Numerical Solution to Belousov – Zhabotinskii

Model and a Comparison with

the Finite Difference Method

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Abstract

In this work, we find a numerical solution to Belousov – Zhabontinskii system, we use the traveling wavelets method. It is well known that this model describes a chemical reaction. The results obtained are compared with those derived from the finite difference method.

The principle of the traveling wavelets method consists in seeking the solution in the form:

\[ u(x,t) = \sum_{i=1}^{N} c_i(t) \Psi \left( x - \frac{b_i(t)}{a_i(t)} \right) \quad , \quad a_i > 0 \quad , \quad b_i , c_i \in R \]

Where the function \( \Psi \) is some wavelet function and \( c_i , a_i , b_i \) are parameters depending on time, amplitude, scale and position respectively. Without loss of generality, we will focus our study only on the one dimensional case.

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1. Introduction

The Belousov-Zhabotinskii model is described by the system:

\[
\begin{align*}
\frac{\partial u_1}{\partial t} &= \frac{\partial^2 u_1}{\partial x^2} + u_1 (1 - u_1 - ru_2) \\
\frac{\partial u_2}{\partial t} &= \frac{\partial^2 u_2}{\partial x^2} - bu_1 u_2
\end{align*}
\]

This system has been studied by a number of authors; in 1979 R. J. Field and W. C. Troy [8] studies the existence of solitary Travelling Wave Solutions, G. B. Yu, C. Z. Xiong [4] and L. Zhibin, S. He [6] has found the solution by the travelling wave method.

In this paper, we use the travelling wavelets method to find the solution of Belousov-Zhabotinskii (for r=b=1), the basics of this method is described bellow (see also[1], [10] for more details), it’s applied in several areas in astrophysics by N.Benhamidouche, B.Torresani and R.Triay [7] and by J.Elezgaray [5] in fluid mechanics.

By using this method we obtain a numerical solution which is exactly the same when we use the finite difference method for some choice of the wavelet.

Global existence in time of solution to reaction diffusion systems: [3]

Global existence in time of solutions to reaction diffusion systems in the form:

\[
\begin{align*}
\frac{\partial u_1}{\partial t} - d_1 \Delta u_1 &= f( u_1, u_2 ) \\
\frac{\partial u_2}{\partial t} - d_2 \Delta u_2 &= g( u_1, u_2 )
\end{align*}
\]

Where \( d_1 = d_2 > 0 \) are the coefficients of diffusion and \( f, g : R^2 \to R \)

Represent the non linear interactions, with the following two properties:

1) \( \forall u_1, u_2 \geq 0 : f(0, u_2), g(u_1, 0) \geq 0 \)

2) \( f(u_1, u_2) + g(u_1, u_2) \leq 0 \)

In the Belousov-Zhabontinskii framework, the global existence in time of solutions is verified with these two properties:
Belousov-Zhabotinskii model

1) \( \forall u_1, u_2 \geq 0 : f(0, u_1, u_2) = g(u_1, 0) = 0 \)

2) \( u_1 + (r + b) u_2 \geq 1 \)

2. The traveling wavelets method (TWM) [1]

The traveling wavelets method seeks an approximate solution of the evolution problem:

\[
\begin{cases}
\frac{\partial u}{\partial t} + A_x u = 0 \\
u(x,0) = u_0(x)
\end{cases}
\]  

(1 - 2)

Under the form

\[
u(x,t) = \sum_{i=1}^{N} c_i(t) \Psi \left( \frac{x - b_i(t)}{a_i(t)} \right), \quad a_i > 0, \quad b_i, c_i \in \mathbb{R}
\]

Where \( u(x, t) \) is a function of space and time variables, and \( A_x \) is a differential linear or nonlinear operator, \( \Psi \) is any wavelet, \( c_i, a_i, b_i \) are the parameters of amplitude, scale, and position depending on time, governess the atom \( \psi \) such that:

\[
\Psi'(x,t) = c_i(t) \Psi \left( \frac{x - b_i(t)}{a_i(t)} \right)
\]

The parameters \( c_i, a_i, b_i \) are obtained by the minimizing problem where the error is calculated at any moment \( t \):

\[
\text{Min} \int_{c_i, a_i, b_i \in \mathbb{R}} \left( \frac{\partial u}{\partial t} + A_x \right)^2 dx,
\]
Therefore, we obtain three equations which read as follows:

\[
\begin{align*}
\frac{\partial}{\partial c_i} \left( \frac{\partial u}{\partial t} + A_x \frac{\partial u}{\partial t} + A_x \right) &= 0 \\
\frac{\partial}{\partial a_i} \left( \frac{\partial u}{\partial t} + A_x \frac{\partial u}{\partial t} + A_x \right) &= 0 \quad \text{for } i = 1, N \\
\frac{\partial}{\partial b_i} \left( \frac{\partial u}{\partial t} + A_x \frac{\partial u}{\partial t} + A_x \right) &= 0
\end{align*}
\]

Where \( \langle \cdot, \cdot \rangle \) is the inner product in \( L^2(R) \).

