Journal of Computational Physics 353 (2018) 407–416

Contents lists available at ScienceDirect

Journal of Computational Physics

www.elsevier.com/locate/jcp

Short note

The scalar auxiliary variable (SAV) approach for gradient flows ☆

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ARTICLE INFO

Article history:
Received 18 June 2017
Received in revised form 17 September 2017
Accepted 17 October 2017
Available online 23 October 2017

Keywords:
Gradient flows
Unconditionally energy stability
Cahn–Hilliard equation

ABSTRACT

We propose a new approach, which we term as scalar auxiliary variable (SAV) approach, to construct efficient and accurate time discretization schemes for a large class of gradient flows. The SAV approach is built upon the recently introduced IEQ approach. It enjoys all advantages of the IEQ approach but overcomes most of its shortcomings. In particular, the SAV approach leads to numerical schemes that are unconditionally energy stable and extremely efficient in the sense that only decoupled equations with constant coefficients need to be solved at each time step. The scheme is not restricted to specific forms of the nonlinear part of the free energy, so it applies to a large class of gradient flows. Numerical results are presented to show that the accuracy and effectiveness of the SAV approach over the existing methods.

1. Introduction

Gradient flows are frequently used in mathematical models for problems in many fields of science and engineering, particularly in materials science and fluid dynamics, see, for instance, [4,1,15,6,13,2,8,25] and the references therein. Hence, it is very important to develop efficient and accurate numerical schemes for their simulation.

A gradient flow is usually determined by a driving free energy $F(\phi)$ and a dissipation mechanism. To fix the idea, we consider a typical free energy functional $E[\phi(\boldsymbol{x})] = \int_\Omega [\frac{1}{2}|\nabla\phi|^2 + F(\phi)]dx$, and the corresponding gradient flow in H^{-1}:

$$\begin{aligned} &\frac{\partial \phi}{\partial t} = \Delta \mu, \\ &\mu = \delta E/\delta\phi = -\Delta\phi + F'(\phi), \end{aligned} \tag{1.1}$$

subject to

$$\text{either periodic boundary conditions or} \quad \frac{\partial \phi}{\partial \boldsymbol{n}}|_{\partial\Omega} = \frac{\partial \mu}{\partial \boldsymbol{n}}|_{\partial\Omega} = 0, \tag{1.2}$$

☆ This work was partially supported by NSF DMS-1620262, AFOSR FA9550-16-1-0102 and by NSFC grants 11371298, 11421110001, 91630204 and 51661135011.

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https://doi.org/10.1016/j.jcp.2017.10.021
0021-9991/

where $\boldsymbol{n}$ is the outward normal of $\partial\Omega$. Taking the inner product of the first equation in (1.1) with μ and the second equation in (1.1) with $\frac{\partial\phi}{\partial t}$, we obtain immediately the energy dissipation law:

$$\frac{d}{dt}E[\phi(\boldsymbol{x})] = -\|\nabla\mu\|^2, \tag{1.3}$$

where $\|\cdot\|$ is the L^2 norm. A time discretization scheme for (1.1)–(1.2) is said to be energy stable if it satisfies a discrete energy dissipation law. The goal of this paper is to present a new approach to construct efficient and accurate energy stable schemes for general gradient flows.

2. A brief review of energy stable schemes for gradient flows

In order to motivate our new approach, we provide below a brief review of several popular numerical approaches to construct energy stable schemes for gradient flows.

2.1. Convex splitting approach

A very popular approach for gradient flow is the so called convex splitting method which appears to be introduced by [9] and popularized by [10]. Assuming the free energy density $F(\phi)$ can be split as the difference of two convex functions, namely, $F(\phi) = F_c(\phi) - F_e(\phi)$ with $F_c''(\phi),\ F_e''(\phi) \geq 0$. Then, the first-order convex splitting scheme reads:

$$\begin{aligned} &\frac{\phi^{n+1}-\phi^n}{\delta t} = \Delta\mu^{n+1}, \\ &\mu^{n+1} = -\Delta\phi^{n+1} + \Big(F_c'(\phi^{n+1}) - F_e'(\phi^n)\Big). \end{aligned} \tag{2.1}$$

One can easily show that the above scheme is unconditionally energy stable in the sense that

$$E(\phi^{n+1}) - E(\phi^n) \leq -\delta t\|\nabla\mu^{n+1}\|^2, \tag{2.2}$$

which is a discrete analog of (1.3). The convex splitting approach enjoys the following advantages: (i) It is unconditionally energy stable; (ii) It is uniquely solvable; and (iii) It leads to a convex minimization problem at each time step. But it also suffers from shortcomings such as (i) A nonlinear system has to be solved at each time step; and (ii) There is no general approach to construct unconditionally stable second-order convex splitting schemes, although such schemes have been developed case-by-case for some problems.

