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Numerical Methods for a Non-linear System Arising in Chemical Kinetics

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ABSTRAK

Dua kaedah berangka dicadangkan sebagai penyelesaian sistem dua dimensi persamaan peressapan tindak balas bersama ketaklinearan kubus, yang dikenali sebagai sistem "Brusselator". Kaedah pertama diperolehi dengan mengguna teknik pembezaan terhingga dan penyelesaiannya dicapai secara selari menggunakan dua pemprosesan yang dijalankan sejajar. Kaedah kedua berasaskan teknik pembetul-peramal. Sistem persamaan ini mempunyai aplikasi penting dalam kinetik kimia.

ABSTRACT

Two numerical methods are proposed for the solution of a system of two-dimensional reaction-diffusion equations with cubic non-linearity, known as the "Brusselator" system. The first method is derived using finite difference techniques and the solution is obtained in paralled using two processors running concurrently. The second method is based on a predictor-corrector technique. This system of equations has important applications in chemical kinetics.

Keywords: numerical methods, non-linear system and chemical kinetics

INTRODUCTION

In the study of chemical kinetics involving two variable intermediates together with a number of initial and final products such as in the formation of ozone by atomic oxygen via a triple collision, enzymatic reactions, and in plasma and

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laser physics in multiple couplings between modes (Adomian 1995), a two-dimensional reaction diffusion system with cubic non-linearity must be solved.

This non-linear oscillator (Tyson 1973), associated with the chemical system

$$\begin{aligned} B &\rightarrow X, && (a)\\ A + X &\rightarrow Y + D, && (b)\\ 2X + Y &\rightarrow 3X, && (c)\\ X &\rightarrow E, && (d) \end{aligned} \qquad (1)$$

in which B and A are input chemicals, D and E are output chemicals and X and Y are intermediates, was analysed by the so-called Brussels school and is known as the "Brusselator" system. The kinetic equations associated with (A) are given by Prigogine and Lefever (1968)

$$\begin{aligned} \frac{\partial X}{\partial t} &= k_i B + k_2 X^2 Y - k_3 AX - K_4 X + D_x \nabla^2 X \\ \frac{\partial Y}{\partial t} &= k_3 AX - k_2 X^2 Y + D_y \nabla^2 Y \end{aligned} \qquad (2)$$

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 (Tyson 1973). Similarly, the rate constant k_3 of the autocatalytic step (1c) can be made unity by scaling time. Following Tyson (1973), the constant k_4 is given the value unity.

A number of authors have discussed the solution and stability of this system (Adomian 1995; Herschkowitz-Kaufman and Nicolis 1968; Lavenda *et al.* 1971; Lefever and Nicolis 1971; Nicolis 1971; Nicolis and Prigogine 1977; Prigogine and Lefever 1968; Tyson 1973). In particular, Adomian (1995) developed a decomposition method for solving the nonlinear system (2) which may be extended to solve general models with wide classes of non-linearities.

In the present paper, the solution of the "Brusselator" system will be obtained first of all using finite difference approximations leading to a parallel algorithm which may be implemented on two processors, each solving a linear algebraic system as opposed to solving non-linear systems, which is often required for integrating non-linear partial differential equations (PDEs), and then by a predictor-corrector technique.

FINITE DIFFERENCE METHOD

Development

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 reactor length.

Then, the partial differential equations associated with the "Brusselator" system may be transformed (see, for instance, Adomian 1995) to the equivalent system

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

$$\frac{\partial u}{\partial t} = A_u - u^2v + \alpha\left(\frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2}\right); \; 0 < x, y < L, \; t > 0 \qquad (3)$$

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

$$\begin{aligned}
\frac{\partial u(0,y,t)}{\partial x} &= \frac{\partial u(L,y,t)}{\partial x} = 0, \; t \geq 0 \\
\frac{\partial u(x,0,t)}{\partial y} &= \frac{\partial u(x,L,t)}{\partial y} = 0, \; t \geq 0 \\
\frac{\partial v(0,y,t)}{\partial x} &= \frac{\partial v(L,y,t)}{\partial x} = 0, \; t \geq 0 \\
\frac{\partial v(x,0,t)}{\partial y} &= \frac{\partial v(x,L,t)}{\partial y} = 0, \; t \geq 0
\end{aligned} \qquad (4)$$

and initial conditions

$$\begin{aligned}
u(x, y, 0) &= f(x,y), \; (x, y) \varepsilon \Omega \cup \partial\Omega \\
v(x, y, 0) &= g(x,y), \; (x, y) \varepsilon \Omega \cup \partial\Omega
\end{aligned} \qquad (5)$$

In (5), $f(x,y)$ and $g(x,y)$ are given continuous functions of x and y (representing the initial concentrations of P_1 and P_2 respectively).

