# Analysis of pattern formation using numerical continuation

V. Janovský

Charles University, Faculty of Mathematics and Physics, Prague

### **Outline**

- Pattern formation: Turing instability
  - Domain size driven instability
- Solution manifolds and numerical continuation
- 3 Critical wavelengths: primary bifurcation
- Symmetries of steady states
- Conclusions
- 6 Supplement: Dynamic simulation

### **Outline**

- Pattern formation: Turing instability
  - Domain size driven instability
- Solution manifolds and numerical continuation
- Critical wavelengths: primary bifurcation
- Symmetries of steady states
- Conclusions
- 6 Supplement: Dynamic simulation

### **Problem**

Consider reaction-diffussion system for two species  $\mathbf{u}$  and  $\mathbf{v}$  in 1D domain  $x \in [0, \ell]$ ,

$$\mathbf{u}_t = d_1 \mathbf{u}_{xx} + \bar{f}(\mathbf{u}, \mathbf{v})$$
  
 $\mathbf{v}_t = d_2 \mathbf{v}_{xx} + \bar{g}(\mathbf{u}, \mathbf{v})$ 

Context: A theory of biological pattern formation. Self-organization in development biology, morphogenesis

Objective: domain size driven instability

V. Klika, M. Kozák and E.A. Gaffney: *Domain Size Driven Instability: Self-Organization in Systems with Advection*, SIAM J. Appl. Math., 2018, pp 2298–2322.

Domain can be scalled to the unit interval  $0 \le x \le 1$  introducing parameter L. Hence, we consider

$$\mathbf{u}_t = \frac{d_1}{L^2} \mathbf{u}_{xx} + f(\mathbf{u}, \mathbf{v})$$
$$\mathbf{v}_t = \frac{d_2}{L^2} \mathbf{v}_{xx} + g(\mathbf{u}, \mathbf{v})$$

in domain  $0 \le x \le 1$ . Here *L* is the length of the interval. We consider Neumann boundary conditions (zero flux)

$$\mathbf{u}_{x}(0,t) = \mathbf{u}_{x}(1,t) = 0, \quad \mathbf{v}_{x}(0,t) = \mathbf{v}_{x}(1,t) = 0.$$

We seek for steady states.

*Homogeneous steady state*: There exists  $u^* \in \mathbb{R}^1$ ,  $v^* \in \mathbb{R}^1$ , such that

$$f(\mathbf{u}(x,0),\mathbf{v}(x,0)) = f(u^*,v^*) = g(\mathbf{u}(x,0),\mathbf{v}(x,0)) = g(u^*,v^*) = 0, \ 0 \le x \le 1.$$

Note that, in this case,  $\mathbf{u}_{xx} = 0$  and  $\mathbf{v}_{xx} = 0$  in the domain  $0 \le x \le 1$ .

5/41

V. Janovský On pattern formation

### **Outline**

- Pattern formation: Turing instability
  - Domain size driven instability
- Solution manifolds and numerical continuation
- Critical wavelengths: primary bifurcation
- Symmetries of steady states
- Conclusions
- 6 Supplement: Dynamic simulation

#### Discretization of the model

*Method of lines*: Define the equidistant mesh on the interval  $0 \le x \le 1$ 

$$x_j = jh, \quad h = \frac{1}{N+1}, \quad j = 1, \dots, N,$$
 (2.1)

where N is the number of meshpoints.

The state variables **u**, **v** are approximated by discrete state variables

$$\mathbf{u} \approx [u_1, \dots, u_i, \dots, u_N]^T \in \mathbb{R}^N, \quad \mathbf{v} \approx [v_1, \dots, v_i, \dots, v_N]^T \in \mathbb{R}^N,$$

We seek for discrete steady states. They depend on the parameter  $L^2$ .

We define

$$F: \mathbb{R}^{2N} \times \mathbb{R}^1 \longrightarrow \mathbb{R}^{2N} \tag{2.2}$$

and seek for the roots

$$F(w, L^2) = 0$$
,  $w \in \mathbb{R}^{2N}$ ,  $w_i = u_i$ ,  $w_{N+i} = v_i$ ,  $i = 1, ..., N$ .

