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Numerical solutions for a coupled non-linear oscillator

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A second-order accurate numerical method has been proposed for the solution of a coupled non-linear oscillator featuring in chemical kinetics. Although implicit by construction, the method enables the solution of the model initial-value problem (IVP) to be computed explicitly. The second-order method is constructed by taking a linear combination of first-order methods. The stability analysis of the system suggests the existence of a Hopf bifurcation, which is confirmed by the numerical method. Both the critical point of the continuous system and the fixed point of the numerical method will be seen to have the same stability properties. The second-order method is more competitive in terms of numerical stability than some well-known standard methods (such as the Runge–Kutta methods of order two and four).

KEY WORDS: numerical method, stability, Hopf bifurcation, coupled oscillator

1. Introduction

A number of authors have reported on the importance of oscillations in chemical systems. For instance, the so-called Brussels school (see [1,2]) developed and analysed the behaviour of a non-linear oscillator (known as the "Brusselator") associated with the chemical system [3]

$$\mathrm{A} \to \mathrm{X}, \tag{1a}$$

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

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

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

in which A and B are input chemicals, D and E are output chemicals and X and Y are intermediates.

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It is known [4] that the trimolecular reaction step (1c) arises in the formation of ozone by atomic oxygen via a triple collision, enzymatic reactions, and in plasma and laser physics in multiple couplings between modes.

Much attention has been devoted in the literature on the ability of non-linear oscillators to synchronize to external influences. In order to carry out a detailed analysis of the interaction of two centres of oscillators in a chemical network, Tyson [3] considers two Brusselators coupled in series in which two outputs of the first provide the two inputs of the second given by

$$\mathrm{A} \to \mathrm{X}, \tag{2a}$$
$$\mathrm{B} + \mathrm{X} \to \mathrm{Y} + \mathrm{U}, \tag{2b}$$
$$2\mathrm{X} + \mathrm{Y} \to 3\mathrm{X}, \tag{2c}$$
$$\mathrm{X} \to \mathrm{E}, \tag{2d}$$
$$\mathrm{E} + \mathrm{U} \to \mathrm{V} + \mathrm{F}, \tag{2e}$$
$$2\mathrm{U} + \mathrm{V} \to 3\mathrm{U}, \tag{2f}$$
$$\mathrm{U} \to \mathrm{G}. \tag{2g}$$

Employing easy-to-use explicit finite-difference methods such as the Runge–Kutta (RK) and Euler methods to discretize non-linear initial-value problems, like the one considered in this paper, is known to lead to contrived chaos and oscillations whenever the discretization parameters exceed certain values (see [5]).

Although such contrived chaos can often be avoided by using small time-steps, the extra computing costs incurred when examining the long-term behaviour of a dynamical system may be substantial. It is therefore essential to use a numerical method which allows the largest possible time steps that are consistent with stability and accuracy. In order to circumvent contrived chaos, whilst retaining accuracy and numerical stability, it may be necessary to forego the ease-of-implementation of inexpensive explicit numerical methods in favour of implicit methods (which are known to be more competitive in terms of numerical stability).

In this paper, a second-order, implicit, finite-difference scheme will be developed and used for the solution of the dynamical system associated with the aforementioned coupled ODE system. Although the method is implicit by construction, the numerical results can be computed explicitly. This method will be seen to have better stability property than the second-and fourth-order Runge–Kutta (RK2 and RK4) methods. Runge–Kutta methods are standard (see, for instance, [5]), so will not be presented here.

A stability and bifurcation of the dynamical system is carried out in section 2. In section 3, a new second-order, implicit, finite-difference method is constructed for the coupled IVP, and its fixed point analysed in section 4. Numerical results are reported in section 5.

2. Stability and bifurcation analyses

2.1. Analysis of critical point of the system

Consider the kinetic equations associated with (2) given by [6]

$$
\begin{aligned}
\frac{\mathrm{d}x}{\mathrm{d}t} &\equiv f_1(x, y) = A - Bx + x^2y - x, && t > 0, \quad x(0) = X^0,\\
\frac{\mathrm{d}y}{\mathrm{d}t} &\equiv f_2(x, y) = Bx - x^2y, && t > 0, \quad y(0) = Y^0,\\
\frac{\mathrm{d}e}{\mathrm{d}t} &\equiv f_3(x, e, u) = x - eu, && t > 0, \quad e(0) = E^0,\\
\frac{\mathrm{d}u}{\mathrm{d}t} &\equiv f_4(x, e, u, v) = Bx - eu + u^2v - u, && t > 0, \quad u(0) = U^0,\\
\frac{\mathrm{d}v}{\mathrm{d}t} &\equiv f_5(e, u, v) = eu - u^2v, && t > 0, \quad v(0) = V^0,
\end{aligned}
\tag{3}
$$

in which $x = x(t)$, $y = y(t)$, $e = e(t)$, $u = u(t)$, $v = v(t)$ and A and B are real constants. It can be shown that the only critical point of the ordinary differential equation (ODE) system is $(x^*, y^*, e^*, u^*, v^*) = (A, B/A, 1/B, AB, 1/(AB^2))$. The Jacobian, J^*, at the critical point $(x^*, y^*, e^*, u^*, v^*)$ is given by

$$
J^* = \begin{bmatrix}
B-1 & A^2 & 0 & 0 & 0\\
-B & -A^2 & 0 & 0 & 0\\
1 & 0 & -AB & -\frac{1}{B} & 0\\
B & 0 & -AB & \frac{1}{B} - 1 & A^2B^2\\
0 & 0 & AB & -\frac{1}{B} & -A^2B^2
\end{bmatrix}. \tag{4}
$$

