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Pattern Prediction in Networks of Diffusively Coupled Nonlinear Systems ^{*}

K. Rogov ^{*} A. Pogromsky ^{*} E. Steur ^{**} W. Michiels ^{***} H. Nijmeijer ^{*}

^{*} Department of Mechanical Engineering, Eindhoven University of Technology, The Netherlands (e-mail: K.Rogov@tue.nl, A.Pogromski@tue.nl, H.Nijmeijer@tue.nl)

^{**} Delft Center for Systems and Control, Delft University of Technology, The Netherlands (e-mail: E.Steur@tudelft.nl)

^{***} Department of Computer Science, Catholic University of Leuven, Belgium (e-mail: Wim.Michiels@cs.kuleuven.be)

Abstract: In this paper, we present a method aiming at pattern prediction in networks of diffusively coupled nonlinear systems. Interconnecting several globally asymptotically stable systems into a network via diffusion can result in diffusion-driven instability phenomena, which may lead to pattern formation in coupled systems. Some of the patterns may co-exist which implies the multi-stability of the network. Multi-stability makes the application of common analysis methods, such as the direct Lyapunov method, highly involved. We develop a numerically efficient method in order to analyze the oscillatory behavior occurring in such networks. We show that the oscillations appear via a Hopf bifurcation and therefore display sinusoidal-like behavior in the neighborhood of the bifurcation point. This allows to use the describing function method in order to replace a nonlinearity by its linear approximation and then to analyze the system of linear equations by means of the multivariable harmonic balance method. The method cannot be directly applied to a network consisting of systems of any structure and here we present the multivariable harmonic balance method for networks with a general system's structure and dynamics.

Keywords: Limit Cycles in Networks of Oscillators, Bifurcations in Chaotic or Complex Systems, Theory and Applications of Complex Dynamical Networks.

1. INTRODUCTION

In recent years, the investigation of complex networks consisting of coupled nonlinear dynamical systems has been an important subject in mathematical biology, control theory, applied physics and interdisciplinary fields. Its relevance is due to several factors: complex networks are prevalent in nature (e.g. Neuroscience, Heart cells synchronization), these networks possess a rich phenomenology and a large number of different applications (see Pikovsky et al. (2001), Strogatz (2003) and references therein). In particular, synchronization and *pattern formation* in coupled systems are subjects of intense research.

Numerous situations in nature exhibit oscillatory behavior and can be described by ensembles of coupled nonlinear oscillators. Due to complex dynamics and different types of coupling, an appearance of different phenomena in the nonlinear networks is a logical consequence. An omnipresent form of interaction is *diffusive coupling* (Hale (1997)), in which the feedback to each (sub)system in the network is a local sum of differences of variables with respect to the neighbors. Diffusively coupled networks exhibit surprisingly rich phenomena, such as synchronization (Pogromsky and Nijmeijer (2001)), partial synchronization (Pogromsky et al. (2011)), waves (Iwasaki (2008)), and patterns arising from a *diffusion-driven instability* discovered

by Turing (1952). Moreover, some of these patterns may co-exist. In his research, Turing (1952) "suggests that a system of chemical substances reacting together and diffusing through a tissue, is adequate to account for the main phenomena of morphogenesis". He introduces several concepts related to the chemical basis of morphogenesis (development of patterns), spatial chemical patterns, and what is now called diffusion-driven instability.

A nonlinear analysis of the diffusion-driven instability phenomena is performed by Smale (1976). In this paper, he studies an example of two systems which are diffusively coupled. Each individual system represents a cell which is inert or dead in the sense that it is globally asymptotically stable. However, when the cells are coupled via diffusion, "the cellular system pulses (or expressed perhaps overdramatically, becomes alive!) in the sense that the concentration of enzymes in each cell will oscillate infinitely". He poses the problem of determining conditions under which diffusive coupling leads to oscillatory behavior in the network of initially globally asymptotically stable systems. Related results can be found in Yakubovich and Tomberg (1989), Tomberg and Yakubovich (2000), and Pogromsky et al. (1999), and references therein.