This set is called solution manifold.

We assume the existence of homogeneous steady state

$$F(w^*, L^2) = 0$$
,  $w^* \in \mathbb{R}^{2N}$ ,  $w_i^* = u^*$ ,  $w_{N+i}^* = v^*$ ,  $i = 1, ..., N$ .

## Primary bifurcation point

<u>Definition</u>. Consider the particular homogeneous steady state  $w^* \in \mathbb{R}^{2N}$ ,  $(L^*)^2 \in \mathbb{R}^1$ ,

$$F(w^*,(L^*)^2) = 0 \in \mathbb{R}^{2N} \,, \quad A \equiv F_w(w^*,(L^*)^2) \,, \quad \dim \operatorname{Ker} A = 1 \,.$$

Let  $\xi$  and  $\eta$  be right and left eigenvectors corresponding to the zero eigenvalue

$$A\xi=0\in\mathbb{R}^{2N}\,,\quad \|\xi\|=1\,,\quad A^T\eta=0\in\mathbb{R}^{2N}\,,\quad \|\eta\|=1\,,\quad \eta^T\xi\neq0,$$

with an algebraic multiplicity equal to one. Then the point  $(w^*, (L^*)^2) \in \mathbb{R}^{2N+1}$  is called *primary bifurcation point*.

... Lyapunov-Schmidt reduction, bifurcation equation

M. Golubitsky, I. Stewart and D.G. Schaeffer: *Singularities and groups in bifurcation theory, Vol II*, Springer, 1988

Example. Consider the Schnackenberg model for the parameter setting  $\overline{a=0.1}$ , b=0.9,  $\gamma=10$ ,  $d_1=0.1$ ,  $d_2=1.6$  and N=20. Homogeneous state state  $w^*$ :  $u^*=a+b=1$ ,  $v^*=b/(a+b)^2=0.9$ . The aim is to compute the branch of inhomogeneous steady states emanating from a particular primary bifurcation point.

The primary bifurcation point  $w^*$ ,  $(L^*)^2$  with least  $(L^*)^2 > 0$  is  $(L^*)^2 = 0.153969537228066$ .

J. Schnakenberg: Simple chemical reaction systems with limit cycle behaviour, J. Theoret. Biol., Vol 81, 1979, pp 389–400.

### Solution manifold via numerical continuation

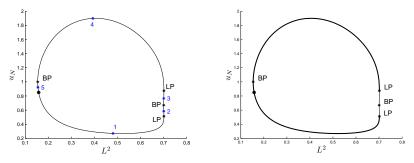


Figure: On the left: Branch of inhomogeneous steady states projected onto pairs  $(u_N, L^2)$ . It is oriented anticlockwise. The branch emanates from the primary bifurcation point  $u_N = 1$ ,  $(L^*)^2 \approx 0.1539$  labeled as BP. The circle on the branch marks the initial point of continuation procedure. In points  $1, \ldots, 5$  we test stability. The indicated bifurcation points are (in clockwise directions) LP, secondary bifurcation point BP, LP and the primary bifurcation point BP. On the right: thick and thin segments of curves indicate stable and unstable steady states.

A. Dhooge, W. Govaerts and Yu.A. Kuznetsov: *MATCONT*: a MATLAB package for numerical bifurcation analysis of ODEs, ACM Transactions on Mathematical Software Vol 29, No.2., 2003, pp 141–164.

### **Outline**

- Pattern formation: Turing instability
  - Domain size driven instability
- Solution manifolds and numerical continuation
- Critical wavelengths: primary bifurcation
- Symmetries of steady states
- Conclusions
- 6 Supplement: Dynamic simulation



# Dispersion equation

Let  $u^* \in \mathbb{R}^1$ ,  $v^* \in \mathbb{R}^1$  be a homogeneous steady i.e.,

$$f(u^*, v^*) = g(u^*, v^*) = 0, 0 \le x \le 1.$$

In particular, in the model Schnakenberg model,

$$u^* = a + b$$
,  $v^* = b/(a+b)^2$ ,  $a > 0, b > 0$ .