2.2. Stabilized approach

Another widely used approach is the stabilized scheme, introduced in [27] (see also [18]). The main idea is to introduce an artificial stabilization term to balance the explicit treatment of the nonlinear term. A first-order stabilized scheme for (1.1) reads:

$$\frac{1}{\delta t}(\phi^{n+1}-\phi^n) = \Delta\mu^{n+1}, \tag{2.3a}$$

$$\mu^{n+1} = -\Delta\phi^{n+1} + S(\phi^{n+1}-\phi^n) + F'(\phi^n), \tag{2.3b}$$

where S is a suitable stabilization parameter. It is shown in [18] that, under the assumption $\|F''(\phi)\|_\infty \leq L$, the above scheme is unconditionally stable for all $S \geq \frac{L}{2}$. The main advantage of the stabilized scheme is its simplicity and efficiency. More precisely, it leads to a system of two coupled second-order equations with constant coefficients. Moreover, it can be decoupled into two sequential second-order equations with constant coefficients [25]. Hence, the stabilized scheme is extremely efficient, particularly when fast Poisson solvers are available. However, it appears difficult to design second-order unconditionally energy stable schemes with a stabilized approach, although some progress has been made recently in [17]. One can also use the spectral deferred correction (SDC) [7] to takes a correction technique to enhance the accuracy of the stabilized scheme, but it still fails to preserve the nonlinear energy stability [11].

2.3. Invariant energy quadratization (IEQ) approaches

An interesting approach is proposed in [12] for dealing with Allen–Cahn and Cahn–Hilliard equations with double well free energy. It is based on a Lagrange multiplier approach introduced in [3]. This approach can lead to unconditionally energy stable, linear, second-order schemes for Allen–Cahn and Cahn–Hilliard equations with double-well free energies. However, it cannot be easily extended to deal with other free energies. Very recently, X. Yang and his collaborators [20,21,23,24,26,22,19] made a big leap in generalizing the Lagrange multiplier approach to the so called invariant energy quadratization (IEQ) approach which is applicable to a large class of free energies. More precisely, assuming that the free energy density $F(\phi)$

is bounded from below, e.g., there exists $C_0 > 0$ such that $F(\phi) \geq -C_0$, one then introduces a Lagrange multiplier (auxiliary variable) $q(t, x; \phi) = \sqrt{F(\phi) + C_0}$, and rewrite (1.1) as

$$\begin{aligned} &\phi_t = \Delta \mu, \\ &\mu = -\Delta \phi + \frac{q}{\sqrt{F(\phi) + C_0}} F'(\phi), \\ &q_t = \frac{F'(\phi)}{2\sqrt{F(\phi) + C_0}} \phi_t. \end{aligned} \tag{2.4}$$

Taking the inner products of the above with μ, ϕ_t and $2q$, respectively, we see that the above system satisfies a modified energy dissipation law:

$$\frac{d}{dt}(\frac{1}{2}\|\nabla \phi\|^2 + \int_\Omega q^2 dx) = -\|\nabla \mu\|^2. \tag{2.5}$$

The above formulation is amenable to simple and efficient numerical schemes. Consider for instance,

$$\frac{\phi^{n+1} - \phi^n}{\delta t} = \Delta \mu^{n+1}, \tag{2.6}$$

$$\mu^{n+1} = -\Delta \phi^{n+1} + \frac{q^{n+1}}{\sqrt{F(\phi^n) + C_0}} F'(\phi^n), \tag{2.7}$$

$$\frac{q^{n+1} - q^n}{\delta t} = \frac{F'(\phi^n)}{2\sqrt{F(\phi^n) + C_0}} \frac{\phi^{n+1} - \phi^n}{\delta t}. \tag{2.8}$$

Taking the inner products of the above with μ^{n+1}, $\frac{\phi^{n+1} - \phi^n}{\delta t}$ and $2q^{n+1}$, respectively, one obtains immediately:

$$\begin{aligned} &\frac{1}{\delta t}\Big[\frac{1}{2}\|\nabla \phi^{n+1}\|^2 + \int_\Omega (q^{n+1})^2 dx - \frac{1}{2}\|\nabla \phi^n\|^2 - \int_\Omega (q^n)^2 dx \\ &\quad + \frac{1}{2}\|\nabla(\phi^{n+1} - \phi^n)\|^2 + \int_\Omega (q^{n+1} - q^n)^2 dx\Big] = -\|\nabla \mu^{n+1}\|^2, \end{aligned} \tag{2.9}$$

which indicates that the above scheme is unconditionally stable with respect to the modified energy. The above approach enjoys the following advantages: (i) One can eliminate q^{n+1} and μ^{n+1} from (2.6) to obtain a linear fourth-order equation with variable coefficients for ϕ^{n+1}, so it is very efficient; (ii) It can be easily extended to higher-order BDF-k scheme, with BDF-2 being unconditionally stable; and (iii) It applies to a large class of gradient flows [20,21,23,24,26,22,19].

However, while the IEQ approach has proven to be a very powerful way to construct energy stable schemes, it does leave some things to be desired: (i) It involves solving linear equations with complicated VARIABLE coefficients; (ii) It requires that the free energy density $F(\phi)$ is bounded from below, and this may not hold for some physically interesting models; and (iii) For gradient flows with multiple components, it leads to a coupled system. These shortcomings can be effectively overcome with a simple modification of the IEQ approach that we present below.