It is easy to verify that its eigenvalues satisfy the fifth-degree stability equation (characteristic equation)

$$
\left[\lambda^2 + \left(A^2 - B + 1\right)\lambda + A^2\right]\left[\lambda^3 + \left(A^2B^2 + AB + 1 - \frac{1}{B}\right)\lambda^2 + \left(A^3B^3 + A^2B^2 + AB - 2A\right)\lambda + A^3B^3\right] = 0. \tag{5}
$$

The quadratic part in (5) is what will be obtained if only the normal isolated Brusselator (first Brusselator) is considered. This is, of course, due to the absence of "back-coupling" in this system.

Using the Routh–Hurwitz criteria (see Lambert [5]), it may be shown that the roots of the cubic part of (5) (the second Brusselator) have negative real parts and the critical point is stable whenever the following inequalities are satisfied:

$$\begin{aligned} g_1(A,B) &= A^2 - B + 1 > 0, \\ g_2(A,B) &= A^2B^3 + AB^2 + B - 1 > 0, \\ g_3(A,B) &= A^4B^6 + 2A^3B^5 + 2A^2B^4 - 3A^2B^3 \\ &\quad + 2AB^3 - 3AB^2 + B^2 - 3B + 2 > 0. \end{aligned} \tag{6}$$

The first Brusselator may either be stationary or oscillate depending on whether $A^2 - B + 1 > 0$ or otherwise.

2.2. Hopf bifurcation

Returning back to the stability equations (5) and (6), it can be shown that when $B = A^2 + 1$, the quadratic part of (5) given by $\lambda^2 + (A^2 - B + 1)\lambda + A^2 = 0$ has a pair of purely imaginary zeros, namely, $\lambda = \pm \mathrm{i}A$. Suppose that B is a Hopf bifurcation parameter, and let $\lambda = \lambda(B)$ be the smooth curve of roots of $\lambda^2 + (A^2 - B + 1)\lambda + A^2 = 0$ with $\lambda(A^2 + 1) = \mathrm{i}A$. Then,

$$\left.\frac{\partial \lambda(B)}{\partial B}\right|_{B=A^2+1} = \left.\frac{\lambda(B)}{2\lambda(B) + (A^2 - B + 1)}\right|_{B=A^2+1}, \tag{7}$$

from which it follows that

$$\mathrm{Re}\left.\frac{\partial \lambda(B)}{\partial B}\right|_{B=A^2+1} = \frac{1}{2} \neq 0.$$

This fact, together with the standard Hopf bifurcation theorem (see, for instance, [6,7]), confirms that the ODE system (3) has a Hopf bifurcation from $(x^*, y^*, e^*, u^*, v^*)$ near $B = A^2 + 1$.

It should be noted that such a Hopf bifurcation is associated with the occurrence of a pair of purely imaginary zeros of the quadratic part of (6) which is exactly what would have been obtained if only the first Brusselator is considered, and hence, a Hopf bifurcation takes place near (x^*, y^*) for the decoupled system

$$\begin{aligned} \frac{\mathrm{d}x}{\mathrm{d}t} &= A - Bx + x^2y - x, \\ \frac{\mathrm{d}y}{\mathrm{d}t} &= Bx - x^2y, \end{aligned} \tag{8}$$

when B is near $A^2 + 1$. To ensure the bifurcating periodic oscillation of the first Brusselator induces non-linear oscillation of the second Brusselator, assume condition (6) as stated and compute the eigenvector of $J^* - \mathrm{i}AI_5$ by solving

$$\left(J^* - \mathrm{i}AI_5\right)\begin{pmatrix} X \\ Y \\ E \\ U \\ V \end{pmatrix} = 0, \tag{9}$$

where I_5 is the identity matrix of order five. It can then be shown that an eigenvector of $J^* - \mathrm{i}AI_5$ is given by $(X, Y, E, U, V)^{\mathrm{T}}$, with

$$X = 1,$$
$$Y = \mathrm{i}\frac{1}{A} + 1,$$
$$\begin{pmatrix} E \\ U \\ V \end{pmatrix} = -\begin{bmatrix} -AB - \mathrm{i}A & -\frac{1}{B} & 0 \\ -AB & \frac{1}{B} - 1 - \mathrm{i}A & A^2B^2 \\ AB & -\frac{1}{B} & -A^2B^2 - \mathrm{i}A \end{bmatrix}^{-1} \begin{pmatrix} 1 & 0 \\ B & 0 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} 1 \\ \frac{\mathrm{i}}{A} + 1 \end{pmatrix}. \quad (10)$$

As the $(E, U, V)^{\mathrm{T}}$ component in (10) is not zero, it can be concluded that the bifurcating periodic solution of system (3) near the fixed point $(x^*, y^*, e^*, u^*, v^*)$ does have a non-constant $(E, U, V)^{\mathrm{T}}$ component, so the second Brusselator is indeed oscillatory.

