Applied Mathematical Sciences, Vol. 3, 2009, no. 8, 351 - 364

Numerical Solution to Belousov – Zhabotinskii Model and a Comparison with the Finite Difference Method

*** S. Benmehdi and **N. Benhamidouche**

*University of Bourdj Bouarerridj, Algeria

**University of M'Sila, Algeria

sabah_benmehdi@yahoo.fr, benhamidouche@yahoo.fr

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:

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

Where the function Ψ 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.

Mathematics Subject Classification: 35B40, 35K55, 35K57, 65T60

Keywords: Traveling wavelets method; reaction- diffusion system; Belousov-Zhabotinskii model; finite difference method

1. Introduction

The Belousov-Zhabotinskii model is described by the system:

$$\begin{cases} \dfrac{\partial u_1}{\partial t} = \dfrac{\partial^2 u_1}{\partial^2 x} + u_1(1 - u_1 - ru_2) \\ \dfrac{\partial u_2}{\partial t} = \dfrac{\partial^2 u_2}{\partial^2 x} - bu_1u_2 \end{cases} \quad r \text{ and } b \text{ are constants} \quad (1\text{-}1)$$

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:

$$\begin{cases} \dfrac{\partial u_1}{\partial t} - d_1 \Delta u_1 = f(u_1, u_2) \\ \dfrac{\partial u_2}{\partial t} - d_2 \Delta u_2 = g(u_1, u_2) \end{cases}$$

Where $d1=d_2>0$ 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:

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

$$\begin{cases} \dfrac{\partial u}{\partial t} + A_x u = 0 \\ u(x,0) = u_0(x) \end{cases} \qquad (1-2)$$

Under the form

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

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

$$\Psi^i(x,t) = c_i(t)\Psi\left(\frac{x - b_i(t)}{a_i(t)}\right)$$

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

$$\underset{c_i, a_i, b_i}{Min} \int_R \left| \frac{\partial u}{\partial t} + A_x \right|^2 dx \quad ,$$

Therefore, we obtain three equations which read as follows:

$$\begin{cases} \dfrac{\partial}{\partial \dot{c}_i}\left\langle \dfrac{\partial u}{\partial t} + A_x , \dfrac{\partial u}{\partial t} + A_x \right\rangle = 0 \\ \dfrac{\partial}{\partial \dot{a}_i}\left\langle \dfrac{\partial u}{\partial t} + A_x , \dfrac{\partial u}{\partial t} + A_x \right\rangle = 0 \qquad for\ i = 1, N \\ \dfrac{\partial}{\partial \dot{b}_i}\left\langle \dfrac{\partial u}{\partial t} + A_x , \dfrac{\partial u}{\partial t} + A_x \right\rangle = 0 \end{cases}$$

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

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

$$\begin{cases} \left\langle \dfrac{\partial u}{\partial t} + A_x u , \Psi^{i} \right\rangle = 0 \\ \left\langle \dfrac{\partial u}{\partial t} + A_x u\ , x\Psi'^{i} \right\rangle = 0 \qquad (1-3) \\ \left\langle \dfrac{\partial u}{\partial t} + A_x u , \Psi'^{i} \right\rangle = 0 \end{cases}$$

This method transforms the problem (1-3) to a system of ordinary differential, equations of unknowns $\dot{c}_i , \dot{a}_i , \dot{b}_i$ given in the form :

$$\mathrm{M}\left(ci\,(t), ai(t)\ ,\ bi\,(t)\right)\begin{pmatrix} \dot{ci} \\ \dot{ai} \\ \dot{bi} \end{pmatrix} = F\left(ci(t), ai\,(t)\ ,\ bi\,(t)\right)$$

Where M is a matrix in order 3N that comes from the term

$\dfrac{\partial u}{\partial t}$, 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:

With $\begin{array}{l} u_1(x,t) = \Psi^1(x,t) \\ u_2(x,t) = \Psi^2(x,t) \end{array}$

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

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

The initial conditions are:

$$u_1(x,0) = c_1(0)\Psi_1\left(\frac{(x-b_1(0)}{a_1(0)}\right) \quad with \quad c_1(0)=1\,, b_1(0)=0\,,\, a_1(0)=1$$

$$u_2(x,0) = c_2(t)\Psi_2\left(\frac{(x-b_2(0)}{a_2(0)}\right) \quad with \quad c_2(0)=1\,, b_2(0)=0\,,\, a_2(0)=1$$

