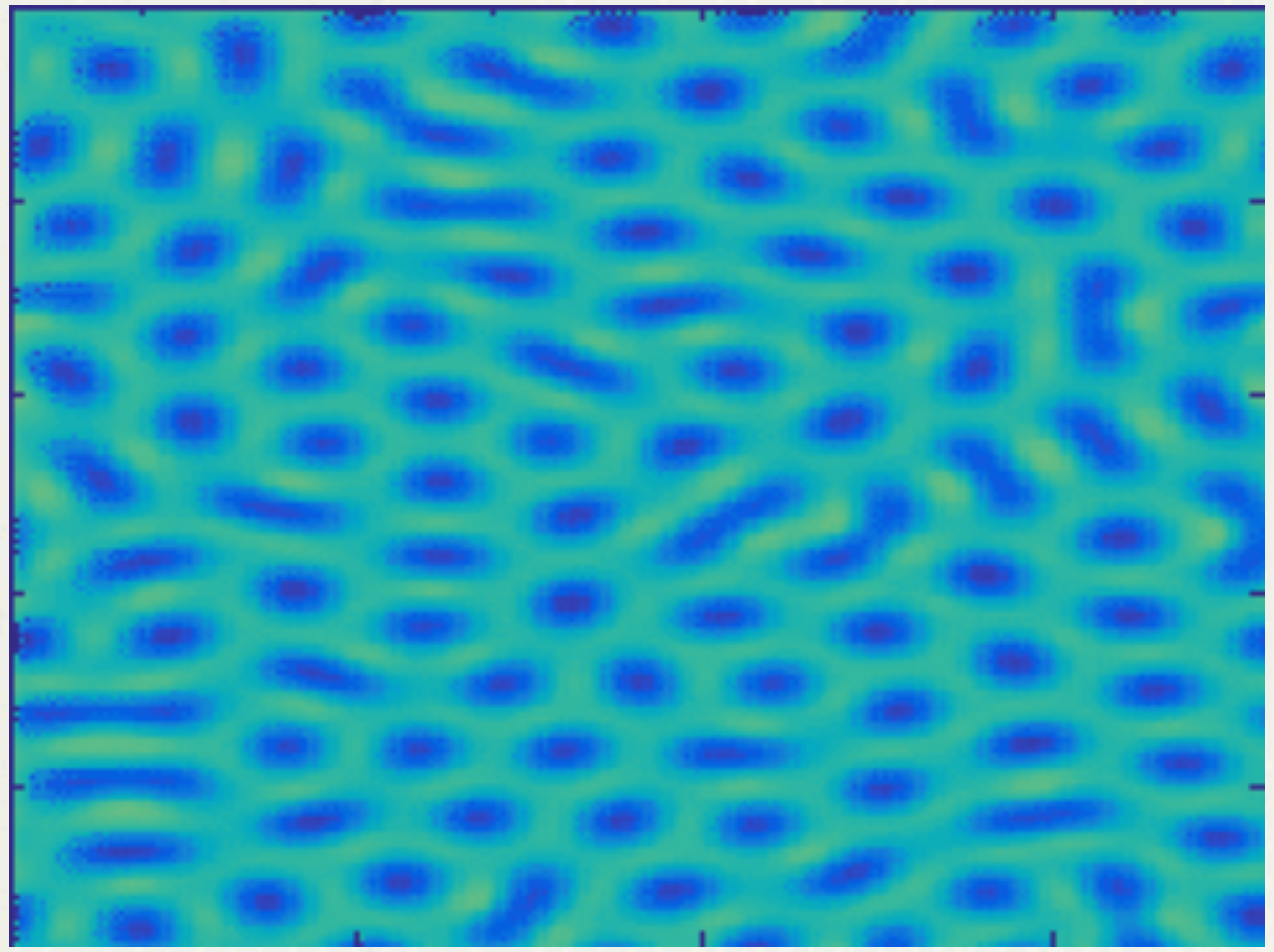


Spatially **homogenous solution is not always stable**, the system evolves towards **complex patterns** (diverse geometries) ! Mathematically, we compute the growth rate of different patterns, the **fastest growing dominates**.

