Spatio-Temporal Structures and Pattern Formation

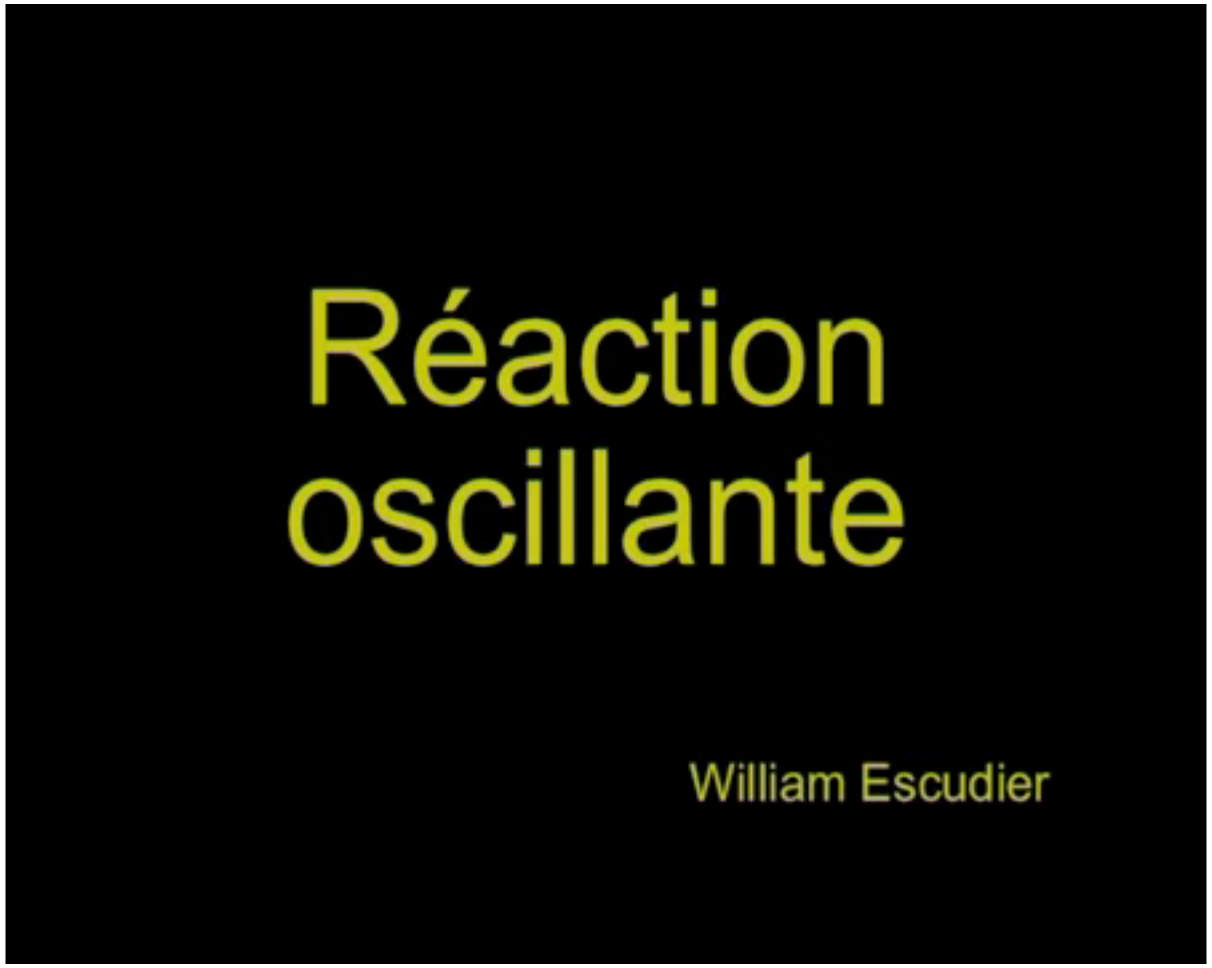
An Overview

this pdf is available online on my home page:
http://itb.biologie.hu-berlin.de/~bordyugov/tut/TBM2010/
or just google up my name and follow the "Teaching" link

What we have done so far: "point systems"

the system under consideration is described by a finite set of dynamical variables

$$\frac{\mathrm{d}u(t)}{\mathrm{d}t} = f(u(t), v(t)),$$
$$\frac{\mathrm{d}v(t)}{\mathrm{d}t} = g(u(t), v(t))$$



well-stirred BZ reaction
http://www.youtube.com/watch?v=Ch93AKJm9os

u, *v*: populations of species, concentrations of chemicals, potential across the cell's membrane, etc.

Next step: Structure in space

BZ reaction in immobilized catalyst

http://www.youtube.com/watch?v=3JAqrRnKFHo

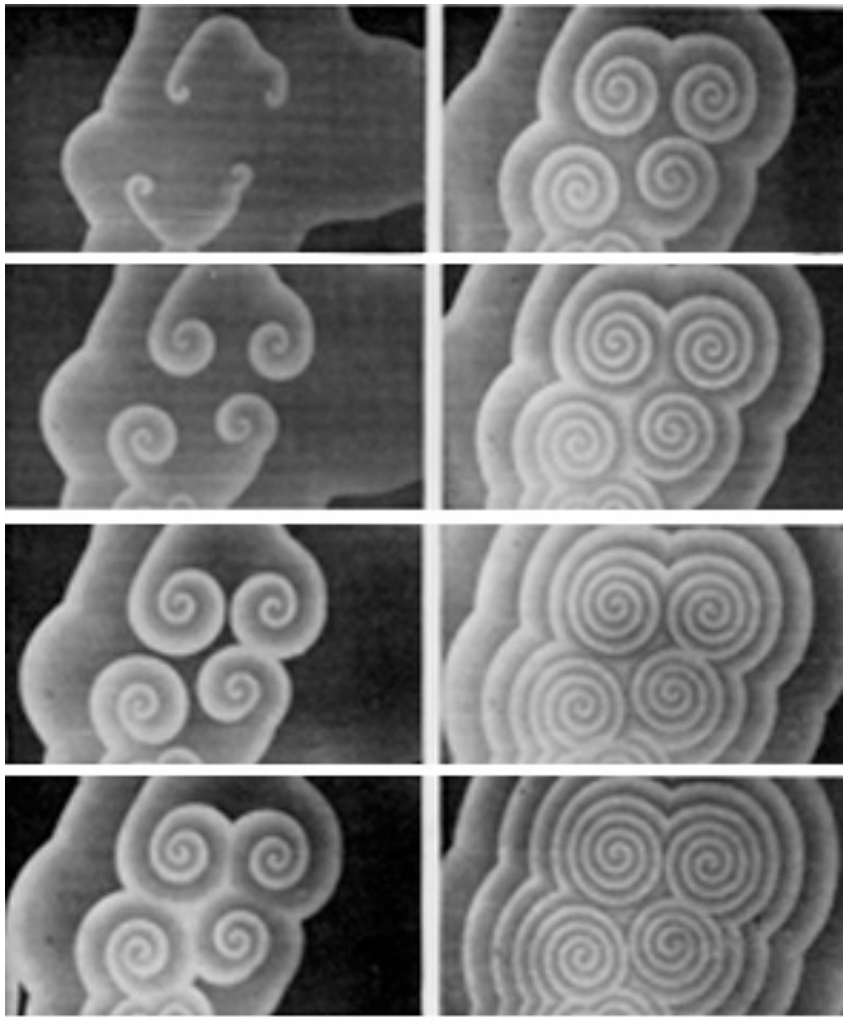


figure from the original Belousov's paper

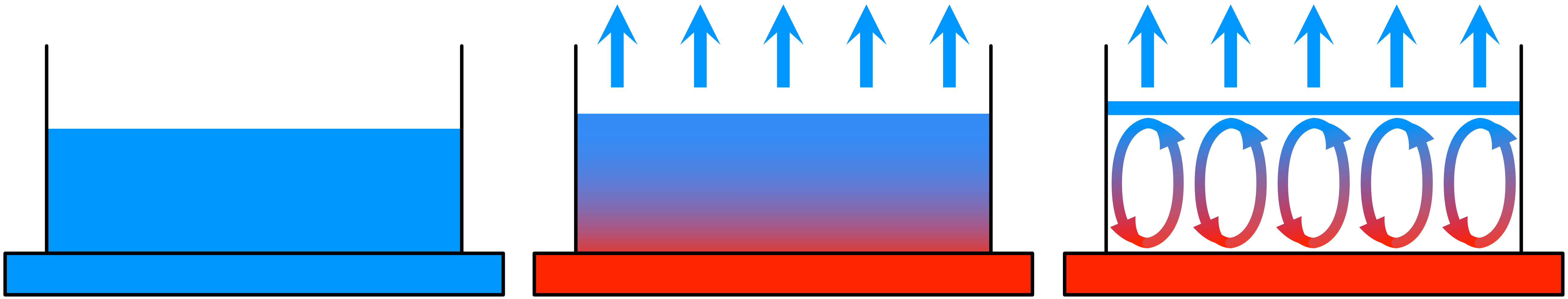
spatial structures in the BZ reaction with non-stirred reactants

$$u\,(t) \longrightarrow u\,(x, y, t)\,,$$

$$v\,(t) \longrightarrow v\,(x, y, t)$$

Rayleigh-Bénard convection

liquid in a temperature gradient



Equilibrium

Conducting solution, macroscopically fluid is not moving

Rolls emerge if temperature diff is too high

Our "observable" is the vertical velocity of the liquid $v(x, z, t)$

Rayleigh-Bénard convection

Benard convection in heated silicone oil

http://www.youtube.com/watch?v=nfvHIfzVnt0

Main idea: due to the interplay of different processes, the homogeneous state can become unstable and a new structure can emerge

