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Multiple bifurcations generated by mode interactions in a reaction–diffusion problem

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Abstract

We study multiple bifurcations in a system of reaction–diffusion equations defined on a unit square with Robin boundary conditions. First we investigate linear stabilities of the system at the uniform steady state solution. Then we discuss how multiple bifurcations can be generated by mode interactions of the system, and how these multiple bifurcations can be preserved in the associated discrete system. A continuation-unsymmetric Lanczos algorithm is described to trace discrete solution curves. Numerical experiments on the Brusselator equations are reported. © 2001 Elsevier Science B.V. All rights reserved.

Keywords: Reaction–diffusion system; Brusselator equations; Bifurcation; Mode interactions; Numerical continuation methods; Unsymmetric Lanczos method

1. Introduction

In this thesis, we will be concerned with the numerical solution branches of a system of two-dimensional reaction–diffusion equations of the form

$$\begin{aligned} \frac{\partial u}{\partial t} &= d_1 \Delta u + f(u, v, \Lambda) \\ &\qquad \text{in } \Omega = [0, \ell] \times [0, \ell], \\ \frac{\partial v}{\partial t} &= d_2 \Delta v + g(u, v, \Lambda) \end{aligned} \tag{1.1}$$

for some positive number $\ell > 0$, for all $t \geqslant 0$. Here the unknowns u, v are state variables which represent concentrations of some intermediate chemicals in the reaction, d_1 and d_2 are diffusion

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rates, while $\Lambda=(\lambda,\alpha,\ldots,\rho)^{\mathrm{T}}\in\mathbb{R}^k$ is the control parameter vector in the system, e.g., initial or final products, catalysts, temperature, etc. As is customary, we shall treat λ as the bifurcation parameter, and the remaining parameters are fixed. Thus when no confusion arises we replace the parameter vector Λ by the single parameter $\lambda\in\mathbb{R}$. A typical example of (1.1) is the well-known Brusselator equations with

$$f(u,v,\lambda)=-(\lambda+1)u+u^2v+\alpha,$$

$$g(u,v,\lambda)=\lambda u-u^2v.$$

Here u,v,λ,α all represent chemical concentrations, see e.g., [10,13, Chapter 7;19,22,24].

In general, one imposes Dirichlet boundary conditions

$$u(x,y,t)=u_0,\quad v(x,y,t)=v_0,\quad (x,y)\in\partial\Omega, \tag{1.2}$$

on Eq. (1.1). Here (u_0,v_0) is a uniform steady-state solution which is independent of the variables x,y,λ and satisfy

$$f(u_0,v_0,\lambda)=g(u_0,v_0,\lambda)=0.$$

On the other hand, one may also consider homogeneous Neumann boundary conditions (see [2])

$$\frac{\partial u}{\partial n}=\frac{\partial v}{\partial n}=0\quad\text{on }\partial\Omega. \tag{1.3}$$

Since we are interested in bifurcations from the trivial solution, we shift the steady-state solution (u_0,v_0) to $(0,0)$ by using suitable linear transformation. Now we impose Robin boundary conditions [4]

$$g_0(\mu)\begin{pmatrix}u\\v\end{pmatrix}+g_1(\mu)\begin{pmatrix}\dfrac{\partial u}{\partial n}\\[2mm]\dfrac{\partial v}{\partial n}\end{pmatrix}=0,\quad (x,y)\in\partial\Omega \tag{1.4}$$

on Eq. (1.1), where g_i, $i=1,2$, are smooth functions which satisfy

$$g_0(0)\cdot g_1(1)\cdot g_0(\mu)\cdot g_1(\mu)\neq 0 \quad \text{for all } \mu\in(0,1).$$
$$g_0(1)=g_1(0)=0$$

For $\mu=0$ we have the homogeneous Dirichlet boundary conditions (1.2), while for $\mu=1$ we obtain the homogeneous Neumann boundary conditions (1.3).

The reaction–diffusion system (1.1) in general exhibits a wide variety of bifurcation phenomena. During the past decades some researchers have used various analytic methods to investigate multiple bifurcation behavior of certain reaction–diffusion systems, see e.g., [10,22,24]. Recently, Adomian [2] has exploited the decomposition method [1] to study solutions of (1.1) with initial conditions $u(x,y,0)=2+0.25y$, $v(x,y,0)=1+0.8x$, $\lambda=3.4$, $\alpha=1$, $d_1=d_2=0.002$, and Neumann boundary conditions $\partial u/\partial n=\partial v/\partial n=0$. On the other hand, Chien and Chen [7] have investigated multiple bifurcations of Eq. (1.1) with Dirichlet boundary conditions by using numerical continuation methods [3,16] to trace solution curves, where both the direct method and the BiCG method are used as linear solvers. In this paper, we study multiple bifurcations of Eq. (1.1) with Robin boundary conditions

(1.4). Of special interest here is the high corank multiple bifurcations generated by mode interactions, see e.g., [5,14, Chapter 19].

This paper is organized as follows. In Section 2 we discuss linear stabilities of Eq. (1.1) with Robin boundary conditions (1.4). The corresponding centered difference approximations of the above equation is described in Section 3. In Section 4 a continuation-unsymmetric Lanczos algorithm is proposed for curve-tracking. Finally, our sample numerical results are reported in Section 5.

2. Linear stability analysis

2.1. General system

To simplify the discussions and the numerical approximations, we shift the homogeneous states (u_0, v_0) to $(0,0)$ by the transformation $(u,v) = (u_0 + \tilde{u}, v_0 + \tilde{v})$ and choose $\ell = 1$. Eqs. (1.1) can be expressed as

$$\begin{aligned} \frac{\partial \tilde{u}}{\partial t} &= d_1 \left(\frac{\partial^2 \tilde{u}}{\partial \tilde{x}^2} + \frac{\partial^2 \tilde{u}}{\partial \tilde{y}^2} \right) + f(u_0 + \tilde{u}, v_0 + \tilde{v}, \lambda) \\ &\qquad \text{in } \Omega = [0,1] \times [0,1]. \\ \frac{\partial \tilde{v}}{\partial t} &= d_2 \left(\frac{\partial^2 \tilde{v}}{\partial \tilde{x}^2} + \frac{\partial^2 \tilde{v}}{\partial \tilde{y}^2} \right) + g(u_0 + \tilde{u}, v_0 + \tilde{v}, \lambda) \end{aligned} \tag{2.1}$$

For simplicity we denote $f(u_0+\tilde{u}, v_0+\tilde{v}, \lambda)$, $g(u_0+\tilde{u}, v_0+\tilde{v}, \lambda)$ and $\tilde{u}, \tilde{v}$ again by $f(u,v,\lambda)$, $g(u,v,\lambda)$ and u, v, respectively, when no confusion arises.

Let

$$C_0^2(\Omega) := \left\{ u \in C^2(\Omega); u|_{\partial\Omega} = -\frac{g_1(\mu)}{g_0(\mu)} \cdot \frac{\partial u}{\partial n} \right\}$$

and

$$X := (C_0^2(\Omega)) \times (C_0^2(\Omega)), \qquad Y := (C(\Omega)) \times (C(\Omega)),$$

where X and Y denote the product spaces of $C_0^2(\Omega)$ and $C(\Omega)$, respectively. We rewrite (2.1) as an operator equation

$$\frac{\partial \boldsymbol{u}}{\partial t} = \Phi(\boldsymbol{u}, \lambda), \tag{2.2}$$

where $\boldsymbol{u} := (u, v)$, and the mapping $\Phi : X \times \mathbb{R} \to Y$ is defined by

$$\Phi(\boldsymbol{u}, \lambda) := \begin{pmatrix} d_1 \left(\dfrac{\partial^2 u}{\partial x^2} + \dfrac{\partial^2 u}{\partial y^2} \right) \\ d_2 \left(\dfrac{\partial^2 v}{\partial x^2} + \dfrac{\partial^2 v}{\partial y^2} \right) \end{pmatrix} + \begin{pmatrix} f(u,v,\lambda) \\ g(u,v,\lambda) \end{pmatrix}.$$

Differentiating Φ with respect to $\boldsymbol{u}$ at the homogeneous equilibrium $\boldsymbol{u}_0 \equiv (u_0, v_0) \equiv (0,0)$, we obtain the linerization L of Φ,

$$L := D_{\boldsymbol{u}}\Phi(\boldsymbol{u}_0, \lambda) = \begin{pmatrix} d_1\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right) & 0 \\ 0 & d_2\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right) \end{pmatrix} + \begin{pmatrix} \frac{\partial f}{\partial u}(0,0,\lambda) & \frac{\partial f}{\partial v}(0,0,\lambda) \\ \frac{\partial g}{\partial u}(0,0,\lambda) & \frac{\partial g}{\partial v}(0,0,\lambda) \end{pmatrix}.$$

Thereafter, stabilities of $\boldsymbol{u}_0$ can be analyzed via solutions of the variational problem

$$\frac{\partial \boldsymbol{u}}{\partial t} = L\boldsymbol{u}.$$

To examine the spectrum of L, we observe that the direct sum

$$X = \sum_{\kappa(\mu)=\kappa_x^2(\mu)+\kappa_y^2(\mu)} \oplus X_{\kappa(\mu)}, \quad X_{\kappa(\mu)} := \left\{ \begin{pmatrix} c_1 \\ c_2 \end{pmatrix} \phi_1 + \begin{pmatrix} c_3 \\ c_4 \end{pmatrix} \phi_2; c_1, c_2, c_3, c_4 \in \mathbb{R} \right\}$$

holds, where

$$\begin{aligned} \phi_1 &= [g_0(\mu)\sin(\kappa_x(\mu)x) + g_1(\mu)\kappa_x(\mu)\cos(\kappa_x(\mu)x)] \\ &\quad \times [g_0(\mu)\sin(\kappa_y(\mu)y) + g_1(\mu)\kappa_y(\mu)\cos(\kappa_y(\mu)y)], \\ \phi_2 &= [g_0(\mu)\sin(\kappa_y(\mu)x) + g_1(\mu)\kappa_y(\mu)\cos(\kappa_y(\mu)x)] \\ &\quad \times [g_0(\mu)\sin(\kappa_x(\mu)y) + g_1(\mu)\kappa_x(\mu)\cos(\kappa_x(\mu)y)], \end{aligned}$$

and κ_x, κ_y satisfy the following equation:

$$2g_0(\mu)g_1(\mu)\kappa\cos\kappa + (g_0^2(\mu) - g_1^2(\mu)\kappa^2)\sin\kappa = 0. \tag{2.3}$$

We refer to [4] for details. Moreover, L maps $X_{\kappa(\mu)}$ into itself. That is,

$$L\left(\begin{pmatrix} c_1 \\ c_2 \end{pmatrix} \phi_1 + \begin{pmatrix} c_3 \\ c_4 \end{pmatrix} \phi_2\right) = \begin{pmatrix} -d_1\kappa(\mu) + f_u^0 & f_v^0 \\ g_u^0 & -d_2\kappa(\mu) + g_v^0 \end{pmatrix} \cdot \left(\begin{pmatrix} c_1 \\ c_2 \end{pmatrix} \phi_1 + \begin{pmatrix} c_3 \\ c_4 \end{pmatrix} \phi_2\right).$$

Here and in the sequel, $f_u^0, f_v^0, \ldots$, represent the partial derivatives of f with respect to u and v at $(0,0,\lambda)$, respectively.