We define Jacobian at the steady state  $u^* \in \mathbb{R}^1$ ,  $v^* \in \mathbb{R}^1$ :

$$\mathbf{J} = \left[ egin{array}{cc} f_u & f_v \ g_u & g_v \end{array} 
ight]_{u,v:=u^*,v^*} \ .$$

In particular, in the model Schnakenberg model,

$$\mathbf{J} = \left[ \begin{array}{cc} 2\gamma b/(a+b) - 1 & (a+b)^2 \\ -2b/(a+b) & -(a+b)^2 \end{array} \right] \,, \quad a > 0, b > 0, \gamma > 0 \,,$$

◆ロト ◆問 → ◆注 > ◆注 > 注 り Q ©

V. Janovský

Let  $d_1$  end  $d_2$  be diffusion parameters. Let **J** be Jacobian corresponding to a steady state. The equation

$$\det \left( \boldsymbol{J} - \boldsymbol{k}^2 \begin{bmatrix} \ d_1 & 0 \\ 0 & d_1 \end{bmatrix} - \lambda \boldsymbol{I} \right) = 0 \,, \quad \boldsymbol{I} = \boldsymbol{I}_{2 \times 2} \in \mathbb{R}^{2 \times 2}$$

is called dispersion relation. It depends on wavenumber  $k^2$  and frequency  $\lambda$ . Dispersion relation implicitly defines the relationship  $\lambda = \lambda(k^2)$ .

Instead of analyzing roots of dispersion relation we analyse the spectrum of the following matrix

$$\mathbf{H} \equiv \mathbf{J} - k^2 \left[ \begin{array}{cc} d_1 & 0 \\ 0 & d_1 \end{array} \right] .$$

The spectrum  $\sigma(\mathbf{H})$  consists of two eigenvalues  $\{\lambda_1(k^2),\lambda_2(k^2)\}$ . These can be numerically computed as a function of  $k^2$ . We use Matlab function eig(H). Note that generally  $\sigma(\mathbf{H})$  consists of either two real eigenvalues or a complex congate pair.

Given  $k^2$ , we define

$$\Re\left(\lambda_*(k^2)\right) = \max\left\{\Re\left(\lambda_i(k^2)\right)\right\}_{i=1,2}$$

which is the right-most eigenvalue of  $\sigma$  (**H**). We call  $\Re$  ( $\lambda_*(k^2)$ ) *maximal growth rate*.

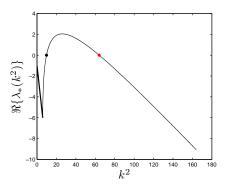


Figure: Maximal growth rate  $k^2 \mapsto \Re(\lambda_*(k^2))$ : thin and thick curve segments refers to two real eigenvalues and complex conjugate pairs, respectively. Case: Schnakenberg model, a=0.1, b=0.9,  $\gamma=10$ ,  $d_1=0.1$ ,  $d_2=1.6$ .

V. Janovský

Let  $k_-^2$  and  $k_+^2$ ,  $k_-^2 \le k_+^2$ , be the roots of function  $k^2 \mapsto \Re(\lambda_*(k^2))$ . We can get the closed-form expressions

$$\mathbf{k}_{-}^{2} = \frac{d_{2}f_{u} + d_{1}g_{v} - \sqrt{\Delta}}{2d_{1}d_{2}}, \quad \mathbf{k}_{+}^{2} = \frac{d_{2}f_{u} + d_{1}g_{v} + \sqrt{\Delta}}{2d_{1}d_{2}}, \quad (3.3)$$

where  $\Delta = (d_2 f_u + d_1 g_v)^2 - 4 d_1 d_2 \det \mathbf{J}$ , and  $\mathbf{J}$ ,  $f_u$ ,  $g_v$  are related to Jacobian.

The open interval  $(k_-^2, k_+^2)$  is called *range of growing wavenumbers*. For a given  $k^2$ ,  $k_-^2 < k^2 < k_+^2$ , the maximal growth rate is positive.

