

STABILITY ANALYSIS AND APPLICATION OF THE EXPONENTIAL TIME DIFFERENCING SCHEMES ^{*1)}

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Dedicated to Professor Zhong-ci Shi on the occasion of his 70th birthday

Abstract

Exponential time differencing schemes are time integration methods that can be efficiently combined with spatial spectral approximations to provide very high resolution to the smooth solutions of some linear and nonlinear partial differential equations. We study in this paper the stability properties of some exponential time differencing schemes. We also present their application to the numerical solution of the scalar Allen-Cahn equation in two and three dimensional spaces.

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1. Introduction

For many time dependent partial differential equations with smooth or regularized solutions, spectral and pseudo-spectral methods have been shown to provide remarkably effective spatial discretization. The application of these discretization methods often results in systems of stiff ordinary differential equations (ODEs) in time and thus make the efficient and stable time integration scheme very essential.

The subject of solving stiff systems has been well studied in the literature [11], including, for instance, linearly implicit methods [1], semi-implicit methods [4], time-splitting methods, projection methods [8], multiscale methods [7, 9], integrating factors (IF), and the exponential time differencing (ETD) methods [6, 12]. In this paper, of particular interests to us are the ETD schemes and their modifications which have been shown to perform extremely well in solving various one dimensional diffusion type problems [12]. ETD schemes have also been used by other authors under different names [2, 15]. In essence, for nonlinear time dependent equations, the ETD schemes provide a systematic coupling of the explicit treatment of nonlinearities and the implicit *and possibly exact* integration of the stiff linear parts of the equations, while achieving high accuracy and maintaining good stability.

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It is natural to expect that ETD like schemes can be very useful in phase field computations that involve more complex physics [4, 16]. In fact, some preliminary numerical studies conducted jointly by us and by a group of material scientists at the Penn State University have indicated that the higher order ETD based schemes can be several orders of magnitude faster than the low-order semi-implicit methods in some simulations of microstructure evolution [17]. This further motivates our theoretical investigation on the various properties of the ETD schemes while carrying out more extensive computational studies for real application problems. As an initial attempt, the work reported here mainly contains an analytical examination of the stability and monotonicity of the ETD type schemes for some model parabolic equations. Until now, the stability of ETD schemes is only studied in [6] for ODEs, while the stability of the modified ETD scheme has not been touched upon in [12]. Using techniques ranging from spectral decomposition, energy estimates, and maximum principles, our study here provides a more detailed theoretical analysis of the ETD schemes. Due to the page limit, we do not include any discussion on the modified ETD schemes proposed in [12], though similar analysis can also be performed. As one of the main applications we are working on, we conduct numerical studies of the the ETD scheme for the solution of a time dependent scalar Ginzburg-Landau equation (also named as the Allen-Cahn equation) in the two and three dimensional spaces. Such a study is often the first step towards a more realistic model for many phase transition problems [3]. Again, only some preliminary two and three dimensional numerical simulation results are provided here to conserve space. Our short presentation merely serves as a hint to the techniques and applications of more detailed theoretical and numerical investigations on the ETD schemes to be carried out in the subsequent study [5].

The rest of the paper is organized as follows. In Section 2, we introduce the original and modified ETD schemes. We then turn to discuss the asymptotic L^2 -stability and L^∞ -stability of those schemes for some model problems in Sections 3 and 4. Some numerical experiments will be given in Section 5.

2. The Exponential Time Differencing Schemes

Given a linear elliptic operator \mathcal{L} , we consider the partial differential equation (PDE) for a scalar function u defined in a spatial domain $\Omega = [0, 2\pi]^d \subset \mathbb{R}^d$ and for time $t > 0$:

$$u_t = \mathcal{L}u + \mathcal{N}(u, t, x), \quad (1)$$

along with suitable initial and boundary conditions. Here, \mathcal{N} denotes a generic nonlinear term. A particular case of our interests in this paper is the dimensionless time-dependent Ginzburg-Landau (Allen-Cahn) equation where $\mathcal{N}(u, t, x) = u(1 - u^2)/\epsilon^2$ for some interfacial parameter ϵ , and Δ being the Laplace operator. It is also convenient for us to introduce a related linear equation of the type

$$u_t = \Delta u + \lambda u. \quad (2)$$

where λ can either be a constant or a function of the time and the spatial variables. In the latter case, λu can represent an approximation of a nonlinear term through either linearization or by frozen coefficients techniques. For most of our discussion, initial boundary value problems with either periodic or homogeneous Dirichlet boundary conditions are considered for the equation (2).