Another related result is obtained by Pogromsky et al. (2011). In that research, the authors present conditions under which the network of systems which are globally asymptotically stable by themselves, being diffusively coupled can display a synchronous state, such as synchronous and partial synchronous

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(oscillatory) behavior. These conditions are shown to be dependent on a coupling strength of the network. When the coupling strength exceeds a threshold, oscillatory behavior appears in the network, which corresponds to a *Hopf bifurcation* in a network. The Hopf bifurcations change the dynamics of the network from a stable equilibrium to oscillatory patterns. However, there are some open questions that are not answered in that paper. One of these is the *prediction* of oscillatory patterns in the neighbourhood of the bifurcation point in the complex networks. Another question arises from the fact that there may exist different oscillatory patterns, which can occur in the networks with diffusive coupling, such as an in-phase and an anti-phase synchronization, and some of patterns can even co-exist, such as clockwise and counterclockwise waves in a ring-like structure. This *co-existence* implies multi-stability of the network. Considering the multi-stability, the application of common methods, such as the direct Lyapunov method, becomes nontrivial.

To answer these questions, we propose an extension of the *multivariable harmonic balance* (MHB) method developed by Iwasaki (2008) for a neuronal circuits called the central pattern generators (CPGs). The method allows to analyse behavior of the complex networks near the bifurcation point and to determine oscillation profiles that approximate the output of the studied network without simulating ordinary differential equations (ODEs). Despite these advantages, the MHB method cannot be directly applied to a network with systems of any structure and provides no information about system's behavior when the system is not in the neighborhood of the bifurcation point. Being inspired by previous results of Pogromsky et al. (2011) and Iwasaki (2008), we develop a new approach in order to analyze oscillatory behavior and predict pattern formation in the complex networks by means of the multivariable harmonic balance method.

The MHB method provides accurate results near the bifurcation point and numerical tools for bifurcation analysis require accurate initial points for the continuation analysis, otherwise, we cannot be sure which solution we follow. This implies that the MHB method can be used as the first step of the continuation analysis. In other words, possessing components of an oscillation profile (i.e. frequency, amplitude and phase) allows us to use these results as initial conditions for the numerical continuation of found patterns in order to determine system behavior when the system is out of the neighbourhood of the bifurcation point.

This paper is organized as follows. The problem formulation is given in section 2. In the third section, we describe the challenges which we encountered during the deriving the MHB equation. The fourth section provides the methodology of solving the derived MHB equation. We finish the paper with numerical examples and a discussion of the results and the further study.

Throughout the paper, the following notations are used. I_k and I_n denote the identity matrices of the size $k \times k$ and $n \times n$, respectively. \top stands for the transposition. i stands for the imaginary unit. $s = i\omega$ is a complex number frequency parameter. The notation \mathbb{R} is the field of the real numbers. \mathbb{R}^+ stands for a vector space over the field of the positive real numbers. \mathbb{R}^n stands for the product of n copies of \mathbb{R} , which is an n -dimensional vector space. The notation \mathbb{C} is the field of

the complex numbers. A function $f : x \rightarrow y$ is C^1 function that stands for a continuously differentiable function.

2. PROBLEM FORMULATION

Coupling several even globally asymptotically stable systems into a network can result in the occurrence of unpredicted patterns called emergent behavior. Moreover, these patterns may co-exist. As mentioned above, the diffusion-driven instability is studied by Smale (1976), who proposes a model of two 4th order diffusively coupled identical cells, despite each independent cell is globally asymptotically stable. Smale shows that connecting the cells via diffusive coupling results in oscillatory behavior.

In this paper we present a method to analyze the behavior of the networks with diffusive coupling in a neighbourhood of the bifurcation point. To do so, we consider a *diffusive cellular network* which describes a network of identical diffusively coupled (sub)systems that cannot be decomposed into two or more uncoupled networks.

To turn the statements above into a mathematical description, consider k identical systems of the following form

$$\begin{aligned} \dot{x}_j &= Ax_j + Bu_j, \\ u_j &= u_{cj} - \psi(z_j), \\ z_j &= Zx_j, \\ y_j &= Cx_j, \end{aligned} \quad (1)$$

where $j = 1, \dots, k$, $x_j(t) \in \mathbb{R}^n$ is the state of the j -th system, $u_j(t) \in \mathbb{R}^1$ is the input of the j -th system, $y_j(t) \in \mathbb{R}^1$ is the output of the j -th system, ψ is a continuously differentiable scalar nonlinear function, $z_j \in \mathbb{R}^1$ and A, B, C, Z are constant matrices of appropriate dimension. We assume that matrix CB is a positive definite matrix and all subsystems are interconnected through mutual linear output coupling

$$u_{cj} = -\gamma_{j1}(y_j - y_1) - \gamma_{j2}(y_j - y_2) - \dots - \gamma_{jk}(y_j - y_k), \quad (2)$$

where γ_{jl} are non-negative constants. Moreover, $\gamma_{jl} > 0$ if and only if j -th and l -th nodes are connected.

