Supplementary Variable Method for Developing Structure-Preserving Numerical Approximations to Thermodynamically Consistent Partial Differential Equations

Yuezheng Gong[a,c], Qi Hong[b,c], Qi Wang[d]

[a] *College of Science, Nanjing University of Aeronautics and Astronautics, Nanjing 210016, China*
[b] *Beijing Computational Science Research Center, Beijing 100193, China*
[c] *Jiangsu Key Laboratory for Numerical Simulation of Large Scale Complex Systems*
[d] *Department of Mathematics, University of South Carolina, Columbia, SC 29208, USA*

Abstract

We present a new temporal discretization paradigm for developing energy-production-rate preserving numerical approximations to thermodynamically consistent partial differential equation systems, called the supplementary variable method. The central idea behind it is to introduce a supplementary variable to the thermodynamically consistent model to make the over-determined equation system, consisting of the thermodynamically consistent PDE system, the energy definition and the energy dissipation equation, structurally stable. The supplementary variable allows one to retain the consistency between the energy dissipation equation and the PDE system after the temporal discretization. We illustrate the method using a dissipative gradient flow model. Among virtually infinite many possibilities, we present two ways to add the supplementary variable in the gradient flow model to develop energy-dissipation-rate preserving algorithms. Spatial discretizations are carried out using the pseudo-spectral method. We then compare the two new schemes with the energy stable SAV scheme and the fully implicit Crank-Nicolson scheme. The results favor the new schemes in the overall performance. This new numerical paradigm can be applied to any thermodynamically consistent models.

Keywords: Supplementary variable method, thermodynamically consistent models, gradient flows, energy-production-rate preserving schemes, finite difference methods, pseudo-spectral methods.

1. Introduction

Nonequilibrium phenomena require dynamical models derived from laws and principles of nonequilibrium thermodynamics to describe. The laws of thermodynamics, especially, the second law of thermodynamics or the equivalent generalized Onsager principle are fundamental laws/principles for developing such models for nonequilibrium phenomena not far from equilibria [12, 13, 16]. Assuming the thermodynamic variables describing nonequilibrium phenomena of a certain system are denoted as $\Phi \in \mathbf{R}^n$, where n is the number of the variables, and the free energy of the system

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is described by a functional $F[\Phi]$ in isothermal cases (for nonisothermal cases, we use an entropy functional instead). The Onsager linear response theory yields the dynamical equation

$$\mathbf{R} \cdot \dot{\Phi} = -\mathbf{M} \cdot \mu, \quad \mu = \frac{\delta F}{\delta \Phi}, \tag{1.1}$$

where $\mathbf{M}$ and $\mathbf{R}$ are operators, $\frac{\delta F}{\delta \Phi}$ is the variation of F, $\mathbf{M}^{-1}\mathbf{R}$ is known as the friction operator and $\mathbf{R}^{-1}\mathbf{M}$ the mobility operator when they exist. This equation system provides relaxation dynamics for the nonequilibirum state to return to equilibria in dissipative systems or to oscillate in nondissipative systems. For simplicity, we consider the case of $\mathbf{R} = \mathbf{I}$ in this paper so that $\mathbf{M}$ is the mobility operator.

In general, the mobility operator can be decomposed into two parts:

$$\mathbf{M} = \mathbf{M}_a + \mathbf{M}_s, \tag{1.2}$$

where $\mathbf{M}_a$ is the antisymmetric part and $\mathbf{M}_s$ is the symmetric part. The time rate of change of the free energy is given by

$$\frac{\mathrm{d}F}{\mathrm{d}t} = -\int_\Omega \frac{\delta F}{\delta \Phi} \mathbf{M} \frac{\delta F}{\delta \Phi} \mathrm{d}\mathbf{x} = -\int_\Omega \frac{\delta F}{\delta \Phi} \mathbf{M}_s \frac{\delta F}{\delta \Phi} \mathrm{d}\mathbf{x}, \tag{1.3}$$

under proper boundary conditions on Φ. If $\mathbf{M}_a = 0$ and $\mathbf{M}_s \geq 0$, the system is called a dissipative system since $\mathrm{d}F/\mathrm{d}t \leq 0$. While only $\mathbf{M}_s = 0$, the system is a conservative system because $\mathrm{d}F/\mathrm{d}t = 0$. Apparently, (1.3) is an equation deduced from (1.1). It can therefore be viewed as a consistent constraint for (1.1). When approximating equation (1.1) numerically, one would like to preserve energy dissipation property at the discrete level, i.e., to arrive at an approximate equation to (1.3) that is derivable from the approximate equation of (1.1). A numerical algorithm of such a property is called an energy stable algorithm or scheme.