The restriction of L in the subspace $X_{\kappa(\mu)}$ is a 2×2 matrix

$$M_{\kappa(\mu)}(\lambda) := L|_{X_{\kappa(\mu)}} = \begin{pmatrix} -d_1\kappa(\mu) + f_u^0 & f_v^0 \\ g_u^0 & -d_2\kappa(\mu) + g_v^0 \end{pmatrix}. \tag{2.4}$$

The eigenvalues of L consist of those of $M_{\kappa(\mu)} \in \mathbb{R}^{2\times 2}$. On the other hand, the eigenvalues ν_1, ν_2 of a matrix $M \in \mathbb{R}^{2\times 2}$ satisfy

$$\det(M) = \nu_1\nu_2, \quad \operatorname{trace}(M) = \nu_1 + \nu_2.$$

In particular, if $\det(M) > 0$ and $\operatorname{trace}(M) = 0$, then ν_1 and ν_2 are pure imaginary. Since

$$\begin{aligned} \det(M_{\kappa(\mu)}(\lambda)) &= (-d_1\kappa(\mu) + f_u^0)(-d_2\kappa(\mu) + g_v^0) - f_v^0 g_u^0, \\ \operatorname{trace}(M_{\kappa(\mu)}(\lambda)) &= (-d_1\kappa(\mu) + f_u^0) + (-d_2\kappa(\mu) + g_v^0), \end{aligned}$$

First, we consider the homogeneous Neumann boundary conditions (1.3), which corresponds to $\beta=0$, or equivalently, $g_0(\mu)=0$, for all $\mu\in(0,1)$. Thus we have

$$A=\begin{pmatrix} A_{N+1} & -2I_{N+1} & & & 0\\ -I_{N+1} & A_{N+1} & -I_{N+1} & & \\ & \ddots & \ddots & \ddots & \\ & & -I_{N+1} & A_{N+1} & -I_{N+1}\\ & 0 & & -2I_{N+1} & A_{N+1}\end{pmatrix}\in\mathbb{R}^{(N+1)^2\times(N+1)^2}, \tag{3.3}$$

with

$$A_{N+1}=\begin{pmatrix} 4 & -2 & & & 0\\ -1 & 4 & -1 & & \\ & \ddots & \ddots & \ddots & \\ & & -1 & 4 & -1\\ & 0 & & -2 & 4\end{pmatrix}=:B_{N+1}+2I_{N+1}\in\mathbb{R}^{(N+1)\times(N+1)},$$

where B_{N+1} is the discretization matrix corresponding to the second-order differential operator $\mathrm{d}^2/\mathrm{d}x^2$ with homogeneous Neumann boundary conditions. The eigenpairs of B_{N+1} are (cf. [15, p. 440])

$$\mu_p=2-2\cos\frac{p\pi}{N},\quad p=0,\dots,N$$

$$V_p=\left[\cos\frac{0p\pi}{N},\cos\frac{p\pi}{N},\dots,\cos\frac{Np\pi}{N}\right]^{\mathrm{T}},\quad p=0,\dots,N. \tag{3.4}$$

Evidently, $H(\mathbf{0},\lambda)\equiv 0$ for all $\lambda\in\mathbb{R}$. The Jacobian matrix corresponding to (3.2) is

$$DH(Z,\lambda)=\begin{pmatrix} d_1A-h^2D_UF & -h^2D_VF & -h^2D_\lambda F\\ -h^2D_UG & d_2A-h^2D_VG & -h^2D_\lambda G\end{pmatrix}, \tag{3.5}$$

where D_UF, D_VF, and D_λ are given by

$$D_UF(Z,\lambda)=\mathrm{diag}(f_u(U_{0,0},V_{0,0},\lambda),\dots,f_u(U_{N,N},V_{N,N},\lambda));\ D_UF(\mathbf{0},\lambda)=f_u^0I_{(N+1)^2},$$

$$D_VF(Z,\lambda)=\mathrm{diag}(f_v(U_{0,0},V_{0,0},\lambda),\dots,f_v(U_{N,N},V_{N,N},\lambda));\ D_VF(\mathbf{0},\lambda)=f_v^0I_{(N+1)^2},$$

$$D_\lambda F(Z,\lambda)=[f_\lambda(U_{0,0},V_{0,0},\lambda),\dots,f_\lambda(U_{N,N},V_{N,N},\lambda)]^{\mathrm{T}};\ D_\lambda F(\mathbf{0},\lambda)\equiv\mathbf{0}.$$

The partial derivatives $D_UG(Z,\lambda)$, $D_VG(Z,\lambda)$, $D_\lambda G(Z,\lambda)$ are defined in a similar way. Along the trivial solution curve $Z\equiv\mathbf{0}$, $\lambda\in\mathbb{R}$, we have

$$DH(\mathbf{0},\lambda)=\begin{pmatrix} d_1A-h^2f_u^0I_{(N+1)^2} & -h^2f_v^0I_{(N+1)^2} & 0\\ -h^2g_u^0I_{(N+1)^2} & d_2A-h^2g_v^0I_{(N+1)^2} & 0\end{pmatrix}:=[L_h\ \mathbf{0}^{\mathrm{T}}], \tag{3.6}$$

where

$$L_h:=\begin{pmatrix} d_1A-h^2f_u^0I_{(N+1)^2} & -h^2f_v^0I_{(N+1)^2}\\ -h^2g_u^0I_{(N+1)^2} & d_2A-h^2g_v^0I_{(N+1)^2}\end{pmatrix}.$$

a stationary bifurcation occurs on $\boldsymbol{u} = (u, v) \equiv \mathbf{0}$ at $\lambda = \lambda_0$ if and only if there exists $\kappa_0(\mu)$ such that

$$\det(M_{\kappa_0(\mu)}(\lambda_0)) = 0.$$

Similarly, a Hopf bifurcation takes place at $\lambda = \lambda^*$ if and only if for some $\kappa_0(\mu)$ we have

$$\operatorname{trace}(M_{\kappa_0(\mu)}(\lambda^*)) = 0, \quad \det(M_{\kappa_0(\mu)}(\lambda^*)) > 0.$$

Let

$$S_{\kappa_1(\mu)} = \{(\kappa_a, \kappa_b)\colon \kappa_a^2 + \kappa_b^2 = \kappa_1(\mu),\ \kappa_a, \kappa_b \text{ satisfy Eq. (2.3)}\}$$

and

$$S_{\kappa_2(\mu)} = \{(\kappa_c, \kappa_d)\colon \kappa_c^2 + \kappa_d^2 = \kappa_2(\mu),\ \kappa_c, \kappa_d \text{ satisfy Eq. (2.3)}\},$$

where $\kappa_1(\mu) \neq \kappa_2(\mu)$. The steady/steady mode interaction of Eq. (2.2) must satisfy

$$\det(M_{\kappa_1(\mu)}(\lambda_0)) = \det(M_{\kappa_2(\mu)}(\lambda_0)) = 0, \tag{2.5}$$

which can be classified as follows. (i) Mode interaction of two simple bifurcations. If there exist $(\kappa_a, \kappa_a) \in S_{\kappa_1(\mu)}$, $(\kappa_b, \kappa_b) \in S_{\kappa_2(\mu)}$ with $\kappa_a \neq \kappa_b$ such that (2.5) holds, then $(\mathbf{0}, \lambda_0)$ is a bifurcation of corank $\geqslant 2$. (ii) Mode interaction of one simple and one double bifurcation. If there exist $(\kappa_a, \kappa_a) \in S_{\kappa_1(\mu)}$, $(\kappa_b, \kappa_c) \in S_{\kappa_2(\mu)}$ with $\kappa_b \neq \kappa_c$, such that (2.5) holds, then $(\mathbf{0}, \lambda_0)$ is a bifurcation point of corank $\geqslant 3$. (iii) Mode interaction of two double bifurcations. If there exist $(\kappa_a, \kappa_b) \in S_{\kappa_1(\mu)}$, $(\kappa_c, \kappa_d) \in S_{\kappa_2(\mu)}$ with $\kappa_a \neq \kappa_b$, $\kappa_c \neq \kappa_d$ and $(\kappa_a, \kappa_b) \neq (\kappa_c, \kappa_d)$ such that (2.5) holds, then $(\mathbf{0}, \lambda_0)$ is a bifurcation point of corank $\geqslant 4$, and so forth.

From (2.5) we have

$$d_1 d_2 \kappa_1^2(\mu) - \kappa_1(\mu)(d_1 g_v^0 + d_2 f_u^0) + f_u^0 g_v^0 - f_v^0 g_u^0 = 0$$

and

$$d_1 d_2 \kappa_2^2(\mu) - \kappa_2(\mu)(d_1 g_v^0 + d_2 f_u^0) + f_u^0 g_v^0 - f_v^0 g_u^0 = 0,$$

which imply that

$$\kappa_1(\mu) + \kappa_2(\mu) = \left(\frac{f_u^0}{d_1} + \frac{g_v^0}{d_2}\right).$$

The Hopf/steady-state mode interaction occurs if there are λ_0 and $(\kappa_a, \kappa_b) \in S_{\kappa_1(\mu)}$, $(\kappa_c, \kappa_d) \in S_{\kappa_2(\mu)}$ such that

$$-\kappa_1(\mu)(d_1 + d_2) + f_u^0 + g_v^0 = 0, \tag{2.6a}$$

$$d_1 d_2 \kappa_1^2(\mu) - \kappa_1(\mu)(d_1 g_v^0 + d_2 f_u^0) + f_u^0 g_v^0 - f_v^0 g_u^0 > 0, \tag{2.6b}$$

$$d_1 d_2 \kappa_2^2(\mu) - \kappa_2(\mu)(d_1 g_v^0 + d_2 f_u^0) + f_u^0 g_v^0 - f_v^0 g_u^0 = 0. \tag{2.6c}$$

Eq. (2.6a) implies that

$$\kappa_1(\mu) = \frac{f_u^0 + g_v^0}{d_1 + d_2}.$$

Substituting the above equation into (2.6b), we obtain

$$\left(\frac{f_u^0+g_v^0}{d_1+d_2}\right)^2-\left(\frac{f_u^0+g_v^0}{d_1+d_2}\right)\left(\frac{f_u^0}{d_1}+\frac{g_v^0}{d_2}\right)+\left(\frac{f_u^0g_v^0-f_v^0g_u^0}{d_1d_2}\right)>0. \tag{2.7}$$

Thus a *Hopf/steady-state* mode interaction occurs at $\boldsymbol{u}=\mathbf{0}$, $\lambda=\lambda_0$, if (2.6c) and (2.7) hold.

