An explicit nonstandard finite difference scheme for the Allen-Cahn equation

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We design explicit nonstandard finite difference schemes for the nonlinear Allen-Cahn reaction diffusion equation in the limit of very small interaction length ε. In the proposed scheme, the perturbation parameter is part of the argument of the functional step size, thereby minimising the restrictions normally associated with standard explicit finite difference schemes. The derivation involves splitting the equation into the space independent and the time independent different models. An exact nonstandard scheme is proposed for the space independent model and energy conservative schemes are proposed for the time independent model. We show the power of the derived scheme over the existing schemes through several numerical examples.

Keywords: Allen-Cahn equation; nonstandard finite difference; explicit scheme.

AMS Subject Classification: 65M06; 65M08; 65L12; 97N40

1. Introduction

The Allen-Cahn equation

$$u_t - \nabla^2 u + \varepsilon^{-2} f(u) = 0, \quad \boldsymbol{x} \in \Omega, \quad t > 0, \tag{1}$$

is a binary alloy model, where $\Omega \subset \mathrm{R}^d$, $u(\boldsymbol{x}, t)$ is an order parameter and ε is the interaction length which is extremely small in practice. The nonlinear term $f(u) = F'(u)$ where $F(u) = 0.25(u^2 - 1)^2$. Equation (1) finds its origin in the work of Allen and Cahn [1] to describe the phase separation process in binary alloy. It has also been used in different areas of applied sciences including image processing, crystal growth, biology, geology, to name just a few. The Allen-Cahn equation is a result of the Ginzburg-Landau free energy

$$E(u) = \int_\Omega \left\{ \frac{1}{2} |\nabla u|^2 + \frac{1}{\varepsilon^2} F(u) \right\} d\Omega, \tag{2}$$

and it is known that the energy decreases with time, [18, 19].

Equation (1) belongs to the class of nonlinear partial differential equations not amenable to analytical solutions. As a result, it has been approximated using vari-

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ous numerical approaches, see for example [8, 9, 17–19], and the literature therein. However, there are two main areas of concern when numerical approximations are used for equation (1). First, it is critical that the nonlinear term is handled properly as this will affect the long term dynamics of the solution such as boundedness and preservation of equilibrium solutions. Secondly, the restriction of standard explicit schemes which require that the step size be $o(\varepsilon^2)$. In particular, the optimal error bound for the equation is dependent upon ε. Therefore, as $\varepsilon \to 0$, spurious oscillations or the non physical effect of ε is reduced provided there is a corresponding reduction in the mesh size.

Recently, nonstandard finite difference (NSFD) methods, first introduced by Mickens [12], has become a very efficient tool for approximating the solutions of several differential equations arising from mathematical physics, see for example [10–12]. In light of the work under investigation here, we highlight the work [6, 14, 15] where NSFD schemes were designed for ordinary differential equations with three distinct fixed points. An extension to a general number of distinct fixed points is given in [14]. In particular, [6] considered the general function $f(u) = \alpha u^3 - \beta u$ with $\beta > 0$ and $\alpha > 0$, and derived a semi-explicit and semi-implicit NSFD schemes. On the other hand the authors in [13] and [14] considered functions of the form $f(u) = \pm u(u-1)(u-\alpha)$ with $0 \leq \alpha \leq 1$. While the first case is applicable here, the second case cannot be used here since it is limited to positive solutions.

Nonstandard finite difference schemes for reaction diffusion equations were considered in [2, 3, 6]. The authors in [6] designed and analysed explicit and implicit nonstandard schemes for a reaction diffusion equation with three fixed points. The diffusion free equation was discretised using different nonstandard schemes while the diffusion term was approximated by standard discretisation. Later in [3] both the diffusion free and the steady state sub equations were discretised via the nonstandard approach. The scheme for the steady state sub equation was derived in such a way as to preserve the conservation of energy. The schemes were carefully assembled together to approximate the solution of the full reaction diffusion equation. In particular, the NSFD approach is credited for the preservation of the qualitative property of the physical models in addition to its inherent stability and boundedness of the solutions.