In many thermodynamical models given in the form of (1.1), the total free energy is given by

$$F = \frac{1}{2}(\Phi, \mathcal{L}\Phi) + \big(f(\Phi, \nabla\Phi), 1\big), \tag{1.4}$$

where $(\bullet, \bullet)$ is the inner product in a L^2 space, $\mathcal{L}$ is a linear, self-adjoint, positive definite operator and f or $(f, 1)$ is bounded below for the physically accessible states of Φ. This is also known as the gradient flow model in the literature. In this model, if we view F as one of the thermodynamical variables, (1.1), (1.3), and (1.4) constitute an *over-determined system* of equations with $n + 2$ equations and $n + 1$ unknowns (Φ, F). This system of equations is consistent and solvable should gradient flow model (1.1) is solvable with free energy (1.4) and proper initial and boundary conditions. However, the structural consistency among the equations in the system can be easily broken under small perturbations to the system, leading to a system that is not solvable because of inconsistency among the equations. We label this scenario in the over-determined system of equations as structural unstable.

Traditionally, to retain consistency among the equations in the over-determined system in numerical approximations, one discretizes (1.1) and (1.4), and then try to put together a consistent discretized energy dissipation equation or inequality for (1.3) to arrive at energy stable algorithms. However, there is no guarantee that this approach would be successful. Then, there came about the convex splitting method for the gradient flow with a free energy given as a difference of two convex functions, in which *one implements a mismatched temporal discretization on the two convex*

parts of the free energy, respectively, to achieve energy stability [6]; and the stabilizer approach [15], in which *one modifies the gradient flow equation by adding higher order perturbations.* All these approaches try to put together a consistent, discrete energy dissipation equation following the traditional approach mentioned above within the over-determined partial differential equation system.

Recently, the energy quadratization (EQ) approach coined by Xiaofeng Yang, Jia Zhao and Qi Wang following the work of Ganzales and Tierra on liquid crystal models, provides a systematic approach to derive energy-dissipation-rate preserving schemes for thermodynamically consistent models [11, 17, 19]. In this approach, *one introduces new unknowns (known as auxiliary variables) to reformulate the energy into a quadratic form and in the meantime supplement the system with the same number of dynamical equations for the new auxiliary variables.* This process is known as the EQ reformulation, which effectively embeds the gradient flow model into a higher dimensional phase space with a quadratic free energy while retaining the thermodynamically consistent structure and property (including the energy dissipation property.) The EQ reformulated gradient flow model together with the definition of the quadratic free energy and the energy dissipation equation constitute *a reformulated over-determined, consistent and solvable gradient flow system.* One designs linear, energy stable schemes from the EQ reformulated gradient flow model. Analogously, the SAV method follows the same idea [14].

We illustrate the idea using an example here. We assume f only depends on Φ, but not its spatial derivatives. In this case, one introduces a q variable to transform the free energy into a quadratic form:

$$q = \sqrt{2\left(f + \frac{A}{|\Omega|}\right)}, \quad F = \frac{1}{2}(\Phi, \mathcal{L}\Phi) + \frac{1}{2}\|q\|^2 - A, \tag{1.5}$$

where A is a constant large enough to make q well-defined. Then, one takes the time derivative of the algebraic equation of q to arrive at an equivalent dynamical equation of q. The EQ-reformulated system in a higher dimensional phase space recasts into

$$\begin{cases} \frac{\partial}{\partial t}\Phi = -\mathbf{M}\left(\mathcal{L}\Phi + q\frac{\partial q}{\partial \Phi}\right), \\ \frac{\partial}{\partial t}q = \frac{\partial q}{\partial \Phi} \cdot \frac{\partial \Phi}{\partial t}. \end{cases} \tag{1.6}$$

Denoting $\Psi = (\Phi, \ q)^T$, the above system is rewritten into [10]

$$\frac{\partial}{\partial t}\Psi = -\mathcal{N}\mathcal{B}\Psi, \tag{1.7}$$

where $\mathcal{N} = \mathcal{A}^*\mathbf{M}\mathcal{A}$, $\mathcal{A}^*$ is the adjoint operator of $\mathcal{A}$,

$$\mathcal{A} = \begin{pmatrix} \mathbf{I}_n & \frac{\partial q}{\partial \Phi} \end{pmatrix}_{n,n+1}, \quad \mathcal{B} = \text{diag}(\mathcal{L}, 1)_{n+1,n+1},$$

