

## Exercise 3 – The Brusselator model

**Deadline 29.3.2004**

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*The objective of this assignment together with the lecture is to introduce to the student some basics ideas of pattern formation in Turing reaction-diffusion systems. In this assignment you will gain insight to basic analytical methods related to nonlinear systems and then carry out numerical simulations of a Brusselator model using the parameters you have predicted analytically. For the interesting historical background and the hypothetical biological relevance of Turing systems the student is referred to literature [1, 2, 3, 4].*

### 1 Introduction to the Brusselator model

British mathematician Alan Turing showed in 1952 that a particular mathematical system could produce spatial patterns from an arbitrary initial state. In its most generic form a Turing model describing chemical diffusion and reactions with respect to the chemical concentrations  $U$  and  $V$  can be written in the form

$$\begin{aligned}\frac{\partial U}{\partial t} &= D_U \nabla^2 U + f(U, V) \\ \frac{\partial V}{\partial t} &= D_V \nabla^2 V + g(U, V),\end{aligned}\tag{1}$$

where  $D_U$  and  $D_V$  are the diffusion coefficients setting the pace of diffusion for chemicals  $U$  and  $V$ , respectively. Notice that for the reaction kinetics  $f(U, V) \equiv g(U, V) \equiv 0$  the system reduces to two independent diffusion equations. The coupling via the reaction kinetics is typically nonlinear.

A reaction-diffusion model often corresponds to real chemical reactions and reaction formulae. The Brusselator model used in this assignment was developed in the 1970s in Brussels by Nobel laureate Ilya Prigogine among others. The Brusselator model is one of the simplest chemical models exhibiting a pattern forming instability called Turing instability. In the case of the Brusselator model the chemical reactions are given as



where  $U$  and  $V$  are spatially and temporally varying chemical concentrations, whereas the concentrations of the chemicals  $A$ ,  $B$  and  $E$  are kept constant. Using the law of mass action [3] one can derive the mathematical equations corresponding to the

reaction scheme defined by Eq. (2). The reaction kinetics of the Brusselator model is given by

$$\begin{aligned} f(U, V) &= A - (B + 1)U + U^2V \\ g(U, V) &= BU - U^2V. \end{aligned} \quad (3)$$

Including the diffusion and time variation (as in Eq. (1)) leads to the Brusselator model given by

$$\begin{aligned} U_t &= D_U \nabla^2 U + A - (B + 1)U + U^2V \\ V_t &= D_V \nabla^2 V + BU - U^2V, \end{aligned} \quad (4)$$

where  $A$  and  $B$  are scalar parameters, which govern the pattern selection in the model by defining the reaction kinetics. The values of  $A$  and  $B$  will be determined in the next section. In order to obtain spatial patterns, it is always required that  $D_U \neq D_V$  (see Refs. [2, 3] for more on this).

## 2 Analysis of the Brusselator model

As one is interested in the pattern forming properties of a nonlinear reaction-diffusion model, one typically first determines the stationary state of the model in the absence of diffusion. This is done by solving the system in Eq. (4) with conditions  $\frac{\partial U}{\partial t} = \frac{\partial V}{\partial t} = 0$  and  $D_U = D_V = 0$ .

**Problem 1: What is the stationary state  $(U_0, V_0)$  of the Brusselator model?**

In order to simplify the further analysis, a change of variables is typically carried out to make  $(0, 0)$  the stationary state. This is achieved by making the substitutions  $U = U_0 + u$  and  $V = V_0 + v$  to Eq. (4).

**Problem 2: Write the Brusselator model using the new scaled concentrations  $u$  and  $v$ , and check that  $(u_0, v_0) = (0, 0)$ .**

The theory by Turing predicts that a spatially uniform stationary state that is stable against perturbations in the absence of diffusion might become unstable against perturbations in the presence of diffusion resulting in a pattern forming instability. This is the most important characteristic of the Turing instability: If there are not any random perturbations from the stationary state, that state will persist. In the absence of diffusion the system will return to the stationary state, if the system is perturbed away from it. In the presence of diffusion, however, the perturbed system will evolve towards another spatially nonuniform steady-state, i.e., a spatial concentration pattern will appear.