Both intervals $0 \leq x \leq L$ and $0 \leq y \leq L$ 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 $u(x,y,t)$ and $v(x,y,t)$ of (3) are sought at each point $(kh, jh, n\ell)$ in Ω x [t > 0], where k, j = 0,1,2,...,N, N +1 and n=0,1,2,.... The notation $U^n_{k,j}$ and $V^n_{k,j}$ will be used to distinguish the solutions of the numerical methods from the theoretical solutions $u(x_k,y_j,t_n)$ and $v(x_k,y_j,t_n)$. The solution vectors $\mathbf{U}^n$ and $\mathbf{V}^n$ will be ordered in the form with T denoting transpose.

$$\begin{aligned}
\boldsymbol{U}^n = \Big(&U^n_{0,0}, U^n_{1,0}, \ldots, U^n_{N,0}, U^n_{N+1,0}; U^n_{0,1}, U^n_{1,1}, U^n_{2,1}, \ldots, U^n_{N,1}, U^n_{N+1,1}; \\
&U^n_{0,2}, U^n_{1,2}, U^n_{2,2}, \ldots, U^n_{N,2}; U^n_{N+1,2}; \ldots; U^n_{0,N+1}, U^n_{1,N+1}, \ldots, U^n_{2,N+1}, \ldots, U^n_{N+1,N+1}\Big)^T \\
\boldsymbol{V}^n = \Big(&V^n_{0,0}, V^n_{1,0}, \ldots, V^n_{N,0}, V^n_{N+1,0}; V^n_{0,1}, V^n_{1,1}, V^n_{2,1}, \ldots, V^n_{N,1}, V^n_{N+1,1}; \\
&V^n_{0,2}, V^n_{1,2}, V^n_{2,2} \ldots, V^n_{N,2}; v^n_{N+1,2}; \ldots; V^n_{0,N+1}, V^n_{1,N+1}, V^n_{2,N+1}, \ldots, V^n_{N+1,N+1}\Big)^T
\end{aligned} \qquad (6)$$

with T denoting transponse. The numerical methods to be developed in this paper are based on approximating the time derivatives in (3) by their first-order forward-difference replacements

$$\frac{\partial u(x,y,t)}{\partial t} = \frac{u(x,y,t+\ell) - u(x,y,t)}{\ell} + O(\ell)$$
$$\frac{\partial v(x,y,t)}{\partial t} = \frac{v(x,y,t+\ell) - v(x,y,t)}{\ell} + O(\ell) \qquad (7)$$

as $\ell \to 0$, and the space derivatives by their second-order central difference approximants

$$\frac{\partial^2 u(x,y,t)}{\partial x^2} = h^{-2}\left[u(x-h,y,t) - 2u(x,y,t) + u(x+h,y,t)\right] + O(h^2),$$
$$\frac{\partial^2 v(x,y,t)}{\partial x^2} = h^{-2}\left[v(x-h,y,t) - 2v(x,y,t) + v(x+h,y,t)\right] + O(h^2),$$
$$\frac{\partial^2 u(x,y,t)}{\partial y^2} = h^{-2}\left[u(x-h,y,t) - 2u(x,y,t) + u(x+h,y,t)\right] + O(h^2), \qquad (8)$$
$$\frac{\partial^2 v(x,y,t)}{\partial y^2} = h^{-2}\left[v(x-h,y,t) - 2v(x,y,t) + v(x+h,y,t)\right] + O(h^2),$$