The *Hopf/Hopf* mode interaction occurs if there are λ_0 and $(\kappa_a,\kappa_b)\in S_{\kappa_1(\mu)}$, $(\kappa_c,\kappa_d)\in S_{\kappa_2(\mu)}$ such that

$$\operatorname{trace}(M_{\kappa_1(\mu)}(\lambda_0))=0,\quad \det(M_{\kappa_1(\mu)}(\lambda_0))>0, \tag{2.8}$$

and

$$\operatorname{trace}(M_{\kappa_2(\mu)}(\lambda_0))=0,\quad \det(M_{\kappa_2(\mu)}(\lambda_0))>0 \tag{2.9}$$

hold. From (2.8) and (2.9) we have

$$-\kappa_1(\mu)(d_1+d_2)+f_u^0+g_v^0=0, \tag{2.10a}$$

$$d_1d_2\kappa_1^2(\mu)-\kappa_1(\mu)(d_1g_v^0+d_2f_u^0)+f_u^0g_v^0-f_v^0g_u^0>0, \tag{2.10b}$$

$$-\kappa_2(\mu)(d_1+d_2)+f_u^0+g_v^0=0, \tag{2.10c}$$

$$d_1d_2\kappa_2^2(\mu)-\kappa_2(\mu)(d_1g_v^0+d_2f_u^0)+f_u^0g_v^0-f_v^0g_u^0>0. \tag{2.10d}$$

Eqs. (2.10a) and (2.10c) imply that

$$\kappa_1(\mu)=\kappa_2(\mu)=\frac{f_u^0+g_v^0}{d_1+d_2}, \tag{2.11}$$

while Eq. (2.10b) and (2.10d) imply that

$$\left(\frac{f_u^0+g_v^0}{d_1+d_2}\right)^2-\left(\frac{f_u^0+g_v^0}{d_1+d_2}\right)\left(\frac{f_u^0}{d_1}+\frac{g_v^0}{d_2}\right)+\left(\frac{f_u^0g_v^0-f_v^0g_u^0}{d_1d_2}\right)>0. \tag{2.12}$$

Thus a *Hopf/Hopf* mode interaction occurs at $\boldsymbol{u}=\mathbf{0},\lambda=\lambda_0$ if (2.11) and (2.12) are satisfied.

2.2. The Brusselator equations

The Brusselator equations have a uniform steady-state solution $(u_0,v_0)\equiv(\alpha,\lambda/\alpha)$. After shifting (u_0,v_0) to the origin $\mathbf{0}$, we obtain

$$f(u,v,\lambda)=(\lambda-1)u+\alpha^2v+\left(\frac{\lambda}{\alpha}u^2+2\alpha uv+u^2v\right),$$

$$g(u,v,\lambda)=-\lambda u-\alpha^2v-\left(\frac{\lambda}{\alpha}u^2+2\alpha uv+u^2v\right).$$

The statement (2.4) becomes

$$M_{\kappa(\mu)}(\lambda)=\begin{pmatrix}-d_1\kappa(\mu)+\lambda-1 & \alpha^2\\ -\lambda & -d_2\kappa(\mu)-\alpha^2\end{pmatrix},$$

where

$$\text{trace}(M_{\kappa(\mu)}(\lambda)) = -\kappa(\mu)(d_1 + d_2) + \lambda - 1 - \alpha^2 \tag{2.13}$$

and

$$\det(M_{\kappa(\mu)}(\lambda)) = d_1 d_2 \kappa^2(\mu) + \kappa(\mu)[d_1\alpha^2 + d_2(1-\lambda)] + \alpha^2. \tag{2.14}$$

The trace of $M_{\kappa(\mu)}$ changes sign at

$$\lambda^* = 1 + \alpha^2 + \kappa(\mu)(d_1 + d_2). \tag{2.15}$$

A *stationary bifurcation* corresponds to $\det(M_{\kappa(\mu)}(\lambda)) = 0$ which is satisfied by

$$\lambda_0 = \frac{\alpha^2}{\kappa(\mu)d_2} + d_1\kappa(\mu) + \frac{d_1}{d_2}\alpha^2 + 1. \tag{2.16}$$

Furthermore, if $\lambda > \lambda^*$, then trace $(M_{\kappa(\mu)}(\lambda)) > 0$, while if $\lambda > \lambda_0$, then $\det(M_{\kappa(\mu)}(\lambda)) < 0$. Thus, we have

$$(\lambda - \lambda_0)\det(M_{\kappa(\mu)}(\lambda)) < 0,$$

$$(\lambda - \lambda^*)\,\text{trace}(M_{\kappa(\mu)}(\lambda)) > 0.$$

Consequently, whenever $\lambda \leqslant \min_{\kappa(\mu)}\{\lambda_0, \lambda^*\}$ at which either a Hopf or a stationary bifurcation takes place, or the uniform steady-state solution becomes unstable.

Lemma 1. *If $d_2\kappa(\mu) < \alpha$ and $d_1 > d_2$, then a Hopf bifurcation point occurs at*

$$\lambda^* = \kappa(\mu)(d_1 + d_2) + \alpha^2 + 1.$$

Proof. First note that from (2.15) we have $\text{trace}(M_{\kappa(\mu)}(\lambda^*) = 0$.

On the other hand, by the assumptions we have

$$d_2\kappa(\mu) < \frac{\alpha^2}{d_2\kappa(\mu)} \quad \text{and} \quad \alpha^2 < \frac{d_1}{d_2}\alpha^2,$$

which implies that

$$\kappa(\mu)(d_1 + d_2) + \alpha^2 + 1 < \frac{\alpha^2}{d_2\kappa(\mu)} + d_1\kappa(\mu) + \frac{d_1}{d_2}\alpha^2 + 1,$$

or equivalently, $\lambda^* < \lambda_0$, from which it follow that

$$\det(M_{\kappa(\mu)}(\lambda^*)) > 0. \qquad \square$$

For steady/steady state mode interaction of the Brusselator equations, the conditions (2.5) must be satisfied. From (2.14) we have

$$d_1 d_2 \kappa_1^2(\mu) + \kappa_1(\mu)(d_1\alpha^2 + d_2(1-\lambda_0)) + \alpha^2 = 0, \tag{2.17a}$$

$$d_1 d_2 \kappa_2^2(\mu) + \kappa_2(\mu)(d_1\alpha^2 + d_2(1-\lambda_0)) + \alpha^2 = 0. \tag{2.17b}$$

Eqs. (2.17a) and (2.17b) imply that

$$\kappa_1(\mu)+\kappa_2(\mu)=\frac{\lambda_0-1}{d_1}-\frac{\alpha^2}{d_2}$$

and

$$\lambda_0=\frac{\alpha^2}{\kappa_1(\mu)d_2}+d_1\kappa_1(\mu)+\frac{d_1}{d_2}\alpha^2+1=\frac{\alpha^2}{\kappa_2(\mu)d_2}+d_1\kappa_2(\mu)+\frac{d_1}{d_2}\alpha^2+1. \tag{2.18}$$

Eq. (2.18) implies that

$$\kappa_1(\mu)\cdot\kappa_2(\mu)=\frac{\alpha^2}{d_1d_2}\quad \text{if } \kappa_1(\mu)\neq\kappa_2(\mu).$$

The *Hopf/steady-state* mode interaction occurs at $\boldsymbol{u}=0$, $\lambda=\lambda_0$, if there are λ_0, $(\kappa_a,\kappa_b)\in S_{\kappa_1(\mu)}$, $(\kappa_c,\kappa_d)\in S_{\kappa_2(\mu)}$ such that

$$\operatorname{trace}(M_{\kappa_1(\mu)}(\lambda))=-\kappa_1(\mu)(d_1+d_2)+\lambda-1-\alpha^2=0,$$

$$\det(M_{\kappa_1(\mu)}(\lambda))=d_1d_2\kappa_1^2(\mu)+\kappa_1(\mu)[d_1\alpha^2+d_2(1-\lambda)]+\alpha^2>0,$$

$$\det(M_{\kappa_2(\mu)}(\lambda))=d_1d_2\kappa_2^2(\mu)+\kappa_2(\mu)[d_1\alpha^2+d_2(1-\lambda)]+\alpha^2=0$$

hold.

Finally, a *Hopf/Hopf* mode interaction occurs at $\boldsymbol{u}=\mathbf{0}$, $\lambda=\lambda_0$, if there exist $(\kappa_a,\kappa_b)\in S_{\kappa_1(\mu)}$, $(\kappa_c,\kappa_d)\in S_{\kappa_2(\mu)}$ such that the following equations

$$\operatorname{trace}(M_{\kappa_1(\mu)}(\lambda_0,1))=0,\quad \det(M_{\kappa_1(\mu)}(\lambda_0,1))>0$$

and

$$\operatorname{trace}(M_{\kappa_2(\mu)}(\lambda_0,1))=0,\quad \det(M_{\kappa_2(\mu)}(\lambda_0,1))>0$$

hold.

3. Centered difference approximations

In this section we discuss discretizations of the system (1.1) with the boundary conditions (1.4) and bifurcations of the discrete problem by using the centered difference method. In particular, we will show how multiple bifurcations of (1.1) may be preserved for the discrete problem. Similar discussions can be found in [7,8,18].