# Spatial pattern: linear stability analysis

Linearization about a homogeneous steady state  $u^* \in \mathbb{R}^1$ ,  $v^* \in \mathbb{R}^1$ :

$$\begin{bmatrix} \mathbf{u}_t \\ \mathbf{v}_t \end{bmatrix} = \mathbf{J} \begin{bmatrix} \mathbf{u} \\ \mathbf{v} \end{bmatrix} + \frac{1}{L^2} \begin{bmatrix} d_1 & 0 \\ 0 & d_1 \end{bmatrix} \begin{bmatrix} \mathbf{u}_{xx} \\ \mathbf{v}_{xx} \end{bmatrix}$$
(3.4)

in domain  $0 \le x \le 1$ . We employ Fourier analysis, setting

$$\begin{bmatrix} \mathbf{u}(x,t) \\ \mathbf{v}(x,t) \end{bmatrix} = \sum_{j=1}^{+\infty} \mathbf{c}_j e^{\lambda t} W_j(x), \quad 0 \le x \le 1, \ t \ge 0,$$
 (3.5)

where  $\mathbf{c}_j \in \mathbb{R}^2$  are coefficients to be determined,  $\lambda \in \mathbb{R}^1$  defines temporal growth.

J.D. Murray: Mathematical biology. II, Springer-Verlag, New York, 2003.

The Fourier functions  $W_j$  are related to 1-D Laplacians with Neumann boundary conditions

$$W_j'' + k^2 W_j = 0$$
,  $0 \le x \le 1$ ,  $W_j'(0) = W_j'(1) = 0$ . (3.6)

The relevant eigenvalues and eigenvectors are  $k^2 = (j\pi)^2$  and  $W_j = \sqrt{2}\cos(j\pi x)$ , for j = 1, 2, ...

We conclude that

$$\det \left( \mathbf{J} - \frac{k^2}{L^2} \begin{bmatrix} d_1 & 0 \\ 0 & d_1 \end{bmatrix} - \lambda \mathbf{I} \right) = 0, \quad \mathbf{I} = \mathbf{I}_{2 \times 2} \in \mathbb{R}^{2 \times 2}. \tag{3.7}$$

This equation is analogous to the dispersion relation. It depends on frequency  $\lambda$ , particular eigenvalue  $k^2=(j\pi)^2, j=1,2,\ldots$  and wavelength  $L^2$ .

The roots of the above dispersion relation are related to the spectrum of the matrix

$$\mathbf{H} \equiv \mathbf{J} - \frac{k^2}{L^2} \begin{bmatrix} d_1 & 0 \\ 0 & d_1 \end{bmatrix} . \tag{3.8}$$

Its spectrum  $\sigma$  (**H**) consists of two eigenvalues  $\left\{\lambda_1\left(\frac{k^2}{L^2}\right), \lambda_2\left(\frac{k^2}{L^2}\right)\right\}$ . We define the maximal growth rate as function

$$\frac{k^2}{L^2} \mapsto \Re\left(\lambda_*\left(\frac{k^2}{L^2}\right)\right) \equiv \max\left\{\Re\left(\lambda_i\left(\frac{k^2}{L^2}\right)\right)\right\}_{i=1,2}.$$
 (3.9)

We ask for  $\frac{k^2}{L^2}$  when  $\Re\left(\lambda_*\left(\frac{k^2}{L^2}\right)\right)$  is positive.

We observe that for parameters  $k^2 = (j\pi)^2$  and  $L^2$  which satisfy

$$k_{-}^2 < \frac{k^2}{L^2} < k_{+}^2$$

we can expect the existence of an inhomogeneous steady state.

V. Janovský

In terms of wavelength  $L^2$ , we arrive at the restriction

$$\frac{k^2}{k_+^2} < L^2 < \frac{k^2}{k_-^2} \,, \quad k^2 = (j\pi)^2 \,. \tag{3.10}$$

The estimate (3.10) of the stable wavelength range is related to the partial differential equation (3.4). The state variables are functions  $\mathbf{u}(x,t)$  and  $\mathbf{v}(x,t)$ , see (3.5).

