Journal of Mathematical Chemistry 26 (1999) 297–316

A second-order scheme for the "Brusselator" reaction–diffusion system

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Received 20 April 1998; revised 2 November 1999

A second-order method is developed for the numerical solution of the initial-value problems $u' \equiv \mathrm{d}u/\mathrm{d}t = f_1(u,v)$, $t > 0$, $u(0) = U^0$ and $v' \equiv \mathrm{d}v/\mathrm{d}t = f_2(u,v)$, $t > 0$, $v(0) = V^0$, in which the functions $f_1(u,v) = B + u^2v - (A+1)u$ and $f_2(u,v) = Au - u^2v$, where A and B are positive real constants, are the reaction terms arising from the mathematical modelling of chemical systems such as in enzymatic reactions and plasma and laser physics in multiple coupling between modes. The method is based on three first-order methods for solving u and v, respectively. In addition to being second-order accurate in space and time, the method is seen to converge to the correct fixed point ($U^* = B$, $V^* = A/B$) provided $1 - A + B^2 \geqslant 0$. The approach adopted is extended to solve a class of non-linear reaction–diffusion equations in two-space dimensions known as the "Brusselator" system. The algorithm is implemented in parallel using two processors, each solving a linear algebraic system as opposed to solving non-linear systems, which is often required when integrating non-linear partial differential equations (PDEs).

1. Introduction

The importance of oscillations in biochemical systems has been emphasized by a number of authors. For instance, Turing [11] showed that when certain reactions are coupled with the process of diffusion, it is possible to obtain a stable spatial pattern (this laid the foundation of the theory of morphogenesis). The so-called Brussels school [5–10] developed and analysed the behaviour of a non-linear oscillator [7,10] associated with the chemical system

$$\mathrm{B_{in}} \to \mathrm{X}, \tag{1a}$$

$$\mathrm{A_{in}} + \mathrm{X} \to \mathrm{Y} + \mathrm{D}, \tag{1b}$$

$$2\mathrm{X} + \mathrm{Y} \to 3\mathrm{X}, \tag{1c}$$

$$\mathrm{X} \to \mathrm{E}, \tag{1d}$$

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in which B_{in} and A_{in} are input chemicals, D and E are output chemicals and X and Y are intermediates. The chemical system (1), known as the "Brusselator" system, is important in that it admits limit-cycle oscillations and yet contains only two dependent variables (X and Y) thus enabling the use of two-dimensional mathematical systems [8].

It is known [1] that the trimolecular reaction step (1c) arises in the formation of ozone by atomic oxygen via a triple collision, in enzymatic reactions, and in plasma and laser physics in multiple couplings between modes. Tyson [13] notes that the system (1) satisfies the necessary (but not sufficient) requirements that "a chemical system be open, non-linear, and far from equilibrium in order to manifest more interesting behaviour other than exponential decay to a homogeneous steady state". The kinetic equations associated with (1) are given by [10]

$$\begin{aligned} \frac{\partial X}{\partial t} &= k_1 B + k_2 X^2 Y - k_3 A X - k_4 X + D_x \nabla^2 X, \\ \frac{\partial Y}{\partial t} &= k_3 A X - k_2 X^2 Y + D_y \nabla^2 Y. \end{aligned} \tag{2}$$

The rate constants k_1 and k_2 are superfluous, since the rate of steps (1a) and (1b) can be varied by changing the parameters B and A [13]. Similarly, the rate constant k_3 of the autocatalytic step (1c) can be made unity by scaling time. Following Tyson [13], the constant k_4 is given the value unity.

Let $u = u(x, y, t)$ and $v = v(x, y, t)$ represent the concentrations of two reaction products P_1 and P_2 at time t, A and B be constant concentrations of two input reagents, and α (a constant) represent D_x and D_y and L the reactor length. Then, the partial differential equations associated with the "Brusselator" system are given by (see, for instance, [1])

$$\frac{\partial u}{\partial t} = B + u^2 v - (A+1)u + \alpha\left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2}\right), \quad 0 < x, y < L,\ t > 0, \tag{3a}$$

$$\frac{\partial v}{\partial t} = Au - u^2 v + \alpha\left(\frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2}\right), \quad 0 < x, y < L,\ t > 0, \tag{3b}$$

subject to Neumann boundary conditions on the boundary $\partial\Omega$ of the square Ω defined by the lines $x = 0$, $y = 0$, $x = L$, $y = L$, given by

$$\begin{aligned} \frac{\partial u(0, y, t)}{\partial x} &= \frac{\partial u(L, y, t)}{\partial x} = 0, \quad t \geqslant 0, \\ \frac{\partial u(x, 0, t)}{\partial y} &= \frac{\partial u(x, L, t)}{\partial y} = 0, \quad t \geqslant 0, \\ \frac{\partial v(0, y, t)}{\partial x} &= \frac{\partial v(L, y, t)}{\partial x} = 0, \quad t \geqslant 0, \\ \frac{\partial v(x, 0, t)}{\partial y} &= \frac{\partial v(x, L, t)}{\partial y} = 0, \quad t \geqslant 0, \end{aligned} \tag{4}$$

and initial conditions

$$\begin{aligned} u(x,y,0) &= f(x,y), \quad (x,y) \in \Omega \cup \partial\Omega, \\ v(x,y,0) &= g(x,y), \quad (x,y) \in \Omega \cup \partial\Omega. \end{aligned} \tag{5}$$

In (5), f and g are given continuous functions of x and y.

A number of methods have been proposed in the literature for the solution and stability analyses of this system, notably by Adomian [1], the Brussels school [5–10], and Tyson [13]. It is common knowledge that, for problems involving reaction terms such as (3), the numerical treatment of such reaction terms has, arguably, the most influence on the numerical results (see, for instance, [12]).

It is therefore important to consider the behaviour of the reaction terms given by (3) with $\alpha = 0$. This will be discussed in section 2 where a novel second-order finite-difference method will be developed. The fixed point of the numerical scheme will be analysed. In section 3, numerical experiments are reported that show that the method converges to the critical point for values of A and B for which $1-A+B^2 > 0$. Extension to the case of non-vanishing α resulting in the full "Brusselator" system, is considered in section 4, where a second-order numerical method is developed which may be implemented in parallel using two processors, each solving a single linear algebraic system at every time step.

2. Numerical method for the diffusion-free case

2.1. *Analysis of the critical point of the system*

Consider the diffusion-free "Brusselator" system given by (3) with $\alpha = 0$

$$\begin{aligned} \frac{\mathrm{d}u}{\mathrm{d}t} &\equiv f_1(u,v) = B + u^2 v - (A+1)u, \quad t > 0, \qquad u(0) = U^0, \\ \frac{\mathrm{d}v}{\mathrm{d}t} &\equiv f_2(u,v) = Au - u^2 v, \qquad\qquad\quad t > 0, \qquad v(0) = V^0, \end{aligned} \tag{6}$$

in which $u = u(t)$, $v = v(t)$ and A and B are positive real constants. It can be shown that the only critical point of the ordinary differential equation (ODE) system is $(u^*, v^*) = (B, A/B)$. The Jacobian, J^*, at the critical point (u^*, v^*) is given by

$$J^* = \begin{bmatrix} A-1 & B^2 \\ -A & -B^2 \end{bmatrix} \tag{7}$$

and its eigenvalues $\lambda_{1,2}$ satisfy the characteristic equation

$$\lambda^2 + \left(1 - A + B^2\right)\lambda + B^2 = 0. \tag{8}$$

The roots of this equation, the eigenvalues of J^*, clearly depend on $1-A+B^2$ and on the quantity $\Delta \equiv (1-A+B^2)^2 - 4B^2$. These eigenvalues govern the stability of the critical point and the existence, or otherwise, of a limit cycle. The stability properties and the existence of a limit cycle are summarized in table 1 in relation to the four

Table 1
Nature of critical point and existence of limit cycle.