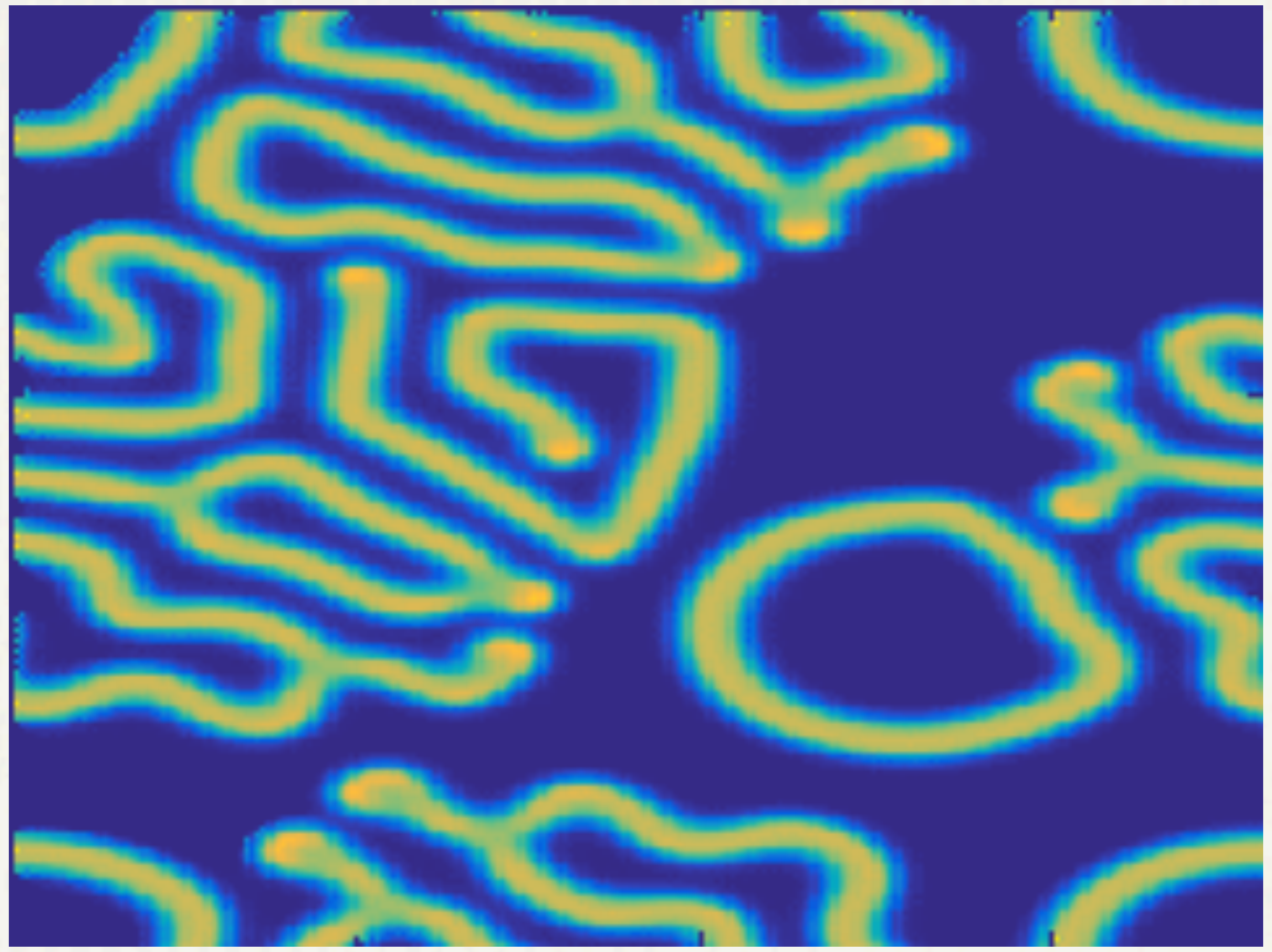
Beyond standard diffusion: patterns



Dominated by **depletion**

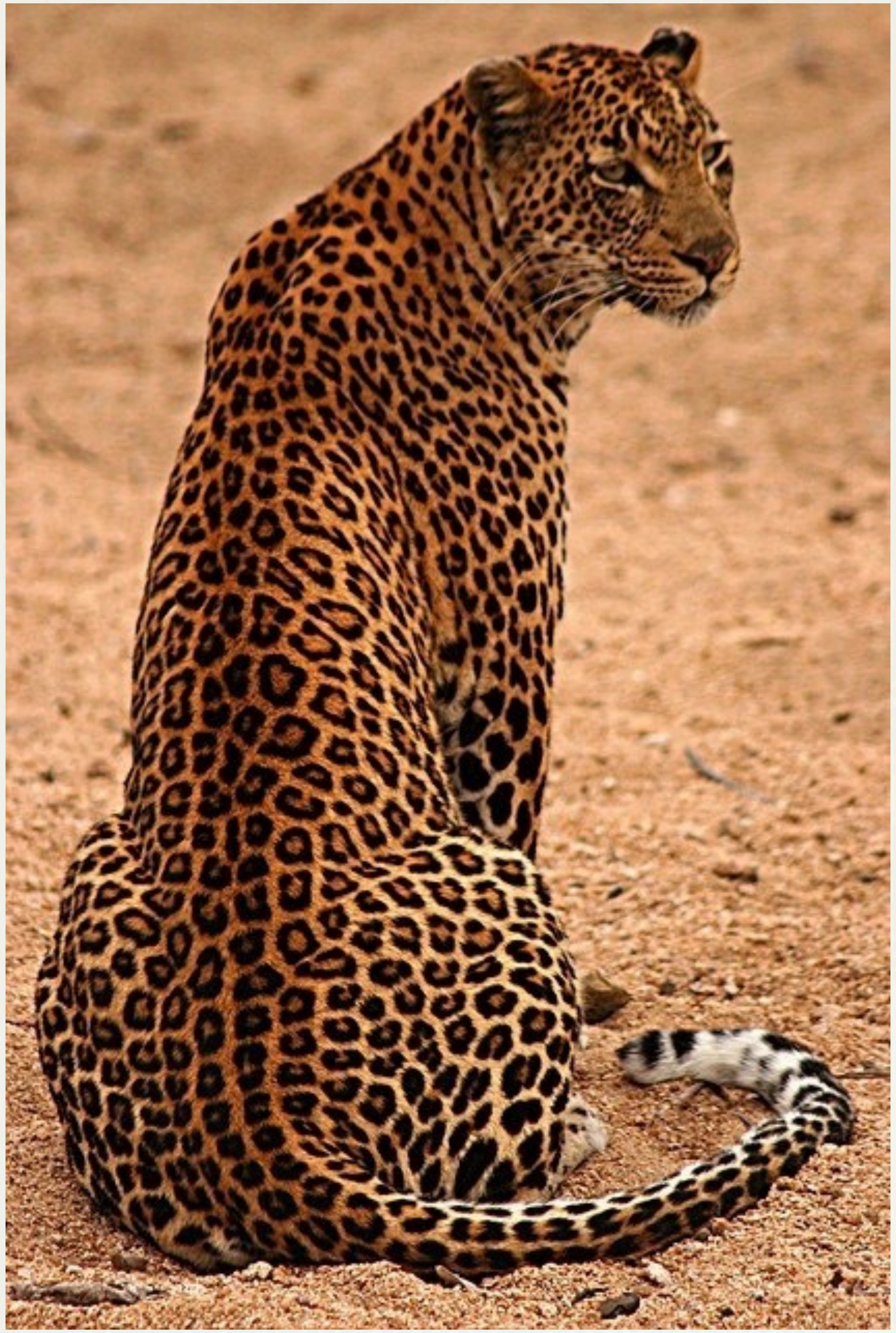


Dominated by **replenishment**

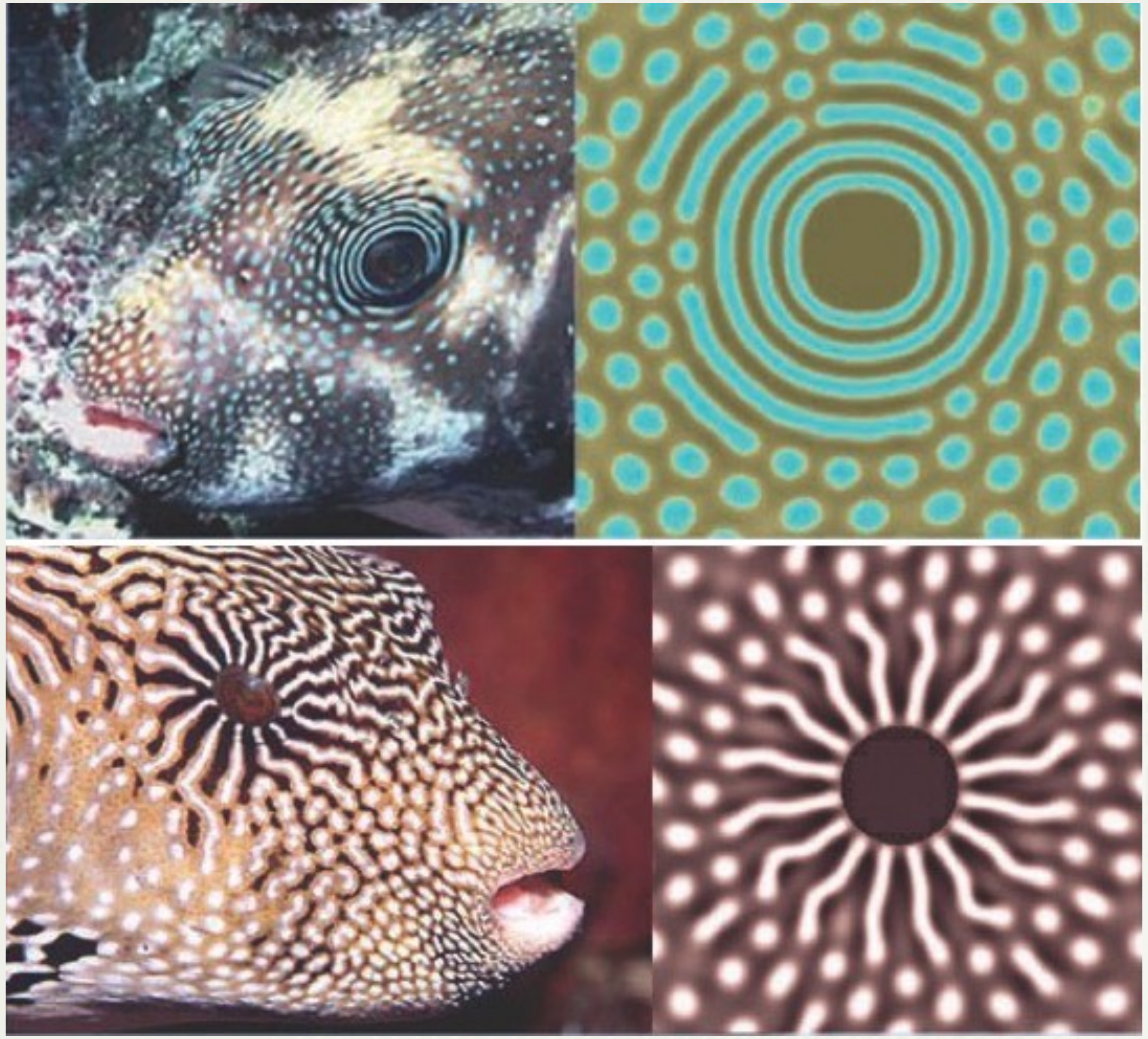


Intermediate case

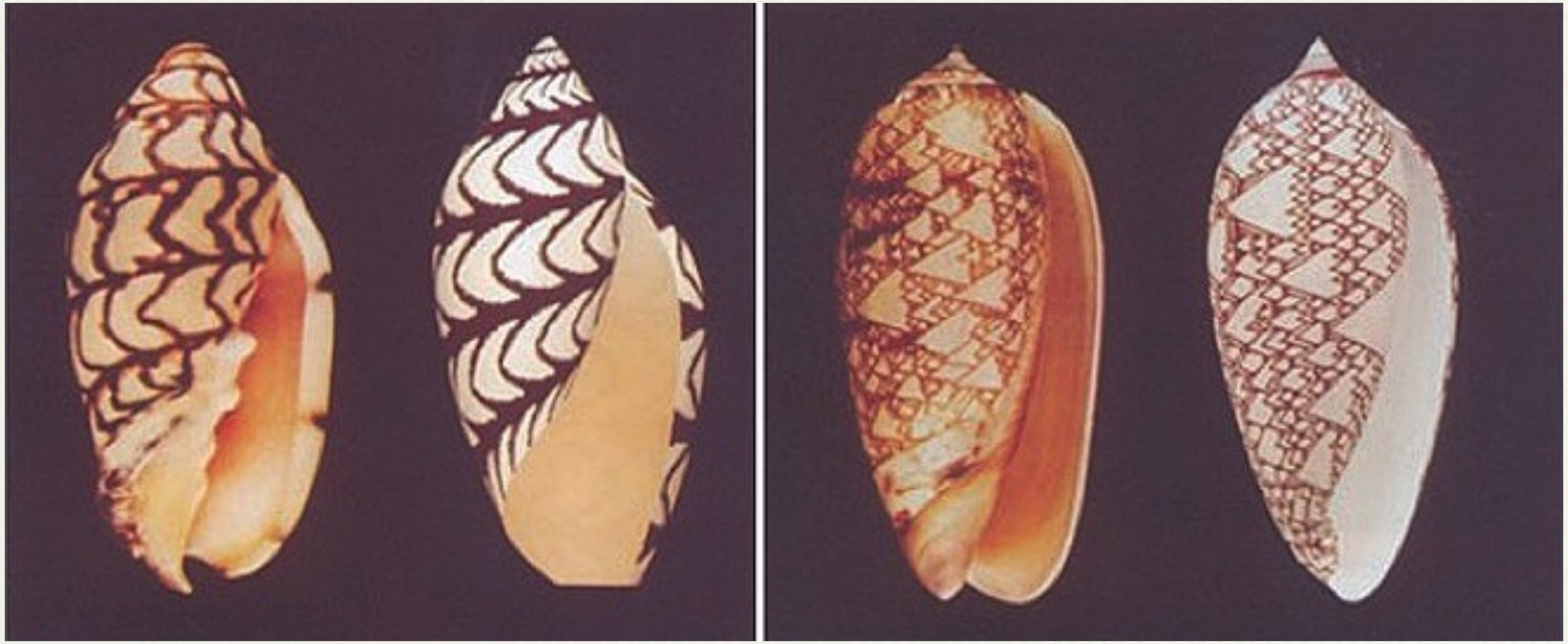
Beyond standard diffusion: patterns



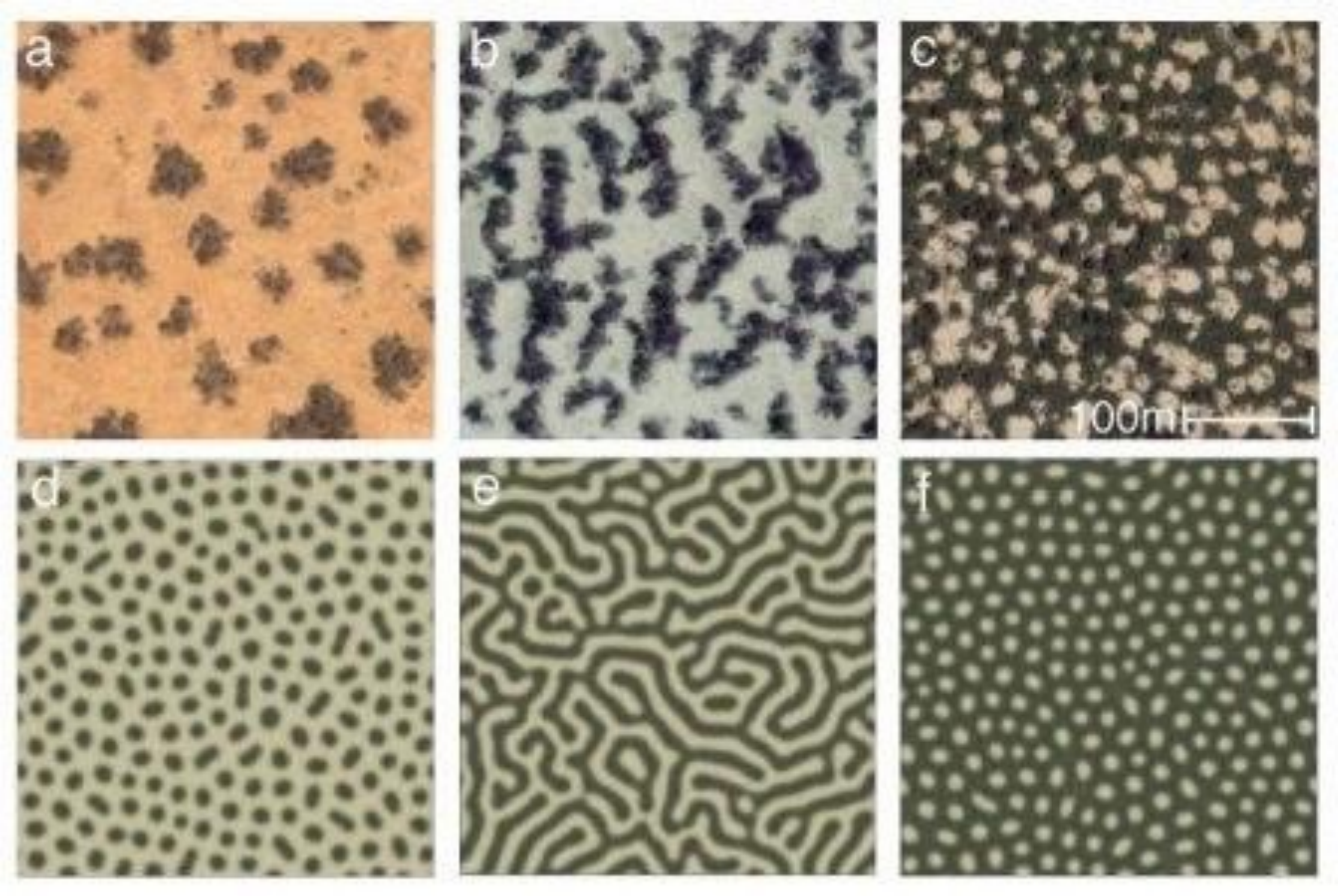
Beyond standard diffusion: patterns



Beyond standard diffusion: patterns



Vegetated patterns, semi-arid environment



Nature

Mathematical model

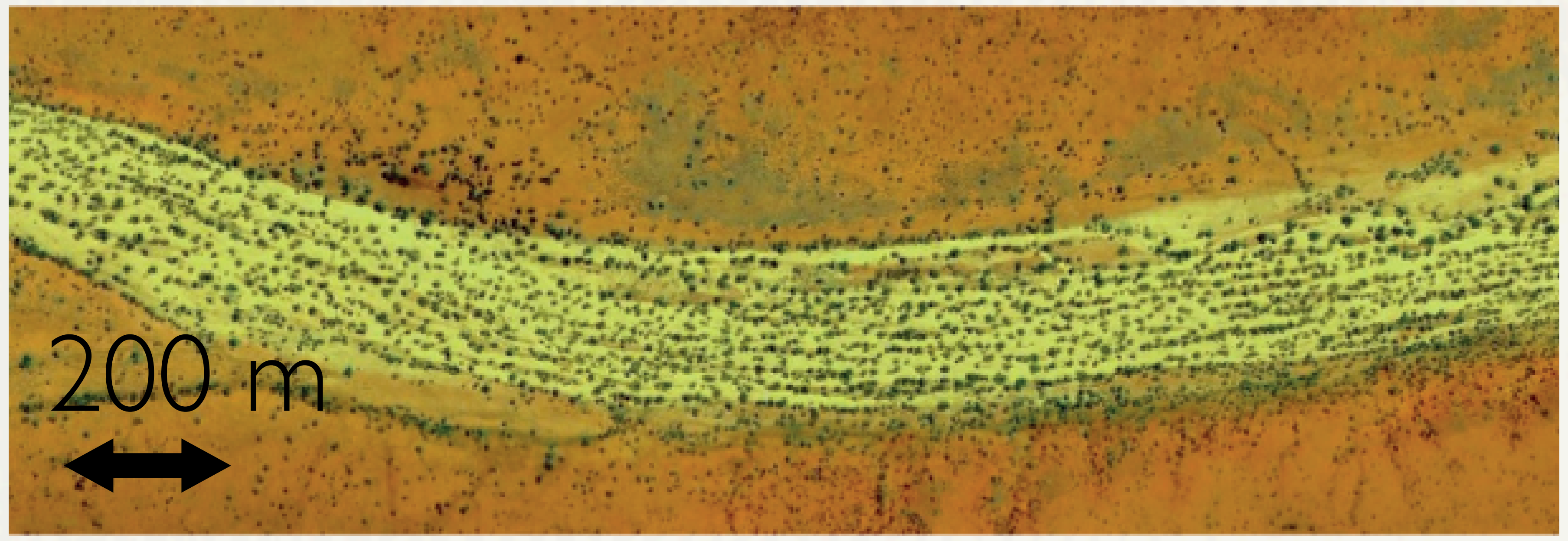
