### Applied Mathematics & Information Sciences An International Journal

http://dx.doi.org/10.18576/amis/100418

# Error Estimates on a Stable and Reliable Numerical Scheme for a Fully Discrete Time-Dependent Allen-Cahn Equation

Pius W. M. Chin\*

Department of Mathematics and Applied Mathematics, University of Pretoria, Pretoria 0002, South Africa

Received: 31 Mar. 2016, Revised: 17 May 2016, Accepted: 18 May 2016

Published online: 1 Jul. 2016

**Abstract:** The stability analysis and error estimates are some of the well-known techniques carried out on a number of commonly used numerical schemes for Allen-Cahn equation. We exploit these techniques and design a reliable fully-discrete scheme consisting of coupling the Non-standard finite difference with the finite element method. We show that the solution obtained from this scheme is stabled and attains its optimal rate of convergence in both the  $H^1$  and  $L^2$ -norms. We further show that this scheme replicates the properties of the exact solution. Some numerical experiments are performed to support our theoretical analysis.

Keywords: Allen-Cahn equation; finite element method; nonstandard finite difference method; error estimates; energy stability.

### 1 Introduction

The time-dependent Allen-Cahn equation aries in the description of a variety of physical phenomena in science and engineering. These phenomena include problems such as the motion by mean curvature [16] and crystal growth [26] to mention a few. In summary, it is well-known for being a basic model equation for the diffuse interface approach developed to study the phase transitions and interfacial dynamics in materials science [7]. For more on the physical background and discussion of the model equation, we refer to [2,6,14,23].

The study of the error analysis of this equation has recently attracted considerable attention. The reason being the dependence of error bounds on the parameter  $\varepsilon \ll 1$ , appearing in the equation which we will clarify later. In this paper we consider the phase field model form of the problem represented by the equation

$$\frac{\partial u}{\partial t} - \Delta u + \frac{1}{\varepsilon^2} f(u) = 0 \text{ in } \Omega \times (0, T),$$
 (1)

with

$$\frac{\partial u}{\partial n} = 0 \text{ on } \partial\Omega \times (0, T)$$
 (2)

and

$$u(\cdot,0) = u_0 \text{ in } \Omega \times \{0\}. \tag{3}$$

where  $\Omega$  is a bounded smooth domain in  $\mathbb{R}^2$  with smooth boundary  $\partial \Omega$ , a fixed constant T > 0,  $\varepsilon$  a parameter representing the "interaction length" lying within the interval  $0 < \varepsilon \le 1$  and f a nonlinear function which will be specifically stated as we progress. Besides, the later specification of f, we will modify f without affecting the solution u and  $f \in C^1(\mathbb{R}^2)$  and assume that f and f' are Lipschitz continuous such that  $||f'(x)||_{L^{\infty}} \leq C$ where C is a Lipschitz constant of f and f' for convenience. Note should be taken at this stage that, since the nonlinear term f(u) in the numerical scheme (19)-(20) could yield some severe stability limitations in the time step, then we minimize these effects by performing a nonlocal approximation of f(u) in a special way as in (35) without affecting the solution of the problem u. An important feature of the Allen-Cahn equation is one which can be viewed as the gradient flow with the Liapunov energy functional

$$\mathscr{J}_{\varepsilon}(u) = \int_{\Omega} \Phi_{\varepsilon}(u) dx, \text{where } \Phi_{\varepsilon}(u) = 1/2 |\nabla u|^2 + \frac{1}{\varepsilon^2} F(u),$$

and F(u) is always positive in  $L^2(\Omega)$  and  $H^{-1}(\Omega)$  and f(u) = F'(u). The precise form in which we will be

<sup>\*</sup> Corresponding author e-mail: pius.chin@up.ac.za



making use of F(u) is as follows:

$$F(u) = 1/4(u^2 - 1)^2 \text{and} f(u) = u^3 - u.$$
 (4)

The numerical methods which have been designed and extensively used in the study of the time-dependent Allen-Cahn equation are among many, the finite difference method found in [8,11] and the a posteriori error estimate for the finite element approximation of the Allen-Cahn equation developed by Feng et al [15]. We also have the Quasi-optimal posteriori error estimate in  $L^{\infty}(0,T;L^2(\Omega))$  derived for the finite element approximation found in [5], the numerical approximation of the celebrated Allen-Cahn equation and related diffuse interface models found in [28] and the stabilized semi-implicit (in time) scheme and the splitting scheme for the Allen-Cahn equation introduced by Yang [27].

Instead of the methods stated above, we exploit a similar conceptual approach and present in this paper, a reliable technique consisting of coupling the nonstandard finite difference (NSFD) method in time and the finite element (FEM) method in the space variables. A similar approach was used for the first time using the diffusion equation in the non-smooth domain in [9] and the wave equation in a smooth domain [10]. Since these two problems were all linear, then our main aim in this paper is to extend the application of the above technique to solve the nonlinear parabolic problems of which the time-dependent Allen-Cahn equation is taken as an example. As regard the comparisons of the standard as well as the Nonstandard coupled with the finite element method we will refer to [9]. For other comparison of the standard and Non-standard finite difference methods we refer to [20]. The NSFD method was initiated by Mickens in [20] and major contributions to the foundation of the NSFD method could be seen in [3,4]. Since its initiation, the NSFD method has been extensively applied to a variety of concrete problems in physics, epidermeology, business sciences, engineering and biological sciences see [18, 19, 20, 21] for more details and also [24] for an overview. In this different framework our primary objective is to prove that the discrete solution obtained from this scheme is stable and attains its optimal rate of convergence in both the  $H^1$  and  $L^2$ -norms. The reliability of the technique comes from the fact that the NSFD-FEM method replicates the monotonicity properties of the solution of the decay equations.

The rest of the paper is organized as follows: In Section 2, we present notations and the function spaces together with some important properties needed for the study of the problem. Section 3 will be devoted to gather essential tools necessary to prove the main result of the paper. In Section 4 we will introduce the theory and state the main result of the paper together with its proof. A numerical example to confirm the validity of our main result will be presented in Section 5 and finally the conclusion and future remarks will be stated in Section 6.

