Chapter 17

Efficient and accurate structure preserving schemes for complex nonlinear systems

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Chapter Outline

Abstract

The scalar auxiliary variable (SAV) approach was recently proposed in Shen et al. (2018) to construct efficient and accurate unconditionally energy stable schemes for gradient flows. We present the SAV approach in a more general setting, and consider a few interesting extensions that enable us to use the SAV approach to deal with a large class of complex dissipative/conservative systems.

Keywords: Scalar auxiliary variable, Gradient flows, Conservative system, Structure preserving, Energy stability, Phase-field model

AMS Classification Codes: 65M12, 35K20, 35K35, 35K55, 65Z05

1 Introduction

The ability of accurate simulation of complex phenomena governed by highly complex dissipative/conservative systems is central to our understanding of

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many important issues, such as advanced materials, quantum mechanics, semiconductors, imaging, optimal transport, nonconvex optimization, etc. Examples of these dissipative systems include Allen–Cahn and Cahn–Hilliard equations, phase-field models (Anderson et al., 1998; Gurtin et al., 1996; Liu and Shen, 2003; Lowengrub and Truskinovsky, 1998; Yue et al., 2004a), thin film models (Giacomelli and Otto, 2001; Otto, 1998), liquid crystal models (Doi and Edwards, 1988; Forest et al., 2004a, b; Larson, 1990; Leslie, 1979; Yu et al., 2010), and examples of conservative systems include nonlinear Schrödinger equations, Sine-Gordon equations, etc.

However, it is a tremendous challenge to numerically solving highly complex nonlinear systems which preserve energy dissipation/conservation, and/or physical constraints such as positivity, mass conservation, etc. Simple explicit or semi-implicit approaches may induce severe stability conditions on the time step so they are not efficient in practice. On the other hand, unconditionally energy stable schemes may be constructed with a fully implicit approach (Du and Nicolaides, 1991) but it leads to nonlinear systems which may not be easy to solve and whose unique solvability may still dictate a time step constraint.

It is in general very challenging to develop efficient and accurate unconditionally structure preserving schemes which preserve essential physical quantities for these stiff systems with highly complex nonlinearities. Many efforts have been made in the last three decades, we refer to Shen et al. (2019) for a brief review on the existing approaches for gradient flows which is a particular class of such problems, and to Du and Feng (2019) for an extensive review. In particular, the recently proposed scalar auxiliary variable (SAV) approach (Shen et al., 2018) enjoys several remarkable advantages (cf. Shen et al., 2019). Thanks to its simplicity, efficiency and generality, the SAV approach can be applied to a large class of problems with energy dissipation/conservation. In addition to the various applications presented in Shen et al. (2019), it has been applied to, among others, the epitaxial thin film growth models in Cheng et al. (2019), the multicomponent two-phase compressible flow in Kou et al. (2018), a phase-field surfactant model in Zhu et al. (2018), a phase-field vesicle membrane model in Cheng and Shen (2018), a phase-field model for solid-state dewetting problems (He et al., 2018), the incompressible Navier–Stokes equations in Yang and Dong (2018), to strongly anisotropic Cahn–Hilliard equations in Yang (2018a), Sine-Gordon equations in Cai et al. (2018), and to compute the stationary solutions of one- and multicomponent Bose–Einstein condensates in Zhuang and Shen (2019).

The aim of this paper is to introduce the recently proposed scalar auxiliary variable (SAV) approach (Shen et al., 2018) in a more general context, discuss how it can be made more effective for a large class of problems, and present a few interesting extensions.

The rest of the paper is organized as follows. In Section 2, we describe the SAV approach in a general context, present its properties. In Section 3, we present several interesting extensions of the SAV approach.

2 The SAV approach

We describe below the scalar auxiliary variable (SAV) approach introduced in Shen et al. (2018). Given a free energy in the form

$$\mathcal{E}(\phi) = \int_\Omega \left[\frac{1}{2}\phi\, \mathcal{L}\phi + F(\phi)\right] dx, \tag{1}$$

where $\mathcal{L}$ is a linear positive definite operator and $F(\phi)$ is a nonlinear free energy, we consider a general gradient flow given by:

$$\begin{aligned} \phi_t &= -\mathcal{G}\mu, \\ \mu &:= \frac{\delta \mathcal{E}}{\delta \phi} = \mathcal{L}\phi + F'(\phi), \end{aligned} \tag{2}$$

where $\mathcal{G}$ is a positive definite operator describing the relaxation process of the gradient flow, e.g., $\mathcal{G} = I$ is the usual L^2-gradient flow while $\mathcal{G} = -\Delta$ is the so-called H^{-1}-gradient flow, μ is the so-called chemical potential. The above system satisfies the energy law:

$$\frac{\partial}{\partial t}\mathcal{E}(\phi) = \frac{\partial}{\partial t}\int_\Omega \left[\frac{1}{2}\phi\, \mathcal{L}\phi + F(\phi)\right] dx = -(\mathcal{G}\mu, \mu) \le 0. \tag{3}$$

Assume that

$$E_1(\phi) := \int_\Omega F(\phi) dx \quad \text{is bounded from below, i.e.,} \quad E_1(\phi) > -C_0 \text{ for some } C_0 > 0. \tag{4}$$

We introduce one scalar auxiliary variable (SAV), $r(t) = \sqrt{E_1(\phi) + C_0}$, and rewrite the original gradient flow (2) as:

$$\begin{aligned} \frac{\partial \phi}{\partial t} &= -\mathcal{G}\mu \\ \mu &= \mathcal{L}\phi + \frac{r(t)}{\sqrt{E_1(\phi) + C_0}} F'(\phi) \\ r_t &= \frac{1}{2\sqrt{E_1(\phi) + C_0}} \int_\Omega F'(\phi)\phi_t dx. \end{aligned} \tag{5}$$

The above system is equivalent to (2) under the initial condition $r(0) = \sqrt{E_1(\phi|_{t=0}) + C_0}$. However, it allows more flexibility in time discretization. For example, with the principle of treating linear terms implicitly and all nonlinear terms explicitly, a second-order scheme for the above reformulated system can be constructed as follows:

$$\begin{aligned} &\frac{\phi^{n+1} - \phi^n}{\Delta t} = -\mathcal{G}\mu^{n+1/2}, \\ &\mu^{n+1/2} = \mathcal{L}\phi^{n+1/2} + \frac{r^{n+1/2}}{\sqrt{E_1\left(\widetilde{\phi}^{n+1/2}\right) + C_0}} F'\left(\widetilde{\phi}^{n+1/2}\right), \\ &\frac{r^{n+1} - r^n}{\Delta t} = \int_\Omega \frac{F'\left(\widetilde{\phi}^{n+1/2}\right)}{2\sqrt{E_1\left(\widetilde{\phi}^{n+1/2}\right) + C_0}} \frac{\phi^{n+1} - \phi^n}{\Delta t}\, dx, \end{aligned} \tag{6}$$

where $h^{n+1/2} := \frac{1}{2}(h^{n+1} + h^n)$ for any sequence $\{h^k\}$, and $\widetilde{\phi}^{n+1/2} := \frac{3}{2}\phi^n - \frac{1}{2}\phi^{n-1}$.

It is clear that the above scheme is second-order accurate. Furthermore, by taking the inner products of three equations in (6) with $\mu^{n+1/2}$, $\phi^{n+1} - \phi^n$, and $2r^{n+1/2}$, respectively, notice that the two terms with $F'(\phi)$ cancel each other regardless the form of $F(\phi)$, so we obtain immediately the following result:

Theorem 1. *The scheme* (6) *is unconditionally energy stable in the sense that*

$$\bar{\mathcal{E}}^{n+1}(\phi, r) - \bar{\mathcal{E}}^n(\phi, r) = -\Delta t(\mathcal{G}\mu^{n+1/2}, \mu^{n+1/2}),$$

where $\bar{\mathcal{E}}^k(\phi, r) := \int_\Omega \frac{1}{2}\phi^k \mathcal{L}\phi^k dx + r^k$ *is the modified free energy at* t^k.

Note that the modified energy $\bar{\mathcal{E}}^n(\phi, r)$ is an approximation of the original energy $\mathcal{E}(\phi^n)$ provided that $(r^n)^2$ is an approximation of $E_1(\phi^n) + C_0$. We observe from the above theorem that not only the scheme (6) is unconditionally energy stable, it also preserve the energy dissipation rate. In particular, it is energy conservative if $\mathcal{G}$ is skew-symmetric.