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

The minimization problem is written as follow:

$$\underset{\dot{c}_1,\dot{a}_1,\dot{b}_1}{Min}\left\|\frac{\partial u_1}{\partial t} - \frac{\partial^2 u_1}{\partial^2 x} - u_1(1-u_1-u_2)\right\|^2$$

$$\underset{\dot{c}_2,\dot{a}_2,\dot{b}_2}{Min}\left\|\frac{\partial u_2}{\partial t} - \frac{\partial^2 u_2}{\partial^2 x} + u_1 u_2\right\|^2$$

Therefore, we obtain six equations:

$$\begin{cases} \left\langle \dfrac{\partial u_1}{\partial t} - \dfrac{\partial^2 u_1}{\partial^2 x} - u_1(1-u_1-u_2), \Psi^1 \right\rangle = 0 \\ \left\langle \dfrac{\partial u_1}{\partial t} - \dfrac{\partial^2 u_1}{\partial^2 x} - u_1(1-u_1-u_2), x\Psi'^1 \right\rangle = 0 \\ \left\langle \dfrac{\partial u_1}{\partial t} - \dfrac{\partial^2 u_1}{\partial^2 x} - u_1(1-u_1-u_2), \Psi'^1 \right\rangle = 0 \\ \left\langle \dfrac{\partial u_2}{\partial t} - \dfrac{\partial^2 u_2}{\partial^2 x} + u_1 u_2, \Psi^2 \right\rangle = 0 \\ \left\langle \dfrac{\partial u_2}{\partial t} - \dfrac{\partial^2 u_2}{\partial^2 x} + u_1 u_2, x\Psi'^2 \right\rangle = 0 \\ \left\langle \dfrac{\partial u_2}{\partial t} - \dfrac{\partial^2 u_2}{\partial^2 x} + u_1 u_2, \Psi'^2 \right\rangle = 0 \end{cases}$$

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

$$\begin{pmatrix} M_1 & 0 \\ 0 & M_2 \end{pmatrix} \begin{pmatrix} \dfrac{\dot{c}_1}{c_1} \\ -\dfrac{\dot{a}_1}{a_1} \\ -\dfrac{\dot{b}_1}{a_1} \\ \dfrac{\dot{c}_2}{c_2} \\ -\dfrac{\dot{a}_2}{a_2} \\ -\dfrac{\dot{b}_2}{a_2} \end{pmatrix} = \begin{pmatrix} F_1 \\ F_2 \end{pmatrix} \qquad (1-4)$$

$$\text{with}: M_i = \begin{pmatrix} \langle \Psi^i, \Psi^i \rangle & \langle \Psi^i, x\Psi''^i \rangle & \langle \Psi^i, \Psi''^i \rangle \\ \langle x\Psi''^i, \Psi^i \rangle & \langle x\Psi''^i, x\Psi''^i \rangle & \langle x\Psi''^i, \Psi''^i \rangle \\ \langle \Psi''^i, \Psi^i \rangle & \langle \Psi''^i, x\Psi''^i \rangle & \langle \Psi''^i, \Psi''^i \rangle \end{pmatrix}$$

and

$$F_1 = \frac{1}{a_1^1}\begin{bmatrix} \langle \Psi''^1 + \Psi^1(1-\Psi^1-\Psi^2), \Psi^1 \rangle \\ \langle \Psi''^1 + \Psi^1(1-\Psi^1-\Psi^2), x\Psi''^1 \rangle \\ \langle \Psi''^1 + \Psi^1(1-\Psi^1-\Psi^2), \Psi''^1 \rangle \end{bmatrix}, \; F_2 = \frac{1}{a_2^2}\begin{bmatrix} \langle \Psi''^2 - \Psi^1\Psi^2, \Psi^2 \rangle \\ \langle \Psi''^2 - \Psi^1\Psi^2, x\Psi''^2 \rangle \\ \langle \Psi''^2 - \Psi^1\Psi^2, \Psi''^2 \rangle \end{bmatrix}$$