### 2 Preliminaries

We specify in this section, the notation, spaces and properties that will be see in this paper. We depart in this section with the Sobolev spaces of real-valued functions defined on  $\Omega$  and denoted for  $r \geq 0$  by  $H^r(\Omega)$ . The norm on  $H^r(\Omega)$  will be denoted by  $\|\cdot\|_r$ . See [17] for the definitions and the relevant properties of these spaces. In a particular case, where r=0 the space  $H^0(\Omega):=L^2(\Omega)$  and its inner product together with the norm will be stated and denoted by

$$(u,v) = \int_{\Omega} u, v dx, \ u, v \in L^2(\Omega),$$

and

$$||u||_{L^2(\Omega)} = \{(u,u)\}^{1/2}, \ u \in L^2(\Omega).$$

Besides,  $C_0^\infty(\Omega)$  will denote the space of infinitely differentiable functions with support compactly contained in  $\Omega$ . The space  $H_0^1(\Omega)$  will denote the subspace of  $H^1(\Omega)$  obtained by completing  $C_0^\infty(\Omega)$  with respect to the norm  $\|\cdot\|_1$ . Following [17], for X a Hilbert space, we will more generally use the Sobolev space  $H^r[(0,t);X]$ , where  $r\geq 0$  and in the case when r=0 we will have  $H^0[(0,T);X]=L^2[(0,T);X]$  with norm

$$\|v\|_{L^2[(0,T);X]} = \left(\int_0^T \|v(\cdot,t)\|_X dt\right)^{1/2}.$$

In practice, X will be the Sobolev space  $H^m(\Omega)$  or  $H_0^1(\Omega)$ . Associated with (1) is the bilinear form

$$a(u,v) = \int_{\Omega} \nabla u \nabla v dx, \ u,v, \in H^{1}(\Omega),$$

and  $a(\cdot, \cdot)$  will be symmetric and positive definite. i.e.,

$$a(u, v) = a(v, u) \text{ and } a(u, u) \ge 0.$$
 (5)

### 3 Finite element method

We proceed under this section to gather essential tools necessary to prove the main result of this paper. We begin first by stating the following weak problem of (1)-(3): find  $u \in L^2[(0,T);H_0^1(\Omega)]$  such that

$$\left(\frac{\partial u(\cdot,t)}{\partial t},v\right) + \left(\nabla u(\cdot,t),\nabla v\right) = \varepsilon^{-2}\left(f(u(\cdot,t)),v\right),\tag{6}$$

$$(u(\cdot,t),v) = (u_0,v), \tag{7}$$

for all  $v \in H_0^1(\Omega)$  and  $t \in (0,T)$  a.e. For the existence and the uniqueness of a solution  $u(\cdot,t)$  of (6)-(7), refer to [13, 22] and [25]. Hence forth, in appropriate places to follow, additional conditions on the regularity of u which guarantee the convergence result will be imposed.

With the above continuous problem in place, we proceed to provide the discrete framework for stating the discrete version of (6)-(7). To this end, we let  $\mathcal{T}_h$  be a regular family of triangulations of  $\bar{\Omega}$  consisting of



compatible triangles  $\mathcal{T}$  of diameter  $h_{\mathcal{T}} \leq h$ , see [12] for more. For each mesh size  $\mathcal{T}_h$ , we associate the finite element space  $V_h$  of continuous piece-wise linear functions that are zero on the boundary

$$V_h := \left\{ v_v \in C^0(\bar{\Omega}); v_h|_{\partial\Omega} = 0, v_h|_{\mathscr{T}} \in P_1, \forall \mathscr{T} \in \mathscr{T}_h \right\}, (8)$$

where  $P_1$  is the space of polynomials of degree less than or equal to 1 and  $V_h$  is a finite dimensional subspace of V which is contained in the Sobolev space  $H_0^1(\Omega)$ . It is well known that, if we let

$$P_h: H_0^1(\Omega) \to V_h$$

to denote the  $L^2$ -projection on  $V_h$ , then for  $w \in V$  we have

$$(\nabla w, \nabla v_h) = (\nabla v_h, \nabla w), \ \forall w \in H_0^1(\Omega) \text{ and } v_h \in V_h$$
 (9)

and

$$\frac{\partial^k (P_h u)}{\partial t^k} = P_h \left( \frac{\partial^k u}{\partial t^k} \right), \ k = 0, 1, 2, \ t \in [0, T]. \tag{10}$$

By the use of the energy method together with the Gronwall's Lemma, there exists a discrete finite element solution  $u_h \in V_h$  such that

$$\left(\frac{\partial u_h}{\partial t}, v_h\right) + (\nabla u_h, \nabla v_h) = -\varepsilon^{-2} \left(f(u_h, v_h), \right)$$
(11)

$$(u_h, v_h) = (P_h u_0, v_h),$$
 (12)

With the above framework in place, it should be recalled that the Liapunov energy of Allen-Cahn equation decay with respect to the time t; that is, according to Feng and Prohl [16], we have  $\frac{d}{dt}\Phi_{\mathcal{E}}(u)$ . In view of this fact, we can show the stability of problem (11)-(12) by using a similar energy stability approach as follows:

If we take  $v_h = \frac{\partial u_h}{\partial t}$  in (11) together with the boundary conditions (12) we have for all  $v_h \in V_h$ 

$$\left(\frac{\partial u_h}{\partial t}, \frac{\partial u_h}{\partial t}\right) + \left(\nabla u_h, \nabla \frac{\partial u_h}{\partial t}\right) + \varepsilon^{-2} \left(f(u_h), \frac{\partial u_h}{\partial t}\right) = 0.$$
(13)

Using (4) and the fact that

$$\int_{\Omega} (F'(u_h), \frac{\partial u_h}{\partial t}) dx = \int_{\Omega} (f(u_h), \frac{\partial u_h}{\partial t}) dx$$

$$= \frac{d}{dt} (F(u_h), I), \tag{14}$$

we have in view of (13) that

$$\left(\frac{\partial u_h}{\partial t}, \frac{\partial u_h}{\partial t}\right) + \frac{d}{dt} \left(1/2 \left(\nabla u_h, \nabla u_h\right) + \frac{1}{\varepsilon^2} \left(F(u), I\right)\right) 
= 0.$$
(15)

Using Cauch-Schwarz inequality on the first term of (15) we have

$$\frac{d}{dt}(u_h, u_h) = \left(u_h, 2\frac{\partial u_h}{\partial t}\right) \le \frac{1}{c}(u_h, u_h) + c\left(\frac{u_h}{\partial t}, \frac{u_h}{\partial t}\right)$$

from where if we take c = 1/2, the above equation combined with (15) will yield

$$\frac{d}{dt}\left((u_h, u_h) + \frac{1}{2}(\nabla u_h, \nabla u_h) + \frac{1}{\varepsilon^2}(F(u_h), I)\right) + \frac{1}{2}\left(\frac{u_h}{\partial t}, \frac{u_h}{\partial t}\right) \le 2(u_h, u_h)$$

and this leads to the following equation:

$$\frac{d}{dt}\left((u_h, u_h) + \frac{1}{2}\left(\nabla u_h, \nabla u_h\right) + \frac{1}{\varepsilon^2}\left(F(u_h), I\right)\right) 
\leq 2\left(u_h, u_h\right).$$
(16)