Region	$1-A+B^2$	Δ	Eigenvalues	Type of critical point	Limit cycle exists
1	>0	$\geqslant 0$	Positive real	Unstable node	Yes
2	>0	<0	Positive real parts	Unstable focus	Yes
	$=0$	<0	Imaginary	Stable fine focus	No
3	<0	<0	Negative real parts	Stable focus	No
4	<0	$\geqslant 0$	Negative real	Stable node	No

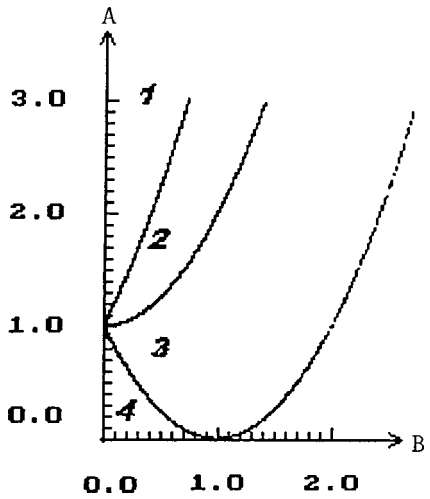

Figure 1. Stability regions of the diffusion-free system.

regions of figure 1. Using Hopf theory [3,4], it may be shown that the critical point loses its stability when A and B move from region 2 to region 3 of figure 1, across the curve $1-A+B^2=0$. A Hopf bifurcation occurs as this curve is crossed and a stable limit cycle exists for A and B in regions 1 and 2 but not for A and B in regions 3 and 4.

2.2. Numerical method for u

Starting with the initial-value problem

$$u' \equiv \frac{\mathrm{d}u}{\mathrm{d}t} = B + u^2 v - (A+1)u, \quad t > 0, \qquad u(0) = U^0, \tag{9}$$

the development of numerical methods may be based on approximating the derivative in (9) by its first-order forward-difference approximant given by

$$\frac{\mathrm{d}u}{\mathrm{d}t} = \frac{u(t+\ell) - u(t)}{\ell} + \mathrm{O}(\ell) \quad \text{as } \ell \to 0, \tag{10}$$

where $\ell > 0$ is an increment in t (time step). Discretizing the interval $t \geqslant 0$ at the points $t_n = n\ell$ ($n = 0, 1, 2, \ldots$), the solution of (9) at the grid point t_n is $u(t_n)$. The

solution obtained by a numerical method at the point t_n will be denoted by U^n. Three numerical methods for solving (9) based on approximating the time derivative in (9) by (10) and making appropriate approximations for the linear and cubic terms in (9) are given below:

$$\begin{aligned} M_u^{(1)}\colon &\quad U^{n+1} = U^n + \ell B + \ell\big(U^n\big)^2 V^n - \ell(A+1)U^n, \\ M_u^{(2)}\colon &\quad U^{n+1} = U^n + \ell B + \ell\big(U^n\big)^2 V^{n+1} - \ell(A+1)U^{n+1}, \\ M_u^{(3)}\colon &\quad U^{n+1} = U^n + \ell B + \ell U^n U^{n+1} V^n - \ell(A+1)U^n. \end{aligned} \tag{11}$$

The associated local truncation errors of these three methods are, respectively,

$$\begin{aligned} L_u^{(1)} &= L_u^{(1)}\big[u(t), v(t), \ell\big] = u(t+\ell) - u(t) - \ell B - \ell\big\{u(t)\big\}^2 v(t) + \ell(A+1)u(t), \\ L_u^{(2)} &= L_u^{(2)}\big[u(t), v(t), \ell\big] = u(t+\ell) - u(t) - \ell B - \ell\big\{u(t)\big\}^2 v(t+\ell) + \ell(A+1)u(t+\ell), \\ L_u^{(3)} &= L_u^{(3)}\big[u(t), v(t), \ell\big] = u(t+\ell) - u(t) - \ell B - \ell u(t)v(t)u(t+\ell) + \ell(A+1)u(t), \end{aligned} \tag{12}$$

in which $t = t_n$. It is easy to show that the Taylor series expansion of the functions in (12) about t leads to

$$\begin{aligned} L_u^{(1)} &= \frac{1}{2}\ell^2 u'' + \mathrm{O}\big(\ell^3\big) && \text{as } \ell \to 0, \\ L_u^{(2)} &= \left[\frac{1}{2}u'' - u^2 v' + (A+1)u'\right]\ell^2 + \mathrm{O}\big(\ell^3\big) && \text{as } \ell \to 0, \\ L_u^{(3)} &= \left(\frac{1}{2}u'' - uu'v\right)\ell^2 + \mathrm{O}\big(\ell^3\big) && \text{as } \ell \to 0, \end{aligned} \tag{13}$$

where u and its derivatives (denoted by primes) are evaluated at some grid point $t = t_n$.

Defining, now, a function $L_u^{(e)}$ by the linear combination

$$L_u^{(e)} = \frac{1}{2}\big[2L_u^{(3)} + L_u^{(2)} - L_u^{(1)}\big], \tag{14}$$

gives

$$L_u^{(e)} = \frac{1}{2}\big[u'' - 2uu'v - u^2 v' + (A+1)u'\big]\ell^2 + \mathrm{O}\big(\ell^3\big) \quad \text{as } \ell \to 0. \tag{15}$$

Differentiating the differential equation in (9) reveals that the coefficient of ℓ^2 in (15) vanishes; thus,

$$L_u^{(e)} = \mathrm{O}\big(\ell^3\big) \tag{16}$$

as $\ell \to 0$. This implies that a second-order method for computing u can be constructed by taking the linear combination $M_u^{(3)} + \frac{1}{2}M_u^{(2)} - \frac{1}{2}M_u^{(1)}$ and is given by

$$\begin{aligned} &\left[1 - \ell U^n V^n + \frac{1}{2}\ell(A+1)\right]U^{n+1} - \frac{1}{2}\,\ell\big(U^n\big)^2 V^{n+1} \\ &\quad = \left[1 - \frac{1}{2}\,\ell(A+1)\right]U^n - \frac{\ell}{2}\big(U^n\big)^2 V^n + \ell B. \end{aligned} \tag{17}$$

This method involves U^{n+1} and V^{n+1}, thus U^{n+1} cannot be calculated explicitly from (17).

2.3. Numerical method for v

Following the approach used in section 2.2, a second-order method for finding v may be shown to be

$$\begin{aligned} -\ell\left(\frac{1}{2}A - U^nV^n\right)U^{n+1} + \left[1 + \frac{1}{2}\ell\big(U^n\big)^2\right]V^{n+1} \\ = V^n + \frac{1}{2}\ell AU^n + \frac{1}{2}\ell\big(U^n\big)^2V^n. \end{aligned} \tag{18}$$

This scheme, like (17), also involves V^{n+1} and U^{n+1}, hence V^{n+1} cannot be obtained explicitly from (18).