3.1. General system

Let

$$\Omega_h=\{(x_i,y_j)\colon 0\leqslant i,j\leqslant N\}$$

be a uniform grid on the unit square with meshsize $h=1/N$. At the discrete points the functions $u(x,y)$ and $v(x,y)$ are approximated by the net functions $U(x_i,y_j):=U_{i,j}$ and $V(x_i,y_j):=V_{i,j}$, $i,j=0,\ldots,N$, where $U,V\in\mathbb{R}^{N^2}$ are defined by

$$U:=(U_{0,0},\ldots,U_{0,N},U_{1,0},\ldots,U_{1,N},\ldots,U_{N,0},\ldots,U_{N,N})^{\mathrm{T}}$$

and

$$V := (V_{0,0}, \ldots, V_{0,N}, V_{1,0}, \ldots, V_{1,N}, \ldots, V_{N,0}, \ldots, V_{N,N})^{\mathrm{T}},$$

respectively. The Robin boundary conditions imply that

$$U_{-1,j} = U_{1,j} - \beta U_{0,j}, \qquad U_{i,-1} = U_{i,1} - \beta U_{i,0},$$
$$U_{N+1,j} = U_{N-1,j} - \beta U_{N,j}, \qquad U_{i,N+1} = U_{i,N-1} - \beta U_{i,N},$$
$$V_{-1,j} = V_{1,j} - \beta V_{0,j}, \qquad V_{i,-1} = V_{i,1} - \beta V_{i,0},$$
$$V_{N+1,j} = V_{N-1,j} - \beta V_{N,j}, \qquad V_{i,N+1} = V_{i,N-1} - \beta V_{i,N},$$

where

$$\beta = 2h\frac{g_0(\mu)}{g_1(\mu)}. \tag{3.1}$$

Discretizing $\partial^2/\partial x^2, \partial^2/\partial y^2$ with the centered difference schemes, and with F, G denoting the net functions associated to the functions f and g, respectively, we obtain the discretization of $\Phi(\boldsymbol{u}, \lambda) \equiv 0$, namely,

$$H(Z,\lambda) := \begin{pmatrix} d_1 AU \\ d_2 AV \end{pmatrix} - h^2 \begin{pmatrix} F(Z,\lambda) \\ G(Z,\lambda) \end{pmatrix} = 0, \quad Z := (U,V)^{\mathrm{T}}. \tag{3.2}$$

Here

$$A = \begin{pmatrix} A_1 & -2I_{N+1} & & & 0 \\ -I_{N+1} & A_2 & -I_{N+1} & & \\ & \ddots & \ddots & \ddots & \\ & & -I_{N+1} & A_N & -I_{N+1} \\ & 0 & & -2I_{N+1} & A_{N+1} \end{pmatrix} \in \mathbb{R}^{(N+1)^2 \times (N+1)^2}$$

with

$$A_1 = A_{N+1} = \begin{pmatrix} 4+2\beta & -2 & & & 0 \\ -1 & 4+\beta & -1 & & \\ & \ddots & \ddots & \ddots & \\ & & -1 & 4+\beta & -1 \\ & 0 & & -2 & 4+2\beta \end{pmatrix} \in \mathbb{R}^{(N+1)\times(N+1)};$$

$$A_i = \begin{pmatrix} 4+\beta & -2 & & & 0 \\ -1 & 4 & -1 & & \\ & \ddots & \ddots & \ddots & \\ & & -1 & 4 & -1 \\ & 0 & & -2 & 4+\beta \end{pmatrix} \in \mathbb{R}^{(N+1)\times(N+1)}, \quad i = 2, \ldots, N$$

and

$$F(Z,\lambda) = (f_{0,0}, \ldots, f_{0,N}, f_{1,0}, \ldots, f_{1,N}, \ldots, f_{N,N})^{\mathrm{T}},$$
$$G(Z,\lambda) = (g_{0,0}, \ldots, g_{0,N}, g_{1,0}, \ldots, g_{1,N}, \ldots, g_{N,N})^{\mathrm{T}}.$$

Let $R=(r_{i,j})\in\mathbb{R}^{m\times n}$ and $S=(s_{i,j})\in\mathbb{R}^{p\times q}$ be arbitrary. We recall that the matrix tensor product of R and S, denoted by $R\otimes S$, is an $mp\times nq$ matrix and is defined by

$$R\otimes S=\begin{pmatrix} r_{11}S & r_{12}S & \dots & r_{1n}S\\ r_{21}S & r_{22}S & \dots & r_{2n}S\\ \vdots & \vdots & & \vdots\\ r_{m1}S & r_{m2}S & \dots & r_{mn}S \end{pmatrix}.$$

We denote the eigenpairs of A defined in (3.3) by $(\mu_{p,q},V_{p,q})$, where

$$\mu_{p,q}=\mu_p+\mu_q=2\left(2-\cos\frac{p\pi}{N}-\cos\frac{q\pi}{N}\right),$$

$$\begin{aligned} V_{p,q}&=V_p\otimes V_q\quad 0\leqslant p,\ q\leqslant N,\\ &=\left[\cos\frac{0p\pi}{N}\cos\frac{0q\pi}{N},\dots,\cos\frac{0p\pi}{N}\cos\frac{Nq\pi}{N},\dots,\cos\frac{Np\pi}{N}\cos\frac{Nq\pi}{N}\right]^{\mathrm{T}}, \end{aligned}\tag{3.7}$$

see [9] for details. Let $X^h_{p,q}:=\mathbb{R}^2V_{p,q}=\{\binom{c_1}{c_2}V_{p,q};c_1,c_2\in\mathbb{R},1\leqslant p,q\leqslant N\}$. We have

$$\mathbb{R}^{2N^2}=\sum_{i,j=1}^{N}\oplus X^h_{i,j}.\tag{3.8}$$

The operator L_h maps $X^h_{p,q}$ into itself, and for $c_1,c_2\in\mathbb{R}$, $0\leqslant p,q\leqslant N$, we have

$$L_h\begin{pmatrix}c_1\\c_2\end{pmatrix}V_{p,q}=\begin{pmatrix} d_1\mu_{p,q}-h^2f^0_u & -h^2f^0_v\\ -h^2g^0_u & d_2\mu_{p,q}-h^2g^0_v\end{pmatrix}\begin{pmatrix}c_1\\c_2\end{pmatrix}V_{p,q}.\tag{3.9}$$

Consequently, under the decomposition (3.8) L_h is a block diagonal matrix, i.e.,

$$L_h=-h^2\,\mathrm{diag}(M^h_{0,0},M^h_{1,0},\dots,M^h_{N,0},M^h_{1,1},M^h_{2,1},\dots,M^h_{N,1},\dots,M^h_{1,N},\dots,M^h_{N,N}),$$

where

$$M^h_{i,j}(\lambda):=\begin{pmatrix}\dfrac{-d_1\mu_{i,j}}{h^2}+f^0_u & f^0_v\\ g^0_u & \dfrac{-d_2\mu_{i,j}}{h^2}+g^0_v\end{pmatrix},\quad 0\leqslant i,j\leqslant N.$$

Hence the spectrum of L_h is the union of the eigenvalues of $M^h_{i,j}$, $0\leqslant i,j\leqslant N$.

Now suppose that $\lambda=\lambda_0$ is a simple bifurcation point of (2.1). There exist $i,j\in\mathbb{N}$, $0\leqslant i,j\leqslant N$ such that $\det(M_{i,j}(\lambda_0))=0$. So we have

$$\begin{aligned}\det(M^h_{i,j}(\lambda_0))&=\det(M^h_{i,j}(\lambda_0))-\det(M_{i,j}(\lambda_0))\\ &=\mathrm{O}\left(\left|\frac{\mu_{i,j}}{h^2}-\pi^2(i^2+j^2)\right|\right)\\ &=\mathrm{O}(h^2).\end{aligned}$$

As expected, λ_0 is no longer a bifurcation point of the discrete problem. Nevertheless, for $h>0$ sufficiently small there exists $\lambda^h_0\in\mathbb{R}$ such that $\det(M^h_{i,j}(\lambda^h_0))=0$ and $|\lambda^h_0-\lambda_0|=\mathrm{O}(h^2)$. In other words,

there exists a simple bifurcation point $(\mathbf{0},\lambda_0)$ of the discrete problem in the $O(h^2)$ neighborhood of the bifurcation point of the continuous problem.

Let $(\mathbf{0},\lambda_0)$ be a double bifurcation point, and let M_{i_1,j_1}, M_{i_2,j_2} be any two matrices which have zero eigenvalues, respectively. It is easy to verify that

$$\det(M^h_{i_1,j_1}(\lambda_0)) = \det(M^h_{i_2,j_2}(\lambda_0)) = O(h^2).$$

That is, we have shown that there exists λ^h_0 in the neighborhood of λ_0 such that

$$\det(M^h_{i_1,j_1}(\lambda^h_0)) = \det(M^h_{i_2,j_2}(\lambda^h_0)) = 0,$$

which corresponds to a double bifurcation of the discrete problem.

Define a map $d:\mathbb{R}^3\to\mathbb{R}^2$ by

$$d(\lambda,h) := \begin{pmatrix} \det(M^h_{i_1,j_1}(\lambda_0)) \\ \det(M^h_{i_2,j_2}(\lambda_0)) \end{pmatrix} = \begin{pmatrix} \left[\dfrac{-d_1\mu_{i_1,j_1}}{h^2} + f^0_u\right]\left[\dfrac{-d_2\mu_{i_1,j_1}}{h^2} + g^0_v\right] - f^0_v g^0_u \\ \left[\dfrac{-d_1\mu_{i_2,j_2}}{h^2} + f^0_u\right]\left[\dfrac{-d_2\mu_{i_2,j_2}}{h^2} + g^0_v\right] - f^0_v g^0_u \end{pmatrix}$$

and note that for $h=0$,

$$d(\lambda,0) := \begin{pmatrix} \det(M_{i_1,j_1}(\lambda)) \\ \det(M_{i_2,j_2}(\lambda)) \end{pmatrix}.$$

If f,g are smooth functions, then so is d. Note that $d(\lambda_0,0)=0$.

3.2. The Brusselator equations

For the Brusselator equations the functions $f(u,v,\lambda), g(u,v,\lambda)$ are given as in Section 2.2 and

$$M^h_{i,j} := \begin{pmatrix} \dfrac{-d_1\mu_{i,j}}{h^2} + (\lambda-1) & \alpha^2 \\ -\lambda & \dfrac{-d_2\mu_{i,j}}{h^2} - \alpha^2 \end{pmatrix}.$$

Theorem 2. *The bifurcation points of the discrete Brusselator equations are*

$$(0,\lambda^h_{i,j}) = \left(0, 1 + \left(d_1 + \frac{h^2}{\mu_{i,j}}\right)\frac{\alpha^2}{d_2} + \frac{d_1}{h^2}\mu_{i,j}\right), \quad 0\leqslant i,j\leqslant N. \tag{3.10}$$

Furthermore, the null vector $(\tilde U_{i,j}, \tilde V_{i,j})$ *of* L_h *in* (3.6) *can be chosen as*

$$\tilde U_{i,j} = U_{i,j}, \quad \tilde V_{i,j} = -\left(\frac{d_1}{d_2} + \frac{h^2}{d_2\mu_{i,j}}\right)\tilde U_{i,j}, \tag{3.11}$$

where $\mu_{i,j}$ *is given as in* (3.7).