Using Gronwall's inequality to (16) yield

$$\left( (u_h, u_h) + \frac{1}{2} (\nabla u_h, \nabla u_h) + \frac{1}{\varepsilon^2} (F(u_h), I) \right) (t)$$

$$\leq e^{2t} \left( (u_h, u_h) + \frac{1}{2} (\nabla u_h, \nabla u_h) + \frac{1}{\varepsilon^2} (F(u_h), I) \right) (0)$$

which completes the proof of the following preliminary result of the paper:

**Proposition 1***The discrete solution of the Allen-Cahn problem (11)-(12) satisfies the energy stability* 

$$\left( (u_h, u_h) + \frac{1}{2} \left( \nabla u_h, \nabla u_h \right) + \frac{1}{\varepsilon^2} \left( F(u_h), I \right) \right) (t)$$

$$\leq e^{2t} \left( (u_h, u_h) + \frac{1}{2} \left( \nabla u_h, \nabla u_h \right) + \frac{1}{\varepsilon^2} \left( F(u_h), I \right) \right) (0) \tag{17}$$

We use the above preliminary results in Proposition 1 to proof the stability result of the next Proposition refwirndzerem.

## 4 Coupled Non-standard finite difference and finite element method

Instead of the features of the traditional combination of the finite difference together with the finite element method manifested by some method listed earlier, we present in this section, a more reliable technique NSFD-FEM, consisting of the Non-standard finite difference method in the time and the finite element method in the space variable. We show in this regard, that the above mentioned scheme is stable and attains its optimal rate of convergence in both the  $H^1$  and  $L^2$ -norms. To achieve this, we start by letting the step size  $t_n = n\Delta t$  for  $n = 0, 1, 2, \dots N$ . For a sufficiently smooth function v(r, t) we set

$$\left(\frac{\partial}{\partial t}\right)^k v^n = \left(\frac{\partial}{\partial t}\right)^k v(\cdot, t_n) \text{ and } v^n = v(\cdot, t_n), \ k \ge 0.$$
 (18)

We proceed with this, to find the fully NSFD-FEM approximation  $\{U_h^n\}$  such that  $U_h^n \approx u_h^n$  at discrete time  $t_n$ . That is, find a sequence  $\{U_h^n\}_{n=0}^N$  in  $V_h$  such that for  $n=1,2,\cdots,N-1$ 

$$(\delta_t U_h^{n+1}, v_h) + (\nabla U_h^{n+1}, \nabla v_h) + \varepsilon^{-2} (f(U_h^n), v_h) = 0, (19)$$



$$(U_h^{n+1}, v_h) = (P_h u^0, v_h) \ \forall \ v_h \in V_h, \tag{20}$$

where

$$\delta_t U_h^n = \frac{U_h^{n+1} - U_h^n}{\phi(\Delta t)},\tag{21}$$

and  $\phi(\Delta t) = \frac{e^{\lambda \Delta t} - 1}{\lambda}$  is restricted between  $0 < \phi(\Delta t) < 1$ .

If the nonlinear function f = 0 in (1), we will have in view of (19) an exact scheme

$$\left(\frac{U_h^{n+1} - U_h^n}{\frac{e^{\lambda \Delta t} - 1}{\lambda}}, \nu_h\right) + \left(\nabla U_h^{n+1}, \nabla \nu_h\right) = 0, \tag{22}$$

which according to Mickens [20] replicates the positivity and the decay to zero, which are the main features of the exact solution of (1)-(3).

For the main goal of this section to be achieved, we first state the afore-mentioned stability result in the next proposition 2.

Proposition 2The solution of a fully-discrete NSFD-FEM scheme (19)-(20) of the Allen-Cahn equation satisfies the energy stability estimate

$$\frac{1}{2} \left( \nabla U_h^{n+1}, \nabla U_h^{n+1} \right) + \frac{1}{\varepsilon^2} \left( F(U_h^{n+1}), I \right) \\
\leq \frac{1}{2} \left( \nabla U_h^n, \nabla U_h^n \right) \\
+ \frac{1}{\varepsilon^2} \left( F(U_h^n), I \right). \tag{23}$$

*Proof.*If we take in (19)  $v_h = \delta_t U_h^{n+1}$  we have

$$\left(\frac{U_{h}^{n+1} - U_{h}^{n}}{\phi(\Delta t)}, \delta_{t} U_{h}^{n+1}\right) + \left(\nabla U_{h}^{n+1}, \nabla \delta_{t} U_{h}^{n+1}\right) + \frac{1}{\varepsilon^{2}} \left(\left(U_{h}^{n+1}\right)^{3} - U_{h}^{n}, \delta_{t} U_{h}^{n+1}\right) = 0.$$
(24)

We have in view of (24) the following equalities using (4)

$$(\delta_{t}U_{h}^{n+1}, \delta_{t}U_{h}^{n+1}) + (\nabla U_{h}^{n+1}, \nabla \delta_{t}U_{h}^{n+1})$$

$$+ \frac{1}{\varepsilon^{2}} ((U_{h}^{n+1})^{3} - U_{h}^{n}, \delta_{t}U_{h}^{n+1})$$

$$= (\nabla U_{h}^{n+1}, \nabla \delta_{t}U_{h}^{n+1})$$

$$+ \frac{1}{4\varepsilon^{2}\phi(\Delta t)} (((U_{h}^{n+1})^{2} - 1)^{2}, \delta_{t}U_{h}^{n+1})$$

$$- \frac{1}{4\varepsilon^{2}\phi(\Delta t)} (((U_{h}^{n+1})^{2} - 1)^{2}, \delta_{t}U_{h}^{n+1})$$

$$+ \frac{1}{4\varepsilon^{2}\phi(\Delta t)} (((U_{h}^{n})^{2} - 1)^{2}, \delta_{t}U_{h}^{n+1})$$

$$- \frac{1}{4\varepsilon^{2}\phi(\Delta t)} (((U_{h}^{n})^{2} - 1)^{2}, \delta_{t}U_{h}^{n+1})$$