However, in both (17) and (18), U^{n+1} and V^{n+1} occur linearly so that (17) and (18) can be solved simultaneously to give

$$U^{n+1} = \frac{\big[1 - \frac{1}{2}\ell(A+1)\big]U^n + \frac{1}{2}\ell^2B(U^n)^2 + \frac{1}{2}\ell(U^n)^3 - \frac{1}{4}\ell^2(U^n)^3 + \ell B}{1 + \frac{1}{2}\ell(A+1) + \frac{1}{2}\ell(U^n)^2 + \frac{1}{4}\ell^2(U^n)^2 - \ell U^nV^n}, \tag{19}$$

and

$$\begin{aligned} V^{n+1} = {} & \frac{V^n + \ell\big[AU^n + \frac{1}{2}(A+1)V^n - \frac{1}{2}(U^n)^2V^n - U^n(V^n)^2\big]}{1 + \frac{1}{2}\ell(A+1) + \frac{1}{2}\ell(U^n)^2 + \frac{1}{4}\ell^2(U^n)^2 - \ell U^nV^n} \\ & + \frac{\ell^2\big[\frac{1}{2}AB - BU^nV^n + \frac{3}{4}(U^n)^2V^n\big]}{1 + \frac{1}{2}\ell(A+1) + \frac{1}{2}\ell(U^n)^2 + \frac{1}{4}\ell^2(U^n)^2 - \ell U^nV^n}. \end{aligned} \tag{20}$$

2.4. Analyses of the fixed point

The expressions for U^{n+1} and V^{n+1} in (19) and (20) are of the forms

$$\begin{aligned} U^{n+1} &= g_1\big(U^n, V^n\big), \\ V^{n+1} &= g_2\big(U^n, V^n\big), \end{aligned} \tag{21}$$

respectively, and it may be verified that the fixed point of (19) and (20) is $U^* = B$, $V^* = A/B$. Thus the fixed point of the numerical method (19), (20) is the same as the critical point of the dynamical system (6). A crucial point of interest is whether or not the fixed point of the difference system has the same stability properties as the critical point of the ODE system (6).

Considering, first, the functions

$$g_1(U,V) = \frac{U - \frac{1}{2}\ell(A+1)U + \frac{1}{2}\ell^2BU^2 + \frac{1}{2}\ell U^3 - \frac{1}{4}\ell^2U^3 + \ell B}{1 + \frac{1}{2}\ell(A+1) + \frac{1}{2}\ell U^2 + \frac{1}{4}\ell^2U^2 - \ell UV}, \tag{22}$$

$$g_2(U,V) = \frac{V + \ell AU + \frac{1}{2}\ell(A+1)V - \frac{1}{2}\ell U^2 V - \ell UV^2 + \frac{1}{2}\ell^2 AB - \ell^2 BUV + \frac{3}{4}\ell^2 U^2 V}{1 + \frac{1}{2}\ell(A+1) + \frac{1}{2}\ell U^2 + \frac{1}{4}\ell^2 U^2 - \ell UV} \tag{23}$$

it may be seen (after some tedious manipulations) that the resulting Jacobian J at the fixed point ($U = B$ and $V = A/B$) is given by

$$J = \frac{1}{Z}\begin{bmatrix} 1 - \frac{1}{2}\ell + \frac{1}{2}\ell A + \frac{1}{2}\ell B^2 - \frac{1}{4}\ell^2 B^2 & \ell B^2 \\ -\ell A & 1 + \frac{1}{2}\ell - \frac{1}{2}\ell A - \frac{1}{2}\ell B^2 - \frac{1}{4}\ell^2 B^2 \end{bmatrix}, \tag{24}$$

where $Z = 1 + \frac{1}{2}\ell - \frac{1}{2}\ell A + \frac{1}{2}\ell B^2 + \frac{1}{4}\ell^2 B^2$, and its eigenvalues are given by

$$\mu_1 = \frac{1 + \frac{1}{2}\ell(1 - A + B^2) - \frac{1}{4}\ell^2 B^2}{1 + \frac{1}{2}\ell(1 - A + B^2) + \frac{1}{4}\ell^2 B^2} \quad \text{and} \quad \mu_2 = \frac{1 - \frac{1}{2}\ell(1 - A + B^2) - \frac{1}{4}\ell^2 B^2}{1 + \frac{1}{2}\ell(1 - A + B^2) + \frac{1}{4}\ell^2 B^2}. \tag{25}$$

It is clear from (25) that the denominators of μ_1 and μ_2 are always positive provided $1 - A + B^2 > 0$ and $\ell > 0$ and it is easy to show then that

$$|\mu_1| < 1 \quad \text{and} \quad |\mu_2| < 1 \tag{26}$$

for any $\ell \in (0, \infty)$. The inequalities in (26) are also true whenever $1 - A + B^2 = 0$. Thus a sufficient condition for the fixed point $(B, A/B)$ to attract the solution sequence generated by (19) and (20) is $1 - A + B^2 \geqslant 0$.

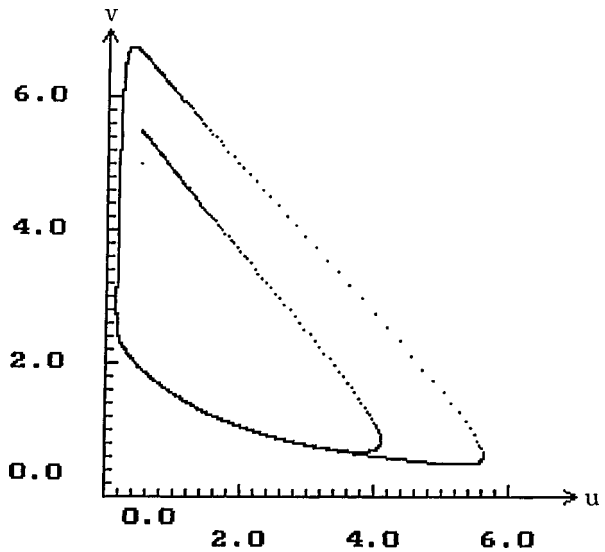

Figure 2. Phase portraits of the diffusion-free system with $A = 2.5$ and $B = 0.5$ (region 1 of figure 1) using the second-order scheme with $\ell = 0.01$.

3. Numerical verification

To verify the convergence properties of the numerical scheme {(19), (20)}, it was tested on the initial-value problem (6). Of particular interest is the behaviour of the method when $1 - A + B^2 \geqslant 0$. Extensive numerical experiments, taking values of A

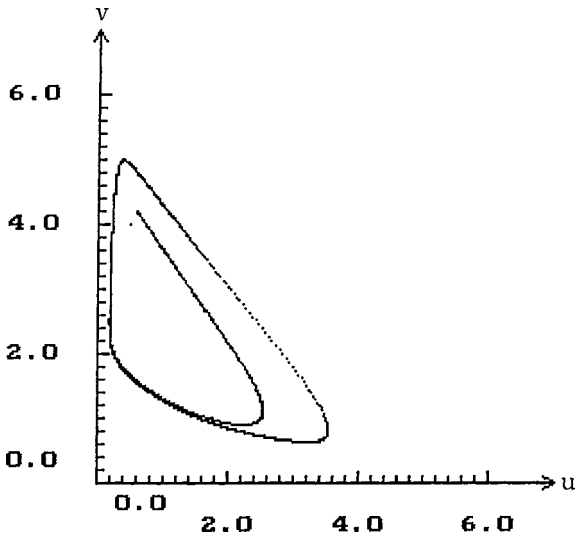

Figure 3. Phase portraits of the diffusion-free system with $A = 2.0$ and $B = 0.5$ (region 2 of figure 1) using the second-order scheme with $\ell = 0.01$.