$\mathcal{B}$ is a linear, self-adjoint, positive definite operator. The energy dissipation rate is given by

$$\frac{\mathrm{d}F}{\mathrm{d}t} = \left(\frac{\delta F}{\delta \Psi}, \frac{\partial \Psi}{\partial t}\right) = -\left(\mathcal{B}\Psi, \mathcal{N}\mathcal{B}\Psi\right) \leq 0. \tag{1.8}$$

Recently, Gong, Zhao and Wang showed that one can devise arbitrarily high order energy stable schemes to solve the over-determined system consisting of (1.5), (1.7) and (1.8) [10, 7, 9, 8]. In

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contrast to the traditional method, the EQ approach guarantees the consistency and solvability in the discretized system due to the reformulated free energy is quadratic whereas the traditional approach may not. Most recently, a class of new methods rooted in the scalar auxiliary variable approach have been devised to ensure linearity as well as energy stability in the numerical schemes developed for gradient flow models [1, 18].

Here, we take look at the issue of developing energy stable numerical approximations from a new perspective. We begin with the over-determined, consistent system of equations consisting of (1.1), (1.3), and (1.4). Now that this system is structurally unstable, it can easily lose the consistency among the equations subject to any small perturbations. How can we make it structurally stable. One way to make it structurally stable is to extend the system by adding supplementary variables to make it well-determined, i.e., the number of unknowns equals to the number of equations. There are virtually unlimited number of ways this can be done. To be consistent with the original problem, we accomplish this using perturbations and require that the well-determined, perturbed system include the original system as a special case. We would like to take a new point of view towards next present a new paradigm to devise energy dissipation rate preserving schemes for the over-determined system consisting of (1.1), (1.3) and (1.4) to retain structural consistency and solvability in the over-determined system. We name it the supplementary variable method (**SVM**). We will show that this includes the newly proposed Lagrange multiplier method based on the SAV approach by Cheng, Liu and Shen as well as the generalized SAV method developed by Yang and Dong lately as special cases [4, 18]. This method originates from the idea on how to enforce structural stability in the over-determined equation system by augmenting it with supplementary variables. Specifically, we perturb the system consisting of (1.1), (1.3) and (1.4) by adding a perturbation:

$$
\begin{cases}
\dot{\Phi} = -\mathbf{M} \cdot \mu, \quad \mu = \frac{\delta F}{\delta \Phi} + \alpha g[\Phi], \\
F = \frac{1}{2}(\Phi, \mathcal{L}\Phi) + \big(f(\Phi, \nabla\Phi), 1\big) + \alpha h(t), \\
\frac{\mathrm{d}F}{\mathrm{d}t} = -\int_\Omega \frac{\delta F}{\delta \Phi} \mathbf{M}_s \frac{\delta F}{\delta \Phi} + \alpha j(t),
\end{cases}
\tag{1.9}
$$

where $\alpha(t)(g[\Phi], h(t), j(t))^T$ is the perturbation, $\alpha(t)$ is a function of time, $g[\Phi]$ is a prescribed functional of Φ, h and j are prescribed functions of t. $\alpha(t)$ is called the supplementary variable. If $\alpha(t) = 0$, this perturbed equation system reduces to the original, consistent and over-determined system. By adding α, however, we lift the dynamical system into a higher dimensional phase space to remove its over-determinedness and to effectively provide it with structural stability. The gained structural stability warrants us to obtain energy-dissipation-rate preserving numerical algorithms for (1.1) under very general conditions so long as we keep the perturbation the same order as the truncation error when we discretize the system. We next detail the implementation of this method in one simple gradient flow case.

2. Supplementary variable method–a new paradigm for developing energy-dissipation-rate preserving numerical algorithms

We explicitly rewrite system (1.1), (1.3) as follows

$$\partial_t \Phi = -\mathbf{M}\big(\mathcal{L}\Phi + f'(\Phi)\big), \tag{2.1}$$

$$\mu = \mathcal{L}\Phi + f'(\Phi), \tag{2.2}$$

$$\frac{\mathrm{d}F}{\mathrm{d}t} = -(\mu, \mathbf{M}\mu). \tag{2.3}$$

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To derive energy-dissipation-rate preserving numerical approximations, we firstly approximate the energy-dissipation-rate equation of the system given in (2.1)-(2.3) as follows