Strategy for survival: **best compromise** between positive (e.g. sheltering from sun) and negative (e.g. competition for water) feedback

Vegetated patterns in rivers

- Observed for various spatial **scales** and **environments**
- Spatial distribution of vegetation correlates with morphology
- Active role in the **formation** or in the **stabilization** of ridges ?

A)

B)



C)

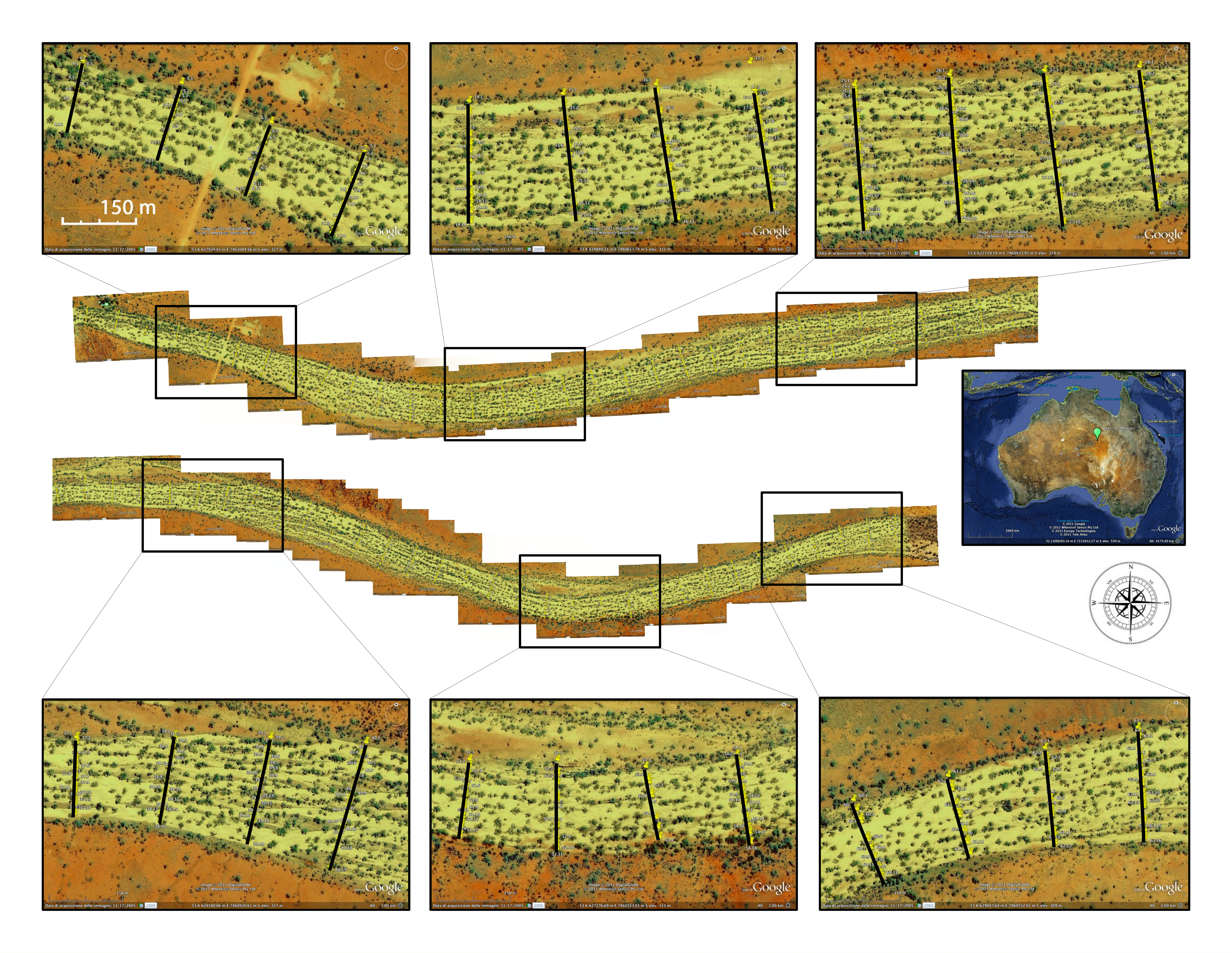
Organization of vegetation

- If the **biomass is mature enough**, it starts to disturb the flow.
- Both **positive and negative interaction** between biomass at different points. Cooperation + competition -> patterns as a compromise