$$+ (\delta_{t}U_{h}^{n+1}, \delta_{t}U_{h}^{n+1})$$

$$= (\nabla U_{h}^{n+1}, \nabla \delta_{t}U_{h}^{n+1})$$

$$+ \frac{1}{4\varepsilon^{2}\phi(\Delta t)} (((U_{h}^{n+1})^{2} - 1)^{2}, \delta_{t}U_{h}^{n+1})$$

$$- \frac{1}{4\varepsilon^{2}\phi(\Delta t)} (((U_{h}^{n+1})^{2} - 1)^{2}, \delta_{t}U_{h}^{n+1})$$

$$+ \frac{1}{4\varepsilon^{2}\phi(\Delta t)} (((U_{h}^{n+1})^{2} - 1)^{2}, \delta_{t}U_{h}^{n+1})$$

$$+ \frac{1}{4\varepsilon^{2}\phi(\Delta t)} (((U_{h}^{n+1})^{2} - 1)^{2}, \delta_{t}U_{h}^{n+1})$$

$$+ \frac{1}{4\varepsilon^{2}\phi(\Delta t)} (((U_{h}^{n+1})^{2}), \delta_{t}U_{h}^{n+1})$$

$$+ \frac{1}{4\varepsilon^{2}\phi(\Delta t)} (((U_{h}^{n+1})^{2}), \delta_{t}U_{h}^{n+1})$$

$$= 0.$$

$$(25)$$

In view of (25) we immediately see using (14) and dropping some positive terms that

$$\begin{split} &\left(\nabla U_h^{n+1}, \nabla \delta_t U_h^{n+1}\right) \\ &+ \frac{1}{4\varepsilon^2 \phi(\Delta t)} \left( \left( (U_h^{n+1})^2 - 1 \right)^2, \delta_t U_h^{n+1} \right) \\ &- \frac{1}{4\varepsilon^2 \phi(\Delta t)} \left( \left( (U_h^n)^2 - 1 \right)^2, I \right) \leq 0. \end{split}$$

Using (21) and (4) in the above inequality we have

$$\begin{split} &\frac{1}{2} \left( \nabla U_h^{n+1}, \nabla U_h^{n+1} \right) + \frac{1}{\varepsilon^2} \left( F(U_h^{n+1}), I \right) \\ &\leq \frac{1}{2} \left( \nabla U_h^n, \nabla U_h^n \right) + \frac{1}{\varepsilon^2} \left( F(U_h^n), I \right) \end{split}$$

which complete the proof.

With this scheme, we are now in the position to state the main Theorem below.

**Theorem 3**Assume that the solution u and its initial data  $u_0$  of the Allen-Cahn equation (6)-(7) are smooth enough and u with its approximate solution  $u_h$  satisfy Proposition 2. Then the solution of the fully-discrete stabled scheme NSFD-FEM of (19) satisfies the energy law together with the following error estimate

$$||u(t_n) - U_h^n||_0 \le C(\Delta t + h^2).$$
 (26)



Furthermore, in the limit case when  $\Delta u = f = 0$  on a subset  $\Omega' \subset \Omega$ , the discrete solution replicates the properties of the solution of the problem (1)-(3).

*Proof.*We depart by decomposing the global error as follows:

$$U_{h}^{n} - u(t_{n}) = U_{h}^{n} - P_{h}u(t_{n}) + P_{h}u(t_{n}) - u(t_{n})$$

$$= \theta^{n} + \rho^{n}$$
(27)

We bound the space error  $\rho^n$  via (19) and (1) by taking the error equation

$$\left(\frac{\partial}{\partial t}(P_h u(t_n) - u(t_n)), v_h\right) + (\nabla(P_h u(t_n) - u(t_n)), \nabla v_h) 
+ \frac{1}{\varepsilon^2} ((f(u) - f(u_h), v_h)) 
= 0,$$
(28)

together with its initial error estimate

$$||u(\cdot,0) - u_h(\cdot,0)|| \le Ch^2.$$
 (29)

If we take  $v_h = P_h \frac{\partial e^n}{\partial t}$  where  $e^n = u - u_h$  then, we have the following equation

$$\left(P_{h}\frac{\partial e^{n}}{\partial t}, P_{h}\frac{\partial e^{n}}{\partial t}\right) + \left(\nabla P_{h}e^{n}, \nabla P_{h}e^{n}\right) 
+ \frac{1}{\varepsilon^{2}}\left(\left(f(u) - f(u_{h})\right), P_{h}\frac{\partial e^{n}}{\partial t}\right) 
= \left(P_{h}\frac{\partial u}{\partial t} - \frac{\partial u}{\partial t}, P_{h}\frac{\partial e^{n}}{\partial t}\right) 
+ \left(P_{h}\nabla\frac{\partial u}{\partial t} - \nabla\frac{\partial u}{\partial t}, P_{h}\nabla e^{n}\right) 
+ \left(P_{h}\frac{\partial u}{\partial t} - \frac{\partial u}{\partial t}\right)$$
(30)

from where we denote the following terms on the right hand side by:

$$A = \left(P_h \frac{\partial u}{\partial t} - \frac{\partial u}{\partial t}, P_h \frac{\partial e^n}{\partial t}\right)$$

$$B = \left(P_h \nabla \frac{\partial u}{\partial t} - \nabla \frac{\partial u}{\partial t}, P_h \nabla e^n\right)$$

and

$$C = \left(P_h \frac{\partial u}{\partial t} - \frac{\partial u}{\partial t}\right).$$

The above terms are then bounded by the use of interpolation error bounds together with the Cauchy-Schwarz inequality as follows:

$$||A|| \le ||\frac{\partial u}{\partial t} - P_h \frac{\partial u}{\partial t}|| ||P_h \frac{\partial e^n}{\partial t}||$$
(31)

$$||B|| \le ||\nabla(\frac{\partial u}{\partial t} - P_h \frac{\partial u}{\partial t})|| ||P_h \nabla e^n||$$
(32)

and

$$||C|| < Ch^2 ||P_h \nabla e^n|| \tag{33}$$

where C is a positive constant depending on  $||u||_{L^{\infty}([0,T];H^2(\Omega))}$  and independent on h. Combining (31), (32) and (33) in (30) yield

$$\|P_{h}\frac{\partial e^{n}}{\partial t}\|^{2} + \frac{1}{2}\frac{d}{dt}\|\nabla P_{h}e^{n}\|^{2} \leq \frac{1}{\varepsilon^{2}}\left((f(u) - f(u_{h})), P_{h}\frac{\partial e^{n}}{\partial t}\right) + Ch^{2}\left(\|P_{h}\frac{\partial e^{n}}{\partial t}\| + \|P_{h}\nabla e^{n}\|\right)$$

$$\leq Ch^{2} + \frac{1}{8}\|P_{h}\frac{\partial e^{n}}{\partial t}\|^{2}$$

$$+ \frac{1}{2}\|P_{h}\nabla e^{n}\|^{2}.$$

$$(34)$$

Since we specified that the nonlinear term on the right hand side of (34) was  $f(u) = u^3 - u$ , then we approximate it by the following cubic expansion

$$f(u) - f(u_h) = f'(u)(u - u_h) + (u - u_h)^3 + 3u(u - u_h)^2.$$
 (35)