Discretizing the PDE (1) in the spatial variables, for instance, by spectral approximations or by finite element approximations, a system of ordinary differential equations (ODEs) is often obtained

$$u_t = \mathbf{L}u + \mathbf{N}(u, t). \quad (3)$$

The exponential time differencing (ETD) methods can be described in the context of solving

(3). Integrating the equation over a single time step from $t = t_n$ to $t_{n+1} = t_n + h$, we get

$$u(t_{n+1}) = e^{\mathbf{L}h}u(t_n) + e^{\mathbf{L}h} \int_0^h e^{-\mathbf{L}s} \mathbf{N}(u(t_n + s), t_n + s) ds. \quad (4)$$

The equation (4) is exact, and the various ETD schemes come from the approximations to the integral [6].

Denote the numerical approximation to $u(t_n)$ by u_n , the first order scheme ETD1 is given by

$$u_{n+1} = e^{\mathbf{L}h}u_n + \mathbf{L}^{-1}(e^{\mathbf{L}h} - \mathbf{I})\mathbf{N}(u_n, t_n). \quad (5)$$

Higher order ETD schemes, for instance, the second, third and fourth order ETD Runge-Kutta schemes (which we refer as ETD2RK, ETD3RK, and ETD4RK respectively) can also be found in [6, 12]. For completeness, we give below the formulae for a fourth-order scheme (ETD4RK):

$$a_n = e^{\mathbf{L}h}/2u_n + \mathbf{L}^{-1}(e^{\mathbf{L}h}/2 - \mathbf{I})\mathbf{N}(u_n, t_n), \quad (6)$$

$$b_n = e^{\mathbf{L}h}/2u_n + \mathbf{L}^{-1}(e^{\mathbf{L}h}/2 - \mathbf{I})\mathbf{N}(a_n, t_n + \frac{h}{2}), \quad (7)$$

$$c_n = e^{\mathbf{L}h}/2a_n + \mathbf{L}^{-1}(e^{\mathbf{L}h}/2 - \mathbf{I})(2\mathbf{N}(b_n, t_n + \frac{h}{2}) - \mathbf{N}(u_n, t_n)), \quad (8)$$

$$\begin{aligned} u_{n+1} &= e^{\mathbf{L}h}u_n + h^{-2}\mathbf{L}^{-3}\{[-4 - \mathbf{L}h + e^{\mathbf{L}h}(4 - 3\mathbf{L}h + (\mathbf{L}h)^2)]\mathbf{N}(u_n, t_n) \\ &+ [4 + 2\mathbf{L}h - 2e^{\mathbf{L}h}(2 - \mathbf{L}h)](\mathbf{N}(a_n, t_n + h/2) + \mathbf{N}(b_n, t_n + h/2)) \\ &+ [-4 - 3\mathbf{L}h - (\mathbf{L}h)^2 + e^{\mathbf{L}h}(4 - \mathbf{L}h)]\mathbf{N}(c_n, t_n + h)\}. \end{aligned} \quad (9)$$

The above formulae may look complicated at the first sight, but the implementation can be carried out efficiently if L is easily diagonalizable. To overcome the vulnerability of error cancellations in the higher-order ETD and ETDRK schemes, and to generalize the ETD schemes to non-diagonal problems, in [12], modified ETD schemes is proposed by using the complex contour integrals

$$f(\mathbf{L}) = \frac{1}{2\pi i} \int_{\Gamma} f(z)(z\mathbf{I} - \mathbf{L})^{-1} dz \quad (10)$$

on a suitable contour Γ to evaluate the coefficients in the update formula for ETD4RK. For more detailed derivations and applications of the ETD and modified ETD schemes, we refer to [6, 12]. Let us note that our recent study has discovered that that only very few nodes are needed in the numerical quadratures in order to preserve the good accuracy to the contour integration and the time integrator. Moreover, the contour integration based modified ETD schemes enjoy even better stability properties than the original ETD schemes. Due to the page limit, these kinds of results are not presented here, and we refer interested readers to our subsequent work [5] for more details.