Alan Turing on morphogenesis

THE CHEMICAL BASIS OF MORPHOGENESIS

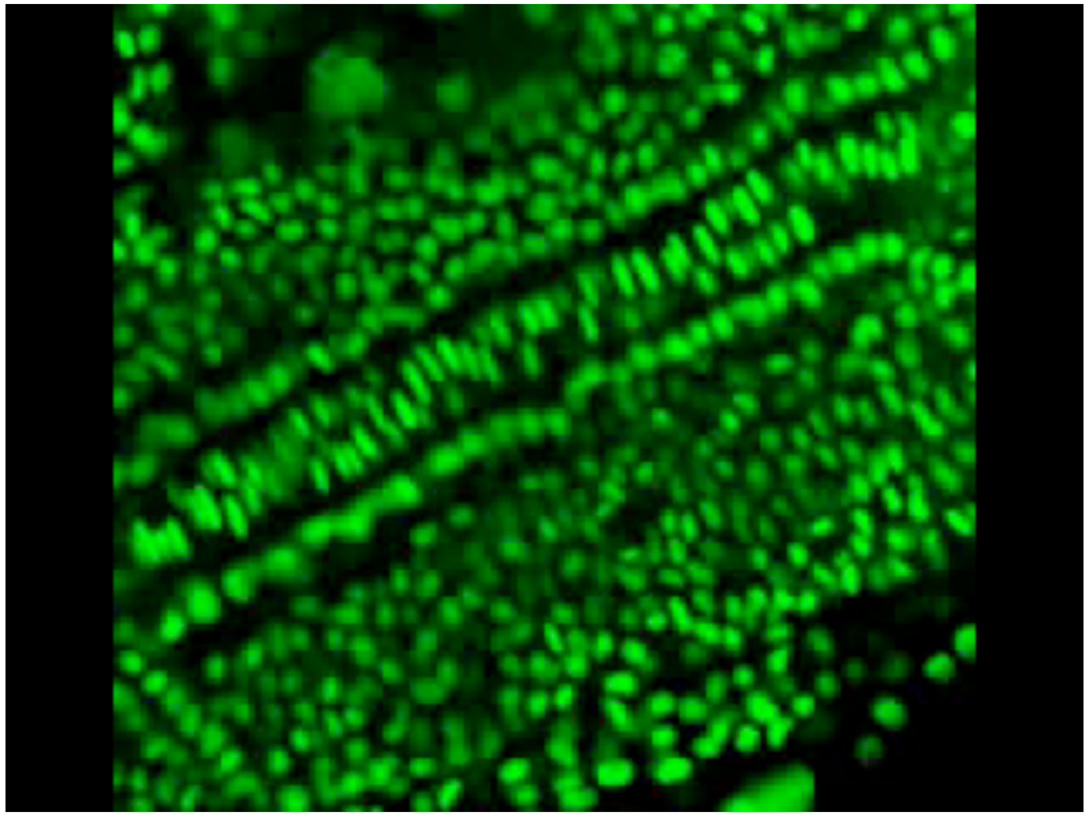
By A. M. TURING, F.R.S. *University of Manchester*

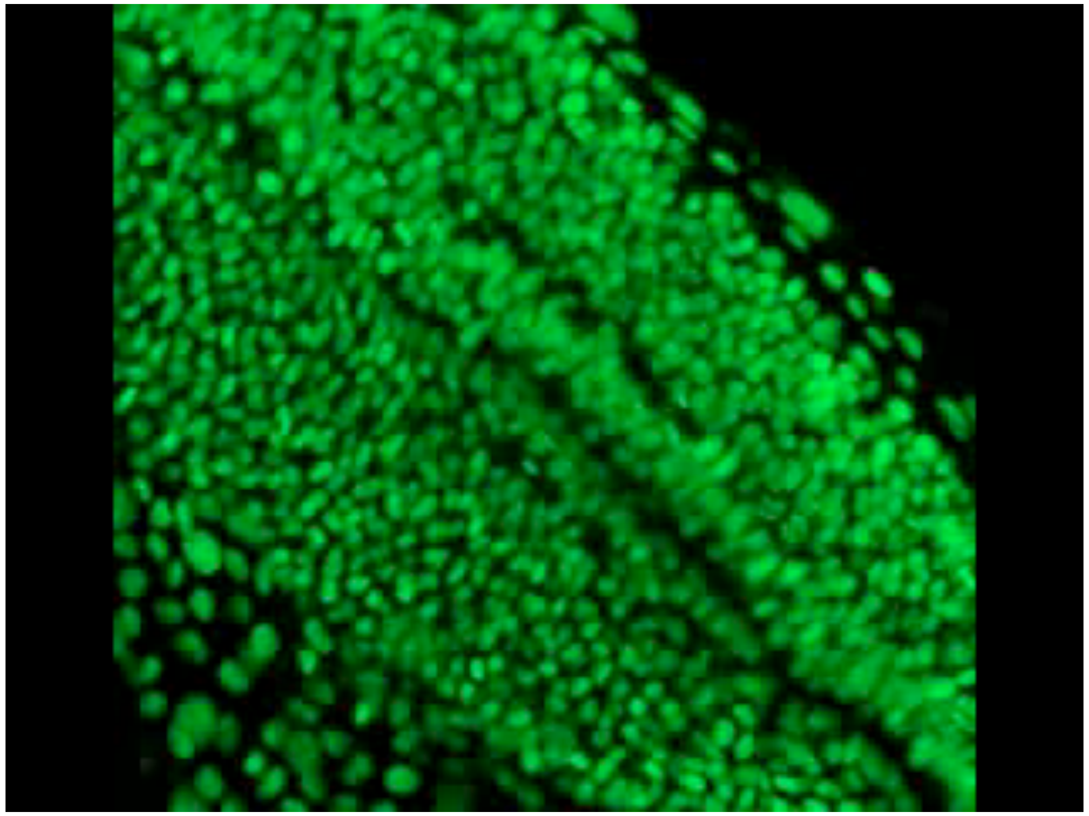
(*Received* 9 *November* 1951—*Revised* 15 *March* 1952)

