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ERROR ANALYSIS OF STABILIZED SEMI-IMPLICIT METHOD OF ALLEN-CAHN EQUATION

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Abstract. We consider in this paper the *stabilized* semi-implicit (in time) scheme and the splitting scheme for the Allen-Cahn equation $\phi_t - \Delta\phi + \varepsilon^{-2} f(\phi) = 0$ arising from phase transitions in material science. For the *stabilized* first-order scheme, we show that it is unconditionally stable and the error bound depends on ε^{-1} in some lower polynomial order using the spectrum estimate of [2, 10, 11]. In addition, the first- and second-order operator splitting schemes are proposed and the accuracy are tested and compared with the semi-implicit schemes numerically.

1. Introduction.

In this paper, we consider numerical schemes in the semi-discrete form (in time) to solve the Allen-Cahn equation

$$\begin{cases} \phi_t - \Delta\phi + \dfrac{1}{\varepsilon^2} f(\phi) = 0, & (x,t) \in \Omega \times (0,T), \\ \dfrac{\partial \phi}{\partial \boldsymbol{n}}|_{\partial\Omega} = 0, \phi(t_0) = \phi_0. \end{cases} \tag{1}$$

where $\Omega \subset \Re^N, N = 1,2,3$ is a bounded domain with $C^{1,1}$ boundary $\partial\Omega$ or a convex polygonal domain, $\boldsymbol{n}$ is the outward normal, $f(\phi) = F'(\phi)$ and $F(\phi) = \frac{1}{4}(\phi^2-1)^2$, a double equal well potential which takes the global minimum value at $\phi = \pm 1$. The equation (1) was originally introduced by Allen-Cahn [1] to describe the motion of anti-phase boundaries in crystalline solids. ϕ represents the concentration of one of the two metallic components of the alloy and the parameter ε represents the interfacial length, which is extremely small compared to the characteristic dimensions on the laboratory scale. The homogenous Neumann boundary condition implies that no mass loss occurs across the boundary walls. The Allen-Cahn equation can also be viewed as a gradient flow with Liapunov energy functional $\int_\Omega \{\frac{1}{2}|\nabla\phi|^2 + \frac{1}{\varepsilon^2}F(\phi)\}dx$. As $\varepsilon \to 0$, the zero level set of ϕ approaches to a surface which evolves according to the geometric law of $V = \kappa$, where V and κ are the normal velocity and the mean curvature of the surface respectively [1]. Recently, the Allen-Cahn equation has been widely applied to many complicated moving interface problems, for example, vesicle membranes, the nucleation of solids and the mixture of two incompressible fluids, etc. (cf.[4, 5, 6, 9, 18, 19, 20]).

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The main difficulty when one wants to design the numerical scheme of (1) is that the nonlinear penalty term $f(\phi)$ will yield a severe stability limitation on the time step when a usual implicit or explicit scheme is adopted (on $f(\phi)$). In particular, the time step constraint relates to $o(\varepsilon^2)$ in both ways. It is also embarrassing if one attempts to obtain error bounds using the straight forward perturbation argument. The error bounds will depend on the factor of $O(e^{1/\varepsilon})$ which tends to infinity when $\varepsilon \to 0$. In [7], the spectrum argument [2, 10, 11] was applied to derive the rigorous error bounds for the implicit scheme (for $f(\phi)$). The optimal error bounds obtained are in terms of some lower polynomial order of ε^{-1}. The same spectral argument is also applied to derive a similar *a posteriori* error estimate in [8]. For the overview on the topic of convergence analysis of the numerical schemes, we refer to [7, 12, 13, 14].

In this article, we consider the first- and second-order (in time) *stabilized* semi-implicit schemes. The nonlinear term $f(\phi)$ is treated explicitly in order to avoid iterations and speed up the numerical computation. An extra stabilizing term is added to alleviate the stability constraint while maintaining accuracy and simplicity. We derive *a priori* energy estimates which show that the first-order scheme is stable if its solution in some norm remains to be bounded as $\delta t \to 0$. Furthermore, using the same spectral argument, the optimal error estimate is also proved for the first-order *stabilized* semi-implicit numerical scheme.

We also consider, as an alternative, the first-order sequential splitting method and the second-order Strang splitting method [15]. The splitting method is unconditionally stable but suffers from a splitting error. For the examples we tested, it is found that the first-order sequential splitting method is more accurate than the first-order semi-implicit scheme when some larger time steps are used. However, for the second-order scheme, the accuracy is reversed.

The paper is organized as follows. In section 2, we describe the *stabilized* first- and second-order semi-implicit schemes as well as the first- and second-order operator splitting schemes. We then establish the *a priori* energy estimates for the first-order semi-implicit scheme and derive the optimal error estimates using the spectrum argument in section 3. Numerical tests of the semi-implicit schemes and the splitting schemes for a classical benchmark problem and some concluding remarks are given finally in section 4.

2. Time discretization of the Allen-Cahn equation.

In this section, we describe two classes of efficient time discretization schemes. A good feature shared by these schemes is that only Poisson-type equations have to be solved at each time step. Hence they are particularly suitable for spatial discretizations with fast Poisson solvers.

2.1. The stabilized semi-implicit method.

The first-order *stabilized* semi-implicit scheme is

$$\begin{cases} \dfrac{\phi_m - \phi_{m-1}}{k} - \Delta\phi_m + \dfrac{1}{\varepsilon^2}(f(\phi_{m-1}) + s(\phi_m - \phi_{m-1})) = 0, \\ \dfrac{\partial \phi_m}{\partial \boldsymbol{n}}|_{\partial\Omega} = 0. \end{cases} \tag{2}$$

The second-order *stabilized* semi-implicit scheme is

$$\begin{cases} \dfrac{3\phi_{m+1}-4\phi_m+\phi_{m-1}}{2\delta t}-\Delta\phi_{m+1}+\dfrac{1}{\varepsilon^2}\big(2f(\phi_m)-f(\phi_{m-1}) \\ \qquad +s(\phi_{m+1}-2\phi_m+\phi_{m-1})\big)=0, \\ \dfrac{\partial\phi_{m+1}}{\partial\boldsymbol{n}}\big|_{\partial\Omega}=0. \end{cases} \tag{3}$$

