Numerical Treatment of Allen's Equation Using Semi Implicit Finite Difference Methods

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Doi: 10.23918/eajse.v8i1p90

Abstract. This paper aims to propose the semi implicit finite difference method for discretizing Cahn-Allen equation. The stability and convergence analysis are proved. It is shown that the suggest scheme is stable for the usage of the Fourier-Von Neumann technique. The accuracy of the proposed method is first order in time and second order in space. A comparison between the numerical and the exact solutions is supported with two examples. Numerical results are shown that there is a good agreement between the approximate solution and exact solution.

Keywords: Allen Equation, Semi Implicit Finite Difference, Stability of Allen Equation

1. Introduction

This paper is devoted to study the numerical analysis of Allen equation. Allen-Cahn equation was originally introduced by Allen and Cahn (1979) and can be regarded as a second-order stiff nonlinear partial differential equation that is utilized in material sciences as a reaction-diffusion equation and in computational fluid dynamics as a convection-diffusion equation. In crystalline materials, the Allen–Cahn model is used to describe the migration of phase boundaries. (Allen & Cahn, 1979).

Consider the following generalized Allen's equation

$$\frac{\partial u(x,t)}{\partial t} - D\frac{\partial^2 u(x,t)}{\partial x^2} = f(u, x, u(x,t)) \quad, (x,t) \in [a,b] \times [0,T], \qquad [1]$$

$$u(x,0) = f(x),$$

$$x \in [a,b], \qquad [2]$$

$$u(a,t) = -1,\ u(b,t) = 1,$$

$$x \in [a,b]. \qquad [3]$$

The nonlinear source term $f(u, x, u(x,t))$ satisfies Lipschtiz condition with respect to u that is

Received: April 2, 2022
Accepted: May 27, 2022
Sabawi, Y.A., Ahmed, S.B., & Hamad, H.Q. (2022). Numerical Treatment of Allen's Equation Using Semi Implicit Finite Difference Methods. *Eurasian Journal of Science and Engineering*, *8*(1), 90-100.

$$|f(u,x,u) - f(u,x,v)| \leq L_F|u-v|.$$

For $f(u) = u(1-u^2)$ Eq. (1) becomes Allen's equation . Most recently, some serious methods have been developed in order to solve nonlinear differential equation for example see, Manaa, Moheemmeed, and Hussien (2010); Hussein (2011); Sabawi, Pirdawood, and Khalaf (2021); Sabawi, Pirdawood, and Rasool (2021); Sabawi, Pirdawood, and Sadeeq (2021); Pirdawood & Sabawi, (2021), Sabawi (2017); Sabawi, Dhumal, & Kiwne, (2018), Sabawi, (2020); Sabawi, (2021). Various numerical methods have been used to solve Allen-Cahn equation one of which is the finite difference method (Huang & Abduwali, 2011; Bulut, 2017; Villarreal, 2020).

The aim of this work is to recommend a numerical method for solving (1-3) that is first order accurate time compound and second order in space. The idea is use Euler's backward method to discretize time derivative and lagging nonlinearity to the previous known level of time. The stability is given. Furthermore, the accuracy in terms of the errors is analyzed.

The rest of this paper is structured as follows. In Section 2, the model problem and semi implicit finite difference method are introduced. Section 3, the stability and convergence analysis are considered. Numerical results are shown in section 4. Finally, conclusion is given in section 5.

2. Semi Implicit Finite Difference Method

We describe the domain with uniform mesh, we can consider a numerical method of implicit-explicit nature: the linear terms are treated implicitly whereas the non-linear coefficients are treated explicitly. More specifically, we seek approximations u_i^n of the function values u(t_n, x_i) for $n = 0, \dots, N_{t-1}$and $i = 1, \dots, N_x$ satisfying the following system of linear equations:

To start with, using Euler's backward method to discretize time derivative and lagging nonlinearity to the previous known level of time, we have the following fully discrete problem:

$$\frac{\partial u}{\partial t} - D\frac{\partial^2 u}{\partial x^2} = u(1-u^2) \quad , (x,t) \in [a,b] \times [0,T], \qquad [4]$$

$$\frac{u_i^{n+1} - u_i^n}{k} - D\frac{u_{i+1}^{n+1} - 2u_i^{n+1} + u_{i-1}^{n+1}}{h^2} = u_i^{n+1}(1-(u_i^n)^2), \qquad [5]$$

which leads to the following

$$u_i^{n+1} - u_i^n = \frac{kD}{h^2}(u_{i+1}^{n+1} - 2u_i^{n+1} + u_{i-1}^{n+1}) + ku_i^{n+1}(1-(u_i^n)^2),$$

$$u_i^{n+1} = R(u_{i+1}^{n+1} - 2u_i^{n+1} + u_{i-1}^{n+1}) + ku_i^{n+1}(1-(u_i^n)^2) + u_i^n,$$

where $R = \frac{kD}{h^2}$. Above equation can be written in tridiagonal form as,

$$A_i u_{i-1}^{n+1} + B_i u_i^{n+1} + C_i u_{i+1}^{n+1} = D_{i,} \qquad [6]$$

where A_i and C_i are constants, so $A_i = C_i = (-R)$ and $B_i = 1 + 2R - k(1-(u_i^n)^2)$.

Assembling the entire system of equations and applied boundary conditions, gives

$$\begin{bmatrix} B_1 & -R & 0 & & \\ -R & B_2 & -R & & \\ & \ddots & \ddots & \ddots & \\ & & -R & B_{M-1} & -R \\ & & 0 & -R & B_M \end{bmatrix} \begin{pmatrix} u_1^{n+1} \\ u_2^{n+1} \\ \vdots \\ \vdots \\ u_{\mathrm{N}-1}^{n+1} \\ u_{\mathrm{N}}^{n+1} \end{pmatrix} = \begin{pmatrix} u_1^{n} \\ u_2^{n} \\ \vdots \\ \vdots \\ u_{\mathrm{N}-1}^{n} \\ u_{\mathrm{N}}^{n} \end{pmatrix}.$$

3. Stability and Convergence Analysis of the of the Semi Implicit Method

3.1 Stability Analysis

In this section, we proved stability of a numerical scheme. The stability of numerical schemes can be investigated by performing von Neumann stability.

$$u_i^n = \xi^n e^{j\alpha i}$$

into the approximate difference scheme and then to find a characteristic equation for the amplification factor ξ.

Lemma 3.1. The semi-implicit finite different scheme for (1) is stable under the condition

$$k \leq \frac{h^2}{(4-h^2)}.$$

Proof: To begin with, we recall (2), such that

$$u_i^{n+1} = u_i^n + R(u_{i+1}^{n+1} - 2u_i^{n+1} + u_{i-1}^{n+1}) + ku_i^{n+1}(1-(u_i^n)^2), \quad [7]$$

which can be rearranged as

$$u_i^{n+1} = \frac{1}{(1+2R)}u_i^n + \frac{R}{(1+2R)}(u_{i+1}^{n+1} + u_{i-1}^{n+1}) + \frac{1}{(1+2R)}ku_i^{n+1}(1-(u_i^n)^2). \quad [8]$$

Using trial solution of the form

$u_i^n = \xi^n e^{j\alpha i}, u_{i+1}^{n+1} = \xi^{n+1} e^{j\alpha(i+1)} = u_i^{n+1}e^{j\alpha}, u_{i-1}^{n+1} = u_i^{n+1}e^{-j\alpha}$ and substituting back in (8) reads

$$\xi u_i^n = \frac{1}{(1+2R)}u_i^n + \frac{R}{(1+2R)}\left(\xi^{n+1}e^{j\alpha(i+1)} + \xi^{n+1}e^{j\alpha(i-1)}\right) + \frac{1}{(1+2R)}k\xi^{n+1}e^{j\alpha i}(1-(\xi^n e^{j\alpha i})^2).$$

Divide the above expression by u_i^n and considering $e^{j\alpha} + e^{-j\alpha} = 2\cos\alpha = 2 - 4sin^2\frac{1}{2}\alpha$, imply that

this gives

$$\xi = \frac{1}{(1+2R)} + \frac{R}{(1+2R)}\xi\left(2 - 4sin^2\frac{1}{2}\alpha\right) + \frac{1}{(1+2R)}k\xi(1-(u_i^n)^2)$$

$$\xi\frac{1}{(1+2R)}\left(R\left(2-4sin^2\frac{1}{2}\alpha\right) - k(1-(u_i^n)^2)\right) = \frac{1}{(1+2R)}$$

$$\xi = \frac{1}{R\left(2 - 4sin^2\frac{1}{2}\alpha\right) - k(1 - (u_i^n)^2)}$$

$$|\xi| \leq 1 \rightarrow \left|\frac{1}{R\left(2 - 4sin^2\frac{1}{2}\alpha\right) - k(1 - (u_i^n)^2)}\right| \leq 1$$

$$-1 \leq \frac{1}{R\left(2 - 4sin^2\frac{1}{2}\alpha\right) - k(1 - (u_i^n)^2)} \leq 1.$$