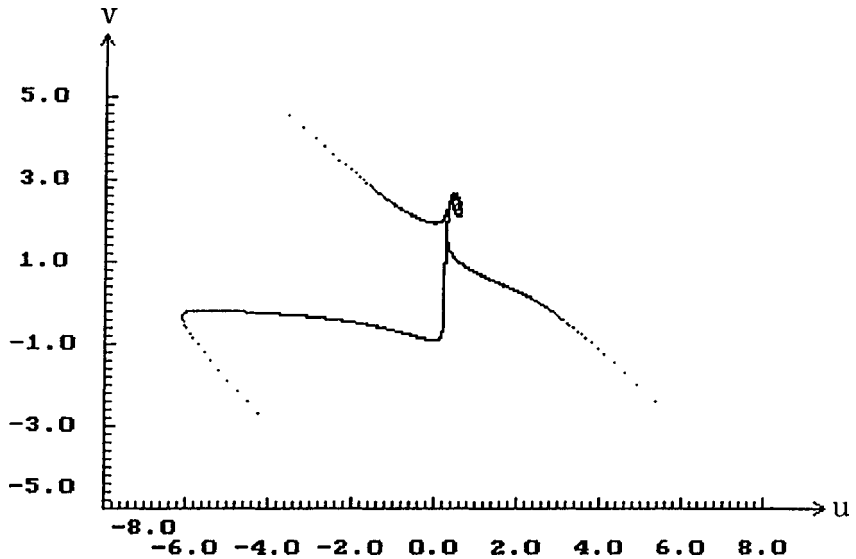

Figure 4. Phase portraits of the diffusion-free system with $A = 1.2$ and $B = 0.5$ (region 3 of figure 1) using the second-order scheme with $\ell = 0.01$.

and B in the four regions of figure 1 with $-8 \leqslant U^0, V^0 \leqslant 8$ and a time-step $\ell = 0.01$ were carried out. Of course, U^0 and V^0 are concentrations so that non-positive values are irrelevant, but the results show that the scheme {(19), (20)} performed well for negative initial conditions, too. It was discovered that the scheme converged to the fixed point $U^* = B$, $V^* = A/B$ whenever $1 - A + B^2 > 0$ (regions 1 and 2 of figure 1). Phase portraits for $B = 0.5$ with $A = 2.5, 2.0, 1.2$ and 0.2 (regions 1, 2, 3

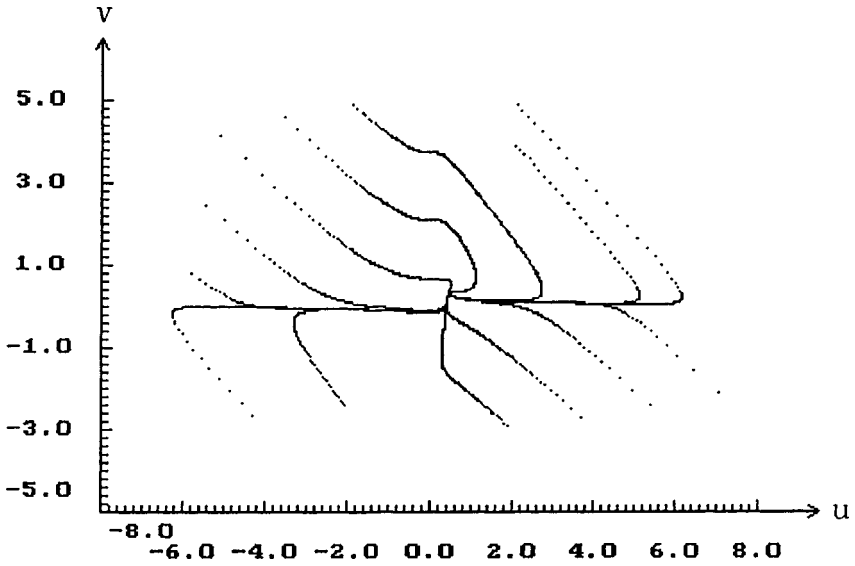

Figure 5. Phase portraits of the diffusion-free system with $A = 0.2$ and $B = 0.5$ (region 4 of figure 1) using the second-order scheme with $\ell = 0.01$.

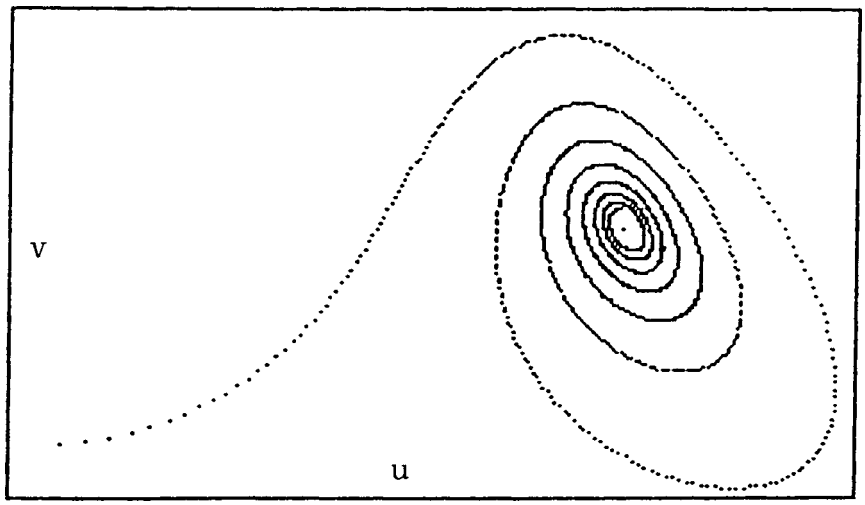

Figure 6. Enlargement of figure 4 in the vicinity of the fixed point $U^* = 0.5$, $V^* = 2.4$.

and 4 of figure 1) are depicted in figures 2, 3, 4 and 5, respectively. An enlargement of the area around the fixed point $(U^*, V^*) = (0.5, 2.4)$ of figure 4 is depicted in figure 6 and shows clearly that the solution sequence spirals into the fixed point. The limit cycles are visible in figures 2 and 3.

4. The "Brusselator" reaction–diffusion equations

4.1. Introduction

The reaction–diffusion equations in the full "Brusselator" system are given by (3) so that, on differentiating with respect to t,

$$u_{tt} - 2uu_tv - u^2v_t + (A+1)u_t - \alpha(u_{xxt} + u_{yyt}) = 0 \tag{27}$$

and

$$v_{tt} - Au_t + 2uu_tv + u^2v_t - \alpha(v_{xxt} + v_{yyt}) = 0, \tag{28}$$

where, now, $u = u(x, y, t)$, $v = v(x, y, t)$, $u_x \equiv \partial u/\partial x$, etc.

4.2. Discretization and notations

Most modern texts on numerical analysis give an introduction to numerical solutions of partial differential equations using the finite-difference approach (see, for example, [2]). In the following sections a linear combination of first-order schemes will be made to obtain second-order approximations to u and v.

Both intervals $0 \leqslant x \leqslant L$ and $0 \leqslant y \leqslant L$ are divided into $N+1$ subintervals each of width h, so that $(N+1)h = L$ and the time variable t is discretized in steps of length ℓ. Thus at each time level $t = t_n = n\ell$ $(n = 0, 1, 2, \ldots)$ the square Ω, and its boundary $\partial\Omega$, have been superimposed by a square mesh with N^2 points within Ω and $N+2$ equally spaced points along each side of $\partial\Omega$.

The solutions $u^n_{k,m} = u(x_k, y_m, t_n)$ and $v^n_{k,m} = v(x_k, y_m, t_n)$ are sought at each point $(kh, mh, n\ell)$ in $\bar{\Omega} \cup \partial\Omega$ where $k, m = 0, 1, 2, \ldots, N, N+1$ and $n = 0, 1, 2, \ldots$. The notation $U^n_{k,m}$ and $V^n_{k,m}$ will be used to distinguish the solutions of the numerical methods from the theoretical solutions $u^n_{k,m}$ and $v^n_{k,m}$. It will be convenient to define the vectors $\mathbf{U}^n$ and $\mathbf{V}^n$ as

$$\begin{aligned}\mathbf{U}^n = \big(&U^n_{0,0}, U^n_{1,0}, \ldots, U^n_{N,0}, U^n_{N+1,0}; U^n_{0,1}, U^n_{1,1}, U^n_{2,1}, \ldots, U^n_{N,1}, U^n_{N+1,1}; U^n_{0,2}, U^n_{1,2},\\ &U^n_{2,2}, \ldots, U^n_{N,2}, U^n_{N+1,2}; \ldots; U^n_{0,N+1}, U^n_{1,N+1}, U^n_{2,N+1}, \ldots, U^n_{N+1,N+1}\big)^{\mathrm{T}}\end{aligned}$$

and

$$\begin{aligned}\mathbf{V}^n = \big(&V^n_{0,0}, V^n_{1,0}, \ldots, V^n_{N,0}, V^n_{N+1,0}; V^n_{0,1}, V^n_{1,1}, V^n_{2,1}, \ldots, V^n_{N,1}, V^n_{N+1,1}; V^n_{0,2}, V^n_{1,2},\\ &V^n_{2,2}, \ldots, V^n_{N,2}, V^n_{N+1,2}; \ldots; V^n_{0,N+1}, V^n_{1,N+1}, V^n_{2,N+1}, \ldots, V^n_{N+1,N+1}\big)^{\mathrm{T}},\end{aligned} \tag{29}$$

with $^{\mathrm{T}}$ denoting transpose.