3. L^2 -stability Analysis

For simplicity, we here mainly present results concerning the application of the first order ETD scheme to the equation (2), with no spatial approximation is made.

Given the solution u_n at the time step t_n , the first order ETD scheme applying directly to (1) is equivalent to solving

$$\begin{cases} \frac{\partial}{\partial t} w(\mathbf{x}, t) &= \Delta w(\mathbf{x}, t) + \mathcal{N}(u_n(\mathbf{x}), t, x), \\ w(\mathbf{x}, 0) &= u_n(\mathbf{x}) \end{cases} \quad (11)$$

with the corresponding boundary condition in a time interval $(0, \tau)$ and setting $u_{n+1} = w(\cdot, \tau)$, $t_{n+1} = \tau + t_n$. Here, we use τ to denote the time step size (same as the h used in the earlier section).

Corresponding to (2), the ETD scheme is reduced to:

$$\begin{cases} \frac{\partial}{\partial t} w(\mathbf{x}, t) &= \Delta w(\mathbf{x}, t) + \lambda u_n(\mathbf{x}), \\ w(\mathbf{x}, 0) &= u_n(\mathbf{x}) \end{cases} \quad (12)$$

with the corresponding boundary condition and $u_{n+1} = w(\cdot, \tau)$. For the spectral approximations of equations (1) and (2), the resulting equations are modified by simply replacing $\mathcal{N}(u_n, t, x)$ and λu_n in (1) and (2) respectively by their Galerkin projections onto the finite dimensional Fourier spaces. In the context of spectral approximation to the nonlinear Allen-Cahn equation (also called the time dependent Ginzburg-Landau equation), the resulting first order ETD scheme becomes very close to the semi-implicit scheme used by [4]. Similarly, for finite element approximations, the operator Δ would have to be replaced by its discrete approximations as well.

We recall some technical terms. Let B denote a Banach space, and u_n denote the numerical solution at the time step n , we call a marching scheme asymptotically B stable, if $\|u_{n+1}\|_B \leq \|u_n\|_B$ for all n . If no restriction needs to be imposed on the time step $\tau = t_{n+1} - t_n$ to achieve such stability bound, then the scheme is called unconditionally asymptotically B stable. For more discussion on the stability of numerical schemes, we refer to [11, 14].

We now proceed with a stability theorem concerning (12). In the case λ being a constant, using a spectral decomposition, the stability issue is related to an analysis of the stabilities of the corresponding system of ODEs for the spectral (Fourier) modes.

Theorem 3.1. *For the first order ETD scheme (12) for the equation (2) with constant λ and periodic boundary condition, we have*

(i) if $|\lambda| = 0$, it is unconditionally asymptotically L^2 -stable.

(ii) if $|\lambda| \neq 0$, it is asymptotically L^2 -stable $\iff \Re\lambda < 0$ and $\tau \leq \frac{-2\Re\lambda}{|\lambda|^2}$.

Proof. Using Fourier expansion let $u_n(\mathbf{x}) = \sum_{\mathbf{k} \in \mathbb{Z}^d} \widehat{u}_{n,\mathbf{k}} e^{i\mathbf{k} \cdot \mathbf{x}}$, where

$$\widehat{u}_{n,\mathbf{k}} = \frac{1}{(2\pi)^{d/2}} \int_{\Omega} u_n(\mathbf{x}) e^{i\mathbf{k} \cdot \mathbf{x}} d\mathbf{x} \quad \mathbf{k} \in \mathbb{Z}^d,$$

and let $w(\mathbf{x}, t) = \sum_{\mathbf{k} \in \mathbb{Z}^d} \widehat{w}_{\mathbf{k}}(t) e^{i\mathbf{k} \cdot \mathbf{x}}$ for any time t , we get