Remark 2.1. The schemes (2) and (3) first appeared in [8, 9, 18, 19]. They are quite stable and robust even in the phase-field model where the Allen-Cahn equation is coupled with the Navier-Stokes equations. It is clear that the explicit (and even fully implicit [7]) treatment of the nonlinear term $f(\phi)$ usually leads to a restriction on the time step δt when $\varepsilon << 1$. Therefore, the extra dissipative term $\frac{s}{\varepsilon^2}(\phi_m-\phi_{m-1})$ (order of $\frac{s\delta t}{\varepsilon^2}$) in (2) and $\frac{s}{\varepsilon^2}(\phi_{m+1}-2\phi_m+\phi_{m-1})$ (order of $\frac{s\delta t^2}{\varepsilon^2}$) in (3) are added to improve the stability while preserving the simplicity. The similar technique of the stabilizer also appeared in [17]. The parameter s is proportional to the amount of artificial dissipation added in the numerical scheme. Larger s will lead to a more stable but less accurate scheme. Numerical results indicate that $s=1$ [9] in the Cartesian coordinates and $s=5$ [18] in the cylindrical coordinates provide a good balance between accuracy and stability.

2.2. **The operator splitting method.** Consider a general evolution equation like

$$\frac{\partial u}{\partial t}=g(u)=Au+Bu, \tag{4}$$

where $g(u)$ is a nonlinear operator. The choices of A and B are arbitrary because A and B do not need commute. The first-order splitting method for (4) [15] is

$$\begin{cases} \dfrac{\partial\tilde{u}}{\partial t}=A\tilde{u}, \quad \tilde{u}(t_m)=u_m, t_m\le t\le t_{m+1}, \\ \dfrac{\partial u}{\partial t}=Bu, \quad u(t_m)=\tilde{u}_{m+1}, t_m\le t\le t_{m+1}. \end{cases} \tag{5}$$

In particular, for the Allen-Cahn equation (1), the first-order splitting method is

$$\frac{\partial\tilde{\phi}}{\partial t}+\frac{1}{\varepsilon^2}f(\tilde{\phi})=0, \tilde{\phi}(t_m)=\phi_m, t_m\le t\le t_{m+1}, \tag{6}$$

$$\frac{\partial\phi}{\partial t}-\Delta\phi=0, \phi(t_m)=\tilde{\phi}_{m+1}, t_m\le t\le t_{m+1}. \tag{7}$$

The second-order splitting method is

$$\frac{\partial\tilde{\phi}}{\partial t}+\frac{1}{\varepsilon^2}f(\tilde{\phi})=0, \tilde{\phi}(t_m)=\phi_m, t_m\le t\le t_{m+\frac{1}{2}}, \tag{8}$$

$$\frac{\partial\phi}{\partial t}-\Delta\phi=0, \phi(t_m)=\tilde{\phi}_{m+1}, t_m\le t\le t_{m+1}, \tag{9}$$

$$\frac{\partial\bar{\phi}}{\partial t}+\frac{1}{\varepsilon^2}f(\bar{\phi})=0, \bar{\phi}(t_{m+\frac{1}{2}})=\phi_{m+1}, t_{m+\frac{1}{2}}\le t\le t_{m+1}. \tag{10}$$

For (6), (8) and (10), the exact solutions are

$$\tilde{\phi}_{m+1}=\frac{\phi_m}{\sqrt{\phi_m^2+(1-\phi_m^2)e^{-\frac{2}{\varepsilon^2}(t_{m+1}-t_m)}}}, \tag{11}$$

$$\tilde{\phi}_{m+1/2}=\frac{\phi_m}{\sqrt{\phi_m^2+(1-\phi_m^2)e^{-\frac{2}{\varepsilon^2}(t_{m+1/2}-t_m)}}}, \tag{12}$$

and

$$\bar{\phi}_{m+1} = \frac{\phi_{m+1}}{\sqrt{\phi_{m+1}^2 + (1-\phi_{m+1}^2)e^{-\frac{2}{\varepsilon^2}(t_{m+1}-t_{m+1/2})}}}, \tag{13}$$

respectively. For (7) and (9), we use the second-order semi-implicit scheme:

$$\frac{\phi_{m+1} - \tilde{\phi}_{m+1}}{\delta t} = \frac{1}{2}(\Delta\phi_{m+1} + \Delta\tilde{\phi}_{m+1}). \tag{14}$$

Remark 2.2. The first- and second-order splitting schemes are unconditionally stable because of the unconditional stability of each sub-step.

3. Energy estimates and error analysis.

In this section, *a priori* energy estimates are established for the Allen-Cahn equation (1) and the first-order *stabilized* numerical scheme (2). The optimal error estimates are also derived thereafter.

3.1. Energy estimates for PDE.

We now introduce some notations. Let $W^{s,p}(\Omega)$ and $W_0^{s,p}(\Omega)$ denote the usual Sobolev spaces equipped with the norm $\|\cdot\|_{s,p}$ for $0 \le s < \infty, 0 \le p \le \infty$. In particular, we denote the Hilbert spaces $W^{s,2}(\Omega)$ by H^s $(s = 0, \pm 1, \cdots)$ with norm $\|\cdot\|_s$ and semi norm $|\cdot|_s$. The norm and inner product of $L^2(\Omega) = H^0(\Omega)$ are denoted by $\|\cdot\|_0$ and $(\cdot,\cdot)$ respectively.

Let $k = \delta t$ be the time step and set $t^n = nk$ for $0 \le n \le N = [\frac{T}{k}]$. For any function which is continuous in time, $u(t)$, we denote $u^n = u(t^n)$ and define the difference operator d_t by $d_t u^n = \frac{u^n - u^{n-1}}{k}$. We denote by c a generic constant that is independent of δt and ε but possibly depends on the data and the solution. We shall use $A \lesssim B$ to say that there is a generic constant that $A \le cB$.

