Efficient and Energy Stable Scheme for an Anisotropic Phase-field Dendritic Crystal Growth Model Using the Scalar Auxiliary Variable (SAV) Approach

Xiaofeng Yang∗
Department of Mathematics, University of South Carolina, Columbia, SC 29208, USA.

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Dedicated to Professor Jie Shen on the Occasion of his 60th Birthday

Abstract. The phase-field dendritic crystal growth model is a highly nonlinear system that couples the anisotropic Allen-Cahn type equation and the heat equation. By combining the recently developed SAV (Scalar Auxiliary Variable) method with the linear stabilization approach, as well as a special decoupling technique, we arrive at a totally decoupled, linear, and unconditionally energy stable scheme for solving the dendritic model. We prove its unconditional energy stability rigorously and present various numerical simulations to demonstrate the stability and accuracy.

AMS subject classifications: 65M12, 65M70, 65Z05
Key words: Phase-field, dendritic, stabilized-SAV method, anisotropy, Allen-Cahn, decoupled.

1 Introduction

The use of the phase-field method for investigating the process of dendritic crystal growth can be attributed to the pioneering modeling work by Halperin, Kobayashi, and Collins et al. in [1–3], and see also the subsequent modeling/simulations in [4–15]. In a typical phase-field dendritic crystal system, an order parameter (called phase-field variable) is usually introduced to define the physical state (liquid or solid) at each point and the total free energy incorporates a specific form of the conformational entropy with anisotropic spatial gradients. The system usually consists of two coupled nonlinear, second-order equations: the Allen-Cahn type equation with a gradient-dependent anisotropic coefficient, and the heat transfer equation.

∗Corresponding author. Email address: xfyang@math.sc.edu (X. Yang)
In this paper, we consider numerical approximations for a phase-field dendritic crystal growth model which was proposed by Karma and Rappel in [12]. It is well known that the main objective of algorithm design for phase-field related models is to construct efficient and easy-to-implement numerical schemes that can verify a discrete energy law. For the particular dendritic model proposed in [12], the associated difficulties to this aim lie on how to discretize three nonlinear terms, including the anisotropic coefficient, the cubic polynomial term, as well as the heat transfer term. Simple explicit treatment for these nonlinear terms will induce large spatial oscillations that may cause the computations easily blow up or loss of accuracy (shown in Figure 2, Figure 4, and Figure 5(b)).

We recall there exist plenty of time discretization methods that had been proved to be effective for solving the phase field models, see [15–38]. However, for this particular model considered in this paper, most of the available schemes are either nonlinear which need some efficient iterative solvers, and/or do not preserve energy stability at all (cf. [7, 39–44] and the references therein). Therefore, in this paper, by combining the recently developed SAV (Scalar Auxiliary Variable) method with the linear stabilization approach, as well as a special decoupling technique, we arrive at a fully-decoupled, stabilized-SAV scheme. The novelty of this scheme is that two linear stabilization terms are added in the SAV scheme, where one is used to remove the oscillations caused by the anisotropic coefficient, and the other is added to the latent heat transfer term in order to realize the decoupling. At each time step, one can only solve an elliptic system for the phase function, and a linear elliptic equation for the temperature. We then prove that the unconditionally energy stability of the scheme and present numerous numerical examples to illustrate its accuracy and stability numerically.

The rest of the paper is organized as follows. In Section 2, we give a brief introduction of the governing PDE system for the phase-field anisotropic dendritic crystal growth model. In Section 3, we develop the scheme for solving the model, and rigorously prove the unconditional energy stability. Various numerical experiments are given in Section 4 to demonstrate the accuracy and efficiency of the proposed numerical scheme. Finally, some concluding remarks are given in Section 5.