The bifurcation direction and stability of bifurcating periodic solution can be determined using the standard algorithm given, for instance, by Hassard et al. [7, pp. 86–90]. The numerical results to be reported in section 5 confirm the existence of a stable limit cycle as suggested (predicted) by the Hopf bifurcation theory together with the bifurcation direction (see table 2).

3. Numerical methods for two Brusselators coupled in series

3.1. Numerical methods for x

Starting with the initial-value problem [given in (3)]

$$x' \equiv \frac{\mathrm{d}x}{\mathrm{d}t} = A - Bx + x^2y - x, \quad t > 0, \quad x(0) = X^0, \tag{11}$$

the development of numerical methods may be based on approximating the time derivative in (11) by its first-order forward-difference approximant given by

$$\frac{\mathrm{d}x}{\mathrm{d}t} = \frac{x(t+\ell) - x(t)}{\ell} + \mathrm{O}(\ell) \quad \text{as } \ell \to 0, \tag{12}$$

where $\ell > 0$ is an increment in t (the time step). Discretizing the interval $t \geqslant 0$ at the points $t_n = n\ell$ $(n = 0, 1, 2, \ldots)$, the solution of (11) at the grid point t_n is $x(t_n)$. The solution obtained by a numerical method at the point t_n will be denoted by X^n. Four first-order numerical methods for solving (11) based on approximating the time derivative in (11) by (12) and making appropriate approximations for the linear and cubic terms in (11) are given below:

$$\begin{aligned}
M_x^{(1)}:&\quad X^{n+1} = X^n + \ell A - \ell B X^n + \ell\big(X^n\big)^2 Y^{n+1} - \ell X^n,\\
M_x^{(2)}:&\quad X^{n+1} = X^n + \ell A - \ell B X^n + \ell X^n Y^n X^{n+1} - \ell X^n,\\
M_x^{(3)}:&\quad X^{n+1} = X^n + \ell A - \ell B X^{n+1} + \ell\big(X^n\big)^2 Y^n - \ell X^{n+1},\\
M_x^{(4)}:&\quad X^{n+1} = X^n + \ell A - \ell B X^n + \ell\big(X^n\big)^2 Y^n - \ell X^n.
\end{aligned} \tag{13}$$

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

$$\begin{aligned}
L_x^{(1)} &= L_x^{(1)}\big[x(t), y(t), \ell\big]\\
&= x(t+\ell) - x(t) - \ell A + \ell B x(t) - \ell\big\{x(t)\big\}^2 y(t+\ell) + \ell x(t),\\
L_x^{(2)} &= L_x^{(2)}\big[x(t), y(t), \ell\big]\\
&= x(t+\ell) - x(t) - \ell A + \ell B x(t) - \ell x(t) y(t) x(t+\ell) + \ell x(t),\\
L_x^{(3)} &= L_x^{(3)}\big[x(t), y(t), \ell\big]\\
&= x(t+\ell) - x(t) - \ell A + \ell B x(t+\ell) - \ell\big\{x(t)\big\}^2 y(t) + \ell x(t+\ell),\\
L_x^{(4)} &= L_x^{(4)}\big[x(t), y(t), \ell\big]\\
&= x(t+\ell) - x(t) - \ell A + \ell B x(t) - \ell\big\{x(t)\big\}^2 y(t) + \ell x(t),
\end{aligned} \tag{14}$$

in which $t = t_n$. It is easy to show that the Taylor series expansion of the functions in (14) about t leads to

$$\begin{aligned}
L_x^{(1)} &= \left(\frac{x''}{2} - x^2 y'\right)\ell^2 + \mathrm{O}\big(\ell^3\big) &&\text{as } \ell \to 0,\\
L_x^{(2)} &= \left(\frac{x''}{2} - xyx'\right)\ell^2 + \mathrm{O}\big(\ell^3\big) &&\text{as } \ell \to 0,\\
L_x^{(3)} &= \left(\frac{1}{2}x'' + Bx' + x'\right)\ell^2 + \mathrm{O}\big(\ell^3\big) &&\text{as } \ell \to 0,\\
L_x^{(4)} &= \frac{1}{2}x''\ell^2 + \mathrm{O}\big(\ell^3\big) &&\text{as } \ell \to 0,
\end{aligned} \tag{15}$$

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

Defining, now, a function $L_x^{(\mathrm{err})}$ by the linear combination

$$L_x^{(\mathrm{err})} = \big[L_x^{(1)} + 2L_x^{(2)} + L_x^{(3)} - 2L_x^{(4)}\big] \tag{16}$$

gives

$$L_x^{(\mathrm{err})} = \big[x'' - 2xx'y - x^2y' + Bx' + x'\big]\ell^2 + \mathrm{O}\big(\ell^3\big) \quad \text{as } \ell \to 0. \tag{17}$$

Differentiating the differential equation in (11) with respect to t reveals that the coefficient of ℓ^2 in (17) vanishes; thus,

$$L_x^{(\mathrm{err})} = \mathrm{O}\big(\ell^3\big) \tag{18}$$

as $\ell \to 0$. This implies that a second-order method for computing x can be constructed by taking the linear combination $M_x^{(1)} + 2M_x^{(2)} + M_x^{(3)} - 2M_x^{(4)}$ and is given by

$$X^{n+1} = \frac{2\ell A + X^n(2 - \ell - \ell B - \ell X^n Y^n) + \ell (X^n)^2 Y^{n+1}}{2 + \ell(1 + B - X^n Y^n)}. \tag{19}$$

This method involves X^{n+1} and Y^{n+1}, thus, X^{n+1} cannot be calculated explicitly from (19).

