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THE FINITE DIFFERENCE METHODS AND ITS STABILITY FOR GLYCOLYSIS MODEL IN ONE DIMENSION

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Abstract: The Glycolysis model has been solved numerically in one dimension by using two finite differences methods: explicit and Crank-Nicolson method and we were found that the explicit method is simpler while the Crank-Nicolson is more accurate. Also, we found that explicit method is conditionally stable while Crank-Nicolson method is unconditionally stable.

Keywords: Glycolysis model, explicit method, Crank-Nicolson method.

2000 AMS Subject Classification: 65N06; 65N12

1. Introduction

Chemical reactions are modeled by non-linear partial differential equations (PDEs) exhibiting travelling wave solutions. These oscillations occur due to feedback in the system either chemical feedback (such as autocatalysis) or temperature feedback due to a non-isothermal reaction.

Reaction-diffusion (RD) systems arise frequently in the study of chemical and

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biological phenomena and are naturally modeled by parabolic partial differential equations (PDEs). The dynamics of RD systems has been the subject of intense research activity over the past decades. The reason is that RD system exhibit very rich dynamic behavior including periodic and quasi-periodic solutions and chaos(see, for example [8]).

Mathematical Model:

A general class of nonlinear-diffusion system is in the form

$$\frac{\partial u}{\partial t} = d_1 \Delta u + a_1 u + b_1 v + f(u, v) + g_1(x)$$
$$\frac{\partial v}{\partial t} = d_2 \Delta v + a_2 u + b_2 v - f(u, v) + g_2(x),$$

with homogenous Dirchlet or Neumann boundary condition on a bounded domain Ω , with locally Lipschitz continuous boundary. It is well known that reaction and diffusion of chemical or biochemical species can produce a variety of spatial patterns. This class of reaction diffusion systems includes some significant pattern formation equations arising from the modeling of kinetics of chemical or biochemical reactions and from the biological pattern formation theory.

In this group, the following four systems are typically important and serve as mathematical models in physical chemistry and in biology:

Brusselator model:

$$a_1 = -(b+1), b_1 = 0, a_2 = b, b_2 = 0, f = u^2 v, g_1 = a, g_2 = 0,$$

where *a* and *b* are positive constants.

Gray-Scott model:

$$a_1 = -(f + K), b_1 = 0, a_2 = 0, b_2 = -F, f = u^2 v, g_1 = 0, g_2 = F,$$

where *F* and *K* are positive constants.

Glycolysis model:

$$a_1 = -1, b_1 = K, a_2 = 0, b_2 = -K, f = u^2 v, g_1 = \rho, g_2 = \delta,$$

where K, ρ and δ are positive constants.

Schnackenberg model:

$$a_1 = -K, b_1 = a_2 = b_2 = 0, f = u^2 v, g_1 = a, g_2 = b,$$

where K, a and b are positive constants.

Then one obtains the following system of two nonlinearly coupled reaction-diffusion equations (the Glycolysis model),

(1)
$$\begin{cases} \frac{\partial u}{\partial t} = d_1 \Delta u - u + Kv + u^2 v + \rho, \ (t, x) \in (0, \infty) \times \Omega, \\ \frac{\partial v}{\partial t} = d_2 \Delta v - Kv - u^2 v + \delta, \quad (t, x) \in (0, \infty) \times \Omega, \end{cases}$$

(2)
$$\begin{cases} u(t, x) = v(t, x) = 0, \quad t > 0, \quad x \in \partial \Omega \\ u(0, x) = u_0(x), \quad v(0, x) = v_0(x), \quad x \in \Omega \end{cases}$$

where ρ , *K* and δ are positive constants [9].

2. Derivation of explicit method for Glycolysis model

Assume that the rectangle $R = \{(x,t): 0 \le x \le a, 0 \le t \le b\}$ is subdivided into *n*-1 by *m*-1 rectangle with sides $\Delta x = h$ and $\Delta t = k$, as shown in Fig. (1). Start at the bottom row, where $t = t_1 = 0$, and the solution is $u(x_p, t_1) = f(x_p)$.