The focus of this work can be summarized with a reference to the work [19], where the authors highlighted the need to choose the spatial step size and the time-step in connection with the small parameter ε. We provide, via the use of NSFD schemes, some insight into how this idea can be captured and we will give numerical simulations supporting our findings for small ε. The structure of this paper is as follows. We discuss the main ideas in the design of numerical schemes and the splitting to sub equations in Section 2. We end the section by testing the the performance of the designed scheme for the space independent differential equation. Some numerical experiments to show the strength of the schemes for the full equation are demonstrated in Section 3 and we summarise our discoveries in Section 4.

2. Numerical schemes derivation

In this section we give a detailed description on the design of nonstandard finite difference schemes for equation (1). For simplicity, we will restrict ourselves to the 1D equation. The numerical approximation of the unknown $u(x,t)$ on a uniform

grid will be written as v_m^n at time $t_n = n\Delta t$ and spatial point $x_m = m\Delta x$, where $m = 0, 1, 2, \cdots, M$ and $n = 0, 1, 2, \cdots$.

Following the rules outlined in [3] and the literature therein, we design the non-standard finite difference schemes for equation (1) using the following three major steps. In the first step, we design a scheme for the space independent equation, followed by the scheme for the time independent equation and we end by assembling the two schemes. The explicit approximation to the solution of the continuous equation will be represented by an explicit finite difference scheme of the form

$$v^{n+1} = F_{\Delta t}(v^n), \tag{3}$$

for some function $F_{\Delta t}$.

2.1. *Space independent equation*

Consider the sub equation

$$\varepsilon^2 \frac{du}{dt} = u(1-u)(1+u), \tag{4}$$

with an initial condition $u(t_0) = u_0$. This space independent equation is an ordinary differential equation with three distinct equilibrium points, i.e., $\tilde{u}^1 = -1$, $\tilde{u}^2 = 0$, $\tilde{u}^3 = 1$. It can be shown that (4) is bistable with stable equilibrium points $\tilde{u}^{1,3} = \pm 1$, while $\tilde{u}^2 = 0$ is unstable. In addition, the solution to (4) enjoys the following properties

- P_1 : If $u_0 \in (-1, 0)$ and $u_0 \in (0, 1)$, then $u(t) \in (-1, 0)$ and $u(t) \in (0, 1)$ respectively.
- P_2 : If $u_0 \in (0, 1)$ or $u_0 \in (-\infty, -1)$ then the solution is monotonically increasing, and if $u_0 \in (-1, 0)$ or $u_0 \in (1, \infty)$ then the solution is monotonically decreasing.
- P_3 : If u_0 coincide with an equilibrium point, then the solution remains on the equilibrium point.

2.1.1. NSFD scheme

In this section we are interested in a finite difference scheme that is stable with respect to these properties, i.e., preservation and stability of fixed points, boundedness of solutions and monotonicity of solutions. We begin with the exact solution of equation (4) as given by

$$u(t) = \frac{1}{\sqrt{1 + (1/u(t_0) - 1)\exp\left(-\frac{2}{\varepsilon^2}(t - t_0)\right)}}, \tag{5}$$

satisfying initial condition $u(t_0)$. Considering the solution at discrete times t_n and t_{n+1} with some mathematical adjustments we derived an exact scheme for equation (4) as stated below

$$\varepsilon^2 \frac{v^{n+1} - v^n}{\phi(\Delta t)} = \frac{2(v^{n+1})^2}{v^{n+1} + v^n}(1 - v^n)(v^n + 1), \tag{6}$$

where

$$\phi = \frac{1 - \exp\left(-2\Delta t/\varepsilon^2\right)}{2/\varepsilon^2}, \tag{7}$$

see [16].

Remark 1. The NSFD scheme (6) is dynamically consistent with equation (4). By this we mean that the scheme (6) reproduces the properties P_1 – P_3 in addition to the preservation of the three fixed points.

In particular, equation (6) leads to an explicit difference scheme with

$$F_{\Delta t}(v^n) = \frac{v^n}{\sqrt{1 - \frac{2}{\varepsilon^2}\phi(1 - v^n)(1 + v^n)}}. \tag{8}$$

The exact scheme (6) preserves all the fixed points, is elementary stable and topologically dynamically consistent with the continuous solution operator of the discussed equation, see [4, 5]. By this, we mean that the value of the derived quantity

$$\frac{dF_{\Delta t}}{dv^n}(\pm 1) = \exp\left(-\frac{2}{\varepsilon^2}\Delta t\right) > 0$$

for the scheme (6).