Since $0 \leq sin^2\frac{1}{2}\alpha \leq 1$, then

$$-1 \leq \frac{1}{-2R - k(1 - (u_i^n)^2)} \leq 1.$$

Subtracting each side by 1 and multiply by -1 we will obtain

Therefore,

$$0 < \frac{1}{2R - k(1 - (u_{min})^2)} < 2.$$

Since $R = \frac{k}{h^2}$, gives

$$0 < \frac{1}{2R - k} < 2$$

$$1 \leq 4R - 2k(1 - (u_i^n)^2) \rightarrow k(1 - (u_i^n)^2) \leq 4\frac{k}{h^2} - 1 \rightarrow kh^2(1 - (u_i^n)^2) \leq 4k - h^2.$$

This gives

$h^2 \leq 4k - kh^2(1 - (u_i^n)^2)$

$$k \leq \frac{h^2}{(4 - h^2)}.$$

3.2 Convergence Analysis

First, we analyze the accuracy of the semi implicit scheme. The scheme is expanded by Taylor series at the point, respectively. To analyse the error of approximation, we assume that the exact solution u is twice continuously exact differentiable with respect to the time variables and four times continuously differentiable with respect to the space variable. We define the truncation error for this method the truncation error is given if we substitute the solution into the numerical scheme. The following lemma describes how well the truncation error approximates the original problem.

Lemma 3.2: Let the exact solution u is twice continuously differentiable with respect to the time variables and four times continuously differentiable with respect to the space variable, then truncation error of (1) defined as

$$T_i^n \leq \frac{k}{2}\mathcal{M}_{tt} + \frac{h^2}{12}\mathcal{M}_{xxxx}$$

$\mathcal{M}_{tt} = max|u_{tt}(\mathrm{t,x})|$, $\mathcal{M}_{xxxx} = max|u_{xxxx}(\mathrm{t,x})|$ and the maxima are taken over all

$$(t,x) \in [0,T_f] \times [a,b]$$

Proof. Recalling

$$T_i^n = \frac{u(t_{n+1},x_i) - u(t_n,x_i)}{k} - \frac{u(t_n,x_{i+1}) - 2u(t_n,x_i) + u(t_n,x_{i-1})}{h^2} - u_i^{n+1}(1-(u_i^n)^2). \quad [9]$$

Applying Taylor's series expansion, this becomes

$$\frac{u(t_{n+1},x_i) - u(t_n,x_i)}{k} = \frac{u(t_{n+\mathrm{k}},x_i) - u(t_n,x_i)}{k} = \frac{u(t_n,x_i) + k\frac{u_t(t_n,x_i)}{1!} + k^2\frac{u_{tt}(t_n,x_i)}{2!} + k^3\frac{u_{ttt}(\rho_n,x_i)}{3!}}{k}$$

$$= u_t(t_n,x_i) + \frac{k}{2}u_{tt}(\rho_n,x_i) + k^2\frac{u_{ttt}(\rho_n,x_i)}{3!}, \quad \rho_n \in (t_n,t_{n+1}) \quad [10]$$

$$u(t_n,x_{i+1}) = u(t_n,x_i) + u_x(t_n,x_i) + \frac{h^2}{2!}u_{xx}(t_n,x_i) + \frac{h^3}{3!}u_{xxx}(t_n,x_i) + \frac{h^4}{4!}u_{xxxx}(t_n,\zeta_i),$$

$$\zeta_i \in (x_i,x_{i+1}), \quad [11]$$

$$u(t_n,x_{i-1}) = u(t_n,x_i) - u_x(t_n,x_i) + \frac{h^2}{2!}u_{xx}(t_n,x_i) - \frac{h^3}{3!}u_{xxx}(t_n,x_i) + \frac{h^4}{4!}u_{xxxx}(t_n,\varepsilon_i),$$

$$\xi_i \in (x_{i-1},x_i). \quad [12]$$

Substituting (7), (8) and (9) in (5), gives

$$T_i^n = \frac{\partial u}{\partial t} - D\frac{\partial^2 u}{\partial x^2} - u_i^{n+1}(1-(u_i^n)^2) + \frac{k}{2}u_{tt}(\rho_n,x_i) - \frac{h^2}{24}\left(u_{xxxx}(t_n,\xi_i) + u_{xxxx}(t_n,\zeta_i)\right).$$

