Reaction-diffusion systems

$$\frac{\partial \mathbf{u}}{\partial t} = D\nabla \mathbf{u} + \vec{F}(\mathbf{u})$$

$\mathbf{u} = (u_1, \ldots u_m)$ is the unknown vector, of densities of different (chemical) species. D is (usually) a diagonal $m \times m$ matrix of (positive) diffusions. Often the boundary conditions are Neumann homogeneous (container walls).

By extension, the term R-D is often used to mean general semilinear parabolic equations like (scalar case)

$$u_t = D\nabla^2 u + f(x, u, \nabla u).$$

The *lumped* or *homogeneous* reaction (stirred, agitated) would be modelled by $\frac{d}{dt}\mathbf{u} = \vec{F}(\mathbf{u})$.

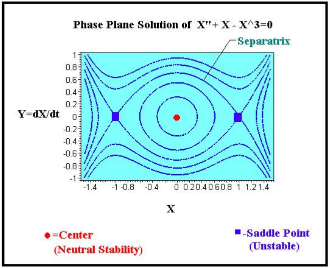
One dimensional scalar reaction-diffusion equations

Example 1: Allen-Cahn nonlinearity, $u_t = u_{xx} + u - u^3$.
It has the form $u_t = u_{xx} - W_u(u)$, with the *(chemical) potential* $W(u) = \frac{1}{4} - \frac{1}{2}u^2 + \frac{1}{4}u^4$.
The *free energy* $H[u] = \int \left(\frac{1}{2}u_x^2 + W(u)\right)\, dx$, Dirichlet + potential, decreases with time except at equilibria. Its critical points are these equilibrium (steady-state) solutions.
There are two absolute minima of H, namely $u \equiv \pm 1$. The equilibrium $u \equiv 0$ is a saddle point.

Problem 4.1:
Prove that $u \equiv 0$ is a saddle point of H (with $W(u) = -\frac{1}{2}u^2 + \frac{1}{4}u^4$).

Allen-Cahn equation is a simplified model for the disaggregation of some metallic alloys. There are two stable states (reaction), and the state of a group of particles is influenced by the state of their neighbours (diffusion). The unknown u is a *phase field* (an *order parameter*). Allen-Cahn is in fact a simplified model of the Cahn-Hilliard model, a pde of 4rth order in space.

But there are more equilibrium solutions. One can look at the phase plane, the curves $\frac{1}{2}u_x^2 - W(u)$ =constant.



Important solutions are these two continua of (monotonic) equilibria of coexistence or *layer* type: $u = U(x - x_0)$ and $u = U(-x + x_0)$ (heteroclinic).

Problem 4.2: Find the analytic expression of $U(x)$.

One can prove that these heteroclinic solutions are local minimizers of H, so they are also stable solutions. The stable solutions are $u = \pm 1$ and the families $u = U$.

There is a simple argument of the Maximum Principle type that shows the stability in some sense of these U-solutions (essentially, a use of sub- and super-solutions): if $u(x, t_0) \leq U(x)$, for all x, then the inequality will continue to hold for $t > t_0$. We will not make a complete proof of this fact, but observe that if $u(t_1, x_0) = U(x_0)$, then

$$u_t(x_0, t_1) = (u(x_0, t_1) - U(x_0))_t = u_{xx}(x_0, t_1) - U_{xx}(x_0) \leq 0$$

This means that if $u(x, t_0)$ is trapped between two of these U solutions, $U(x + C_1) \leq u(x, t_0) \leq U(x + C_2)$, then it will continue to be trapped for $t > t_0$.

We can imagine a typical time evolution as a fast approximation to a multiple layer solution and then a slow change to merging among layers to a simple layer or to a homogeneous state

https://www.youtube.com/watch?time_continue=1&v=WsnloyUQnjE

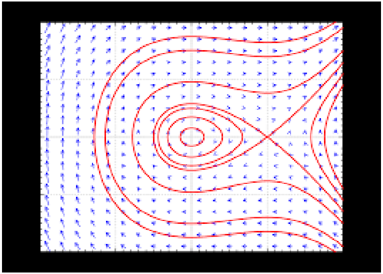
https://www.youtube.com/watch?v=QQCr2g6jDsM