Another important fact is that the SAV scheme (6) is easy to implement. To this end, we write (6) in the following matrix form:

$$\begin{pmatrix} \frac{1}{\Delta t} I & \frac{1}{2}\mathcal{G} & 0 \\ \mathcal{L} & -I & * \\ * & 0 & \frac{1}{\Delta t} \end{pmatrix} \begin{pmatrix} \phi^{n+1} \\ \mu^{n+1} \\ r^{n+1} \end{pmatrix} = \overline{b}^n, \tag{7}$$

where $\overline{b}^n$ is the vector with known quantities, and * represents known vectors with variable coefficients. Hence, we can solve r^{n+1} with a block Gaussian elimination, which requires solving a system with constant coefficients of the form

$$\begin{pmatrix} \frac{1}{\Delta t} I & \frac{1}{2}\mathcal{G} \\ \mathcal{L} & -I \end{pmatrix} \begin{pmatrix} \phi \\ \mu \end{pmatrix} = \overline{b}. \tag{8}$$

Once r^{n+1} is known, we can obtain (ϕ^{n+1}, μ^{n+1}) by solving one more equation in the above form.

Remark 1. Several remarks are in order:

- It should be noted that the SAV approach is inspired by the IEQ/EQ methods (Yang, 2016; Zhao et al., 2017). However, with the IEQ/EQ approach, one has to solve a coupled linear system with time dependent variable coefficients, so in this sense the SAV approach is computationally more efficient.
- While, for the sake of simplicity, we described the scheme and its stability in semidiscrete form, the above stability result carries over to any consistent Galerkin type approximations, e.g. finite-elements or finite-differences, which respect proper integration by parts.
- The linear system (8) can be reduced to

$$\left(\frac{1}{\Delta t} I + \frac{1}{2}\mathcal{G}\mathcal{L}\right)\phi = \psi, \tag{9}$$

  with some known ψ. With any consistent Galerkin approximations of $\mathcal{G}$ and $\mathcal{L}$, the corresponding linear system for (9) is positive definite so can be efficiently solved by one's favourite method, e.g., preconditioned conjugate gradient method. In many common situations such as $\mathcal{L} = -\Delta$ and $\mathcal{G} = I$ or $-\Delta$ with suitable boundary conditions, the corresponding linear system for (9) can even be solved by fast direct methods such as fast Poisson solvers. Hence, the scheme (6) is very efficient.
- Note that in a linearly implicit scheme with or without stabilization, one also has to solve (8) at each time step. Therefore, the cost of the SAV scheme is essentially twice of linearly implicit schemes which are usually conditionally stable, and the benefit is that the scheme becomes unconditionally stable so an adaptive time stepping can be employed to further reduce the computational cost.

For dissipative systems, it is usually better to use BDF type schemes rather than the Crank–Nicolson scheme. For example, a semi-implicit second-order scheme based on BDF2 formula is

$$\frac{3\phi^{n+1} - 4\phi^n + \phi^{n-1}}{2\Delta t} = \mathcal{G}\mu^{n+1}, \tag{10a}$$

$$\mu^{n+1} = \mathcal{L}\phi^{n+1} + \frac{r^{n+1}}{\sqrt{E_1(\overline{\phi}^{n+1})}} F'(\overline{\phi}^{n+1}), \tag{10b}$$

$$\frac{3r^{n+1} - 4r^n + r^{n-1}}{2\Delta t} = \int_\Omega \frac{F'(\overline{\phi}^{n+1})}{2\sqrt{E_1(\overline{\phi}^{n+1})}} \frac{3\phi^{n+1} - 4\phi^n + \phi^{n-1}}{2\Delta t}\, d\boldsymbol{x}, \tag{10c}$$

where $\overline{\phi}^{n+1} := 2\phi^n - \phi^{n-1}$.

Taking the inner products of the three equations with μ^{n+1}, $(3\phi^{n+1} - 4\phi^n + \phi^{n-1})/(2\Delta t)$, $2r^{n+1}$, respectively, and using the identity:

$$\begin{aligned} 2(a^{k+1}, 3a^{k+1} - 4a^k + a^{k-1}) = {} & |a^{k+1}|^2 + |2a^{k+1} - a^k|^2 + |a^{k+1} - 2a^k + a^{k-1}|^2 \\ & - |a^k|^2 - |2a^k - a^{k-1}|^2, \end{aligned} \tag{11}$$

we can obtain the following result:

Theorem 2. *The scheme* (10) *is second-order accurate, and unconditionally energy stable in the sense that*

$$\begin{aligned} \widetilde{\mathcal{E}}^{n+1}(\phi, r) - \widetilde{\mathcal{E}}^n(\phi, r) = {} & -\Delta t(\mathcal{G}\mu^{n+1}, \mu^{n+1}) \\ & - \left\{ \frac{1}{4}\left(\phi^{n+1} - 2\phi^n + \phi^{n-1}, \mathcal{L}(\phi^{n+1} - 2\phi^n + \phi^{n-1})\right) \right. \\ & \left. + \frac{1}{2}(r^{n+1} - 2r^n + r^{n-1})^2 \right\}, \end{aligned}$$

where the modified discrete energy at t^{n+1} *is defined as*

$$\begin{aligned} \widetilde{\mathcal{E}}^{n+1}(\phi, r) = {} & \frac{1}{4}\left((\phi^{n+1}, \mathcal{L}\phi^{n+1}) + \left(2\phi^{n+1} - \phi^n, \mathcal{L}(2\phi^{n+1} - \phi^n)\right)\right) \\ & + \frac{1}{2}\left((r^{n+1})^2 + (2r^{n+1} - r^n)^2\right). \end{aligned}$$

Note that the modified discrete energy $\mathcal{E}^{n+1}(\phi, r)$ Comparing with (6), the scheme (10) introduces extra dissipation terms so the dissipation rate is not exactly preserved as in (6). On the other hand, we can easily construct higher-order SAV schemes by replacing BDF2 approximation with BDF-k ($k \leq 6$) approximation. Numerical results (Shen et al., 2019) indicate that these BDF-k ($k \leq 6$) schemes are also unconditionally energy stable although a rigorous proof is still elusive.

We note that while the SAV schemes such as (6) and (10) are unconditionally energy stable for any type of free energies as long as we can split the free energy in the form of (1) satisfying (4). However, for the SAV schemes to be most effective, the following two considerations are very important.

2.1 Suitable energy splitting

The unconditional energy stability does not necessarily mean that the corresponding SAV schemes such as (6) and (10) will be effective. For example, if we take $\mathcal{L}=0$, the SAV schemes (6) and (10) are still unconditionally energy stable, but they are fully explicit so exceedingly small time steps are required to obtain reasonable accurate approximations. Therefore, the performance of the SAV schemes depend intrinsically on how to split the free energy. In principle, the splitting should be such that the linear term $\frac{1}{2}\phi\mathcal{L}\phi$ should "dominate" the other term $F(\phi)$. Otherwise, accurate approximate solutions can only be obtained with very small time steps. Hence, it is important to find suitable splittings such that good approximations can be obtained with reasonably large time steps.

Consider, for instance, a typical example with free energy

$$\mathcal{E}[\phi]=\int\frac{1}{2}|\nabla\phi|^2+\frac{1}{4\epsilon^2}(1-\phi^2)^2d\boldsymbol{x}, \tag{12}$$

where ϵ is a small parameter. This type of free energy is often used in Allen–Cahn (Allen and Cahn, 1979) and Cahn–Hilliard equations (Cahn and Hilliard, 1958, 1959), and in the study of interfacial dynamics (Ainsworth and Mao, 2017; Allen and Cahn, 1979; Anderson et al., 1998; Gurtin et al., 1996; Kim, 2012; Liu and Shen, 2003; Lowengrub and Truskinovsky, 1998; Rogers and Desai, 1989; Yue et al., 2004a). In typical situation, ϵ, representing the interfacial width, is usually small so that the nonlinear term is not "small" compared with the linear term. The consequence is that very small time steps are needed for the approximate solution to be accurate. However, this situation can be easily dealt with by using a suitable splitting of the free energy as follows:

$$\mathcal{E}(\phi)=\int\left[\frac{1}{2}|\nabla\phi|^2+\frac{\beta}{\epsilon^2}\phi^2\right]+\left[\frac{1}{4\epsilon^2}(1-\phi^2)^2-\frac{\beta}{\epsilon^2}\phi^2\right]d\boldsymbol{x}, \tag{13}$$

where β is a parameter of our choice. It can be easily shown that $E_1(\phi)=\int[\frac{1}{4\epsilon^2}(1-\phi^2)^2-\frac{\beta}{\epsilon^2}\phi^2]\,d\boldsymbol{x}$ has a lower bound for any β so SAV approach can be applied.