$$\frac{\widetilde{\Phi}^{n+\frac{1}{2}} - \Phi^n}{\tau/2} = -\mathbf{M}\left(\mathcal{L}\widetilde{\Phi}^{n+\frac{1}{2}} + f'(\overline{\Phi}^{n+\frac{1}{2}})\right), \tag{2.4}$$

$$\mu^* = \mathcal{L}\widetilde{\Phi}^{n+\frac{1}{2}} + f'(\widetilde{\Phi}^{n+\frac{1}{2}}), \tag{2.5}$$

$$\frac{\widetilde{F}^{n+1} - F[\Phi^n]}{\tau} = -(\mu^*, \mathbf{M}\mu^*), \tag{2.6}$$

where τ is the time step,

$$\overline{\Phi}^{n+\frac{1}{2}} = \frac{3\Phi^n - \Phi^{n-1}}{2}, \quad F[\Phi^n] = \frac{1}{2}(\Phi^n, \mathcal{L}\Phi^n) + \left(f(\Phi^n), 1\right). \tag{2.7}$$

It follows from (2.4) that

$$\widetilde{\Phi}^{n+\frac{1}{2}} = \left(1 + \frac{\tau}{2}\mathbf{M}\mathcal{L}\right)^{-1}\left(\Phi^n - \frac{\tau}{2}\mathbf{M}f'(\overline{\Phi}^{n+\frac{1}{2}})\right), \quad \widetilde{F}^{n+1} = F[\Phi^n] - \tau(\mu^*, \mathbf{M}\mu^*). \tag{2.8}$$

This is a 2th order approximation to the energy-dissipation-rate equation with a truncation error in the order of $O(\tau^2)$.

Secondly, we modify (2.1) by a time-dependent supplementary variable $\alpha(t)$ together with a user supplied functional $g[\Phi]$:

$$\begin{cases} \partial_t \Phi = -\mathbf{M}\left(\mathcal{L}\Phi + f'(\Phi)\right) + \alpha g[\Phi], \ t \in (t^n, t^{n+1}], \\ F[\Phi(t^{n+1})] = \widetilde{F}^{n+1}, \end{cases} \tag{2.9}$$

where $g[\Phi]$ is a given functional that may depend on Φ and its derivatives. There is a grate deal of flexibility in determining how to modify the gradient flow model with a supplementary variable. It is clearly an open problem for this approach. We simply present two special implementations in this study to illustrate the idea.

- One is

$$g[\Phi] = \mathbf{M}f'(\Phi), \tag{2.10}$$

  which leads to

$$\partial_t \Phi = -\mathbf{M}\left(\mathcal{L}\Phi + (1-\alpha)f'(\Phi)\right). \tag{2.11}$$

  Here, the chemical potential is modified into

$$\mu = \mathcal{L}\Phi + (1-\alpha)f'(\Phi). \tag{2.12}$$

- The other is

$$g[\Phi] = -\mathbf{M}\left(\mathcal{L}\Phi + f'(\Phi)\right), \tag{2.13}$$

  which implies

$$\partial_t \Phi = -(1+\alpha)\mathbf{M}\left(\mathcal{L}\Phi + f'(\Phi)\right). \tag{2.14}$$

  Here, the mobility is modified into $(1+\alpha)\mathbf{M}$.

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We note that a system consisting of (2.3), (2.11) and (2.12) is equivalent to the reformulated model proposed in [4] using what they call the Lagrange multiplier method. The supplementary variable α can also be viewed as a perturbation variable since when $\alpha(t) = 0$, the modified/perturbed system reduces to the original one. *By supplementing the over-determined system with a new variable without introducing an equation, we effectively remove the over-determinedness by making the modified system a well-determined in a higher dimensional phase space!* In addition, the modified model reduces to the original one at $\alpha = 0$. We reiterate that there is a great deal of flexibility to place the supplementary variable in the gradient flow model, which differentiates it from the Lagrange multiplier method and the generalized SAV method.

