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Research Article

Numerical Solutions of 2-Dimensional Schrödinger Equation Using Modified Gauss Elimination Method

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Abstract

In this study, modifed Gauss elimination method will be used to obtain solution of first order Rothe difference scheme and second order Crank-Nicholson difference scheme for numerical approximation of two-dimensional Schrödinger equation in space variable. One example is given, and an approximate solution is found by three approaches. Modified Gauss elimination method is used with respect to time variable and with respect to space variable. In order to compare the difference schemes are also solved by the classical inverse matrix method.

Keywords: Modified Gauss elimination method, Rothe difference scheme, Self-adjoint operator.

Modifiye Gauss Eleme Yöntemi Kullanarak 2-Boyutlu Schrödinger Denklemine Sayısal Yaklaşım

Öz

Bu çalışmada, uzay değişkeninde iki boyutlu Schrödinger denkleminin sayısal yaklaşımı için birinci mertebeden Rothe fark şemasının ve ikinci mertebeden Crank-Nicholson fark şemasının çözümünü elde etmek için modifiye Gauss eliminasyon yöntemi kullanılmıştır. Bir örnek verilmiş ve üç yöntemle yaklaşık çözüm bulunmuştur. Modifiye Gauss eliminasyon yöntemi, zaman değişkenine ve uzay değişkenine göre kullanılmıştır. Karşılaştırma yapmak için fark şemaları, klasik ters matris yöntemi ile de çözülmüştür.

Anahtar Kelimeler: Modifiye Gauss eleme metodu, Rothe fark şeması, Öz-eşlenik operator.

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1. Introduction

Modified Gauss elimination method is used for solving linear difference equations correspond to linear partial differential equations. Detail of this method can be seen in Ashyaralyev and Sırma (2008) and Yıldirim (2007). In Ashyaralyev and Sırma (2008), the modified Gauss elimination method is used for solving first order of accuracy Rothe difference scheme and second order of accuracy Crank-Nicholson difference scheme to find approximate solution of nonlocal boundary value problem for the Schrödinger equation. In Ashyaralyev and Sırma (2009), the modified Gauss elimination method is used for solving modified Crank-Nicholson difference scheme to find approximate solution of nonlocal boundary value problem for the Schrödinger equation. In Ashyralyyev (2017), Ashyralyyev and Akyuz (2018) in order to find approximate solution of Bitsadze-Samarskii equation, in Ashyralyyev and Cay (2020) in order to find approximate solution of elliptic-inverse problem two-dimensional in space variable modified Gauss elimination method is used to find the solution of corresponding difference schemes. Ashyralyyev C., used this method in his some other articles also. Beside these, for the numerical solution of two-dimensional Schrödinger equation different numerical methods can be investigated in the literature. For example Dehghan and Shokri (2007), proposed a numerical scheme to solve two-dimensional linear homogeneous Schrödinger equation using collocation points and approximating the solution using multiquadrics and thing plate splines radial basis function. Zhang & Chen (2016), used a meshless symplectic method for linear two-dimensional Schrödinger equation with radial basis functions. Gülkaç (2003), extended Boadway's transformation technique to obtain numerical solution for linear two-dimensional Schrödnger equation. Zhang & Zhang (2019), suggests a meshless symplectic procedure bases on highly accurate multiquadric quasi-interpolation for two-dimensional time-dependent linear Schrödinger equation.

In this study, applicability of modified Gauss elimination in first order of accuracy Rothe difference scheme and second order of accuracy Crank-Nicholson difference scheme for finding approximate solution of two-dimensional Schrödinger equation is shown. In addition, the modified Gauss elimination method is implemented with respect to time variable and with respect to space variable as well. Standart inverse matrix method is also implemented to compare performance requirements of each approach.