As an illustrative example, we implemented the SAV scheme (10) for the Cahn–Hilliard equation, which is the gradient flow with the above free energy and $\mathcal{L}=\mathcal{G}=-\Delta$. We assume the periodic boundary conditions in the domain $[0,\ 2\pi)$, and use the Fourier-spectral method in space with initial condition $\phi(x,0)=0.2\sin x$. In the right of Fig. 1, we plot the numerical solutions of the scheme with $\beta=0$ (no stabilization) and $\beta=1$ (with stabilization) using a small $\Delta t=10^{-4}$. We observe that both solutions have the correct profile. However, with a relatively large $\Delta t=4\times10^{-3}$, see the left of Fig. 1, the solution with no stabilization exhibits oscillations while that with stabilization is still accurate.

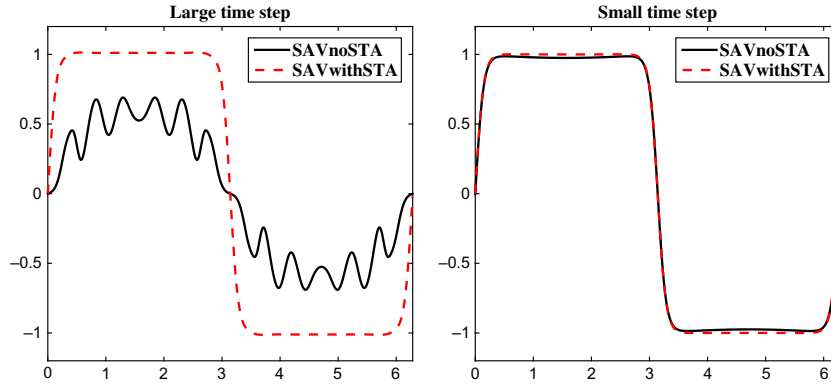

FIG. 1 The solution at $T = 0.1$ with $\epsilon = 0.1$. *Left*: $\Delta t = 4 \times 10^{-3}$; *Right*: $\Delta t = 10^{-4}$. The *red dashed lines* represent solutions with stabilization, while the *black solid lines* represent solutions without stabilization.

2.2 Adaptive time stepping

A main advantage of unconditional energy stable schemes is that they can be easily implemented with an adaptive time stepping strategy so that the time step is only dictated by accuracy rather than by stability as with conditionally stable schemes. This is particularly important for those situations where the solution may vary drastically in certain time intervals, but changes very little elsewhere.

It should be noted that variation of energy alone does not provide enough information to determine appropriate time steps. A suitable time adaptive strategy similar to that employed in Gomez and Hughes (2011) is proposed in Shen et al. (2016) (see also Shen et al. (2019)). In particular, the formula for updating the time step size is given by

$$A_{dp}(e,\tau) = \rho\left(\frac{tol}{e}\right)^{1/2}\tau, \tag{14}$$

along with prescribed minimum and maximum time steps. In the above, ρ is a default safety coefficient, tol is a reference tolerance, and e is the relative error at each time level. As an illustrative example, we consider the 2D Cahn–Hilliard equation with $\mathcal{L} = \mathcal{G} = -\Delta$ on $[0, 2\pi) \times [0, 2\pi)$ with periodic boundary conditions and random initial data. We take $\epsilon = 0.1$, and use the Fourier-spectral method with $N_x = N_y = 256$. We choose $\rho = 0.9$ and $tol = 10^{-3}$. The minimum and maximum time steps are taken as $\tau_{min} = 10^{-5}$ and $\tau_{max} = 10^{-2}$, respectively. The initial time step is taken as τ_{min}. Numerical results are shown in Fig. 2. We observe that the adaptive time stepping leads to correct energy evolution with the largest time step being several hundred times larger than the smallest time step. This indicates that savings up to several orders of magnitude times

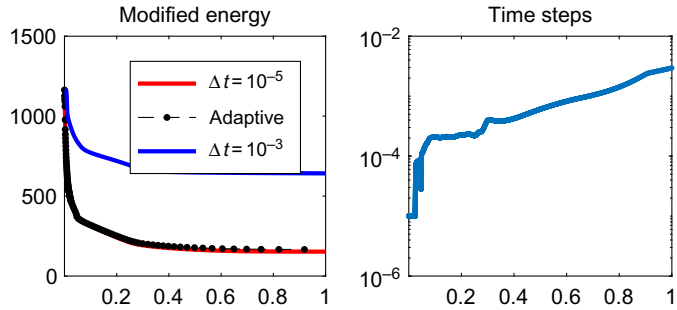

FIG. 2 Adaptive time stepping. *Left*: Energy evolution with small time steps, adaptive time steps, and large time steps; *Right*: step sizes of adaptive time stepping.

can be achieved by combining SAV schemes with an adaptive time stepping compared with semi-implicit schemes whose time steps are dictated by stability constraint.

In summary, the SAV schemes possess some amazing advantages such as: (i) it only requires solving elliptic systems with constant coefficients at each time step; (ii) it is second-order accurate, unconditionally energy stable and can be extended to higher-order. Ample numerical results in Shen et al. (2019, 2018) have shown its advantages compared with other schemes. Furthermore, it has been shown in Shen and Xu (2018) that the SAV schemes converge under essentially the same conditions as are required for the well posedness of the system (2), thanks to the unconditionally energy stability. On the other hand, convergence of linearly implicit schemes (Condette et al., 2011; Kessler et al., 2004; Shen and Yang, 2010b) usually requires that the derivative of nonlinear free energy, $F'(\phi)$ is uniformed bounded, a condition which is not even satisfied by the double well potential. The convergence results and error estimates in Shen and Xu (2018) for the semidiscrete case have also been extended to fully discrete cases with finite-differences in Li et al. (2019) and with finite-elements in Chen and Shen (2019).

3 Several extensions of the SAV approach

In the following, we present a few interesting extensions which enable us to use the SAV approach for a larger class of complex nonlinear systems.

3.1 Problems with global constraints

Many complex systems not only obey energy dissipation/conservation but also are constrained with other conservations such as mass, volume, surface area, etc. A popular and effective approach is to introduce penalty terms in the free energy so as to enforce, approximately, these constraints. Then, we can apply the SAV approach.

Consider, for example, the phase-field vesicle membrane model in Du et al. (2004) with the elastic bending energy

$$\begin{aligned} E_b(\phi) &= \frac{\epsilon}{2}\int_\Omega \left(-\Delta\phi + \frac{1}{\epsilon^2}G(\phi)\right)^2 d\boldsymbol{x} \\ &= \frac{\epsilon}{2}\int_\Omega \left(|\Delta\phi|^2 - \frac{2}{\epsilon^2}|\nabla\phi|^2 + \frac{6}{\epsilon^2}\phi^2|\nabla\phi|^2 + \frac{1}{\epsilon^4}(G(\phi))^2\right) d\boldsymbol{x}, \end{aligned} \tag{15}$$

where $G(\phi) = F'(\phi)$ with $F(\phi) = \frac{1}{4}(\phi^2-1)^2$, and subject to volume and surface area conservation:

$$A(\phi) = \frac{1}{2}\int_\Omega (\phi+1)d\boldsymbol{x} \equiv \alpha, \quad \text{and} \quad B(\phi) = \int_\Omega \left(\frac{\epsilon}{2}|\nabla\phi|^2 + \frac{1}{\epsilon}F(\phi)\right) d\boldsymbol{x} \equiv \beta, \tag{16}$$

where α, β represent the initial volume and surface area.

There is no mechanism in the SAV approach to enforce these constraints directly. However, we can penalize the free energy to approximately enforce them. More precisely, we consider the following free energy with additional penalization terms:

$$E_{tot}(\phi) = E_b(\phi) + \frac{1}{2\gamma}(A(\phi)-\alpha)^2 + \frac{1}{2\eta}(B(\phi)-\beta)^2, \tag{17}$$

where γ and η are two small parameters. In order to apply the SAV approach, we split $E_{tot}(\phi)$ as follows

$$\begin{aligned} E_{tot}(\phi) = &\frac{\epsilon}{2}\int_\Omega \left\{\frac{\epsilon}{2}\left(|\Delta\phi|^2 - \frac{2}{\epsilon^2}|\nabla\phi|^2\right) + \frac{1}{2\gamma}(A(\phi)-\alpha)^2\right\} \\ &+ \int_\Omega \left\{\frac{\epsilon}{2}\left(\frac{6}{\epsilon^2}\phi^2|\nabla\phi|^2 + \frac{1}{\epsilon^4}(G(\phi))^2\right) + \frac{1}{2\eta}(B(\phi)-\beta)^2\right\}. \end{aligned} \tag{18}$$

Note that the volume constraint is linear, so it is included in the first part. Then, we can apply the SAV approach to the above energy to construct unconditional energy stable SAV schemes. Usually such schemes would be effective, but due to the three small parameters in the free energy, it is observed in Cheng and Shen (2018) that such SAV schemes, while unconditionally energy stable, require exceedingly small time steps to obtain reasonable approximate solutions.