$$\begin{cases} \frac{d}{dt} \widehat{w}_{\mathbf{k}}(t) &= -|\mathbf{k}|^2 \widehat{w}_{\mathbf{k}}(t) + \lambda \widehat{u}_{n,\mathbf{k}}, \\ \widehat{w}_{\mathbf{k}}(0) &= \widehat{u}_{n,\mathbf{k}} \end{cases} \quad (13)$$

for all $\mathbf{k} \in \mathbb{Z}^d$. By the variation of constants formula,

$$\widehat{w}_{\mathbf{k}}(\tau) = \widehat{u}_{n,\mathbf{k}} e^{-|\mathbf{k}|^2 \tau} + \int_0^\tau \lambda e^{-|\mathbf{k}|^2(\tau-s)} \widehat{u}_{n,\mathbf{k}} ds.$$

Define, for any $\mathbf{k} \in \mathbb{Z}^d$,

$$g_{\mathbf{k}}(\tau) = \begin{cases} 1 + \lambda \tau & \text{if } |\mathbf{k}|^2 = 0, \\ 1 + \frac{1 - e^{-|\mathbf{k}|^2 \tau}}{|\mathbf{k}|^2} (\lambda - |\mathbf{k}|^2) & \text{if } |\mathbf{k}|^2 \neq 0, \end{cases}$$

then we get $\widehat{w}_{\mathbf{k}}(\tau) = g_{\mathbf{k}}(\tau) \widehat{u_{n,\mathbf{k}}}$, for all $\mathbf{k} \in \mathbb{Z}^d$. Therefore,

$$w(\mathbf{x}, \tau) = \frac{1}{(2\pi)^{d/2}} \int_{\Omega} \sum_{\mathbf{k} \in \mathbb{Z}^d} g_{\mathbf{k}}(\tau) u_n(\mathbf{y}) e^{i\mathbf{k} \cdot (\mathbf{x} - \mathbf{y})} d\mathbf{y} \quad (14)$$

and $\|w(\cdot, \tau)\|_{L^2(\Omega)}^2 = \sum_{\mathbf{k} \in \mathbb{Z}^d} |g_{\mathbf{k}}(\tau)|^2 |\widehat{u_{n,\mathbf{k}}}|^2$.

To get the asymptotic L^2 -stability, we need $|g_{\mathbf{k}}(\tau)| \leq 1$ for all $\mathbf{k} \in \mathbb{Z}^d$, i.e.,

$$|1 + \lambda \tau| \leq 1, \quad (15)$$

and

$$|1 + r_{\mathbf{k}}(\lambda - |\mathbf{k}|^2)| \leq 1 \quad \forall \mathbf{k} \in \mathbb{Z}^d, |\mathbf{k}|^2 \neq 0, \quad (16)$$

where $r_{\mathbf{k}} = (1 - e^{-|\mathbf{k}|^2 \tau})/|\mathbf{k}|^2$. Note that the above two inequalities hold trivially when $|\lambda| = 0$, we then turn to the case when $|\lambda| \neq 0$.

First, (15) is equivalent to $\tau|\lambda|^2 + 2\Re\lambda \leq 0$, and one must have

$$\Re\lambda < 0 \quad \text{and} \quad \tau \leq \bar{\tau}_0 \stackrel{\text{def}}{=} \frac{-2\Re\lambda}{|\lambda|^2}. \quad (17)$$

Next, direct computation shows that (16) is equivalent to

$$r_{\mathbf{k}}(|\lambda|^2 - 2\Re\lambda |\mathbf{k}|^2 + |\mathbf{k}|^4) + 2(\Re\lambda - |\mathbf{k}|^2) \leq 0, \quad (18)$$

which holds if $|\mathbf{k}|^2 \geq |\lambda|$. Now for those $\mathbf{k} \in \mathbb{Z}^d$, $|\mathbf{k}|^2 < |\lambda|$, and $|\mathbf{k}|^2 \neq 0$, the equation (18) is equivalent to

$$e^{-|\mathbf{k}|^2 \tau} \geq \frac{|\lambda|^2 - |\mathbf{k}|^4}{|\lambda|^2 - 2\Re\lambda |\mathbf{k}|^2 + |\mathbf{k}|^4},$$

namely,

$$\tau \leq \bar{\tau}_{\mathbf{k}} \stackrel{\text{def}}{=} \frac{1}{|\mathbf{k}|^2} \ln \left(1 + \frac{2(|\mathbf{k}|^2 - \Re\lambda)|\mathbf{k}|^2}{|\lambda|^2 - |\mathbf{k}|^4} \right) = f(|\mathbf{k}|^2) \quad (19)$$