Fig. (1) The grid

A method for computing the approximations to u(x,t) at grid points in successive rows $\{u(x_p,t_q): p=1,2,...,n\}$, for q=2,3,...,m. The difference formulas used for approximation $u_t(x,t), u_x(x,t)$ and $u_{xx}(x,t)$ are

(3)
$$u_t(x,t) = \frac{u(x,t+k) - u(x,t)}{k} + O(k),$$

(4)
$$u_x(x,t) = \frac{u(x+h,t) - u(x,t)}{h} + O(h),$$

(5)
$$u_{xx}(x,t) = \frac{u(x-h,t) - 2u(x,t) + u(x+h,t)}{h^2} + O(h^2).$$

The grid spacing is uniform in every row: $x_{p+1} = x_p + h$ and $(x_{p-1} = x_p - h)$, and it is uniform in every column: $t_{q+1} = t_q + k$ and $(t_{q-1} = t_q - k)$. Next, we drop the terms O(k), O(h) and $O(h^2)$ [4], and use the approximation $u_{p,q}$ for $u(x_p, t_q)$ in equations (3) and (5), and substituted into equation (1) to obtain

$$\begin{aligned} \frac{u_{p,q+1} - u_{p,q}}{k} &= d_1 \frac{u_{p+1,q} - 2u_{p,q} + u_{p-1,q}}{h^2} - u_{p,q} + Kv_{p,q} + u_{p,q}^2 v_{p,q} + \rho, \\ \frac{v_{p,q+1} - v_{p,q}}{k} &= d_2 \frac{v_{p+1,q} - 2v_{p,q} + v_{p-1,q}}{h^2} - Kv_{p,q} - u_{p,q}^2 v_{p,q} + \delta, \\ u_{p,q+1} &= \frac{d_1 k}{h^2} (u_{p+1,q} - 2u_{p,q} + u_{p-1,q}) - Ku_{p,q} + Kkv_{p,q} + ku_{p,q}^2 v_{p,q} + u_{p,q} + \rho k, \\ v_{p,q+1} &= \frac{d_2 k}{h^2} (v_{p+1,q} - 2v_{p,q} + v_{p-1,q}) - Kkv_{p,q} - ku_{p,q}^2 v_{p,q} + k\delta + v_{p,q}, \end{aligned}$$
Let $\frac{d_1 k}{h^2} = r_1$ and $\frac{d_2 k}{h^2} = r_2$, then
$$\begin{cases} u_{p,q+1} = r_1 (u_{p+1,q} + u_{p-1,q}) + (1 - 2r_1 - k)u_{p,q} + Kkv_{p,q} + ku_{p,q}^2 v_{p,q} + \rho k, \\ v_{p,q+1} &= r_2 (v_{p+1,q} + v_{p-1,q}) + (1 - 2r_2 - Kk)v_{p,q} - ku_{p,q}^2 v_{p,q} + k\delta, \end{cases}$$

the result is the explicit forward difference equation to the Glycolysis model .

3. Derivation of implicit Crank-Nicholson method for Glycolysis

model

This method was invented by John Crank and Phyllis Nicholson, in (1947), and is based on numerical approximations for solutions, they replace u_{xx} by the mean of its finite difference representation of the $(q)^{th}$ and $(q+1)^{th}$ time rows [7]

$$\begin{split} u_{p,q+1} &= r_1(u_{p+1,q} - 2u_{p,q} + u_{p-1,q} + u_{p+1,q+1} - 2u_{p,q+1+}u_{p-1,q+1}) - ku_{p,q} + \\ & Kkv_{p,q} + ku_{p,q}^2 v_{p,q} + k\rho, \\ v_{p,q+1} &= r_2(v_{p+1,q} - 2v_{p,q} + v_{p-1,q} + v_{p+1,q+1} - 2v_{p,q+1} + v_{p-1,q+1}) + Kkv_{p,q} + \\ & \delta k - ku_{p,q}^2 v_{p,q}. \end{split}$$

Rearranging the last two equations give

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(7)
$$\begin{cases} (1+2r_1)u_{p,q+1} - r_1(u_{p+1,q+1}+u_{p-1,q+1}) = r_1(u_{p-1,q}+u_{p+1,q}) - (1-2r_1-k)u_{p,q} + Kkv_{p,q} \\ +ku_{p,q}^2v_{p,q} + k\rho, \\ (1+2r_2)v_{p,q+1} - r_2(v_{p+1,q+1}+v_{p-1,q+1}) = r_2(v_{p-1,q}+v_{p+1,q}) - (1+Kk+2r_2)v_{p,q} - ku_{p,q}^2v_{p,q} + \delta k. \end{cases}$$

The system of equations (7) represents the implicit difference approximation for Glycolysis model, where the left hand side of the system contains three unknown values, while the right hand side contains three known values for p=2,3,...,n-1.

Hence the first equations in (7) form a tridiagonal linear system in the form

$$(8) \qquad AX = B.$$

The boundary conditions are used in the first and last equation (i.e. $u_{1,q} = u_{n,q} = 0$ and $u_{1,q+1} = u_{n,q+1} = 0$ respectively). The equation (7) is especially pleasing to view in their tri-diagonal matrix form

(9)
$$A_1 X_1 = B_1,$$

Also we can similarly solve the second equation of (7).