The boundedness condition P_1 for scheme (8) follows from the observation that the function

$$g(z) = \frac{z}{\sqrt{1 - (1 - \exp(-2\Delta t/\varepsilon^2))(1 - z^2)}},$$

is monotonically increasing on the interval $-1 \leq z \leq 1$ with $g(-1) = -1$ and $g(1) = 1$. Since $(1 - \exp(-2\Delta t/\varepsilon^2))(1 - (v^n)^2) \geq 0$ then $\sqrt{1 - (1 - \exp(-2\Delta t/\varepsilon^2))(1 - (v^n)^2)} < 1$, therefore from (8),

$$|v^n| < |v^{n+1}|,$$

and scheme (6) satisfies property P_2. In addition, if $v^n = \tilde{v}^n$, it can be shown from scheme (6) via (8) that $\tilde{v}^{n+1} = \tilde{v}^n$. Therefore, scheme (6) reproduces all the properties of the continuous problem.

2.1.2. Chen et al. *(2003) scheme*

For completeness we will also consider the NSFD scheme derived under *Method 2* in [6] with $\alpha = \beta = 1/\varepsilon^2$. The scheme is given by

$$\varepsilon^2 \frac{v^{n+1} - v^n}{\Delta t} = 2v^n - v^{n+1} - (v^n)^2 v^{n+1}. \tag{9}$$

The schemes (6) and (9) satisfy the NSFD rules highlighted for nonstandard schemes in [12].

2.1.3. *Forward Euler scheme*

On the other hand, recall the standard forward Euler scheme for equation (4), i.e.,

$$v^{n+1} = v^n + \frac{\Delta t}{\varepsilon^2} v^n (1 - v^n)(1 + v^n). \tag{10}$$

Scheme (10) preserves the fixed points of the continuous equation but it is not elementary stable. Consider

$$\frac{dF_{\Delta t}}{dv^n}(\pm 1) = 1 - \frac{2\Delta t}{\varepsilon^2}.$$

Hence the Euler scheme requires that $\Delta t < \frac{\varepsilon^2}{2}$, to preserve the stability of the equilibrium points.

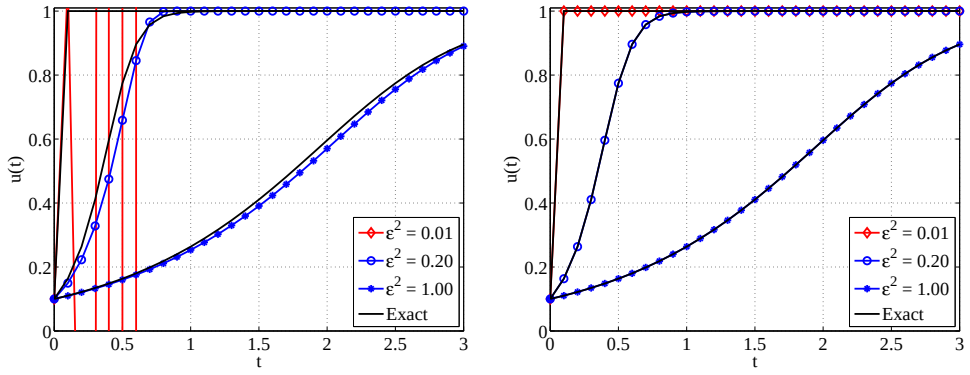
2.1.4. *Numerical simulations of the ODE subproblem*

In this section we compare the performance of schemes (6), (10) and (9) using the following example.

Experiment 1. Consider the following ordinary differential equation subproblem

$$\varepsilon^2 \frac{du}{dt} = u(1 - u)(1 + u), \quad u(0) = u_0. \tag{11}$$

We solve equation (11) using schemes (10), (6) and (9). Fig. 1 compares the performance of the standard finite difference scheme and the derived nonstandard scheme as $\varepsilon \to 0$. In both cases, the solid line represent the exact solution. As expected, the standard scheme requires many grid points to avoid the spurious oscillations in Fig. 1(a).



(a) Standard scheme (10). (b) Exact scheme (6).