Define the $k \times k$ matrix Γ as

$$\Gamma = \begin{pmatrix} \sum_{l=2}^k \gamma_{1l} & -\gamma_{12} & \dots & -\gamma_{1k} \\ -\gamma_{21} & \sum_{l=1, l \neq 2}^k \gamma_{2l} & \dots & -\gamma_{2k} \\ \vdots & \vdots & \ddots & \vdots \\ -\gamma_{k1} & -\gamma_{k2} & \dots & \sum_{l=1}^{k-1} \gamma_{kl} \end{pmatrix}, \quad (3)$$

where all row sums are zero.

The goal of this section is to present conditions that guarantee that the network (1)-(2) exhibits oscillatory behavior in the following sense:

Definition 1. (Yakubovich (1973)) A scalar function $\zeta : \mathbb{R}^1 \rightarrow \mathbb{R}^1$ is called oscillatory in the sense of Yakubovich (or Y-oscillatory) for $t \rightarrow +\infty$ if $\zeta(t)$ is bounded on \mathbb{R}^+ and

$$\overline{\lim}_{t \rightarrow +\infty} \zeta(t) \geq \mathcal{B}, \quad \underline{\lim}_{t \rightarrow +\infty} \zeta(t) \leq \mathcal{A}$$

for some $\mathcal{B} > \mathcal{A}$.

Definition 2. The system (1)-(2) is called *Y-oscillatory with respect to a scalar output* y_j if each solution $x_j(t)$ is bounded and for almost all initial conditions $x_j(0)$

$$\lim_{t \rightarrow +\infty} y_j(t) < \overline{\lim}_{t \rightarrow +\infty} y_j(t).$$

We call the system Y-oscillatory if it is Y-oscillatory with respect to at least one component of the vector x_j .

Define two transfer functions

$$W_y(s) = C(sI - A)^{-1}B, \quad (4)$$

$$W_z(s) = Z(sI - A)^{-1}B, \quad (5)$$

where $W_y(s)$ is the transfer function from u_j to $y_j = Cx$ taking $\psi(z_j) = 0$ and $W_z(s)$ is the transfer function from u_j to z_j taking $u_{cj} = 0$.

Following Pogromsky et al. (2011), we impose a set of assumptions.

Assumption 1. The following conditions hold

- i) The matrix A is Hurwitz, so there is a positive definite matrix $P = P^\top$, so that $A^\top P + PA = -I_k$;
- ii) $z_j = Zx_j$, where $Z^\top = PB$ with matrix P as in i);
- iii) ψ is an odd, strictly increasing C^1 function with the following property
$$\forall L > 0 \exists \sigma > 0 \forall z_j > \sigma \psi(z_j) > Lz_j;$$
- iv) The transfer function $W_y(s)$ is nondegenerate, has an even number of zeros with positive real part and $W_y(0) > 0$;
- v) The transfer function $W_z(s)$ is such that $W_z(0) > 0$.

The following theorem is presented in Pogromsky et al. (2011).

Theorem 1. Consider a network of diffusively coupled systems of the form (1)-(2) with a symmetric Γ as in (3) that satisfy Assumption 1.

There is a number $\bar{\lambda} > 0$ so that if the largest non-zero eigenvalue of Γ exceeds $\bar{\lambda}$ then the network is oscillatory in the sense of Yakubovich.

The proof of theorem captures three points:

- i) The origin is the unique equilibrium point of the closed loop system;
- ii) The system is uniformly ultimately bounded (see Khalil (1996));
- iii) The origin is hyperbolically unstable if $\lambda_{max} > \bar{\lambda}$, where λ_{max} is the largest eigenvalue of Γ .