However, when it comes to the discrete model (2.2) of reality, we must consistently consider Laplacian on an equidistant grid (2.1):

#### Definition.

# Discrete Laplacian on an equidistant grid

Properties.  $[e\_val, e\_vec] = Lap\_neum(N, No)$ 

- N is number of meshpoints
- No is serial number of eigenmode,  $No = j \in \{1, ..., N-1\}$

The function  $Lap\_neum$  returns corresponding eigenvalue  $e\_val \in \mathbb{R}^1$  and eigenvector  $e\_vec \in \mathbb{R}^N$ . By definition: If No = 0 then  $e\_val = 0$ . Positive eigenvalues are arranged:  $No \in \{1, \dots, N-1\}$  from the smallest to the largest.

We formulate appropriate discrete analogies of (3.7), (3.8), (3.9) and (3.10). In particular, we set

$$k^2 = e_val = Lap_neum(N, No), No = j \in \{1, ..., N-1\}$$
 (3.11)

In order to simplify notation, e\_val and e\_vec are generic value variables.

# Critical wavelengths

<u>Definition</u>. Given a mode number  $No = j \in \{1, ..., N-1\}$ , we define interval

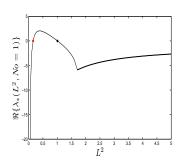
$$\frac{e_{-}val}{k_{+}^{2}} < L^{2} < \frac{e_{-}val}{k_{-}^{2}}$$
 (3.12)

and call it stable wavelength range. We define

$$L2\_No\_up = \frac{e\_val}{k_+^2}$$
,  $L2\_No\_down = \frac{e\_val}{k_-^2}$  (3.13)

as *critical wavelengths* related to mode number  $No = j \in \{1, ..., N-1\}$ .

V. Janovský



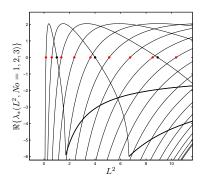


Figure: Critical wavelengths, see Example: On the left:  $L2\_1\_up \approx 0.1542$ ,  $L2\_1\_down \approx 1.0098$ . On the right: sorted in ascending order:  $L2\_1\_up$ ,  $L2\_2\_up$ ,  $L2\_1\_down$ ,  $L2\_3\_up$ ,  $L2\_4\_up$ ,  $L2\_5\_up$ ,  $L2\_2\_down$ ,  $L2\_6\_up$ , etc.

# Critical wavelengths: primary bifurcation

<u>Theorem</u>. For a given  $j \in \{1, ..., N-1\}$ , let  $L2\_j\_up$  and  $L2\_j\_down$  be the critical wavelengths. Then  $L2\_j\_up$  and  $L2\_j\_down$  are connected to the following primary bifurcation points:

$$\begin{aligned} \bullet & F(w^*, L2\_j\_up) = 0 \in \mathbb{R}^N, \\ F_w(w^*, L2\_j\_up) \left[ \begin{array}{c} a_{up} \\ b_{up} \end{array} \right] \otimes e\_vec \in \mathbb{R}^{2N} = 0 \in \mathbb{R}^{2N} \end{aligned}$$

$$\begin{array}{l} \bullet \ \ F(w^*, L2\_j\_down) = 0 \in \mathbb{R}^N, \\ F_w(w^*, L2\_j\_down) \left[ \begin{array}{c} a_{down} \\ b_{down} \end{array} \right] \, \otimes \, e\_vec \in \mathbb{R}^{2N} = 0 \in \mathbb{R}^{2N} \\ \end{array}$$

The coefficients  $a_{up} \in \mathbb{R}^1$ ,  $b_{up} \in \mathbb{R}^1$  and  $a_{down} \in \mathbb{R}^1$ ,  $b_{down} \in \mathbb{R}^1$  are defined by a formula.

Therefore, we can identify the critical wavelength with the primary bifurcation point. We can compute and sort all 2(N-1) bifurcation points.

### **Outline**

- Pattern formation: Turing instability
  - Domain size driven instability
- Solution manifolds and numerical continuation
- Critical wavelengths: primary bifurcation
- Symmetries of steady states
- Conclusions
- 6 Supplement: Dynamic simulation

# Matrix representation

Consider abstract group  $\Gamma = \mathbb{Z}_2 \oplus \mathbb{Z}_2 = \{\iota, \kappa_1, \kappa_2, \kappa_1 \kappa_2\}, \kappa_1 \kappa_2 = \kappa_2 \kappa_1$ . Here

- Z<sub>2</sub> is a cyclic group of order 2
- $\mathbb{Z}_2 \oplus \mathbb{Z}_2$  is a direct sum of groups.