Increased deposition (positive interaction) or sediment anchoring

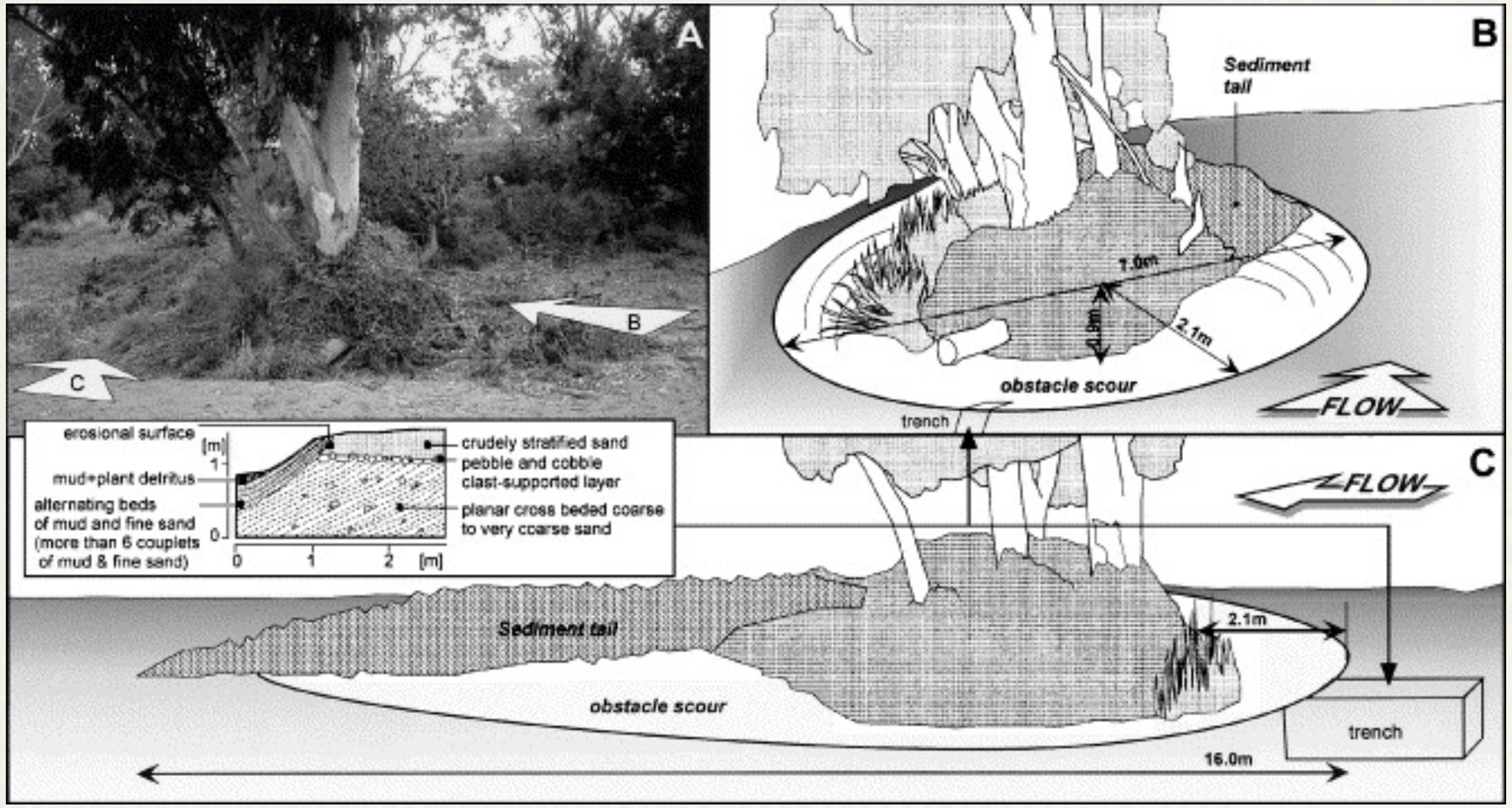
Increased scouring due to flow deflection (negative interaction)

Vegetated patterns: anabranching patterns in ephemeral rivers



Interaction Kernel (model hypotheses)

Obstacle cross-section proportional to the local biomass (deposition).

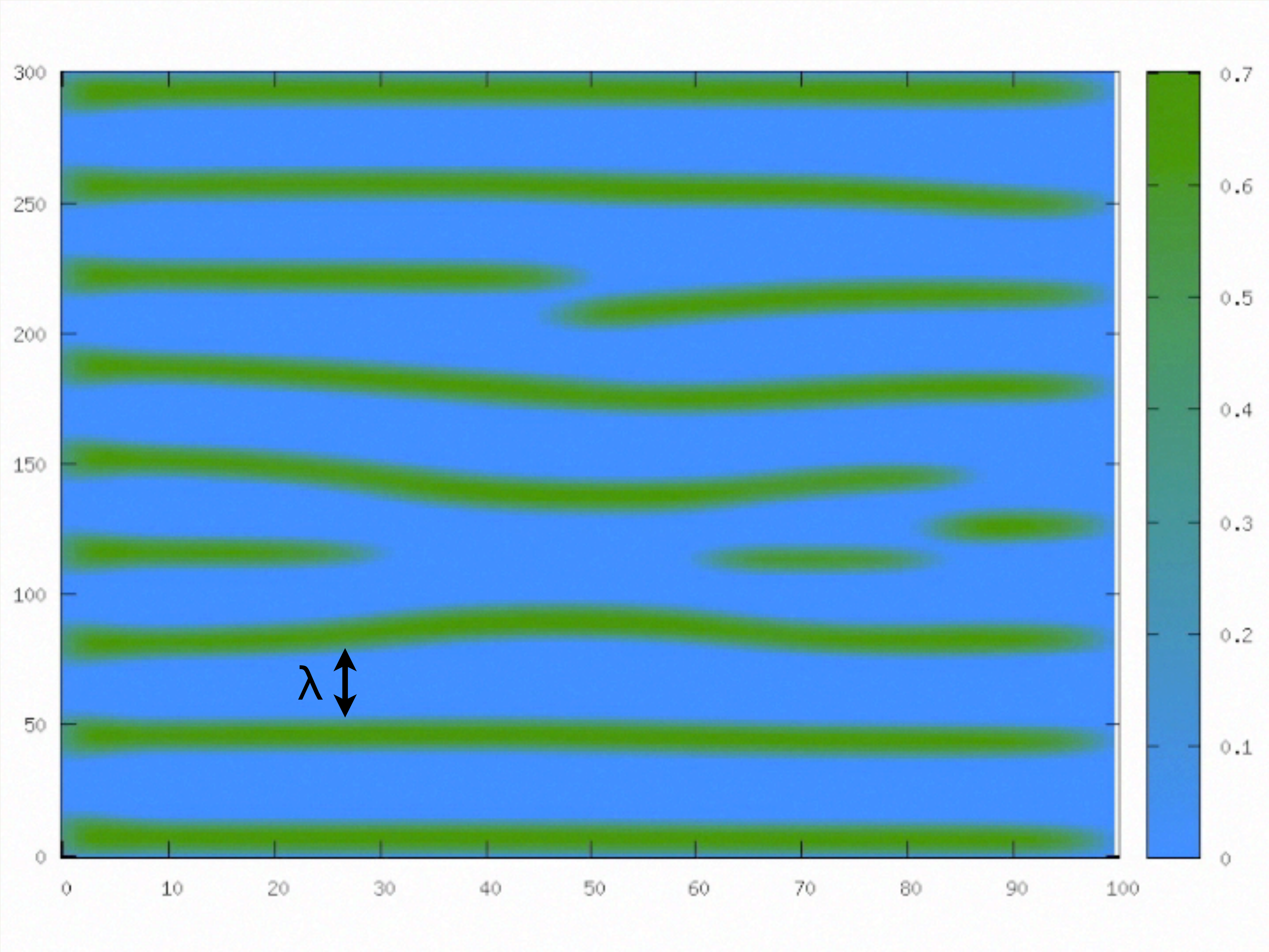


Nakayama, Fielding and Alexander, Sedimentary Geology (2002)

Local positive interaction
(sediment anchoring by vegetation)

$$\int\int dx'dy'\phi(x',y')W_+(x-x',y-y') \approx A\phi(x,y) + B\nabla_y\phi(x,y) + D_s\nabla^2\phi(x,y)$$

Vegetated patterns: model evolution



https://www.sciencedirect.com/science/article/abs/pii/S030917081500158X

Stability analysis (Turing 1952): set of analytical conditions under which the **homogeneous solution becomes unstable** and evolves towards periodic patterns.