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

http://www.dna.caltech.edu/courses/cs191/paperscs191/turing.pdf

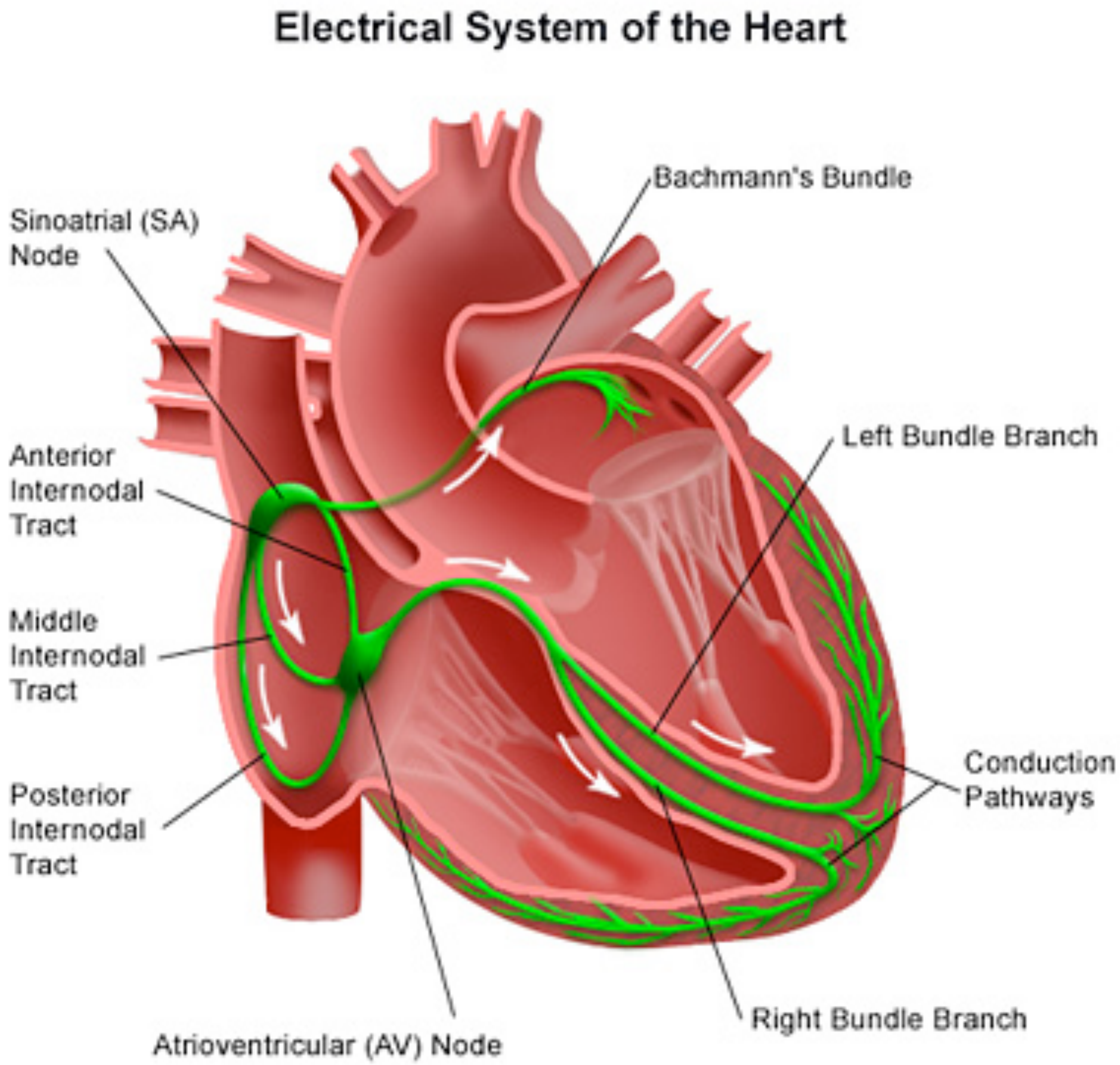
Somite formation in zebrafish

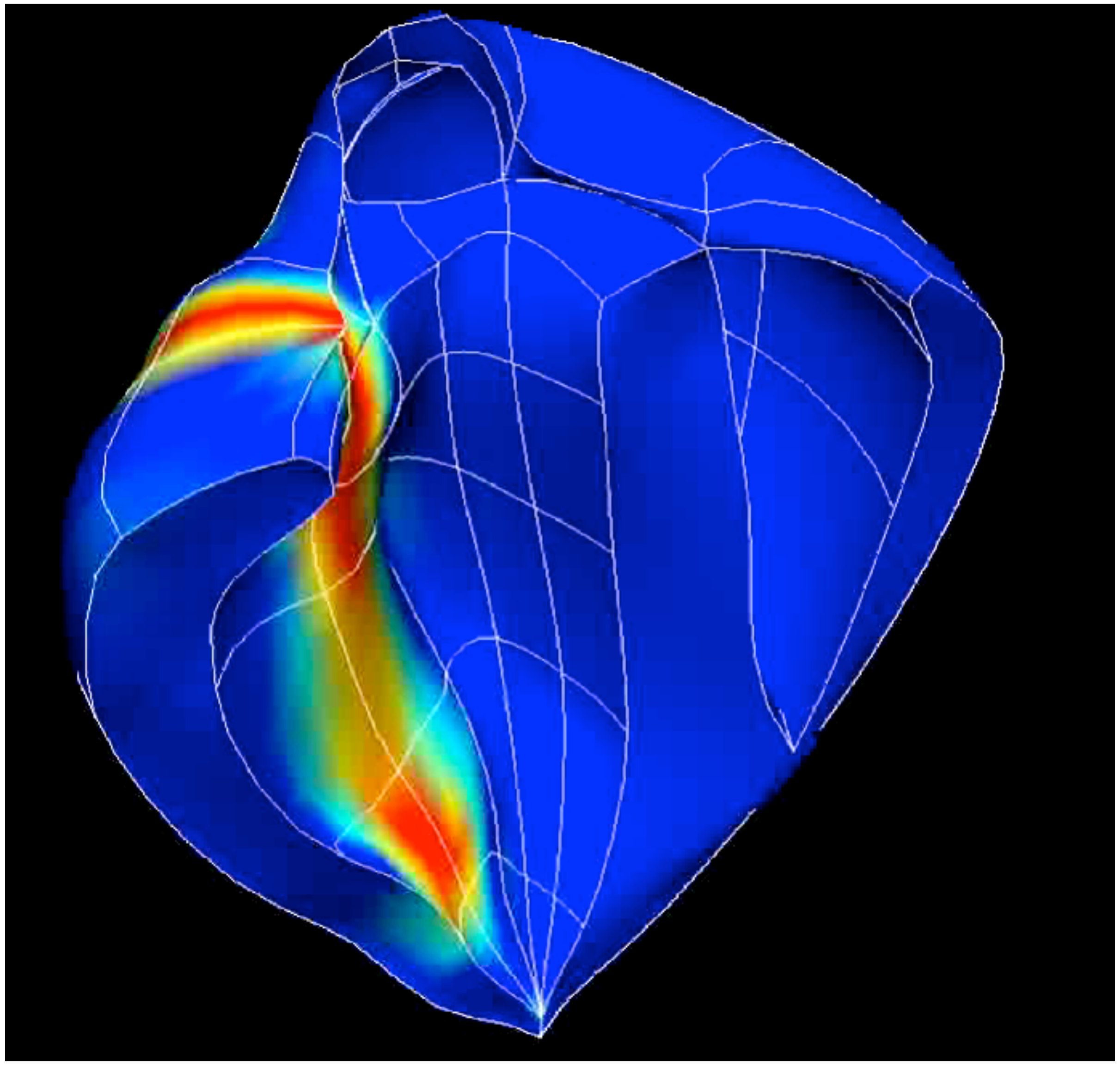




http://www.youtube.com/watch?v=JmLhEd73jRw

Spiral waves in human heart can cause arrhythmias





Computer simulation of human heart by A Panfilov et al

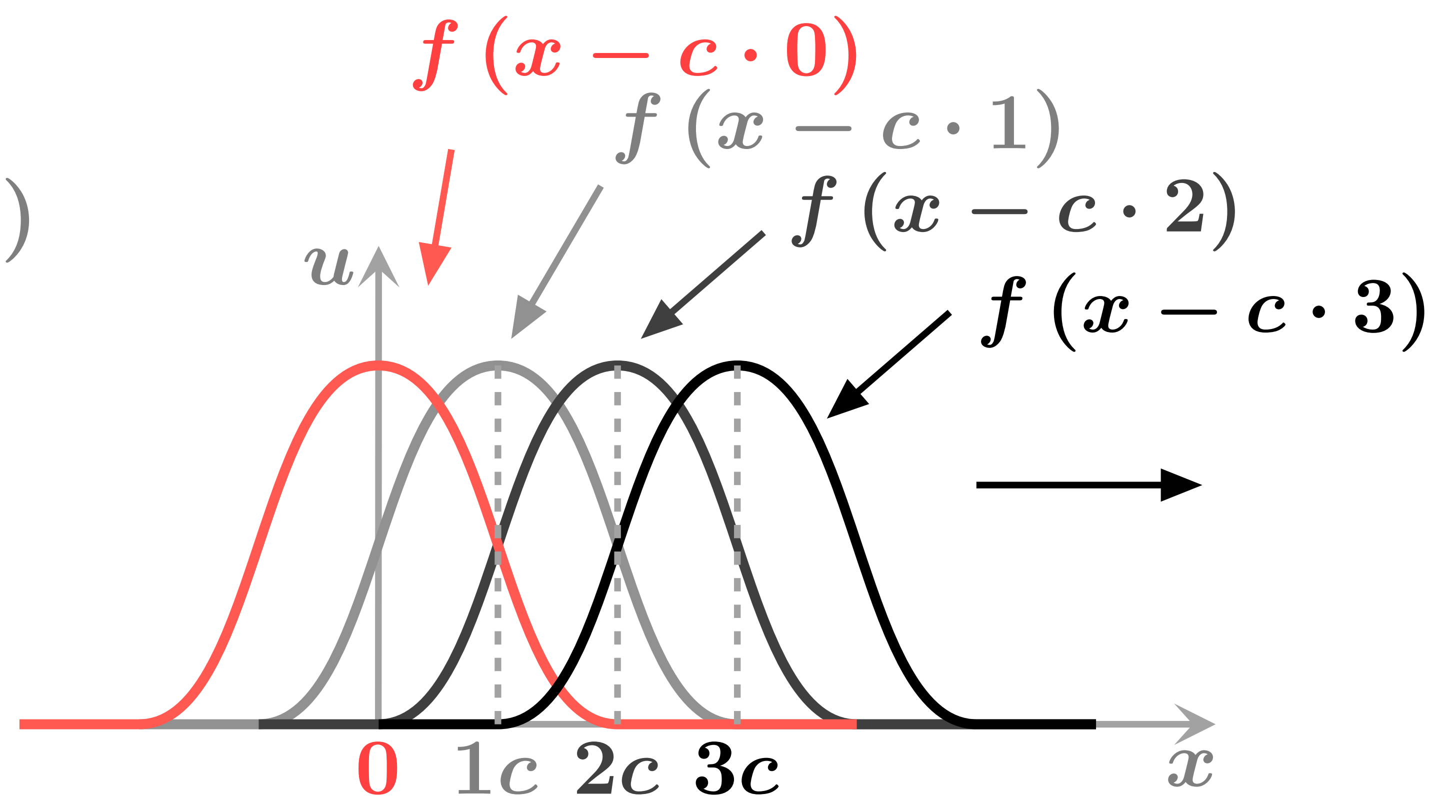
What we have learned:

- structures and patterns are ubiquitous in the (living) nature
- they can spontaneously emerge from homogeneous states under homogeneous conditions
- one obviously needs a more involving mathematics to describe temporal evolution of spatial structures, ODEs are not enough :-(
- modeling of spatio-temporal structures hence needs:
  - more mathematics (PDEs instead of ODEs)
  - more computer power
  - better resolved experimental data to compare to (for instance, a normal ECG cannot resolve the spatial structure of the heart activity)

Example of PDE: Wave equation in 1d

string profile: $u = u(x, t)$

$$u_{tt} = c^2 u_{xx}$$



wave running down the string with a speed c

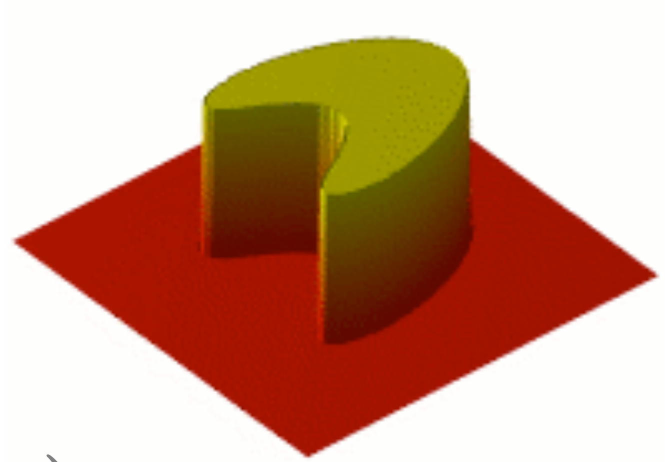
any function in the form of $u(x, t) = f(x - ct)$ will be a solution to the wave equation. Indeed:

$$u_{tt} = (f(x - ct))_{tt} = (-cf'(x - ct))_t = c^2 f''(x - ct)$$
$$u_{xx} = (f(x - ct))_{xx} = (f'(x - ct))_x = f''(x - ct)$$