We assume that the initial value of ϕ_0 in (1) satisfies $\|\phi_0\|_{L^\infty} \le 1$ so that the following maximum principle for the solution of (1) holds (cf. [1, 2, 3, 7, 9]):

Lemma 3.1. *If $\phi_0 \in [-1,1]$ a.e. in Ω, then $\phi \in [-1,1]$ a.e in $\Omega \times [0,T]$.*

In order to trace the dependence of the solution on ε, we also assume $\phi_0 \in H^1(\Omega) \cap H^2(\Omega)$ and satisfies the following assumptions:
There exist nonnegative constants $\sigma_1, \sigma_2, \sigma_3$ such that

$$\Gamma_\varepsilon(\phi_0) = \frac{1}{2}\|\nabla\phi_0\|_0^2 + \frac{1}{\varepsilon^2}\int_\Omega F(\phi_0)dx \lesssim \varepsilon^{-2\sigma_1}. \tag{H1}$$

$$\|\Delta\phi_0 - \varepsilon^{-2} f(\phi_0)\|_0 \lesssim \varepsilon^{-\sigma_2}. \tag{H2}$$

$$\lim_{x\to 0^+} \|\nabla\phi_t(x)\|_0 \lesssim \varepsilon^{-\sigma_3}. \tag{H3}$$

Lemma 3.2. *$\forall t \in [0,T]$, the solution of (1) satisfies the following energy estimates,*

$$\frac{1}{2}\|\nabla\phi(t)\|_0^2 + \frac{1}{\varepsilon^2}\int_\Omega |F(\phi(t))|dx + \int_0^t \|\phi_t\|_0^2 d\tau = \Gamma_\varepsilon(\phi_0), \tag{15}$$

$$\int_0^t \|\Delta\phi\|_0^2 d\tau \lesssim \varepsilon^{-2\sigma_1 - 2}, \tag{16}$$

$$\|\phi_t(t)\|_0^2 + \|\Delta\phi(t)\|_0^2 + \int_0^t \|\nabla\phi_t(\tau)\|_0^2 d\tau \lesssim \varepsilon^{2\min(-\sigma_1-1,-\sigma_2)}, \tag{17}$$

$$\int_0^t \|\phi_{tt}(\tau)\|_{-1}^2 d\tau \lesssim \varepsilon^{2\min(-\sigma_1-2,-\sigma_2)}, \tag{18}$$

$$\int_0^t \|\phi_{tt}(\tau)\|_0^2 d\tau \lesssim \varepsilon^{2\min(-\sigma_1-2,-\sigma_3)}. \tag{19}$$

Proof. Taking the inner product of (1) with ϕ_t, we derive

$$\|\phi_t\|_0^2 + \frac{1}{2}\partial_t\|\nabla\phi\|_0^2 + \frac{1}{\varepsilon^2}\partial_t\int_\Omega |F(\phi)|dx = 0. \tag{20}$$

After the integration over $[0,t]$, we obtain (15). Taking the inner product of (1) with $-\Delta\phi$ and using the Schwarz inequality and Lemma 3.1, we obtain

$$\begin{aligned}\|\Delta\phi\|_0^2 &= (\phi_t, \Delta\phi) - \varepsilon^{-2}(f(\phi), -\Delta\phi)\\ &\le \frac{1}{2}\|\phi_t\|_0^2 + \frac{1}{2}\|\Delta\phi\|_0^2 - \varepsilon^{-2}((3\phi^2-1)\nabla\phi,\nabla\phi)\\ &\le \frac{1}{2}\|\phi_t\|_0^2 + \frac{1}{2}\|\Delta\phi\|_0^2 + 2\varepsilon^{-2}\|\nabla\phi\|_0^2.\end{aligned} \tag{21}$$

After integrating over $[0,t]$ and using (15), we derive

$$\int_0^t \|\Delta\phi\|_0^2 d\tau \le \int_0^t \|\phi_t\|_0^2 d\tau + 4\varepsilon^{-2}\int_0^t \|\nabla\phi\|_0^2 d\tau \lesssim \varepsilon^{-2\sigma_1-2}. \tag{22}$$

We differentiate (1) in time to obtain

$$\phi_{tt} - \Delta\phi_t + \frac{1}{\varepsilon^2}f'(\phi)\phi_t = 0. \tag{23}$$

After taking the inner product with ϕ_t, we infer

$$\frac{1}{2}\partial_t\|\phi_t\|_0^2 + \|\nabla\phi_t\|_0^2 + \varepsilon^{-2}(f'(\phi)\phi_t,\phi_t) = 0. \tag{24}$$

We then integrate over $[0,t]$ to derive

$$\begin{aligned}\frac{1}{2}\|\phi_t\|_0^2 + \int_0^t \|\nabla\phi_t\|_0^2 d\tau &\le \frac{1}{2}\|\phi_t(0)\|_0^2 + 2\varepsilon^{-2}\int_0^t \|\phi_t\|_0^2 d\tau\\ &\lesssim \varepsilon^{-2\sigma_2} + \varepsilon^{-2\sigma_1-2}.\end{aligned} \tag{25}$$

Also from (15), (17) and (21), we derive that

$$\|\Delta\phi\|_0^2 \le \|\phi_t\|_0^2 + 4\varepsilon^{-2}\|\nabla\phi\|_0^2 \lesssim \varepsilon^{2\min(-\sigma_1-2,-\sigma_2)}. \tag{26}$$

From (23) and Lemma 3.1, we obtain

$$\begin{aligned}\|\phi_{tt}\|_{-1} &\le \|\nabla\phi_t\|_0 + \varepsilon^{-2}\sup_{\psi\in H^1(\Omega)}\frac{(f'(\phi)\phi_t,\psi)}{\|\psi\|_1}\\ &\lesssim \|\nabla\phi_t\|_0 + \varepsilon^{-2}\|f'(\phi)\|_{L^\infty}\|\phi_t\|_0\\ &\lesssim \|\nabla\phi_t\|_0 + \varepsilon^{-2}\|\phi_t\|_0.\end{aligned} \tag{27}$$

After squaring the above inequality and integrating over $[0,t]$, we obtain (18). Finally, taking the inner product of (23) with ϕ_{tt}, we derive

$$\|\phi_{tt}\|_0^2 + \frac{1}{2}\partial_t\|\nabla\phi_t\|_0^2 + \frac{1}{\varepsilon^2}(f'(\phi)\phi_t,\phi_{tt}) = 0. \tag{28}$$

By Schwarz inequality, the last term of the left hand side can be bounded as

$$\frac{1}{\varepsilon^2}(f'(\phi)\phi_t,\phi_{tt}) \le \frac{1}{2}\|\phi_{tt}\|_0^2 + \frac{1}{2\varepsilon^4}\|f'(\phi)\|_{L^\infty}\|\phi_t\|_0^2. \tag{29}$$

After integrating over $[0,t]$, we obtain (19). ∎

3.2. *A priori* **energy estimates for the first-order stabilized scheme.** Thanks to the maximum principle, we can modify the nonlinear function f to be

$$\tilde{f}(x) = \begin{cases} f(x), |x| \leq 2; \\ 11x - 16, x \geq 2; \\ 11x + 16, x \leq -2; \end{cases} \tag{30}$$

without affecting the solution and $\tilde{f} \in C^1(\Re)$. The function $\tilde{f}$ is now Lipschitz continuous with Lipschitz constant L_0. We can also assume $\|f'(x)\|_{L^\infty} \leq L_0$. For convenience, we consider the problem formulated with the substitute $\tilde{f}$, but omit the tilde in the notation. The symbol F is still used to be the nonlinear potential such that $F'(x) = f(x)$. Furthermore, f' is also Lipschitz continuous. Hence, we will use L to represent the Lipschitz constant of f and f' for convenience.