(10)
$$A_2 X_2 = B_2$$
,

When the Crank-Nicholson method is implemented with a computer, the linear system AX=B can be solved by either direct methods or by iterations method.

In this study we use the direct methods (Gaussian Elimination Method) to solve the linear system in equation (7). The numerical stability of the numerical methods is studying the errors introduced by the truncation of the series which are used to represent the derivatives in the process of replacing the differential equations by finite difference equation and the growth of these errors and finding the conditions for which the errors will be decay from one time step to the next [6].

4. Numerical stability of explicit method

The numerical stability of the numerical methods is studying the errors introduced by the truncation of the series which are used to represent the derivatives in the process of replacing the differential equations by finite difference equation and the growth of these errors and finding the conditions for which the errors will be decay from one time step to the next [5].

The Von Neumann analysis is the most commonly used method of determining

stability criteria as it is generally the easiest to apply, the most straight-forward and most dependable. This method developed by Von Neumann during World War II, was first discussed in detail by O'Brien, Hyman and Kaplan in a paper published in 1951 [5].

The general form of this method is to substitute the solution in finite difference method at the time t by $\psi(t)e^{i\alpha x}$, when $\alpha >0$ and $i = \sqrt{-1}$ [5]. To apply the Von Neumann method, it will take the following form

$$u_{p,q+1} = r_1(u_{p+1,q} + u_{p-1,q}) + (1 - 2r_1 - k)u_{p,q}$$

$$v_{p,q+1} = r_2(v_{p+1,q} + v_{p-1,q}) + (1 - 2r_2 - Kk)v_{p,q}$$

where $r_1 = \frac{d_1k}{h^2}$, $r_2 = \frac{d_2k}{h^2}$, $\Delta x = h$ and $\Delta y = k$ for the first equation of the system, neglecting for some values of *K*, ρ the terms $Kkv_{p,q}$ and ρ linearizing the system, the non linear terms can be neglected [3]. So

$$\psi(t+\Delta t)e^{i\alpha x} = r_1(\psi(t)e^{i\alpha(x+\Delta x)} + \psi(t)e^{i\alpha(x-\Delta x)}) + (1-2r_1-k)\psi(t)e^{i\alpha x}$$

Dividing both sides by $e^{i\alpha x}$, to obtain

$$\psi(t + \Delta t) = r_1 [e^{i\alpha\Delta x} + e^{-i\alpha\Delta x}]\psi(t) + (1 - 2r_1 - k)\psi(t).$$

For some values of α , we can assume that $\sin^2(\alpha \Delta x/2)$ is unity [3], and

$$\frac{\psi(t+\Delta t)}{\psi(t)} = (1-4r_1-k) = \xi.$$

It is stable if $\left|\frac{\psi(t+\Delta t)}{\psi(t)}\right| \le 1$, so

 $|(1-4r_1-k)| \le 1$, which implies $-1 \le (1-4r_1-k) \le 1$.

Case 1:
$$-1 \le (1-4r_1-k) \Rightarrow 4r_1 \le 2-k \Rightarrow r_1 \le \frac{2-k}{4}$$
, or

Case 2:
$$1-4r_1-k \le 1 \Rightarrow r_1 \ge \frac{-\kappa}{4}$$
.

The equation is stable under the conditions $r_1 \le \frac{2-k}{4}$ and we will neglect $r_1 \ge \frac{-k}{4}$ because r_1 is positive.

And for the second equation

$$v_{p,q+1} = r_2(v_{p+1,q} + v_{p-1,q}) + (1 - 2r_2 - Kk)v_{p,q}.$$

To study the stability of the second equation we let $v_{p,q} = \phi(t)e^{i\beta x}$ so the equation will be in the form

$$\phi(t+\Delta t)e^{i\beta x} = r_2[\phi(t)e^{i\beta(x+\Delta x)} + \phi(t)e^{i\beta(x-\Delta x)}] + (1-2r_2-Kk)\phi(t)e^{i\beta x}.$$

Dividing both sides of the equation by $\phi(t)e^{i\beta x}$ to obtain

$$\frac{\phi(t+\Delta t)}{\phi(t)} = r_2(2\cos(\beta\Delta x)) + (1-2r_2 - Kk) = 2r_2(1-2\sin^2(\beta\Delta x/2)) + (1-2r_2 - Kk)$$
$$= 1-4r_2 - Kk = \xi.$$