Heat equation in 2D

Since the observables depend on both time and space, PDEs involve (higher-order) partial derivative with respect to them, for example, the **heat equation**:

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2}$$



temperature at *(x,y)* at moment *t*: $u = u(x, y, t)$

initial condition at *t=0* is a function:

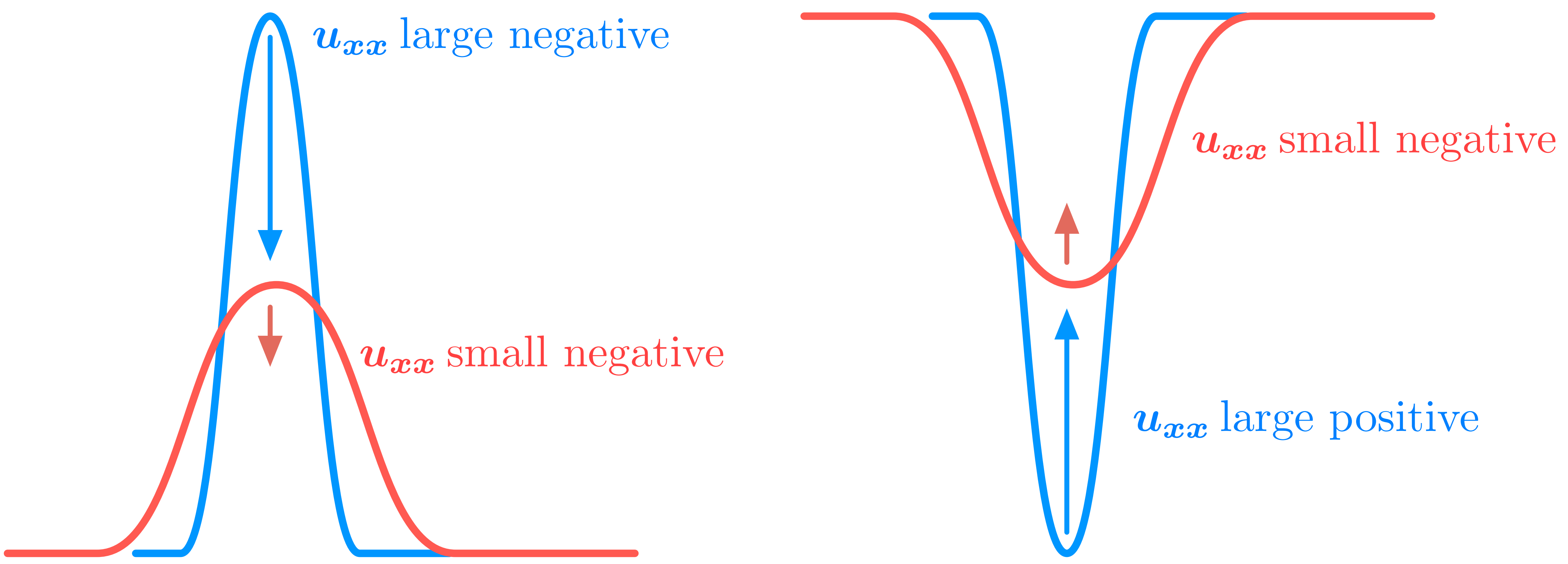
$$u(x, y, t = 0) = u_0(x, y)$$

Reaction-diffusion systems (RDS)

$$u_t = f(u) + D u_{xx}$$

$f(u)$ describes the local reaction kinetics, can be nonlinear!

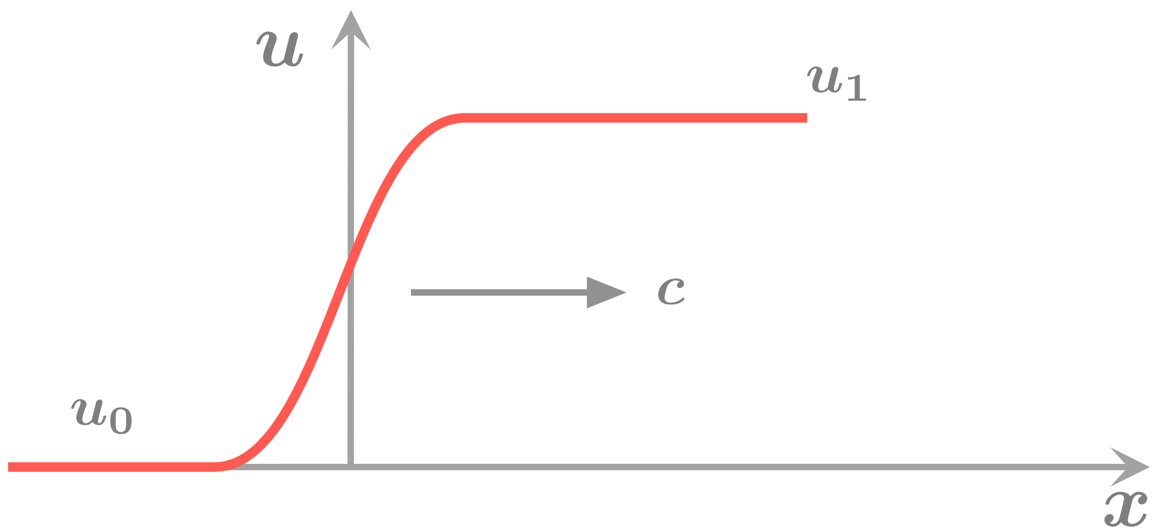
$D u_{xx}$ describes the diffusion of u, D - diffusion coef.



the role of diffusion in smoothening out the inhomogeneities

Fronts in RDS

$$u_t = f(u) + Du_{xx}$$



$f(u_{0,1}) = 0$ homogeneous stable steady states

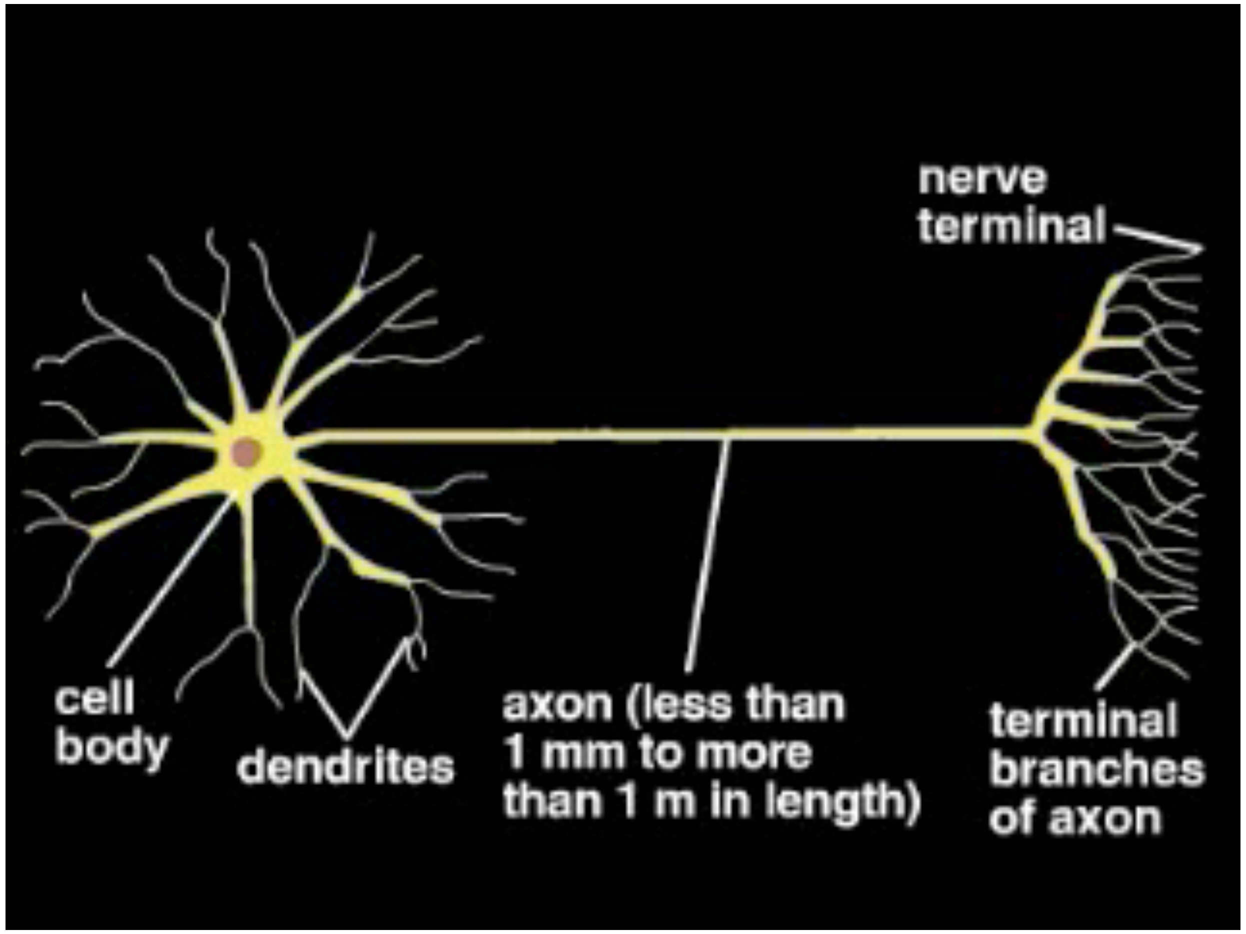
wave of transition between two otherwise stable states

propagation of fire fronts

the front profile and its speed doesn't depend on the initial conditions!!!