We are now in position to establish the following:

Theorem 3.1. *When $s \geq \frac{3}{2}L$, the scheme (2) is stable and the solution satisfies the following energy estimates:*

$$k\sum_{m=1}^{M} \|d_t\phi_m\|_0^2 + \frac{k}{2}\sum_{m=1}^{M} k\|d_t\nabla\phi_m\|_0^2 + \Gamma_\varepsilon(\phi_M) \leq \Gamma_\varepsilon(\phi_0).$$

Proof. First, we rewrite (2) for convenience,

$$\begin{cases} d_t\phi_m - \Delta\phi_m + \varepsilon^{-2}f(\phi_{m-1}) + sk\varepsilon^{-2}d_t\phi_m = 0, \\ \dfrac{\partial\phi_m}{\partial \boldsymbol{n}}|_{\partial\Omega} = 0. \end{cases} \tag{31}$$

Second, we take the inner product of (31) with $d_t\phi_m$, we obtain

$$\begin{aligned} \|d_t\phi_m\|_0^2 + \frac{1}{2}d_t\|\nabla\phi_m\|_0^2 + \frac{k}{2}\|d_t\nabla\phi_m\|_0^2 + sk\varepsilon^{-2}\|d_t\phi_m\|_0^2 \\ + \varepsilon^{-2}(f(\phi_m), d_t\phi_m) = \varepsilon^{-2}(f(\phi_m) - f(\phi_{m-1}), d_t\phi_m). \end{aligned} \tag{32}$$

From the Taylor expansion, we derive

$$\begin{aligned} (f(\phi_m), d_t\phi_m) =& \frac{1}{k}(F(\phi_m) - F(\phi_{m-1}), 1) \\ &+ \frac{1}{2k}(f'(\xi)(\phi_m - \phi_{m-1}), \phi_m - \phi_{m-1}) \\ \geq& d_t\int_\Omega |F(\phi_m)|dx - \frac{kL}{2}\|d_t\phi_m\|_0^2, \end{aligned} \tag{33}$$

here ξ is a value between ϕ_m and ϕ_{m-1}. By the Lipschitz continuity of f, we have

$$\varepsilon^{-2}(f(\phi_m) - f(\phi_{m-1}), d_t\phi_m) \leq L\varepsilon^{-2}k\|d_t\phi_m\|_0^2. \tag{34}$$

After combining the above inequalities together, we obtain

$$\begin{aligned} (1 + (s - \frac{3}{2}L)k\varepsilon^{-2})\|d_t\phi_m\|_0^2 + \frac{1}{2}d_t\|\nabla\phi_m\|_0^2 + \frac{k}{2}\|d_t\nabla\phi_m\|_0^2 \\ + \varepsilon^{-2}d_t\int_\Omega |F(\phi_m)|dx \leq 0. \end{aligned} \tag{35}$$

Finally, after multiplying by k and taking the summation from $m = 0$ to M, we can obtain

$$
\begin{aligned}
&k\sum_{m=0}^{M}(1+(s-\frac{3}{2}L)k\varepsilon^{-2})\|d_t\phi_m\|_0^2+\frac{1}{2}\|\nabla\phi_M\|_0^2\\
&+\frac{1}{2}k\sum_{m=0}^{M}k\|d_t\nabla\phi_m\|_0^2+\varepsilon^{-2}\int_\Omega|F(\phi_M)|dx\\
\le&\frac{1}{2}\|\nabla\phi_0\|_0^2+\varepsilon^{-2}\int_\Omega|F(\phi_0)|dx=\Gamma_\varepsilon(\phi_0).
\end{aligned}\tag{36}
$$

□

Remark 3.1. For the explicit scheme, i.e. $s=0$, the constraint of the time step comes from the condition of $1-\frac{3}{2}Lk\varepsilon^{-2}\ge 0$, i.e. $k\le\frac{2\varepsilon^2}{3L}$. Actually, for the implicit scheme ($s=0$ and replace $f(\phi^{m-1})$ by $f(\phi^m)$ in (2)), there still exists the time step constraint of $k\le\varepsilon^2$, the detailed proof is in [7].

In order to obtain the error bounds, we also need the following two energy estimates in H^2-norm.

Lemma 3.3. *If $k\lesssim\varepsilon^2$, the following energy estimates hold:*

$$
k\sum_{m=1}^{M}\|\Delta\phi_m\|_0^2\lesssim\varepsilon^{-2\sigma_1-2},\tag{37}
$$

$$
\|\Delta\phi_m\|_0^2+\|d_t\phi_M\|_0^2+k\sum_{m=0}^{M}\|\nabla d_t\phi_m\|_0^2\lesssim\varepsilon^{2\min(-\sigma_2,-\sigma_1-1)}.\tag{38}
$$

Proof. We take the inner product of (31) with $-\Delta\phi_m$ and use the Schwarz inequality, we obtain

$$
\begin{aligned}
\|\Delta\phi_m\|_0^2=&(d_t\phi_m,\Delta\phi_m)-\varepsilon^{-2}(f(\phi_{m-1}),-\Delta\phi_m)+sk\varepsilon^{-2}(d_t\phi_m,\Delta\phi_m)\\
\le&\frac{1}{2}\|\Delta\phi_m\|_0^2+(1+s^2k^2\varepsilon^{-4})\|d_t\phi_m\|_0^2\\
&+\frac{1}{2}L\varepsilon^{-2}(\|\nabla\phi_m\|_0^2+\|\nabla\phi_{m-1}\|_0^2).
\end{aligned}\tag{39}
$$