Let $b = |\lambda|$, $a = -\Re\lambda$, $x = |\mathbf{k}|^2$, we have

$$f(x) = \frac{1}{x} \ln \left(\frac{b^2 + 2ax + x^2}{b^2 - x^2} \right)$$

Notice that $b > x > 0$, and $b > a > 0$, we get from a direct computation that $f'(x) > 0$ which implies that $f = f(x)$ is an increasing function of x . Moreover, since $\lim_{x \rightarrow 0^+} f(x) = 2a/b^2$, we get that $\bar{\tau}_{\mathbf{k}}$ is an increasing function of $|\mathbf{k}|^2$, and $\bar{\tau}_{\mathbf{k}} < \bar{\tau}_0$. This proves the theorem.

Clearly, the above analysis can be adapted to more general domain and boundary conditions. A suitable eigen-decomposition corresponding to the differential operator can be used in place of the Fourier series. We omit the details.

Before we move on, let us consider a slight variation of the above theorem. Since for the spectral approximation of the ETD schemes, a linear shift in the operator \mathcal{L} can be easily implemented, we thus establish in the following the fact that a *good* shift, or a suitable operator splitting, can improve the stability. For $\alpha > 0$, consider the ETD scheme with $\mathcal{L} = \Delta - \alpha$ which is equivalent to solve

$$\begin{cases} \frac{\partial}{\partial t} w(\mathbf{x}, t) &= (\Delta - \alpha)w(\mathbf{x}, t) + (\lambda + \alpha) u_n(\mathbf{x}), \\ w(\mathbf{x}, 0) &= u_n(\mathbf{x}) \end{cases}. \quad (20)$$

Following similar discussions as that given in the above theorem, we can show that:

Corollary 3.1. *The first order ETD scheme with splitting (20) is unconditionally asymptotically L^2 -stable for the equation (2) with constants $\alpha > 0$, λ and periodic boundary condition if either $|\lambda| = 0$ or if $\Re\lambda < 0$ together with $\alpha \geq -|\lambda|^2/(2\Re\lambda)$.*

This is a particularly useful fact when solving nonlinear equations. With a suitable splitting of its linear part, stability can often be improved for ETD like schemes.

We can easily extend the stability conditions to the first order ETD scheme applied to problem (2) with homogeneous Dirichlet boundary conditions:

$$w(\mathbf{x}, t) = 0 \quad \mathbf{x} \in \partial\Omega, \quad (21)$$

Corollary 3.2. *For the first order ETD scheme (12) with (21),*

(i) *if $|\lambda| \leq 1$, then it is unconditionally asymptotically L^2 -stable.*

(ii) *if $|\lambda| \geq 1$, then it is asymptotically L^2 -stable if and only if $\Re\lambda < 0$ and*

$$\tau \leq \ln \left(\frac{|\lambda|^2 - 2\Re\lambda + 1}{|\lambda|^2 - 1} \right).$$

Proof. Note that with homogeneous Dirichlet boundary conditions (21), the Fourier series becomes sine series, and we have the Fourier mode $\mathbf{k} \in \mathbb{Z}^d \setminus \{\mathbf{0}\}$. Hence, if $|\lambda| \leq 1$, then (18) holds; if $|\lambda| \geq 1$, then (18) holds if and only if $\Re\lambda < 0$ and (19) holds. Noting that for all $\bar{\tau}_{\mathbf{k}}$'s defined in (19), where $\mathbf{k} \in \mathbb{Z}^d \setminus \{\mathbf{0}\}$, the minimum is obtained at $|\mathbf{k}|^2 = 1$; and then the corollary follows.