The stability of a state can be studied by using linear analysis [2, 3]. The linearized system can be written in the form  $\vec{w}_t = (\mathbf{D} + \mathbf{A})\vec{w}$  and reads as

$$\begin{pmatrix} u_t \\ v_t \end{pmatrix} = \left( \begin{pmatrix} D_u \nabla^2 & 0 \\ 0 & D_v \nabla^2 \end{pmatrix} + \begin{pmatrix} f_u & f_v \\ g_u & g_v \end{pmatrix}_{(u_0, v_0)} \right) \begin{pmatrix} u \\ v \end{pmatrix}, \quad (5)$$

where  $f_u, f_v, g_u$  and  $g_v$  in the matrix  $\mathbf{A}$  denote the partial derivatives of the reaction kinetics, which are evaluated at the stationary state  $(u_0, v_0) = (0, 0)$ .

**Problem 3: How does the linearized matrix  $\mathbf{A}$  look like (use the kinetics of the scaled model you calculated in Problem 2)?**

In the absence of diffusion the stability of the system can be studied by calculating the eigenvalues of the matrix  $\mathbf{A}$  defined in Eq. (5). In the presence of diffusion one can solve the eigenvalues by substituting a trial solution of the form  $w(\vec{r}, t) \propto e^{\lambda(k)t} e^{i\vec{k}\cdot\vec{r}}$  into the linearized system (Eq. (5)). This yields the characteristic equation  $|\mathbf{A} - \mathbf{D}k^2 - \lambda\mathbf{I}| = 0$ , i.e.,

$$\begin{vmatrix} f_u - D_u k^2 - \lambda & f_v \\ g_u & g_v - D_v k^2 - \lambda \end{vmatrix} = 0, \quad (6)$$

where  $k^2 = \vec{k} \cdot \vec{k}$  is the modulus of the wave vector.

**Problem 4: Write the characteristic equation (Eq. (6)) in the form  $\lambda^2 + B(k)\lambda + C(k) = 0$  and substitute the values defined by the matrix  $\mathbf{A}$  (calculated in Problem 3) to the equation.**

From the characteristic equation one can solve the dispersion relation, i.e., the two eigenvalues  $\lambda_1(k)$  and  $\lambda_2(k)$ . By plotting the real part of the bigger eigenvalue as a function of the wave number  $k$  one can study the stability of the wave vectors  $\vec{k}$  corresponding to the wave number  $|\vec{k}| = k$ . Stable wave vectors are those for which  $\lambda(k) < 0$  and for the unstable ones  $\lambda(k) > 0$ . We want to find such parameter values that there is a narrow wave window, i.e., there is only a limited amount of unstable wave numbers  $k$ , which fix the spatial length of the pattern  $\ell = 2\pi/k$ .

At the onset of the instability, which corresponds to the critical wave number  $k_c$  the eigenvalue or growth rate  $\lambda(k_c) = 0$ . Thus the characteristic equation must satisfy  $C(k_c) = 0$ , which is a second order equation with respect to  $k_c^2$ . *The discriminant  $\mathcal{D}$  defined by the equation  $C(k_c^2) = 0$  must be zero at the onset for the equation to have only one solution.* The modulus of the critical wave number  $k_c^2$  can be solved from the condition  $C(k_c^2) = 0$  given that  $\mathcal{D} = 0$ . In the case of the Brusselator model it is given by  $k_c^2 = \frac{A}{\sqrt{D_u D_v}}$ .

In the Brusselator model the instability is governed by the bifurcation parameter  $B$ . At the onset of the instability  $B = B_c$ . For  $B < B_c$  the stationary state is stable and for  $B > B_c$  there is a critical unstable mode corresponding to the wave number  $k_c$ . Figure 1 in the appendix shows the dispersion relations corresponding to these three different cases. The critical value  $B_c$  can be found from the characteristic equation. To ease the search of  $B_c$  resulting in Turing instability, fix  $A = 4.5$  and  $D_v = 8D_u = 16$ .

**Problem 5: Solve analytically the critical value  $B_c$  of the bifurcation parameter  $B$  with respect to the parameters  $A$ ,  $D_u$  and  $D_v$  from the condition  $\mathcal{D} = 0$ . Calculate also the numerical value of  $B_c$  using the given parameters.**

Now you should have all the parameter values required for starting numerical simulations of the Brusselator model. To get spatial patterns you must use  $B > B_c$ . Linear analysis predicts very efficiently the stability of a particular stationary states. It does not, however, answer to the question about pattern selection, i.e., whether one will obtain stripes or spots. Studying the pattern selection involves highly complex mathematical techniques, which will not be discussed here. Those, who are interested in the nonlinear bifurcation analysis are suggested to study Ref. [2] and refereces therein.