Local Truncation error for above equation can be written as,

$$T_i^n = \lim_{k,h\to 0}\left(\frac{k}{2}u_{tt}(\rho_n,x_i)\frac{k^2}{6}u_{tt}(\rho_n,x_i) - \frac{h^2}{12}u_{xxxx}(t_n,\xi)\right) + \cdots = 0$$

Tkeorem 3.1. Suppose that $u(x,t)$ satisfies the smooth condition of lemma 3.2 and the semi implicit scheme for Allan Eq (1) is convergent, and we have

$$\max_{1\le i\le N_x}|u(t_n,x_i) - u_i^n| \le \frac{exp(L_F T_f) - 1}{L_F}\left(\frac{k}{2}\mathcal{M}_{tt} + \frac{h^2}{12}\mathcal{M}_{xxxx}\right),$$

for $i = 1,\ldots N_t$.

Proof. For brevity, we shall denote by $e_i^n := u(t_n,x_i) - u_i^n$ the error on each node (t_n,x_i); notice that $e_i^0 := u_0(x_i) - u_i^0 = 0$. From the definition of the truncation error (4), we obtain

$$T_i^n := \frac{u(t_{n+1},x_i) - u(t_n,x_i)}{k} - \frac{u(t_{n+1},x_{i+1}) - 2u(t_{n+1},x_i) + u(t_{n+1},x_{i-1})}{h^2} - f(u_i^n), \quad [13]$$

and our numerical scheme (5) is equivalent to

$$\frac{U_i^{n+1}-U_i^n}{k}-D\,\frac{U_{i+1}^{n+1}-2U_i^{n+1}+U_{i-1}^{n+1}}{h^2}=f(U_i^n). \quad [14]$$

Subtracting (10) from (11), gives

$$\frac{u(t_{n+1},x_i)-U_i^{n+1}-u(t_n,x_i)+U_i^n}{k}-\frac{u(t_{n+1},x_{i+1})-U_i^n-2u(t_{n+1},x_i)-2U_i^{n+1}+u(t_{n+1},x_{i-1})-U_{i-1}^{n+1}}{h^2}$$
$$-f(u_i^n)+f(U_i^n),$$

Setting $e_i^n := u(t_n,x_i)-u_i^n$, this gives

$$T_i^n=\frac{e_i^{n+1}-e_i^n}{k}-\frac{e_{i+1}^{n+1}-2e_i^{n+1}+e_{i-1}^{n+1}}{h^2}-f(u_i^n)+f(U_i^n)$$

$$\mathrm{k}\big(f(u_i^n)-f(U_i^n)\big)+kT_i^n+e_i^n=(1+2\mathrm{R})e_i^{n+1}+Re_{i+1}^{n+1}+\mathrm{R}e_{i-1}^{n+1}.$$

Define

$$E^n=\max_{1\le i\le N_x}\{|e_i^{n+1}|\}$$

i.e., the maximum error at the n-th time-step, then taking the maximum with respect to i on the right-hand side of (4.12), we arrive to

Applying Lipchitz condition on the nonlinear term, gives

$$|f(u_i^n)-f(U_i^n)|\le L_F|u_i^n-U_i^n|\le L_F|e_i^n|$$

which implies

$$e_i^{n+1}\le\tfrac{(1+\mathrm{k}L_F)}{(1+2\mathrm{R})}E^n+kT_i^n,$$

Or taking the maximum with respect to i, and using lemma 3.1, gives

$$E^{n+1}\le\frac{(1+\mathrm{k}L_F)}{(1+2\mathrm{R})}E^n+k\mathcal{T}_E,$$

where $\mathcal{T}_E=\frac{k}{2}\mathcal{M}_{tt}+\frac{h^2}{12}\mathcal{M}_{xxxx}$,

for $n=0,\dots,N_t-1$. This means that we have inductively

$$E^{n+1}\le(1+\mathrm{k}L_F)E^n+k\mathcal{T}_E,$$

showing that

$$E^n\le\left(\frac{(1+\mathrm{k}L_F)}{(1+2\mathrm{R})}\right)^n E^0+\left[1+\left(\frac{(1+\mathrm{k}L_F)}{(1+2\mathrm{R})}\right)+\cdots+\left(\frac{(1+\mathrm{k}L_F)}{(1+2\mathrm{R})}\right)^{n-1}\right]k\mathcal{T}$$