Ecomorphodynamic equations

- Couple the equation for the evolution of vegetation with the equations of the morphodynamics (Shallow water equations + Exner + Vegetation).

$$\frac{\partial U}{\partial t} = -U\frac{\partial U}{\partial s} - V\frac{\partial U}{\partial n} - g\left[\frac{\partial Y}{\partial s} + \frac{\partial \eta}{\partial s}\right] - \frac{g}{Y}\left[\frac{1}{\chi_b^2} + \frac{c_D d Y \phi}{2g}\right] U||\mathbf{U}||$$

$$\frac{\partial V}{\partial t} = -U\frac{\partial V}{\partial s} - V\frac{\partial V}{\partial n} - g\left[\frac{\partial Y}{\partial n} + \frac{\partial \eta}{\partial n}\right] - \frac{g}{Y}\left[\frac{1}{\chi_b^2} + \frac{c_D d Y \phi}{2g}\right] V||\mathbf{U}||$$

$$\frac{\partial Y}{\partial t} = -\nabla \cdot (Y\mathbf{V})$$

Friction induced by vegetation

$\mathbf{V} = (U, V)$ Flow velocity

(s, n) longitudinal / transverse coordinates

η riverbed elevation $\mathbf{Q_s}$ sediment flux

Y flow depth p porosity

ϕ vegetation density d vegetation diameter

$$\frac{\partial \eta}{\partial t} = -\frac{\nabla \cdot \mathbf{Q_s}}{(1-p)}$$

$$\frac{\partial \phi}{\partial t} = \alpha_g \phi(\phi_m - \phi) + D\nabla^2\phi - \alpha_d Y \mathbf{U}^2 \phi$$

logistic growth + diffusion - mortality

Perona et al. ESPL, 2014

Vegetated patterns: model evolution

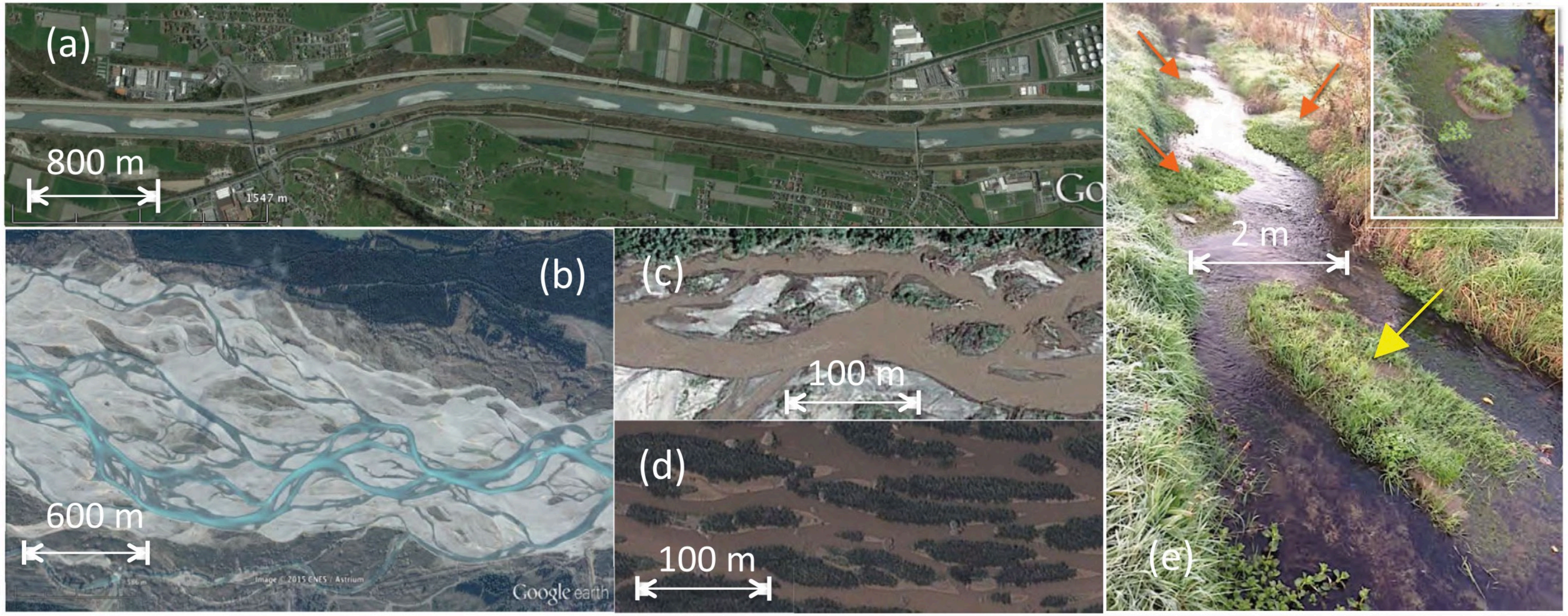
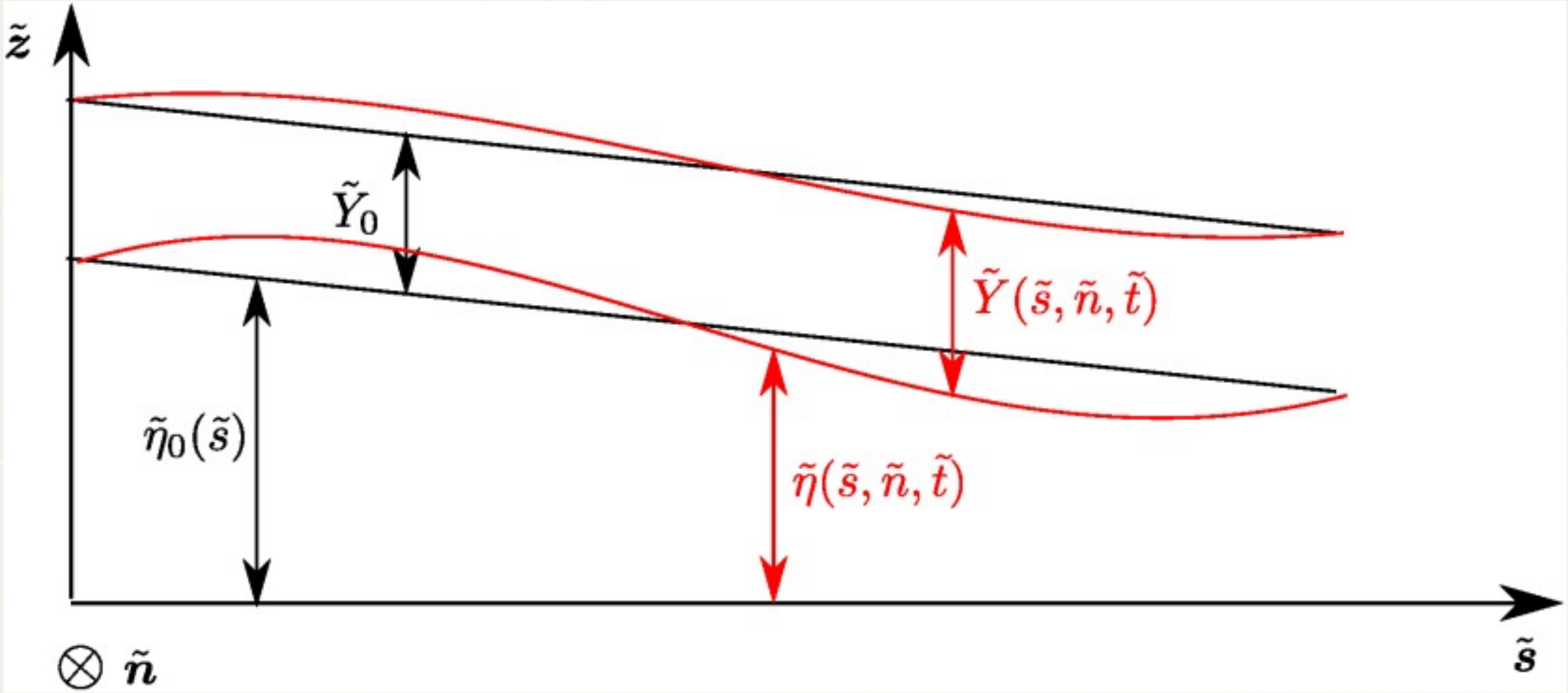


Figure 1. Examples of river bed patterns emerging in different environments: (a) regular series of unvegetated alternate bars on the Rhine River (Haag, Switzerland); (b) braided river in absence of vegetation (Waimakariri River, New Zealand); (c) moderately vegetated multiple bars (Awash River, Ethiopia); (d) anabranching patterns in the form of completely vegetated multiple bars (Awash River, Ethiopia). Map data: Google, Digitalglobe. (e) Alternate bars (orange arrows) and islands (yellow arrow) in a small creek near Schwarzenburg, Switzerland (Photo: P.Perona).