To remedy this situation, a multiple SAV approach is introduced in Cheng and Shen (2018). The basic strategy is to introduce one SAV for each small parameter in the nonlinear part of the free energy. So we are led to introduce two SAVs:

$$U = B(\phi) - \beta, \quad V = \sqrt{\int_\Omega \left(\frac{6}{\epsilon^2}\phi^2|\nabla\phi|^2 + \frac{1}{\epsilon^4}(G(\phi))^2\right) d\boldsymbol{x} + C}, \tag{19}$$

where C is a positive constant, so the total energy becomes

$$E_{tot}(\phi,U,V)=\frac{\epsilon}{2}\int_\Omega\left(|\Delta\phi|^2-\frac{2}{\epsilon^2}|\nabla\phi|^2\right)d\boldsymbol{x}+\frac{1}{2\gamma}(A(\phi)-\alpha)^2+\frac{U^2}{2\eta}+\frac{\epsilon}{2}(V^2-C).$$

Then, the L^2 gradient flow with a mobility M can be written as:

$$\phi_t=-M\mu, \tag{20}$$

$$\mu=\frac{\delta E_{tot}}{\delta\phi}=\epsilon\Delta^2\phi+\frac{2}{\epsilon}\Delta\phi+\frac{1}{\gamma}(A(\phi)-\alpha)+\frac{1}{\eta}U\frac{\delta U}{\delta\phi}+\epsilon V\frac{\delta V}{\delta\phi}, \tag{21}$$

$$U_t=\int_\Omega\frac{\delta U}{\delta\phi}\phi_t d\boldsymbol{x},\quad V_t=\int_\Omega\frac{\delta V}{\delta\phi}\phi_t d\boldsymbol{x}. \tag{22}$$

We can then apply the SAV approach to construct efficient energy stable schemes. For example, a second-order SAV scheme based on Crank–Nicolson is

$$\frac{\phi^{n+1}-\phi^n}{\Delta t}=-M\frac{\mu^{n+1}+\mu^n}{2}, \tag{23}$$

$$\frac{\mu^{n+1}+\mu^n}{2}=\epsilon\Delta^2\frac{\phi^{n+1}+\phi^n}{2}+\frac{2}{\epsilon}\Delta\frac{\phi^{n+1}+\phi^n}{2}+\frac{1}{\gamma}\left(A\left(\frac{\phi^{n+1}+\phi^n}{2}\right)-\alpha\right) \tag{24}$$

$$\begin{aligned}&+\frac{1}{\eta}\frac{U^{n+1}+U^n}{2}\frac{\delta U}{\delta\phi}\left(\phi^{\star,n+\frac{1}{2}}\right)+\epsilon\frac{V^{n+1}+V^n}{2}\frac{\delta V}{\delta\phi}\left(\phi^{\star,n+\frac{1}{2}}\right),\\ \frac{U^{n+1}-U^n}{\Delta t}&=\int_\Omega\frac{\delta U}{\delta\phi}\left(\phi^{\star,n+\frac{1}{2}}\right)\frac{\phi^{n+1}-\phi^n}{\Delta t}d\boldsymbol{x},\end{aligned} \tag{25}$$

$$\frac{V^{n+1}-V^n}{\Delta t}=\int_\Omega\frac{\delta V}{\delta\phi}\left(\phi^{\star,n+\frac{1}{2}}\right)\phi^{n+1}-\phi^n\Delta t d\boldsymbol{x}, \tag{26}$$

where $\phi^{\star,n+\frac{1}{2}}=\frac{3}{2}\phi^n-\frac{1}{2}\phi^{n-1}$. Taking the inner products of (23) with $\frac{\mu^{n+1}+\mu^n}{2}$, (24) with $\frac{\phi^{n+1}-\phi^n}{\Delta t}$, (25) with $\frac{U^{n+1}+U^n}{2}$ and (26) with $\frac{V^{n+1}+V^n}{2}$, respectively, and summing up the results, we obtain the following results:

Theorem 3. *The scheme (23)–(26) is unconditionally energy stable in the sense that*

$$E^{n+1}(\phi,U,V)-E^n(\phi,U,V)=-\Delta tM\parallel\mu^{n+\frac{1}{2}}\parallel^2,$$

where

$$E^{n+1}(\phi,U,V)=\frac{\epsilon}{2}\parallel\Delta\phi^{n+1}\parallel^2-\frac{1}{\epsilon}\parallel\nabla\phi^{n+1}\parallel^2+\frac{1}{2\eta}(U^{n+1})^2+\frac{\epsilon}{2}(V^{n+1})^2+\frac{1}{2\gamma}(A(\phi^{n+1})-\alpha)^2.$$

The above scheme can also be implemented as in the case with one SAV. Indeed, we can write it as a matrix system

$$\begin{pmatrix} \frac{1}{\Delta t}I & \frac{M}{2} & 0 \\ -\frac{\epsilon}{2}\Delta^2 - \epsilon\Delta - \frac{1}{4\gamma}I & \frac{1}{2}I & * \\ * & 0 & I_2 \end{pmatrix} \begin{pmatrix} \phi^{n+1} \\ \mu^{n+1} \\ \overline{r}^{n+1} \end{pmatrix} = \overline{b}^n,$$

where $\overline{r}^{n+1} = (U^{n+1}, V^{n+1})^t$, I is the identity operator, I_2 is the identity matrix of order 2, $*$ and $\overline{b}^n$ include only the terms from previous time steps. Therefore, we can first solve $\overline{r}^{n+1}$ using a block Gaussian elimination, which requires solving two systems with constant coefficients of the form

$$\begin{pmatrix} \frac{1}{\Delta t}I & \frac{M}{2} \\ -\frac{\epsilon}{2}\Delta^2 - \epsilon\Delta - \frac{1}{4\gamma}I & \frac{1}{2}I \end{pmatrix} \begin{pmatrix} \phi \\ \mu \end{pmatrix} = \overline{b},$$

which is a fourth-order equation with constant coefficients. With $\overline{r}^{n+1}$ known, we can obtain (ϕ^{n+1}, μ^{n+1}) by solving one more system in the above form. We refer to Cheng and Shen (2018) for more details with numerical validations.

3.2 L^1 minimization via hyper regularization

In imaging processing and many other applications, one often considers minimization of the free energy (Rudin et al., 1992)

$$E(\phi) = \int_\Omega \left[|\nabla\phi| + \frac{\lambda}{2}(\phi - g)^2 \right] dx, \tag{27}$$

where g is a given function. Oftentimes, one attempts to find the minimizer by finding the steady state solution of its gradient flow:

$$\frac{\partial\phi}{\partial t} = \nabla \cdot \frac{1}{|\nabla\phi|}\nabla\phi - \lambda(\phi - g). \tag{28}$$

However, there is no suitable energy splitting which would make the SAV approach effective. Therefore, we consider a hyper regularized free energy

$$E_\epsilon(\phi) = \int_\Omega \left\{ \frac{\epsilon}{2}|(-\Delta)^\beta\phi|^2 + \frac{\lambda}{2}(\phi - g)^2 + F_\epsilon(\phi) - \epsilon^2 \right\} dx, \tag{29}$$

where $\epsilon \ll 1$ and $\beta \geq 1$ are two parameters of our choice, and $F_\epsilon(\phi) = \sqrt{|\nabla\phi|^2 + \epsilon^2}$. Its gradient flow takes the form

$$\frac{\partial\phi}{\partial t} = -\epsilon(-\Delta)^{2\beta}\phi - \lambda(\phi - g) - F_\epsilon'(\phi). \tag{30}$$

We can then introduce a SAV $r(t)=\sqrt{E_{1,\epsilon}(\phi)}$ with $E_{1,\epsilon}(\phi)=\int_\Omega F_\epsilon(\phi)$, and rewrite the hyper regularized gradient flow (30) as

$$\begin{aligned}\frac{\partial\phi}{\partial t}&=-\epsilon(-\Delta)^{2\beta}\phi-\lambda(\phi-g)-\frac{r(t)}{\sqrt{E_{1,\epsilon}(\phi)}}F'_\epsilon(\phi),\\ r_t&=\frac{1}{2\sqrt{E_{1,\epsilon}(\phi)}}\int_\Omega F'_\epsilon(\phi)\phi_t dx.\end{aligned}\tag{31}$$

Then, a first-order scheme based on the above regularized SAV formulation is:

$$\begin{aligned}\frac{\phi^{n+1}-\phi^n}{\Delta t}&=-\epsilon(-\Delta)^{2\beta}\phi^{n+1}-\lambda(\phi^{n+1}-g)-\frac{r^{n+1}}{\sqrt{E_{1,\epsilon}(\phi^n)}}F'_\epsilon(\phi^n),\\ \frac{r^{n+1}-r^n}{\Delta t}&=\frac{1}{\sqrt{E_{1,\epsilon}(\phi^n)}}\int_\Omega F'_\epsilon(\phi^n)\frac{\phi^{n+1}-\phi^n}{\Delta t}dx.\end{aligned}\tag{32}$$

Second- and higher-order SAV schemes can be constructed as usual.