as $\ell \to 0$. The cubic reaction terms u^2v and $-u^2v$ in (3) will be approximated by $U^n_{k,j} V^n_{k,j} U^{n+1}_{k,j}$ and $-\left(U^n_{k,j}\right)^2 V^{n+1}_{k,j}$, respectively, and the linear terms $-(A+1)u$ and Au by $-(A+1)U^{n+1}_{k,j}$ and $AU^n_{k,j}$ respectively. Using these replacements together with the approximations (7) and (8) in (3) leads to the fully-implicit $O(h^2 + \ell)$ schemes

$$-paU^{n+1}_{k-1,j} - paU^{n+1}_{k,j-1} + \left[1 + 4pa - \ell U^n_{k,j} V^n_{k,j} + \ell(A+1)\right]U^{n+1}_{k,j} - paU^{n+1}_{k+1,j}$$
$$- paU^{n+1}_{k,j+1} = U^n_{k,j} + \ell B \qquad (9)$$

and

$$-p\alpha V^{n+1}_{k-1,j} - p\alpha U^{n+1}_{k,j-1} + \left[1 + 4p\alpha + \ell(U^n_{k,j})^2\right]V^{n+1}_{k,j} - p\alpha V^{n+1}_{k+1,j} - p\alpha U^{n+1}_{k,j+1}$$
$$= V^n_{k,j} + \ell A U^n_{k,j} \qquad (10)$$

for k, j = 1,2,...., N and n=0,1,..., where $p = \frac{\ell}{h^2}$. In the cases k, j = 0 and equations (9) and (10) introduce 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,

$$U^n_{k,-1} = U^n_{k,1},\ U^n_{k,N+2} = U^N_{k,N};\ k = 0,1,\ldots,N+1$$
$$U^n_{-1,j} = U^n_{1,j},\ U^n_{N+2,j} = U^N_{N,j};\ j = 0,1,\ldots,N+1$$
$$V^n_{k,-1} = V^n_{k,1},\ V^n_{k,N+2} = V^N_{k,N};\ k = 0,1,\ldots,N+1 \qquad (11)$$
$$V^n_{-1,j} = V^n_{1,j},\ V^n_{N+2,j} = V^N_{N,j};\ j = 0,1,\ldots,N+1$$

for all n=0,1,2,... The relations in (11) will be used in the implementation of the numerical methods (9) and (10) which will be discussed in Section 2.2.It is easy to show that the principal part of the local truncation error of the implicit schemes (9) and (10) are

$$L_u(u,v;h,\ell)=\left[\frac{1}{2}\frac{\partial^2 u}{\partial t^2}+(A+1-uv)\frac{\partial u}{\partial t}-\alpha\left(\frac{\partial^3 u}{\partial x^2\partial t}+\frac{\partial^3 u}{\partial y^2\partial t}\right)\right]\ell-\frac{\alpha h^2}{12}\left(\frac{\partial^4 u}{\partial x^4}+\frac{\partial^4 u}{\partial y^4}\right) \quad (12)$$

and

$$L_u(u,v;h,\ell)=\left[\frac{1}{2}\frac{\partial^2 u}{\partial t^2}+u^2\frac{\partial u}{\partial t}-\alpha\left(\frac{\partial^3 u}{\partial x^2\partial t}+\frac{\partial^3 u}{\partial y^2\partial t}\right)\right]\ell-\frac{\alpha h^2}{12}\left(\frac{\partial^4 u}{\partial x^4}+\frac{\partial^4 u}{\partial y^4}\right) \quad (13)$$

respectively, in which $x = x_k$, $y=y_j$ and $t=t_n$.

A linearized von-Neumann analysis shows that the necessary conditions for the numerical schemes (9) and (10) to be stable at the point (x_k,y_j, t_n) are

$$p \geq \frac{\ell\,(UV-A-1)}{8\alpha} \quad (14)$$

dan

$$p \geq \frac{\ell\,(A-1)}{8\alpha} \quad (15)$$

respectively. Equations (14) and (15) are trivial restrictions for small values of h and ℓ. A similar restriction was reported by Fakhr and Twizell(1997) for a chemical system model with pure cubic autocatalysis in one space dimension.