 $\Gamma$  is therefore an Abelian group.

#### **Preliminaries**

We consider the following matrices:

identity matrix end zero matrix and exchange matrix of the proper size:

$$\mathbf{I}_{2N\times 2N} \in \mathbb{R}^{2N\times 2N}\,, \quad \mathbf{O}_{N\times N} \in \mathbb{R}^{N\times N}\,, \quad \mathbf{E} = \left[ \begin{array}{ccc} 0 & & 1 \\ & \ddots & \\ 1 & & 0 \end{array} \right] \in \mathbb{R}^{N\times N}$$

We define matrix representation of the group  $\Gamma$  in the state space  $\mathbb{R}^{2N}$ :

$$\begin{split} \mathbf{G}(\iota) &= \mathbf{I}_{2N\times 2N} \in \mathbb{R}^{2N\times 2N} \,, \quad \mathbf{G}(\kappa_1) = -\mathbf{I}_{2N\times 2N} \in \mathbb{R}^{2N\times 2N} \,, \\ \mathbf{G}(\kappa_2) &= \left[ \begin{array}{cc} \mathbf{E} & \mathbf{O}_{N\times N} \\ \mathbf{O}_{N\times N} & \mathbf{E} \end{array} \right] \in \mathbb{R}^{2N\times 2N} \,, \\ \mathbf{G}(\kappa_1\kappa_2) &= \mathbf{G}(\kappa_1)\mathbf{G}(\kappa_2) = -\mathbf{G}(\kappa_2) = \mathbf{G}(\kappa_2\kappa_1) \,. \end{split}$$

We conclude, that  $\Gamma = \{\mathbf{G}(\iota), \mathbf{G}(\kappa_1), \mathbf{G}(\kappa_2), \mathbf{G}(\kappa_1\kappa_2)\}$  is Abelian group with faithful representation on state space  $\mathbb{R}^{2N}$ . Each group element  $\gamma \in \Gamma$  is identified with its action namely a linear transformation on  $\mathbb{R}^{2N}$ .

In order to simplify notation, we identify the mentioned linear transformations with group elements  $\Gamma = \{\iota, \kappa_1, \kappa_2, \kappa_1 \kappa_2\}$ .

V. Janovský

# Maximal isotropy subgroups

#### The group Γ has proper subgroups

$$\Sigma_{\kappa_1} = \{\iota, \kappa_1\}, \Sigma_{\kappa_2} = \{\iota, \kappa_2\}, \Sigma_{\kappa_1 \kappa_2} = \{\iota, \kappa_1 \kappa_2\} \text{ and } \Sigma_0 = \{\iota\}.$$
 We need to recall two notions of representation theory:

- the isotropy subgroup  $\Sigma$
- the fixed point subspace  $Fix \Sigma$  of a subgroup  $\Sigma$ .

#### It holds

$$\begin{cases} \operatorname{Fix}_{\mathbb{R}^{2N}} \Sigma_{\kappa_{1}} &= \operatorname{Fix}_{\mathbb{R}^{2N}} \Gamma = 0 \in \mathbb{R}^{2N} \,, \\ \operatorname{Fix}_{\mathbb{R}^{2N}} \Sigma_{\kappa_{2}} &= \left\{ w \in \mathbb{R}^{2N} : w_{i} = w_{N-i+1} \,, \, w_{N+i} = w_{2N-i+1} \,, \right. \\ \left. i = 1, \dots, N \right\} \,, \\ \operatorname{Fix}_{\mathbb{R}^{2N}} \Sigma_{\kappa_{1}\kappa_{2}} &= \left\{ w \in \mathbb{R}^{2N} : w_{i} = -w_{N-i+1} \,, \, w_{N+i} = -w_{2N-i+1} \,, \right. \\ \left. i = 1, \dots, N \right\} \,, \\ \operatorname{Fix}_{\mathbb{R}^{2N}} \Sigma_{0} &= \mathbb{R}^{2N} \,. \end{cases}$$

 $\Sigma_{\kappa_2}$ ,  $\Sigma_{\kappa_1\kappa_2}$  and  $\Sigma_0$  are isotropy subgroups of  $\Gamma$ . Moreover,  $\Sigma_{\kappa_2}$  and  $\Sigma_{\kappa_1\kappa_2}$  are maximal isotropy subgroups.