3.2. *Numerical methods for y*

Recalling the ODE [given in (3)]

$$\frac{\mathrm{d}y}{\mathrm{d}t} \equiv y' = Bx - x^2 y, \tag{20}$$

a second-order method for solving (20) may be obtained by approximating its derivative with (12) and evaluating the linear and cubic forcing terms in ways which lead to the following numerical methods for finding y:

$$\begin{aligned} M_y^{(1)}&: \quad Y^{n+1} = Y^n + \ell B X^n - \ell \left(X^n\right)^2 Y^n, \\ M_y^{(2)}&: \quad Y^{n+1} = Y^n + \ell B X^{n+1} - \ell \left(X^n\right)^2 Y^{n+1}, \\ M_y^{(3)}&: \quad Y^{n+1} = Y^n + \ell B X^n - \ell Y^n X^n X^{n+1}. \end{aligned} \tag{21}$$

The principal parts of the local truncation errors associated with (21) are given by, respectively,

$$\begin{aligned} L_y^{(1)} &= \frac{1}{2} y'' \ell^2 + \mathrm{O}\left(\ell^3\right) && \text{as } \ell \to 0, \\ L_y^{(2)} &= \left(\frac{1}{2} y'' - Bx' + x^2 y'\right) \ell^2 + \mathrm{O}\left(\ell^3\right) && \text{as } \ell \to 0, \\ L_y^{(3)} &= \left(\frac{1}{2} y'' + yxx'\right) \ell^2 + \mathrm{O}\left(\ell^3\right) && \text{as } \ell \to 0. \end{aligned} \tag{22}$$

Defining, as in (16), the function

$$L_y^{(\mathrm{err})} = \left[2L_y^{(3)} + L_y^{(2)} - L_y^{(1)}\right], \tag{23}$$

gives

$$L_y^{(\mathrm{err})} = \left(y'' - Bx' + 2xx'y + x^2 y'\right)\ell^2 + \mathrm{O}\left(\ell^3\right) \quad \text{as } \ell \to 0. \tag{24}$$

Differentiating (20) with respect to t reveals that $L_y^{(\mathrm{err})} = \mathrm{O}(\ell^3)$ as $\ell \to 0$ and the resulting second-order method for finding y (obtained by taking the combination $2M_y^{(3)} + M_y^{(2)} - M_y^{(1)}$) is

$$Y^{n+1} = \frac{2Y^n + \ell B X^n + X^{n+1}\left(\ell B - 2\ell Y^n X^n\right) + \ell\left(X^n\right)^2 Y^n}{2 + \ell\left(X^n\right)^2}. \tag{25}$$

This scheme, like (19), also involves Y^{n+1} and X^{n+1}, hence, Y^{n+1} cannot be obtained explicitly from (25).

In both (19) and (25), however, X^{n+1} and Y^{n+1} occur linearly so that (19) and (25) can be solved simultaneously to give

$$X^{n+1} = \frac{4X^n + \ell[4A + 2(X^n)^3 - 2X^n - 2BX^n] + \ell^2[2A(X^n)^2 - (X^n)^3]}{4 + 2\ell[1 + B - 2X^n Y^n + (X^n)^2] + \ell^2 (X^n)^2} \tag{26}$$

and

$$\begin{aligned} Y^{n+1} = {} & \frac{4Y^n + \ell[2Y^n + 2BY^n + 4BX^n - 4X^n(Y^n)^2 - 2Y^n(X^n)^2]}{4 + 2\ell[1 + B - 2X^n Y^n + (X^n)^2] + \ell^2(X^n)^2} \\ & + \frac{\ell^2[3Y^n(X^n)^2 - 4AX^nY^n + 2AB]}{4 + 2\ell[1 + B - 2X^n Y^n + (X^n)^2] + \ell^2(X^n)^2}. \end{aligned} \tag{27}$$

3.3. *Numerical methods for e*

Consider the ODE [given in (3)]

$$\frac{\mathrm{d}e}{\mathrm{d}t} \equiv e' = x - eu, \tag{28}$$

a second-order method for solving (28) may be obtained by approximating its derivative with (12) and evaluating the linear and quadratic forcing terms in ways which lead to the following numerical methods for finding e:

$$\begin{aligned} M_e^{(1)}: \quad & E^{n+1} = E^n + \ell X^n - \ell E U^{n+1}, \\ M_e^{(2)}: \quad & E^{n+1} = E^n + \ell X^{n+1} - \ell U^n E^{n+1}. \end{aligned} \tag{29}$$