4.3. The numerical method for u

The equations in (11) will be adapted to obtain approximations to $\partial u(x_k, y_m, t_n)/\partial t$ for use in (3a). The space derivative will be replaced by the approximation

$$\begin{aligned}
&\alpha\left(\frac{\partial^2 u(x,y,t)}{\partial x^2}+\frac{\partial^2 u(x,y,t)}{\partial y^2}\right)\\
&\quad\approx \alpha\xi_u u(x,y,t)\\
&\quad\equiv \alpha h^{-2}\left[\frac{1}{2}\big\{u(x-h,y,t+\ell)-2u(x,y,t+\ell)+u(x+h,y,t+\ell)\big\}\right.\\
&\qquad\quad+\frac{1}{2}\big\{u(x-h,y,t)-2u(x,y,t)+u(x+h,y,t)\big\}\\
&\qquad\quad+\frac{1}{2}\big\{u(x,y-h,t+\ell)-2u(x,y,t+\ell)+u(x,y+h,t+\ell)\big\}\\
&\qquad\quad\left.+\frac{1}{2}\big\{u(x,y-h,t)-2u(x,y,t)+u(x,y-h,t)\big\}\right] \qquad (30)
\end{aligned}$$

in which $(x,y,t)=(x_k,y_m,t_n)$. Expanding $u(x\pm h,y,t+\ell)$, $u(x\pm h,y,t)$, $u(x,y\pm h,t+\ell)$ and $u(x,y\pm h,t)$ about (x,y,t) reveals that

$$\begin{aligned}
&\alpha\left(\frac{\partial^2 u(x,y,t)}{\partial x^2}+\frac{\partial^2 u(x,y,t)}{\partial y^2}\right)-\alpha\xi_u u(x,y,t)\\
&\quad=-\alpha\left(\frac{1}{2}\,\ell u_{xxt}+\frac{1}{4}\,\ell^2 u_{xxtt}+\cdots+\frac{1}{12}\,h^2 u_{xxxx}+\cdots+\frac{1}{2}\,\ell u_{yyt}\right.\\
&\qquad\left.+\frac{1}{4}\,\ell^2 u_{yytt}+\cdots+\frac{1}{12}\,h^2 u_{yyyy}+\cdots\right). \qquad (31)
\end{aligned}$$

Using the expression for $M_u^{(1)}$ in (11) and (30) in (3a) gives

$$\frac{U_{k,m}^{n+1}-U_{k,m}^{n}}{\ell}-B-\big(U_{k,m}^{n}\big)^2 V_{k,m}^{n}+(A+1)U_{k,m}^{n}-\alpha\xi_u u(x_k,y_m,t_n)=0, \qquad (32)$$

adapting $M_u^{(2)}$ in (11) and using (30) in (3a) gives

$$\frac{U_{k,m}^{n+1}-U_{k,m}^{n}}{\ell}-B-\big(U_{k,m}^{n}\big)^2 V_{k,m}^{n+1}+(A+1)U_{k,m}^{n+1}-\alpha\xi_u u(x_k,y_m,t_n)=0, \qquad (33)$$

while adapting $M_u^{(3)}$ in (11) and using (30) in (3a) gives

$$\frac{U_{k,m}^{n+1}-U_{k,m}^{n}}{\ell}-B-U_{k,m}^{n}U_{k,m}^{n+1}V_{k,m}^{n}+(A+1)U_{k,m}^{n}-\alpha\xi_u u(x_k,y_m,t_n)=0. \qquad (34)$$

It follows from the analysis of section 2.2 and noting (27) that

$$\text{Eq. (34)}+\frac{1}{2}\,\text{Eq. (33)}-\frac{1}{2}\,\text{Eq. (32)} \qquad (35)$$

will give a second-order approximation to (3a). This method is given by

$$
\begin{aligned}
&-\frac{1}{2}\,\alpha p U^{n+1}_{k,m-1} - \frac{1}{2}\,\alpha p U^{n+1}_{k-1,m} + \left[1 - \ell U^n_{k,m} V^n_{k,m} + \frac{1}{2}\,\ell(A+1) + 2\alpha p\right] U^{n+1}_{k,m} \\
&\quad - \frac{1}{2}\,\alpha p U^{n+1}_{k+1,m} - \frac{1}{2}\,\alpha p U^{n+1}_{k,m+1} - \frac{1}{2}\,\ell\big(U^n_{k,m}\big)^2 V^{n+1}_{k,m} \\
&= \frac{1}{2}\,\alpha p U^n_{k,m-1} + \frac{1}{2}\,\alpha p U^n_{k-1,m} + \left[1 - \frac{1}{2}\,\ell U^n_{k,m} V^n_{k,m} - \frac{1}{2}\,\ell(A+1) - 2\alpha p\right] U^n_{k,m} \\
&\quad + \frac{1}{2}\,\alpha p U^n_{k+1,m} + \frac{1}{2}\,\alpha p U^n_{k,m+1} + \ell B
\end{aligned}
\tag{36}
$$

and it may be shown that it has local truncation error given by

$$
\begin{aligned}
L_u[u,v;h,\ell] = &-\frac{1}{12}\,\alpha h^2 (u_{xxxx} + u_{yyyy}) + \left[\frac{1}{6}\,u_{tt} - \frac{1}{2}\,uvu_{tt} - \frac{1}{4}\,u^2 v_{tt} + \frac{1}{4}(A+1)u_{tt}\right. \\
&\left. - \frac{1}{4}\,u_{xxtt} - \frac{1}{4}\,u_{yytt}\right]\ell^2 + \mathrm{O}\big(h^4 + \ell^3\big) \quad \text{as } h,\ell \to 0.
\end{aligned}
\tag{37}
$$

The finite difference method (36) may be applied with $k,\ m = 1, 2, \ldots, N$. In the cases $k,\ m = 0$ and $k,\ m = N+1$, (36) introduces mesh points outside $\Omega \cup \partial\Omega$ for which the problem is not defined. However, the boundary conditions (4) give, to second order in h,

$$
\begin{aligned}
&U^n_{k,-1} = U^n_{k,1}, \quad U^n_{k,N+2} = U^n_{k,N}; \quad k = 0, 1, \ldots, N+1, \\
&U^n_{-1,m} = U^n_{1,m}, \quad U^n_{N+2,m} = U^n_{N,m}; \quad m = 0, 1, \ldots, N+1,
\end{aligned}
\tag{38}
$$

for all $n = 0, 1, 2, \ldots$. The relations in (38) will be needed in the implementation of (36) which will be discussed in section 5. It should be noted that, because of the appearance of the term $V^{n+1}_{k,m}$, equation (36) with (38) does not enable the vector $\mathbf{U}^{n+1}$ to be computed until the equivalent numerical method for v has been developed.