Proof. Note that the operator L_h is singular if and only if there exist two positive integers i and j with $0 \leqslant i, j \leqslant N$ such that $\det(M_{i,j}^h) = 0$. Solving it for λ, we obtain

$$\lambda_{i,j}^h = 1 + \left(d_1 + \frac{h^2}{\mu_{i,j}}\right)\frac{\alpha^2}{d_2} + \frac{d_1}{h^2}\mu_{i,j}.$$

Recall the statements (3.7) and (3.8). We see the null vectors of L_h are of the form $\binom{c_1}{c_2}U_{i,j}$ with $(c_1, c_2)^{\mathrm{T}}$ as a null vector of $M_{i,j}^h(\lambda_{i,j}^h)$, which can be chosen as $c_1 = 1, c_2 = -(d_1/d_2 + h^2/\mu_{i,j}d_2)$. The statement (3.11) follows immediately. □

Theorem 3. $(\mathbf{0}, \lambda_{i_1,j_1}^h) = (\mathbf{0}, \lambda_{i_2,j_2}^h)$ *is a multiple bifurcation of the discrete Brusselator equations if and only if one of the following statements hold*:

(i) $\mu_{i_1,j_1} = \mu_{i_2,j_2}$; *or*

(ii) $\mu_{i_1,j_1} \neq \mu_{i_2,j_2}$ *and* $\mu_{i_1,j_1} \cdot \mu_{i_2,j_2} = \alpha^2 h^4/d_1 d_2$.

Proof. (i) This follows from (3.10).

(ii) If $\mu_{i_1,j_1} \neq \mu_{i_2,j_2}$, then by Theorem 2 we have

$$\frac{d_1}{h^2}(\mu_{i_1,j_1} - \mu_{i_2,j_2}) = \alpha^2 \frac{h^2}{d_2}\left(\frac{\mu_{i_1,j_1} - \mu_{i_2,j_2}}{\mu_{i_1,j_1} \cdot \mu_{i_2,j_2}}\right),$$

and the result follows immediately. □

4. Linear solvers for reaction–diffusion problems

Linear systems which arise from the discretization of a reaction–diffusion problem are in general nonsymmetric. In this section we are concerned with conjugate gradient(CG) type methods for solving nonsymmetric linear systems of the form

$$Ax = b, \tag{4.1}$$

where $A \in \mathbb{R}^{N\times N}$ is nonsingular and $b \in \mathbb{R}^N$. For example, the generalized minimal residual method (GMRES) of Saad and Schultz [21] is widely used for solving (4.1). By incorporating some techniques on GMRES, Brown and Walker [6] show that it can be used to detect ill conditioning of the coefficient matrix A. On the other hand, some Krylov subspace methods that are based on the unsymmetric Lanczos process are developed for solving (4.1), see [12, Chapter 9; 20] and the references cited therein for details.

Several well-known curve-tracking algorithms have been developed during the past decade, e.g., the HOMPACKg0 of Watson et al. [23]. Recently, some conjugate gradient type methods have been incorporated in the context of continuation algorithms for curve-tracking, see e.g., [7–9,17]. We are interested in the generalized CG methods which can be used to solve (4.1) as well as to monitor ill conditioning of the coefficient matrices in path-following problems. This in turn leads to the possibility of detecting singular points along solution curves of the associated discrete bifurcation problem. In [11] Day has proposed some techniques called maintaining semiduality, which can be exploited to implement the unsymmetric Lanczos process more efficiently. We will show how the

unsymmetric Lanczos algorithm described in [11] can be incorporated in the context of continuation methods for curve-tracking. The implementation of GMRES together with the techniques of Brown and Walker will be given elsewhere.

To start with, let $V_j = [v_1, v_2, \ldots, v_j]$ and $W_j = [w_1, w_2, \ldots, w_j]$ be the two biorthogonal systems generated by the two unsymmetric Lanczos process [20] such that $W_j^{\mathrm{T}} A V_j = T_j$ is tridiagonal. Let x_0 be the initial guess, and $r_0 = b - Ax_0$ the initial residual. We seek an approximate solution x_j by requiring

$$(b - Ax_j, w_j) = 0, \quad i = 1, 2, \ldots, j, \tag{4.2}$$

and

$$x_j = x_0 + z_j, \tag{4.3}$$

where $z_j = V_j y_j \in \operatorname{span}\{v_1, v_2, \ldots, v_j\} =: K_j$ for some $y_j \in \mathbb{R}^j$, where $(\cdot, \cdot)$ denotes the inner product in $\mathbb{R}^N$. It follows from (4.2) that

$$(r_0 - Az_j, w_i) = 0, \quad i = 1, 2, \ldots, j. \tag{4.4}$$

Assume that $\det(T_j) \neq 0$. Then (4.4) implies that

$$W_j^{\mathrm{T}}(r_0 - Az_j) = 0. \tag{4.5}$$

Replacing z_j by $V_j y_j$ in (4.5) yields an equation for y_j,

$$T_j y_j = W_j^{\mathrm{T}} r_0, \tag{4.6}$$

where

$$T_j = \begin{pmatrix} \alpha_1 & \beta_2 w_2 & & & 0 \\ \gamma_2 w_2 & \ddots & \ddots & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & \ddots & \beta_j w_j \\ & 0 & & \gamma_j w_j & \alpha_j \end{pmatrix}.$$

The entries α_j, β_j and γ_j will be determined later. If we set $w_1 = v_1 = r_0 / \|r_0\|_2$ and $\beta = \|r_0\|_2$, it follows from the biorthogonality that the equalities

$$W_j^{\mathrm{T}} r_0 = \beta W_j^{\mathrm{T}} w_1 = \beta e_1$$

hold, where $e_1 = [1, 0, \ldots, 0]^{\mathrm{T}} \in \mathbb{R}^j$ is the first standard unit vector. Thereafter, via (4.6) the approximate solution x_j in (4.3) is calculated as

$$x_j = x_0 + V_j y_j = x_0 + \beta V_j T_j^{-1} e_1. \tag{4.7}$$

In exact arithmetic $W_j^{\mathrm{T}}V_j$ is a diagonal matrix. However, Lanczos vectors computed in finite precision arithmetic by the three-term recurrence tend to lose their mutual biorthogonality. Thus $W_j^{\mathrm{T}}V_j$ is not diagonal any more. In order to compensate for this phenomenon, Day proposed a compromise approach called maintaining semiduality, which has the advantage that the computed tridiagonal is a perturbation of a matrix that is exactly similar to the appropriate projection of the matrix A onto the computed subspace. Therefore, we can use the condition number of T_j to approximate the singularity of the coefficient matrix A. The following algorithm clearly can be incorporated in the context of continuation algorithm for curve-tracking, which is more stable than the continuation-Arnoldi algorithm in [8], or the continuation-BCG algorithm in [7].

Algorithm 4.1. Lanczos algorithm maintaining semiduality
Start: Choose v_1 and w_1 such that $\omega_1 = (v_1, w_1) = 1, \omega_0 = 1, \beta_1 = \gamma_1 = 0$
Iterate: For $i = 1, \ldots, m$ do

1. $r_i = Av_i - (\beta_i\omega_i/\omega_{i-1})v_{i-1}, s_i = A^{\mathrm{T}}w_i - (r_i\omega_i/\omega_{i-1})w_{i-1}$
2. $\alpha_i = (v_i, s_i)$
3. $r_i = r_i(\alpha_i/\omega_i)v_i,\ s_i = s_i - (\alpha_i/\omega_i)w_i$
4. Maintain extended local duality
5. $\alpha_i^r = (w_i, r_i), \alpha_i^l = (v_i, s_i)$ (*small correction to* α_i)
6. $r_i := r_i - (\alpha_i^r/\omega_i)v_i,\ s_i := s_i - (\alpha_i^l/\omega_i)w_i$
7. $\gamma_{i+1} = \|r_i\|_2,\ \beta_{i+1} = \|s_i\|_2$
8. Check for invariant subspace
9. $v_{i+1} = r_i/\gamma_{i+1}, w_{i+1} = s_i/\beta_{i+1}$
10. $\omega_{i+1} = (v_{i+1}, w_{i+1})$
11. Check for breakdown: $|w_{i+1}| < (n + 10(i+1))\varepsilon$
12. Monitor duality loss
13. Correct duality loss only if necessary
14. Check for convergence after a correction step only.

5. Numerical results

We have performed extensive numerical experiments to trace solution branches of the Brusselator via the predictor-corrector continuation methods, where a local perturbation technique is used for branch-switching. Examples 1–7 show our sample numerical results, where we choose $g_0(\mu) = 1 - \mu, g_1(\mu) = \mu$ in (1.4). All computations of our numerical experiments were performed on an IBM RS/6000 SP2 machine with High Performance Fortran Compiler and with 64 bit IEEE arithmetic at National Chung-Hsing University. All of the examples were discretized by the centered-difference formulae with diffusion rates $d_1 = 1, d_2 = 2$ and uniform meshsize $h = 0.05$ on the x- and y-axis, respectively. For convenience we only considered $\mu = 1$. Additionally, we chose $\alpha = 4$ in Examples 1–4. All of the bifurcation diagrams in Figs. 1a–6a were obtained by choosing the values of the function U (respectively V) at the point (0.25, 0.25).