3. The scalar auxiliary variable (SAV) approach

We observe that the main reason for the above shortcomings of IEQ approach is that the auxiliary variable q depends on the space variable. Therefore, instead of assuming $F(\phi)$ is uniformly bounded from below, we now only assume $E_1(\phi) := \int_\Omega F(\phi) dx$ is bounded from below, i.e., $E_1(\phi) \geq -C_0$, which is necessary for the free energy to be physically sound, and introduce a *scalar* auxiliary variable (SAV):

$$r(t) = \sqrt{E_1(\phi) + C_0}.$$

Then, (1.1) can be rewritten as:

$$\begin{aligned} &\frac{\partial \phi}{\partial t} = \Delta \mu, \\ &\mu = -\Delta \phi + \frac{r(t)}{\sqrt{E_1[\phi] + C_0}} F'(\phi), \\ &r_t = \frac{1}{2\sqrt{E_1[\phi] + C_0}} \int_\Omega F'(\phi) \phi_t dx. \end{aligned} \tag{3.1}$$

Taking the inner products of the above with μ, $\frac{\partial \phi}{\partial t}$ and $2r$, respectively, we obtain the modified energy dissipation law:

$$\frac{d}{dt}(\frac{1}{2}\|\nabla\phi\|^2 + r^2(t)) = -\|\nabla\mu\|^2. \tag{3.2}$$

We now construct a semi-implicit second-order BDF scheme for the above system.

$$\frac{3\phi^{n+1} - 4\phi^n + \phi^{n-1}}{2\delta t} = \Delta\mu^{n+1}, \tag{3.3a}$$

$$\mu^{n+1} = -\Delta\phi^{n+1} + \frac{r^{n+1}}{\sqrt{E_1[\phi^{n+1/2}] + C_0}} F'(\phi^{n+1/2}), \tag{3.3b}$$

$$\frac{3r^{n+1} - 4r^n + r^{n-1}}{2\delta t} = \int_\Omega \frac{F'(\phi^{n+1/2})}{2\sqrt{E_1[\phi^{n+1/2}] + C_0}} \frac{3\phi^{n+1} - 4\phi^n + \phi^{n-1}}{2\delta t}\, dx, \tag{3.3c}$$

where $\phi^{n+1/2}$ is any explicit $O(\delta t^2)$ approximation for $\phi(t^{n+1})$, which can be flexible according to the problem, and which we will specify in our numerical results.

Theorem 3.1. *The scheme (3.3) is unconditionally energy stable in the sense that*

$$\begin{aligned}&\frac{1}{4\delta t}[(\|\nabla\phi^{n+1}\|^2 + \|\nabla(2\phi^{n+1} - \phi^n)\|^2) - (\|\nabla\phi^n\|^2 + \|\nabla(2\phi^n - \phi^{n-1})\|^2)] \\ &\quad + \frac{1}{2\delta t}[(|r^{n+1}|^2 + |2r^{n+1} - r^n|^2) - (|r^n|^2 + |2r^n - r^{n-1}|^2)] \le -\|\nabla\mu^{n+1}\|^2.\end{aligned} \tag{3.4}$$

Proof. By taking the inner products of the above with μ^{n+1}, $\frac{3\phi^{n+1} - 4\phi^n + \phi^{n-1}}{2\delta t}$ and $2r^{n+1}$ with (3.3a), (3.3b) and (3.3c) respectively, using the identity:

$$\begin{aligned}2(a^{k+1}, 3a^{k+1} - 4a^k + a^{k-1}) =& |a^{k+1}|^2 + |2a^{k+1} - a^k|^2 + |a^{k+1} - 2a^k + a^{k-1}|^2 \\ &- |a^k|^2 - |2a^k - a^{k-1}|^2,\end{aligned} \tag{3.5}$$

and dropping some unnecessary terms, one obtains immediately (3.4). □

Remark 3.2.

(i) The semi-implicit BDF2 in (3.3) can be replaced by semi-implicit Crank–Nicolson scheme with a similar stability result.
(ii) For the H^{-1} gradient flow, we have the conservation of $\int_\Omega \phi dx$. With this fact and the Poincaré inequality, (3.4) implies that ϕ is bounded in H^1.
(iii) For the L^2 gradient flow, if there exists an $\beta > 0$ such that $\int dx[F(\phi) - \beta\phi^2] \ge -C_0$, one may define $E_1 = \int dx[F(\phi) - \beta\phi^2]$ and replace $-\Delta\phi^{n+1}$ by $-\Delta\phi^{n+1} + \beta\phi^{n+1}$ in (3.3b). In this case, the corresponding stability result immediately gives the H^1 bound. Note in particular that the commonly used double well potential $F = (\phi^2 - 1)^2/4\epsilon^2$ satisfies the condition.
(iv) With some further assumptions, it can be shown that the modified numerical energy converges to the exact energy, which will be discussed in a forthcoming paper.