https://agupubs.onlinelibrary.wiley.com/doi/full/10.1002/2015WR017492

Vegetated patterns: model evolution

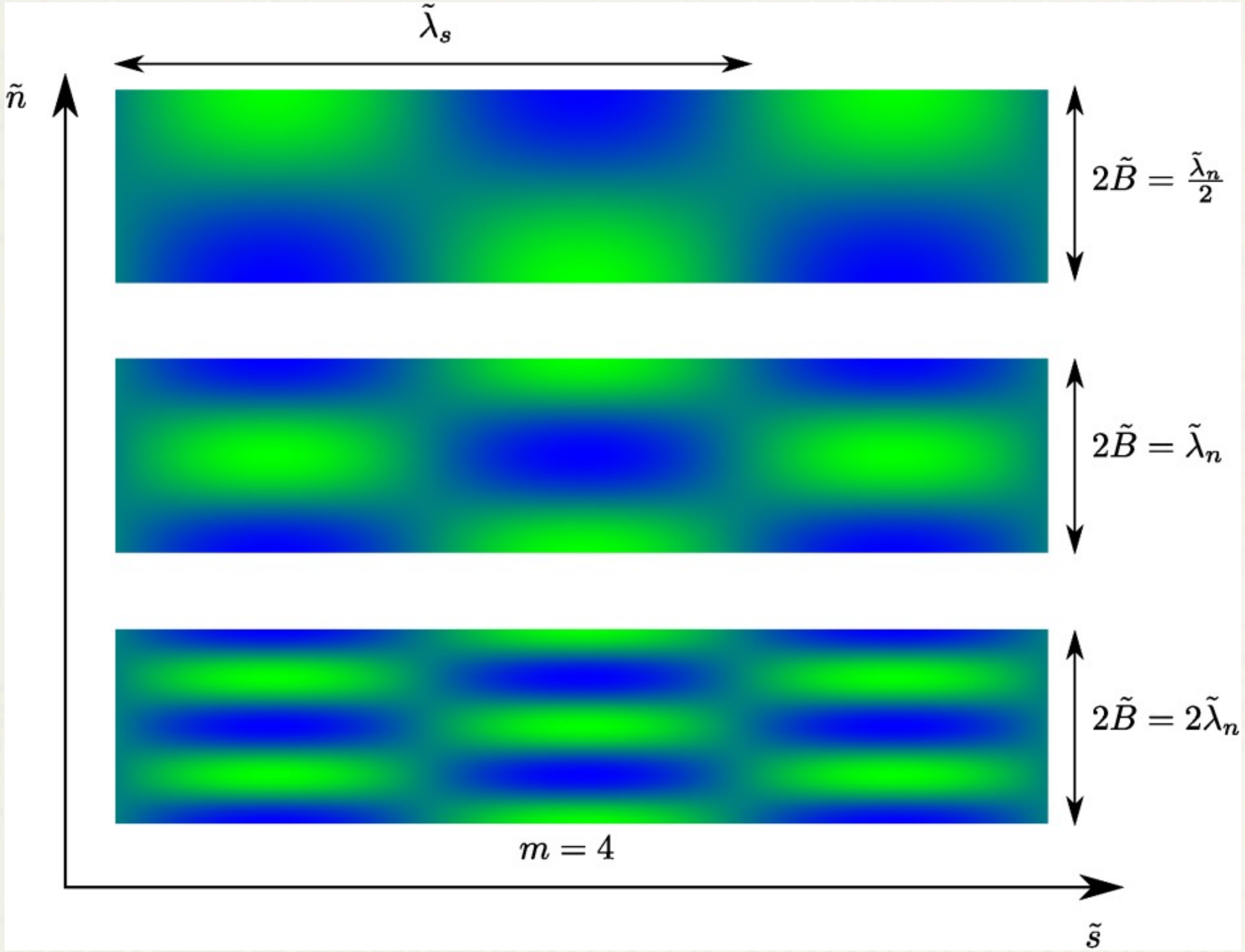


Following Turing's method, we introduce a **perturbation** to the homogeneous solution and study its evolution (damping or exponential growth.

Vegetated patterns: model evolution

$$\begin{pmatrix} U_1 \\ V_1 \\ Y_1 \\ \eta_1 \\ \phi_1 \end{pmatrix} = \begin{pmatrix} u(t)\ \cos(k_n n+\psi_u) \\ v(t)\ \cos(k_n n+\psi_v) \\ y(t)\ \cos(k_n n+\psi_y) \\ h(t)\ \cos(k_n n+\psi_h) \\ f(t)\ \cos(k_n n+\psi_f) \end{pmatrix} \exp(ik_s s) + \text{c.c.}.$$

perturbation to the homogeneous solution



Stability analysis (Turing 1952): set of analytical conditions under which the **homogeneous solution becomes unstable (perturbation grows exponentially)** and evolves towards periodic patterns (alternate or multiple bars).

Take-home message on diffusion and patterns

Complex patterns are **ubiquitous** in Nature (other examples: epidemics, invasions by species). Components needed for the emergence of patterns:

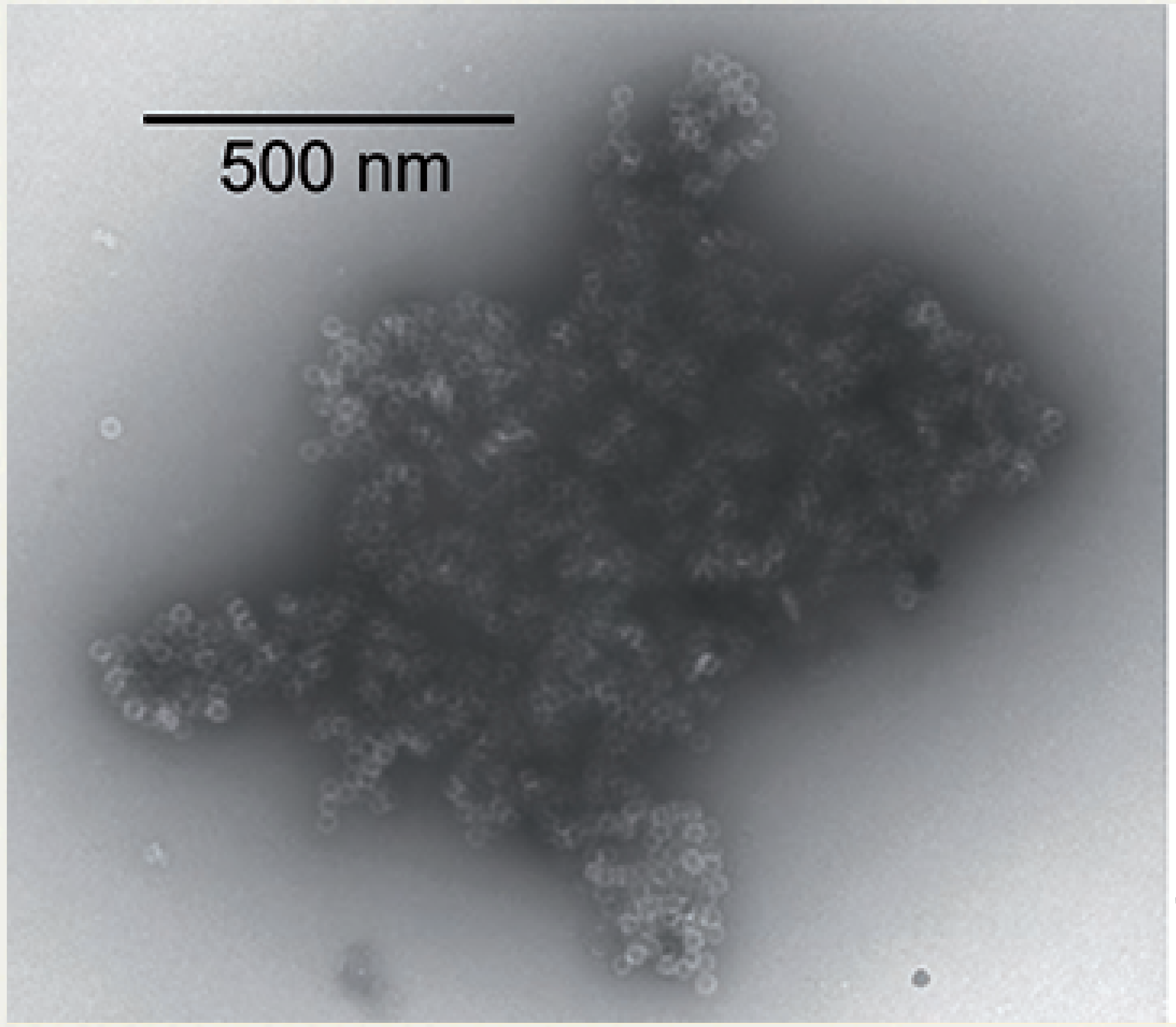
- **Diffusion** can turn a stable state (reaction equilibrium) into an unstable one (instability towards patterns)
- Depletion-replenishment / **activation-inhibition** / cooperation-competition are needed for the emergence of the patterns
- The pattern scale that **grows the fastest** will dominate (method described in Turing's paper).