Action potential propagation and excitable media

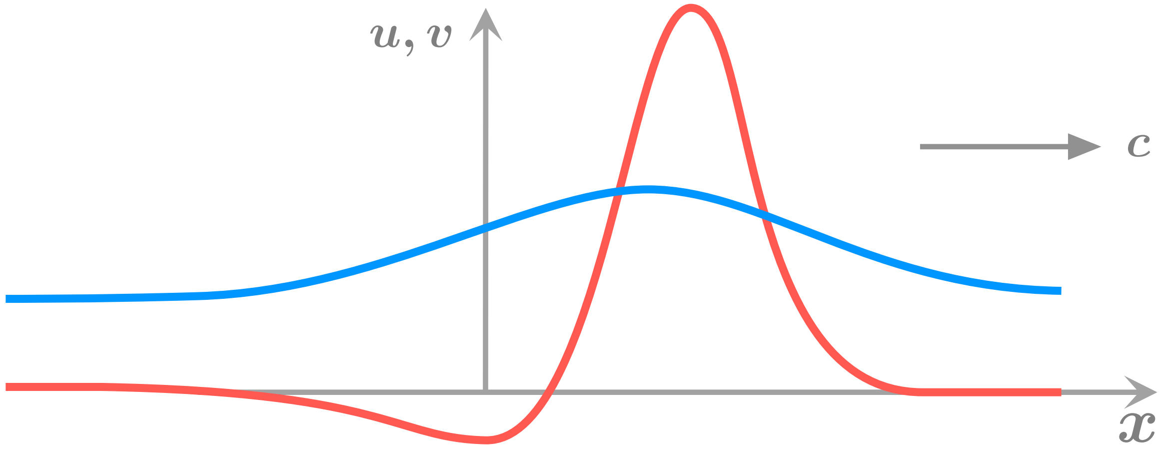
$$u_t = f(u,v) + D_u u_{xx},$$
$$v_t = g(u,v) + D_v v_{xx}$$



models propagation of the action potential along the axons of giant squids

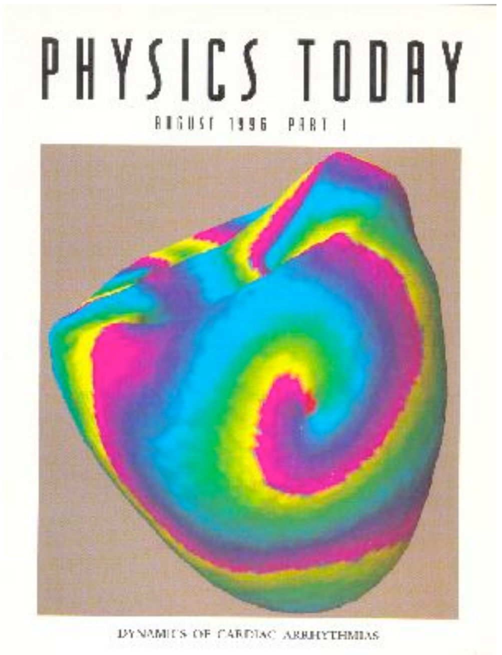
u - action potential variable

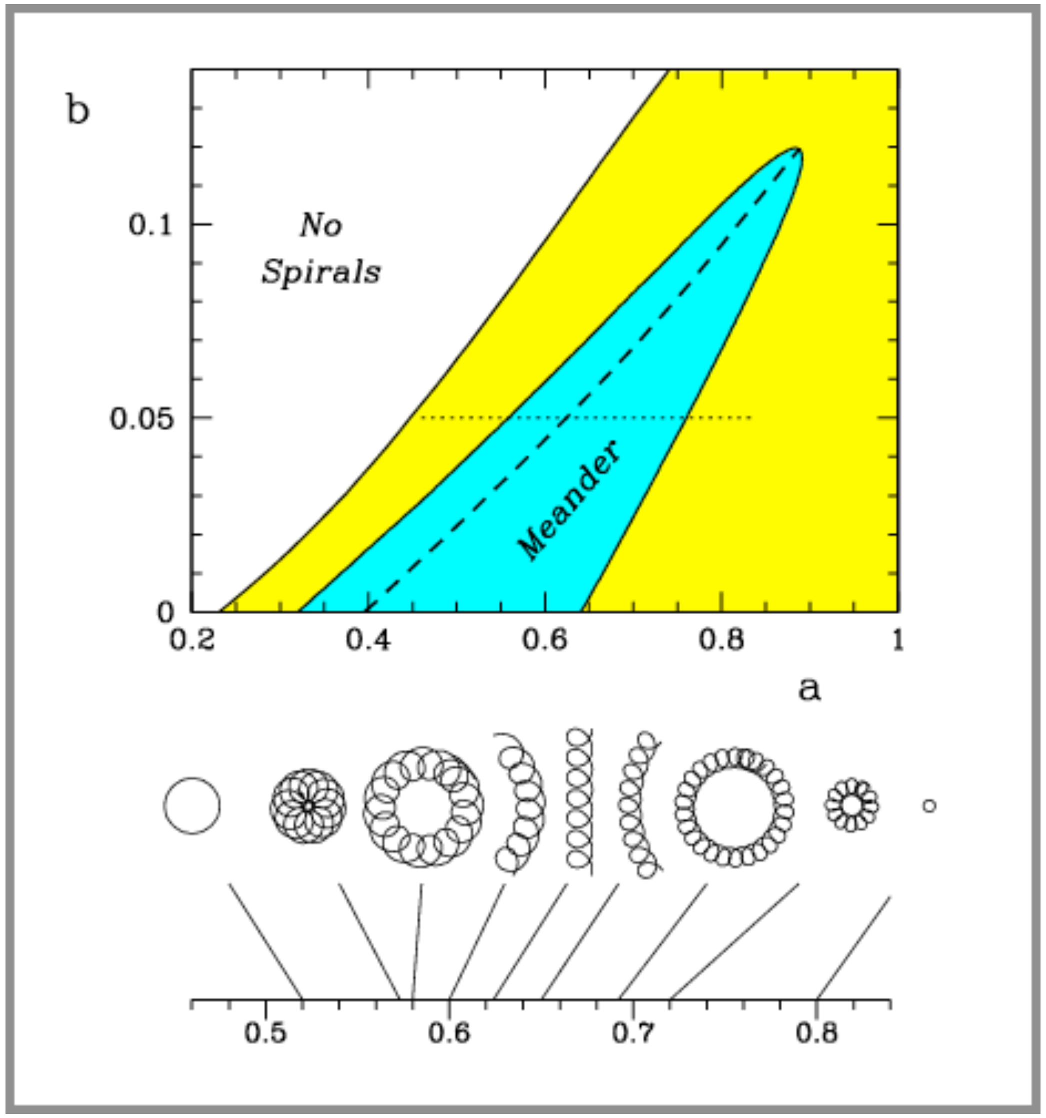
v - the recovery (slow) variable



Spiral waves in 2D Barkley model

$$u_t = \epsilon^{-1} u \left(1 - u\right) \left(u - \left(v + b\right)/a\right) + \Delta u,$$
$$v_t = u - v.$$