Besides its unconditional stability, a most remarkable thing about the above scheme is that it can be solved very efficiently. Indeed, we can eliminate μ^{n+1} and r^{n+1} from (3.3) to obtain

$$\begin{aligned}\frac{3\phi^{n+1} - 4\phi^n + \phi^{n-1}}{2\delta t} =& -\Delta^2\phi^{n+1} + \frac{\Delta F'(\phi^{n+1/2})}{3\sqrt{E_1[\phi^{n+1/2}] + C_0}}\Big(4r^n - r^{n-1} \\ &+ \int_\Omega \frac{F'(\phi^{n+1/2})}{2\sqrt{E_1[\phi^{n+1/2}] + C_0}}(3\phi^{n+1} - 4\phi^n + \phi^{n-1})\, dx\Big).\end{aligned} \tag{3.6}$$

Denote

$$b^n = \frac{F'(\phi^{n+1/2})}{\sqrt{E_1[\phi^{n+1/2}] + C_0}}.$$

Then the above equation can be written as

$$\begin{aligned}&(I+\frac{2\delta t}{3}\Delta^2)\phi^{n+1}-\frac{\delta t}{3}(b^n,\phi^{n+1})\Delta b^n\\&=\frac{1}{3}(4\phi^n-\phi^{n-1})+\frac{2\delta t}{9}\left[4r^n-r^{n-1}-\frac{1}{2}(b^n,4\phi^n-\phi^{n-1})\right]\Delta b^n:=g^n.\end{aligned}\tag{3.7}$$

We shall first determine (b^n,ϕ^{n+1}) from the above. To this end, multiplying (3.7) with $(I+(2\delta t/3)\Delta^2)^{-1}:=A^{-1}$, then taking the inner product with b^n, we obtain

$$(b^n,\phi^{n+1})+\frac{\delta t}{3}\gamma^n(b^n,\phi^{n+1})=(b^n,A^{-1}g^n),\tag{3.8}$$

where $\gamma^n=-(b^n,A^{-1}\Delta b^n)\geq 0$ since $-A^{-1}\Delta$ is a positive definite operator. We then obtain from the above that

$$(b^n,\phi^{n+1})=\frac{(b^n,A^{-1}g^n)}{1+\delta t\gamma^n/3}.\tag{3.9}$$

Finally, we can solve ϕ^{n+1} from (3.7). To summarize, the SAV scheme (3.3b) can be easily implemented in the following manner:

(i) Compute $\gamma^n=-(b^n,A^{-1}\Delta b^n)$. This can be accomplished by solving a fourth-order equation with *constant coefficients*.
(ii) Compute (b^n,ϕ^{n+1}) using (3.9). This requires solving another fourth-order equation $A^{-1}g^n$, which has *constant coefficients*.
(iii) Finally, with (b^n,ϕ^{n+1}) known, $A^{-1}\Delta b^n$ and $A^{-1}g^n$ computed from (i) and (ii), we can find ϕ^{n+1} from (3.7) as

$$\phi^{n+1}=\frac{\delta t}{3}(b^n,\phi^{n+1})A^{-1}\Delta b^n+A^{-1}g^n.\tag{3.10}$$

Hence, the total cost at each time step are essentially solving two fourth-order equations with *constant coefficients*. We note that these fourth-order equations can be reduced to two decoupled Poisson type equations with some algebraic manipulations (cf. [25]), hence, this scheme is extremely efficient and easy to implement.

4. SAV approach for gradient flows of several functions

We consider, as an example of gradient flows of several functions, the following energy functional (cf. [14]):

$$E(\phi_1,\dots,\phi_k)=\sum_{i=1}^{k}\int_\Omega\frac{1}{2}|\nabla\phi_i|^2dx+E_1(\phi_1,\dots,\phi_k).\tag{4.1}$$

Denote $\Phi=(\phi_1,\dots,\phi_k)^t$, and assume $E_1(\Phi)\geq -C_0$ is a nonlinear energy functional bounded from below. We set $U_i=\delta E_1/\delta\phi_i$, and introduce $r(t)=\sqrt{E_1(\Phi)+C_0}$ as the scalar auxiliary variable. Then the H^{-1} gradient flow is given by

$$\frac{\partial\phi_i}{\partial t}=\Delta\mu_i,\tag{4.2}$$

$$\mu_i=-\Delta\phi_i+\frac{r}{\sqrt{E_1+C_0}}U_i,\tag{4.3}$$

$$r_t=\frac{1}{2\sqrt{E_1+C_0}}\int_\Omega\sum_{i=1}^{k}U_i\frac{\partial\phi_i}{\partial t}dx.\tag{4.4}$$

Then a semi-implicit second-order SAV scheme based on Crank–Nicolson is as follows:

$$\frac{\phi_i^{n+1}-\phi_i^n}{\delta t}=\Delta\mu_i^{n+1/2},\tag{4.5a}$$

$$\mu_i^{n+1/2}=-\Delta\frac{1}{2}(\phi_i^{n+1}+\phi_i^n)+\frac{r^{n+1}+r^n}{2\sqrt{E_1[\bar\Phi^{n+1/2}]+C_0}}U_i[\bar\Phi^{n+1/2}],\tag{4.5b}$$

$$\frac{r^{n+1}-r^n}{\delta t}=\int_\Omega\sum_{i=1}^{k}\frac{U_i[\bar\Phi^{n+1/2}]}{2\sqrt{E_1[\bar\Phi^{n+1/2}]+C_0}}\frac{\phi_i^{n+1}-\phi_i^n}{\delta t}dx,\tag{4.5c}$$

where $\bar\Phi^{n+1/2}$ is any explicit $O(\delta t^2)$ approximation for $\Phi(t^{n+1/2})$.