Concerning the stability of the actual numerical scheme, we note that same conclusions can be drawn when solving the model problem (12) with periodic or homogeneous Dirichlet boundary conditions (21) using the first order ETD scheme in the time variable and spectral or pseudo-spectral methods in the space variables. The method of finite Fourier (or sine) series can still be used; and it is not hard to see that all the assertions in the above theorem still remain true for constant λ .

For the case that the coefficient λ is a function dependent on the spatial variables, we have the following sufficient condition for the stability in a modified energy norm.

Theorem 3.2. *For the first order ETD scheme with operator splitting (20) for the equation (2) with the periodic boundary condition or (21) and λ be dependent on x , if $\max_x \Re\{\lambda\} \leq 0$ and $2\tau(\max_x \Re\{-\lambda\} - \alpha) \leq 1$, then,*

$$\int_{\Omega} \left(|\nabla w(\tau)|^2 - \Re\{\lambda\} |w(\tau)|^2 \right) d\Omega \leq \int_{\Omega} \left(|\nabla w_n|^2 - \Re\{\lambda\} |w_n|^2 \right) d\Omega. \quad (22)$$

Proof. Multiplying the equation (12) by w_t^* , integrating in both space and time, taking the real part and using integration by parts, we get

$$\begin{aligned} \int_0^\tau \int_{\Omega} |w_s(s)|^2 d\Omega ds &+ \int_{\Omega} \left(\frac{1}{2} (|\nabla w(s)|^2 + \alpha |w(s)|^2) - \Re\{\lambda w(\tau)^* w_n\} \right) d\Omega \\ &= \int_{\Omega} \left(\frac{1}{2} (|\nabla w_n|^2 - \Re\{\lambda\} |w_n|^2) \right) d\Omega. \end{aligned} \quad (23)$$

We multiply the above by 2τ and take note that,

$$\int_0^\tau \int_{\Omega} \tau |w_s(s)|^2 d\Omega ds \geq \int_{\Omega} |w(\tau) - w_n|^2 d\Omega.$$

Rearranging terms, we get

$$\begin{aligned} \int_{\Omega} (\tau \Re\{\lambda\} + \tau\alpha + 2) |w(\tau) - w_n|^2 d\Omega &+ \int_{\Omega} \left(\tau |\nabla w(s)|^2 - \tau \Re\{\lambda\} |w(\tau)|^2 \right) d\Omega \\ &= \int_{\Omega} \left(\tau |\nabla w_n|^2 - \tau \Re\{\lambda\} |w_n|^2 \right) d\Omega. \end{aligned}$$

Thus, by the assumption on λ and the α , (22) follows.

Remark 3.1. The above theorem also holds for the spatial discretization of (12) via either spectral or finite element Galerkin approximations since the relation (23) remains valid in such cases.

4. L^∞ -stability

Next, we turn to study the point-wise behavior of the first order ETD scheme. When modeling phase transition problems, point-wise estimates are usually desirable so that a proper physical interpretation of the solution can be made.

Recall that the equation (2) often shares maximum principle. We thus examine similar properties of the ETD scheme. This part of our discussion is limited only to the one space dimensional case and with no spatial discretization.

First of all, let us establish the monotonicity property for linear equations. In order to extend to some nonlinear problems, we again allow λ to vary with respect to \mathbf{x} but not to t . Moreover, we only consider the case λ being real.

Theorem 4.1. *For the initial Cauchy value problem (12) with $\max \lambda \leq 0$ on the real line, we have*

i) if $1 + 2\tau \min \lambda \geq 0$, and $u_n \geq 0$ for all x , then $w(\mathbf{x}, t) \geq 0$ for all x .

ii) if $1 + \tau \min \lambda \geq 0$, then $|w(\mathbf{x}, \tau)| \leq \sup_{\mathbf{x} \in R^1} |u_n(\mathbf{x})|$.