Figure 1. Solution for problem (11) using standard finite difference scheme (10) and NSFD scheme (6) with $\Delta t = 0.1$ and $u_0 = 0.1$.

We also compared the performance of the derived NSFD scheme (6) against the NSFD scheme (9) from *Method 2* of [6]. Fig. 2 shows that our new scheme (6) converges faster than scheme (9) for the same number of points. We highlight that, though scheme (9) does not exhibit oscillations in the solution, it also requires a sufficient number of grid points to converge to the exact solution.

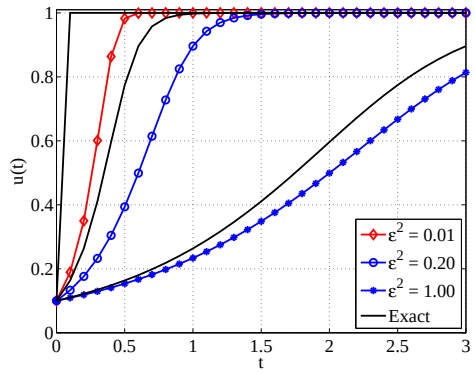


Figure 2. Comparison of the exact solution with NSFD scheme (9) for $\Delta t = 0.1$ and $u_0 = 0.1$.

2.2. *Time independent equation*

In this section we discuss the design of nonstandard finite difference scheme for the time independent equation

$$0 = \varepsilon^2 \frac{d^2u}{dx^2} + u(1+u)(1-u). \tag{12}$$

The derivation follows the procedures highlighted in [3] and [12]. The stability of this scheme is inherent in its conservation of energy. The total energy for equation (12) is given by

$$\frac{\varepsilon^2}{2}\left(\frac{du}{dx}\right)^2 + \frac{u^2}{2} - \frac{u^4}{4} = E, \tag{13}$$

where E is a constant. First, following the procedure in [12], we discretize equation (13) as follows

$$\frac{\varepsilon^2}{2}\left(\frac{v_m - v_{m-1}}{\psi(\Delta x)}\right)^2 + \frac{1}{2}v_m v_{m-1} - \frac{1}{4}v_m^2 v_{m-1}^2 = E, \tag{14}$$

where $\psi(\Delta x) \sim \Delta x + O(\Delta x^2)$. We highlight here that equation (14) is invariant under the transformation $v_m \leftrightarrow v_{m-1}$. Imposing the difference operator $\Delta r_m = r_{m+1} - r_m$ on equation (14) yields the time independent scheme

$$\varepsilon^2 \frac{v_{m-1} - 2v_m + v_{m+1}}{\psi(\Delta x)^2} + v_m - (v_m)^2 \frac{v_{m+1} + v_{m-1}}{2} = 0, \tag{15}$$

with

$$\psi(\Delta x) = 2\varepsilon \sin\left(\frac{\Delta x}{2\varepsilon}\right). \tag{16}$$

In the second procedure, we first write $f(u)$ as a product $ug(x)$ where $g(x) =$

$(1+x)(1-x)$. The scheme takes the form

$$0 = \frac{v_{m-1} - 2v_m + v_{m+1}}{\Delta x^2} + \frac{1}{\varepsilon^2} v_m \frac{K(v_m v_{m+1}) - K(v_m v_{m-1})}{v_m(v_{m+1} - v_{m-1})}, \tag{17}$$

where

$$K(z) = \int_0^z g(x) = -z + \frac{1}{2}z^2.$$

Therefore

$$K(v_m v_{m+1}) = -v_m v_{m+1} + \frac{1}{2}(v_m v_{m+1})^2.$$

Finally, we propose the scheme for steady state equation (12) as follows

$$0 = \varepsilon^2 \frac{v_{m-1} - 2v_m + v_{m+1}}{(\Delta x)^2} + v_m \left(1 - \frac{(v_{m+1} + v_{m-1})}{2} v_m\right). \tag{18}$$

The above derivation yields similar schemes which are stable with regard to the conservation of energy. The only difference is the existence of a complex denominator in (15) as compared to (18). This stability is a result of $\Delta E = 0$. The next step is to carefully assemble the time independent and the space independent schemes to approximate the solution of equation (1).