In view of this, we bound the nonlinear term in (34) as follows:

$$\begin{split} &\frac{1}{\varepsilon^2}\left((f(u)-f(u_h)),P_h\frac{\partial e^n}{\partial t}\right)\\ &=\frac{1}{\varepsilon^2}\left((f(u)-f(P_hu)),P_h\frac{\partial e^n}{\partial t}\right)\\ &+\frac{1}{\varepsilon^2}\left((f(P_hu)-f(u_h)),P_h\frac{\partial e^n}{\partial t}\right)\\ &=\frac{1}{\varepsilon^2}\left(f'(\xi)(u-P_hu),P_h\frac{\partial e^n}{\partial t}\right)\\ &+\frac{1}{\varepsilon^2}\left(f(P_hu)-f(u_h),P_h\frac{\partial e^n}{\partial t}\right)\\ &=E+G \end{split}$$

where

$$E = \frac{1}{\varepsilon^2} \left( f'(\xi)(u - P_h u), P_h \frac{\partial e^n}{\partial t} \right)$$

$$G = \frac{1}{\varepsilon^2} \left( f(P_h u) - f(u_h), P_h \frac{\partial e^n}{\partial t} \right)$$

and  $\xi$  is between u and  $P_h u$ .

Using Young inequality for any positive  $\varepsilon' > 0$  we have

$$|E| \leq \frac{1}{\varepsilon^{2}} \|f'\|_{L^{\infty}(\Omega)} |(u - P_{h}u), P_{h} \frac{\partial e^{n}}{\partial t}|$$

$$\leq \frac{1}{\varepsilon^{2}} \left( \varepsilon' \|P_{h} \frac{\partial e^{n}}{\partial t}\|^{2} + \frac{\|f'\|_{L^{\infty}(\Omega)}}{4\varepsilon'} \|u - P_{h}u\|^{2} \right)$$

and if we take  $\varepsilon' = \frac{\varepsilon^2}{4}$  the above inequality yields

$$|E| \le \frac{1}{4} \|P_h \frac{\partial e^n}{\partial t}\|^2 + \frac{Ch^4}{\varepsilon^4} \tag{36}$$

where C>0 is depending on  $\|f'\|_{L^{\infty}(\Omega)}$  and  $\|u\|_2$  and independent on h. To bound G we use (35) as follows:

$$G = \frac{1}{\varepsilon^{2}} \left( f'(P_{h}u)(P_{h}u - u_{h}), P_{h} \frac{\partial e^{n}}{\partial t} \right)$$

$$+ \frac{1}{\varepsilon^{2}} \left[ (P_{h}u - u_{h})^{3} + 3P_{h}u(P_{h}u - u_{h})^{2}, P_{h} \frac{\partial e^{n}}{\partial t} \right]$$

$$= \frac{1}{\varepsilon^{2}} \left[ f'(P_{h}u)P_{h}e^{n} + (P_{h}e^{n})^{n} + 3P_{h}u(P_{h}e^{n})^{2}, P_{h} \frac{\partial e^{n}}{\partial t} \right]$$

$$= \frac{1}{4\varepsilon^{2}} \frac{d}{dt} \left( (P_{h}e^{n})^{2}, (P_{h}e^{n})^{2} \right)$$

$$+ \frac{1}{4\varepsilon^{2}} \left( f'(P_{h}u)P_{h}e^{n} + 3P_{h}u(P_{h}e^{n})^{2}, P_{h} \frac{\partial e^{n}}{\partial t} \right)$$

$$= \frac{1}{4\varepsilon^{2}} \frac{d}{dt} \left( (P_{h}e^{n})^{2}, (P_{h}e^{n})^{2} \right) + S$$

$$(37)$$

where S in (37) is bounded as follows:

$$|S| \le \frac{1}{4} \|P_h \frac{\partial e^n}{\partial t}\|^2 + \frac{C}{\varepsilon^4} (\|P_h e^n\|^2 + ((P_h e^n)^2, (P_h e^n)^2)).$$
(38)

Assembling the inequalities (36), (37) and (38) into (34) we have

$$||P_{h}\frac{\partial e^{n}}{\partial t}||^{2} + \frac{1}{2}\frac{d}{dt}||\nabla P_{h}e^{n}||^{2} \leq \frac{-1}{4\varepsilon^{2}}\frac{d}{dt}||(P_{h}e^{n})^{2}||^{2} + \frac{5}{8}||P_{h}\frac{\partial e^{n}}{\partial t}||^{2} + \frac{1}{2}||P_{h}\nabla e^{n}||^{2} + \frac{C}{\varepsilon^{4}}(||(P_{h}e^{n})^{2}||^{2} + ||P_{h}e^{n}||^{2}) + Ch^{4} + \frac{C}{\varepsilon^{2}}h^{4}.$$
(39)

Using Young inequality for any positive constant  $\varepsilon' > 0$  on the first term of the left hand side yield

$$\frac{d}{dt}\left(\frac{1}{\varepsilon^2}\|P_he^n\|^2\right) \leq \frac{1}{\varepsilon^2}\left(\frac{1}{\varepsilon'}\|P_he^n\|^2 + \varepsilon'\|P_h\frac{\partial e^n}{\partial t}\|^2\right)$$

and setting  $\varepsilon' = \frac{\varepsilon^2}{8}$  we have

$$\frac{d}{dt}\left(\frac{1}{\varepsilon^2}\|P_he^n\|^2\right) \leq \frac{8}{\varepsilon^4}\|P_he^n\|^2 + \frac{1}{8}\|P_h\frac{\partial e^n}{\partial t}\|^2$$

and re-introducing it to (39) and gathering the common terms together yield

$$\begin{split} & \frac{d}{dt} \left( \frac{1}{\varepsilon^2} \|P_h e^n\|^2 + \frac{1}{2} \|\nabla P_h e^n\|^2 + \frac{1}{4\varepsilon^2} \|(P_h e^n)^2\|^2 \right) \\ & \leq \frac{1}{2} \|P_h \nabla e^n\|^2 + Ch^4 + \frac{C}{\varepsilon^4} h^4 + \frac{C}{\varepsilon^4} \left( \|P_h e^n\|^2 + \|(P_h e^2)^2\|^2 \right). \end{split}$$