Algorithm

Applying (9) and (10) to all the $(N+2)^2$ mesh points of the square Ω, and its boundary $\partial\Omega$, at time level $t=t_n=n\ell$ and using the boundary conditions (4) (in which each first-order derivative is approximated by its second-order central difference approximant as in (11))leads to the linear algebraic systems of the form

$$E_1\,\mathbf{U}(t+\ell)=\mathbf{Q}_1,\ t=0,\ell,2\ell,\ \ldots$$
$$E_2\,\mathbf{V}(t+\ell)=\mathbf{Q}_2,\ t=0,\ell,2\ell,\ \ldots \quad (16)$$

where the block quin-diagonal matrices E_1 and E_2 are each of order $(N+2)^2$. The matrix E_1 is given by

$$E_1=h^{-2}\begin{bmatrix} E_1^* & 2cI & & & & \mathbf{0} \\ cI & E_1^* & cI & & & \\ & cI & E_1^* & cI & & \\ & & \ddots & \ddots & \ddots & \\ & & & cI & E_1^* & cI \\ \mathbf{0} & & & & 2cI & E_1^* \end{bmatrix} \quad (17)$$

in which E_1^* is a tridiagonal matrix of order N+2 given by

$$E_i^* = \begin{bmatrix} e & 2c & & & \mathbf{0} \\ c & e & c & & \\ & \ddots & \ddots & \ddots & \\ & & c & e & c \\ \mathbf{0} & & & 2c & e \end{bmatrix} \tag{18}$$

with c = -pα, *e=1 - 4c -* $\ell U_{k,j}^n V_{k,j}^n + \ell(A+1)$ for *k, j=0,1,2,...,N+1; n = 0*,1,.... The vectors $\mathbf{Q}_1$ and $\mathbf{Q}_2$ in (16) are obtained from (9) and (10) and *I* is the identity matrix of order *N+2*. The matrix E_2 takes the form of E_1 with *e* replaced by *1-4C +* $\ell(U_{k,j}^n)^2$. The solution vectors $\mathbf{U}(t+\ell)$ and $\mathbf{V}(t+\ell)$ in (16) may now be obtained using a parallel architecture involving two processors operating concurrently with each processor employing a quin-diagonal solver to solve a linear algebraic system at every time-step as follows

$$\begin{aligned} &\text{Processor 1 : } E_1\ \mathbf{U}(t+\ell) = \mathbf{Q}_1 \\ &\text{Processor 2 : } E_2\ \mathbf{V}(t+\ell) = \mathbf{Q}_2 \end{aligned} \tag{19}$$

The decomposition of the coefficient matrices E_1 and E_2 into upper and lower triangular forms are carried out by Processors 1 and 2 respectively and the solution vectors $U(t+\ell)$ and $V(t+\ell)$ are determined by forward and backward substitutions at every time level. It is worth mentioning that in the computational implementation of algorithm (19), only the five nonzero diagonals are stored and used in computing the solution vectors at every time step thus minimizing computer storage and CPU time.

Predictor-corrector Method

A predictor-corrector algorithm for the determination of the fully discrete solutions $\mathbf{U}^{n+1}$ and $\mathbf{V}^{n+1}$ is given below.

Predicting u and v

Let $\hat{U}_{k,j}^{n+1}$ and $\hat{V}_{k,j}^{n+1}$ denote the predicted approximations to $u(kh, jh,(n+1)\ell)$ and $v(kh, jh,(n+1)\ell)$ respectively. Then it follows from (3), (7), and (8) $\hat{U}_{k,j}^{n+1}$ and $\hat{V}_{k,j}^{n+1}$ may be obtained explicitly using the formulae

$$\hat{U}_{k,j}^{n+1} = U_{k,j}^n + \ell\left[B + \left(U_{k,j}^n\right)^2 V_{k,j}^n - (A+1)U_{k,j}^n + \frac{\alpha}{h^2}\right.$$
$$\left.\left\{U_{k-1,j}^n - 2U_{k,j}^n + U_{k+1,j}^n + U_{k,j-1}^n - 2U_{k,j}^n + U_{k,j+1}^n\right\}\right]$$

$$\hat{V}_{k,j}^{n+1} = V_{k,j}^{n} + \ell \left[AU_{k,j}^{n} - \left(U_{k,j}^{n}\right)^2 V_{k,j}^{n} + \frac{\alpha}{h^2} \right.$$
$$\left. \left\{ V_{k-1,j}^{n} - 2V_{k,j}^{n} + V_{k+1,j}^{n} + V_{k,j-1}^{n} - 2V_{k,j}^{n} + V_{k,j+1}^{n} \right\} \right] \qquad (20)\}$$