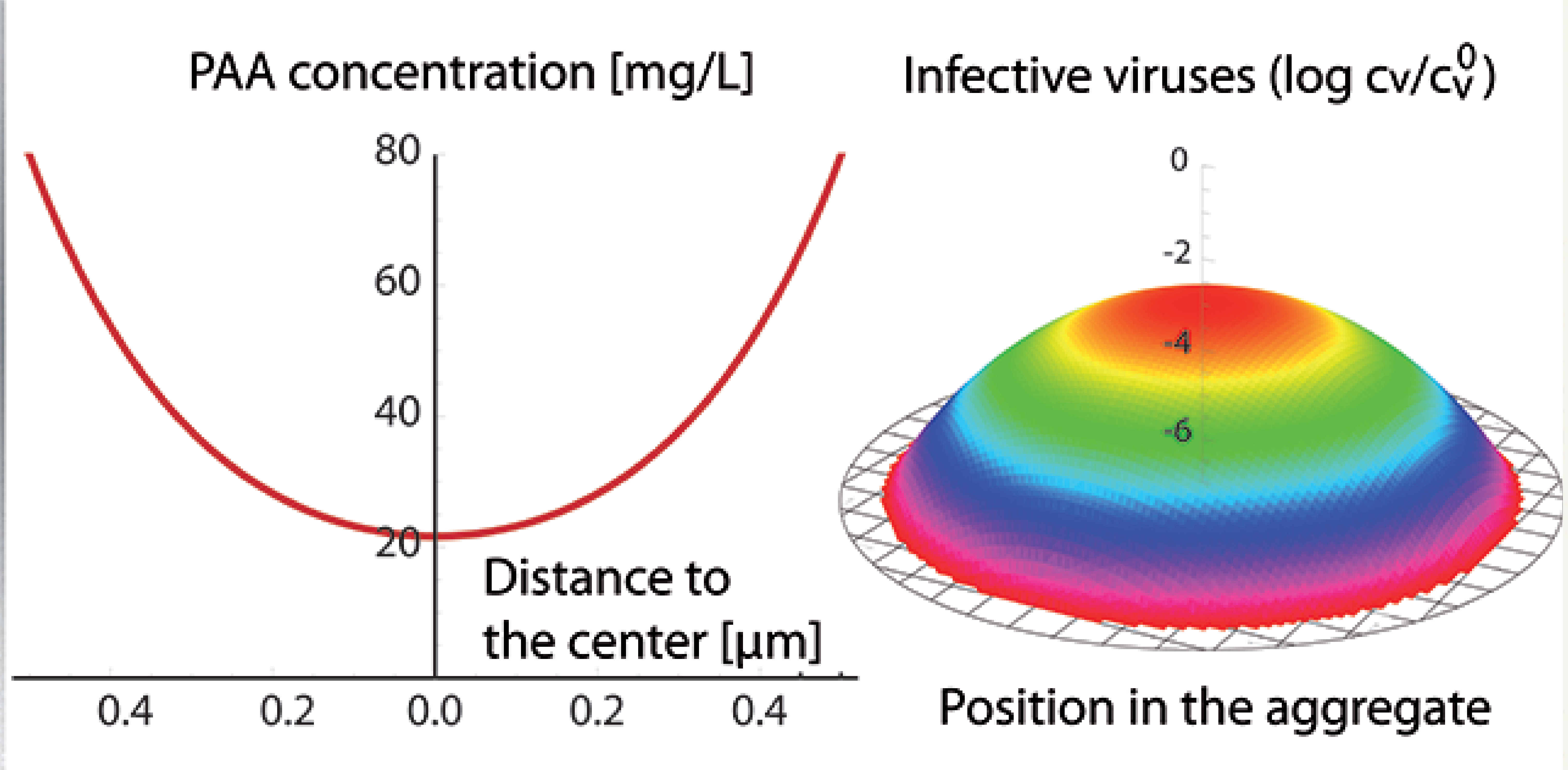
II) 3D diffusion-reaction: disinfection of virus aggregates

Paper by ETP student: *M. J. Mattle, B. Crouzy, M. Brennecke, K. Wigginton, P. Perona, and T. Kohn. Impact of virus aggregation on inactivation by peracetic acid and implications for other disinfectants. Environmental Science and Technology, 45(18):7710-7717, 2011*

Impact of aggregation on virus disinfection

Disinfection doses are determined for dispersed viruses. Viruses are known to aggregate, what are the consequences for disinfection ?





Viruses may form **aggregates**

Concentration of disinfectant **smaller close to aggregate center**

Viruses survive **longer** close to the center

Model for aggregate disinfection

$$\partial_t c_v = -k_1 c_d^a c_v$$

Disinfection, known from experiments with dispersed viruses (“slave equation”)

$$\partial_t c_d = D\nabla^2 c_d - k_2 c_d$$

Diffusion-Consumption of disinfection in the aggregates (“master equation”)

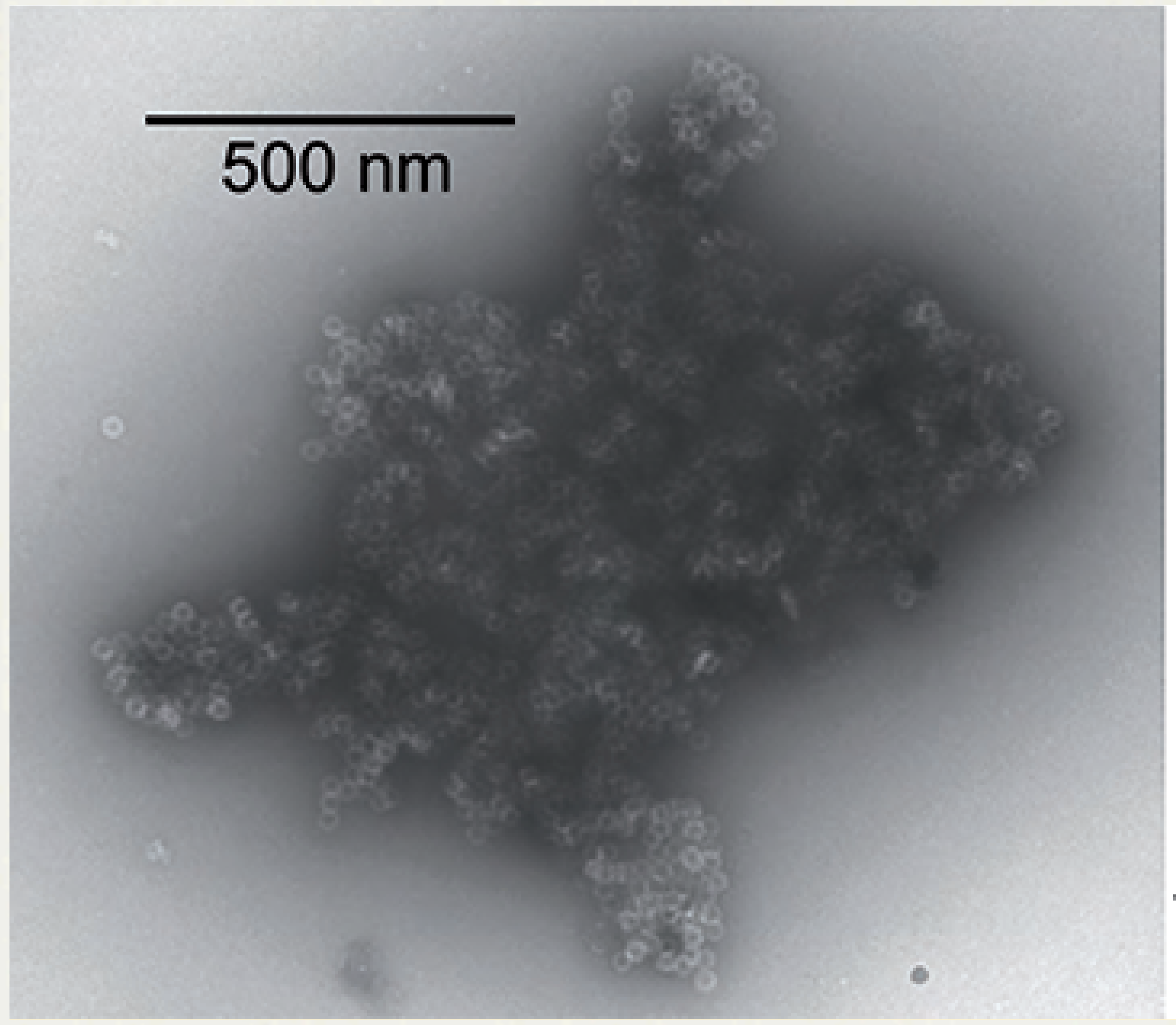
Spherical aggregates (Radius R) $\nabla^2 = \partial_r^2 + \frac{2}{r}\partial_r$

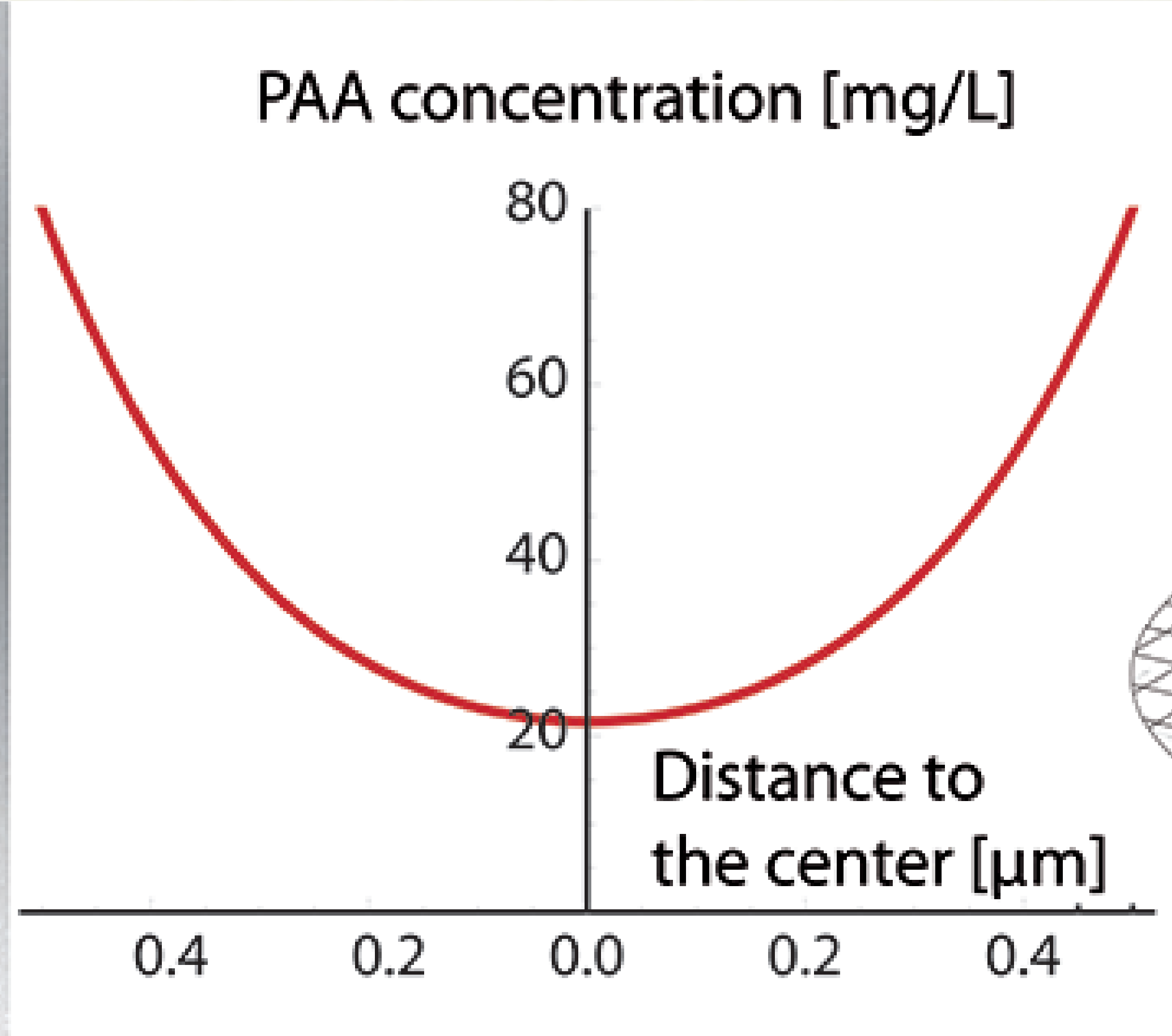
change to spherical coordinates, symmetric aggregates