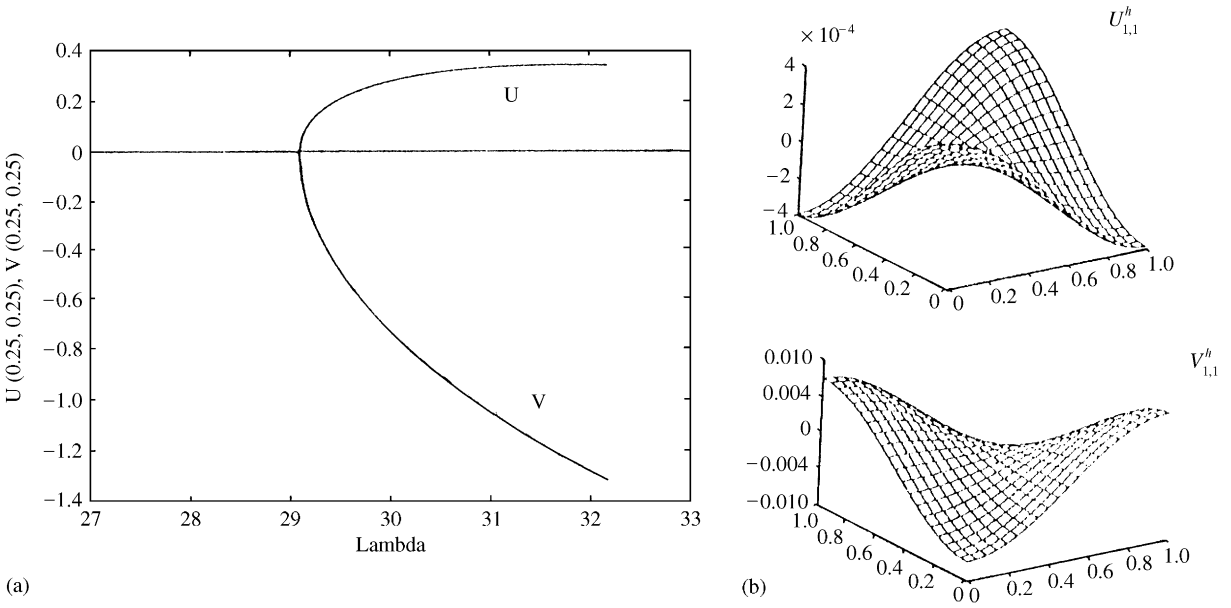


Fig. 1. Bifurcation scenario at the simple bifurcation point $(0, \lambda^h_{1,1}) = (0, 29.1047714)$: (a) bifurcation diagram; (b) contours of the solution curves at $\lambda = 28.279912$.

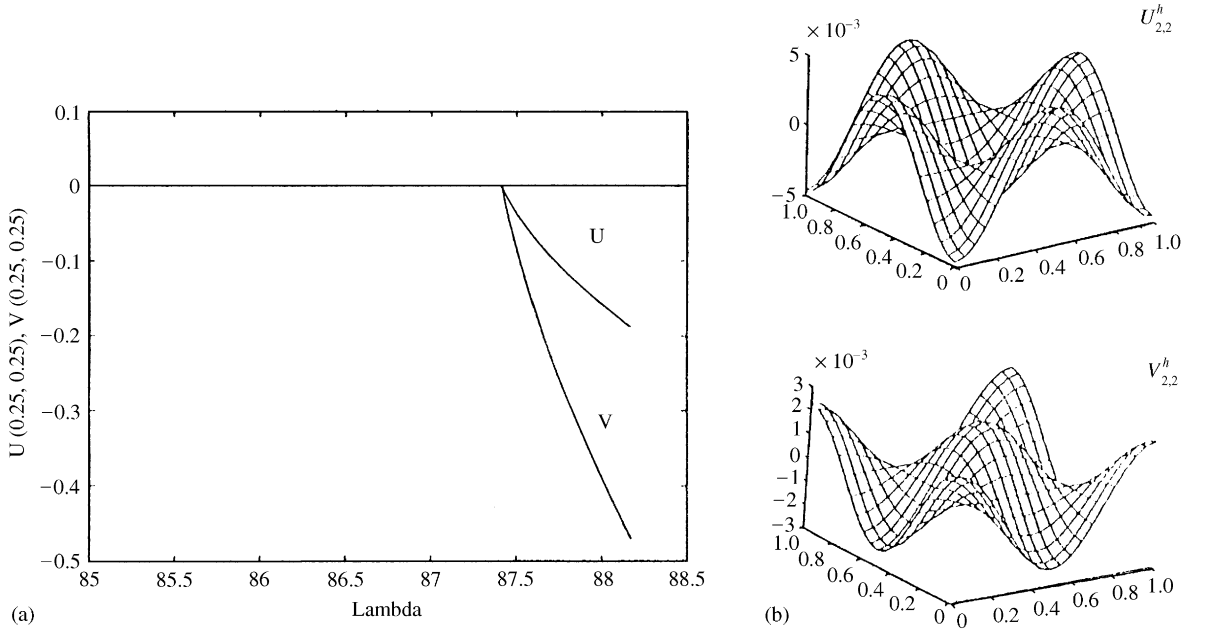


Fig. 2. Bifurcation scenario at the simple bifurcation point $(0, \lambda^h_{2,2}) = (0, 87.4117325)$: (a) bifurcation diagram; (b) contours of the solution curves at $\lambda = 88.576421$.

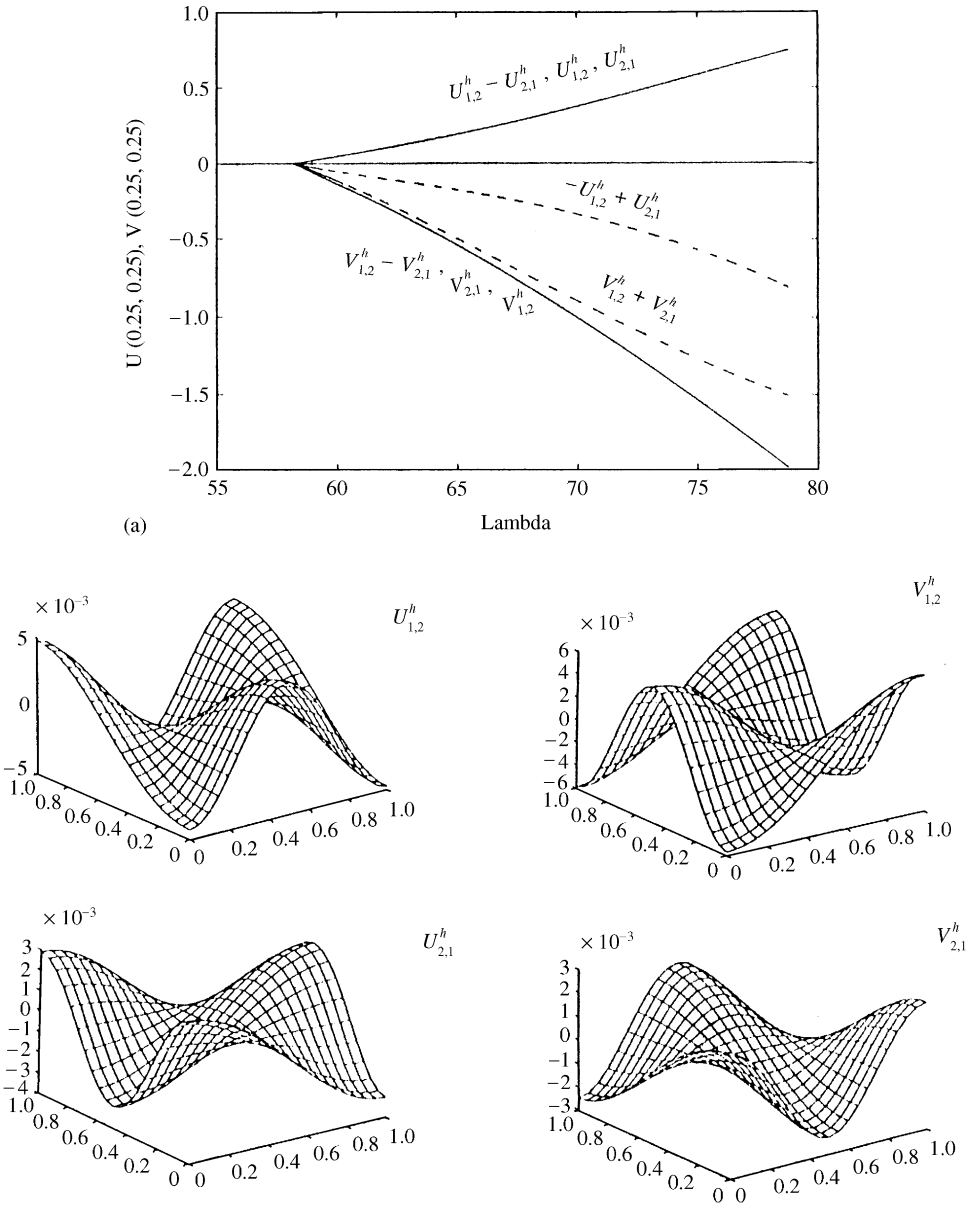
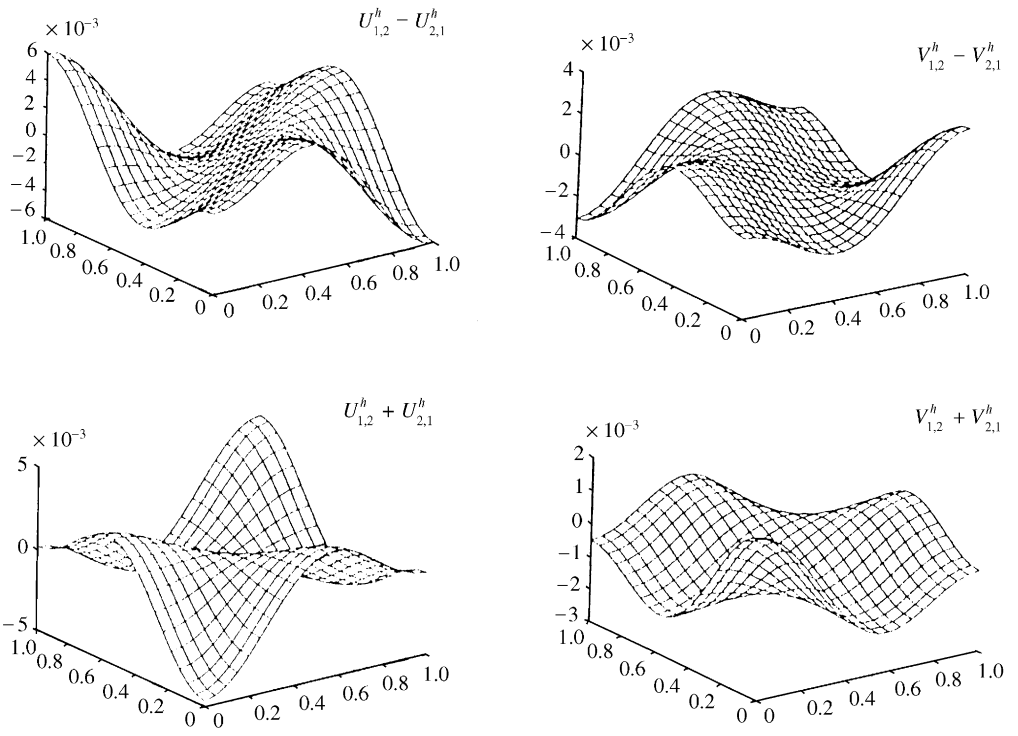


Fig. 3. Bifurcation scenario at the double bifurcation point $(0, \lambda^h_{1,2}) = (0, \lambda^h_{2,1}) = (0, 58.167366)$: (a) bifurcation diagram; (b) contours of the solution curves at $\lambda = 57.213542$.