Multiplying both sides of the above inequality by  $\varepsilon^2$  and using the Gronwall's inequality together with the initial error (29) we have the required results

$$\|\rho^{n}\| = \|u - P_{h}u\|^{2} + \frac{\varepsilon^{2}}{2} \|\nabla(u - P_{h}u)\|^{2} + \frac{1}{4} \|(u - P_{h}u)^{2}\|^{2}$$

$$< Ch^{2}. \tag{40}$$

On the other hand, we bound  $\theta^n$  in (27) via (19) as follows:

$$(\delta_{t}\theta^{n}, v_{h}) + (\nabla\theta^{n}, \nabla v_{h}) = (\delta_{t}(U_{h}^{n} - P_{h}u(t_{n})), v_{h})$$

$$+ (\nabla(U_{h}^{n} - P_{h}u(t_{n})), \nabla v_{h})$$

$$= - (P_{h}\delta_{t}u(t_{n}), v_{h})$$

$$- \frac{1}{\varepsilon^{2}}(f(u(t_{n})), v_{h})$$

$$- (\nabla P_{h}u(t_{n}), \nabla v_{h})$$

$$= - (P_{h}\delta_{t}u(t_{n}), v_{h})$$

$$+ \left(\frac{\partial u(t_{n})}{\partial t}, v_{h}\right)$$

$$= ((I - P_{h})\delta_{t}u(t_{n}), v_{h})$$

$$+ \left(\frac{\partial u(t_{n})}{\partial t} - \delta_{t}u(t_{n}), v_{h}\right)$$

$$= (W_{1}^{n}, v_{h}) + (W_{2}^{n}, v_{h}).$$

$$(41)$$

Taking  $v_h = \theta^n$  and (21) we have

$$\begin{split} (\delta_t \theta^n, \theta^n) &= \phi^{-1}(\Delta t) \left( \theta^{n+1} - \theta^n, \theta^n \right) \\ &= \phi^{-1}(\Delta t) \|\theta^{n+1}\|^2 - \phi^{-1}(\Delta t) \left( \theta^n, \theta^{n+1} \right) \end{split}$$

which when combined with (41) will yield

$$\phi^{-1} \left[ \|\theta^{n+1}\|^2 - \left(\theta^n, \theta^{n+1}\right) \right] \le (W_1^n, \theta^n) + (W_2^n, \theta^n). \tag{42}$$

Using Cauchy-Schwarz inequality we have

$$\|\theta^{n+1}\|_{0} \le \phi(\Delta t) \|W_{1}^{n}\|_{0}^{2} + \phi(\Delta t) \|W_{2}^{n}\|_{0}^{2} + \|\theta^{n}\|_{0}$$

which yield the next result after the use of mathematical induction

$$\|\theta^{n}\|_{0} \leq \|\theta^{0}\|_{0} + \phi(\Delta t) \sum_{j=1}^{n} \|W_{1}^{j}\|_{0}^{2} + \phi(\Delta t) \sum_{j=1}^{n} \|W_{2}^{j}\|_{0}^{2}.$$

$$(43)$$

Bounding estimate (43) in view of (29) since  $u_0 \in H^2(\Omega)$  we have

$$\|\theta^0\|_0 = \|u_{h,0} - P_h u_0\|_0 \le Ch^2 \|u_0\|_0. \tag{44}$$

The bound on  $\phi(\Delta t) \sum_{j=1}^{n} ||W_1^j||_0$  will be equivalent to that on  $\rho^n$  since  $u \in L^2[(0, +\infty); H^2(\Omega)]$ .

Finally we bound  $\phi(\Delta t) \sum_{j=1}^{n} \|W_2^j\|_0$  via (41) as follows:

$$W_2^j = \delta_t u(t_{j+1}) - \frac{\partial u(t_{j+1})}{\partial t}$$
  
=  $\phi^{-1}(\Delta t) \left( u(t_{j+1}) - u(t_j) \right) - \frac{\partial u(t_{j+1})}{\partial t}$ 



from where we have using Taylor theorem with the integral expansion on the remainder term

$$\begin{aligned} \phi(\Delta t) \sum_{j=1}^{n} \|W_{2}^{j}\|_{0}^{2} &\leq \sum_{j=1}^{n} \|\int_{t_{j}}^{t_{j+1}} (s - t_{j}) \frac{\partial^{2} u(s)}{\partial s^{2}} \|_{0}^{2} \\ &+ C(\phi(\Delta t))^{2} \sum_{j=1}^{2} \|\frac{\partial u(t_{j+1})}{\partial t} \|_{0}^{2} \\ &\leq (\Delta t)^{2} \int_{0}^{t_{n}} \|\frac{\partial^{2} u(s)}{\partial s^{2}} \|_{0}^{2} \\ &+ C(\phi(\Delta t))^{2} \sup_{1 \leq j \leq n} \|\frac{\partial u(t_{j})}{\partial t} \|_{0}^{2} \\ &\leq C\Delta t, \end{aligned}$$

$$(45)$$

since  $u \in L^2\left[(0,+\infty);H^2(\Omega)\right]$  and  $\Delta t \approx \phi(\Delta t)$  as  $\Delta t \to 0$ . Combining (44) and (45) in (43) and taking note that the second term on the right hand side of (43) is equivalent to (40) then we have proved

$$\|\theta^n\|_0 \le C\left(\Delta t + h^2\right). \tag{46}$$

Hence in view of (40) and (46) we have proved the first part of the Theorem that show the solution of the Allen-Cahn equation converges optimally in both  $H^1(\Omega)$  and  $L^2$ -norms using the coupled Non-standard finite difference with finite element method.