2. Material and Method

To show applicability of modified Gauss elimination method for two dimensional Schrödinger equation in space let us take the following example:

$$i\frac{\partial u(t,x,y)}{\partial t} - \left[\frac{\partial^2 u(t,x,y)}{\partial x^2} + \frac{\partial^2 u(t,x,y)}{\partial x^2}\right] = f(t,x,y) \quad (1)$$

$$u(0,x,y) = \sin(\pi xy), \quad 0 < x,y < 1, \quad (2)$$

$$u(t,0,y) = u(t,x,0) = 0, \quad 0 < t,x,y < 1, \quad (3)$$

$$u(t,1,y) = e^{it}\sin(\pi y), \quad 0 < t,y < 1, \quad (4)$$

$$u(t,x,1) = e^{it}\sin(\pi x), \quad 0 < t,x < 1, \quad (5)$$

where $f(t,x,y) = [\pi^2(x+y) - 1]e^{it}\sin(\pi xy)$. Exact solution of this problem is $u(t,x,y) = e^{it}\sin(\pi xy)$. We consider this problem in a Hilbert space $H = L_2([0,1]\times[0,1])$ of all integrable functions defined on $[0,1]\times[0,1]$, equipped with the norm $\|u\|_{[0,1]\times[0,1]} = \left(\int_0^1\int_0^1 |u(x,y)|^2\,dxdy\right)^{1/2}$. But unfortunately in our example the operator $A(u(.,x,y)) = -\left[\frac{\partial^2 u(.,x,y)}{\partial x^2} + \frac{\partial^2 u(.,x,y)}{\partial x^2}\right]$, $u(.,0,y) = u(.,x,0) = 0$, $0 < x,y < 1$, $u(.,1,y) = e^{it}\sin(\pi y)$, $0 < y < 1$, $u(.,x,1) = e^{it}\sin(\pi x)$, $0 < x < 1$, is not a self-adjoint operator. But we still have numerically good convergence results. In order to obtain numerical approximation of this problem let us use first order of accuracy Rothe difference scheme as follows:

$$i\frac{u_{n,m}^k - u_{n,m}^{k-1}}{\tau} - \left[\frac{u_{n+1,m}^k - 2u_{n,m}^k + u_{n-1,m}^k}{h^2} + \frac{u_{n,m+1}^k - 2u_{n,m}^k + u_{n,m-1}^k}{\sigma^2}\right] = f(t_k,x_n,y_m), 1 \le k \le N,\ 1 \le n \le M-1,\ 1 \le m \le L-1, \quad (6)$$

$$u_{n,m}^0 = \sin(\pi x_n y_m), 1 \le n \le M-1,\ 1 \le m \le L-1 \quad (7)$$

$$u_{0,m}^k = u_{n,0}^k = 0, 1 \le k \le N, 1 \le n \le M-1,\ 1 \le m \le L-1, \quad (8)$$

$$u_{M,m}^k = e^{it_k}\sin(\pi y_m), 1 \le k \le N, 1 \le m \le L-1, \quad (9)$$

$$u_{n,L}^k = e^{it_k}\sin(\pi x_n), 1 \le k \le N, 1 \le n \le M-1, \quad (10)$$

In order to solve this difference scheme using modified Gauss elimination method we followed two ways. First way is as follows:

2.1. Modified Gauss elimination with respect to time

Write the difference scheme as

For $1 \le k \le N$

$$au_{n,m-1}^k + \left[bu_{n-1,m}^k + cu_{n,m}^k + bu_{n+1,m}^k\right] + au_{n,m+1}^k = f(t_k,x_n,y_m) + du_{n,m}^{k-1} \quad (11)$$

Where $a = -\frac{1}{\sigma^2}$, $b = -\frac{1}{h^2}$, $c = \frac{i}{\tau} + \frac{2}{h^2} + \frac{2}{\sigma^2}$, $d = \frac{i}{\tau}$