4.4. The numerical method for v

Following the approach used in section 4.3, it may be shown that the unique $\mathrm{O}(h^2 + \ell^2)$ method for v (as $h, \ell \to 0$), analogous to (36), takes the form

$$
\begin{aligned}
&-\left(\frac{1}{2}\,A - U^n_{k,m} V^n_{k,m}\right)\ell U^{n+1}_{k,m} - \frac{1}{2}\,\alpha p V^{n+1}_{k,m-1} - \frac{1}{2}\,\alpha p V^{n+1}_{k-1,m} \\
&\quad + \left[1 + \frac{1}{2}\,\ell\big(U^n_{k,m}\big)^2 + 2\alpha p\right] V^{n+1}_{k,m} - \frac{1}{2}\,\alpha p V^{n+1}_{k+1,m} - \frac{1}{2}\,\alpha p V^{n+1}_{k,m+1} \\
&= \frac{1}{2}\,\ell A U^n_{k,m} + \frac{1}{2}\,\alpha p V^n_{k,m-1} + \frac{1}{2}\,\alpha p V^n_{k-1,m} + \left[1 + \frac{1}{2}\,\ell\big(U^n_{k,m}\big)^2 - 2\alpha p\right] V^n_{k,m} \\
&\quad + \frac{1}{2}\,\alpha p V^n_{k+1,m} + \frac{1}{2}\alpha p V^n_{k,m+1}
\end{aligned}
\tag{39}
$$

and that it has local truncation error given by

$$L_v[u,v;h,\ell] = -\frac{1}{12}\,\alpha h^2(v_{xxxx}+v_{yyyy}) + \left[\frac{1}{6}\,v_{ttt} - \frac{1}{4}\,Au_{tt} + \frac{1}{2}\,uvu_{tt} + \frac{1}{4}\,u^2v_{tt} - \frac{1}{4}\alpha v_{xxtt} - \frac{1}{4}\,\alpha v_{yytt}\right]\ell^2 + \mathrm{O}\big(h^4+\ell^3\big) \quad \text{as } h,\ell \to 0. \tag{40}$$

The boundary conditions (4) give, to second-order in h,

$$\begin{aligned} &V^n_{k,-1} = V^n_{k,1}, \quad V^n_{k,N+2} = V^n_{k,N}; \quad k = 0,1,\ldots,N+1,\\ &V^n_{-1,m} = V^n_{1,m}, \quad V^n_{N+2,m} = V^n_{N,m}; \quad m = 0,1,\ldots,N+1, \end{aligned} \tag{41}$$

for all $n = 0,1,2,\ldots$ which may be used when k, $m = 0$ and k, $m = N+1$. It should be noted that, because of the occurrence of the term $U^{n+1}_{k,m}$, equation (39) with (41) does not enable the vector $\mathbf{V}^{n+1}$ to be computed directly. Equations $\{$(36), (38)$\}$ and $\{$(39), (41)$\}$ are solved simultaneously to find $\mathbf{U}^{n+1}$ and $\mathbf{V}^{n+1}$. To do so, they must be written in matrix–vector form first of all.

Assuming convergence, it is easy to check that, as $n \to \infty$, $U_{k,m} = B$ and $V_{k,m} = A/B$ $(k,m = 0,1,\ldots,N,N+1)$ is the only steady-state solution of (36), (39) for any $\ell \in (0,\infty)$.

5. Implementation

It may be shown that equation (36) with (38) may be written in matrix–vector form as

$$E^n\mathbf{U}^{n+1} + D^n\mathbf{V}^{n+1} = Q^n\mathbf{U}^n + \ell\beta; \quad n = 0,1,2,\ldots, \tag{42}$$

where E^n, D^n and Q^n are square matrices of order $(N+2)^2$ given by

$$E^n = \begin{bmatrix} C^n_0 & -\alpha pI & & & & & 0 \\ -\frac{1}{2}\,\alpha pI & C^n_1 & -\frac{1}{2}\,\alpha pI & & & & \\ & -\frac{1}{2}\,\alpha pI & C^n_2 & -\frac{1}{2}\,\alpha pI & & & \\ & & \ddots & \ddots & \ddots & & \\ & & & -\frac{1}{2}\,\alpha pI & C^n_N & -\frac{1}{2}\,\alpha pI & \\ 0 & & & & -\alpha pI & C^n_{N+1} & \end{bmatrix}, \tag{43}$$

$$D^n = \begin{bmatrix} d^n_0 & & & & 0 \\ & d^n_1 & & & \\ & & d^n_2 & & \\ & & & \ddots & \\ 0 & & & & d^n_{N+1} \end{bmatrix}, \quad d^n_m = \mathrm{diag}\big\{d^n_{k,m}\big\}, \tag{44}$$

$$Q^n = \begin{bmatrix} Q_0^n & \alpha pI & & & & 0 \\ \frac{1}{2}\alpha pI & Q_1^n & \frac{1}{2}\alpha pI & & & \\ & \frac{1}{2}\alpha pI & Q_2^n & \frac{1}{2}\alpha pI & & \\ & & \ddots & \ddots & \ddots & \\ & & & \frac{1}{2}\alpha pI & Q_N^n & \frac{1}{2}\alpha pI \\ 0 & & & & \alpha pI & Q_{N+1}^n \end{bmatrix}, \tag{45}$$

in which I is the identity matrix of order $N+2$,

$$C_m^n = \begin{bmatrix} c_{0,m}^n & -\alpha p & & & & 0 \\ -\frac{1}{2}\alpha p & c_{1,m}^n & -\frac{1}{2}\alpha p & & & \\ & -\frac{1}{2}\alpha p & c_{2,m}^n & -\frac{1}{2}\alpha p & & \\ & & \ddots & \ddots & \ddots & \\ & & & -\frac{1}{2}\alpha p & c_{N,m}^n & -\frac{1}{2}\alpha p \\ 0 & & & & -\alpha p & c_{N+1,m}^n \end{bmatrix}, \tag{46}$$

$$Q_m^n = \begin{bmatrix} q_{0,m}^n & \alpha p & & & & 0 \\ \frac{1}{2}\alpha p & q_{1,m}^n & \frac{1}{2}\alpha p & & & \\ & \frac{1}{2}\alpha p & q_{2,m}^n & \frac{1}{2}\alpha p & & \\ & & \ddots & \ddots & \ddots & \\ & & & \frac{1}{2}\alpha p & q_{N,m}^n & \frac{1}{2}\alpha p \\ 0 & & & & \alpha p & q_{N+1,m}^n \end{bmatrix}, \tag{47}$$

are square matrices of order $N+2$ with

$$\begin{aligned} c_{k,m}^n &= 1 - \ell U_{k,m}^n V_{k,m}^n + \frac{1}{2}\ell(A+1) + 2\alpha p, \\ d_{k,m}^n &= -\frac{1}{2}\ell\big(U_{k,m}^n\big)^2, \\ q_{k,m}^n &= 1 - \frac{1}{2}\ell U_{k,m}^n V_{k,m}^n - \frac{1}{2}\ell(A+1) - 2\alpha p \end{aligned} \tag{48}$$