as $E^0=0$, being the maximum of $e_i^0=0$ with respect to i and $nk\le nN_t=T_f$, so we have

$$E^n\le\frac{\left(\frac{(1+\mathrm{k}L_F)}{(1+2\mathrm{R})}\right)^n-1}{\mathrm{k}L_F}\;k\mathcal{T}_E\le\frac{\left(\frac{(1+\mathrm{k}L_F)}{(1+2\mathrm{R})}\right)^{\frac{T_f}{k}}-1}{L_F}\;\mathcal{T}_E\le\frac{exp\big(L_FT_f\big)-1}{L_F}\;\mathcal{T}_E$$

The result now follows

4. Numerical Results

The goal of this section is to illustrate the performance of a presented method, through an implementation based on Mathematica programming. We measure the error between exact and approximation by

$$L_{abc} = |u(x_i) - u_h|$$

4.1 Example 1

We consider the initial boundary value problem (IBVP), the initial condition and boundary condition are

$$u_t - Du_{xx} = 0$$

$$u(x,0) = sinx$$

$$u(0,t)$$

$$u(1,t) = 0 \quad t > 0.$$

The exact solution to this IBVP is $u(x,t) = e^{-D\pi^2 t}\sin(\pi x)$.

Table 1: Semi implicit finite difference method where the number of intervals is *N* = 20, *D* = 0.01, *t* = 0.01.

xi	Semi implicit	Exact	present	Munguia, M., & Bhatta, D. (2015).
0.05	0.1562805251	0.1562801466	0.0000003785	0.0006416721
0.10	0.3087129049	0.3087121573	0.0000007477	0.0012675441
0.15	0.4535437485	0.4535426501	0.0000010984	0.0018622049
0.20	0.5872068398	0.5872054177	0.0000014221	0.0024110121
0.25	0.7064109499	0.7064092390	0.0000017108	0.0029004522
0.30	0.8082208779	0.8082189205	0.0000019574	0.0033184735
0.35	0.8901297256	0.8901275698	0.0000021558	0.0036547829
0.40	0.9501206252	0.9501183242	0.0000023011	0.0039010995
0.45	0.9867164018	0.9867140122	0.0000023897	0.0040513581
0.50	0.9990159459	0.9990135264	0.0000024195	0.0041018588
0.55	0.9867164018	0.9867140122	0.0000023897	0.0040513581
0.60	0.9501206252	0.9501183242	0.0000023011	0.0039010995
0.65	0.8901297256	0.8901275698	0.0000021558	0.0036547829
0.70	0.8082208779	0.8082189205	0.0000019574	0.0033184735
0.75	0.7064109499	0.7064092390	0.0000017108	0.0029004522
0.80	0.5872068398	0.5872054177	0.0000014221	0.0024110121
0.85	0.4535437485	0.4535426501	0.0000010984	0.0018622049
0.90	0.3087129049	0.3087121573	0.0000007477	0.0012675441
0.95	0.1562805251	0.1562801466	0.0000003785	0.0006416721

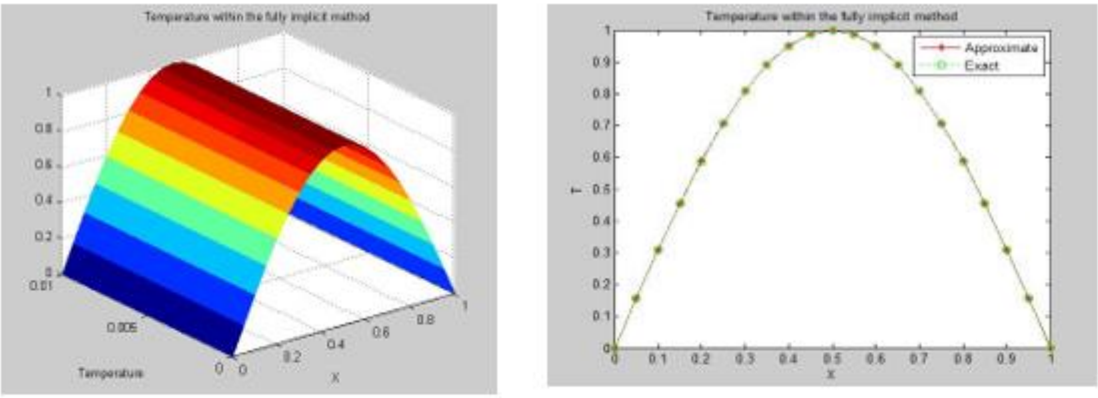

Figure 1: Numerical solution for 4.1 Example 1 by using semi implicit finite difference method