Hence this system can be written in matrix form as

$$AU_{m-1}^k + BU_m^k + AU_{m+1}^k = D\varphi_m^k, 1 \le m \le L-1, \quad (12)$$

$U_0^k = 0$ and $U_L^k = \begin{bmatrix} e^{it_k}\sin(\pi x_0) \\ e^{it_k}\sin(\pi x_1) \\ \vdots \\ e^{it_k}\sin(\pi x_M) \end{bmatrix}$.

where

$$\varphi_m^k = \begin{bmatrix} \varphi_{0,m}^k \\ \varphi_{1,m}^k \\ \dots \\ \varphi_{M,m}^k \end{bmatrix}$$

$$\varphi_{n,m}^k = \begin{cases} 0, & n = 0 \\ f(t_k,x_n,y_m) + du_{n,m}^{k-1}, & 1 \le n \le M-1 \\ e^{it_k}\sin(\pi y_m), & n = M \end{cases}$$

$$A=\begin{bmatrix}0&0&0&\dots&0&0&0\\0&a&0&\dots&0&0&0\\0&0&a&\dots&0&0&0\\..&\dots&\dots&\dots&\dots&\dots&\dots\\0&0&0&\dots&0&a&0\\0&0&0&\dots&0&0&a\\0&0&0&\dots&0&0&0\end{bmatrix},$$

$$B=\begin{bmatrix}1&0&0&0&\dots&0&0&0\\0&b&c&b&\dots&0&0&0\\0&0&b&c&\dots&0&0&0\\0&0&0&b&\dots&0&0&0\\0&..&\dots&\dots&\dots&\dots&\dots&\dots\\0&0&0&0&\dots&c&b&0\\0&0&0&0&\dots&b&c&b\\0&0&0&0&\dots&0&0&1\end{bmatrix}$$

D is an identity matrix of order $M+1$ and $U_s^k=\begin{bmatrix}u_{0,s}^k\\u_{1,s}^k\\..\\u_{M,s}^k\end{bmatrix}$, $s=m-1,m,m+1$.

In order to solve the matrix equation (12), we have applied a modified Gauss elimination method with respect to m with matrix coefficients. According this method we are looking for a solution in the form, $U_m^k=\alpha_{m+1}^k U_{m+1}^k+\beta_{m+1}^k, m=L-1,\dots,2,1,0,$ Here $\alpha_j^k,(j=1,\dots,L-1)$ are square matrices of order $M+1$ and $\beta_j^k,(j=1,\dots,L-1)$ are column vectors with dimension $M+1$. Using the fact that $U_0^k=0$, we have α_1^k is a zero matrix of order $M+1$ and β_1^k is zero column vector of dimension $M+1$. For α_j^k and $\beta_j^k,(j=1,\dots,L-1)$ and for the detail the reader is referred to the article Ashyaralyev and Sırma (2008).

For each k, starting from $U_L^k=\begin{bmatrix}e^{it_k}\sin(\pi x_0)\\e^{it_k}\sin(\pi x_1)\\..\\e^{it_k}\sin(\pi x_M)\end{bmatrix}$, we obtain U_m^k $m=L-1,\dots,2,1$. So for each $k,(k=1,\dots N)$ obtaining the solution U_m^k $m=L-1,\dots,2,1$, we obtained the approximate solution of Eqn. (1) with corresponding intial and boundary conditions.

2.2. Modified Gauss elimination with respect to space

In order to solve the Rothe difference scheme (6)-(10) we will apply modifed Gauss elimination method with respect to space variable. For this write the difference scheme as

$$au_{n,m-1}^k+\left[bu_{n-1,m}^k+au_{n,m}^{k-1}+cu_{n,m}^k+bu_{n+1,m}^k\right]+au_{n,m+1}^k=f(t_k,x_n,y_m) \qquad (13)$$