2.3. *The full equation*

We carefully bring both the space independent scheme (6), and the time independent schemes (15), together to obtain a scheme for equation (1). To this end, we propose

$$\frac{v_m^{n+1} - v_m^n}{\phi(\Delta t)} = \frac{v_{m-1}^n - 2v_m^n + v_{m+1}^n}{\psi(\Delta x)^2} + \varepsilon^{-2} \frac{2(v_m^{n+1})^2}{v_m^{n+1} + v_m^n} \left(1 - \frac{v_{m-1}^n + v_{m+1}^n}{2} v_m^n\right), \tag{19}$$

where $\phi(\Delta)$ and $\psi(\Delta x)$ are given in (7) and (16) respectively. This is a quadratic equation in v_m^{n+1} which can be solved to get

$$v_m^{n+1} = \frac{-B_m^n \pm \sqrt{{B_m^n}^2 + A_m^n C_m^n}}{A_m^n},$$

where

$$A_m^n = 1 - \phi_\varepsilon(1 - \bar{v}_m^n v_m^n), \quad B_m^n = R(v_m^n - \bar{v}_m^n), \quad C_m^n = R\bar{v}_m^n v_m^n - (2R-1)(v^n)^2,$$

$R = \phi(\Delta t)/[\psi(\Delta x)]^2$, $\phi_\varepsilon(\Delta t) = 2\phi(\Delta t)/\varepsilon^2$ and $\bar{v}_m^n = (v_{m-1}^n + v_{m+1}^n)/2$. If we impose the condition $R = \frac{1}{2}$, and consider the definition of $\phi(\Delta t)$, then $A_m^n > 0$ and $C_m^n > 0$, hence, the sign of v_m^{n+1} depends mainly on the sign of the square root. Therefore, we are able to control the positivity and negativity of the solution as the case requires.

On the other hand, combining schemes (9) and (18), we have

$$\frac{v_m^{n+1}-v_m^n}{\Delta t} = \frac{v_{m-1}^n - 2v_m^n + v_{m+1}^n}{(\Delta x)^2} + \varepsilon^{-2}\left([2v_m^n - v_m^{n+1}] - v_m^n \frac{v_{m-1}^n + v_{m+1}^n}{2} v_m^{n+1}\right). \tag{20}$$

We note that scheme (20) is different from *Method B* in [6]. The current scheme can be rewritten as

$$v_m^{n+1} = \frac{\varepsilon^2(1-2R)v_m^n + 2\varepsilon^2(\Delta t)v_m^n + 2\varepsilon^2 R\bar{v}_m^n}{\varepsilon^2 + \varepsilon^2(\Delta t) + \varepsilon^2(\Delta t)v_m^n\bar{v}_m^n/2}. \tag{21}$$

Equation (21) reveals that v_m^{n+1} remains positive given that $v_m^n > 0$ and negative if $v_m^n \leq 0$. Imposing the condition $R = \frac{1}{2}$, equation (21) takes the form

$$v_m^{n+1} = \frac{2\varepsilon^2(\Delta t)v_m^n + \varepsilon^2\bar{v}_m^n}{\varepsilon^2 + \varepsilon^2(\Delta t) + \varepsilon^2(\Delta t)v_m^n\bar{v}_m^n/2}.$$

3. Numerical simulations of the full equation

The performance of the derived schemes is demonstrated by applying them to solve the Allen-Cahn equation. Three schemes will be considered, i.e., our derived scheme (19), scheme (20) and scheme *Method B* from [6]. Note that scheme (20) is a result of [6] for the space independent problem and our energy formulation for the time independent problem. For all the simulations, we will impose the condition $R = \frac{1}{2}$.

Experiment 2. Consider the Allen-Cahn equation

$$\begin{aligned} \frac{\partial u}{\partial t} &= \frac{\partial^2 u}{\partial x^2} + \varepsilon^{-2}u(1-u)(1+u), \\ u(x,0) &= u_0(x), \quad u_x(-2,t) = u_x(2,t) = 0. \end{aligned} \tag{22}$$