As regard the second part of the above proof which is purely the replication of the properties of the exact solution of (19)-(20), we proceed thanks to Adams [1] Corollary 2.11 as follows: We use the fart that the convergence in the  $L^2$  as well as  $H^1$ -norms of the discrete solution  $U_h^n$  to the exact solution u in (26) implies that, there exists a subsequence of  $U_h^n$  still denoted by  $U_h^n$  that converges point-wise to u as  $h \to 0$  and  $n \to +\infty$ . In view of this, if we assume that  $\Delta u = 0$  near a point  $a \in \Omega$  and  $v_h$  in (19) is chosen in such a way that its support containing the point a is very small and  $v_h = 1$  near a, then we use the approximation

$$\int_{\Omega} (f(U_h^n)) v_h dx = f(U_h^n(a) \cdot \mathbf{K})$$

where **K** is the measure of the  $supp(v_h)$ . Using the above approximation in (19), it follows that the solution  $U_h^n$  is really the discrete solution of the exact scheme (22) if we also have

$$f(U_h^n(a,t)) = 0$$

and hence we complete the second part of the proof and therefore completing the proof of the Theorem.

### **5** Numerical experiments

Under this section, we present the numerical experiments carried out using problem (1) and (19). Our expectations are indeed to obtain in the  $L^2$ -norm, the best rate convergence of approximately 2 and in the  $H^1$ -norm the

best rate of convergence of approximately 1 of the discrete to the exact solution of Allen-Cahn equation. To achieve this, we begin by considering the equation

$$\frac{\partial u}{\partial t} - \Delta u + \frac{1}{\varepsilon^2} f(u) = g(x, t) \tag{47}$$

with the Dirichlet boundary conditions on the domain  $\Omega = [0,1] \times [0,1]$  where  $\Omega$  is discretized using regular meshes of sizes h = 1/M in the space and  $\Delta t = T/N$  in the time space. The forcing function g(x,t) was taken in such a way that it would yield an exact solution u(x,t). If g(x,t) is considered in such a way that

$$u(x,t) = e^{-2\varepsilon^2 t} \sin(x_1) \sin(x_2) \tag{48}$$

where  $\varepsilon=0.3$  and the following data are considered with the following values:  $\Delta t=\varepsilon^2, N=5, \lambda=3$  and T=0.1, then using a Mathlab 7.10.0(R2010a) code, we obtained the following figures from 1 to 6 for various values of t=0.08, 0.1 and 0.12:

We exploit the data obtained from the numerical computations to find the errors for T=0.12 with mesh sizes varying from 10,15,20 and 25. The results from these computations are illustrated in table 1. Making use of the error values of the solution u(x,t) from the table 1, we compute for T=0.12 with the same mesh sizes, the rate of convergence of u(x,t) using the formular

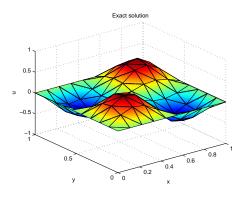
$$Rate = \frac{\ln(\frac{e_2}{e_1})}{\ln(\frac{h_2}{h_1})}$$

where  $h_1$  and  $h_2$  together with  $e_1$  and  $e_2$  are successive triangle diameters and errors respectively. Furthermore, the clarification of the convergence of the solution to be more specific in the  $L^2$ -norm can be illustrated in figure 7.

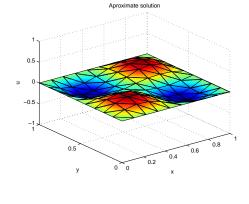
In view of figure 1 to 6, we observed that the exact solutions for each time t are almost identical to the approximate solutions. Besides, table 1 shows that the solution u(x,t) has an approximate rate of almost 2 for the  $L^2$ -norm and 1 for the  $H^1$ -norm. All these results are self explanatory and we would like to conclude that the results as shown by all these experiments exhibit the desired theoretical analysis as expected.

**Table 1** Error in  $L^2$  and  $H^1$ -norms of u using NSFD-FEM method

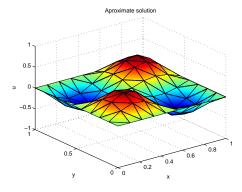
| М  | L <sup>2</sup> -error | L <sup>2</sup> -Rate | H <sup>1</sup> -error | H <sup>1</sup> -Rate |
|----|-----------------------|----------------------|-----------------------|----------------------|
| 10 | 2.9856E-2             |                      | 5.0853E-1             |                      |
| 15 | 1.4216E-2             | 1.83                 | 3.5722E-1             | 0.86                 |
| 20 | 8.2775E-3             | 1.87                 | 2.6923E-1             | 0.98                 |
| 25 | 5.3570E-3             | 1.95                 | 2.1538E-1             | 0.99                 |



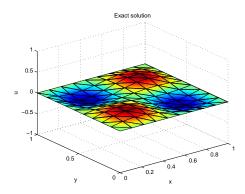
**Fig. 1** Exact Solutions of u(x,t) at t = 008



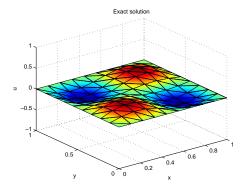
**Fig. 4** Approximate Solutions of u(x,t) at t = 0.1



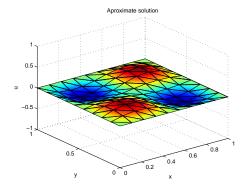
**Fig. 2** Approximate Solutions of u(x,t) at t = 008



**Fig. 5** Exact Solutions of u(x,t) at t = 0.12



**Fig. 3** Exact Solutions of u(x,t) at t = 0.1



**Fig. 6** Approximate Solutions of u(x,t) at t = 0.12

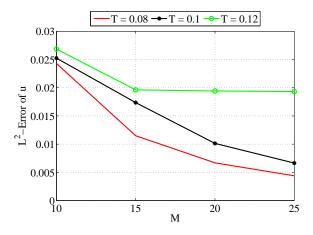


Fig. 7 Unit Square

### **6 Conlusion**

A stable and reliable numerical scheme of a fully-discrete time-dependent Allen-Cahn equation was presented. The method used in the analysis of the above scheme was a coupled non-standard finite difference method in the time and the finite element method in the space variables (NSFD-FEM). With this, we proved theoretically that the discrete solution obtained from this scheme was stabled and it's optimal rates of convergence in the both  $H^1$  and  $L^2$ -norms were obtained. Furthermore, we showed that the said scheme replicates the properties of the exact solution of the problem under investigation. We proceeded by the help of a numerical example, to justify our theoretical analysis.