◆ロト ◆個 ト ◆ 恵 ト ◆ 恵 ・ 夕 Q ○

# The symmetry of the solution: how it manifests itself

A key feature of Schnackenberg's model is its Γ-equivariance:

$$F(\gamma w, L^2) = \gamma F(w, L^2)$$

for  $(w, L^2) \in \mathbb{R}^{2N} \times \mathbb{R}^1$ , for all  $\gamma \in \{\iota, \kappa_1, \kappa_2, \kappa_1 \kappa_2\}$ .

Consider Schnakenberg model, see Example, assuming N = 40:

From the homogeneous steady state bifurcate the following inhomogeneous steady states (in ascending order)

L2\_1\_up, L2\_2\_up, L2\_1\_down, L2\_3\_up, L2\_4\_up, L2\_5\_up, L2\_2\_down, L2\_6\_up, etc.

Consider the branches emanating from *L*2\_3\_*up* and *L*2\_4\_*up*. We ask for a comparison.

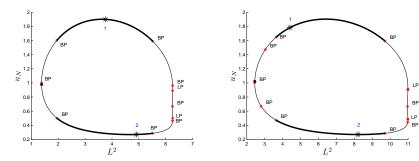


Figure: Schnakenberg model, see Example, N=40. Branches of inhomogeneous steady states projected onto pairs  $(u_N, L^2)$ , emanating from  $L2\_3\_up$  (on the left) and  $L2\_4\_up$  (on the right). Thick and thin segments of curves indicate stable and unstable steady states. Placement of random test points \* on stable segments.

### $\sum_{\kappa_1 \kappa_2}$ discrete odd functions = antisymmetric

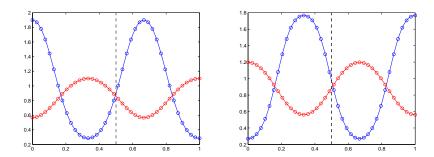


Figure: Schnakenberg model, see Example, N=40, the branch  $L2\_3\_up$ : Consider the steady states  $[u_1,\ldots,u_N,v_1,\ldots,v_N]\in\mathbb{R}^{2N}$  related the two marked test points \* in the branch  $L2\_3\_up$ . Both steady states  $[u_1,\ldots,u_N]$  (in blue), and  $[v_1,\ldots,v_N]$  (in red) have rotational symmetry with respect to the center line x=1/2.

#### activator/inhibitor = red/blue

### discrete even functions = symmetric

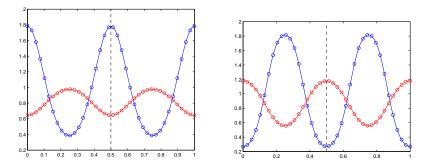


Figure: Schnakenberg model, see Example, N=40, the branch  $L2\_4\_up$ : Consider the steady states  $[u_1,\ldots,u_N,v_1,\ldots,v_N]\in\mathbb{R}^{2N}$  related the two marked test points \* in the branch  $L2\_4\_up$ . Both steady states  $[u_1,\ldots,u_N]$  (in blue), and  $[v_1,\ldots,v_N]$  (in red) have symmetry of reflection with respect to the center line x=1/2.

activator/inhibitor = red/blue

$$L^2$$
, asym  $\equiv \frac{u_1 - u_N}{2}$ , sym  $\equiv \frac{u_1 + u_N}{2}$ .

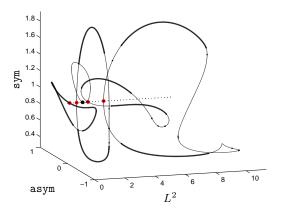


Figure: Schnakenberg model, see Example. Homogeneous steady states (dashed). Branches of inhomogeneous steady states emanating from L2\_1\_up, L2\_2\_up, L2\_1\_down, L2\_3\_up, L2\_4\_up.