with $\varepsilon \ll 1$. For comparison, we use the traveling wave solution

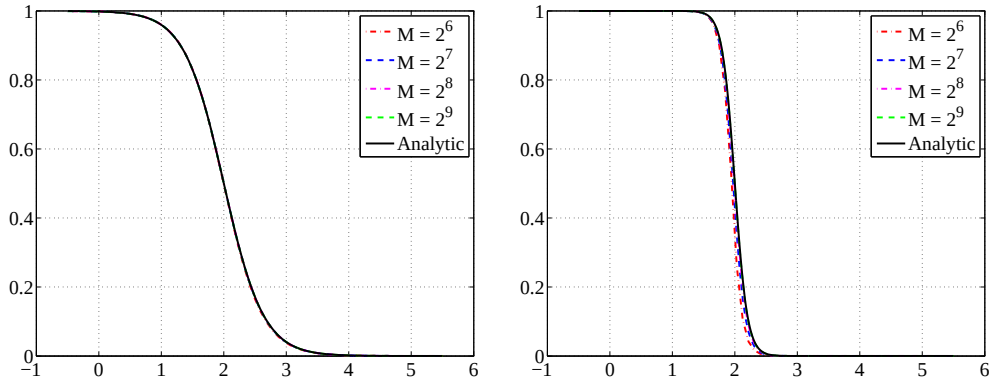
$$u(x,t) = \frac{1}{2}\left(1 - \tanh\frac{x-st}{\varepsilon 2\sqrt{2}}\right),$$

where the traveling wave speed is $s = 3/(\varepsilon\sqrt{2})$, see [7].

The approximations using scheme (19) are shown in Figs. 3 and 4 with the error values tabulated in Table 1. Fig. 3(a) confirms that the convergence of our scheme is very fast to the extent that the curves for different number of grid point are indistinguishable. However, while no spurious oscillations can be seen in Fig. 4, the convergence is much slower. We also highlight that the performance of *Method B* of [6] is equally the same as scheme (20) as can be seen in the table of errors albeit they being two different schemes. Table 1 also confirms the better performance of the derived scheme.

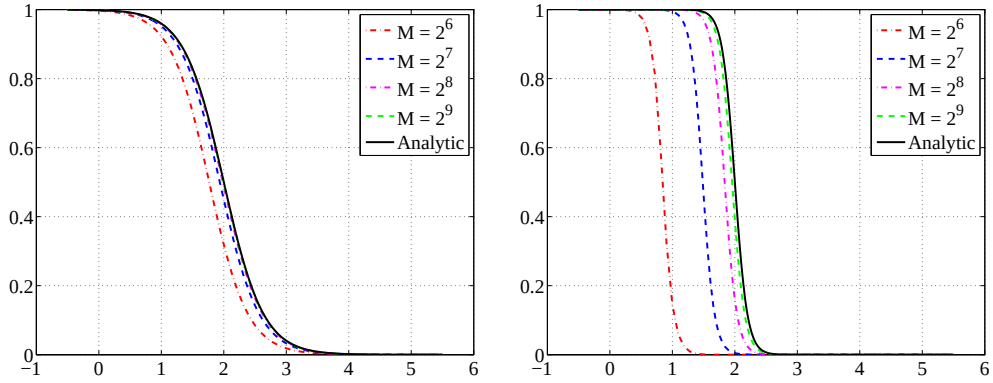
Table 1. Error values of the nonstandard scheme for different values of ε

M	L_∞ Norm error					
	$\varepsilon^2 = 0.05$			$\varepsilon^2 = 0.005$		
	Scheme (19)	Scheme (20)	[6]	Scheme (19)	Scheme (20)	[6]
2^6	$6.58e-3$	$1.86e-1$	$1.86e-1$	$1.63e-1$	$9.94e-1$	$9.94e-1$
2^7	$1.34e-3$	$5.09e-2$	$5.10e-2$	$7.09e-2$	$8.66e-1$	$8.66e-1$
2^8	$6.92e-4$	$1.24e-2$	$1.24e-2$	$2.40e-2$	$3.90e-1$	$3.90e-1$
2^9	$3.54e-4$	$3.48e-3$	$3.48e-3$	$7.24e-3$	$1.01e-1$	$1.01e-1$



(a) $\varepsilon^2 = 0.05$ (b) $\varepsilon^2 = 0.005$

Figure 3. The convergence of the scheme (19).



(a) $\varepsilon^2 = 0.05$ (b) $\varepsilon^2 = 0.005$

Figure 4. The convergence of the scheme (20).