Proof. First, we have

$$w(\mathbf{x}, t) = \int_{R^d} u_n(\mathbf{x} - \mathbf{y}) \left(\int_0^t \lambda \Phi(\mathbf{y}, s) ds + \Phi(\mathbf{y}, t) \right) d\mathbf{y}, \quad (24)$$

where $\Phi(\mathbf{y}, s) = \frac{e^{-|\mathbf{y}|^2/4s}}{(4\pi s)^{d/2}}$. Since

$$\int_0^t \Phi(\mathbf{y}, s) ds = (2\pi)^{-\frac{d}{2}} \int_{\frac{|\mathbf{y}|}{\sqrt{2t}}}^\infty u^{d-3} |\mathbf{y}|^{2-d} e^{-\frac{u^2}{2}} du. \quad (25)$$

If $d = 1$, then integrating by parts shows

$$\int_0^t \Phi(\mathbf{y}, s) ds = \frac{1}{\sqrt{2\pi}} |\mathbf{y}| \left(|\mathbf{y}|^{-1} \sqrt{2t} e^{-\frac{|\mathbf{y}|^2}{4t}} - \int_{\frac{|\mathbf{y}|}{\sqrt{2t}}}^\infty e^{-\frac{u^2}{2}} du \right) \leq 2t \Phi(\mathbf{y}, t),$$

therefore, if $\max \lambda \leq 0$, we have

$$(1 + 2\min \lambda t) \Phi(\mathbf{y}, t) \leq \int_0^t \lambda \Phi(\mathbf{y}, s) ds + \Phi(\mathbf{y}, t) \leq \Phi(\mathbf{y}, t). \quad (26)$$

Hence from (24) and (26), depending on whether $1 + 2\min \lambda \tau \geq 0$ or $1 + 2\min \lambda \tau \geq -1$, we get respectively either $0 \leq w(x, \tau) \leq u_n(x)$ if $u_n(x) \geq 0$ or $|w(x, \tau)| \leq |u_n(x)|$. Thus, the assertions of the theorem follow.

We can also obtain similar results for the linear equation (12) with periodic boundary conditions.

Corollary 4.1. *For the initial boundary value problem (12) with periodic boundary condition, if λ is also periodic with $\max_x \lambda \leq 0$, then*

i) for $2\tau \min_x(\lambda) \geq -1$, $w(\mathbf{x}, \tau) \geq 0$ for all $\mathbf{x} \in (0, 2\pi)$ if $u_n \geq 0$ in $(0, 2\pi)$;

ii) for $\tau \min_x(\lambda) \geq -1$, $\sup_{\mathbf{x} \in (0, 2\pi)} |w(\mathbf{x}, \tau)| \leq \sup_{\mathbf{x} \in (0, 2\pi)} |u_n(\mathbf{x})|$.

Proof. Extend u_n and λu_n periodically (with period 2π) to \tilde{u}_n and $\lambda \tilde{u}_n$ to the whole space; and notice that $\sup_{\mathbf{x} \in R^1} |\tilde{u}_n(\mathbf{x})| = \sup_{\mathbf{x} \in (0, 2\pi)} |u_n(\mathbf{x})|$ the assertion follows exactly from the proof in Theorem 4.1 with u_n replaced by \tilde{u}_n .

L^∞ stability analysis can also be carried out for semi-implicit schemes that use a time difference to replace the time differentiation. In fact, such analysis for semi-implicit schemes are generally valid also in multi-dimensional spaces by invoking a maximum principle type arguments for elliptic equations.

5. Numerical Results

We now turn our attention to the application of the ETD scheme and its modifications to the solution of the time dependent Ginzburg-Landau equation (also called the Allen-Cahn equation) that often forms a core component of the phase field modeling of the microstructure evolution in a binary or multicomponent alloy. One of our ultimate goals is to make the high order ETD scheme work very efficiently for such complex phase field models.

The unknown function u in the time dependent Ginzburg-Landau equation

$$u_t = \Delta u + \frac{1}{\epsilon^2} u(1 - u^2), \quad (27)$$

represents an order parameter, and the nonlinear term $N(u) = (u - u^3)/\epsilon^2$ is obtained from the standard double-well free energy potential [13] with ϵ measuring the interface thickness.

In our simulations, periodic boundary condition is used as it often is the case in practice where the bulk properties are of central interests. This leads, conveniently, to the application of the Fourier pseudo-spectral approximation in space. At $t = 0$, an initial condition is given with a circular (spherical) interface boundary centered at the center of a square (cubic) domain. The order parameter values inside the circle (sphere) are assigned $+1$ and -1 outside. Such a circular (spherical) interface will undergo the mean curvature motion and eventually disappear.