### 3 Numerical simulations of the Brusselator model

Solving reaction-diffusion models by hand is not possible due to their time-dependent nature. Numerical simulations of reaction-diffusion models, on the other hand, are not very complicated. Nevertheless, in this assignment most of the simulation code (`brusselator.c`) is given and it requires only a few additions by the student.

In the numerical simulation the spatial dimension of the problem is discretized into a lattice by using the finite difference method. In a two-dimensional system the laplacian with respect to the concentration field  $U$  in the node  $(i, j)$  is calculated by

$$\nabla_{i,j}^2 U = \frac{U_{i+1,j} + U_{i-1,j} + U_{i,j+1} + U_{i,j-1} - 4U_{i,j}}{dx^2}, \quad (7)$$

where  $dx$  is the lattice constant corresponding to the length of spatial discretization. The boundary conditions can be either zero-flux or periodic. The calculation of the laplacian using periodic boundary conditions is already implemented in the given simulation code.

The time iteration is carried out by using the basic Euler's method, where the time derivative (LHS of Eq. (4)) is approximated with a difference. In this case it is  $(U^{t+dt} - U^t)/dt$ , where the superscripts denote time and  $dt$  is the time step (suitable numerical value is given in the code). Now the update step for the concentration fields  $U$  and  $V$  may be written as follows

$$\begin{aligned} U_{i,j}^{t+dt} &= U_{i,j}^t + dt \cdot (D_U \nabla_{i,j}^2 U^t + f_{i,j}^t), \\ V_{i,j}^{t+dt} &= V_{i,j}^t + dt \cdot (D_V \nabla_{i,j}^2 V^t + g_{i,j}^t), \end{aligned} \quad (8)$$

where  $f_{i,j}^t$  and  $g_{i,j}^t$  are the reaction kinetics at point  $(i, j)$  at time  $t$  defined by Eq. (3). Initial conditions  $U^0$  and  $V^0$  typically used in simulations of Turing systems are random perturbations around the stationary state  $(U_0, V_0)$ . This comes down to the most fascinating characteristic of Turing instability, i.e., the fact that it can create organized patterns from a random initial state.

**Problem 6: Complete the given code (`brusselator.c`) by adding the values of the stationary states (Problem 1), an amplitude for the initial random deviations from these states (`var`) and the time iteration for both  $U$  and  $V$  according to Eq. (8). See the code for more instructions.**

Now the code should be completed and ready to work. You must have four files in order to carry out the simulations and visualize the results: `brusselator.c` (the simulation code), `ranmar.c` (random number generator), `Makefile` (for compiling the program), and `visual.m` (for visualization using Matlab). To compile the program type `make` in the directory. After the compilation succeeds you can start the simulation by typing e.g. `simu 12345 12345 A B`, where `A` and `B` are the numerical values for the parameters you want to use (Problem 5). See the comments of the code for more guidance.

In the code the system size has been fixed to  $100 \times 100$  and the number of iterations is 50000. You can change these and see what happens. The simulation program writes a data file named `data.m`, which can be visualized using the Matlab script `visual.m`. This script visualizes both concentration fields ( $U$  and  $V$ ). Notice that the fields are in anti-phase, i.e., the high concentration of  $U$  means low concentration of  $V$  and vice versa.

**Problem 7: Carry out simulations for  $A = 4.5$ ,  $D_V = 8D_U = 16$  and try out different values for the parameter  $B > B_c$  according to your calculations (Problem 5). What kind of patterns do you get? Try to get at least stripes and spots, save the figures and write down the corresponding parameter values.**

One can check the agreement of the numerical results with the analytical prediction by studying the characteristic length scale of the resulting pattern. The modulus of the critical wave vector  $k_c^2$  with respect to the system parameters was calculated previously. The characteristic wave length corresponding to this critical mode is given by  $\ell = 2\pi/k_c$  since  $dx = 1$ . By calculating the predicted characteristic length  $\ell$  for the parameters that one uses, one can approximately check the agreement between theory and the results of the numerical simulations. The distance between stripes or spots should correspond to  $\ell$ .

To conclude the assignment let us once more repeat the main point of Turing instability. Turing predicted that a stationary state that is stable against perturbations in the absence of diffusion may become unstable against perturbations in the presence of diffusion. Using the code you have completed this theory is easy to test. In the following problem, use the parameter values that you used in Problem 7 to obtain spatial patterns. You can decrease the number of iterations to 1000.

**Problem 8: Test of Turing's theory: 1) Keep  $D_V = 8D_U = 16$  and set variable `var` in the code equal to zero. What happens and why? 2) Fix  $D_U = D_V = 0$  and use non-zero amplitude of random perturbations (`var`). What happens and why?**

## 4 Report requirements

Return a short report (handwritten or PS/PDF). The report should consist of answers to all the problems and contain at least two figures of the simulation results (stripes&spots).