Theorem 4.1. *The scheme (4.5) is unconditionally energy stable in the sense that*

$$\frac{1}{2\delta t}[(\sum_{i=1}^{k}\|\nabla\phi_i^{n+1}\|^2+|r^{n+1}|^2)-(\sum_{i=1}^{k}\|\nabla\phi_i^{n}\|^2+|r^{n}|^2)]=-\sum_{i=1}^{k}\|\nabla\mu_i\|^2. \tag{4.6}$$

Proof. Multiplying the above three equations with $\delta t\mu_i^{n+1/2}$, $\frac{\phi_i^{n+1}-\phi_i^n}{\delta t}$, $r^{n+1}+r^n$ and taking the sum over i, we obtain immediately the desired result. □

Next, we describe how the scheme (4.5) can be efficiently implemented. Denote

$$b_i^n=\frac{U_i[\bar{\Phi}^{n+1/2}]}{2\sqrt{E_1[\bar{\Phi}^{n+1/2}]+C_0}},\quad A=I+\frac{\delta t}{2}\Delta^2.$$

By substituting (4.5b) and (4.5c) into (4.5a), we obtain linear equations of the following form

$$A\phi_i^{n+1}-\sum_{j=1}^{k}(\phi_j^{n+1},b_j^n)\Delta b_i^n=g_i^n,\quad i=1,\cdots,k. \tag{4.7}$$

Denote $\alpha_j=(\phi_j^{n+1},b_j^n)$, $\gamma_i^n=(b_i^n,A^{-1}\Delta b_i^n)\geq 0$, and $\alpha=\sum_{j=1}^{k}\alpha_j$. Taking inner product with $A^{-1}b_i$, then taking the summation over i, we obtain

$$\sum_{i=1}^{k}\alpha_i+\sum_{i=1}^{k}\gamma_i^n\sum_{j=1}^{k}\alpha_j=\sum_{i=1}^{k}(b_i^n,A^{-1}g_i^n), \tag{4.8}$$

which gives

$$\alpha=\Big(\sum_{i=1}^{k}(p_i^n,A^{-1}g_i^n)\Big)\Big/\Big(1+\sum_{i=1}^{k}\gamma_i^n\Big). \tag{4.9}$$

Finally, we can solve Φ^{n+1} from (4.7) by

$$\phi_i^{n+1}=\alpha A^{-1}\Delta b_i^n+A^{-1}g_i^n. \tag{4.10}$$

To summarize, the SAV scheme (4.5) can be easily implemented in the following manner:

(i) Compute $\{\gamma_i^n\}$, which requires solving k decoupled four-order equations with constant coefficients.
(ii) Compute α from (4.9), which requires solving k decoupled four-order equations with constant coefficients;
(iii) Finally, using $A^{-1}\Delta b_i^n$ and $A^{-1}g_i^n$ computed from (i) and (ii), we obtain $\{\phi_i^{n+1}\}$ from (4.10).

The total cost is essentially solving $2k$ four-order equations with constant coefficients, each of which can be further reduced to two decoupled Poisson type equations (cf. [25]). Hence, this scheme is extremely efficient and easy to implement. We note that with the IEQ approach, we will need to solve k coupled four-order equations with variable coefficients.

5. Numerical results and discussions

In this section, we present some numerical examples of the Cahn–Hilliard equation (1.1) with periodic boundary conditions and where the free energy is given by $E[\phi(\boldsymbol{x})]=\int_\Omega[\frac{1}{2}|\nabla\phi|^2+(\phi^2-1)^2/4\epsilon^2]dx$. We rewrite it as

$$E[\phi(\boldsymbol{x})]=\int_\Omega[\frac{1}{2}|\nabla\phi|^2+\frac{\beta}{\epsilon^2}\phi^2+\frac{1}{4\epsilon^2}(\phi^2-1-\beta)^2-\frac{\beta^2+2\beta}{4\epsilon^2}]dx.$$

We drop the constant in the free energy and let $E_1[\phi]=\int_\Omega F(\phi)dx=\int_\Omega(\phi^2-1-\beta)^2/4\epsilon^2dx$, and modify (for example, for the BDF2 scheme) (3.3b) into

$$\mu^{n+1}=-\Delta\phi^{n+1}+\frac{\beta}{\epsilon^2}\phi^{n+1}+\frac{r^{n+1}}{\sqrt{E_1[\phi^{n+1/2}]+C_0}}F'(\phi^{n+1/2}). \tag{5.1}$$