https://en.wikipedia.org/wiki/Cahn-Hilliard_equation

https://www.youtube.com/watch?v=dhn1QIzHYsU

Example 2: Fisher or Kolmogorov-Petrovsky-Piskounof nonlinearity, $u_t = u_{xx} + u - u^2$. One restricts to nonegative solutions (u is a concentration or a probability density).
It also has the form $u_t = u_{xx} - W_u(u)$, with the *potential* $W(u) = -\frac{1}{2}u^2 + \frac{1}{3}u^3$. Here also the *free energy* $\int \left(\frac{1}{2}u_x^2 + W(u)\right)\ dx$, Dirichlet + potential, decreases with time. Its critical points are equilibrium (steady-state) solutions, $u \equiv 1$ is the absolute minimum (among non-negative solutions), and $u = 0$ is a saddle-point.
For the ODE ($u \equiv u(t)$) $u_t = u - u^2$ we have two equilibrium points, $u = 0$ (unstable) and $u = 1$ (stable) and a connection between them (from $u = 0$ to $u = 1$). So, the system has a trend to leave the value zero and go to the value one.
Problem 4.3: Find the analytic expression of this connection. Has it something to do with the *Logistic model*?
FKPP is a model for invasions. Either of biological populations or of chemical species. Population $u = 1$, with a lower potential, invades population $u = 0$, less prepared for the competition.

In FKPP we look for *Traveling Wave* solutions $u(x,t) = V(x-ct)$ with $V(-\infty) = 1$ and $V(+\infty) = 0$, when $c > 0$, or $V(-\infty) = 0$ and $V(+\infty) = 1$, when $c < 0$. These are solutions of $V_{xx} + cV_x + V - V^2 = 0$ The phase portrait can be drawn after that of $c = 0$ ($\frac{1}{2}u_x^2 - W(u) =$const.), if we imagine cV_x as a dissipation/activation term ($x \sim$ auxiliary time).



Problem 4.4: In FKPP, show that for each $c > 0$ there exists a traveling wave solution of speed c. Show that they are oscillatory for $c < 2$ (with sign oscillations too) and monotonically decreasing for $c \geq 2$.

It is known that the traveling wave with $c = 2$ is more relevant, in the sense that if an initial condition $u(x, 0)$ is monotonic and continuous with $u(x, 0) = 1$ for $x < x_0$ and $u(x, 0) = 0$ for $x > x_1$ then the solution $u(x, t)$ approaches the $c = 2$ traveling wave as $t \to \infty$.

One can also imagine initial conditions being zero except between x_0 and x_1 and evolving into two traveling waves, one moving forwards and the other backwards.

In the *fractional diffusion* F/KPP equation $u_t = -(-\partial_x^2)^\alpha u + u - u^2$, $0 < \alpha < 1$ similar phenomena occur, but the "traveling waves" move with a speed that grows exponentially in time (Cabré and Roquejoffre, 2013).

Reaction-diffusion systems

Example 3: Consider the reaction $u + v \rightleftharpoons 2v$ (called *autocatalytic*).

$$\frac{d}{dt}u = -uv + v^2$$

$$\frac{d}{dt}v = uv - v^2,$$

when the stechiometric coefficients are 1. (affinity=product of concentrations, law of mass action).
If we take diffusions into account, we get the R-D system

$$\frac{\partial}{\partial t}u = D_u \nabla^2 u - uv + v^2$$

$$\frac{\partial}{\partial t}v = D_v \nabla^2 v + uv - v^2$$

Let's consider the more general case

$$\frac{\partial}{\partial t}u = D_u \nabla^2 u + f(u, v)$$

$$\frac{\partial}{\partial t}v = D_v \nabla^2 v + g(u, v).$$

Suppose $f(u_0, v_0) = g(u_0, v_0) = 0$, so $u \equiv u_0, v \equiv v_0$ is an equilibrium solution of the homogeneous ODE system.
Suppose that (u_0, v_0) is stable for the ODE. It is a quite surprising fact that (u_0, v_0) can be unstable for the PDE, if the diffusion coefficients D_u and D_v are different, and chosen appropriately. This is Turing instability.
To observe Turing instability is enough to look at the linearized system around (u_0, v_0).

Theorem (A. Turing, 1952): Suppose that M is a 2×2 matrix with all of its eigenvalues satisfying $Re(\lambda) < 0$ and of one of the following four sign-types

$$\begin{pmatrix} + & - \\ + & - \end{pmatrix}, \begin{pmatrix} - & + \\ - & + \end{pmatrix}, \begin{pmatrix} + & + \\ - & - \end{pmatrix} \text{ or } \begin{pmatrix} - & - \\ + & + \end{pmatrix}.$$