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:

$$\int_R x^m K_l(x)dx = 0 \quad for \;\; m = 0, l-1$$

$$\int_R K_m(x)K_n(x)K_l(x)dx = 0 \quad for \;\; m+n+l \; is\, an \; odd$$

-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:

$$M_1 = \frac{a_1 c^2{}_1 \sqrt{\pi}}{2^{2m}} \frac{2m!}{m!} \begin{pmatrix} 1 & -\frac{1}{2} & 0 \\ -\frac{1}{2} & m+\frac{3}{4} & 0 \\ 0 & 0 & m+\frac{1}{2} \end{pmatrix}, \quad M_2 = \frac{a_2 c^2{}_2 \sqrt{\pi}}{2^{2n}} \frac{2n!}{n!} \begin{pmatrix} 1 & -\frac{1}{2} & 0 \\ -\frac{1}{2} & n+\frac{3}{4} & 0 \\ 0 & 0 & n+\frac{1}{2} \end{pmatrix}$$

The following notation will be used:

with $T_{mn}(u,v) = a_1 c_1 c_2 \int_R K_m(ux+v) K_n(x) dx$

$w = \dfrac{a_1}{a_2}, v = \dfrac{b_1 - b_2}{a_2}$

and the second member is

$$F_1 = \begin{pmatrix} \frac{c^2{}_1}{a_1} T_{m+2,m}(1,0) + a_1 c^2{}_1 T_{m,m}(1,0) - c^3{}_1 J_{m,m,m}(1,0,a_1) - \\ c_2 c_1^2 J_{m,n,m}(u,v,a_1) \\ -\frac{c^2{}_1}{a_1}\left(T_{m+2,m+2}(1,0) + (m+1) T_{m+2,m}(1,0)\right) - \\ a_1 c^2{}_1 \left(T_{m+2,m}(1,0) + (m+1) T_{m,m}(1,0)\right) + \\ c^3{}_1 \left(J_{m,m,m+2}(1,0,a_1) + (m+1) J_{m,m,m}(1,0,a_1)\right) + \\ c_2 c^2{}_1 \left(J_{m,n,m+2}(u,v,a_1) + (m+1) J_{m,n,m}(u,v,a_1)\right) \\ c^3{}_1 J_{m,m,m+1}(1,0,a_1) + c_1 c^2{}_2 J_{m,n,m+1}(u,v,a_1) \end{pmatrix},$$

$$F_2 = \begin{pmatrix} \frac{c^2{}_2}{a_2} T_{n+2,n}(1,0) - c^2{}_2 c_1 J_{m,n,n}(u,v,a_1) \\ -\frac{c^2{}_2}{a_2}\left(T_{n+2,n+2}(1,0) + (n+1) T_{n+2,n}(1,0)\right) + \\ c^2{}_2 c_1 \left(J_{m,n,n+1}(u,v,a_1) + (n+1) J_{m,n,n}(u,v,a_1)\right) \\ c^2{}_2 c_1 J_{m,n,n+1}(u,v,a_1) \end{pmatrix}$$

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 : $V(t) = \{\Psi^{(i)}, \Psi'^{(i)}, x\Psi'^{(i)} \ i = 1,2\}$

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

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

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

and thus if also $A_x u$ belongs to *V(t)* then the method provides us an exact solution. In our problem $A_x u$ 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

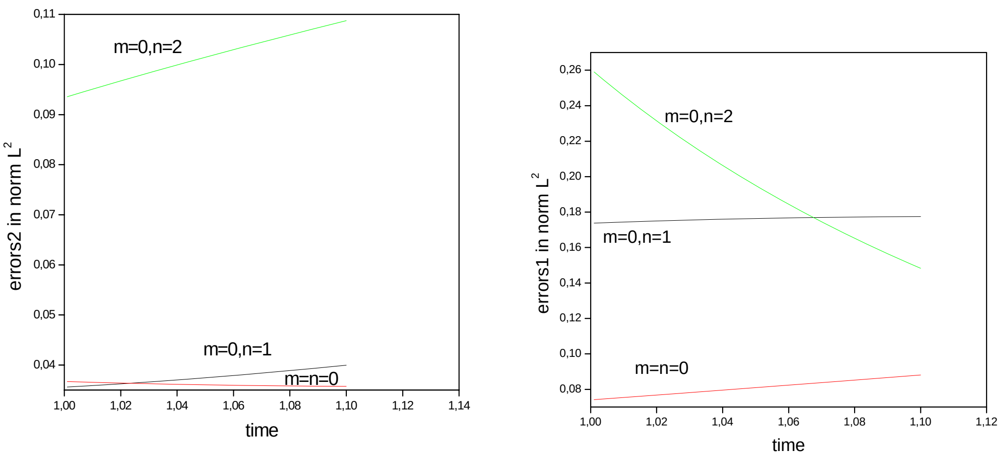
$$\Delta_2(u_2) = \left\| \frac{\partial u_2}{\partial t} - \frac{\partial^2 u_2}{\partial^2 x} + u_1 u_2 \right\|^2$$