($k, m = 0, 1, \ldots, N, N+1$), and β is an $(N+2)$-vector given by

$$\beta = [B, B, \ldots, B, B]^{\mathrm{T}}. \tag{49}$$

Similarly, equation (39) with (41) may be written in matrix–vector form as

$$\Gamma^n \mathbf{U}^{n+1} + T^n \mathbf{V}^{n+1} = R\mathbf{U}^n + \Psi^n \mathbf{V}^n; \quad n = 0, 1, 2, \ldots, \tag{50}$$

where Γ^n, T^n, R and Ψ^n are square matrices of order $(N+2)^2$ given by

$$T^n = \begin{bmatrix} F_0^n & -\alpha pI & & & & & 0 \\ -\frac{1}{2}\alpha pI & F_1^n & -\frac{1}{2}\alpha pI & & & & \\ & -\frac{1}{2}\alpha pI & F_2^n & -\frac{1}{2}\alpha pI & & & \\ & & \ddots & \ddots & \ddots & & \\ & & & -\frac{1}{2}\alpha pI & F_N^n & -\frac{1}{2}\alpha pI & \\ 0 & & & & -\alpha pI & F_{N+1}^n & \end{bmatrix}, \tag{51}$$

$$\Gamma^n = \begin{bmatrix} G_0^n & & & & 0 \\ & G_1^n & & & \\ & & G_2^n & & \\ & & & \ddots & \\ 0 & & & & G_{N+1}^n \end{bmatrix}, \tag{52}$$

$$\Psi^n = \begin{bmatrix} S_0^n & \alpha pI & & & & 0 \\ \frac{1}{2}\alpha pI & S_1^n & \frac{1}{2}\alpha pI & & & \\ & \frac{1}{2}\alpha pI & S_2^n & \frac{1}{2}\alpha pI & & \\ & & \ddots & \ddots & \ddots & \\ & & & \frac{1}{2}\alpha pI & S_N^n & \frac{1}{2}\alpha pI \\ 0 & & & & \alpha pI & S_{N+1}^n \end{bmatrix}, \tag{53}$$

$$R = \begin{bmatrix} \frac{1}{2}\ell AI & & & & 0 \\ & \frac{1}{2}\ell AI & & & \\ & & \frac{1}{2}\ell AI & & \\ & & & \ddots & \\ 0 & & & & \frac{1}{2}\ell AI \end{bmatrix}, \tag{54}$$

in which

$$F_m^n = \begin{bmatrix} f_{0,m}^n & -\alpha p & & & & 0 \\ -\frac{1}{2}\alpha p & f_{1,m}^n & -\frac{1}{2}\alpha p & & & \\ & -\frac{1}{2}\alpha p & f_{2,m}^n & -\frac{1}{2}\alpha p & & \\ & & \ddots & \ddots & \ddots & \\ & & & -\frac{1}{2}\alpha p & f_{N,m}^n & -\frac{1}{2}\alpha p \\ 0 & & & & -\alpha p & f_{N+1,m}^n \end{bmatrix} \tag{55}$$

and

$$S_m^n = \begin{bmatrix} s_{0,m}^n & \alpha p & & & & 0 \\ \frac{1}{2}\alpha p & s_{1,m}^n & \frac{1}{2}\alpha p & & & \\ & \frac{1}{2}\alpha p & s_{2,m}^n & \frac{1}{2}\alpha p & & \\ & & \ddots & \ddots & \ddots & \\ & & & \frac{1}{2}\alpha p & s_{N,m}^n & \frac{1}{2}\alpha p \\ 0 & & & & \alpha p & s_{N+1,m}^n \end{bmatrix} \tag{56}$$

are square matrices of order $N+2$ with

$$\begin{aligned} f_{k,m}^n &= 1 + \ell\big(U_{k,m}^n\big)^2 + 2\alpha p, \\ s_{k,m}^n &= 1 + \frac{1}{2}\,\ell\big(U_{k,m}^n\big)^2 - 2\alpha p \end{aligned} \tag{57}$$

($k, m = 0, 1, \ldots, N, N+1$), and

$$G_m^n = \operatorname{diag}\big\{g_{k,m}^n\big\} = \operatorname{diag}\left\{\ell\left(U_{k,m}^n V_{k,m}^n - \frac{1}{2}\,A\right)\right\} \tag{58}$$

is a diagonal matrix of order $N+2$.

Since D^n and Γ^n are diagonal matrices, equations (42) and (50) may be solved for $\mathbf{U}^{n+1}$ and $\mathbf{V}^{n+1}$, which may then be computed in parallel on an architecture with two processors as follows:

Processor 1: Solve for $\mathbf{U}^{n+1}$:

$$\big(T^n\big(D^n\big)^{-1}E^n - \Gamma^n\big)\mathbf{U}^{n+1} = \big(T^n\big(D^n\big)^{-1}Q^n - R\big)\mathbf{U}^n - \Psi^n\mathbf{V}^n + \ell T^n\big(D^n\big)^{-1}\beta. \tag{59}$$

Processor 2: Solve for $\mathbf{V}^{n+1}$:

$$\big(E^n\big(\Gamma^n\big)^{-1}T^n - D^n\big)\mathbf{V}^{n+1} = \big(E^n\big(\Gamma^n\big)^{-1}R - Q^n\big)\mathbf{U}^n + E^n\big(\Gamma^n\big)^{-1}\Psi^n\mathbf{V}^n - \ell\beta.$$

It should be noted that each processor solves a linear algebraic system of order $(N+2)^2$ at each time level $t_n = n\ell$ ($n = 0, 1, 2, \ldots$) even though the system of PDEs (3) is non-linear.

6. Stability and convergence

Writing (42) and (50) as one system of order $2(N+2)^2$ gives

$$K^n\mathbf{Y}^{n+1} = M^n\mathbf{Y}^n + \ell\mathbf{b}, \tag{60}$$

in which

$$K^n = \left[\begin{array}{c|c} E^n & D^n \\ \hline \Gamma^n & T^n \end{array}\right], \tag{61}$$

$$M^n = \left[\begin{array}{c|c} Q^n & O \\ \hline R & \Psi^n \end{array}\right], \tag{62}$$

and

$$\mathbf{Y}^n = \big[\big(\mathbf{U}^n\big)^{\mathrm{T}}, \big(\mathbf{V}^n\big)^{\mathrm{T}}\big]^{\mathrm{T}}, \qquad \mathbf{Y}^{n+1} = \big[\big(\mathbf{U}^{n+1}\big)^{\mathrm{T}}, \big(\mathbf{V}^{n+1}\big)^{\mathrm{T}}\big]^{\mathrm{T}}, \qquad \mathbf{b} = \big[\beta^{\mathrm{T}}, \mathbf{0}^{\mathrm{T}}\big]^{\mathrm{T}}. \tag{63}$$

In (62), O is the zero matrix of order $N+2$ and in (63), $\mathbf{0}$ is the zero column vector of order $N+2$. The matrix method requires

$$\big\|\big(K^n\big)^{-1}M^n\big\|_S \leqslant 1 \tag{64}$$

for stability, S denoting the spectral norm. This localized condition must be satisfied at every time step. The inverse matrix $(K^n)^{-1}$ can be determined using, for instance, NAG (Numerical Algorithms Group) routine F01ACF following which its spectral norm may be calculated using NAG routine F02AFF. It is not possible to find in closed form a necessary condition for stability involving A, B, h and ℓ using, say, a linearization of the von Neumann method. This is because $\mathbf{U}^n$ and $\mathbf{V}^n$ are coupled in (59).

Assuming that a steady-state is reached, diffusion no longer takes place ($\alpha = 0$) and equations (36) and (39) reduce to

$$\left[1 - \ell U_{k,m}^n V_{k,m}^n + \frac{1}{2}\ell(A+1)\right] U_{k,m}^{n+1} - \frac{1}{2}\ell\left(U_{k,m}^n\right)^2 V_{k,m}^{n+1} = \left[1 - \frac{1}{2}\ell U_{k,m}^n V_{k,m}^n - \frac{1}{2}\ell(A+1)\right] U_{k,m}^n + \ell B \tag{65}$$

and

$$-\left(\frac{1}{2}A - U_{k,m}^n V_{k,m}^n\right)\ell U_{k,m}^{n+1} + \left[1 + \frac{1}{2}\ell\left(U_{k,m}^n\right)^2\right] V_{k,m}^{n+1} = \frac{1}{2}\ell A U_{k,m}^n + \left[1 + \frac{1}{2}\ell\left(U_{k,m}^n\right)^2\right] V_{k,m}^n, \tag{66}$$

respectively. Equations (65) and (66) are clearly equivalent to (17) and (23) and it follows from the analysis of section 2.4 that $U_{k,m}^n \to B$ and $V_{k,m}^n \to A/B$ ($k, m = 0, 1, \ldots, N, N+1$) as $n \to \infty$ for any $\ell \in (0, \infty)$ provided $1 - A + B^2 > 0$. The pair $(U, V) = (B, A/B)$ is the unique steady-state of (36) and (39).