It follows from the proof that a Hopf bifurcation occurs at $\lambda_{max} = \bar{\lambda}$ in the network of given form (1)-(2). According to normal form theory (see Han and Yu (2012) and references therein), the oscillations are sinusoidal-like near the bifurcation point. It allows to use the describing function method to replace the nonlinearity by its linear approximation and then to analyze the system of linear equations by means of the multivariable harmonic balance method.

The MHB method is based on the approximation of a periodic solution to the system by a sinusoidal signal, and nonlinearity ψ by its describing function. Suppose a system has a periodic solution. Then, by Fourier series expansion, we obtain

$$q_j(t) = \sum_{m=0}^{\infty} a_m \sin(\omega m t) + b_m \cos(\omega m t)$$

for some real vectors a_m and b_m and frequency ω . The signal $q_j(t)$ can then be rewritten as

$$q_j(t) \cong \alpha_j \sin(\omega t + \phi_0 + \phi_j), \quad (6)$$

where α_j is the amplitude, ω is the frequency, ϕ_0 is the initial phase and ϕ_j is the phase shift for the j -th subsystem of the

network. For the autonomous system we can take ϕ_0 to be equal to 0. Let us approximate nonlinearity ψ by its describing function k

$$\psi(q_j) \cong k(\alpha_j)q_j, \quad (7)$$

$$k(\alpha_j) := \frac{2}{\pi \alpha_j} \int_0^\pi \psi(\alpha_j \sin \theta) \sin \theta d\theta. \quad (8)$$

The describing function $k(\alpha_j)$ stands for the gain of ψ when the input is a sinusoidal signal of amplitude α_j and the output is approximated by its first harmonic (Khalil (1996)). In this paper, we focus on determining the waves with *equal amplitudes*. We thus look for $\alpha_j = \alpha_e \forall j$, with $\alpha_e \in \mathbb{R}^+$.

The MHB method for networks of specific structure is described by Iwasaki (2008), and here we present the multivariable harmonic balance method for networks with a more general system's structure and dynamics.

3. DERIVING THE MHB EQUATION

The multivariable harmonic balance (MHB) method turns the problem of determining an oscillation profile (frequency ω , amplitudes α_j , phases ϕ_j) into an easily solvable eigenvalue problem rather than doing a dynamical analysis by means of the direct Lyapunov method. The network of identical interconnected (sub)system can be described by a dynamical mapping from the input u_j to the output of interest q_j :

$$v_j = \Psi(q_j), \quad u_j = \sum_{l=1}^k \mu_{jl}(s)v_l, \quad q_j = f_j(s)u_j,$$

where $f(s)$ is a complex valued rational transfer function which represents the linear time-invariant part of each subsystem, $\Psi(q_j)$ is the continuously differentiable odd static nonlinear function, $q_j \in \mathbb{C}^1$ is the output and $\mu_{jk}(s)$ is a transfer function of connection from k -th system to j -th system. In a vector form, the dynamics can be written as

$$v = \Psi(q), \quad q = \mathcal{M}(s)v, \quad \mathcal{M}(s) = F(s)M(s), \quad (9)$$

where $q := \text{col}[q_1, \dots, q_k]$ $M(s)$ is the transfer matrix of the coupling whose (j, k) entry is $\mu_{jk}(s)$, $F(s) := f(s)I_k$ and $\Psi := \text{col}[\Psi(q_1), \dots, \Psi(q_k)]$.

With approximations (6)-(8), the dynamical equations reduce to the MHB equation

$$(\mathcal{M}(s)\mathcal{K}(\alpha) - I_k)q = 0, \quad q_j := \alpha_j e^{i\phi_j}, \quad q \in \mathbb{C}^k, \quad (10)$$

where $\mathcal{K}(\alpha) := k(\alpha_j)I_k$ is a diagonal matrix of the describing functions. The MHB equation characterizes the oscillation profile for (9).

In general, the MHB equation does not have a unique solution and we want to identify the stable oscillation. In order to examine the stability of the determined oscillatory profile, we can use an argument from Glad and Ljung (2000) as follows. Consider the linear systems obtained by replacing the nonlinearity Ψ with a constant gain K

$$q = \mathcal{M}(s)v, \quad v = Kv, \quad (11)$$

with $K := \mathcal{K}(\alpha)$. Name this linear system L_K . The oscillation with certain ω, α, ϕ is expected stable if L_K is stable/unstable when small perturbations in positive/negative direction ($\alpha \pm \delta\alpha$) are applied to α so that the perturbed orbit tends to the original one.