We put

$$resd_i = \sqrt{\varepsilon_i} \quad i = 1,2 \;\; with \;\; \varepsilon_1 = \frac{\left\| \frac{\partial u_1}{\partial t} - \frac{\partial^2 u_1}{\partial^2 x} - u_1(1 - u_1 - u_2) \right\|^2}{\left\| \frac{\partial u_1}{\partial t} \right\|^2} \;\; and \;\; \varepsilon_2 = \frac{\left\| \frac{\partial u_2}{\partial t} - \frac{\partial^2 u_2}{\partial^2 x} + u_1 u_2 \right\|^2}{\left\| \frac{\partial u_2}{\partial t} \right\|^2}$$

5. The numerical results

The numerical results obtained by this method are found on board



Comparison of errors2 in L^2 norm

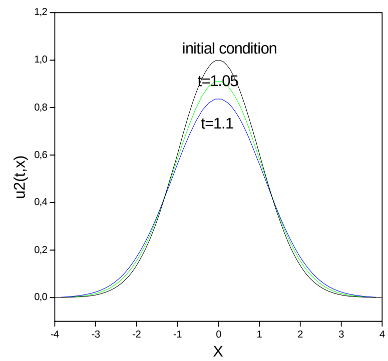
comparison of errors1 in L^2norm

Figure (5-1)

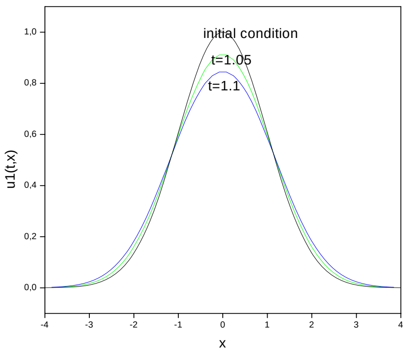
Comment

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:



The solution u2(t,x) by the TWM for varoius time
for m=n=0 with dt=0.001,number of time steps=100



The solution u1(t,x) by the TWM for various time
for m=n=0 with dt =0.001,number of time steps =100

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

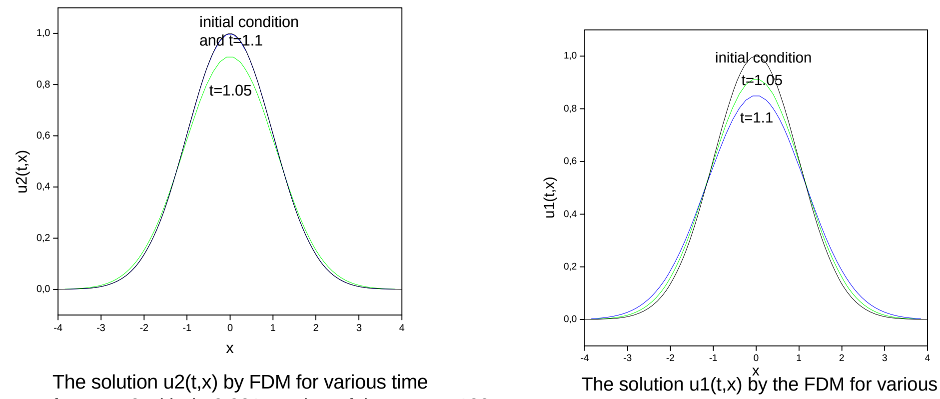
6. B-Z solving by the finite differences method (FDM)

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 u2(t,x) by FDM for various time
for m=n=0 with dt=0.001,number of time steps=100