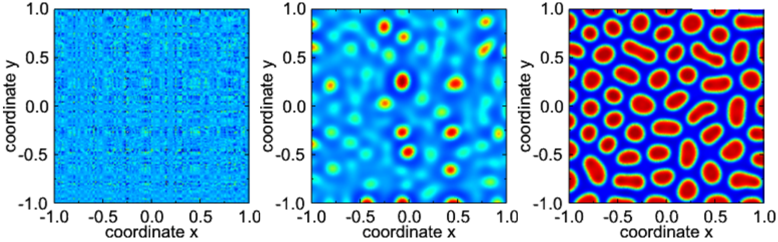
Then, there exist positive numbers D_u and D_v such $(u, v) = (0, 0)$ is an unstable solution of

$$\frac{\partial}{\partial t}\begin{pmatrix} u \\ v \end{pmatrix} = \begin{pmatrix} D_u \nabla^2 u \\ D_v \nabla^2 v \end{pmatrix} + M \begin{pmatrix} u \\ v \end{pmatrix}$$

Problem 4.5: Prove Turing's Theorem in the first of the four sign-type cases. Hint: look for unstable solutions of the PDE system of the form $u = A(t)e^{i\omega x}, v = B(t)e^{i\omega x}$ for some ω (one space dimension). Take one of the diffusivities to be ε and the other 1.

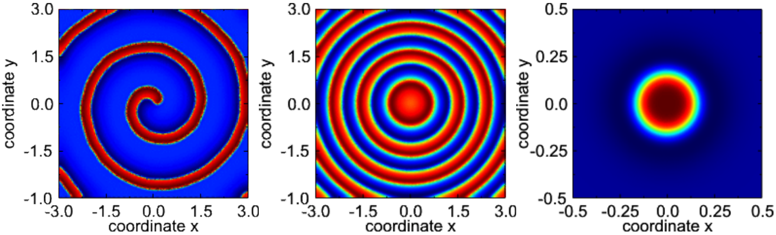
Problem 4.6: Do the same for the last of the four sign-type cases.

Turing instability induces the growth of *spatial* perturbations of the equilibrium, and the appearance of new stable (bifurcated) equilibria that are seen as spatial patterns (morphogenesis).



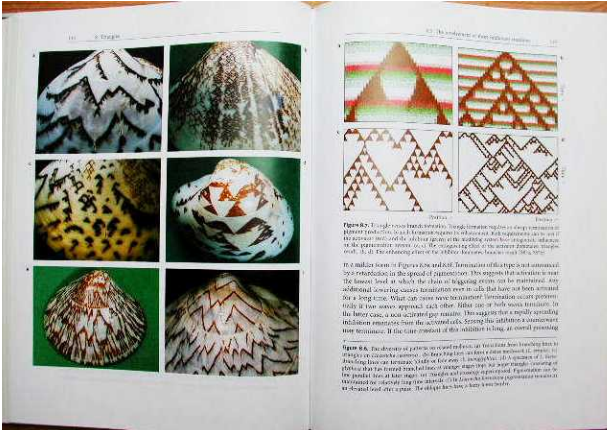
Evolution to an hexagonal pattern: $t = 0, t = 10, t = 100$.
Fitzhugh-Nagumo nonlinearity

https://en.wikipedia.org/wiki/FitzHugh-Nagumo_model



(spiral wave, target solution, dissipative soliton)
Fitzhugh-Nagumo nonlinearity

http://en.wikipedia.org/wiki/Reaction%E2%80%93diffusion_system
http://www.cgjennings.ca/toybox/turingmorph/



The algoritmic beauty of sea shells
Hans Meinhardt, 2009

$$\frac{\partial a}{\partial t} = s\left(\frac{a^2}{b} + b_a\right) - r_a a + D_a \frac{\partial^2 a}{\partial x^2}$$

$$\frac{\partial b}{\partial t} = s\, a^2 + b_b - r_b b + D_b \frac{\partial^2 b}{\partial x^2}$$

Where:

x : spatial coordinates

t: time

D_a , D_b: diffusion coefficients

r_a, r_b : decay rates of a and b respectively

s: source density: Ability of cells to perform autocatalysis

$s\frac{a^2}{b}$: production rate: The activator has a non-linear autocatalytic influence as two molecules must form a complex. The production is slowed down by the inhibitor

$r_a a$: removal rate: Rate at which molecules disappear is proportional to number of molecules present

$D_a \frac{\partial^2 a}{\partial x^2}$: exchange by diffusion. No diffusion takes place when the molecules have the same concentration or a linear concentration gradient as here the loss of substance = gain of substance so no net diffusion takes place

b_a : basic activator production. This initiates the system at low activator concentrations as it is activator independent. It is required for pattern regeneration, insertion of a new maxima during growth or for sustained oscillations.

b_b : basic inhibitor production. A small activator independent inhibitor production can cause a second homogenous stable state at low activator concentrations.

From the same book

More references

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