Example 1. *Simple bifurcation*, $(i, j)=(1, 1)$. Fig. 1a shows the first solution curve $U^h_{1,1}$ (respectively $V^h_{1,1}$) branching from $(0, \lambda^h_{1,1})=(0, 29.1047741)$ is barely transcritical, see [13, p. 233]. Fig. 1b shows the 3-D contours of the solution curve $U_{1,1}$ and $V_{1,1}$ at $\lambda = 30.0837$.



(b)

Fig. 3. (*Continued.*)

Example 2. *Simple bifurcation*, $(i, j) = (2, 2)$. Fig. 2a shows the solution curve bifurcating at $(0, \lambda^h_{2,2}) = (0, 87.4117325)$ is transcritical, while Fig. 2b shows the contours of the solution curves $U^h_{2,2}$ and $V^h_{2,2}$ at $\lambda = 88.9421$, respectively.

Example 3. *Multiple bifurcation*, $(i, j) = (1, 2)$. Fig. 3a shows four solution curves branching from the double bifurcation point $(0, \lambda^h_{1,2}) = (0, \lambda^h_{2,1}) \approx (0, 58.167366)$, namely, $U^h_{1,2}, U^h_{2,1}, U^h_{1,2} + U^h_{2,1}$, and $U^h_{1,2} - U^h_{2,1}$ (respectively, $V^h_{1,2}, V^h_{2,1}, V^h_{1,2} + V^h_{2,1}$, and $V^h_{1,2} - V^h_{2,1}$). Note that the solution curves of $U^h_{1,2}, U^h_{2,1}$, and $U^h_{1,2} - U^h_{2,1}$ (respectively $V^h_{1,2}, V^h_{2,1}$, and $V^h_{1,2} - V^h_{2,1}$) coincide with one another. Fig. 3b shows the contours of the solution curves at $\lambda = 57.213542$.

Example 4. *Multiple bifurcation*, $(i, j) = (1, 3)$. Fig. 4a shows four solution curves bifurcating at $(0, \lambda^h_{1,3}) = (0, \lambda^h_{3,1}) = (0, 106.126545)$, namely, $U^h_{1,3}, U^h_{3,1}, U^h_{1,3} + U^h_{3,1}$ and $U^h_{1,3} - U^h_{3,1}$ (respectively $V^h_{1,3}, V^h_{3,1}, V^h_{1,3} + V^h_{3,1}$, and $V^h_{1,3} - V^h_{3,1}$). Note that the solution curves of $U^h_{1,3}$ and $U^h_{3,1}$ (respectively $V^h_{1,3}$ and $V^h_{3,1}$) coincide with each other. Fig. 4b shows the contours of these solution curves at $\lambda = 107.3492$.

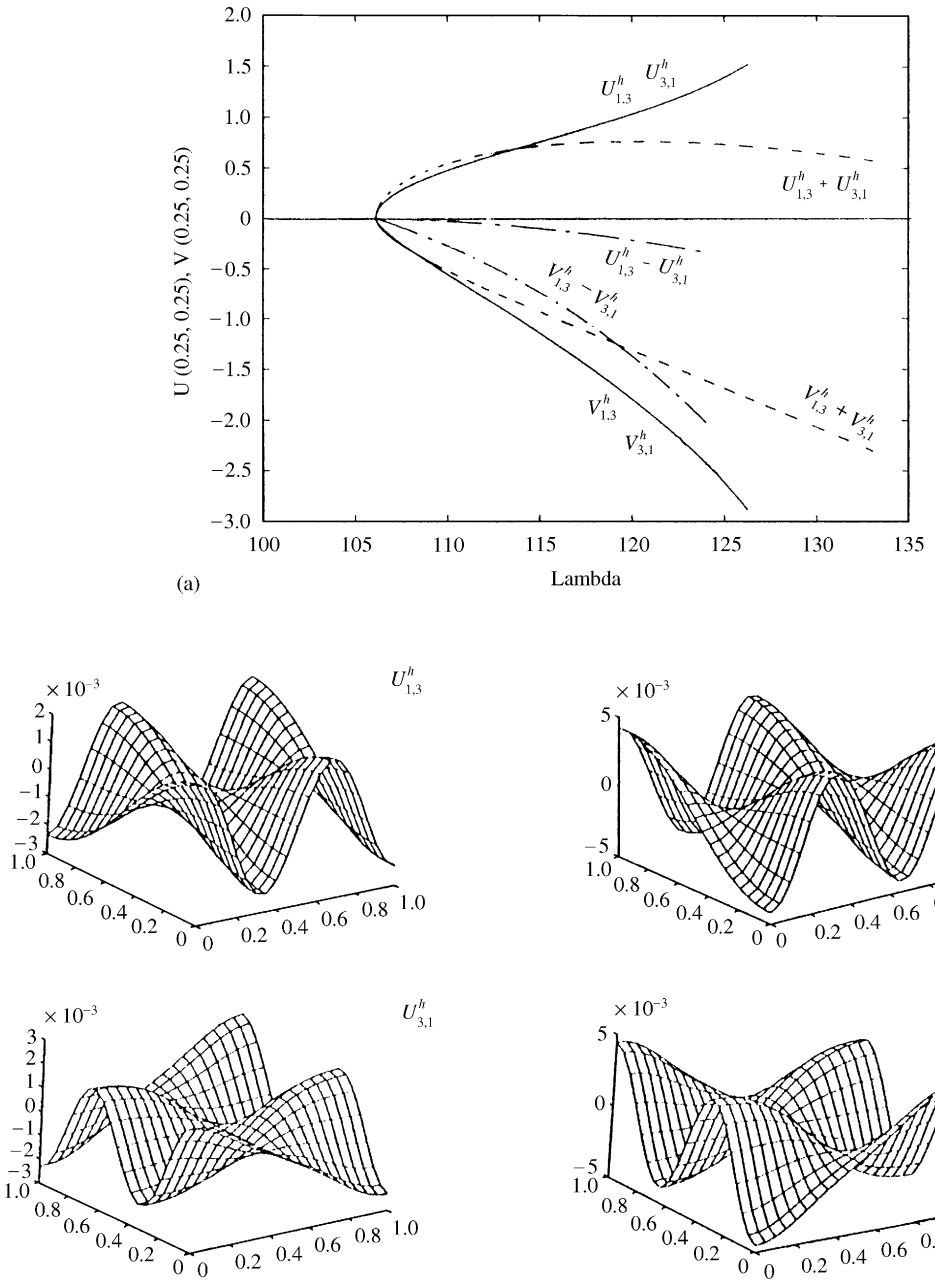
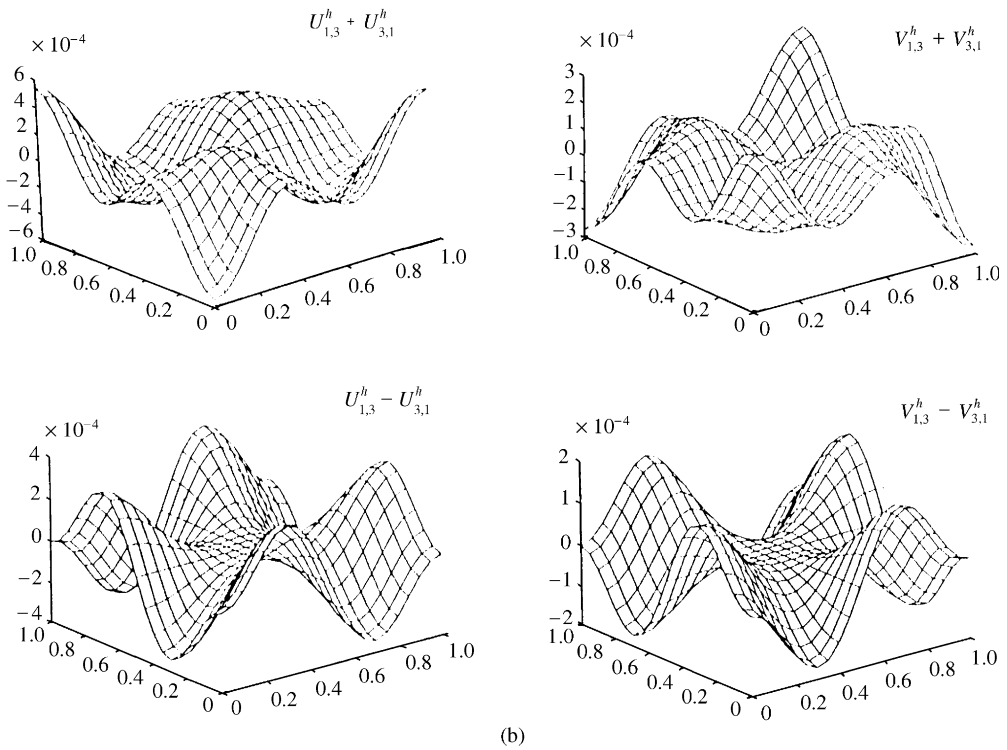


Fig. 4. Bifurcation scenario at the double bifurcation point $(0, \lambda^h_{1,3}) = (0, \lambda^h_{3,1}) = (0, 106.126545)$: (a) bifurcation diagram; (b) contours of the solution curves at $\lambda = 107.349207$.



(b)

Fig. 4. (*Continued.*)

Example 5. *Steady/steady-state* mode interaction of two simple bifurcations, where $(i_1, j_1) = (1, 1)$, and $(i_2, j_2) = (2, 2)$. By choosing $\alpha = 55.544456$ we obtain $(0, \lambda^h_{1,1}) = (0, \lambda^h_{2,2}) = (0, 1641.601512)$ which is a double bifurcation point. Fig. 5a shows that two solution curves branching from this double bifurcation point. Fig. 5b shows the contours of the solution curves at $\lambda = 1640.2643$ and 1640.2884, respectively.

Example 6. *Steady/steady-state* mode interaction of one simple and one double bifurcations, where $(i_1, j_1) = (1, 1)$ and $(i_2, j_2) = (1, 2)$. If we choose $\alpha = 43.938938$, then $(0, \lambda^h_{1,1}) = (0, \lambda^h_{1,2}) = (0, 1035.017916)$ is a bifurcation point of corank 3. Fig. 6a shows six solution curves branching from this bifurcation point. Similar to the case of Example 3, the solution curves of $U^h_{1,2}, U^h_{2,1}$, and $U^h_{1,2} - U^h_{2,1}$ (respectively $V^h_{1,2}, V^h_{2,1}$, and $V^h_{1,2} - V^h_{2,1}$) coincide with each other. Fig. 6b shows the contours of these five solution curves at $\lambda = 1036.134529$.

