Computer Experiment
Pattern Formation in Reaction-Diffusion Systems

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Systems of interacting chemical components able to diffuse are denoted reaction-diffusion systems. Complex spatio-temporal patterns may spontaneously form in a reaction-diffusion system, a classical example for a self-organizing process.

This computer experiment deals with a basic and abstract reaction diffusion system, with the task to develop a first understanding of underlying terms of complex system theory, such as the stability of fixpoints and bifurcation diagrams, together with hands-on numerical simulation using an existing Java applet.

The Gray-Scott Reaction-Diffusion system

Consider two scalar fields, $\rho(\mathbf{x},t)$ and $\sigma(\mathbf{x},t)$, representing the concentrations of two chemical substances in space $\mathbf{x} = (x, y)$ and time t. The Gray-Scott system is defined by

$$\begin{array}{rcl} \dot\rho &=& -\rho\sigma^2 + F(1-\rho) + D_\rho\Delta\rho \\ \dot\sigma &=& \rho\sigma^2 - (F+k)\sigma + D_\sigma\Delta\sigma \end{array} , \qquad (1)$$

where $F, k > 0$ are parameters of the reaction system and D_ρ/D_σ the respective diffusion constants. Remember, that the diffusion equation for a field $n(\mathbf{x},t)$ has the form

$$\frac{\partial}{\partial t}n = \dot n = D\Delta n, \qquad \Delta = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial x^2} ,$$

with D being the diffusion constant.

1. Task: Understanding what it's about

Study the literature given and obtain a first understanding of what pattern formation in reaction diffusion systems is about. Find several examples of self-organized pattern formation occurring in the real world. Play around with the applets provided in order to obtain a first intuition of what's going on.

2. Task: Analytic understanding

Study analytically the reaction part of (1),

$$\begin{array}{rcl} \dot{\rho} & = & -\rho\sigma^2 \,+\, F(1-\rho) \\ \dot{\sigma} & = & \rho\sigma^2 \,-\, (F+k)\sigma \end{array} \,. \tag{2}$$

The system (2) has, for all parameters $F, k > 0$ the fixpoint $\mathbf{p}_0^* = (1, 0)$. It may have two additional fixpoints $\mathbf{p}_i^*$, determined by

$$\rho_i^*\sigma_i^* \,=\, K, \qquad F\rho_i^* + K\sigma_i^* \,=\, F, \qquad i \,=\, 1,\, 2\ .$$

Perform the following studies.

1. For which parameters k and F has the reaction system (2) only a single fixpoint?
2. Examine the stability of $\mathbf{p}_0^*$.
3. Examine the stability of $\mathbf{p}_i^*$, $i = 1, 2$, whenever present.
4. For which parameters is $\mathbf{p}_i^*$, $i = 1, 2$ a stable node/focus or a saddle?

Explanation. In order to investigate the stability of a fixpoint one linearizes the dynamical system around the fixpoint and studies the eigenvalues $\lambda_{1,2}$ of the linear system. For a two dimensional system the following possibilities occur:

- <u>real eigenvalues</u> $\lambda_{1,2} \neq 0$.
  ($\lambda_1\lambda_2 < 0$): saddle
  ($\lambda_1\lambda_2 > 0$): node which is stable / unstable if both eigenvalues are negative / positive.
- <u>complex conjugate eigenvalues</u> $\lambda_{1,2} = \lambda' \pm \lambda''$.
  stable / unstable focus if λ' is negative / positive.

3. Task: Numerical simulations

Run the provided Java simulation applets for certain sets of parameters k and F, while keeping the preset diffusion constants D_ρ and D_σ. Describe the observed dynamics and illustrate them by selected screenshots. Repeatedly disturb the patterns observed in order to examine their stability.

3.1 For $F = 0.025$ consider

$$k \,=\, 0.048,\, 0.049,\, 0.050,\, \ldots,\, 0.058,\, 0.60,\, 0.62,\, \ldots, 0.68\ .$$

3.1(a) Go through the series upwards consecutively.

3.1(b) Start every time with a single dot in the middle.

3.1(c) Try to make a single dot stable for $k = 0.068$.

3.2 For $F = 0.05$ consider

$$\begin{aligned} k &= 0.058,\, 0.060,\, \dots,\, 0.062 \\ k &= 0.062,\, 0.064,\, \dots,\, 0.076 \end{aligned} \quad .$$

3.2(a) Go through the first series from right to left consecutively.

3.2(b) Go through the second series from left to right consecutively.

Links and Literature

- `http://itp.uni-frankfurt.de/~gros/JavaApplets/Gray-Scott`
  The Java simulation applet to be used for the Gray-Scott reaction-diffusion system.
- C. Gros, *Complex and Adaptive Dynamical Systems, a Primer.*
  Springer (2008); (second and third editions 2010 and 2013).
- `http://itp.uni-frankfurt.de/~gros/Vorlesungen/SO`
  Lecture course on self-organization and complex systems containing downloadable scripts dealing with fixpoint analysis and reaction diffusion systems.
- `http://en.wikipedia.org/wiki/Reaction%E2%80%93diffusion_system`
  Wikipedia article regarding the Gray-Scott reaction-diffusion system.
- `http://www.joakimlinde.se/java/ReactionDiffusion`
  An alternative Java simulation applet for the Gray-Scott reaction-diffusion system.