Then the minimization problem leads to the system of 3N equations given by:

\[
\begin{align*}
\left( \frac{\partial u}{\partial t} + A_x u, \Psi' \right) &= 0 \\
\left( \frac{\partial u}{\partial t} + A_x u, x \Psi'' \right) &= 0 \quad (1-3) \\
\left( \frac{\partial u}{\partial t} + A_x u, \Psi'' \right) &= 0
\end{align*}
\]

This method transforms the problem (1-3) to a system of ordinary differential, equations of unknowns \( c_i, a_i, b_i \) given in the form:

\[
\begin{pmatrix}
\dot{c}_i \\
\dot{a}_i \\
\dot{b}_i
\end{pmatrix} = M \begin{pmatrix}
c_i \\
a_i \\
b_i
\end{pmatrix} = F \left( c_i(t), a_i(t), b_i(t) \right)
\]

Where \( M \) is a matrix in order 3N that comes from the term \( \frac{\partial u}{\partial t} \), and \( F \) the second member comes from the term \( A_x u \).

3. The traveling wavelets method to solving the model of Bélousov-Zhabontinskii
With the traveling wavelets method we will seek the solutions of the system (1-1) (for $r=b=1$) in the following form:

$$u_1(x,t) = \Psi^1(x,t)$$
$$u_2(x,t) = \Psi^2(x,t)$$

$$\Psi^1(x,t) = c_1(t)\Psi_1 \left( \frac{x-b_1(t)}{a_1(t)} \right)$$
$$\Psi^2(x,t) = c_2(t)\Psi_2 \left( \frac{x-b_2(t)}{a_2(t)} \right)$$

The initial conditions are:

$$u_1(x,0) = c_1(0)\Psi_1 \left( \frac{x-b_1(0)}{a_1(0)} \right) \text{ with } c_1(0) = 1, b_1(0) = 0, a_1(0) = 1$$
$$u_2(x,0) = c_2(0)\Psi_2 \left( \frac{x-b_2(0)}{a_2(0)} \right) \text{ with } c_2(0) = 1, b_2(0) = 0, a_2(0) = 1$$

We note: $(x\Psi')^i = \left( \frac{x-b_i(t)}{a_i(t)} \right)\Psi^u$

The minimization problem is written as follow:

$$\min_{c_1, a_1, b_1} \left| \frac{\partial u_1}{\partial t} - \frac{\partial^2 u_1}{\partial^2 x} - u_1 \left( 1 - u_1 - u_2 \right) \right|^2$$
$$\min_{c_2, a_2, b_2} \left| \frac{\partial u_2}{\partial t} - \frac{\partial^2 u_2}{\partial^2 x} + u_1 u_2 \right|^2$$

Therefore, we obtain six equations:
Which are written as a linear system of ordinary differential equation in the form:

\[
\begin{bmatrix}
\frac{\partial u_1}{\partial t} - \frac{\partial^2 u_1}{\partial^2 x} - u_1(1-u_1-u_2), \Psi^1
\frac{\partial u_1}{\partial t} - \frac{\partial^2 u_1}{\partial^2 x} - u_1(1-u_1-u_2), \Psi^1
\frac{\partial u_1}{\partial t} - \frac{\partial^2 u_1}{\partial^2 x} - u_1(1-u_1-u_2), \Psi^1
\frac{\partial u_2}{\partial t} - \frac{\partial^2 u_2}{\partial^2 x} + u_2, \Psi^2
\frac{\partial u_2}{\partial t} - \frac{\partial^2 u_2}{\partial^2 x} + u_2, \Psi^2
\frac{\partial u_2}{\partial t} - \frac{\partial^2 u_2}{\partial^2 x} + u_2, \Psi^2
\end{bmatrix} = 0
\]

Which are written as a linear system of ordinary differential equation in the form:

\[
\begin{pmatrix}
M_1 & 0
0 & M_2
\end{pmatrix}
\begin{pmatrix}
c_1 \\
c_1 \\
a_1 \\
a_1 \\
b_1 \\
b_1 \\
-\frac{a_2}{a_2} \\
-\frac{a_2}{a_2} \\
-\frac{b_2}{a_2}
\end{pmatrix}
= \begin{pmatrix} F_1 \\ F_2 \end{pmatrix}
\]