The associated local truncation errors are given by

$$\begin{aligned} L_e^{(1)} &= \left(\frac{e''}{2} + eu'\right)\ell^2 + \mathrm{O}\left(\ell^3\right) \qquad \text{as } \ell \to 0, \\ L_e^{(2)} &= \left(\frac{e''}{2} - x' + ue'\right)\ell^2 + \mathrm{O}\left(\ell^3\right) \quad \text{as } \ell \to 0. \end{aligned} \tag{30}$$

It may be shown that the linear combination

$$L_e^{(\mathrm{err})} = \left[L_e^{(1)} + L_e^{(2)}\right] \tag{31}$$

gives

$$L_e^{(\mathrm{err})} = \bigl(e'' - x' + eu' + ue'\bigr)\ell^2 + \mathrm{O}\bigl(\ell^3\bigr) \quad \text{as } \ell \to 0. \tag{32}$$

Differentiating (28) with respect to t reveals that $L_e^{(\mathrm{err})} = \mathrm{O}(\ell^3)$ as $\ell \to 0$ and the resulting second-order method for finding e (obtained by adding $M_e^{(1)}$ and $M_e^{(2)}$) is

$$E^{n+1} = \frac{2E^n + \ell X^n + \ell X^{n+1} - \ell E^n U^{n+1}}{2 + \ell U^n}. \tag{33}$$

This scheme, like (19) and (25), also involves E^{n+1}, X^{n+1} and U^{n+1}, hence, E^{n+1} cannot be obtained explicitly from (33).

3.4. *Numerical methods for u*

Returning to the ODE system (3) where

$$\frac{\mathrm{d}u}{\mathrm{d}t} \equiv u' = Bx - eu + u^2 v - u, \tag{34}$$

a second-order method for solving (34) may be obtained by approximating its derivative with (12) and evaluating the reaction terms in ways which lead to the following numerical methods for finding u:

$$\begin{aligned}
M_u^{(1)}:&\quad U^{n+1} = U^n + \ell B X^n - \ell E^n U^n + \ell U^n V^n U^{n+1} - \ell U^n,\\
M_u^{(2)}:&\quad U^{n+1} = U^n + \ell B X^n - \ell E^n U^{n+1} + \ell\bigl(U^n\bigr)^2 V^{n+1} - \ell U^{n+1},\\
M_u^{(3)}:&\quad U^{n+1} = U^n + \ell B X^{n+1} - \ell U^n E^{n+1} + \ell\bigl(U^n\bigr)^2 V^n - \ell U^n,\\
M_u^{(4)}:&\quad U^{n+1} = U^n + \ell B X^n - \ell U^n E^n + \ell\bigl(U^n\bigr)^2 V^n - \ell U^n.
\end{aligned} \tag{35}$$

The associated local truncation errors are given by

$$\begin{aligned}
L_u^{(1)} &= \left(\frac{u''}{2} - uvu'\right)\ell^2 + \mathrm{O}\bigl(\ell^3\bigr) && \text{as } \ell \to 0,\\
L_u^{(2)} &= \left(\frac{u''}{2} + eu' - u^2 v' + u'\right)\ell^2 + \mathrm{O}\bigl(\ell^3\bigr) && \text{as } \ell \to 0,\\
L_u^{(3)} &= \left(\frac{u''}{2} - Bx' + ue'\right)\ell^2 + \mathrm{O}\bigl(\ell^3\bigr) && \text{as } \ell \to 0,\\
L_u^{(4)} &= \frac{u''}{2}\ell^2 + \mathrm{O}\bigl(\ell^3\bigr) && \text{as } \ell \to 0.
\end{aligned} \tag{36}$$

Similarly, defining the function $L_u^{(\mathrm{err})}$ by

$$L_u^{(\mathrm{err})} = \bigl[2L_u^{(1)} + L_u^{(2)} + L_u^{(3)} - 2L_u^{(4)}\bigr] \tag{37}$$

leads to

$$L_u^{(\mathrm{err})} = \bigl(u'' - Bx' - 2uvu' + eu' - u^2 v' + u' + ue'\bigr)\ell^2 + \mathrm{O}\bigl(\ell^3\bigr) \quad \text{as } \ell \to 0. \tag{38}$$

Differentiating (34) with respect to t reveals that $L_u^{(\mathrm{err})} = \mathrm{O}(\ell^3)$ as $\ell \to 0$ and the resulting second-order method for finding u is

$$U^{n+1} = \frac{2U^n + \ell[BX^n + BX^{n+1} - U^n E^{n+1} + (U^n)^2 V^{n+1} - U^n - U^2 V^n]}{2 + \ell(1 + E^n - 2U^n V^n)}. \tag{39}$$

This scheme also involves U^{n+1}, X^{n+1}, E^{n+1} and V^{n+1}, hence, U^{n+1} cannot be obtained explicitly from (39).