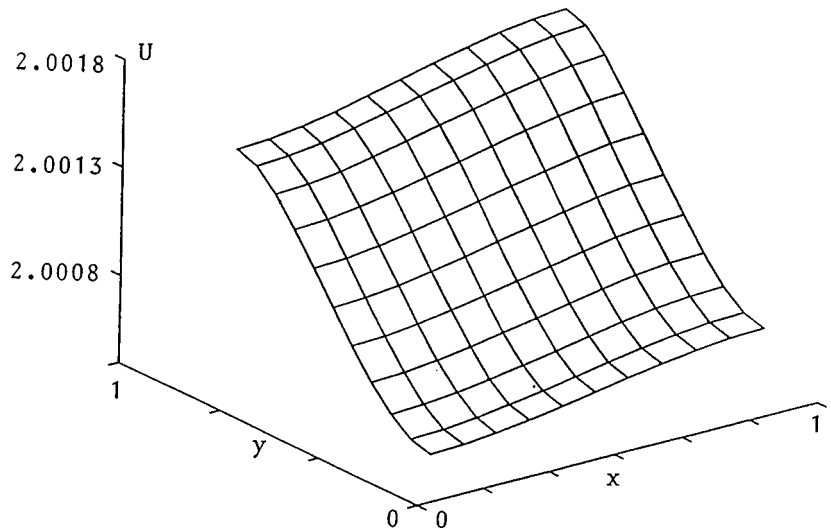

Figure 7. Profile of U at $t = 5$ for $A = 1$, $B = 2$ and $\alpha = 0.002$ with $h = 0.1$ and $\ell = 0.001$.

7. Numerical experiments

Following Adomian [1], the PDEs (3) subject to the boundary conditions (4) and initial conditions (5) with $f(x, y, 0) = 2 + 0.25y$ and $g(x, y, 0) = 1 + 0.8x$ are solved using the second-order methods (36) and (39). The constants A, B and α are given the values 1, 2 and 0.002, respectively. The discretization parameters h and ℓ are given the values $1/10$ and $1/1000$, respectively. The concentration profiles of u and v computed at time $t = 1$ are depicted in figures 7 and 8, respectively. It is clear from figures 7 and 8 that, for these values of h, ℓ and α, the numerical method is stable for this combination of A and B. Figures 9 and 10 depict profiles for U and V at

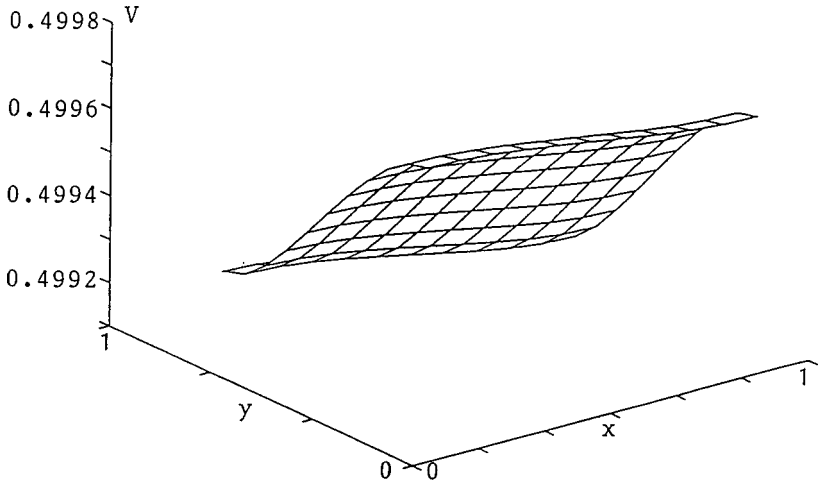

Figure 8. Profile of V at $t = 5$ for $A = 1$, $B = 2$ and $\alpha = 0.002$ with $h = 0.1$ and $\ell = 0.001$.

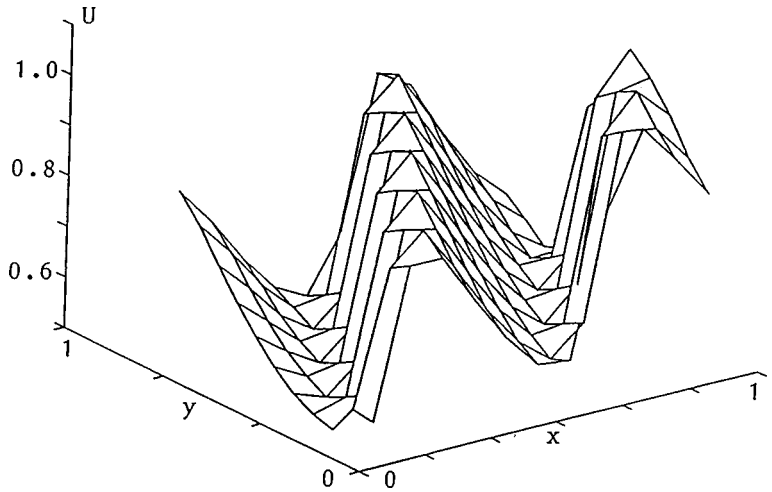

Figure 9. Profile of U at $t = 1$ for $A = 3.4$, $B = 1$ and $\alpha = 0.002$ with $h = 0.1$ and $\ell = 0.001$.

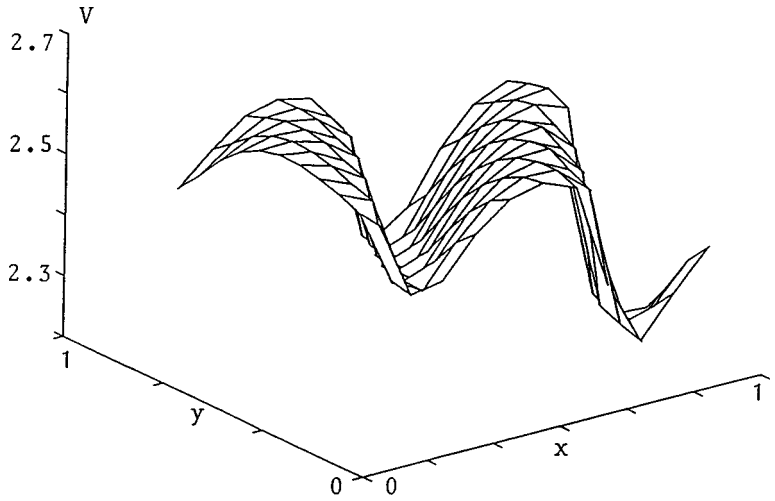

Figure 10. Profile of V at $t = 1$ for $A = 3.4$, $B = 1$ and $\alpha = 0.002$ with $h = 0.1$ and $\ell = 0.001$.

time $t = 1$ for $A = 3.4$ and $B = 1$, using the same values of α, h and ℓ. It is clear from these figures that the solution is unstable. This experiment was repeated with various combinations of A and B within the interval $1 \leqslant A, B \leqslant 5$. The computed results at $t = 5$ reveal that, like in the diffusion-free "Brusselator" system, whenever the parameters A and B are chosen such that $1 - A + B^2 > 0$, the concentration profiles of u and v converge to the fixed point $(u, v) = (B, A/B)$, and for values of A and B such that $1 - A + B^2 < 0$, the numerical method is seen not to converge to any fixed concentration.

8. Conclusion

A second-order numerical method has been developed for the initial-value problems $u_t = A + u^2v - (A + 1)u$ and $v_t = Au - u^2v$ in which $u(0) = U^0$, $v(0) = V^0$ and A and B are real constants. The approach adopted was extended to solve two non-linear two-dimensional reaction–diffusion equations known as the "Brusselator" system. The numerical solution is obtained using two processors running concurrently, each solving a single linear algebraic system by employing a quin-diagonal solver at every time step.

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