Here, due to page limitations, we only compare the results of the Ginzburg-Landau simulation using ETD4RK with that of a sharp interface model. We take a two dimensional square of size 8×8 and an initial circle of radius 3.125 and solve the equation (27) with various values of ϵ . Let $A(t)$ be the area (volume) of the circle (sphere) at time t with positive u values and A_0 be the initial area, then in the limit as $\epsilon \rightarrow 0$, that is, in the sharp interface limit, the mean curvature motion gives

$$A(t) = A_0 - 2\pi t. \quad (28)$$

First, we show in Fig1 that as ϵ decreases from 0.5 to 0.25 and 0.125, the plot of $A(t)$ in time based on a modified ETD4RK scheme (which is the ETD4RK implemented with a complex integration proposed in [12]) becomes closer and closer to the asymptotic value given by (28).

The fact that ETD4RK is able to simulate small interface thickness ϵ with a relatively coarse mesh clearly demonstrates the effectiveness of the spectral-ETD coupled approximation schemes in the simulation of interface dynamics. Other convergence and accuracy tests will be presented in our future works.

Finally, we present a simulation with $\epsilon = 1$ and a fixed spatial domain size of $32 \times 32 \times 32$ cube in the three dimensional space. The numerical solution is computed with a $128 \times 128 \times 128$ grid and a time step size of 0.2. The snapshots of the isosurface with value $1.0E-12$ of the solution in the three dimensional space are shown in Fig2. It can be observed that the sphere shrinks and eventually disappears, just as predicted theoretically.

6. Conclusion

In this paper, we presented some preliminary stability analysis of the exponential time

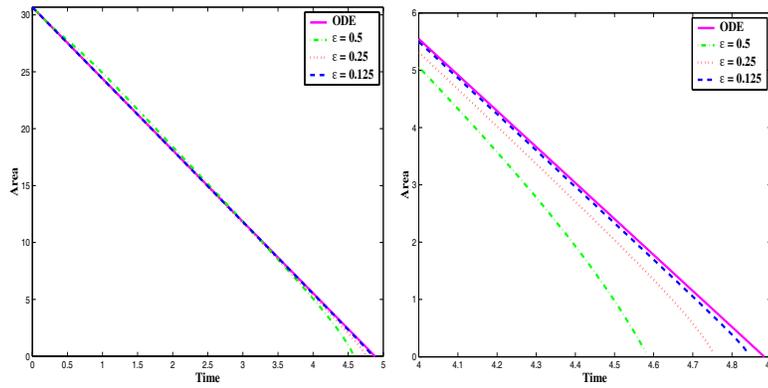


Figure 1: Left: computed values of area $A(t)$ by (28), and by a modified ETD4 scheme for (27) using $\epsilon = 0.5, 0.25$ and 0.125 . The picture on the right is a zoomed-in part of the left figure.

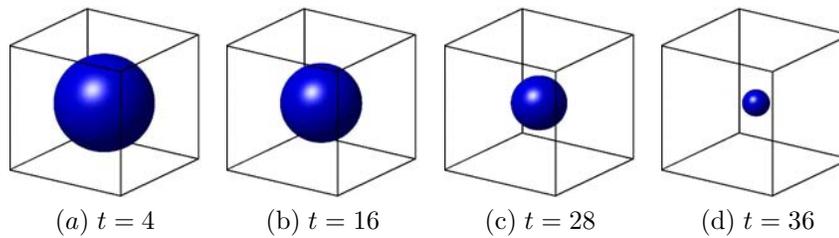


Figure 2: Isosurface plots at the value $1.0E - 12$

differencing schemes for some parabolic type equations. Though only results for the first order scheme were stated, their generalizations to higher order schemes are also possible. More recently, we have also shown that the contour integration suggested in [12] has the effect of improving the stability of the time integration. These theoretical analysis along with other extensive numerical simulations of more complex equations that model phase transition problems will be reported elsewhere.

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