## References

- [1] P. Ball, *The self-made tapestry: Pattern formation in nature*, (Oxford University Press, Oxford 2001).
- [2] T. Leppänen, *The theory of Turing pattern formation*, available online at [http://www.lce.hut.fi/research/polymer/turing\\_review.pdf](http://www.lce.hut.fi/research/polymer/turing_review.pdf)
- [3] J.D. Murray, *Mathematical Biology*, 2nd. ed., (Springer-Verlag, Berlin 1993); J.D. Murray, *Mathematical Biology II: Spatial models and biomedical applications*, (Springer-Verlag, Berlin 2003)
- [4] T. Leppänen, *Matemaatikko selätti seepran raidat* (in Finnish), Tiede 1/2004. Extended version available online at [http://www.lce.hut.fi/research/polymer/turing\\_popular.pdf](http://www.lce.hut.fi/research/polymer/turing_popular.pdf)

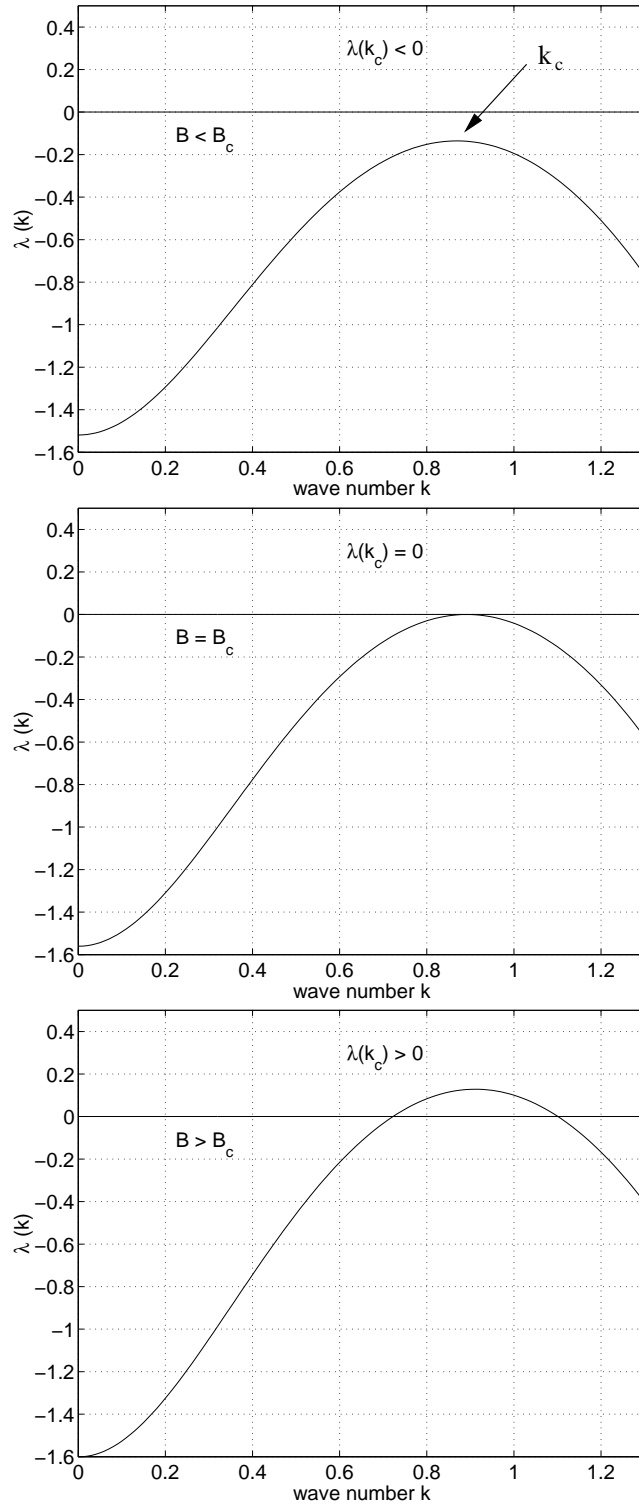


Figure 1: The dispersion relation  $\lambda(k)$  for three different cases. Top: the stationary state is stable for  $B < B_c$ . Middle: At the onset  $B = B_c$ . Bottom: Turing instability with  $B > B_c$  (unstable wave vectors are those with  $\lambda(|\vec{k}|) > 0$ ).