(1.4)
Belousov-Zhabotinskii model

\[ M_i = \begin{pmatrix}
\langle \Psi^i, \Psi^i \rangle & \langle \Psi^i, x \Psi^i \rangle & \langle \Psi^i, x^2 \Psi^i \rangle \\
\langle x \Psi^i, \Psi^i \rangle & \langle x \Psi^i, x \Psi^i \rangle & \langle x \Psi^i, x^2 \Psi^i \rangle \\
\langle \Psi^i, \Psi^i \rangle & \langle \Psi^i, x \Psi^i \rangle & \langle \Psi^i, x^2 \Psi^i \rangle 
\end{pmatrix} \]

and

\[
F_1 = \frac{1}{a_1} \begin{pmatrix}
\langle \Psi^i + \Psi^i (1 - \Psi^i - \Psi^2), \Psi^i \rangle \\
\langle \Psi^i + \Psi^i (1 - \Psi^i - \Psi^2), x \Psi^i \rangle \\
\langle \Psi^i + \Psi^i (1 - \Psi^i - \Psi^2), x^2 \Psi^i \rangle 
\end{pmatrix},
F_2 = \frac{1}{a_2} \begin{pmatrix}
\langle \Psi^i + \Psi^i (1 - \Psi^i - \Psi^2), \Psi^2 \rangle \\
\langle \Psi^i + \Psi^i (1 - \Psi^i - \Psi^2), x \Psi^2 \rangle \\
\langle \Psi^i + \Psi^i (1 - \Psi^i - \Psi^2), x^2 \Psi^2 \rangle 
\end{pmatrix}
\]

To calculate the solution, it is necessary to make a choice of wavelets. The family of the following functions:

\[ K_m(x) = (-1)^m \frac{d^m}{dx^m} \exp\left(-\frac{x^2}{2}\right), m \geq 1, \]

Where \( K_m \) is a derivative of a Gaussian function, are good wavelet candidates for the following reasons:

- The inner product in the matrix and the second member expressed analytically by the function of unknown \( c_i, a_i, b_i \).

- The following properties of the integral are very interesting:

\[
\int K_m(x) dx = 0 \text{ for } m = 0, l - 1
\]

\[
\int K_m(x) K_n(x) K_l(x) dx = 0 \text{ for } m + n + l \text{ is an odd}
\]

- These wavelets have another property due mainly to which properties of Hermite polynomials.

Then for \( \Psi_1(x) = K_m(x), \Psi_2(x) = K_n(x) \).

In this case, our matrix will becomes as follows:
\[ M_1 = \frac{a_1 c_1^2 \sqrt{\pi} 2m!}{2^{2m} m!} \begin{pmatrix} 1 & -1 & 0 \\ -1 & m + \frac{3}{4} & 0 \\ 0 & 0 & m + \frac{1}{2} \end{pmatrix}, \quad M_2 = \frac{a_2 c_2^2 \sqrt{\pi} 2n!}{2^{2n} n!} \begin{pmatrix} 1 & -1 & 0 \\ -1 & n + \frac{3}{4} & 0 \\ 0 & 0 & n + \frac{1}{2} \end{pmatrix} \]

The following notation will be used:

\[ T_m(u, v) = a_1 c_1^2 \int \limits_{R} K_m(ux + v)K_n(x)dx \]

\[ w = \frac{a_1}{a_2}, \quad \nu = \frac{b_1 - b_2}{a_2} \]

and the second member is

\[
F_1 = \begin{cases} 
\frac{c_1^2}{a_1} T_{m+2,m+1}(1,0) + a_1 c_1^2 T_{m,m}(1,0) - c_1^3 J_{m,m,m}(1,0, a_1) - \\
- \frac{c_1^2}{a_1} (T_{m+2,m+1}(1,0) + (m + 1)T_{m+2,m}(1,0)) + \\
a_1 c_1^2 (T_{m,m,m}(1,0) + (m + 1)T_{m,m,m}(1,0)) + \\
c_1^3 (J_{m,m,m+2}(1,0, a_1) + (m + 1)J_{m,m,m}(1,0, a_1)) + \\
c_2 c_1^2 (J_{m,m,m+2}(u,v,a_1) + (m + 1)J_{m,m,m}(u,v,a_1)) + \\
c_1^3 J_{m,m,m+1}(1,0, a_1) + c_1 c_2^2 J_{m,m,m+1}(u,v,a_1) 
\end{cases}
\]

\[
F_2 = \begin{cases} 
\frac{c_2^2}{a_2} T_{n+2,n+1}(1,0) - c_2^2 c_1 J_{m,n,n}(u,v,a_1) - \\
- \frac{c_2^2}{a_2} (T_{n+2,n+1}(1,0) + (n + 1)T_{n+2,n}(1,0)) + \\
c_2^2 c_1 (J_{m,n,n+1}(u,v,a_1) + (n + 1)J_{m,n,n}(u,v,a_1)) + \\
c_2^2 c_1 J_{m,n,n+1}(u,v,a_1) 
\end{cases}
\]
The system (1-4) is a system of nonlinear differential equations that can be integrated by classical numeric method of integration. For the solution, we will process by calculating the reverse of the matrix $M_1, M_2$ by using an idea of the conjugate gradient method. Then we integrate the system obtained, which gives $X = M^{-1}F$ by using the method of Adams-Bashfors, (Ref [7]).