Thirdly, we apply the implicit-explicit Crank-Nicolson scheme in time to (2.9) to arrive at the following semi-discrete system

$$\begin{cases} \delta_t^+ \Phi^n = -\mathbf{M}\left(\mathcal{L}\Phi^{n+\frac{1}{2}} + f'(\widetilde{\Phi}^{n+\frac{1}{2}}) \right) + \alpha^{n+\frac{1}{2}} g[\widetilde{\Phi}^{n+\frac{1}{2}}], \\ F[\Phi^{n+1}] = \widetilde{F}^{n+1}, \quad \delta_t^+ \Phi^n = \frac{\Phi^{n+1} - \Phi^n}{\tau}, \quad \Phi^{n+\frac{1}{2}} = \frac{\Phi^{n+1} + \Phi^n}{2}, \end{cases} \tag{2.15}$$

where $\widetilde{\Phi}^{n+\frac{1}{2}}$, $\widetilde{F}^{n+1}$ have been obtained from (2.8).

Remark 1. *We apply a special implicit-explicit Crank-Nicolson scheme to the system consisting of* (2.11), (2.12) *and* (2.3) *and obtain the following discrete method*

$$\begin{cases} \delta_t^+ \Phi^n = -\mathbf{M}\mu^{n+\frac{1}{2}}, \\ \mu^{n+\frac{1}{2}} = \mathcal{L}\Phi^{n+\frac{1}{2}} + (1 - \alpha^{n+\frac{1}{2}})f'(\overline{\Phi}^{n+\frac{1}{2}}), \\ \frac{F[\Phi^{n+1}] - F[\Phi^n]}{\tau} = -(\mu^{n+\frac{1}{2}}, \mathbf{M}\mu^{n+\frac{1}{2}}). \end{cases} \tag{2.16}$$

It is not difficult to prove that the scheme (2.16) *is equivalent to the Lagrange multiplier approach proposed in [4].*

Next we discuss how to solve system (2.15) efficiently . Let

$$\widehat{\Phi}^{n+1} = (1 + \frac{\tau}{2}\mathbf{M}\mathcal{L})^{-1}\left((1 - \frac{\tau}{2}\mathbf{M}\mathcal{L})\Phi^n - \tau\mathbf{M}f'(\widetilde{\Phi}^{n+\frac{1}{2}}) \right), \tag{2.17}$$

$$w^n = (1 + \frac{\tau}{2}\mathbf{M}\mathcal{L})^{-1}g[\widetilde{\Phi}^{n+\frac{1}{2}}], \tag{2.18}$$

$$\beta = \tau\alpha^{n+\frac{1}{2}}. \tag{2.19}$$

It follows from the first equation of (2.15) that

$$\Phi^{n+1} = \widehat{\Phi}^{n+1} + \beta w^n. \tag{2.20}$$

Then we plug Φ^{n+1} into the second equation in (2.15) to obtain

$$F[\widehat{\Phi}^{n+1} + \beta w^n] = \widetilde{F}^{n+1}, \tag{2.21}$$

which is an algebraic equation for β. In general, it can have multiple solutions, but one of them must be close to 0 and it approaches to zero as $\tau \to 0$. So, we solve for this solution using an iterative method such as the Newton iteration with 0 as the initial condition, it generally converges to a solution close to 0 when τ is not too large. After obtaining β, we update Φ^{n+1} using (2.20). Following the work of Refs. [2, 3], the existence of solution β is guaranteed under the conditions of the following theorem.

Theorem 2.1. *If $\left(\frac{\delta F}{\delta \Phi}[\Phi^n], g[\Phi^n]\right) \neq 0$, there exists a $\tau^* > 0$ such that (2.21) defines a unique function $\beta = \beta(\tau)$ for all $\tau \in [0, \tau^*]$ and scheme (2.15) with (2.4)-(2.6) is of order $O(\tau^2)$.*

Proof. For τ, β in a neighborhood of $(0,0)$, we define the real function

$$u(\tau, \beta) = F[\widehat{\Phi}^{n+1} + \beta w^n] - \widetilde{F}^{n+1} = F[\widehat{\Phi}^{n+1} + \beta w^n] - F[\Phi^n] + \tau(\mu^*, \mathbf{M}\mu^*), \tag{2.22}$$

where μ^* is calculated in the first step. It follows from (2.5), (2.8), (2.17) and (2.18) that

$$u(0,0) = 0, \quad \frac{\partial u}{\partial \beta}(0,0) = \left(\frac{\delta F}{\delta \Phi}[\Phi^n], g[\Phi^n]\right) \neq 0. \tag{2.23}$$

According to the implicit function theorem, there exists a $\tau^* > 0$ such that equation $u(\tau, \beta) = 0$ defines a unique smooth function $\beta = \beta(\tau)$ satisfying $\beta(0) = 0$ and $u\left(\tau, \beta(\tau)\right) = 0$ for all $\tau \in [0, \tau^*]$.