After multiplying by k and taking the summation from $m=1$ to M, we derive

$$
\begin{aligned}
k\sum_{m=1}^{M}\|\Delta\phi_m\|_0^2\le&2L\varepsilon^{-2}k\sum_{m=1}^{M}\|\nabla\phi_m\|_0^2+L\varepsilon^{-2}k\|\nabla\phi_0\|_0^2\\
&+2(1+s^2k^2\varepsilon^{-4})\sum_{m=1}^{M}k\|d_t\phi_m\|_0^2.
\end{aligned}\tag{40}
$$

Let $C_{k,\varepsilon}=k\varepsilon^{-2}\le 1$, from Theorem 3.1 and (H1), we obtain

$$
\begin{aligned}
k\sum_{m=1}^{M}\|\Delta\phi_m\|_0^2&\le 2\Gamma_\varepsilon(\phi_0)(1+LC_{k,\varepsilon}+s^2C_{k,\varepsilon}^2+2LT\varepsilon^{-2})\\
&\lesssim\varepsilon^{-2\sigma_1-2}.
\end{aligned}\tag{41}
$$

We apply d_t to both sides of (31) and do the inner product with $d_t\phi_m$, we have

$$
\begin{aligned}
(1+sk\varepsilon^{-2})(\frac{1}{2}d_t\|d_t\phi_m\|_0^2+\frac{k}{2}\|d_t^2\phi_m\|_0^2)+\|\nabla d_t\phi_m\|_0^2&\\
+\varepsilon^{-2}(d_tf(\phi_{m-1}),d_t\phi_m)=0.&
\end{aligned}\tag{42}
$$

From the Lipschitz continuity of f and Schwarz inequality,

$$\varepsilon^{-2}(d_t f(\phi_{m-1}), d_t\phi_m) \leq \frac{L\varepsilon^{-2}}{2}(\|d_t\phi_m\|_0^2 + \|d_t\phi_{m-1}\|_0^2). \tag{43}$$

After multiplying k and taking the summation from $m=2$ to M, we obtain

$$\begin{aligned} &\|d_t\phi_M\|_0^2 + k\sum_{m=2}^{M} k\|d_t^2\phi_m\|_0^2 + k\sum_{m=2}^{M}\|\nabla d_t\phi_m\|_0^2 \\ \lesssim&\|d_t\phi_1\|_0^2 + \varepsilon^{-2}\Gamma_\varepsilon(\phi_0). \end{aligned} \tag{44}$$

From (39), we have

$$\begin{aligned} \|\Delta\phi_m\|_0^2 &\leq 2(1+s^2k^2\varepsilon^{-4})\|d_t\phi_m\|_0^2 + L\varepsilon^{-2}(\|\nabla\phi_m\|_0^2 + \|\nabla\phi_{m-1}\|_0^2) \\ &\lesssim \|d_t\phi_1\|_0^2 + \varepsilon^{-2}\Gamma_\varepsilon(\phi_0). \end{aligned} \tag{45}$$

Finally, taking the inner product with $d_t\phi_1$ with (31) when $m=1$, we obtain

$$\|d_t\phi_1\|_0^2 + k\|\nabla d_t\phi_1\|_0^2 \leq \|\Delta\phi_0 - \varepsilon^{-2}f(\phi_0)\|_0^2 \lesssim \varepsilon^{-2\sigma_2}, \tag{46}$$

then we complete the proof. □

Remark 3.2. This time step constraint condition $k \lesssim \varepsilon^2$ is inevitable for the energy estimates in higher norm and the error estimates in the following subsection.

3.3. **Error analysis for the first-order scheme.** In this subsection, we give the error bounds for the first-order scheme (2). In order to avoid the dependence of $e^{1/\varepsilon}$ caused by the Gronwall's lemma, we have to use the spectral estimate [2, 10, 11].

Lemma 3.4 (Spectral estimate). *Define*

$$\mathrm{L}_{\mathrm{AC}} = -\Delta + \mathrm{f}'(\phi)\mathrm{I}, \tag{47}$$

where I *is the identity operator and* ϕ *is the solution of the Allen-Cahn equation. There exists a positive* ε*-independent constant* C_0 *such that the principle eigenvalue of the linearized Allen-Cahn operator* L_{AC} *satisfies for* $\varepsilon \geq 0$

$$\lambda_{AC} \equiv \inf_{\psi\in \mathrm{H}^1,\psi\neq 0}\frac{\|\nabla\psi\|^2 + \frac{1}{\varepsilon^2}(\mathrm{f}'(\phi)\psi,\psi)}{\|\psi\|^2} \geq -\mathrm{C}_0. \tag{48}$$

From the maximum principle, the spectral estimate is still suitable for the current modified function f in (30). Hence we have the error estimate of the first-order scheme (31) as follows.

Theorem 3.2. *Under the assumptions (*H1 − H3*) and suppose*

$$k \lesssim \min(\varepsilon^2, \varepsilon^{\alpha_1}, \varepsilon^{\alpha_2}), \tag{49}$$

the solution of (2) satisfies the following error estimates

$$\|\phi(t_m) - \phi_m\|_0 \quad\lesssim\quad k\varepsilon^{\min(-\sigma_1-2,-\sigma_3)}, \tag{50}$$

$$\Big(k\sum_{m=0}^{M}\|\nabla(\phi(t_m)-\phi_m)\|_0^2\Big)^{\frac{1}{2}} \quad\lesssim\quad k\varepsilon^{\min(-\sigma_1-3,-\sigma_3-1)}. \tag{51}$$

Proof. Let $e_m = \phi(t_m) - \phi_m$ and subtract (31) from (1), we can obtain

$$d_t e_m - \Delta e_m + \varepsilon^{-2}(f(\phi(t_m)) - f(\phi_{m-1})) - sk\varepsilon^{-2}d_t\phi_m = R_m, \tag{52}$$

where

$$R_m = -\frac{1}{k}\int_{t_m-1}^{t_m}(s-t_{m-1})\phi_{tt}(s)ds. \tag{53}$$

From (19), we have

$$
\begin{aligned}
k\sum_{m=0}^{M}\|R_m\|_0^2 \leq & \frac{1}{k}\int_{t_{m-1}}^{t_m}\|\phi_{tt}(s)\|_0^2 ds\sum_{m=0}^{M}\int_{t_{m-1}}^{t_m}(s-t_m)^2 ds \\
& \lesssim k^2\varepsilon^{2\min(-\sigma_1-2,-\sigma_3)}.
\end{aligned}
\tag{54}
$$