Taking the inner products of two equations above with $\frac{\phi^{n+1}-\phi^n}{\Delta t}$ and $2r^{n+1}$, respectively, one obtains:

Theorem 4. *The scheme* (32) *is unconditionally energy diminishing in the sense that*

$$E^{n+1}(\phi,r)-E^n(\phi,r)=-\Delta t\,\|\frac{\phi^{n+1}-\phi^n}{\Delta t}\|^2-\frac{\epsilon}{2}\|\,(-\Delta)^\beta(\phi^{n+1}-\phi^n)\|^2-|r^{n+1}-r^n|^2,$$

where $E^{n+1}(\phi,r)=\frac{\epsilon}{2}\|\,(-\Delta)^\beta\phi^{n+1}\|^2+\frac{\lambda}{2}\|\,\phi^{n+1}-g\|^2+|r^{n+1}|^2$.

Note that at each time step, one only need to solve, twice, a system of the form

$$\alpha\phi+\epsilon(-\Delta)^{2\beta}\phi=h,$$

with suitable boundary conditions. For imaging processing, periodic boundary condition can be used so the above equation can be solved fast a Fourier spectral method. One can then tune ϵ and β to achieve desired results.

3.3 Free energies with highly nonlinear terms

For problems with nonlinear terms in the highest derivative terms, such as in anisotropic Cahn–Hilliard equations (Torabi et al., 2009), it may not be easy or even possible to find a suitable splitting. In these cases, one may combine the SAV approach with a suitable regularization (Yang, 2018b). Consider for example an free energy with a nonlinear operator $\mathcal{L}$:

$$E(\phi)=\int_\Omega[\gamma(\phi)|\nabla\phi|^2+F(\phi)]dx,\tag{33}$$

where $\gamma(\phi) \geq 0$ is certain nonlinear function of ϕ. The corresponding anisotropic Cahn–Hilliard equation is

$$\phi_t = \Delta\mu; \;\; \mu = \frac{\delta E}{\delta \phi}. \tag{34}$$

We shall approximate the above equation with the following regularized equation:

$$\phi_t = \Delta\mu; \;\; \mu = -\sum_{k=0}^{2} \epsilon_k (-1)^k \Delta^k \phi_{tt} + \frac{\delta E}{\delta \phi}, \tag{35}$$

where $\epsilon_k \ll 1$ are free parameters and their choices depend on $\gamma(\phi)$ and $F(\phi)$. Introducing a SAV $r(t) = \sqrt{E(\phi) + C_0}$ where C_0 is a suitable constant such that $E(\phi) + C_0 > 0$, we can rewrite (35) as

$$\begin{aligned} \phi_t &= \Delta\mu, \\ \mu &= -\sum_{k=0}^{2} \epsilon_k (-1)^k \Delta^k \phi_{tt} + \frac{r(t)}{\sqrt{E(\phi) + C_0}} \frac{\delta E}{\delta \phi}, \\ r_t &= \frac{1}{2\sqrt{E(\phi) + C_0}} \int_\Omega \frac{\delta E}{\delta \phi} \phi_t dx. \end{aligned} \tag{36}$$

Then, a second-order SAV Crank–Nicolson scheme is

$$\begin{aligned} &\frac{\phi^{n+1} - \phi^n}{\Delta t} = \Delta \mu^{n+1/2}, \\ &\mu^{n+1/2} = -\sum_{k=0}^{2} \frac{\epsilon_k}{\Delta t^2} (-1)^k \Delta^k \left(\phi^{n+1} - 2\phi^n + \phi^{n-1}\right) + \frac{r^{n+1/2}}{\sqrt{E\left(\widetilde{\phi}^{n+1/2}\right) + C_0}} \frac{\delta E}{\delta \phi}\left(\widetilde{\phi}^{n+1/2}\right), \\ &\frac{r^{n+1} - r^n}{\Delta t} = \frac{1}{2\sqrt{E(\widetilde{\phi}^{n+1/2}) + C_0}} \int_\Omega \frac{\delta E}{\delta \phi}\left(\widetilde{\phi}^{n+1/2}\right) \frac{\phi^{n+1} - \phi^n}{\Delta t} \, dx, \end{aligned} \tag{37}$$

where $h^{n+1/2} := \frac{1}{2}(h^{n+1} + h^n)$ for any sequence $\{h^k\}$, and $\widetilde{\phi}^{n+1/2} = \frac{3}{2}\phi^n - \frac{1}{2}\phi^{n-1}$.

Taking the inner products of the first equation with $\mu^{n+1/2}$, the second equation with $\frac{\phi^{n+1} - \phi^n}{\Delta t}$ and the third equation with $2r^{n+1/2}$, summing up the results, we obtain immediately the following results:

Theorem 5. *The scheme* (37) *is unconditionally energy stable in the sense that*

$$\bar{\mathcal{E}}^{n+1}(\phi, r) - \bar{\mathcal{E}}^n(\phi, r) = -\Delta t \| \nabla \mu^{n+1/2} \|^2 - \sum_{k=0}^{2} \frac{\epsilon_k}{2\Delta t} \| \Delta^{k/2} (\phi^{n+1} - 2\phi^n + \phi^{n-1}) \|^2,$$

where $\bar{\mathcal{E}}^{j+1}(\phi, r) := \sum_{k=0}^{2} \frac{\epsilon_k}{2\Delta t^2} \| \Delta^{k/2} (\phi^{j+1} - \phi^j) \|^2 + (r^{j+1})^2$ *is the modified free energy at* t^{j+1}.

The above approach was successfully used in Yang (2018b) to approximate the strongly anisotropic Cahn–Hilliard equation proposed in Torabi et al. (2009). We refer to Yang (2018b) for details on the choice of ϵ_k and their effects on the accuracy.

3.4 Coupling with other physical conservation laws

In complex thermodynamic systems, e.g., phase-field models of multiphase complex fluids (Liu and Shen, 2003; Yue et al., 2004b), only the order parameters such as the phase variable (Liu and Shen, 2003) and/or director field (Yue et al., 2004b), are governed by gradient flows which are coupled to other physical conservation laws such as momentum, mass, and energy conservations. The SAV approach can be used to deal with the nonlinear terms in gradient flow part to construct efficient numerical schemes for the coupled thermodynamic systems (see also Zhu et al. (2018) and Kou et al. (2018)).

Consider for example a phase-field model for the mixture of two incompressible, immiscible fluids. Let ϕ be a labelling function to identify the two fluids, i.e.,

$$\phi(x,t) = \begin{cases} 1 & x \in \text{in fluid 1}, \\ -1 & x \in \text{in fluid 2}, \end{cases} \tag{38}$$

with a smooth interfacial layer of thickness η. Consider a mixing free energy

$$E_{mix}(\phi) = \lambda \int_\Omega \left(\frac{1}{2} |\nabla \phi|^2 + F(\phi) \right) d\boldsymbol{x},$$

where $F(\phi) = \frac{1}{4\eta^2}(\phi^2 - 1)^2$ and λ is a mixing coefficient. For the sake of simplicity, we consider the two fluids having the same density $\rho_0 = 1$. Then, the Navier–Stokes Cahn–Hilliard phase-field model for the two-phase incompressible flow is as follows (cf., for instance, Anderson et al., 1998; Liu and Shen, 2003):

$$\frac{\partial \phi}{\partial t} + \nabla \cdot (u\phi) = \nabla \cdot (\gamma \nabla \mu), \tag{39}$$

$$\mu = \frac{\delta E_{mix}}{\delta \phi} = -\lambda \Delta \phi + \lambda F'(\phi); \tag{40}$$

$$\frac{\partial u}{\partial t} + (u \cdot \nabla) u = \nu \Delta u - \nabla p - \phi \nabla \mu; \tag{41}$$

$$\nabla \cdot u = 0; \tag{42}$$

subject to suitable boundary conditions for ϕ, μ, u. In the above, γ is a relaxation coefficients and ν is the viscosity coefficient; the unknown are ϕ, μ, u,

p with u being the velocity and p the pressure. Taking the inner products of (39), (40) and (53) with μ, $\frac{\partial\phi}{\partial t}$ and u, respectively, we obtain the following energy dissipation law:

$$\frac{d}{dt}\int_\Omega \left\{\frac{1}{2}|u|^2+\frac{\lambda}{2}|\nabla\phi|^2+\lambda F(\phi)\right\}d\boldsymbol{x}=-\int_\Omega\{\nu|\nabla u|^2+\gamma|\nabla\mu|^2\}\,d\boldsymbol{x}.$$