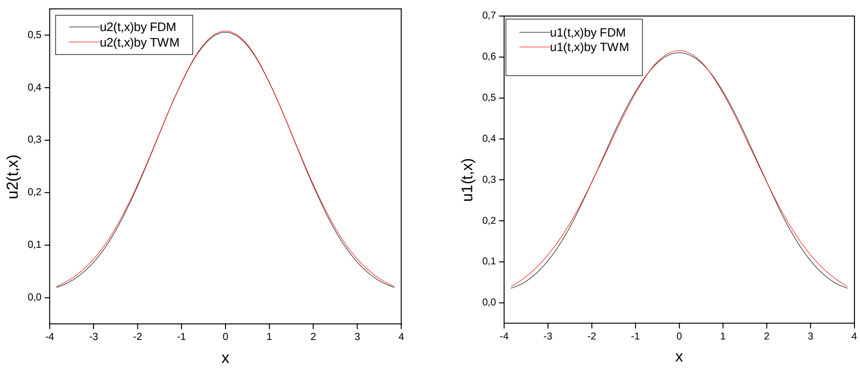
The solution u1(t,x) by the FDM for various time
for m=n=0 with dt = 0.001,number of time steps=100

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 notes 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].

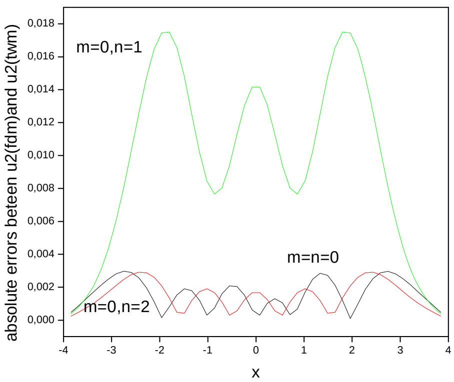


The solution u2(t,x)by the FDM and TWM
for iteration:500

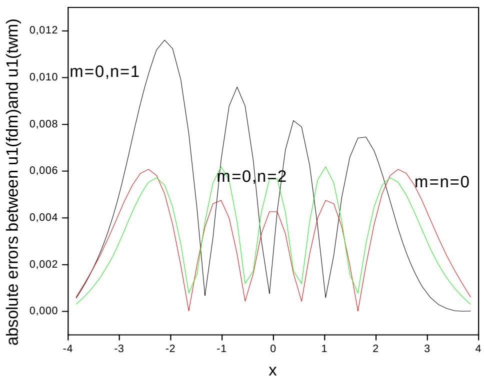
The solution u1(t,x) by the FDM and by the TWM
for iteration 500

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



Comparison of the errors for varoius value of m and n



Comparison of the errors for various value of m and n

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 Bélousov-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

[1] C. Basdevant , M. Holschneider et V. Perrier, La méthode des ondelettes mobiles , C.R.Acad .Sci.Paris, (1990) , 647-652.

[2] D. Euvrard, Résolution numériques des équations aux dérivées partielles. Paris, 1994.

[3] D. Schmith, Existence globales pour des systèmes de réaction diffusion avec contrôle de masse, Nancy I , 1995 .

[4] G. B. Yu, C. Z. Xiong: Analytic solutions of Noyes-Field system for Belousov-Zhabotinskii reaction, Partial Differential Equations, 2(1995), 174- 192.

[5] J. Elezgaray , Traveling wavlets for the simulation of a Hele-Shaw Flow with surface tension, Applied and Computational Harmonic analysis , 6 (1999) , 103-108.

[6] L. Zhibin, S. He: Exact solutions for Belousov-Zhabotinskii reaction-diffusion system, Gaoxiao Yingyong Shuxue Xuebao , 1 (1996) , 125.

[7] N. Benhamidouche, Instabilité gravitationnelle et ondelettes mobiles, AIX-Marseille II, 1995.

[8] R. J. Field , W. C. Troy, The Existence of Solitary Travelling Wave Solutions of a Model of the Belousov-Zhabotinskii Reaction. Journal on Applied Mathematics, 3(1979), 561-587.

[9] S. Benmehdi, Application de la méthode des ondelettes mobiles aux systèmes de réaction diffusion non linéaires, M'Sila, 2001.

[10] V. Perrier, Ondelettes et simulations numérique. Paris 6, 1990.

Received : June 16, 2008