$\Delta = \partial_{xx} + \partial_{yy}$

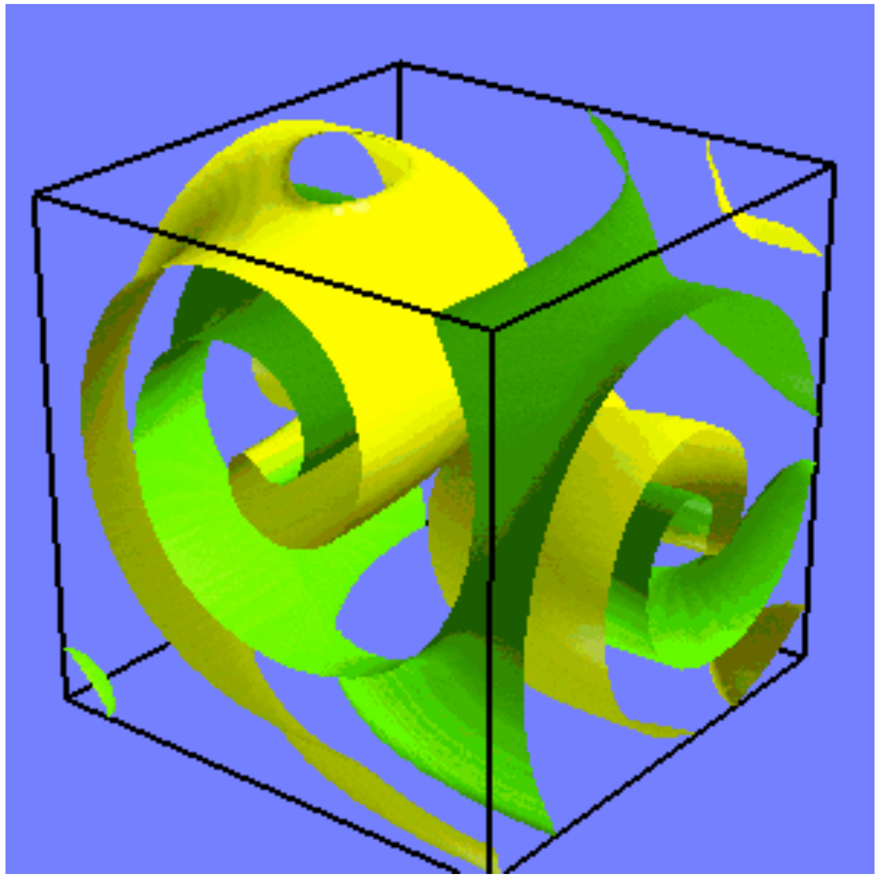
$\epsilon \ll 1$ time-scale separation

a, b parameters

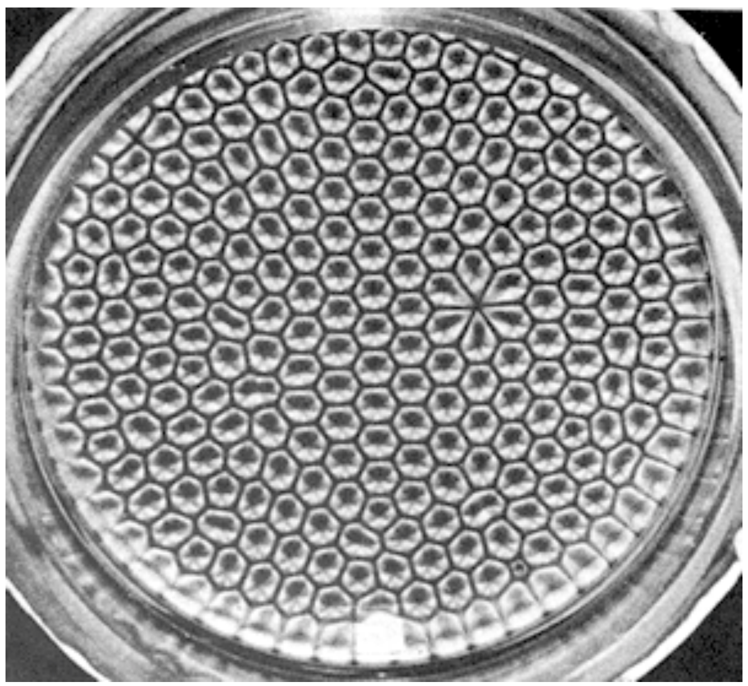
spirals come in two flavors:
rigidly rotating
and meandering

Questions about spirals

- How their rotational frequency is chosen?
- The reason spirals don't care about boundaries being non-localized
- Why they start to meander
- Inward/outward meander
- 3D scroll waves



Symmetries



another picture
of Benard cells

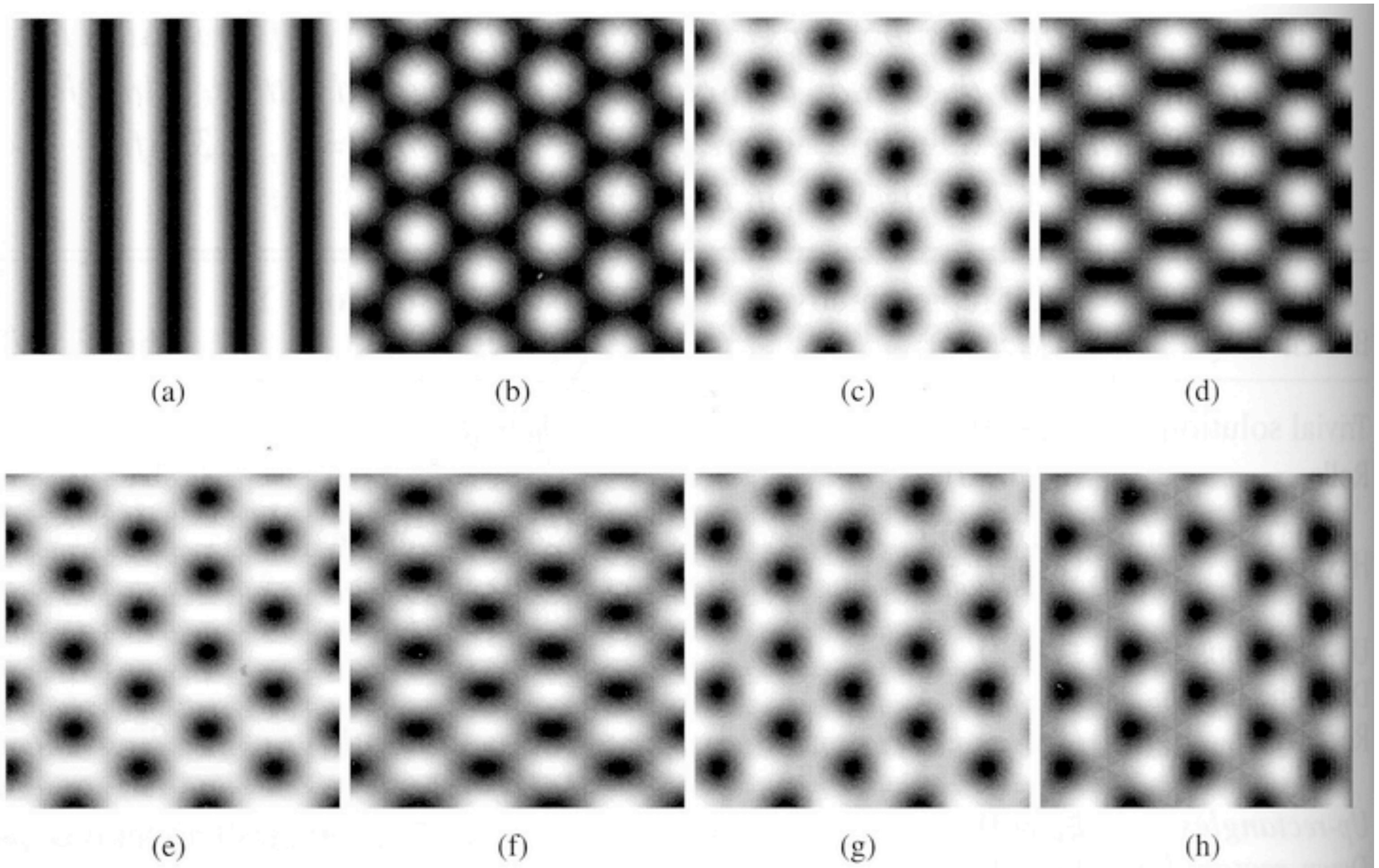


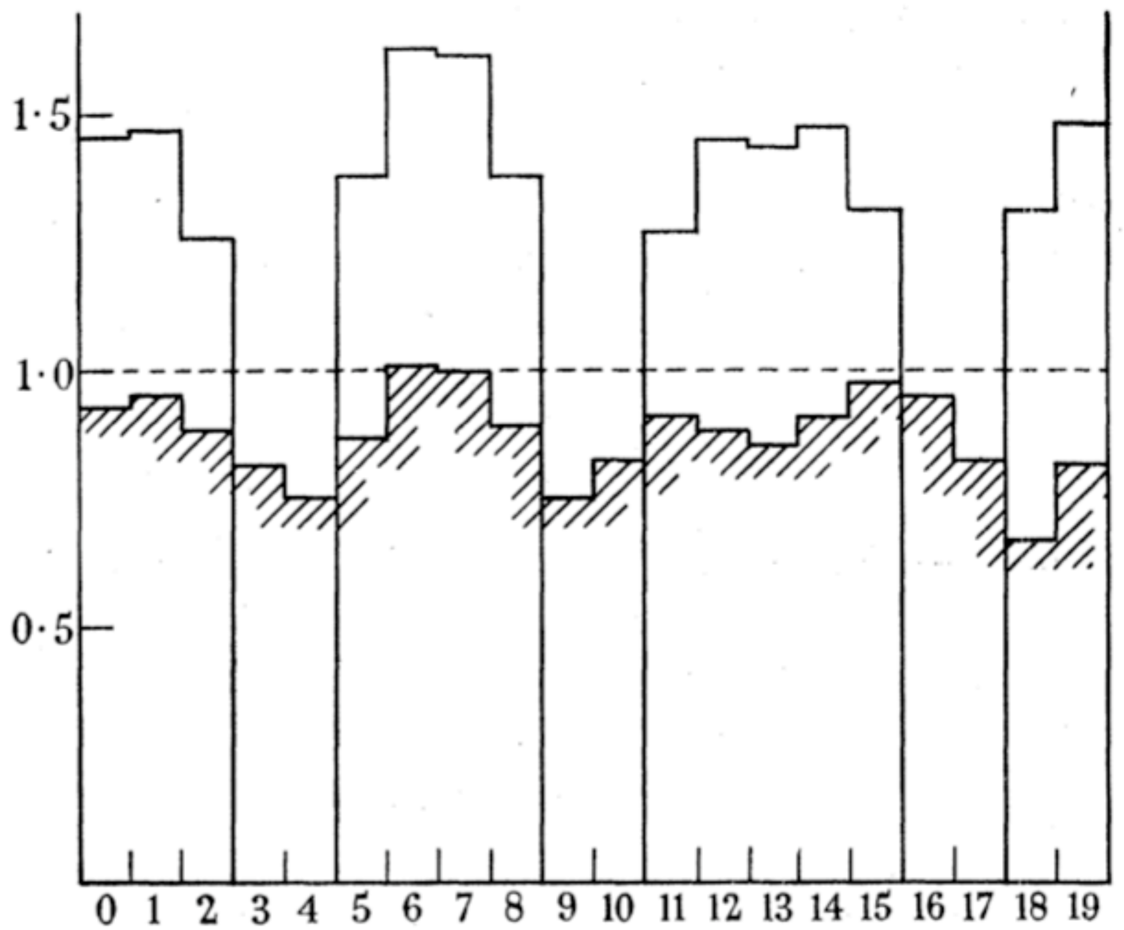
Fig. 5.7. Greyscale plots of some solutions on the hexagonal lattice: (a) rolls, (b) up hexagons, (c) down hexagons, (d) up rectangles, (e) down rectangles, (f) patchwork quilt, (g) triangles and (h) regular triangles.