The stability analysis and error estimates are based on a weak formulation thus we could be tempted to ask that natural question which is, whether or not we can easily extend the technique to other domains like non-smooth domains? The tempting answer might be yes provided we stick to the procedure as proposed by Mickens [20] but it might not be true. Another concern of interest is the comparison studies which will be able to reveal the technique's strength and limitations. We set aside this later studies to be addressed in our future works.

We would like in future, to also study system of nonlinear time-dependent decoupled parabolic problems using the same technique. The subject for considering these same problems in domains which are non-smooth using the same technique is very challenging but interesting and it is ongoing now.

### Acknowledgement

The author acknowledges the financial support by the University of Pretoria, South African and also to the

anonymous referee for a careful checking of the details and for helpful comments that improved this paper.

#### References

- R.A. Adams, Sobolev Space. Academic Press, New York, 1975.
- [2] S.M. Allen, and J.W. Cahn, A microscopic theory for antiphase boundary motion and its application to antiphase domain coarsening. *Acta Metallurgica*, 27(6):1085–1095, 1979.
- [3] R. Anguelov, and J.M-S. Lubuma, Contributions to the mathematics of the nonstandard finite difference method and applications. *Numerical Methods for Partial Differential Equations*, 17(5):518–543, 2001.
- [4] R. Anguelov and J.M-S Lubuma, Nonstandard finite difference method by nonlocal approximation. *Mathematics* and Computers in Simulation, 61(3):465–475, 2003.
- [5] S. Bartels, and R. Müller, Quasi-optimal and robust a posteriori error estimates in  $L^{\infty}(L^2)$  for the approximation of Allen-Cahn equations past singularities. *Mathematics of Computation*, 80(274):761–780, 2011.
- [6] J.W. Cahn, and J.E. Hilliard, Free energy of a nonuniform system. I. Interfacial free energy. J. Chem. Phys., 28(2):258-267, 1996.
- [7] L.Q. Chen, Phase-field models for microstructure evolution. Annual Review of Materials Research, 32(1):113–140, 2002.
- [8] X. Chen, and C.M. Elliott, and A. Gardiner, and J. JING ZHAO, Convergence of numerical solutions to the Allen-Cahn equation. *Applicable analysis*, 69(1-2): 47–56, 1998.
- [9] P.M.W. Chin, J.K. Djoko and J.M-S. Lubuma, Reliable numerical schemes for a linear diffusion equation on a nonsmooth domain. *Applied Mathematics Letters*, 23(5): 544–548, 2010.
- [10] P.W.M. Chin, Optimal Rate of Convergence for a Nonstandard Finite Difference Galerkin Method Applied to Wave Equation Problems. *Journal of Applied Mathematics*, vol 213: 2013.
- [11] J.W. Choi, and H.G. Lee, and D. Jeong, and J. Kim, An unconditionally gradient stable numerical method for solving the Allen–Cahn equation. *Physica A: Statistical Mechanics and its Applications*, 388(9): 1791–1803, 2009.
- [12] P.G. Ciarlet, *The finite element method for elliptic problems*. Elsevier, 1978.
- [13] P. Colli, and G. Gilardi, and P. Podio-Guidugli, and J. Sprekels, Existence and uniqueness of a global-in-time solution to a phase segregation problem of the Allen–Cahn type. *Mathematical Models and Methods in Applied Sciences*, 20(04), 519–541, 2010.
- [14] P. De Mottoni, and M. Schatzman, Geometrical evolution of developed interfaces *Transactions of the American Mathematical Society*, 347(5):1533–1589, 1995.
- [15] X. Feng, and H.J. Wu, A posteriori error estimates and an adaptive finite element method for the Allen–Cahn equation and the mean curvature flow. *Journal of Scientific Computing*, 24(2):121–146, 2005.
- [16] X. Feng, and A. Prohl, Numerical analysis of the Allen-Cahn equation and approximation for mean curvature flows. *Numerische Mathematik*, 94(1):33–65, 2003.



- [17] J.L. Louis, E. Magenes, and P. Kenneth, Non-homogeneous Boundary Value Problems and Applications, volume 1. Springer Berlin, 1972.
- [18] J.M.S, Lubuma, E. Mureithi and Y.A, Terefe. Analysis and dynamically consistent numerical scheme for the SIS model and related reaction diffusion equation volume 168. AIP Conf. Proc., 1404: 2011.
- [19] Jean M.-S, Lubuma, Eunice W. Mureithi and Yibeltal A. Terefe. Nonstandard discretization of the SIS Epidemiological model with and without diffusion. *Contemporary Mathematics*, vol 618: 2014.
- [20] R.E. Mickens, Nonstandard finite difference models of differential equations. World Scientific, 1994.
- [21] S.M. Moghadas, and M.E. Alexander, and B.D. Corbett, and A.B. Gumel, A positivity-preserving Mickens-type discretization of an epidemic model. *The Journal of Difference Equations and Applications*, 9(11): 1037–1051, 2003.
- [22] H. Ninomiya, and M. Taniguchi, Existence and global stability of traveling curved fronts in the Allen–Cahn equations. *Journal of Differential Equations*, 2139(1); 204-233, 2005.
- [23] A. Novick-Cohen, Triple-junction motion for an Allen–Cahn/Cahn–Hilliard system. *Physica D: Nonlinear Phenomena*, 137(1): 1–24, 2000.
- [24] K.C. Partidar, On the use of nonstandard finite difference methods. *Journal of Difference Equations and Applications*, 11(8): 735–758, 2005.
- [25] M. Taniguchi, The uniqueness and asymptotic stability of pyramidal traveling fronts in the Allen–Cahn equations. *Journal of Differential Equations*, 246(5); 2103-2130, 2009.
- [26] A.A. Wheeler, W.J. Boettinger, and G.B. McFadden, Phase-field model for isothermal phase transitions in binary alloys. *Phys. Rev.*, 45(A): 7424-7439, 1992.
- [27] X. Yang, Error analysis of stabilized semi-implicit method of Allen-Cahn equation. *Discrete Contin. Dyn. Syst. Ser. B.*, 11(4): 1057–1070, 2009.
- [28] J. Zhang, and Q. Du, Numerical studies of discrete approximations to the Allen-Cahn equation in the sharp interface limit. SIAM Journal on Scientific Computing, 31(4): 3042–3063, 2009.



W. Pius M., Chin received the PhD degree Applied Mathematics at the University of Pretoria, South Africa and presently is lecturing in the said University in the Department of Mathematics and Applied Mathematics. His research interests are in the areas of finite element method both theory and numerical. He has published research articles in

reputed international journals in Applied Mathematics. In addition, he is a referee of some international journals.