To apply the SAV approach, we set $E_1(\phi)=\int_\Omega F(\phi)$, introduce $r(t)=\sqrt{E_1(\phi)+\delta}$ with $\delta>0$, and replace (40) by

$$\begin{aligned}\mu&=-\lambda\Delta\phi+\lambda\frac{r(t)}{\sqrt{E_1(\phi)+\delta}}F'(\phi),\\ \frac{dr}{dt}&=\frac{1}{2\sqrt{E_1(\phi)+\delta}}\int_\Omega F'(\phi)\,\frac{\partial\phi}{\partial t}\,d\boldsymbol{x}.\end{aligned}\tag{43}$$

Then, we can combine the scheme (3.9) in Shen and Yang (2010a) and the SAV approach to construct the following scheme for (39)–(42):

$$\begin{aligned}&\frac{3\phi^{n+1}-4\phi^n+\phi^{n-1}}{2\Delta t}+\hat{u}^{n+1}\cdot\nabla\overline{\phi}^{n+1}=\gamma\Delta\mu^{n+1},\\ &\mu^{n+1}=-\lambda\Delta\phi^{n+1}+\frac{\lambda r^{n+1}}{\sqrt{E_1(\overline{\phi}^{n+1})+\delta}}F'(\overline{\phi}^{n+1}),\\ &\frac{3r^{n+1}-4r^n-r^{n-1}}{2\Delta t}=\int_\Omega\frac{F'(\overline{\phi}^{n+1})}{2\sqrt{E_1(\overline{\phi}^{n+1})+\delta}}\frac{3\phi^{n+1}-4\phi^n+\phi^{n-1}}{2\Delta t}\,dx;\end{aligned}\tag{44}$$

$$\begin{aligned}&\frac{3\tilde{u}^{n+1}-4u^n+u^{n-1}}{2\Delta t}+\bar{u}^{n+1}\cdot\nabla\tilde{u}^{n+1}\\ &-\nu\Delta\tilde{u}^{n+1}+\nabla p^n-\mu^{n+1}\nabla\overline{\phi}^{n+1}=0;\end{aligned}\tag{45}$$

$$\begin{aligned}&\frac{3}{2\Delta t}(u^{n+1}-\tilde{u}^{n+1})+\nabla(p^{n+1}-p^n)=0,\\ &\nabla\cdot u^{n+1}=0;\quad u^{n+1}\cdot\boldsymbol{n}|_{\partial\Omega}=0.\end{aligned}\tag{46}$$

In the above, $\overline{\psi}^{n+1}:=2\psi^n-\psi^{n-1}$ for any sequence $\{\psi^k\}$. As for $\hat{u}^{n+1}$, we can choose $\hat{u}^{n+1}=\tilde{u}^{n+1}$ or $\hat{u}^{n+1}=2u^n-u^{n-1}$.

If $\hat{u}^{n+1}=\tilde{u}^{n+1}$, we can show that the scheme is unconditionally energy stable. More precisely, we have the following result:

Theorem 6. *The scheme (44)–(46) with $\hat{u}^{n+1}=\tilde{u}^{n+1}$ is unconditionally energy stable in the sense that*

$$\mathcal{E}^{n+1}(\phi,u,p)-\mathcal{E}^n(\phi,u,p)\le-\Delta t[\gamma\,\|\,\nabla\mu^{n+1}\|^2+\nu\,\|\,\nabla\tilde{u}^{n+1}\|^2],$$

where $\mathcal{E}^{n+1}(\phi,u,p)$ is the modified total energy at t^{n+1} given by

$$\mathcal{E}^{n+1}(\phi,\mu,u,p)=\frac{\lambda}{4}(\|\nabla\phi^{n+1}\|^2+\|\nabla(2\phi^{n+1}-\phi^n)\|^2)+\frac{\lambda}{2}(|r^{n+1}|^2+|2r^{n+1}-r^n|^2)$$
$$+\frac{1}{4}(\|u^{n+1}\|^2+\|2u^{n+1}-u^n\|^2)+\frac{\Delta t^2}{3}\|\nabla p^{n+1}\|^2.$$

Proof. Taking the inner products of three equations in (44) with $\Delta t\mu^{n+1}$, $\frac{1}{2}(3\phi^{n+1}-4\phi^n+\phi^{n-1})$ and $2\Delta t\lambda r^{n+1}$, respectively, using the identity (11), we obtain

$$\left[\frac{\lambda}{4}(\|\nabla\phi^{n+1}\|^2+\|\nabla(2\phi^{n+1}-\phi^n)\|^2)+\frac{\lambda}{2}(|r^{n+1}|^2+|2r^{n+1}-r^n|^2)\right]$$
$$-\left[\frac{\lambda}{4}(\|\nabla\phi^n\|^2+\|\nabla(2\phi^n-\phi^{n-1})\|^2)+\frac{\lambda}{2}(|r^n|^2+|2r^n-r^{n-1}|^2)\right]+\Delta t(\tilde{u}^{n+1}\nabla\overline{\phi}^{n+1},\mu^{n+1})$$
$$=-\Delta t\gamma\|\mu^{n+1}\|^2-\frac{\lambda}{4}\|\nabla(\phi^{n+1}-2\phi^n+\phi^{n-1})\|^2-\frac{\lambda}{2}|r^{n+1}-2r^n+r^{n-1}|^2. \tag{47}$$

Next, taking the inner product of (45) with Δtu^{n+1}, and using the property

$$(u\cdot\nabla v,v)=0,\ \forall u\in H,\ v\in(H_0^1(\Omega))^d, \tag{48}$$

where $H=\{u\in(L^2(\Omega))^d\colon \nabla\cdot u=0,\ u\cdot n|_{\partial\Omega}=0\}$, we obtain

$$\frac{1}{2}(3\tilde{u}^{n+1}-4u^n+u^{n-1},\tilde{u}^{n+1})+\Delta t(\nabla p^n,\tilde{u}^{n+1})-\Delta t(\mu^{n+1}\nabla\overline{\phi}^{n+1},\tilde{u}^{n+1})=-\mu\Delta t\|\nabla\tilde{u}^{n+1}\|^2. \tag{49}$$

Then, we rearrange (46) as

$$\frac{\sqrt{3}}{2}u^{n+1}+\frac{\Delta t}{\sqrt{3}}\nabla p^{n+1}=\frac{\sqrt{3}}{2}\tilde{u}^{n+1}+\frac{\Delta t}{\sqrt{3}}\nabla p^n, \tag{50}$$

and take the inner products of both side with itself to get

$$\frac{3}{4}\|u^{n+1}\|^2+\frac{\Delta t^2}{3}\|p^{n+1}\|^2=\frac{3}{4}\|\tilde{u}^{n+1}\|^2+\frac{\Delta t^2}{3}\|p^n\|^2+\Delta t(\nabla p^n,\tilde{u}^{n+1}). \tag{51}$$

Since the term $\Delta t(\nabla p^n,\tilde{u}^{n+1})$ in (51) and (49) cancel each other, and the term $\Delta t(\mu^{n+1}\nabla\overline{\phi}^{n+1},\tilde{u}^{n+1})$ in (49) and (47) cancel each other, it remains to deal with the first term in (49), which we write as

$$\frac{1}{2}(3\tilde{u}^{n+1}-4u^n+u^{n-1},\tilde{u}^{n+1})=\frac{3}{2}(\tilde{u}^{n+1}-u^{n+1},\tilde{u}^{n+1})$$
$$+\frac{1}{2}(3u^{n+1}-4u^n+u^{n-1},\tilde{u}^{n+1}-u^{n+1}) \tag{52}$$
$$+\frac{1}{2}(3u^{n+1}-4u^n+u^{n-1},u^{n+1}):=I_1+I_2+I_3.$$