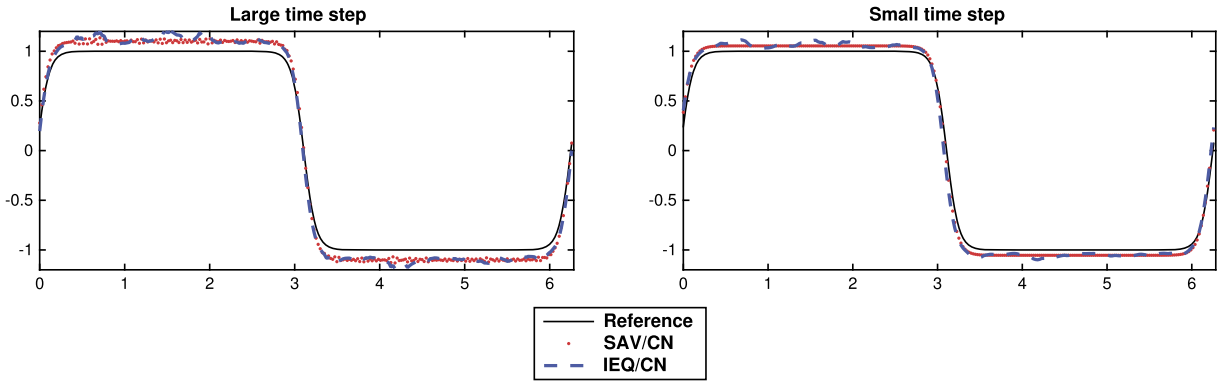

Fig. 1. (Example 1) Comparison of SAV and IEQ. Left: $\Delta t = 10^{-4}$; Right: $\Delta t = 10^{-5}$.

Note that this modification does not affect the implementation procedure we described above. We compute $\phi^{n+1/2}$ by using the following simple scheme:

$$\frac{\phi^{n+1/2} - \phi^n}{\delta t} = \Delta\Big(- \Delta\phi^{n+1/2} + \frac{\beta}{\epsilon^2}\phi^{n+1/2} + F'(\phi^n)\Big), \tag{5.2}$$

where we only need to solve another Poisson type equation.

The reference solutions are computed using the fourth order scheme ETDRK4 (see [5]) with sufficiently small time steps. In the first example, we compare IEQ and SAV schemes, and in the other examples we focus on other aspects of SAV approach.

Example 1 *(Comparison of IEQ and SAV approach).* We consider the Cahn–Hilliard equation in $[0, 2\pi)$ with $\epsilon^2 = 0.01$, using the finite difference method for spatial discretization with $h = 2\pi/256$. The parameters in the scheme are chosen as $\beta = 4$ and $C_0 = 0$.

We run BDF schemes for both IEQ and SAV approaches with one more regular initial condition

$$\phi(x, 0) = 0.5 \sin x + 0.1\text{Rand}(x), \tag{5.3}$$

and one less regular initial condition

$$\phi(x, 0) = 0.1 \sin x + 0.5\text{Rand}(x), \tag{5.4}$$

where Rand(x) stands for the random values in $[-1, 1]$.

First, we compare IEQ/CN and SAV/CN schemes. We use two time steps $\Delta t = 10^{-4}, 10^{-5}$, and plot in Fig. 1 the results at $T = 0.04$. We observe oscillations when $\Delta t = 10^{-4}$ for both IEQ and SAV approaches, but more pronounced for IEQ. With $\Delta t = 10^{-5}$, oscillations are still visible for IEQ but vanish for SAV. This indicates that the SAV/CN scheme can be more accurate than the IEQ/CN scheme, possibly due to the fact that the SAV function is directly related to the energy functional, not the energy density as in the IEQ approach.

Next, we compare IEQ/BDF2 and SAV/BDF2 schemes. We use two time steps $\delta t = 10^{-3}, 10^{-5}$, and plot the results at $T = 0.1$ in Fig. 2.

We observe that both schemes produce non oscillatory solutions for both large time step and small time step, but SAV is still more accurate than IEQ with the larger time step.

To further test the robustness of SAV approach, we take $\epsilon^2 = 0.0001$ with two time steps $\delta t = 10^{-4}$, 10^{-7}, and plotted the results in Fig. 3. We observe that while $\delta t = 10^{-4}$ is not sufficient small for accuracy but the modified energy and original energy are kept dissipative.

Example 2 *(Convergence rates of SAV).* We perform a simulation in $[0, 2\pi)^2$ with $\epsilon^2 = 0.01$, $\beta = 2$, $C_0 = 0$ and the initial condition:

$$\phi(x, y, 0) = 0.05 \sin x \sin y. \tag{5.5}$$

The space is discretized by the Fourier spectral method with 128×128 modes so the spatial discretization error is negligible compared to the time discretization. The errors at $T = 0.016$, measured in the L^2 norm, are plotted in Fig. 4, where we can clearly observe the second-order convergence for both SAV/BDF2 and SAV/CN schemes. As expected, the SAV/CN scheme is slightly more accurate than the SAV/BDF scheme.