We take the inner product of (52) with e_m, we obtain

$$
\begin{aligned}
&\frac{1}{2}d_t\|e_m\|_0^2+\frac{k}{2}\|d_te_m\|_0^2+\|\nabla e_m\|_0^2+\frac{1}{\varepsilon^2}(f(\phi(t_m))-f(\phi_m),e_m)\\
&+\frac{1}{\varepsilon^2}(f(\phi_m)-f(\phi_{m-1}),e_m)-sk\varepsilon^{-2}(d_t\phi_m,e_m)\\
=&(R_m,e_m).
\end{aligned}
\tag{55}
$$

Notice that $f(a)-f(b)=\int_0^{a-b}f'(a-\xi)d\xi$, we derive

$$
\begin{aligned}
(f(\phi(t_m))-f(\phi_m),e_m)=&(\int_0^{e_m}f'(\phi(t_m)-\xi)d\xi,e_m)\\
=&(\int_0^{e_m}(f'(\phi(t_m)-\xi)-f'(\phi(t_m)))d\xi,e_m)\\
&+(\int_0^{e_m}f'(\phi(t_m))d\xi,e_m)\\
\geq&-\frac{L}{2\varepsilon^2}\|e_m\|_{L^3}^3+(f'(\phi(t_m))e_m,e_m).
\end{aligned}
\tag{56}
$$

By the Schwarz inequality, we obtain

$$
\begin{aligned}
sk\varepsilon^{-2}(d_t\phi_m,e_m)&\leq\frac{1}{2}k^2\varepsilon^{-4}\|d_t\phi_m\|_0^2+\frac{1}{2}s^2\|e_m\|_0^2,\\
-\frac{1}{\varepsilon^2}(f(\phi_m)-f(\phi_{m-1}),e_m)&\leq\frac{1}{2}k^2\varepsilon^{-4}\|d_t\phi_m\|_0^2+\frac{1}{2}L^2\|e_m\|_0^2,\\
(R_m,e_m)&\leq\frac{1}{2}\|R_m\|_0^2+\frac{1}{2}\|e_m\|_0^2.
\end{aligned}
\tag{57}
$$

From the Lemma 3.4, we obtain

$$
\begin{aligned}
\frac{1}{2}d_t\|e_m\|_0^2+\frac{k}{2}\|d_te_m\|_0^2\leq&(C_0+\frac{1+L^2+s^2}{2})\|e_m\|_0^2\\
&+k^2\varepsilon^{-4}\|d_t\phi_m\|_0^2+\frac{1}{2}\|R_m\|_0^2+\frac{L}{2\varepsilon^2}\|e_m\|_{L^3}^3.
\end{aligned}
\tag{58}
$$

After multiplying $2k$, taking the summation from $m=0$ to M and using (54), we obtain

$$
\begin{aligned}
\|e_M\|_0^2+k\sum_{m=0}^{M}k\|d_te_m\|_0^2\leq&(1+2C_0+L^2+s^2)k\sum_{m=0}^{M}\|e_m\|_0^2\\
&+k^2\varepsilon^{-2(\sigma_1+2)}+k^2\varepsilon^{2\min(-\sigma_1-2,-\sigma_3)}\\
&+L\varepsilon^{-2}\|e_m\|_{L^3}^3.
\end{aligned}
\tag{59}
$$

To handle the L^3 space, we apply a shift in the sub-index to obtain

$$
\|e_m\|_{L^3}^3\leq C(\|e_{m-1}\|_{L^3}^3+k^3\|d_te_m\|_{L^3}^3).
\tag{60}
$$

We interpolate L^3 between L^2 and H^2 and use (17) and (38) to get

$$\begin{aligned}\|e_m\|_{L^3}^3 &\lesssim (\|\Delta e_m\|_0^{\frac{N}{4}}\|e_m\|_0^{3-\frac{N}{4}} + \|e_m\|_0^3)\\ &\lesssim \varepsilon^{\frac{N}{4}\min(-\sigma_1-1,-\sigma_2)}\|e_m\|_0^{3-\frac{N}{4}}.\end{aligned} \tag{61}$$

Similarly, the second term of (60) can be bounded by

$$\begin{aligned}k^3\|d_te_m\|_{L^3}^3 &\lesssim k^3(\|\Delta d_te_m\|_0^{\frac{N}{4}}\|d_te_m\|_0^{3-\frac{N}{4}} + \|d_te_m\|_0^3)\\ &\lesssim k^3\|d_te_m\|_0^{3-\frac{N}{4}}(\|\Delta d_te_m\|_0^{\frac{N}{4}} + \|d_te_m\|_0^{\frac{N}{4}})\\ &\lesssim k^{3-\frac{N}{4}}\varepsilon^{\frac{N}{4}\min(-\sigma_1-1,-\sigma_2)}\|d_te_m\|_0^{3-\frac{N}{4}}\\ &\lesssim k^{3-\frac{N}{4}}\varepsilon^{\min(-\sigma_1-1,-\sigma_2)}\|d_te_m\|_0^2.\end{aligned} \tag{62}$$

We multiply $k\varepsilon^{-2}$ to (60) and sum it up over m from 0 to ℓ, we obtain

$$\begin{aligned}k\varepsilon^{-2}\sum_{m=0}^{\ell}\|e_m\|_{L^3}^3 \lesssim&\varepsilon^{\frac{N}{4}\min(-\sigma_1-1,-\sigma_2)-2}k\sum_{m=0}^{\ell}\|e_m\|_0^{3-\frac{N}{4}}\\ &+ k^{3-\frac{N}{4}}\varepsilon^{\min(-\sigma_1-1,-\sigma_2)-2}k\sum_{m=0}^{\ell}\|d_te_m\|_0^2.\end{aligned} \tag{63}$$

The second term can be absorbed by the corresponding term on the left hand side of (59) if

$$k \lesssim \varepsilon^{\alpha_1}, \text{with } \alpha_1 = \frac{4\max(\sigma_1+1,\sigma_2)+8}{8-N}. \tag{64}$$

Then (59) turns to

$$\begin{aligned}\|e_M\|_0^2 + k\sum_{m=0}^{M}k\|d_te_m\|_0^2 \lesssim& k\sum_{m=0}^{M}\|e_m\|_0^2 + k^2\varepsilon^{2\min(-\sigma_1-2,-\sigma_3)}\\ &+ \varepsilon^{\frac{N}{4}\min(-\sigma_1-1,-\sigma_2)-2}k\sum_{m=0}^{M}\|e_m\|_0^{3-\frac{N}{4}}.\end{aligned} \tag{65}$$