It is stable if $|\xi| \le 1$, or $\left|\frac{\phi(t+\Delta t)}{\phi(t)}\right| \le 1 \Longrightarrow |1-4\mathbf{r}_2-\mathbf{K}\mathbf{k}| \le 1$.

$$\begin{aligned} \left|1-4r_2-Kk\right| &\leq 1 \Longrightarrow -1 \leq (1-4r_2-Kk) \leq 1, \\ -1 &\leq (1-4r_2-Kk) \Longrightarrow 4r_2 \leq 2-Kk \Longrightarrow r_2 \leq \frac{2-Kk}{4}, \end{aligned}$$
or
$$(1-4r_2Kk) \leq 1 \Longrightarrow 4r_2 \geq -Kk \Longrightarrow r_2 \geq \frac{-Kk}{4}.$$

Finally the system is conditionally stable under the conditions

$$\frac{-k}{4} \le r_1 \le \frac{2-k}{4}$$
 and $\frac{-Kk}{4} \le r_2 \le \frac{2-Kk}{4}$.

5. Numerical stability of implicit (Crank-Nicolson) method

We use Crank-Nicolson finite difference in equation (1) to obtain

$$\frac{u_{p,q+1} - u_{p,q}}{k} = \frac{d_1}{2h^2} [u_{p-1,q} - 2u_{p,q} + u_{p+1,q} + u_{p-1,q+1} - 2u_{p,q+1} + u_{p+1,q+1}] - u_{p,q} + Kv_{p,q} + \rho + kv_{p,q} + \rho + kv_{p,q}]$$

Substituting $u_{p,q}$ by $\psi(t)e^{i\gamma x}$ in the above equation, yields

$$\frac{\psi(t+\Delta t)e^{i\gamma x} - \psi(t)e^{i\gamma x}}{k} = \frac{d_1}{2h^2} [\psi(t)e^{i\gamma(x-\Delta x)} - 2\psi(t)e^{i\gamma x} + \psi(t)e^{i\gamma(x+\Delta x)} + \psi(t+\Delta t)e^{i\gamma(x-\Delta x)} - 2\psi(t+\Delta t)e^{i\gamma x} + \psi(t+\Delta t)e^{i\gamma(x+\Delta x)}] - \psi(t)e^{i\gamma x}.$$

Neglecting for some values of k, ρ and linearizing the nonlinear term can be neglected.

Dividing both sides of the equation by $e^{i\gamma x}$ to obtain

$$[\psi(t+\Delta t) - \psi(t)] - \frac{d_1 k \psi(t)}{2h^2} [e^{-i\gamma \Delta x} - 2 + e^{i\gamma \Delta x}] - \frac{d_1 k \psi(t+\Delta t)}{2h^2} [e^{-i\gamma \Delta x} - 2 + e^{i\gamma \Delta x}] = -k \psi(t).$$

Assuming $r_1 = \frac{d_1k}{h^2}$, from the above equation, we get

$$[\psi(t+\Delta t)-\psi(t)] - \frac{r_{\mathrm{l}}\psi(t)}{2} [2\cos(\gamma\Delta x)-2] - \frac{r_{\mathrm{l}}\psi(t+\Delta t)}{2} [2\cos(\gamma\Delta x)-2]$$
$$= [\psi(t+\Delta t)-\psi(t)] + r_{\mathrm{l}}\psi(t) [2\sin^{2}(\gamma\Delta x/2)] + r_{\mathrm{l}}\psi(t+\Delta t) [2\sin^{2}(\gamma\Delta x/2)] = -k\psi(t)$$

and

$$[1+2r_1\sin^2(\gamma\Delta x/2)]\psi(t+\Delta t) = [1-2r_1\sin^2(\gamma\Delta x/2)-k]\psi(t),$$

which implies that
$$\frac{\psi(t + \Delta t)}{\psi(t)} = \frac{1 - (2r_1 \sin^2(\gamma \Delta x/2) + k)}{1 + 2r_1 \sin^2(\gamma \Delta x/2)} = \xi$$

For stability we need
$$\left| \frac{\psi(t + \Delta t)}{\psi(t)} \right| \le 1$$
, i.e.
 $\left| \frac{1 - (2r_{1} \sin^{2}(\gamma \Delta x/2) + k)}{1 + 2r_{1} \sin^{2}(\gamma \Delta x/2)} \right| \le 1$, for all r_{1}, k, b .