Correcting u and v

Once $\hat{U}_{k,j}^{n+1}$ and $\hat{V}_{k,j}^{n+1}$ have been determined, the solutions $U_{k,j}^{n+1}$ and $V_{k,j}^{n+1}$ may be obtained *via* the equivalent corrector formulation

$$U_{k,j}^{n+1} = U_{k,j}^{n} + \ell \left[B + \left(\hat{U}_{k,j}^{n}\right)^2 \hat{V}_{k,j}^{n+1} - (A+1)\hat{U}_{k,j}^{n+1} + \frac{\alpha}{h^2} \right.$$
$$\left. \left\{ \hat{U}_{k-1,j}^{n+1} - 2\hat{U}_{k,j}^{n+1} + \hat{U}_{k+1,j}^{n+1} + \hat{U}_{k,j-1}^{n+1} - 2\hat{U}_{k,j}^{n+1} + \hat{U}_{k,j+1}^{n+1} \right\} \right]$$
$$V_{k,j}^{n+1} = V_{k,j}^{n} + \ell \left[A\hat{U}_{k,j}^{n+1} - \left(\hat{U}_{k,j}^{n+1}\right)^2 \hat{V}_{k,j}^{n+1} + \frac{\alpha}{h^2} \right. \qquad (21)$$
$$\left. \left\{ \hat{V}_{k-1,j}^{n+1} - 2\hat{V}_{k,j}^{n+1} + \hat{V}_{k+1,j}^{n+1} + \hat{V}_{k,j-1}^{n+1} - 2\hat{V}_{k,j}^{n+1} + \hat{V}_{k,j+1}^{n+1} \right\} \right]$$

This predictor-corrector combination {(20), (21)} is $O(h^2+\ell)$as $h, \ell \rightarrow 0$ and correcting to convergence gives unconditional stability.

COMPARISONS BETWEEN METHODS

It has already been noted that both methods are $O(h^2+\ell)$as $h, \ell \rightarrow 0$ so that neither is superior to the other with respect to accuracy.

The parallel algorithm developed above is subject to a trivial stability requirement given by (14) and (15). The predictor-corrector method, on the other hand, has a more restricting stability condition if used in *PECE* mode and requires correcting to convergence for unconditional stability (Twizell and Khaliq 1981).

The parallel algorithm requires the application of quin-diagonal solvers (with minimum storage) to solve two linear algebraic systems at every time step, whereas the predictor-corrector technique may be applied explicitly using (20) and (21). The predictor-corrector method is therefore faster particularly if used in *PECE* mode.

Numerical Experiments

Following Adomian(1995), the PDE's (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 parallel algorithm (19) and the predictor-corrector combination {(20), (21)}. The constants A, B, and a are given the values 2.4, 1, and 0.002 respectively. The discretization parameters h and ℓ are given the values $\frac{1}{10}$ and $\frac{1}{1000}$ respectively. The concentration profiles of u and v at t=5 computed using the two algorithms are depicted in *Figures 1-4.* It is clear from the figures that,