Finally, we do the inductive argument as the following: Suppose for $0 \leq m \leq \ell$, we have the following inequality

$$\|e_m\|_0^2 + k\sum_{m=1}^{\ell}k\|d_te_m\|_0^2 \lesssim k^2\varepsilon^{2\min(-\sigma_1-2,-\sigma_3)}. \tag{66}$$

Notice that the exponent of the last term in (65) is bigger than 2, hence, we can recover (66) by using the discrete Gronwall's inequality, provided k satisfies

$$\begin{aligned}&\varepsilon^{\frac{N}{4}\min(-\sigma_2,-\sigma_1-1)-2}\big[k^2\varepsilon^{2\min(-\sigma_2-2,-\sigma_3)}\big]^{\frac{3}{2}-\frac{N}{8}}\\ \lesssim& k^2\varepsilon^{2\min(-\sigma_2-2,-\sigma_3)}.\end{aligned} \tag{67}$$

This provide another constraint of $k \lesssim \varepsilon^{\alpha_2}$ with

$$\alpha_2 = \max(\sigma_1+2,\sigma_3) + \frac{N\max(\sigma_1+1,\sigma_2)+8}{4-N}, \tag{68}$$

then we have (50).

To obtain the estimate of H^1 norm, in (55), we use Schwarz inequality as follows.

$$\begin{aligned}\varepsilon^{-2}(f(\phi(t_m)) - f(\phi_m), e_m) &\lesssim \varepsilon^{-2}\|e_m\|_0^2,\\ k\varepsilon^{-2}(f(\phi_m) - f(\phi_{m-1}), e_m) &\lesssim k^2\varepsilon^{-2}\|d_t\phi_m\|_0^2 + \varepsilon^{-2}\|e_m\|_0^2,\\ sk\varepsilon^{-2}(d_t\phi_m, e_m) &\lesssim k^2\varepsilon^{-2}\|d_t\phi_m\|_0^2 + \varepsilon^{-2}\|e_m\|_0^2.\end{aligned} \tag{69}$$

Then we have

$$\frac{1}{2}d_t\|e_m\|_0^2 + \|\nabla e_m\|_0^2 \lesssim k^2\varepsilon^{-2}\|d_t\phi_m\|_0^2 + \varepsilon^{-2}\|e_m\|_0^2 + \|R_m\|_0^2. \tag{70}$$

After multiplying k and taking the summation from $m = 0$ to M, we obtain (51). ☐

3.4. **Second-order scheme.** Numerical results reported in section 4 clearly indicate that the second-order scheme is more accurate than the first-order scheme under the same time step. However, the rigorous proof of the stability and the accuracy are still elusive.

4. **Numerical results and discussions.** In this section, we compare the accuracy between the splitting schemes and the *stabilized* semi-implicit schemes for the classical benchmark problem in [3]. The problem is described as follows. At the initial state, there is a circular interface boundary with a radius of $R_0 = 100$ in the rectangular domain of $[0, 256] \times [0, 256]$. Such a circular interface is unstable and the driving force will shrink and eventually disappear. It is easily shown, in the limit that the radius of the circle is much larger than the interfacial thickness, the velocity of the moving interface V is given by

$$V = \frac{dR}{dt} = -\frac{1}{R}, \tag{71}$$

where R is the radius of the circle at a given time t. After taking the integration, we obtain

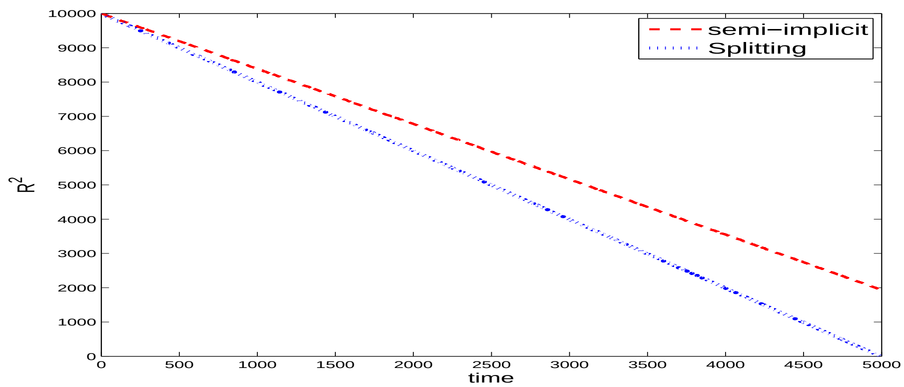
$$R^2 = R_0^2 - 2t. \tag{72}$$

We use Spectral-Galerkin method to handle the spatial discretization [16]. In order to omit the error induced from the space, 513×513 Legendre-Gauss-Lobatoo points are used. After we map the domain to $[-1, 1] \times [-1, 1]$, we obtain the following phase equation

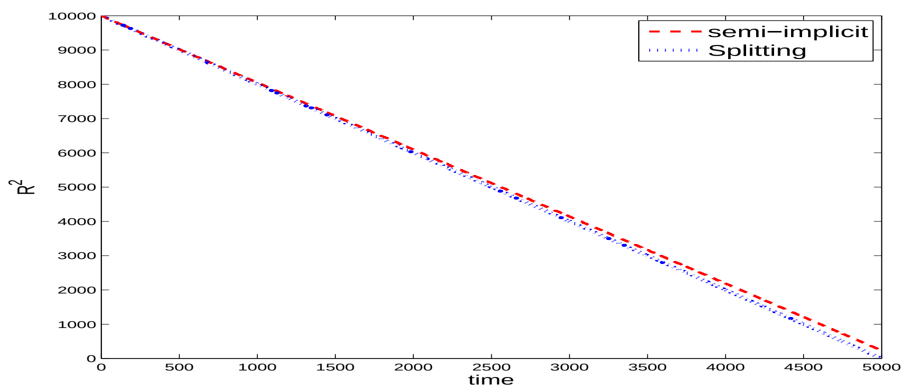
$$\phi_t - \gamma(\Delta\phi - \frac{f(\phi)}{\varepsilon^2}) = 0, \tag{73}$$

where $\gamma = 6.10351 \times 10^{-5}$ and $\varepsilon = 0.0078$. The square of the radius as a function of time obtained from the splitting scheme and the semi-implicit scheme are shown in Figure 1 and Figure 2. Three time steps $\delta t = 0.1, 0.01, 0.001$ and $\delta t = 0.5, 0.1, 0.01$ are used to test the accuracy of the first- and second-order schemes, respectively. For the first-order scheme, the splitting method shows the competence especially when time steps are larger. When time step is smaller, both of these schemes are very accurate, for example, Figure 1 (c) and Figure 2 (b),(c). However, the semi-implicit method shows its advantage for the second-order scheme at larger time steps, for example, Figure 2 (a).