3.5. *Numerical methods for v*

Recalling the ODE

$$\frac{\mathrm{d}v}{\mathrm{d}t} \equiv v' = eu - u^2 v, \tag{40}$$

a second-order method for solving (40) may be obtained by approximating its derivative with (12) and evaluating the quadratic and cubic forcing terms in ways which lead to the following numerical methods for finding v:

$$\begin{aligned}
M_v^{(1)}:&\quad V^{n+1} = V^n + \ell E^n U^n - \ell V^n \big(U^n\big)^2,\\
M_v^{(2)}:&\quad V^{n+1} = V^n + \ell E^n U^{n+1} - \ell \big(U^n\big)^2 V^{n+1},\\
M_v^{(3)}:&\quad V^{n+1} = V^n + \ell E^n U^n - \ell U^n V^n U^{n+1},\\
M_v^{(4)}:&\quad V^{n+1} = V^n + \ell U^n E^{n+1} - \ell V^n \big(U^n\big)^2.
\end{aligned} \tag{41}$$

The principal parts of the local truncation errors are given by

$$\begin{aligned}
L_v^{(1)} &= \frac{v''}{2}\ell^2 + \mathrm{O}\big(\ell^3\big) && \text{as } \ell \to 0,\\
L_v^{(2)} &= \left(\frac{v''}{2} - eu' + u^2 v'\right)\ell^2 + \mathrm{O}\big(\ell^3\big) && \text{as } \ell \to 0,\\
L_v^{(3)} &= \left(\frac{v''}{2} + uvu'\right)\ell^2 + \mathrm{O}\big(\ell^3\big) && \text{as } \ell \to 0,\\
L_v^{(4)} &= \left(\frac{v''}{2} - ue'\right)\ell^2 + \mathrm{O}\big(\ell^3\big) && \text{as } \ell \to 0.
\end{aligned} \tag{42}$$

Letting

$$L_v^{(\mathrm{err})} = \big[L_v^{(2)} + 2L_v^{(3)} + L_v^{(4)} - 2L_v^{(1)}\big] \tag{43}$$

gives

$$L_v^{(\mathrm{err})} = \big(v'' - ev' + u^2 v' - ue' + 2uvu'\big)\ell^2 + \mathrm{O}\big(\ell^3\big) \quad \text{as } \ell \to 0. \tag{44}$$

Differentiating (40) with respect to the t reveals that $L_v^{(\mathrm{err})} = \mathrm{O}(\ell^3)$ as $\ell \to 0$ and the resulting second-order method for finding v is

$$V^{n+1} = \frac{2V^n + \ell U^n(U^n V^n + E^{n+1}) - \ell(2U^n V^n - E^n)U^{n+1}}{2 + \ell(U^n)^2}. \tag{45}$$

This scheme also involves E^{n+1}, U^{n+1} and V^{n+1}, hence, V^{n+1} cannot be obtained explicitly from (45).

It may be seen that, in both (33), (39) and (45), E^{n+1}, U^{n+1} and V^{n+1} occur linearly, thus, the three equations can be solved simultaneously (in terms of the already computed X^{n+1}) to give (using the Maple software package)

$$E^{n+1} = \frac{C_1 + D_1 + R_1}{W}, \tag{46}$$

$$U^{n+1} = \frac{C_2 + D_2 + R_2}{W} \tag{47}$$

and

$$V^{n+1} = \frac{C_3 + D_3 + R_3}{W}, \tag{48}$$

where

$$\begin{aligned}
C_1 &= \ell^3 (U^n)^2 \left[X^{n+1} + X^n + U^n E^n - BX^n E^n - BX^{n+1} E^n\right],\\
Q_1 &= 2\left[(U^n)^2 X^{n+1} + X^{n+1} + X^n + E^n X^n + E^n X^{n+1} + U^n E^n\right.\\
&\quad \left. - BX^{n+1} E^n - 2U^n V^n X^n\right],\\
D_1 &= \ell^2 \left\{Q_1 - 2\left[2U^n V^n X^{n+1} + BX^n E^n - (U^n)^2 X^n - (U^n)^2 E^n + (U^n)^3 E^n\right]\right\},\\
R_1 &= 8E^n + 4\ell\left[X^n + X^{n+1} + E^n + (U^n)^2 E^n - U^n E^n + (E^n)^2 - 2U^n V^n E^n\right],\\
C_2 &= -\ell^3 (U^n)^3 \left[U^n - BX^n - BX^{n+1}\right],\\
D_2 &= -2\ell^2 U^n \left[(U^n)^2 - BU^n X^n - BU^n X^{n+1} + U^n - BX^n - (U^n)^3\right.\\
&\quad \left. + X^n + X^{n+1} - BX^{n+1}\right],\\
R_2 &= 8U^n - 4\ell\left[U^n E^n + U^n - BX^n - BX^{n+1} - (U^n)^3 - (U^n)^2\right],\\
C_3 &= \ell^3 U^n \left[3(U^n)^2 V^n - 2BU^n V^n X^n - 2BU^n V^n X^{n+1} + X^n + X^{n+1}\right],\\
Q_2 &= 2\left[BE^n X^{n+1} + U^n V^n + BX^n E^n - (U^n)^3 V^n + 3(U^n)^2 V^n\right],\\
D_3 &= \ell^2 \left\{Q_2 + 2\left[U^n X^n - 2BU^n V^n X^n - 2BU^n V^n X^{n+1} - 2(U^n V^n)^2 + U^n X^{n+1}\right]\right\},\\
R_3 &= 8V + 4\ell\left[2U^n E^n - (U^n)^2 V^n + E^n V^n + V^n - 2U^n (V^n)^2 + U^n V^n\right],\\
W &= 8 + 4\ell\left[1 + E^n + U^n - 2U^n V^n + (U^n)^2\right]\\
&\quad + 2\ell^2 U^n \left[1 + (U^n)^2 + U^n - 2U^n V^n\right] + \ell^3 (U^n)^3.
\end{aligned} \tag{49}$$

The second-order method {(26), (27), (46), (47), (48)} is denoted GLTW2.