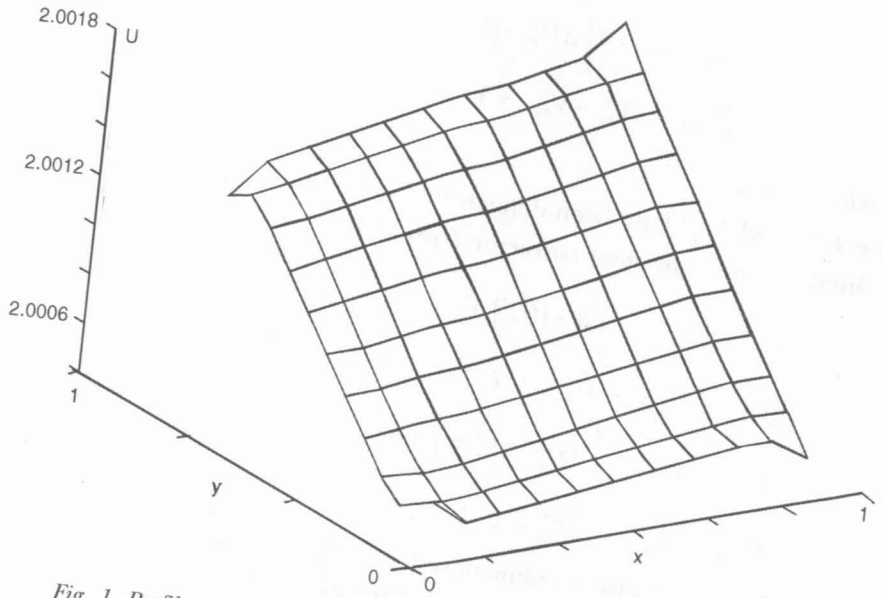

Fig. 1. Profile of U at $t = 5$ for $A = 1$, $B = 2$ and $\alpha = 0.002$ using the finite-difference method with $h = 0.1$ and $\ell = 0.001$

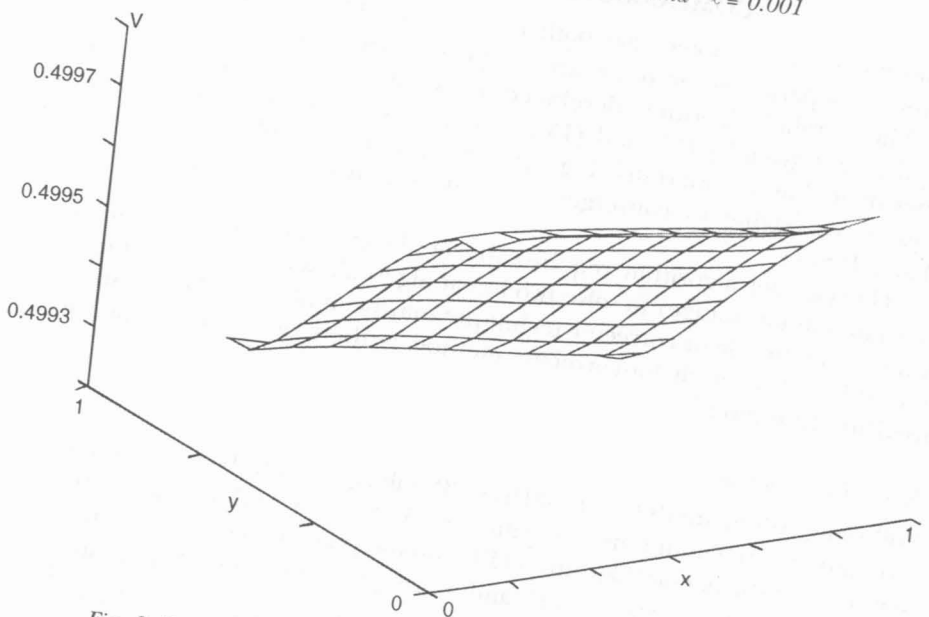

Fig. 2. Profile of V at $t = 5$ for $A = 1$, $B = 2$ and $\alpha = 0.002$ using the finite-difference method with $h = 0.1$ and $\ell = 0.001$