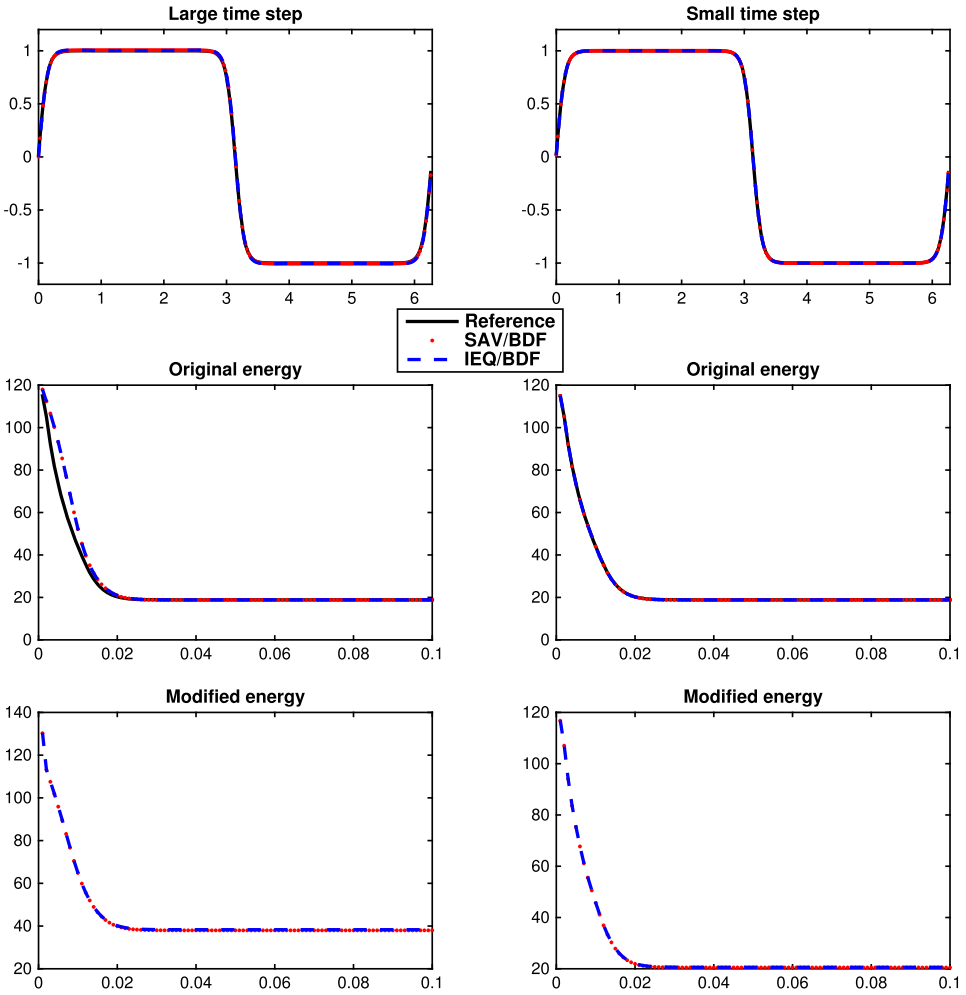

Fig. 2. (Example 1) Comparison of SAV and IEQ with more regular initial value. Left: $\delta t = 10^{-3}$; Right: $\delta t = 10^{-5}$.

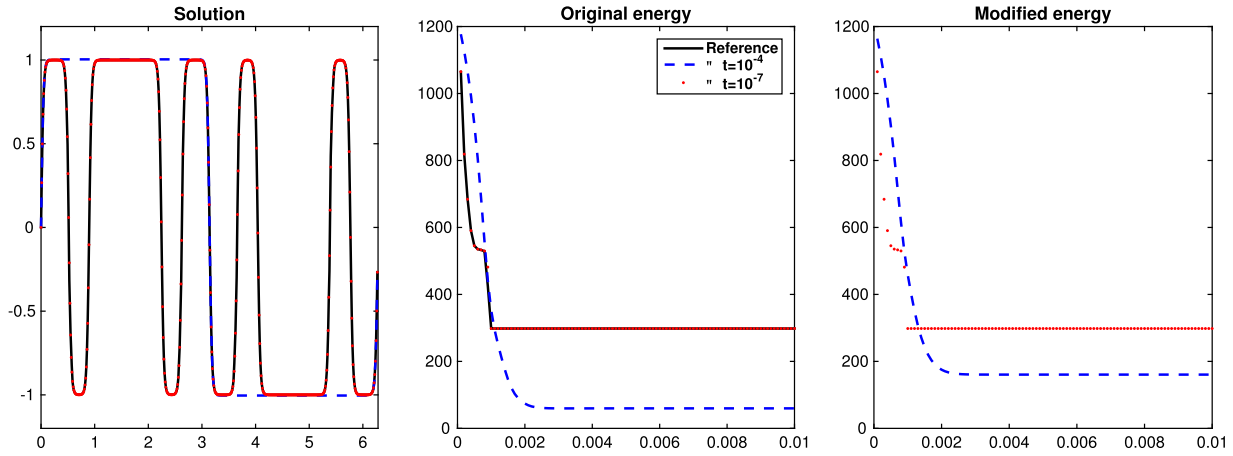

Fig. 3. (Example 1) Solution profiles and energy evolutions of SAV/BDF2 with $\epsilon^2 = 0.0001$. Left: $\delta t = 10^{-4}$; Right: $\delta t = 10^{-7}$.

Example 3 *(Evolutions of coarsening process and of energy).* In this example, we simulate the Cahn–Hilliard equation on $[0, 2\pi)^2$, starting from

$$\phi(x, y, 0) = 0.25 + 0.4\text{Rand}(x, y). \tag{5.6}$$

We choose $\beta = 4$, $C_0 = 0$, and discretize the space by the Fourier spectral method with 256×256 modes.