4.2 Example 2

Consider the following Allen's equation

$$u_t - \varepsilon u_{xx} = u - u^3 \qquad x \in [-1,1]\,, t \in (0,T]$$

$$\Omega = [-1,1] \times (0,T]$$

Initial condition:

$$u(x,0) = 0.53x + 0.47\sin(-1.5\pi x)$$

Boundary condition: $u(-1,t) = -1, \quad u(1,t) = 1$

Exact Solution:

$$u(x,t) = 0.53x + 0.47\sin(t - 1.5\pi x)$$

Table 2: Semi implicit finite difference method where the number of intervals is $N = 20$, $D = 0.01$, $t = 0.01$.

xi	Semi implicit	Exact	Absolute Error
-0.9	-0.8992193047	-0.8978858477	0.0013334570
-0.8	-0.7037407666	-0.7040475722	0.0003068057
-0.7	-0.4467567832	-0.4491625802	0.0024057971
-0.6	-0.1736673927	-0.1772391656	0.0035717730
-0.5	0.0676087332	0.0640002238	0.0036085094
-0.4	0.2360882955	0.2335218573	0.0025664381
-0.3	0.3066566963	0.3059255393	0.0007311570
-0.2	0.2755426936	0.2769815203	0.0014388267
-0.1	0.1611404822	0.1645525271	0.0034120448
0	0.0000000000	0.0046999217	0.0046999217
0.1	-0.1611404822	-0.1561772053	0.0049632769
0.2	-0.2755426936	-0.2714564310	0.0040862626
0.3	-0.3066566963	-0.3044550799	0.0022016164
0.4	-0.2360882955	-0.2364265687	0.0003382732
0.5	-0.0676087332	-0.0706469168	0.0030381836
0.6	0.1736673927	0.1682993834	0.0053680093
0.7	0.4467567832	0.4398784646	0.0068783186
0.8	0.7037407666	0.6964429392	0.0072978273
0.9	0.8992193047	0.8936184081	0.0056008966

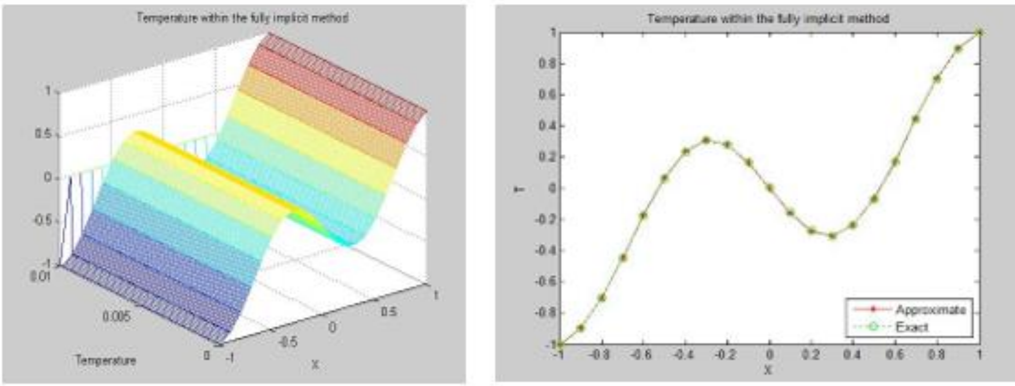

Figure 2: Numerical solution for 4.2 Example 2 by using semi implicit finite difference method

In Table 1, we have compared the absolute error with Munguia, M., & Bhatta, D. (2015). As it is seen from the table, the results obtained in the present study agree with in other studies and become better as time increases. In table 2, it is seen that there is a good agreement between approximate and exact solution that is mesh size decreases, the error decreases.

4. Conclusion

This study aims to apply semi implicit finite difference method in combination with the method of lagging in approximating the numerical solutions to the Cahn-Allen equation. Error analysis and stability are analyzed. The proposed method is first order in time and second order in space.

Furthermore, the behavior of the exact solution and approximate solution are examined graphically. The numerical results obtained by the proposed method are quite satisfactory from exact solution.

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