3.6. Implementation

The solution of the ODE system (3) may be obtained at every time step via the following sequential algorithm:

$$\begin{array}{ll} \text{(a)} & \text{compute } X^{n+1} \text{ using (26)},\\ \text{(b)} & \text{compute } Y^{n+1} \text{ using (27)},\\ \text{(c)} & \text{compute } E^{n+1} \text{ using (46) with (49)},\\ \text{(d)} & \text{compute } U^{n+1} \text{ using (47) with (49)},\\ \text{(e)} & \text{compute } V^{n+1} \text{ using (48) with (49).} \end{array} \tag{50}$$

4. Analyses of the fixed point

The expressions for X^{n+1} and Y^{n+1} in (26) and (27) for solving the first Brusselator are of the forms

$$\begin{aligned} X^{n+1} &= h_1\bigl(X^n, Y^n\bigr),\\ Y^{n+1} &= h_2\bigl(X^n, Y^n\bigr), \end{aligned} \tag{51}$$

respectively. It is easy to verify that the fixed point of (26) and (27) is $X^* = A$, $Y^* = B/A$. Thus, the fixed point of the numerical method (26), (27) is the same as the corresponding critical point of the dynamical system (3). It is worth investigating, at this point, whether or not the fixed point of the difference systems has the same stability properties as the critical point of the first Brusselator.

Starting first with the functions

$$h_1(X,Y) = \frac{4X + \ell(4A + 2X^3 - 2X - 2BX) + \ell^2(2AX^2 - X^3)}{4 + 2\ell(1 + B - 2XY + X^2) + \ell^2X^2}, \tag{52}$$

$$\begin{aligned} h_2(X,Y) &= \frac{4Y + \ell(2Y + 2BY + 4BX - 4XY^2 - 2YX^2)}{4 + 2\ell(1 + B - 2XY + X^2) + \ell^2X^2}\\ &\quad + \frac{\ell^2(3YX^2 - 4AXY + 2AB)}{4 + 2\ell(1 + B - 2XY + X^2) + \ell^2X^2}, \end{aligned} \tag{53}$$

it may be seen (after some tedious manipulations) that the resulting Jacobian J_1 at the fixed point ($X^* = A$ and $Y^* = B/A$) is the matrix

$$J_1 = \frac{1}{\alpha}\begin{bmatrix} 4 + 2\ell\bigl(A^2 + B - 1\bigr) - 4\ell^2A^2 & 4\ell A^2\\ -4\ell B & 4 + 2\ell\bigl(A^2 + B - 1\bigr) - \ell^2A^2 \end{bmatrix}, \tag{54}$$

in which $\alpha = 4 + 2\ell(1 - B + A^2 + \ell^2A^2)$. The eigenvalues of (54) are given by

$$\begin{aligned} \lambda_1 &= \frac{4 + 2\ell\sqrt{(A^2 - B + 1)^2 - 4A^2} - \ell^2A^2}{4 + 2\ell(A^2 - B + 1) + \ell^2A^2},\\ \lambda_2 &= \frac{4 + 2\ell\sqrt{(A^2 - B + 1)^2 - 4A^2} - \ell^2A^2}{4 + 2\ell(A^2 - B + 1) + \ell^2A^2}. \end{aligned} \tag{55}$$

It is clear from (55) that the denominators of λ_1 and λ_2 are always positive provided $A^2 - B + 1 > 0$ and it is easy to show then that

$$|\lambda_1| < \frac{4 + 2\ell(A^2 - B + 1) - \ell^2 A^2}{4 + 2\ell(A^2 - B + 1) + \ell^2 A^2} < 1 \tag{56}$$

and

$$|\lambda_2| < \frac{4 - 2\ell(A^2 - B + 1) - \ell^2 A^2}{4 + 2\ell(A^2 - B + 1) + \ell^2 A^2} < 1. \tag{57}$$

The inequalities in (56) and (57) are also true whenever $A^2 - B + 1 = 0$. Thus, a sufficient condition for (26) and (27) to converge to the fixed point $(A, B/A)$ is $A^2 - B + 1 \geqslant 0$. Similarly, it may be shown that the second Brusselator converges to the fixed point $(E, U, V) = (1/B, AB, 1/(AB^2))$ whenever the inequalities in (6) are satisfied.

5. Numerical verification

In order to verify the convergence properties of the implicit, second-order GLTW2 numerical method {(26), (27), (46), (47), (48)}, it was tested on the initial-value problem (3). Extensive numerical experiments were carried out with various values of time-steps ℓ and initial conditions within the interval $-8 \leqslant X^0, Y^0, E^0, U^0, V^0 \leqslant 8$. Of course, X^0, Y^0, E^0, U^0, and V^0 are concentrations so that non-positive values are irrelevant, but the results show that the numerical method GLTW2 performed well for negative initial conditions, too. Comparisons were made with the standard explicit Runge–Kutta methods of order two and four.