a priori knowledge of the problem symmetries can help to predict the emerging pattern

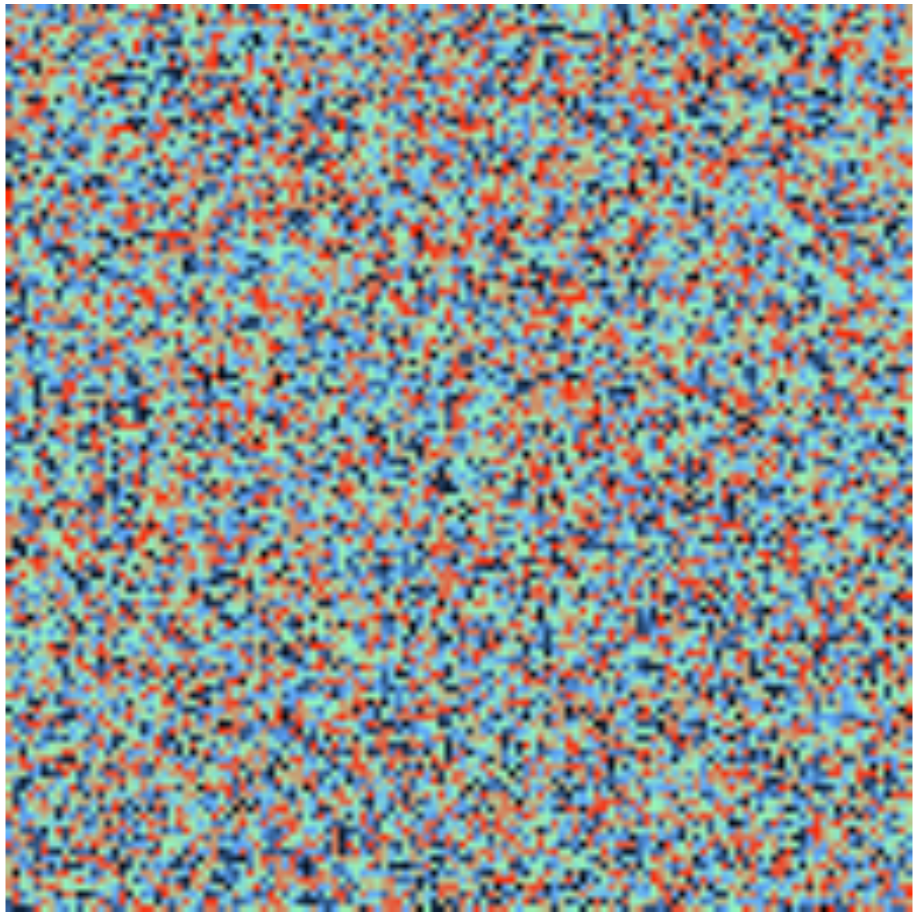
Numerics for PDEs

- even stiff ODEs can be solved by brute force with small time steps, this doesn't apply to PDEs. For example, the explicit Euler scheme for the simplest PDE $u_t = u_x$ is unstable, no matter how small your time step is.
- implicit schemes (backward Euler or Crank-Nicolson) are needed, they involve heavy linear algebra calculations: solving linear systems with large number of unknowns
- you are happy if doubling the number of grid points just doubles your computation time (and not multiplies it by four or eight, as it often is the case)
- much fewer standard tools for numerical analysis, full-scale bifurcation analysis software must be hand-coded

Turing instability



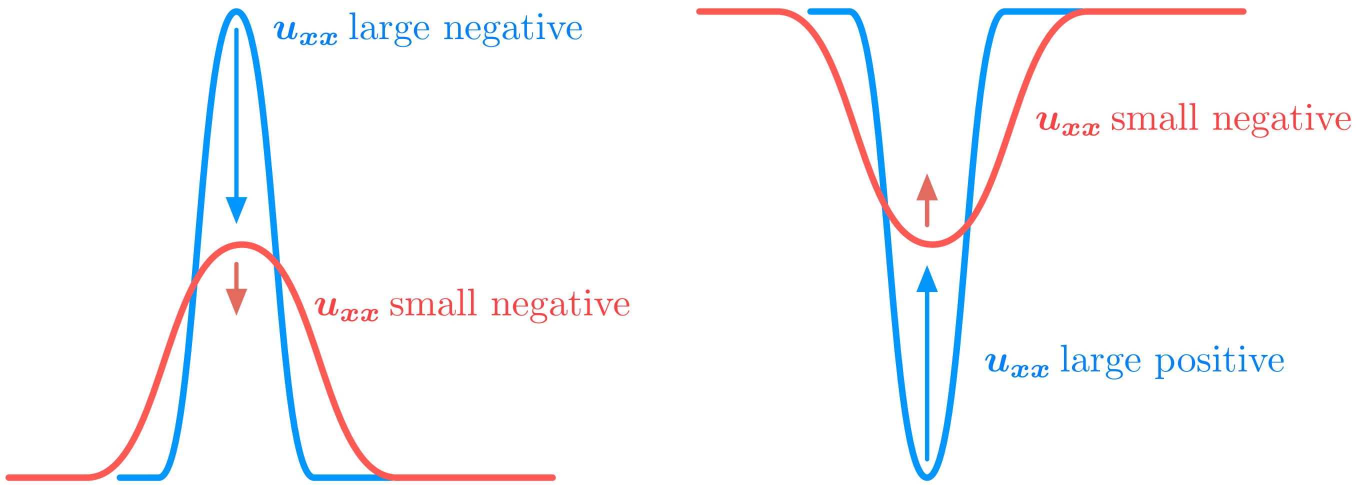
from original paper by A Turing



modern computer simulation

Turing instability

$$u_t = f(u,v) + D_u u_{xx},$$
$$v_t = g(u,v) + D_v v_{xx}$$



Suppose that $u = v = 0$ is a steady state without diffusion:

$$f(0,0) = g(0,0) = 0$$

Can diffusion (smoothening process by itself) lead to an instability of the zero steady state?

Turing instability

Now concentrate on small perturbation of the zero steady state

$$|u|, |v| \ll 1$$

$$f(u,v) = \underbrace{f(0,0)}_{=0} + \underbrace{f_u(0,0)}_{\overset{\text{def}}{=} a} u + \underbrace{f_v(0,0)}_{\overset{\text{def}}{=} -b} v,$$

$$g(u,v) = \underbrace{g(0,0)}_{=0} + \underbrace{g_u(0,0)}_{\overset{\text{def}}{=} c} u + \underbrace{g_v(0,0)}_{\overset{\text{def}}{=} -d} v$$

Taylor expansion of the first order at *(u,v)* = *(0,0)*

Turing instability: linearized Eqs

close to the steady state we have

$$u_t = au - bv + D_u u_{xx},$$
$$v_t = cu - dv + D_v v_{xx}$$

stability without diffusion:

$$u_t = au - bv,$$
$$v_t = cu - dv$$

$$u(t) = u_0 \mathrm{e}^{\sigma t}, \quad v(t) = v_0 \mathrm{e}^{\sigma t}$$

$$\sigma = \frac{a - d \pm \sqrt{(a+d)^2 - 4bc}}{2} < 0$$

by the imposed stability w/o diff ==> $a < d, \quad ad < bc$

Turing instability: linearized Eqs

$$u_t = au - bv + D_u u_{xx},$$
$$v_t = cu - dv + D_v v_{xx}$$

solution Ansatz:

$$u(x,t) = u_0 \mathrm{e}^{\mathrm{i}kx+\sigma t},$$
$$v(x,t) = v_0 \mathrm{e}^{\mathrm{i}kx+\sigma t}$$

$$\partial_{xx} u(x,t) = -k^2 u_0 \mathrm{e}^{\mathrm{i}kx+\sigma t}$$

$$\boxed{\sigma \begin{pmatrix} u_0 \\ v_0 \end{pmatrix} = \begin{pmatrix} a - D_u k^2 & -b \\ c & -d - D_v k^2 \end{pmatrix} \begin{pmatrix} u_0 \\ v_0 \end{pmatrix}}$$

results in the characteristic equation for σ:

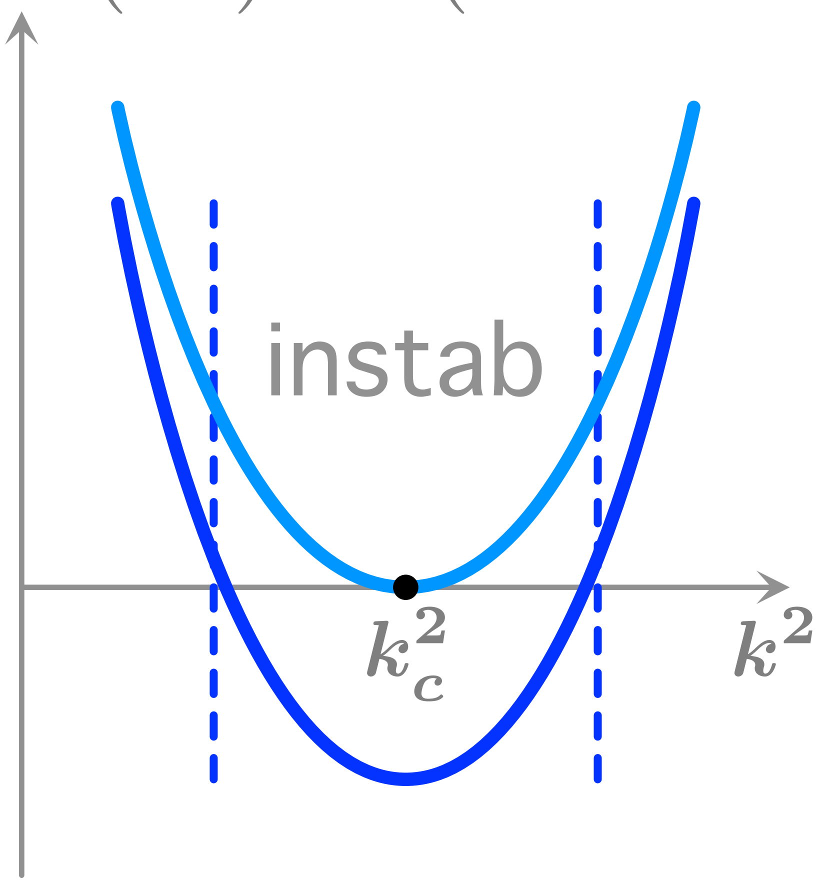
$$\sigma^2 + \sigma\left((D_u + D_v)k^2 - a + d\right) + \\ + \left(D_u k^2 - a\right)\left(D_v k^2 + d\right) + bc = 0$$

product of roots is given by the free term:

$$h\left(k^2\right) = \left(D_u k^2 - a\right)\left(D_v k^2 + d\right) + bc$$

Turing instability: the critical wave number

$$h\left(k^2\right) = \left(D_u k^2 - a\right)\left(D_v k^2 + d\right) + bc$$



critical condition:

$$\frac{\left(dD_u - aD_v\right)^2}{4D_u D_v} = bc - ad$$

critical wave number:

$$k_c^2 = \frac{1}{2}\left(\frac{a}{D_u} - \frac{d}{D_v}\right)$$

minimal value of h:

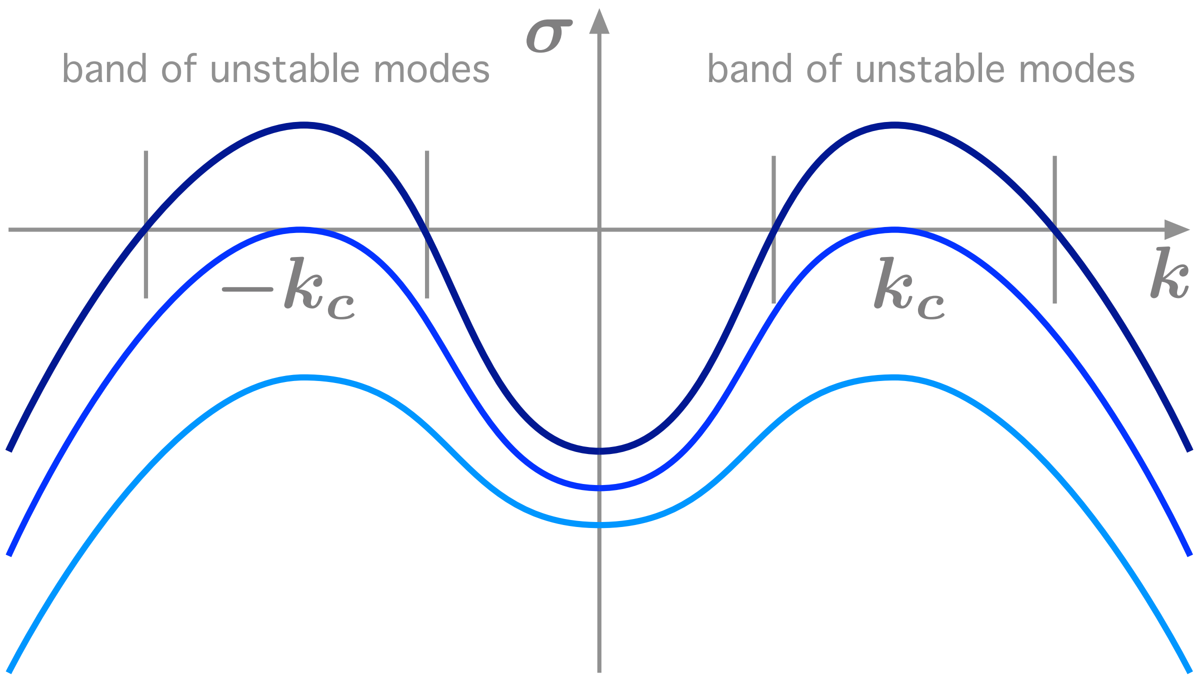
$$h_{\min} = -\frac{\left(dD_u - aD_v\right)^2}{4D_u D_v} - ad + bc$$

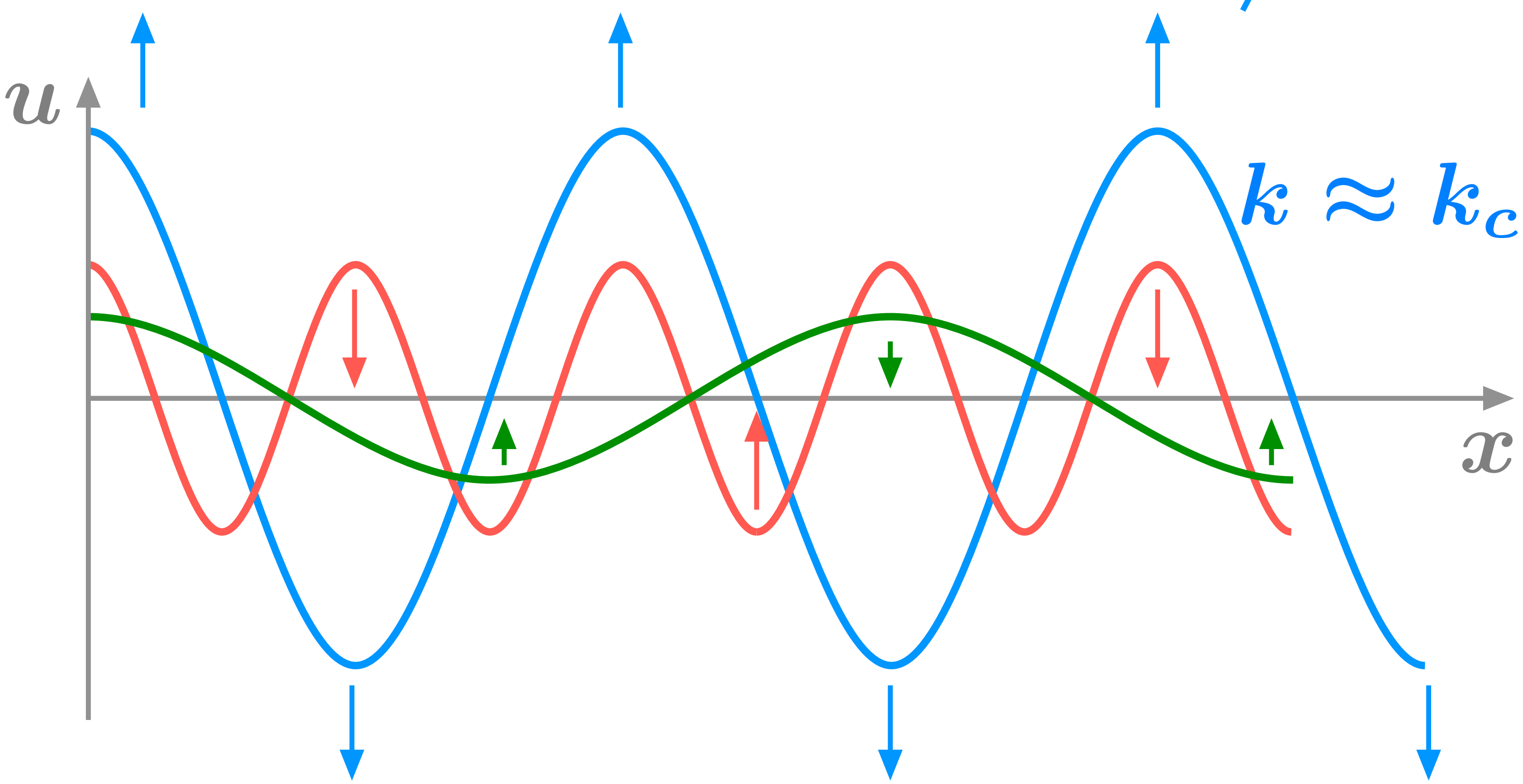
Turing instability: the dispersion relation

solution Ansatz:

$$u(x,t) = u_0 \mathrm{e}^{\mathrm{i}kx+\sigma t},$$

$$v(x,t) = v_0 \mathrm{e}^{\mathrm{i}kx+\sigma t}$$





modes with wave numbers close to the critical one grow, others decay, thus a preferred wavelength of the pattern is selected

Turing instability: Conclusions

- contra-intuitively, diffusion can result in an instability with a characteristic wave length
- linear stability analysis can predict this length scale
- beyond instabilities, further analysis is needed (reduced equations for the amplitude of the emerging mode, expansions in higher-order terms)