For the accuracy of our solution, we need to evaluate the error depending on the choice of $m$ and $n$.

4. Evaluation of error [7], [9], [10]

Let: $V(t) = \{\Psi^{(i)}, \Psi^{(i+1)} \} i = 1, 2$

From relations (1-2), we deduce that $\frac{\partial u}{\partial t} + A_u u$ is orthogonal to $V(t)$

and as $\frac{\partial u}{\partial t}$ belongs to $V(t)$

We find: $\left\langle \frac{\partial u}{\partial t} + A_u u, \frac{\partial u}{\partial t} \right\rangle = 0$

and thus if also $A_u u$ belongs to $V(t)$ then the method provides us an exact solution. In our problem $A_u u$ does not belong to $V(t)$ and we must evaluate the errors:

Consider

$$\Delta_1(u_1) = \left\| \frac{\partial u_1}{\partial t} - \frac{\partial^2 u_1}{\partial^2 x} - u_1(1 - u_1 - u_2) \right\|^2$$

And

$$\Delta_2(u_2) = \left\| \frac{\partial u_2}{\partial t} - \frac{\partial^2 u_2}{\partial^2 x} + u_1 u_2 \right\|^2$$

We put
\[ resd_i = \sqrt{\varepsilon_i} \quad i = 1,2 \] with \( \varepsilon_i = \left\| \frac{\partial u_1}{\partial t} - \frac{\partial^2 u_1}{\partial x^2} - u_1(1 - u_1 - u_2) \right\|^2 \) and \( \varepsilon_2 = \left\| \frac{\partial u_2}{\partial t} - \frac{\partial^2 u_2}{\partial x^2} + u_1 u_2 \right\|^2 \)

5. The numerical results

The numerical results obtained by this method are found on board

![Comparison of errors in L^2 norm](image1)

![Comparison of errors in L^2 norm](image2)

Figure (5-1)

Comment

The errors corresponding to the cases \( m=n=0 \) is the weakest compared to the other case \( m=0, n=1 \), \( m=0, n=2 \) therefore the approximate solution \( m=n=0 \) is the best solution.
This is the behavior of the solution for the case $m=n=0$, for various iteration:

![Graph of solution $u_2(t,x)$](image1)

![Graph of solution $u_1(t,x)$](image2)

Figure (5-2)

**Conclusion:**

The evaluation of the errors ensures us that the best solution obtained by the TWM is the case $m=n=0$

**6. B-Z solving by the finite differences method (FDM)**

There are three types of basic methods for solving such equations: explicit, implicit and Crank-Nicholson type methods.

We will solve our system by schema implicit.

The numerical results obtained by the FDM for $m=n=0$

For iteration 100
The solution $u_2(t,x)$ by FDM for various time for $m=n=0$ with $dt=0.001$, number of time steps=100.

The solution $u_1(t,x)$ by the FDM for various time for $m=n=0$ with $dt = 0.001$, number of time steps=100.

Figure (6-1)

Comparison with the finite differences method:

By comparing our solutions obtained with those of the finite differences method for various values of $m$ and $n$, we note that the case corresponding $m=n=0$, provides practically the same solution, i.e. the behavior for the two methods is the same (Figure (5-2)).

And for a detailed account of this step see the Ref [9].

Figure (6-2)

We will compare the absolute errors between the solutions obtained by the TWM and the solution obtained by the FDM for various choices of $m$ and $n$. 

The solution $u_2(t,x)$ by the FDM and TWM for iteration:500

The solution $u_1(t,x)$ by the FDM and by the TWM for iteration 500
Belousov-Zhabotinskii model

Figure (6-3)

For example the absolute error between the solutions obtained by the two methods, for the case \( m=n=0 \) is of order 0.006 for the first solution and 0.003 for the second solution (figure (5-3)), on the other hand for the other cases, we notice significant differences between various solutions obtained by the two methods, the absolute error between the solutions for the case \( m=0, n=1 \) is of order 0.012 for the first solution and 0.004 for the second solution, for the case \( m=0, n=2 \) are of order 0.006 for the first solution and 0.018 for the second solution.

Conclusion:

The traveling wavelets method gives us a very rich choice to represent the solution of the system of Béloousov-Zhabotinskii. It appears that the \( m=n=0 \) choice gives the best approximation compared to other choices of \( m \) and \( n \) and that corresponds to the condition of existence and uniqueness of the positive solution.
References


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