The key ideas of the MHB analysis can be summarised as follows:

Substituting (4) and (5) into the equation above, we obtain

$$k(\alpha_e)Z(i\omega I_k - A)^{-1}B + 1 + \lambda_{max}C(i\omega I_n - A)^{-1}B = 0,$$

$$1 + (k(\alpha_e)Z + \lambda_{max}C)(i\omega I_n - A)^{-1}B = 0.$$

Since $\det(i\omega I_n - A) \neq 0$, we have

$$\det(i\omega I_k - A)[1 + (k(\alpha_e)Z + \lambda_{max}C)(i\omega I_n - A)^{-1}B] = 0.$$

Using Schur's Lemma (see Dummit and Foote (1999)), we arrive at

$$\det[i\omega I_n - A + B(k(\alpha_e)Z + \lambda_{max}C)] = 0.$$

Thus matrix of a relatively low order $A - B(k(\alpha_e)Z + \lambda_{max}C)$ has imaginary eigenvalues for $\pm i\omega$, where ω stands for frequency of the oscillations. In other words $k(\alpha_e)$ and ω can be derived from the Hopf bifurcation condition.

We now have two components of the oscillation profile α_e which is computed by (8) and ω . The phases ϕ_j are encoded in the eigenvector that corresponds to the largest eigenvalue λ_{max} of the topology matrix Γ . Substitute $(k(\alpha_e)W_z(i\omega) + 1)/W_y(i\omega) = -\lambda_{max}$ in (14) in order to obtain

$$[\Gamma - \lambda_k I_k]q = 0.$$

Since we look for the equal amplitudes, we need such eigenvector q from $\Lambda := span[q]$ that all entries of q have the same modulus. In order to determine the phases from the eigenvector the following equation is used

$$\phi_j = \text{angle}(q_j).$$

We now have all components of the oscillation profile and can construct the approximation of the output of the network using (6). The equal amplitude case is fully investigated and the oscillation profile is determined. In the next section the numerical examples are presented.

5. NUMERICAL EXAMPLES

As examples we study ring networks of three and four diffusively coupled identical (sub)systems.

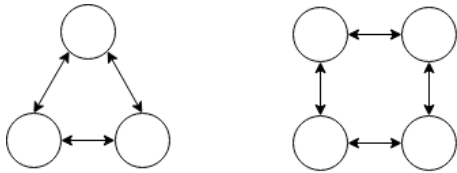


Fig. 2. A ring-like structure of networks of identical diffusively coupled systems

The individual dynamics of the nodes, as in Pogromsky et al. (2011), is given in (1) with

$$A = \begin{pmatrix} 1 & -1 & 1 \\ 1 & 0 & 0 \\ -4 & 2 & -3 \end{pmatrix}$$

$$B = (0 \ 0 \ 1)^T, \quad C = (0 \ 0 \ 1), \quad Z = B^T P,$$

where P is the solution to the Lyapunov equation

$$A^T P + PA = -I_3.$$

This setting satisfies the conditions imposed in *Assumption 1*.

The topology of the network is given by matrices Γ_3 and Γ_4 where subscript denotes the number of nodes in the network

$$\Gamma_3 = \gamma_3 \begin{pmatrix} 2 & -1 & -1 \\ -1 & 2 & -1 \\ -1 & -1 & 2 \end{pmatrix}, \quad \Gamma_4 = \gamma_4 \begin{pmatrix} 2 & -1 & 0 & -1 \\ -1 & 2 & -1 & 0 \\ 0 & -1 & 2 & -1 \\ -1 & 0 & -1 & 2 \end{pmatrix},$$

where $\gamma_{3,4}$ are positive parameters. One can also conclude that there are positive numbers a_3, a_4 so that if $a_3 < \gamma_3$ and $a_4 < \gamma_4$ for the three node and four node systems, respectively, (a_3, a_4 can be calculated from the Hopf bifurcation condition: $a_3 = 0.4343$ and $a_4 = 0.3257$) the systems are Y-oscillatory.