Hence this system can be written in matrix form as

$$EU_{m-1}+FU_m+EU_{m+1}=D\varphi_m, 1\le m\le L-1, \qquad (14)$$

U_0 =0 and $U_L=\begin{bmatrix}e^{it_0}\sin(\pi x_0)\\e^{it_0}\sin(\pi x_1)\\..\\e^{it_0}\sin(\pi x_M)\\e^{it_1}\sin(\pi x_0)\\e^{it_1}\sin(\pi x_1)\\..\\e^{it_1}\sin(\pi x_M)\\\dots\\\dots\\e^{it_N}\sin(\pi x_0)\\e^{it_N}\sin(\pi x_1)\\..\\e^{it_N}\sin(\pi x_M)\end{bmatrix}$.

where

$$\varphi_m=\begin{bmatrix}\varphi_{0,m}^0\\\varphi_{1,m}^0\\\dots\\\varphi_{M,m}^0\\\varphi_{0,m}^1\\\varphi_{1,m}^1\\\dots\\\varphi_{M,m}^1\\\dots\\\dots\\\varphi_{0,m}^N\\\varphi_{1,m}^N\\\dots\\\varphi_{M,m}^N\end{bmatrix}$$

$$\varphi_{n,m}^k=\begin{cases}0,\ n=0\\f(t_k,x_n,y_m), \quad 1\le n\le M-1\\e^{it_k}\sin(\pi y_m),n=M\\\sin(\pi x_n y_m),k=0\end{cases}$$

$$E=\begin{bmatrix}0&0&0&\dots&0&0&0\\0&A&0&\dots&0&0&0\\0&0&A&\dots&0&0&0\\..&\dots&\dots&\dots&\dots&\dots&\dots\\0&0&0&\dots&A&0&0\\0&0&0&\dots&0&A&0\\0&0&0&\dots&0&0&A\end{bmatrix}$$

$$F=\begin{bmatrix}I&0&0&0&\dots&0&0&0\\0&A&B&0&\dots&0&0&0\\0&0&A&B&\dots&0&0&0\\0&0&0&A&\dots&0&0&0\\\dots&\dots&\dots&\dots&\dots&\dots&\dots&\dots\\0&0&0&0&\dots&B&0&0\\0&0&0&0&\dots&A&B&0\\0&0&0&0&\dots&0&A&B\end{bmatrix}$$

$$U_s = \begin{bmatrix} u_{0,s}^0 \\ u_{1,s}^0 \\ \cdot\cdot \\ u_{M,s}^0 \\ u_{0,s}^1 \\ u_{1,s}^1 \\ \cdot\cdot \\ u_{M,s}^1 \\ \cdots \\ \cdots \\ u_{0,s}^N \\ u_{1,s}^N \\ \cdot\cdot \\ u_{M,s}^N \end{bmatrix}, s = m-1, m, m+1.$$

and D is an identity matrix of order $(N+1)\times(M+1)$.

In order to solve the matrix equation (14), we have applied a modified Gauss elimination method with respect to m with matrix coefficients. According this method we are looking for a solution in the form,

$$U_m = \alpha_{m+1}U_{m+1} + \beta_{m+1}, m = L-1, \ldots, 2,1,0.$$

Here $\alpha_j, (j = 1, \ldots, L-1)$ are square matrices of order $(N+1)(M+1)$ and $\beta_j, (j = 1, \ldots, L-1)$ are column vectors with dimension $M+1$. Using the fact that $U_0^k = 0$, we have α_1 is a zero matrix of order $(N+1)(M+1)$and β_1 is zero column vector of dimension $(N+1)(M+1)$. For α_j and $\beta_j, (j = 1, \ldots, L-1)$ and for the detail the reader is referred to the article Ashyaralyev and Sırma (2008).

For each k, starting from U_L, we obtain U_m $m = L-1, \ldots, 2,1$. So for each $k, (k = 1, \ldots N)$ obtaining the solution U_m $m = L-1, \ldots, 2,1$, we obtained the approximate solution of Eqn. (1) with corresponding initial and boundary conditions.