We have $I_1 = \frac{3}{4}(\| \tilde{u}^{n+1}\|^2 - \| u^{n+1}\|^2 + \| \tilde{u}^{n+1} - u^{n+1}\|^2)$, and for I_3 we use (11). On the other hand, by using (46), we derive that $I_2 = 0$. Finally, collect all the results in the above identities, we obtain the desired result. □

Several remarks are in order:

- The pressure-correction step (46) is decoupled from the rest. More precisely, if $\tilde{u}^{n+1}$ is known, one can determine (p^{n+1}, u^{n+1}) from (46) by solving a Poisson equation for $p^{n+1} - p^n$ with a homogeneous Neumann boundary condition.
- If we take $\hat{u}^{n+1} = 2u^n - u^{n-1}$, one can eliminate r^{n+1} from (44) as before, so the scheme is linear, decoupled, second-order, and only requires solving a sequence of elliptic type equations at each time step, but not unconditionally energy stable.
- On the other hand, if we take $\hat{u}^{n+1} = \tilde{u}^{n+1}$, the scheme is unconditionally energy stable, linear and second-order. However, it is weakly coupled between $(\phi^{n+1}, w^{n+1}, \tilde{u}^{n+1})$ by the term $\tilde{u}^{n+1} \cdot \nabla \overline{\phi}^{n+1}$. The weakly coupled linear system is positive definite, and one can use the decoupled scheme with $\hat{u}^{n+1} = 2u^n - u^{n-1}$ as a preconditioner for the coupled scheme with $\hat{u}^{n+1} = \tilde{u}^{n+1}$.

3.5 Dissipative/conservative systems which are not driven by free energy

In a recent work (Lin and Dong (2018)), the authors presented an interesting extension of the SAV approach to the following incompressible Navier–Stokes equations (NSE):

$$\begin{aligned} u_t + (u \cdot \nabla)u &= \nu \Delta u - \nabla p, \\ \nabla \cdot u = 0, \quad u|_{\partial\Omega} &= 0, \end{aligned} \tag{53}$$

which is not a gradient flow but consists of only physical conservation laws and satisfies an energy dissipation law:

$$\frac{1}{2}\frac{d}{dt}\int |u|^2 dx = -\nu \int_\Omega |\nabla u|^2. \tag{54}$$

A usual semi-implicit scheme for (53) is

$$\begin{aligned} \frac{u^{n+1} - u^n}{\Delta t} + (u^n \cdot \nabla)u^n &= \nu \Delta u^{n+1} - \nabla p^{n+1}, \\ \nabla \cdot u^{n+1} = 0, \quad u^{n+1}|_{\partial\Omega} &= 0. \end{aligned} \tag{55}$$

However, it is not unconditionally energy stable.

Let $E(t) = \int_\Omega \frac{1}{2}|u|^2 dx + \delta$ with any $\delta > 0$, and introduce a SAV variable $R(t) = \sqrt{E(t)}$. We can rewrite the NSE (53) as

$$\begin{aligned} u_t + \frac{R(t)}{\sqrt{E(t)}}(u\cdot\nabla)u &= \nu\Delta u - \nabla p, \quad u|_{\partial\Omega} = 0; \\ \nabla\cdot u &= 0; \\ 2R(t)R'(t) = (u_t, u) &= \left(u_t + \frac{R(t)}{\sqrt{E(t)}}(u\cdot\nabla)u, u\right). \end{aligned} \tag{56}$$

In the last equation, we have used the property $((u\cdot\nabla)u, u) = 0$ for all u such that $\nabla\cdot u = 0$ and $u|_{\partial\Omega} = 0$. With $R(0) = \sqrt{E(0)}$, the above system is equivalent to the original NSE (53).

The following semi-implicit SAV scheme based on the above reformulation is proposed in Lin and Dong (2018):

$$\begin{aligned} \frac{u^{n+1}-u^n}{\Delta t} + \frac{R^{n+1}}{\sqrt{E(t^{n+1})}}(u^n\cdot\nabla)u^n &= \nu\Delta u^{n+1} - \nabla p^{n+1}, \\ \nabla\cdot u^{n+1} = 0, \quad u^{n+1}|_{\partial\Omega} &= 0; \\ 2R^{n+1}\frac{R^{n+1}-R^n}{\Delta t} &= \left(\frac{u^{n+1}-u^n}{\Delta t} + \frac{R^{n+1}}{\sqrt{E(t^{n+1})}}(u^n\cdot\nabla)u^n, u^{n+1}\right). \end{aligned} \tag{57}$$

Taking the inner product of the first equation with u^{n+1} and sum up with the third equation, we obtain:

Theorem 7. *The scheme (57) is unconditionally energy stable in the sense that all its solutions satisfy*

$$\frac{1}{\Delta t}(|R^{n+1}|^2 - |R^n|^2 + |R^{n+1}-R^n|^2) + \nu\,\|\nabla u^{n+1}\|^2 = 0.$$

The above result is very surprising since the nonlinear term is treated explicitly.

The above scheme can also be implemented very efficiently. Indeed, denote $S^{n+1} = \frac{R^{n+1}}{\sqrt{E(t^{n+1})}}$ and set

$$u^{n+1} = u_1^{n+1} + S^{n+1}u_2^{n+1},\ p^{n+1} = p_1^{n+1} + S^{n+1}p_2^{n+1}.$$

Plugging the above in (57), we find that (u_i^{n+1}, p_i^{n+1}) $(i = 1, 2)$ can be determined separately from:

$$\begin{aligned} \frac{u_1^{n+1}-u^n}{\Delta t} &= \nu\Delta u_1^{n+1} - \nabla p_1^{n+1}, \quad u_1^{n+1}|_{\partial\Omega} = 0; \\ \nabla\cdot u_1^{n+1} &= 0; \end{aligned} \tag{58}$$

and

$$\frac{u_2^{n+1}}{\Delta t} + (u^n \cdot \nabla)u^n = \nu \Delta u_2^{n+1} - \nabla p_2^{n+1}, \quad u_2^{n+1}|_{\partial\Omega} = 0; \qquad \nabla \cdot u_2^{n+1} = 0. \tag{59}$$

Once (u_i^{n+1}, p_i^{n+1}) $(i = 1,2)$ are known, the last equation in (57) becomes a nonlinear algebraic equation for S^{n+1} which can be solved by a Newton iteration.

Several remarks are in order:

- The cost of solving the nonlinear algebraic equation for S^{n+1} is negligible. The main cost at each time step is to solve (58) and (59). So the computational cost is about twice of that for the usual semi-implicit scheme (55) but it has the advantage of being unconditionally energy stable.
- Existence of a positive solution for S^{n+1} is still elusive. But in practice, this is always true as long as Δt is not "too" large. Since S^{n+1} is designed to be an approximation to 1, the difference $|S^{n+1} - 1|$ provides a "free" estimator for adaptive time stepping: if $|S^{n+1} - 1|$ is not "sufficiently small", then, one needs to reduce Δt.
- Ample numerical results in Lin and Dong (2018) show that the SAV approach is more efficient and robust than the usual semi-implicit schemes.
- This approach is not restricted to the Navier–Stokes equations and can be applied to other nonlinear systems. For example, we can couple this approach with the scheme (44)–(46) to construct new efficient schemes for two-phase phase-field models, we refer to Yang and Dong (2018) for an attempt in this direction.

4 Conclusion

We provided an updated account for the recently proposed SAV approach for complex dissipative/conservative systems. The SAV approach was originally developed for dealing with gradient flows. But as shown in the last section, the idea can be extended to deal with a large class of complex dissipative/conservative systems which are not gradient flows, and still lead to efficient and accurate numerical schemes.

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References

Ainsworth, M., Mao, Z., 2017. Analysis and approximation of a fractional Cahn-Hilliard equation. SIAM J. Numer. Anal. 55 (4), 1689–1718. ISSN 0036-1429.

Allen, S.M., Cahn, J.W., 1979. A microscopic theory for antiphase boundary motion and its application to antiphase domain coarsening. Acta Metall. 27 (6), 1085–1095.

Anderson, D.M., McFadden, G.B., Wheeler, A.A., 1998. Diffuse-interface methods in fluid mechanics. Annu. Rev. Fluid Mech. 30 (1), 139–165.

Cahn, J.W., Hilliard, J.E., 1958. Free energy of a nonuniform system. I. Interfacial free energy. J. Chem. Phys. 28 (2), 258–267.

Cahn, J.W., Hilliard, J.E., 1959. Free energy of a nonuniform system. III. Nucleation in a two-component incompressible fluid. J. Chem. Phys. 31 (3), 688–699.

Cai, W., Jiang, C., Wang, Y., 2018. Structure-preserving algorithms for the two-dimensional sine-Gordon equation with Neumann boundary conditions. arXiv preprint arXiv:1809.02704.