33 / 41

### **Outline**

- Pattern formation: Turing instability
  - Domain size driven instability
- Solution manifolds and numerical continuation
- Critical wavelengths: primary bifurcation
- Symmetries of steady states
- Conclusions
- 6 Supplement: Dynamic simulation

#### Conclusions

Algorithmic contribution to the continuation algorithm: a) initialization of the branch (via Taylor expansion of the bifurcation equation), b) segmenting the branch, distinquishing stable and unstable branch segments.

#### Results

- classification of model symmetries
- construction of a global bifurcation diagram

### **Outline**

- Pattern formation: Turing instability
  - Domain size driven instability
- Solution manifolds and numerical continuation
- Critical wavelengths: primary bifurcation
- Symmetries of steady states
- Conclusions
- 6 Supplement: Dynamic simulation

# Supplement: Dynamic simulation

Recall

$$F: \mathbb{R}^{2N} \times \mathbb{R}^1 \longrightarrow \mathbb{R}^{2N}$$

$$F(w, L^2) = 0$$
,  $w \in \mathbb{R}^{2N}$ ,  $w_i = u_i$ ,  $w_{N+i} = v_i$ ,  $i = 1, ..., N$ .

Dynamic simulation. Define the initial value problem

$$w'(t) = F(w(t), L^2),$$

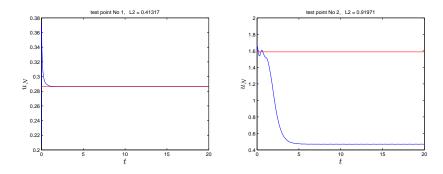
$$t \in \mathbb{R}^1 \longmapsto w(t) = \left[u_1(t), \ldots, u_N(t), v_1(t), \ldots, v_N(t)\right]^T \in \mathbb{R}^{2N}$$
.

*L* is fixed. The initial condition  $w^0 \in \mathbb{R}^{2N}$  is usually considered to be randomly perturbed *homogeneous steady state*.

It is expected that  $w(t) \in \mathbb{R}^{2N} \longmapsto [u_1, \dots, u_N, v_1, \dots, v_N]^T \in \mathbb{R}^{2N}$  as  $t \in \mathbb{R}^1 \longmapsto \infty$ . Thus, in the case of convergence, the vector  $[u_1, \dots, u_N, v_1, \dots, v_N]^T$  can be an *inhomogeneous* steady state related to the selected parameter L.

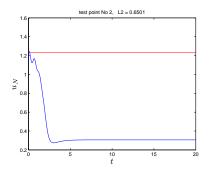
#### We are going to illustrate that

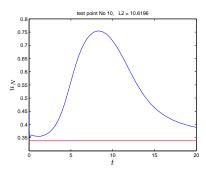
- dynamic simulations can converge to steady states that are not unique,
- it may not converge at all.
- in principle, the dynamic simulation can only provide stable steady states.



On the left: Consider the branch *L2\_1\_up*. Dynamic simulation: random perturbation at stable test point No 1. Steady state (red), resulting trajectory (blue).

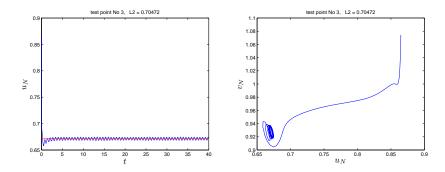
On the right: Consider the branch  $L2_1$ -down. Dynamic simulation: random perturbation at an unstable test point No 2. Steady state (red), resulting trajectory (blue).





On the left: Consider the branch  $L2\_2\_up$ . Dynamic simulation: random perturbation at unstable test point No 2. Steady state (red), resulting trajectory (blue).

On the right: Consider the branch *L2\_5\_up*. Dynamic simulation: random perturbation at stable test point No 10. Steady state (red), resulting trajectory (blue). Observe the *Transient growth*.



The branch *L*2\_1\_*up*. Dynamic simulation: random perturbation at unstable test point No 3. On the left: Steady state (red), resulting oscillation (blue). On the right: Phase portrait of the oscillations.