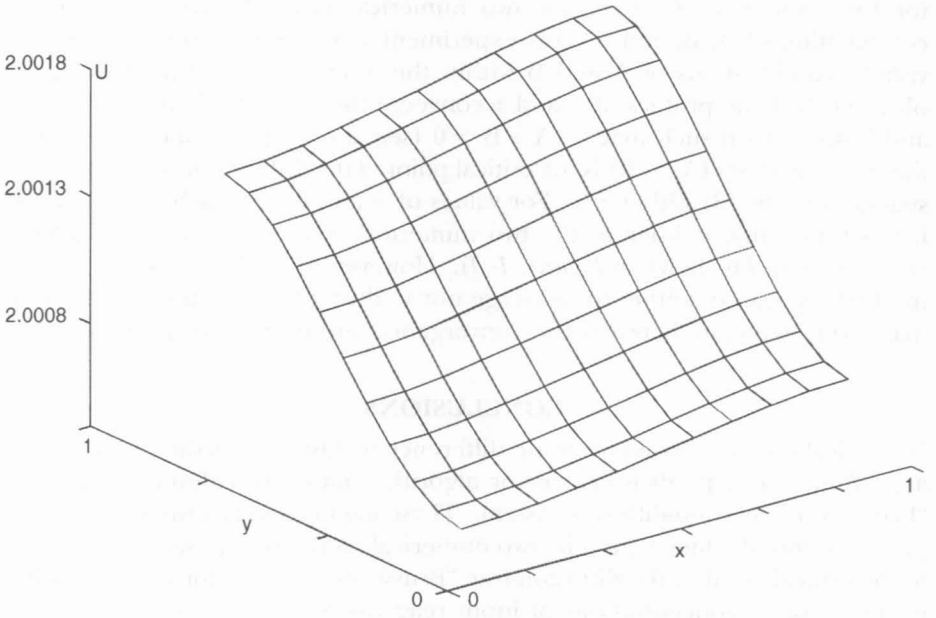

Fig. 3. Profile of U at t = 5 for A = 1, B = 2 and α = 0.002 using the predictor-corrector method with h = 0.1 and ℓ = 0.001

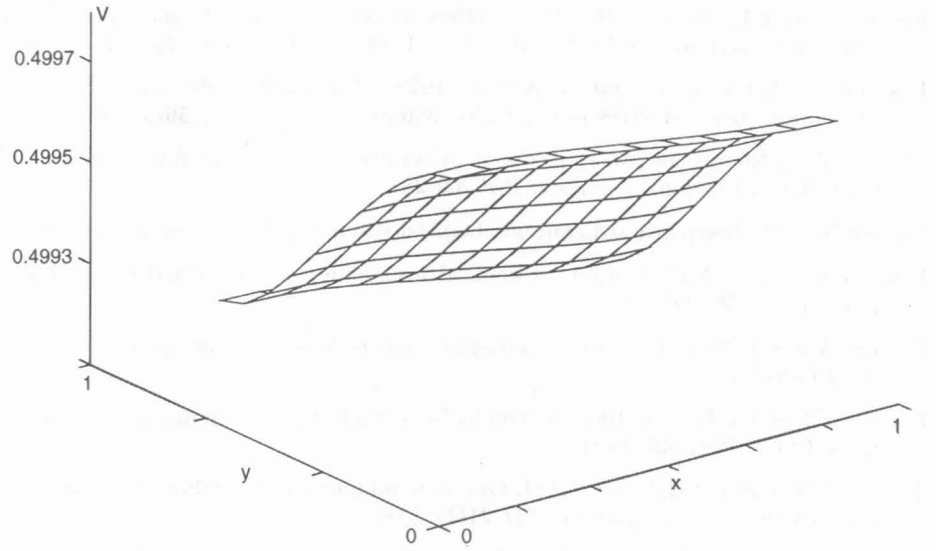

Fig. 4. Profile of V at t = 5 for A = 1, B = 2 and α = 0.002 using the predictor-corrector method with h = 0.1 and ℓ = 0.001

for these values of h and ℓ, the two numerical methods are stable for this combination of A, B, and a. This experiment was repeated to time t=10 with various combinations of A and B within the interval 1<A, B< 5 where it was observed that the profiles of u and v converge to(u,v)= (B , A/B) whenever A and B are chosen such that $1 - A + B^2 > 0$ (see also [10]). It should be noted that the pair (u,v)=(A, A/B) is the critical point of the diffusion-free "Brusselator" system given by (3) with a = 0. For values of A and B for which $1 - A + B^2 < 0$, it was found that neither of the two numerical methods converge to a fixed concentration (as shown in *Figures. 1- 4*). However, when $1 - A + B^2 = 0$, the two methods appeared neither to converge nor to diverge. This is because this case marks the boundary between the convergence and divergence criteria.

CONCLUSIONS

Numerical methods based on finite difference techniques, leading to a parallel algorithm, and a predictor-corrector algorithm have been developed for the "Brusselator" reaction-diffusion system. These methods were tested on a model problem from the literature. The two numerical methods were seen to converge to the critical point of the diffusion-free "Brusselator" system for certain choices of the constant concentrations of input reagents A and B.

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