Chen, H., Shen, J., 2019. Optimal error estimates for SAV finite-element schemes for gradient flows. Numer. Math. (submitted for publication).

Cheng, Q., Shen, J., 2018. Multiple scalar auxiliary variable (MSAV) approach and its application to the phase-field vesicle membrane model. SIAM J. Sci. Comput. 40 (6), A3982–A4006.

Cheng, Q., Shen, J., Yang, X., 2019. Highly efficient and accurate numerical schemes for the epitaxial thin film growth models by using the SAV approach. J. Sci. Comput. 78 (3), 1467–1487.

Condette, N., Melcher, C., Süli, E., 2011. Spectral approximation of pattern-forming nonlinear evolution equations with double-well potentials of quadratic growth. Math. Comp. 80 (273), 205–223. ISSN 0025-5718. https://doi.org/10.1090/S0025-5718-10-02365-3.

Doi, M., Edwards, S.F., 1988. The Theory of Polymer Dynamics. vol. 73. Oxford University Press.

Du, Q., Feng, X., 2019. The phase field method for geometric moving interfaces and their numerical approximations. arXiv preprint arXiv:1902.04924.

Du, Q., Nicolaides, R.A., 1991. Numerical analysis of a continuum model of phase transition. SIAM J. Numer. Anal. 28 (5), 1310–1322. ISSN 0036-1429. https://doi.org/10.1137/0728069.

Du, Q., Liu, C., Wang, X., 2004. A phase field approach in the numerical study of the elastic bending energy for vesicle membranes. J. Comput. Phys. 198 (2), 450–468.

Forest, M.G., Wang, Q., Zhou, R., 2004. The flow-phase diagram of Doi-Hess theory for sheared nematic polymers II: finite shear rates. Rheol. Acta 44 (1), 80–93.

Forest, M.G., Wang, Q., Zhou, R., 2004. The weak shear kinetic phase diagram for nematic polymers. Rheol. Acta 43 (1), 17–37.

Giacomelli, L., Otto, F., 2001. Variatonal formulation for the lubrication approximation of the Hele-Shaw flow. Calc. Var. 13 (3), 377–403.

Gomez, H., Hughes, T.J.R., 2011. Provably unconditionally stable, second-order time-accurate, mixed variational methods for phase-field models. J. Comput. Phys. 230 (13), 5310–5327. ISSN 0021-9991. https://doi.org/10.1016/j.jcp.2011.03.033.

Gurtin, M.E., Polignone, D., Vinals, J., 1996. Two-phase binary fluids and immiscible fluids described by an order parameter. Math. Models Methods Appl. Sci. 6 (06), 815–831.

He, Z., Chen, J., Chen, Z., 2018. Efficient linearly and unconditionally energy stable schemes for the phase field model of solid-state dewetting problems. In: International Conference on Computational Science, pp. 102–112.

Kessler, D., Nochetto, R.H., Schmidt, A., 2004. A posteriori error control for the Allen-Cahn problem: circumventing Gronwall's inequality. M2AN Math. Model. Numer. Anal. 38 (1), 129–142. ISSN 0764-583X. https://doi.org/10.1051/m2an:2004006.

Kim, J., 2012. Phase-field models for multi-component fluid flows. Commun. Comput. Phys. 12 (03), 613–661.

Kou, J., Sun, S., Wang, X., 2018. Linearly decoupled energy-stable numerical methods for multicomponent two-phase compressible flow. SIAM J. Numer. Anal. 56 (6), 3219–3248.

Larson, R.G., 1990. Arrested tumbling in shearing flows of liquid crystal polymers. Macromolecules 23 (17), 3983–3992.

Leslie, F.M., 1979. Theory of flow phenomena in liquid crystals. Adv. Liq. Cryst. 4, 1–81.

Li, X., Shen, J., Rui, H., 2019. Energy stability and convergence of SAV block-centered finite difference method for gradient flows. Math. Comp. 88 (319), 2047–2068.

Lin, L., Dong, S., 2018. Numerical approximation of incompressible Navier-Stokes equations based on an auxiliary energy variable. arXiv:1804.10859.

Liu, C., Shen, J., 2003. A phase field model for the mixture of two incompressible fluids and its approximation by a Fourier-spectral method. Physica D 179 (3), 211–228.

Lowengrub, J., Truskinovsky, L., 1998. Quasi-incompressible Cahn-Hilliard fluids and topological transitions. In: Proceedings of the Royal Society of London A: Mathematical, Physical and Engineering Sciences, vol. 454. The Royal Society, pp. 2617–2654.

Otto, F., 1998. Lubrication approximation with prescribed nonzero contact angle. Commun. Partial Differ. Equ. 23 (11–12), 2077–2164.

Rogers, T.M., Desai, R.C., 1989. Numerical study of late-stage coarsening for off-critical quenches in the Cahn-Hilliard equation of phase separation. Phys. Rev. B 39 (16), 11956.

Rudin, L.I., Osher, S., Fatemi, E., 1992. Nonlinear total variation based noise removal algorithms. Physica D 60 (1–4), 259–268.

Shen, J., Xu, J., 2018. Convergence and error analysis for the scalar auxiliary variable (SAV) schemes to gradient flows. SIAM J. Numer. Anal. 56 (5), 2895–2912. ISSN 0036-1429. https://doi.org/10.1137/17M1159968.

Shen, J., Yang, X., 2010. Energy stable schemes for Cahn-Hilliard phase-field model of two phase incompressible flows equations. Chin. Ann. Math. B 31, 743–758.

Shen, J., Yang, X., 2010. Numerical approximations of Allen-Cahn and Cahn-Hilliard equations. Discrete Contin. Dynam. Systems. A 28, 1669–1691.

Shen, J., Tang, T., Yang, J., 2016. On the maximum principle preserving schemes for the generalized Allen-Cahn equation. Comm. Math. Sci. (14), 1517–1534.

Shen, J., Xu, J., Yang, J., 2019. A new class of efficient and robust energy stable schemes for gradient flows. SIAM Rev. (submitted for publication).

Shen, J., Xu, J., Yang, J., 2018. The scalar auxiliary variable (SAV) approach for gradient flows. J. Comput. Phys. 353, 407–416. ISSN 0021-9991. https://doi.org/10.1016/j.jcp.2017.10.021.

Torabi, S., Lowengrub, J., Voigt, A., Wise, S., 2009. A new phase-field model for strongly anisotropic systems. In: Proceedings of the Royal Society of London A: Mathematical, Physical and Engineering Sciences. The Royal Society. pp. rspa–2008.

Yang, X., 2016. Linear, first and second-order, unconditionally energy stable numerical schemes for the phase field model of homopolymer blends. J. Comput. Phys. 327, 294–316.

Yang, X., 2018. Efficient schemes with unconditionally energy stability for the anisotropic Cahn-Hilliard equation using the stabilized-scalar augmented variable (S-SAV) approach. arXiv preprint arXiv:1804.02619.

Yang, X., 2018. Efficient schemes with unconditionally energy stability for the anisotropic Cahn-Hilliard equation using the stabilized-scalar augmented variable (S-SAV) approach. arXiv preprint arXiv:1804.02619.

Yang, Z., Dong, S., 2018. An unconditionally energy-stable scheme based on an implicit auxiliary energy variable for incompressible two-phase flows with different densities involving only precomputable coefficient matrices. arXiv preprint arXiv:1811.07888.

Yu, H., Ji, G., Zhang, P., 2010. A nonhomogeneous kinetic model of liquid crystal polymers and its thermodynamic closure approximation. Commun. Comput. Phys. 7 (2), 383.

Yue, P., Feng, J.J., Liu, C., Shen, J., 2004. A diffuse-interface method for simulating two-phase flows of complex fluids. J. Fluid Mech. 515, 293–317.
Yue, P., Feng, J.J., Liu, C., Shen, J., 2004. A diffuse-interface method for simulating two-phase flows of complex fluids. J. Fluid Mech. 515, 293–317.
Zhao, J., Wang, Q., Yang, X., 2017. Numerical approximations for a phase field dendritic crystal growth model based on the invariant energy quadratization approach. Int. J. Numer. Methods Eng. 110 (3), 279–300.
Zhu, G., Kou, J., Sun, S., Yao, J., Li, A., 2018. Decoupled, energy stable schemes for a phase-field surfactant model. Comput. Phys. Commun. 233, 67–77.
Zhuang, Q., Shen, J., 2019. Efficient SAV approach for imaginary time gradient flows with applications to one- and multi-component Bose-Einstein Condensates. J. Comput. Phys. (submitted for publication).