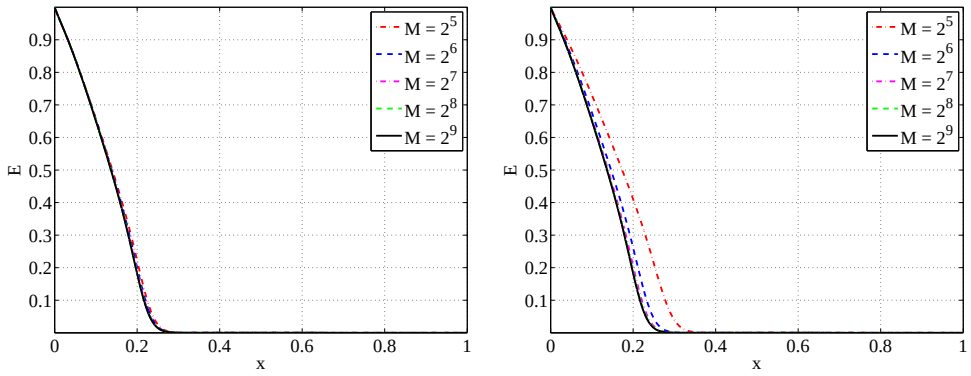
Experiment 3. Consider the Allen-Cahn equation

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} + \varepsilon^{-2} u(1-u)(1+u), \tag{23}$$
$$u(x,0) = \exp\left(-5x^2\right), \quad u_x(-2,t) = u_x(2,t) = 0.$$

for $\varepsilon \in (0,1)$.

A major property of any scheme designed for the Allen-Cahn equation is the dissipation of Ginzburg-Landau energy, see equation (2). Here we consider Experiment 3 to verify this property. The results are shown in Fig. 5 for both schemes (19) and (20). The faster convergence of scheme (19) is evident in Fig. 5(a). In the last ex-

periment we changed the initial condition for Experiment 3 to $u(x,0) = \sin\left(\frac{5\pi}{2}x\right)$. Figure 6 shows the absorption of interphases. Initially, there exists four crests, with the solution fluctuating between the two stable fixed points. At $t = 1$, all the crests are absorbed and we only remain with the widest crest which is the traveling wave solution indicated in [7].



(a) Scheme (19) . (b) Scheme (20)

Figure 5. This shows the dissipation of the nondimensionalized energy functional $E(u)/E(u_0)$ where $u(x,0) = \exp\left(-5x^2\right)$.

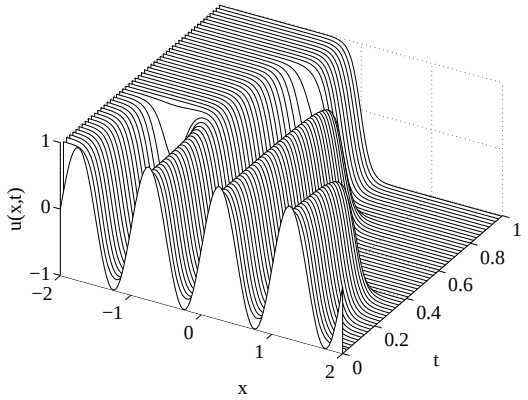


Figure 6. Numerical solution for Experiment 3 with initial condition $u(x,0) = \sin\left(\frac{5\pi}{2}x\right)$.

4. Discussion and conclusion

In this work we designed an explicit nonstandard finite difference scheme for the Allen-Cahn reaction diffusion equation. Our analysis centered on the strength of the schemes to preserve the qualitative properties of the isolated equations. We highlighted that the difference schemes (6) and (9) preserve the stable fixed points of the equation (4). Figure 1 shows that the stability of scheme (6) is independent of ε but this is not true of the standard finite difference scheme. The standard scheme requires many grid points in order to prevent spurious oscillations. Therefore, as $\varepsilon \to 0$ simulation with the standard scheme will become expensive. Also, the schemes designed for the steady state equation are stable with respect to the conservation of energy. Schemes (6) and (9) were carefully assembled with the time

independent scheme (15). We claim that these explicit schemes have better time restriction compared to the standard finite difference scheme. Work on the global stability analysis of the scheme (19) is under investigation and will be submitted soon.

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