2.3 Standart Inverse Matrix Method

In order to solve the system (6)-(10) using standart inverse matrix method, write the system (6)-(10) in a form $GU = \varphi$, where G is coefficient matrix of dimension $(L+1)(M+1)(N+1)$, $U = \{u_{n,m}^k,\ 0 \le k,n,m \le N,M,L\}$ unknown vector and φ is a right hand side. Then $U = G^{-1}\varphi$ give us the solution of the system (6)-(10).

Now let us give another example with a self-adjoint operator:

$$i\frac{\partial u(t,x,y)}{\partial t} - \left[\frac{\partial^2 u(t,x,y)}{\partial x^2} + \frac{\partial^2 u(t,x,y)}{\partial x^2}\right] = f(t,x,y) \quad (15)$$

$$u(0,x,y) = \sin(\pi x)\sin(\pi y),\ 0 < x,y < 1, \quad (16)$$

$$u(t,0,y) = u(t,x,0) = 0,\ \ 0 < t,x,y < 1, \quad (17)$$

$$u(t,1,y) = u(t,x,1) = 0,\ \ 0 < t,y < 1, \quad (18)$$

where $f(t,x,y) = [2\pi^2 - 1]e^{it}\sin(\pi x)\sin(\pi y)$. Exact solution of this problem is $u(t,x,y) = e^{it}\sin(\pi x)\sin(\pi y)$. In this case, the operatör $A(u(.,x,y)) = -\left[\frac{\partial^2 u(.,x,y)}{\partial x^2} + \frac{\partial^2 u(.,x,y)}{\partial x^2}\right]$, $u(.,0,y) = u(.,x,0) = 0,\ \ 0 < x,y < 1,\ \ \ u(.,1,y) = u(.,x,1) = 0,\ 0 < x,y < 1,$ is self-adjoint in a Hilbert space $H = L_2([0,1]\times[0,1])$. So this problem satisfies the conditions given in Ashyaralyev and Sırma (2008). Hence it satisfies all the stability results given there.

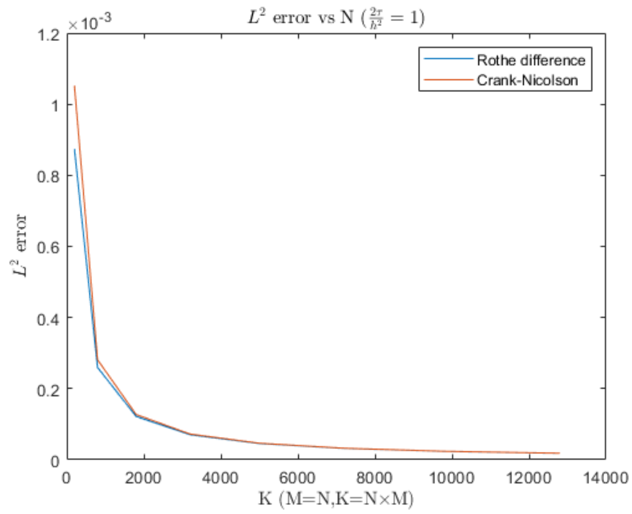
Now, in the next section we will also apply the three methods given above to find the solution of Rothe difference scheme related to two dimensional in space Schrödinger equation (1) with the corresponding initial and boundary conditions (2)-(5). Numerical results will be given below.

3. Results and Discussion

In this section we will give the numerical results for the approximate solution of problem (1)-(4). To find approximate solution of problem (1)-(4), we have applied first order of accuracy Rothe difference scheme (Rt) and second order of accuracy Crank-Nicholson difference scheme (C-N). In order to solve these difference schemes, we have applied the three methods mentioned above, namely modified Gauss elimination method with respect to time, modified Gauss elimination method with respect to space and standart inverse matrix method. Then Matlab is used to find the approximate solution by these three methods. Since equations are linear and finite these three methods give the same results. The results are given by the following tables and graphs.

Table 1. Errors between exact solution and numerical solutions with different space (N,M) and time (K) discretizations.