Hence the Crank-Nicolson method is unconditionally stable for the first equation of Glycolysis model, and for the second equation

$$\begin{aligned} \frac{\partial v}{\partial t} &= d_2 \frac{\partial^2 v}{\partial x^2} - Kkv_{p,q}, \\ \frac{v_{p,q+1} - v_{p,q}}{k} &= \frac{d_2}{2h^2} [v_{p-1,q} - 2v_{p,q} + v_{p+1,q} + v_{p-1,q+1} - 2v_{p,q+1} + v_{p+1,q+1}] - Kkv_{p,q}. \end{aligned}$$

Substitute $v_{p,q} = \phi(t)e^{i\varphi x}$ in the above equation to obtain

$$[\frac{\phi(t+\Delta t)-\phi(t)}{k}]e^{i\beta x} = \frac{d_2\phi(t)}{2h^2}[e^{i\beta(x-\Delta x)} - 2e^{i\beta x} + e^{i\beta(x+\Delta x)}] + \frac{d_2\phi(t+\Delta t)}{2h^2}[e^{i\beta(x-\Delta x)} - 2e^{i\beta x} + e^{i\beta(x+\Delta x)}] - Kk\phi(t)e^{i\beta x}.$$

Multiplying both sides of the above equation by $ke^{-i\beta x}$ to obtain

$$\phi(t+\Delta t) - \phi(t) = \frac{d_2 k \phi(t)}{2h^2} \left[e^{-i\beta\Delta x} - 2 + e^{i\beta\Delta x} \right] + \frac{d_2 k \phi(t+\Delta t)}{2h^2} \left[e^{-i\beta\Delta x} - 2 + e^{i\beta\Delta x} \right] - Kk\phi(t).$$

In the above equation, let $\frac{d_2k}{h^2} = r_2$, yields

$$\phi(t + \Delta t) - \phi(t) = \frac{r_2 \phi(t + \Delta t)}{2} [2\cos(\beta \Delta x) - 2] + r_2 \frac{\phi(t)}{2} [2\cos(\beta \Delta x) - 2] - Kk\phi(t)$$

= $-r_2 \phi(t + \Delta t) [1 - (1 - 2\sin^2(\beta \Delta x/2)] - r_2 \phi(t) [1 - (1 - 2\sin^2(\beta \Delta x/2)] - Kk\phi(t)]$
= $-2r_2 \phi(t + \Delta t) \sin^2(\beta \Delta x/2) - 2r_2 \phi(t) \sin^2(\beta \Delta x/2) - Kk\phi(t).$

Hence,

$$\phi(t+\Delta t) + 2r_2\phi(t+\Delta t)\sin^2(\beta\Delta x/2) = \phi(t) - 2r_2\phi(t)\sin^2(\beta\Delta x/2) - Kk\phi(t),$$

and after simplification, we get

$$\frac{\phi(t+\Delta t)}{\phi(t)} = \frac{\left[1-\text{Kk}-2r_2\sin^2\left(\beta\Delta x/2\right)\right]}{\left[1+2r_2\sin^2\left(\beta\Delta x/2\right)\right]} = \xi.$$

Thus $\left|\frac{\phi(t+\Delta t)}{\phi(t)}\right| = |\xi| \le 1$, so
 $\left|\frac{\left[1-\text{Kk}-2r_2\sin^2\left(\beta\Delta x/2\right)\right]}{\left[1+2r_2\sin^2\left(\beta\Delta x/2\right)\right]}\right| \le 1, \forall r_2, k, K.$

Since for both equations of the system we have $|\xi| \le 1$, the Crank-Nicolson method is unconditionally stable.

6. Numerical example

We solved the following example numerically to illustrate efficiency of the presented methods

Example:

$$\frac{\partial u}{\partial t} = d_1 \Delta u - u + Kv + u^2 v + p, \qquad t > 0, \quad x \in \Omega,$$
$$\frac{\partial v}{\partial t} = d_1 \Delta v - v - u \quad v + \mu, \qquad t > 0, \qquad x \in \Omega,$$

with the initial conditions

$$U(x, 0) = Us + 0.01 \sin(\pi x/L) \quad \text{for} \quad 0 \le x \le L$$

$$V(x, 0) = Vs - 0.12 \sin(\pi x/L) \quad \text{for} \quad 0 \le x \le L$$

$$U(0, t) = Us, \quad U(L, t) = Us \quad \text{and} \quad V(0, t) = Vs, \quad V(L, t) = Vs.$$

We will take

$$d_1 = d_2 = 0.01$$
, $K = 0.5$, $del = p = 0.5$, $U_s = 0$, $V_s = 1$.



Fig. 2a The Implicit method of the concentration V



Fig.2b The Explicit method of concentration V

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