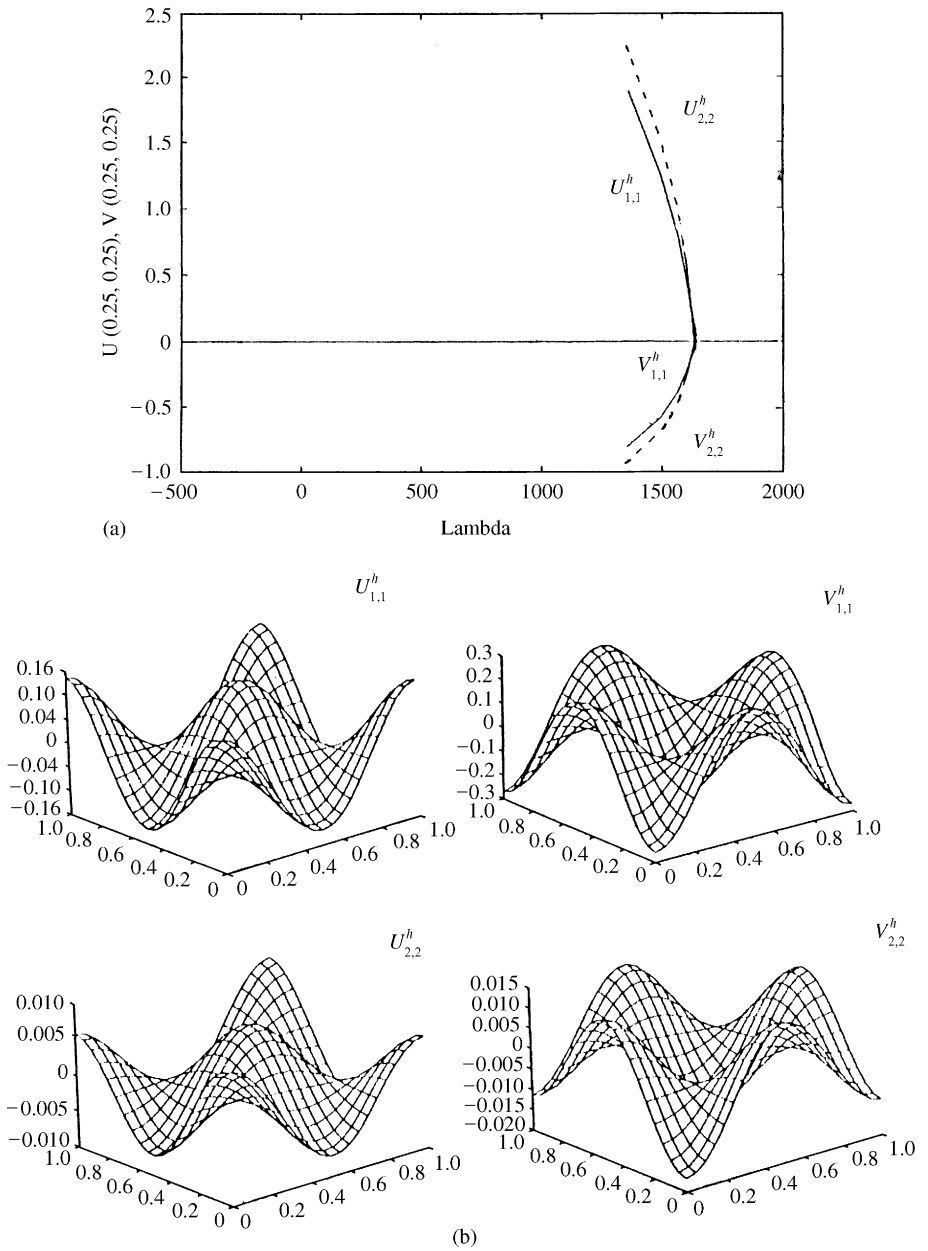


Fig. 5. Bifurcation scenario at the double bifurcation point $(0, \lambda^h_{1,1}) = (0, \lambda^h_{2,2}) = (0, 1641.601512)$, $\alpha = 55.47742$: (a) bifurcation diagram; (b) contours of the solution curves at $\lambda = 1640.288436$.

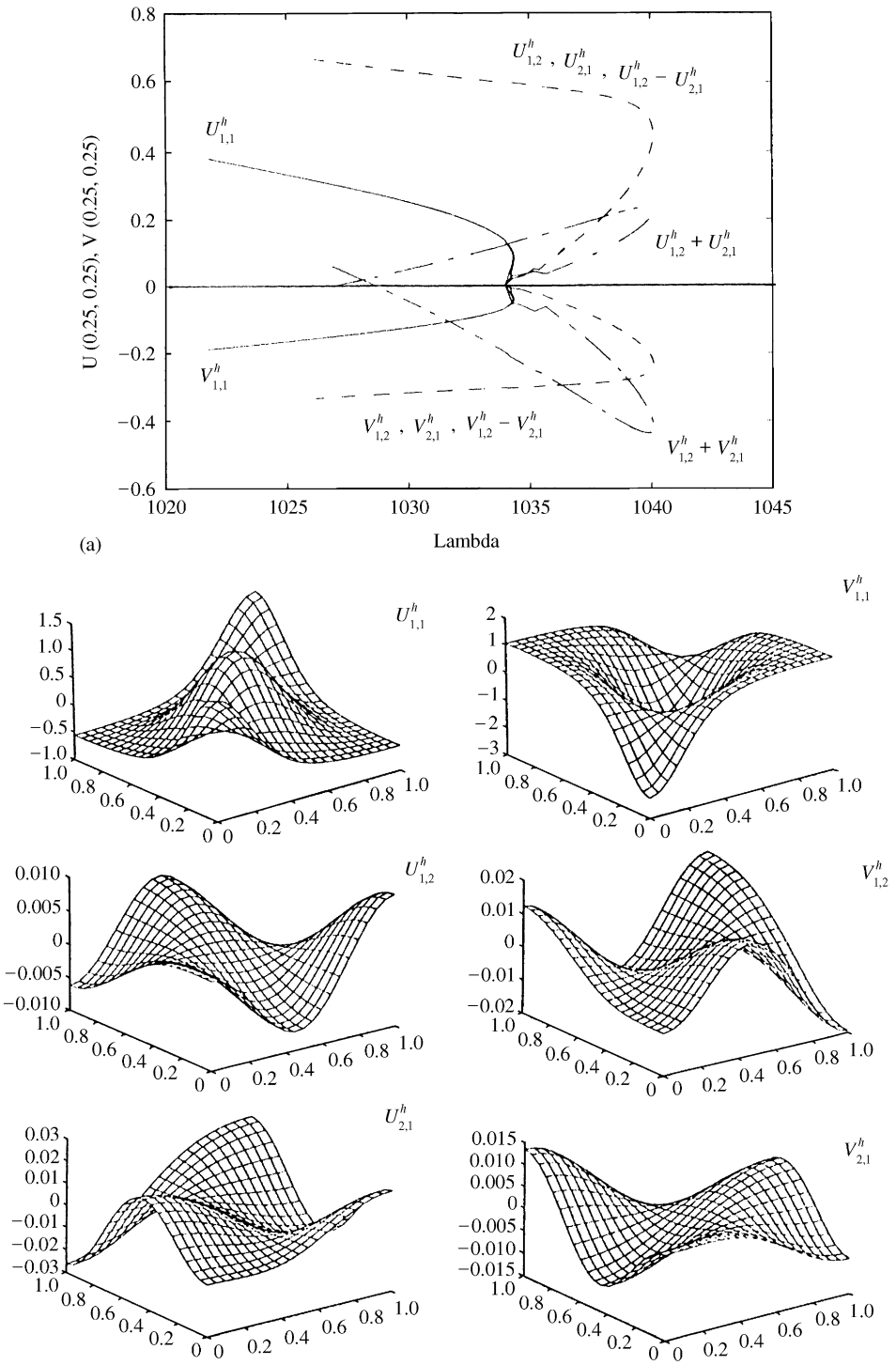


Fig. 6. Bifurcation scenario at the triple bifurcation point $(0, \lambda^h_{1,1}) = (0, \lambda^h_{1,2}) = (0, \lambda^h_{2,1}) = (0, 1035.017916)$, $\alpha = 43.89231$: (a) bifurcation diagram; (b) contours of the solution curves at $\lambda = 1036.134529$.

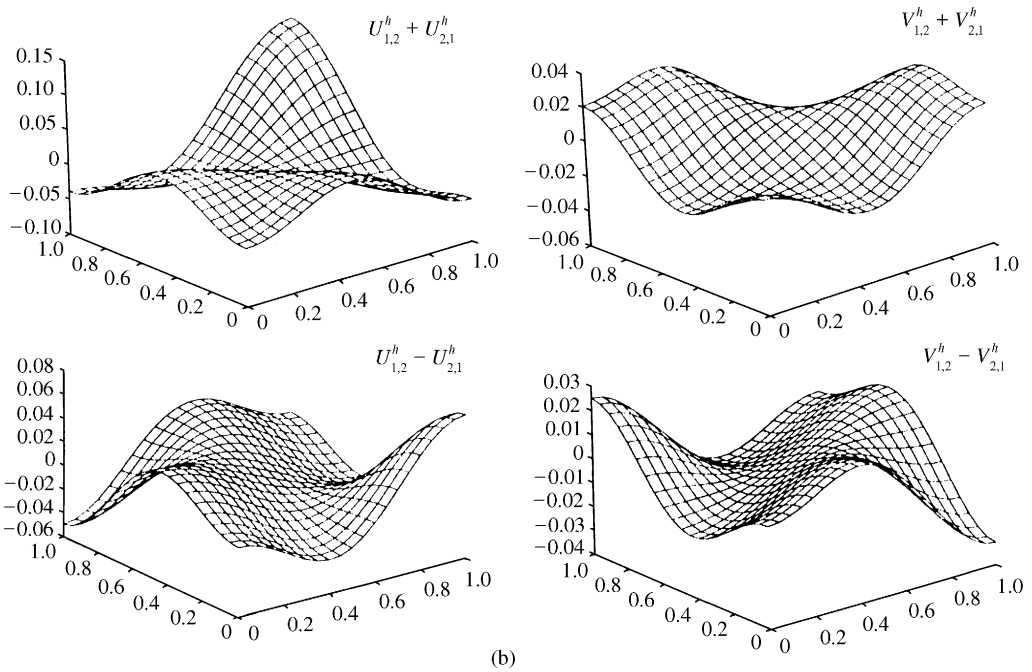


Fig. 6. (*Continued.*)

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