Since $\widehat{\Phi}^{n+1}$ satisfies the following scheme

$$\frac{\widehat{\Phi}^{n+1} - \Phi^n}{\tau} = -\mathbf{M}\left(\mathcal{L}\frac{\widehat{\Phi}^{n+1} + \Phi^n}{2} + f'(\widetilde{\Phi}^{n+\frac{1}{2}})\right), \tag{2.24}$$

through local truncation error analysis we have

$$\widehat{\Phi}^{n+1} = \Phi(t^{n+1}) + O(\tau^3), \quad F[\widehat{\Phi}^{n+1}] = F[\Phi(t^{n+1})] + O(\tau^3). \tag{2.25}$$

In addition, we expand

$$u(\tau, \beta) = u(\tau, 0) + \beta\frac{\partial u}{\partial \beta}(\tau, 0) + O(\beta^2), \tag{2.26}$$

with

$$\begin{aligned}
u(\tau, 0) &= F[\widehat{\Phi}^{n+1}] - \widetilde{F}^{n+1} = O(\tau^3), \\
\frac{\partial u}{\partial \beta}(\tau, 0) &= \frac{\partial u}{\partial \beta}(0,0) + O(\tau).
\end{aligned} \tag{2.27}$$

Then $\beta = \beta(\tau) = O(\tau^3)$ and the proposed scheme is of order $O(\tau^2)$. $\qquad\square$

Remark 2. *If (2.13) is chosen, i.e. $g[\Phi] = -\mathbf{M}\frac{\delta F}{\delta \Phi}[\Phi]$, then the sufficient condition in Theorem 2.1 reduces to $\left(\frac{\delta F}{\delta \Phi}[\Phi^n], \mathbf{M}\frac{\delta F}{\delta \Phi}[\Phi^n]\right) \neq 0$, which is usually satisfied when the steady state is not reached.*

3. Numerical results

We present a numerical example to demonstrate the practicability, accuracy, as well as energy stability of the proposed schemes. For simplicity, we use periodic boundary conditions for the numerical example below and name the resulting scheme **SVM-I** and **SVM-II** when (2.10) and (2.13) are adopted, respectively.

Example 1 (Cahn-Hilliard model)**.** *We consider the following Cahn-Hilliard phase field model with phase variable ϕ*

$$\partial_t \phi = \lambda \Delta \left(-\varepsilon^2 \Delta \phi + \phi^3 - \phi \right),$$

where the free energy is given by

$$F = \frac{\varepsilon^2}{2} \|\nabla \phi\|^2 + \frac{1}{4}(\phi^2 - 1)^2.$$

First of all, we present the mesh refinement test in time to confirm the order of accuracy of the schemes. We set the computational domain as $\Omega = [0,1]^2$ and the parameter values as $\varepsilon = 10^{-2}$ and $\lambda = 10^{-3}$, respectively. This model is discretized spatially using a Fourier pseudo-spectral method with 256×256 spatial meshes. We use initial condition $\phi = 0.25 \sin(2\pi x) \cos(2\pi y)$ and time steps $\tau = 1.25e - 2 \times \frac{1}{2^{k-1}}$, $k = 1, 2, 3, \cdots$. The errors are calculated as the difference between the solution of the coarse time step and that of the adjacent finer time step. Both the discrete L^2 and L^∞ errors of numerical solution ϕ at $t = 1$ are shown in Figure 1, where we observe that the proposed schemes yield second order convergence rates in time.

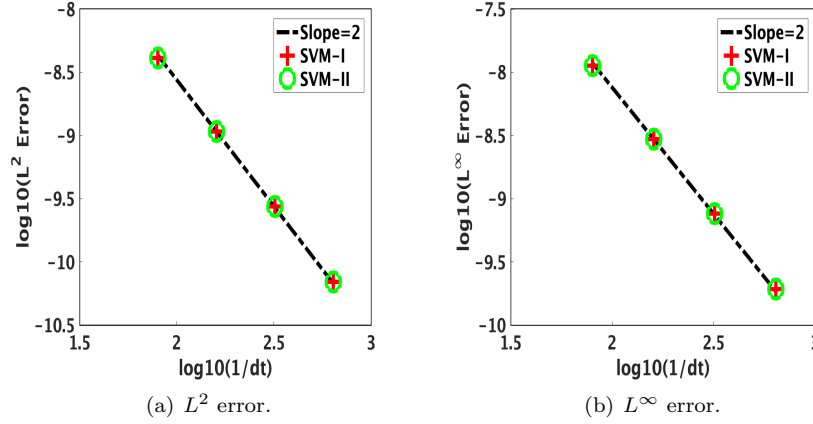(a) L^2 error.　　　　(b) L^∞ error.