The behaviours of the two Brusselators for many different combinations of A and B satisfying or violating the stability conditions (g_1, g_2 and g_3) using $\ell = 0.001$ are tabulated in table 1.

As expected, both methods (GLTW2, RK2 and KR4) gave solution sequences that converge to the fixed point $(X, Y, E, U, V) = (A, B/A, 1/B, AB, 1/(AB^2))$ whenever the inequalities in (6) are satisfied, and give oscillatory or divergent results otherwise. For instance, when the parameters A and B were given the values 2 and 1.5, respectively, thereby satisfying the condition $1 - B + A^2 = 3.5 > 0$, the first Brusselator is stationary. In the case when $A = 0.5$ and $B = 1$, satisfying the stability condition g_1

Table 1
Convergence properties of two Brusselators using GLTW2 with $\ell = 0.001$.

A	B	g_1	g_2	g_3	Brusselator 1	Brusselator 2
2	1.5	3.5	18.500	303.500	stationary	stationary
0.5	1	0.25	0.750	−0.438	stationary	oscillatory
1	3	−1.0	38	1325	oscillatory	non-autonomous oscillation
1	0.8	1.2	0.952	−0.455	stationary	oscillatory
0.2	1.2	−0.160	0.557	−0.330	oscillatory	oscillatory

Table 2
Hopf bifurcation analysis of Brusselator 1 using GLTW2 with A fixed at 1, B varied and $\ell = 0.001$.

A	B	g_1	Brusselator 1
1	0	2	stationary
1	1	1	stationary
1	2	0	neither stationary nor oscillatory
1	3	-1	oscillatory
1	4	-2	oscillatory

(for the first Brusselator) and violating g_3 (for the second Brusselator), the second Brusselator oscillates autonomously (oscillation of the second Brusselator when the first is stationary). The absence of back-coupling in the system is responsible for ensuring that the first Brusselator remains stationary even when the second Brusselator is oscillating.

The phenomenon of non-autonomous oscillation of the second Brusselator (forced oscillation of the second due to the oscillation of the first) is illustrated in table 1 by choosing $A = 1$ and $B = 3$. With these choices, condition g_1 is violated whereas g_2 and g_3 are both satisfied. Hence, Brusselator 2, if acting alone (without coupling), will be expected to be stationary. The oscillation of the first Brusselator drives the second Brusselator to oscillate. This confirms the prediction and analysis of section 2.2. Another important observation to make is the case $A = 0.2$ and $B = 1.2$ in which both the two Brusselators are oscillatory. This is an interesting case which the authors hope to investigate (for the possibility of modulated oscillation) in the near future.

In table 2, the Hopf bifurcation of the first Brusselator was investigated by fixing the value of A at $A = 1$ and varying B. Values of B to the left of (less than) the bifurcating value ($B = 2$) lead to the first Brusselator being stationary, whereas values of B to the right of (greater than) $B = 2$ make the first Brusselator to oscillate, thereby causing the second to oscillate non-autonomously. Thus, the numerical method GLTW2 confirms the bifurcation direction of the first Brusselator.

The effect of the time-step on the numerical methods was monitored by solving (3) using both the RK2, RK4 and GLTW2 methods with various time-steps. The concentration parameters A and B were assigned the values 2 and 1.5 respectively, and the results tabulated in table 3. Clearly, from table 3, the method GLTW2 has superior stability property (admit large time steps) than the RK2 (which fails when $\ell \geqslant 0.3$) and the RK4 (which fails for $\ell \geqslant 0.5$). This, of course, is consistent with the known fact that implicit methods, unlike explicit schemes, are very suited for solving non-linear initial value problems.

It is worth mentioning that using values of A and B for which the convergence criteria becomes zero, it was observed that the methods appeared neither to converge nor to diverge. This is because this case marks the boundary between the convergence and divergence criteria. Detailed analytical study on the possibility of a double-Hopf bifurcation will be carried out in a separate study.

Table 3
Convergence properties of GLTW2, RK2 and RK4 using various time-steps with $A = 2$ and $B = 1.5$.

ℓ	GLTW2	RK2	RK4
0.001	converge	converge	converge
0.01	converge	converge	converge
0.1	converge	converge	converge
0.2	converge	converge	converge
0.3	converge	diverge (method failed)	converge
0.5	converge	diverge	diverge (method failed)
1	converge	diverge	diverge
2	converge	diverge	diverge
3	converge	diverge	diverge

6. Conclusion

A competitive, implicit, second-order accurate numerical method has been developed for the coupled Brusselator system introduced by Tyson [3]. The numerical method converges to its correct fixed point whenever the input chemicals A and B are chosen such that a certain convergence criterion is satisfied. The fixed point of the numerical method was seen to have the same stability properties as the critical point of the ODE system arising from coupling two Brusselators in series. The second-order method was seen to be more competitive (in terms of numerical stability) than Runge–Kutta methods of order two and four. The numerical method confirms the existence of oscillatory solutions as suggested by the Hopf bifurcation analysis.

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