N	M	K ($\times 100$)	Rt L_2 *error* ($\times \mathbf{10^{-3}}$)	C-N L_2 *error* ($\times \mathbf{10^{-3}}$)
10	10	2	0.8740	1.100
20	20	8	0.2596	0.2811
30	30	18	0.1219	0.1274
40	40	32	0.0704	0.0723
50	50	50	0.0457	0.0466
60	60	72	0.0320	0.0324
70	70	98	0.0237	0.0239
80	80	128	0.0182	0.0183



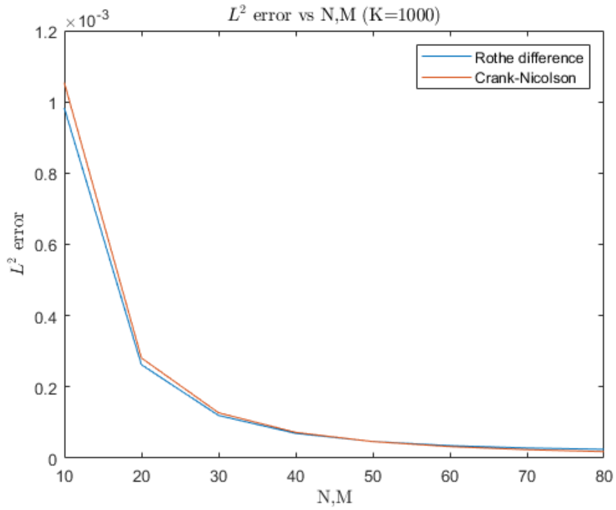
Graph 1. Convergence of Rothe and Crank Nicholson difference schemes with respect to time while keeping $\frac{2\tau}{h^2}$ ratio is equal to 1

In Table 1 and Graph 1, the errors between exact solution and numerical solution in L_2 norm for the two-dimensional

Schrodinger equation (1) with the initial and boundary conditons (2)-(4) using Rothe difference scheme and Crank Nicholson difference scheme for different number of space and time discretizations are given. In Table 1 and Graph 1, the number of time and space discretizations $\boldsymbol{K}$, $\boldsymbol{N}$ and $\boldsymbol{M}$ are chosen in such a way that $\boldsymbol{N}=\boldsymbol{M}$ and $\frac{2\tau}{h^2}=\mathbf{1}$. With these settings for the number of discretizations, it is seent that for both Rothe difference scheme and Crank-Nicholson difference scheme numerical solution converges to exact solution with the same rate of convergence and nearly quadratically.

Table 2. Errors between exact solution and numerical solutions with different space (N, M) discretizations

N	M	K (×1000)	Rt L_2 *error* (× 10^{-3})	C-N L_2 *error* (× 10^{-3})
10	10	1	0.9829	1.0541
20	20	1	0.2623	0.2812
30	30	1	0.1199	0.1274
40	40	1	0.0696	0.0723
50	50	1	0.0468	0.0465
60	60	1	0.0351	0.0324
70	70	1	0.0286	0.0239
80	80	1	0.0248	0.0183

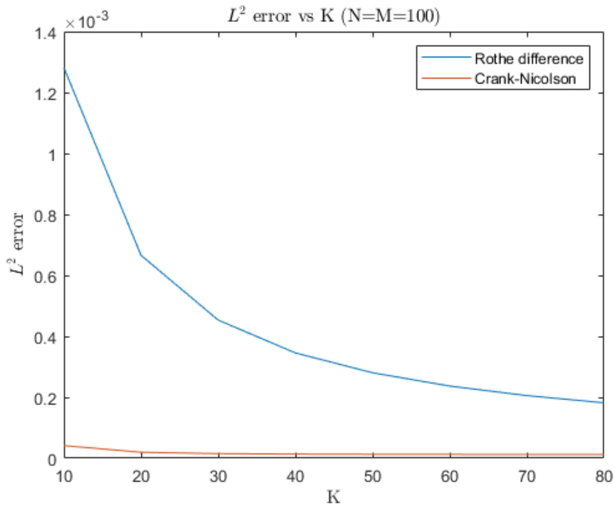


Graph 2. Convergence of Rothe and Crank Nicholson difference schemes with respect to space