Figure 1: Mesh refinement test in time for the two schemes. Here, we fix the number of spatial meshes at $N = 256$. Second order convergence rates are confirmed.

Next, we examine the computational efficiency of the two schemes: **SVM-I** *and* **SVM-II***. We compare the two proposed schemes with the SAV scheme using the Crank-Nicolson method* **SAV-CN** *[14] and the fully implicit Crank-Nicolson scheme* **FICN** *[5]. The result in the total CPU time to solve for the solution using each scheme is summarized in Figure 2. We observe that* **SVM-I** *and* **SVM-II** *for this model are less efficient than scheme* **SAV-CN***, but much more efficient than scheme* **FICN***. The price we pay using the proposed scheme in CPU time is that we have to solve a scalar nonlinear equation at each time step. In contrast,* **SAV** *scheme solves a linear system while* **FICN** *solves a nonlinear system.*
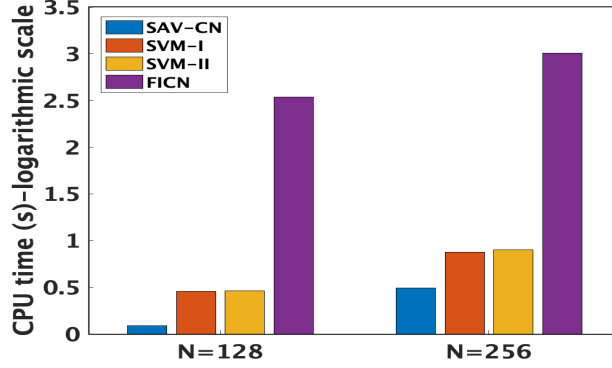
Figure 2: Comparison of CPU time in logarithmic scale using the four different numerical methods with two sets of spatial meshes up to $t = 1$, where the time step is chosen as $\tau = 1.0e - 2$. The charts show that the two proposed schemes performs equally well, more slowly than **SAV-CN**, but much faster than **FICN**.

Finally, we compare **SVM-I**, **SVM-II** and **SAV-CN** in their accuracy in resolving the energy-dissipation-rate. We do it using a spatial discretization on 128^2 meshes in $\Omega = [0,1]^2$. The parameter values are $\lambda = 1$ and $\varepsilon = 1.0e - 2$. We use the following initial condition [8]

$$\phi(x, y, 0) = 0.05 \left(\cos(6\pi x) \cos(8\pi y) + (\cos(8\pi x) \cos(6\pi y))^2 + \cos(2\pi x - 10\pi y) \cos(4\pi x - 2\pi y) \right).$$

The initial profile undergoes a fast coarsening dynamics such that the algorithms must use small time steps in order to capture the correct coarsening dynamics. The simulation results are depicted in Figure 3, where the snapshots of $\phi(x, y, t)$ at $t = 0.1$ are shown using different schemes and time steps. We observe that scheme **SAV-CN** predicts the correct solution at time step $\tau = 1.5625e - 6$ but fails at time step $\tau = 3.125e - 6$. For **SVM-I**, it predicts correct numerical result at time step $\tau = 5.0e - 5$, and **SVM-II** performs even better with time step $\tau = 2.0e - 4$. The errors in the total volume and the energy are plotted in Figure 4. The numerical results show that both schemes conserve the total volume and capture the energy-dissipation-rate correctly using relatively larger time steps compared to the **SAV** scheme. In addition, the supplementary variable $\alpha(t)$ remains close to zero except at a few initial time spots.