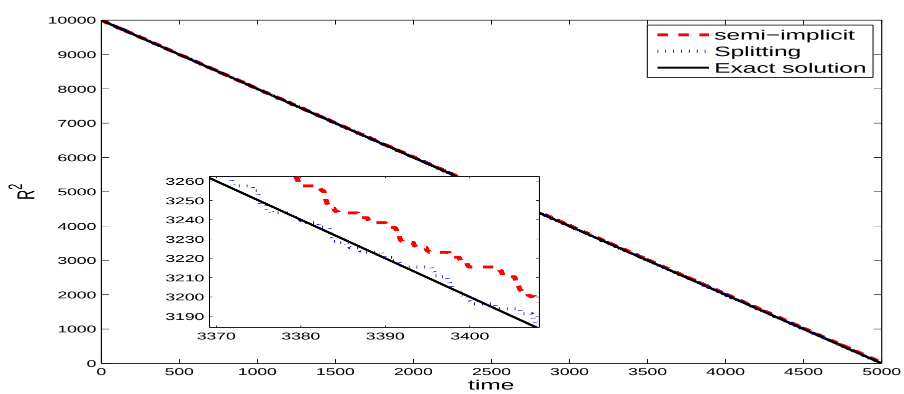
To conclude, we show in this paper that the first-order semi-implicit *stabilized* scheme is unconditionally stable and derive the optimal error estimates with polynomial growth in ε^{-1}. However, for the second-order scheme (3), the stability and error analysis appear to be very difficult. The main difficulty happens when one attempts to estimate the upper bound of the inner product of the nonlinear term:



(a) $\delta t = 0.1$

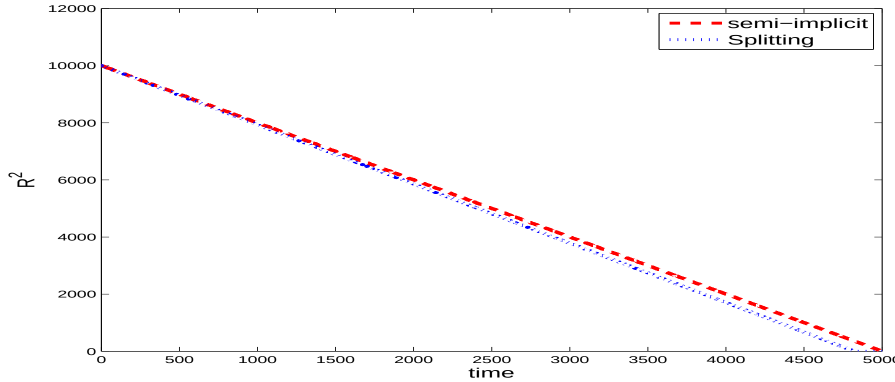


(b) $\delta t = 0.01$

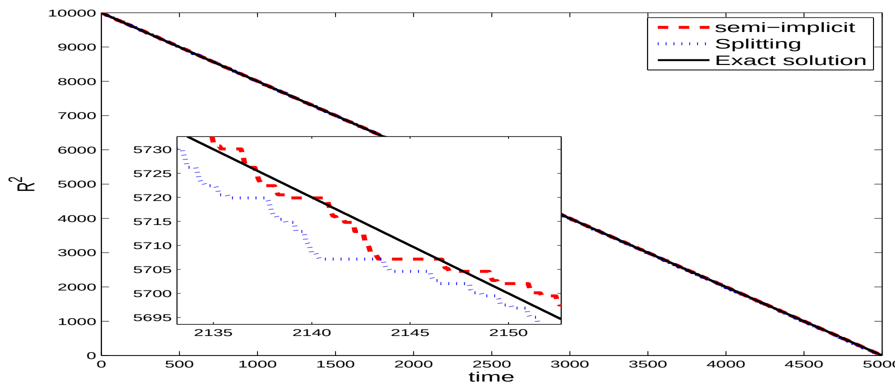


(c) $\delta t = 0.001$

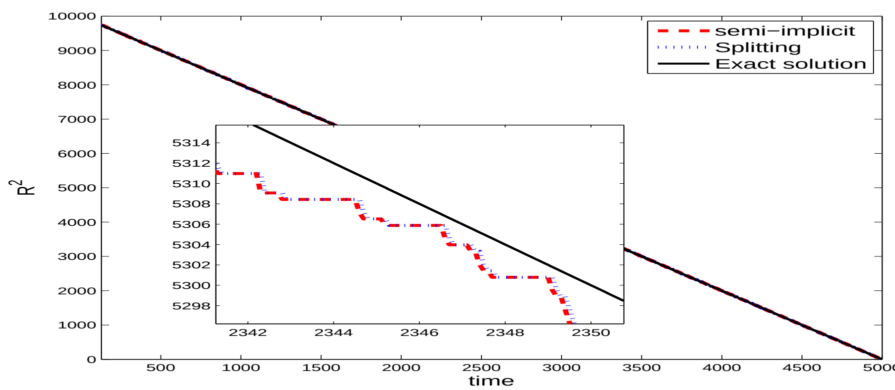
FIGURE 1. The comparison of the first-order semi-implicit scheme and the first-order splitting scheme using $\delta t = 0.1, 0.01, 0.001$.



(a) $\delta t = 0.5$



(b) $\delta t = 0.1$



(c) $\delta t = 0.01$

FIGURE 2. The comparison of the second-order semi-implicit scheme and the second-order Strang splitting scheme using $\delta t = 0.5, 0.1, 0.01$.

$(f(\phi_{m+1}) - 2f(\phi_m) + f(\phi_{m-1}), d_t\phi_{m+1})$. And also, rigorous error estimates for the first- and second-order splitting method are still open problems.

We have also performed numerical tests to compare the accuracy for the numerical schemes considered in this paper. These numerical tests indicated that the *stabilized* semi-implicit scheme is accurate, efficient and easy to implement.

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