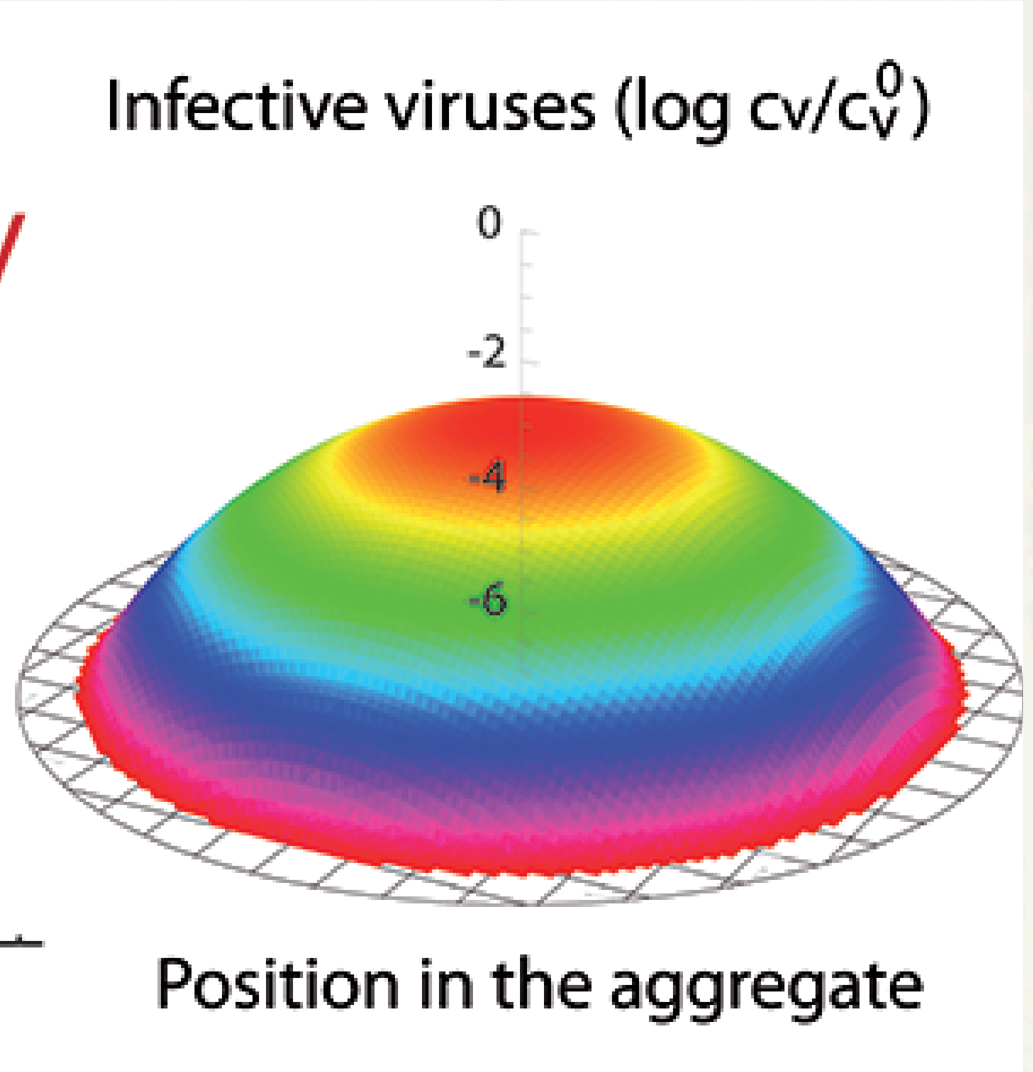
$$\begin{aligned} c_v(r \leq R, t=0) &= c_v^0 \\ \partial_r c_d(r,t)|_{r=0} &= 0 \\ c_d(R,t) &= c_d^0 \end{aligned}$$

Boundary conditions (model: spherical aggregates, no flux at the center, fixed disinfectant concentration at the boundary)

Model for aggregate disinfection





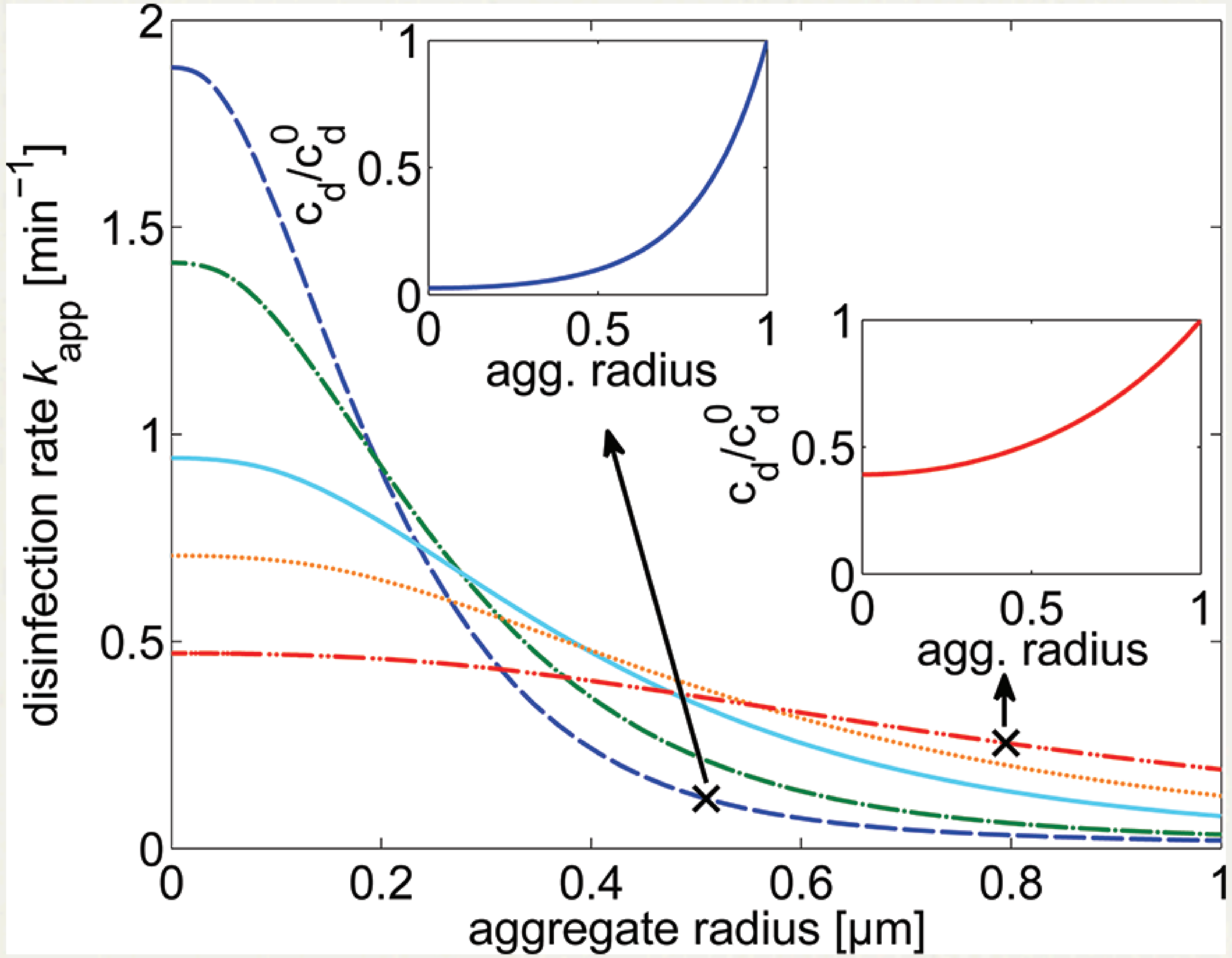


For realistic values of $D \sim 10^{-9}\frac{m^2}{s}$ the disinfectant would reach the center in $t \sim 10^{-3}min$.

Consumption of disinfectant however results in lower disinfectant concentrations towards the center of aggregates (steady state, **equilibrium between diffusion flux and consumption**).

Solution of the equations, see paper on Moodle.

Conclusion on virus disinfection



Red to blue: stronger disinfectants

Stronger disinfectants lead on one hand to a **faster local disinfection** (increased k_1) but on the other hand also to the **disinfectant being consumed faster** (increased k_2). As a result, depending on the aggregate size, **stronger disinfectants can lead to a slower disinfection**.