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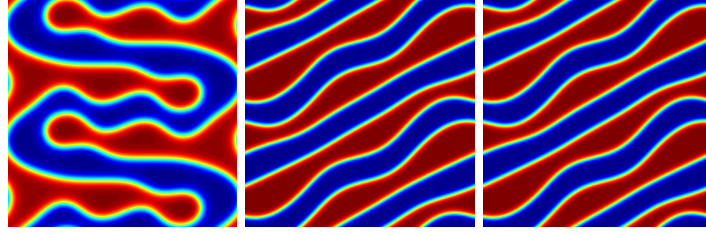
(a) ϕ at $t = 0.1$ using **SAV-CN** with time steps: $\tau = 3.125e - 6$, $\tau = 1.5625e - 6$ and $\tau = 1.0e - 6$ (reference) (from left to right).
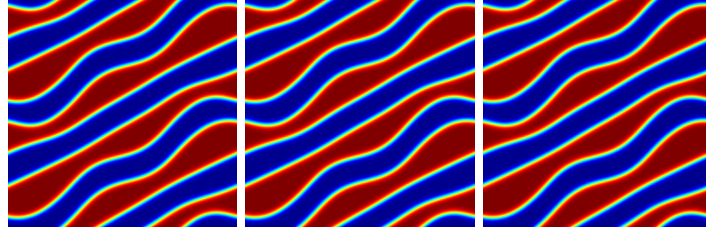
(b) ϕ at $t = 0.1$ using **SVM-I** with time steps: $\tau = 5.0e - 5$, $\tau = 4.0e - 5$ and $\tau = 1.0e - 6$ (reference) (from left to right).
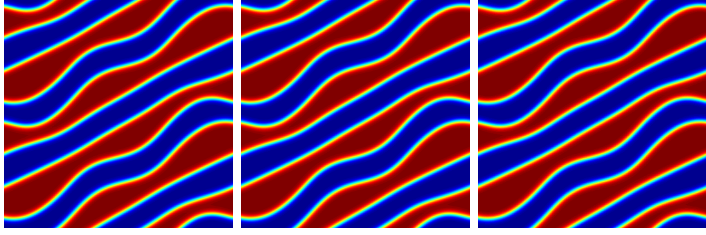
(c) ϕ at $t = 0.1$ using **SVM-II** with time steps: $\tau = 2.0e - 4$, $\tau = 1.5625e - 4$ and $\tau = 1.0e - 6$ (reference) (from left to right).

Figure 3: Comparison of three schemes at different time steps. The first sub-figure in each row indicates the "maximum possible" time step to predict correct dynamics. These snapshots show that both schemes **SVM-I** and **SVM-II** perform better than **SAV-CN** and **SVM-II** performs the best.
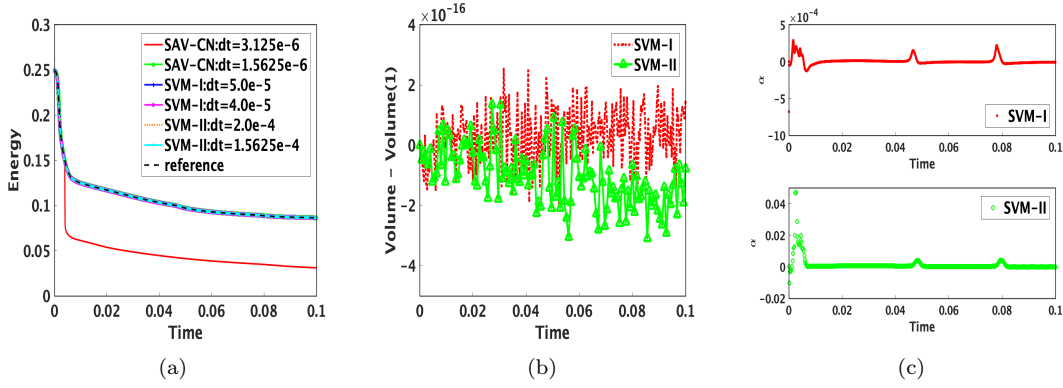
Figure 4: (a)Time evolution of the free energy computed using the three schemes with various time steps. The subfigure shows that **SVM-I** and **SVM-II** can work well with much larger time steps than **SAC-CN** does, while **SVM-II** performs the best. (b) Time evolution of the error in the total volume using **SVM-I** and **SVM-II** with $\tau = 5.0e - 5$ and $\tau = 2.0e - 4$, respectively. The results show that the proposed schemes preserve the total volume very well. (c) The evolution of supplementary variable α. This subfigure indicates α may fluctuate near zero initially, but eventually, settles down close to zero.

4. Conclusion

The numerical results demonstrate the proposed schemes based on the supplementary variable approach can predict fast coarsening dynamics of the Cahn-Hilliard model accurately and outperform **SAV-CN** in solution accuracy and **FICN** in efficiency. Here we simply present two convenient implementations of supplementary variables for developing energy-dissipation-rate preserving schemes. There can be many other ways guided by this paradigm to achieve energy stability, better computational efficiency and accuracy. We expect to see more property preserving numerical algorithms developed for thermodynamically consistent models guided by this paradigm in the future.

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