In Table 2 and Graph 2, the errors between exact solution and numerical solution in L_2 norm for the two-dimensional Schrodinger equation (1) with the initial and boundary conditons (2)-(4) using Rothe difference scheme and Crank Nicholson difference scheme for the time discretizations $\boldsymbol{K}=\mathbf{1000}$ but for different space discretizations are given. In Table 2 and Graph 2, for the number of spaces discretizations $\boldsymbol{N}=\boldsymbol{M}=$10, 20, 30, …, 80 the errors are given. Here also for both Rothe difference scheme and Crank-Nicholson difference scheme error behaves with the same pattern. With this choice of number of discretizations, it is seen that error decreases quadratically for both Rothe difference scheme and Crank-Nicholson difference scheme. This result is in line with the theory.

Table 3. Errors between exact solution and numerical solutions with different time (K) discretizations

N	M	K	Rt L_2 *error* (× 10^{-3})	C-N L_2 *error* (× 10^{-3})
100	100	10	1.2819	0.0415
100	100	20	0.6659	0.0197
100	100	30	0.4533	0.0152
100	100	40	0.3456	0.0136
100	100	50	0.2805	0.0129
100	100	60	0.2369	0.0125
100	100	70	0.2056	0.0123
100	100	80	0.1820	0.0122



Graph 3. Convergence of Rothe and Crank Nicholson difference schemes with respect to time

In Table 3 and Graph 3 the errors are given for fixed value of $\boldsymbol{N}=\boldsymbol{M}=\mathbf{100}$ but for different value of time discretizations. From Table 3 and Graph 3 it is seen that the for the Rothe difference scheme numerical solution converges to exact solution with the order one but unfortunately for the Crank-Nicholson difference scheme the rate of converges is so slow.

Table 4. Running times of each approach, (Modified Gauss Elimination with respect to space MG_S*, Modified Gauss elimination with respect to time* MG_T *and Inverse Matrix method InvM)*

N	M	K	MG_S (s)	MG_T (s)	InvM (s)
10	10	10	0.005	0.030	0.008
20	20	20	0.031	0.420	0.032
30	30	30	0.113	3.515	0.114
40	40	40	0.292	18.494	0.346
50	50	50	0.735	82.497	0.691

In Table 4, running times of each approach is given to compare their computational complexities. As seen in the table, standard inverse matrix method has lowest computational complexity. Modified Gaussian method requires to use more memory space and computational resourse for square matrices $\boldsymbol{\alpha}$ and column vectors $\boldsymbol{\beta}$. As a result, running times are higher for Modified Gauss Elimination methods. Further, the size of matrix $\boldsymbol{\alpha}$ for Modified Gauss Elimination with respect to space is in the order of $\boldsymbol{N}$ whereas it is is in the order of $\boldsymbol{NxK}$ for Modified Gauss Elimination with respect to time. This affects the running times as seen in the Table.

4. Conclusions and Recommendations

In this article, to find approximate solution of Schrödinger equation in two dimension, Rothe difference scheme and Crank-Nicholson difference scheme are applied. To solve these difference schemes three approaches are used. The first approach is the modified Gauss elimination method with respect to time, second one is the modified Gauss elimination method with respect to space and last is the standart inverse matrix method. Using these methods, the same numerical results are obtained. When spaces discretizations are fixed but the time discretizations are increasing the Crank-Nicholson difference scheme converges quadratically and reaches steady state. The cases are in line with theory. Running times of each approaches are compared. These three approaches can be applied to solve difference schemes for obtaining approximate solutions of nonlocal boundary value problem for the Schrödinger equation in two dimensions. But in this problem, one should be careful about obtaining approximation for the initial value.

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