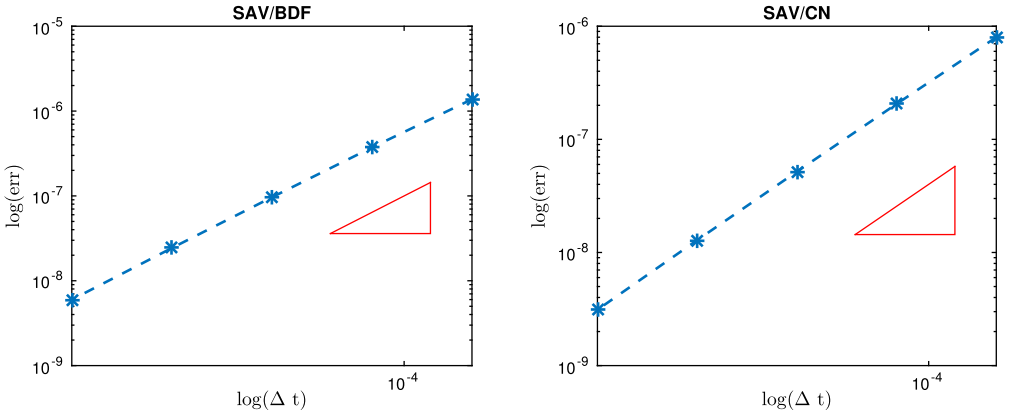

Fig. 4. (Example 2) Numerical convergence rate of SAV schemes. The triangle represents the second-order convergence rate.

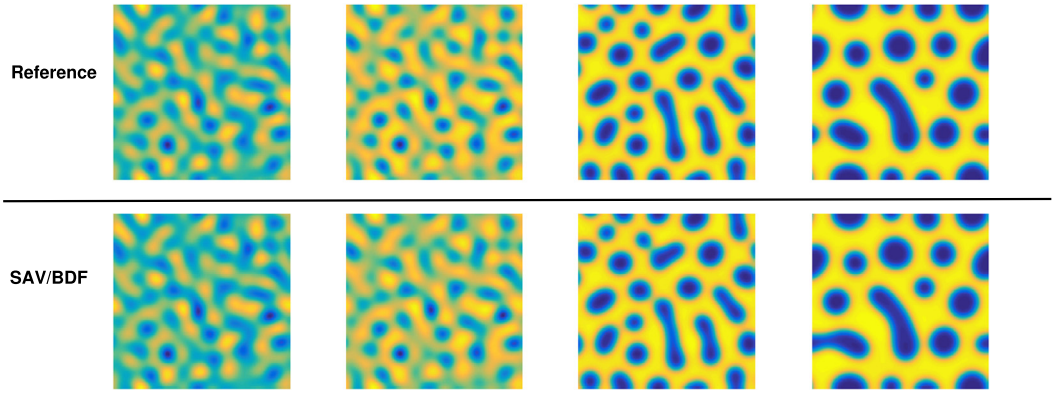

Fig. 5. (Example 3) Coarsening process with SAV/BDF2.

We investigate the coarsening process with $\epsilon^2 = 0.01$ and $\delta t = 2 \times 10^{-5}$. The reference solution and the results of SAV/BDF2 are shown in Fig. 5, no visible difference is observed.

6. Summary

We presented in this note a new approach, termed as scalar auxiliary variable (SAV) approach, for gradient flows. The SAV approach enjoys all the advantages of the invariant energy quadratization (IEQ) method which has shown, with ample numerical evidences, to be superior to existing approaches such as convex splitting and stabilization methods. Furthermore, it possesses the following additional advantages:

- For H^{-1} gradient flows of a single function, the total computational cost is essentially solving two fourth-order equations, or two systems of two second-order equations, with *constant* coefficients;
- For H^{-1} gradient flows of k functions, the SAV scheme will lead to, at each time step, $2k$ *decoupled* fourth-order equations with constant coefficients;
- It only requires $E_1(\phi) := \int_\Omega F(\phi)dx$, instead of $F(\phi)$, be bounded from below, so it applies to a larger class of gradient flows. For example, the free energy density in the epitaxial thin film growth model without slope selection [16] is unbounded from below, but its integral is bounded from below so SAV approach can be applied.

It is obvious that the SAV approach applies also to L^2 gradient flows for which one only requires solving second-order equations with constant coefficients. Thus, the SAV schemes are extremely efficient, its second-order versions are unconditionally energy stable, applicable to a large class of gradient flows, and can be extended to higher-order with BDF and Adam–Bashforth schemes. Numerical results show that the SAV approach is not only much more efficient and easy to implement, it also outperforms, in terms of accuracy, the IEQ approach.

In a forthcoming paper, we shall present applications of SAV approach to a variety of challenging gradient flows, including Q tensor models for liquid crystal, gradient flows with non-local dissipation operators, multi-phase phase-field models, molecular beam epitaxial without slope selection (where the free energy density is unbounded from below), phase-field crystals, etc.

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