The nonlinear function is given as follows

$$\psi(z_j) = z_j^3;$$

and computing the describing function by (8), we obtain

$$k(\alpha_e) = \frac{3}{4} \alpha_e^2.$$

For the three node network, two wave-like oscillatory patterns (clockwise and counterclockwise waves) are found and the oscillation parameters are successfully determined. The derived oscillation profiles for coupling strength $\gamma_3 = 0.4386$ are presented in the table below

Table 1. Oscillatory profiles for Γ_3 structure

Wave	ω	α_e	ϕ_1	ϕ_2	ϕ_3
Clockwise	0.8365	0.1296	0	-120	120
Counterclockwise	0.8365	0.1296	0	120	-120

For the four node network, the one wave-like solution is predicted. The solution predicts the partial synchronization. We can observe synchronous behavior between pairs of nodes 1 and 3, and 2 and 4. Moreover, these pairs are in anti-phase synchronization with respect to each other. The predicted oscillation profile is provided in the following table

Table 2. Oscillatory profile for Γ_4 structure

γ_4	ω	α_e	ϕ_1	ϕ_2	ϕ_3	ϕ_4
0.3290	0.8362	0.1159	0	180	0	180

Figures 3 and 4 display outputs $y(t)$ and $q(t)$ of the simulation and the MHB method for the clockwise wave for the ring of three nodes and for the ring of four nodes, respectively. Offsets $y_j(t) + 2(j-1)$ and $q_j(t) + 2(j-1)$ are added for the visibility.

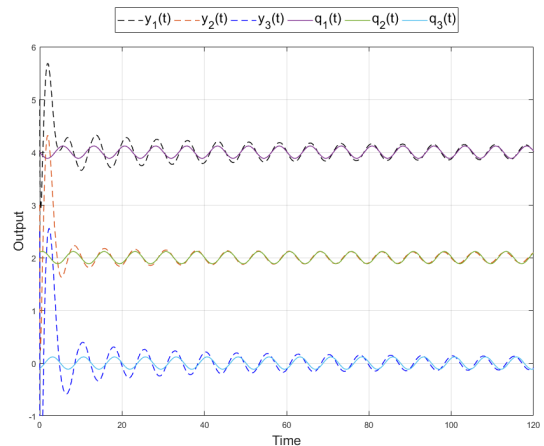


Fig. 3. Output of simulation and output of the MHB method for the ring of three nodes

In the case of the four node network, the MHB method predicts the result which was previously obtained by the direct Lyapunov method in Pogromsky et al. (2011). For the three node

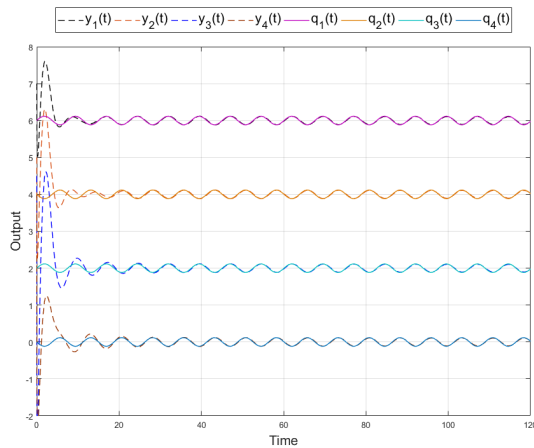


Fig. 4. Output of simulation and output of the MHB method for the ring of four nodes

case, the analysis by means of the direct Lyapunov method can be nontrivial due to the co-existence of two stable solutions.

One can notice that in the beginning the output of simulation and the output of the MHB method do not match because of the transient process. After decay of transients the outputs are almost identical which clarifies the accuracy of the approximations. For some initial conditions, the outputs of the simulation and of the MHB method can mismatch in initial phase and in order to avoid it, we did add initial phase offset ϕ_0 .

6. CONCLUSION

The paper addresses the problem of predicting oscillatory patterns in a network. We developed the multivariable harmonic balance method for the networks with a more general structure and dynamics, which allows to predict the oscillatory patterns appearing in such networks even if some of patterns co-exist. Our approach determines the oscillation profile (i.e. frequency, amplitudes, phases) which is encoded in the largest eigenvalue and its corresponding eigenvector of the coupling matrix in the equal amplitudes case. In this work, we show that the MHB method provides a very accurate approximation of the ODEs simulation in the neighborhood of the bifurcation point. Moreover, the oscillation profile components obtained by the approach can be used as initial points for the further numerical continuation analysis.

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