## 2 Model equations

We give a brief description of the anisotropic phase-field dendritic crystal growth model proposed in [12]. Let \( \Omega \) be a smooth, open, bounded, connected domain in \( \mathbb{R}^d \) with \( d = 2, 3 \). A scalar phase-field function \( \phi(x,t) \) is introduced to label the liquid and solid phase, where \( \phi = 1 \) for the solid and \( \phi = -1 \) for the fluid. These two regions are connected by a smooth transitional layer with the thickness \( \epsilon \). The total free energy is postulated as follows,

\[
E(\phi, T) = \int_{\Omega} \left( \frac{1}{2} \kappa (\nabla \phi) \nabla \phi \right)^2 + \frac{\lambda}{2 \epsilon K} T^2 + \frac{1}{4 \epsilon^2} F(\phi) \, dx,
\]

(2.1)
in which, $T(x,t)$ is the temperature, $\epsilon$, $\lambda$, and $K$ are all positive parameters, $F(\phi) = (\phi^2 - 1)^2$ is the Ginzburg-Landau double well potential, $\kappa(\nabla \phi)$ is a function describing the anisotropic property that depends on the direction of the outer normal vector $n$ which is the interface normal defined as $n = -\frac{\nabla \phi}{|\nabla \phi|}$. For the 2D system, the anisotropy coefficient $\kappa(\nabla \phi)$ is usually given by

$$\kappa(\nabla \phi) = 1 + \epsilon_4 \cos(m \theta), \quad (2.2)$$

where $m$ is the number of folds of anisotropy, $\epsilon_4$ is the parameter for the anisotropy strength, and $\theta = \arctan(\frac{\phi_y}{\phi_x})$. When $m = 4$ (i.e., fourfold anisotropy), for instance, $\kappa(\nabla \phi)$ can be easily reformulated in terms of the phase field variable $\phi$, namely,

$$\kappa(\nabla \phi) = \begin{cases} (1 - 3\epsilon_4) \left( 1 + \frac{4\epsilon_4}{1 - 3\epsilon_4} \frac{\phi_x^4 + \phi_y^4}{|\nabla \phi|^4} \right) & \text{for 2D}; \quad \text{and} \\ (1 - 3\epsilon_4) \left( 1 + \frac{4\epsilon_4}{1 - 3\epsilon_4} \frac{\phi_x^4 + \phi_y^4 + \phi_z^4}{|\nabla \phi|^4} \right) & \text{for 3D}. \end{cases} \quad (2.3)$$

By adopting the $L^2$-gradient flow relaxation dynamics for the dendritic crystal growth, one obtains the governing dynamical equations via the variational approach, which reads as follows:

$$\tau(\phi) \phi_t = -\frac{\delta E}{\delta \phi} - \frac{\lambda}{\epsilon} \frac{p'(\phi)}{\epsilon} T,$$

$$= \nabla \cdot (\kappa^2(\nabla \phi) \nabla \phi + \kappa(\nabla \phi) |\nabla \phi|^2 H(\phi)) - \frac{f(\phi)}{\epsilon^2} - \frac{\lambda}{\epsilon} p'(\phi) T,$$

$$T_t = D \Delta T + K p'(\phi) \phi_t, \quad (2.4)$$

where, $\tau(\phi) > 0$ is the mobility parameter that is chosen either as a constant [11, 12] or a function of $\phi$ [12], $D$ is the diffusion rate of the temperature, $\frac{\delta E}{\delta \phi}$ is the variational derivative of the total energy with respect to $\phi$,

$$H(\phi) = \frac{\delta \kappa(\nabla \phi)}{\delta \phi}$$

is the variational derivative of $\kappa(\nabla \phi)$ that reads as

$$H(\phi) = \begin{cases} 4\epsilon_4 \frac{4}{|\nabla \phi|^6} \left( \phi_x (\phi_x^2 \phi_y^2 - \phi_y^4), \phi_y (\phi_x^2 \phi_y^2 - \phi_x^4) \right), & \text{for 2D}; \quad \text{and} \\ 4\epsilon_4 \frac{4}{|\nabla \phi|^6} \left( \phi_x (\phi_x^2 \phi_y^2 + \phi_y^2 \phi_z^2 - \phi_x^4 - \phi_y^4), \phi_y (\phi_y^2 \phi_z^2 + \phi_x^2 \phi_y^2 - \phi_x^4 - \phi_y^4), \phi_z (\phi_z^2 \phi_x^2 + \phi_y^2 \phi_z^2 - \phi_x^4 - \phi_y^4) \right), \quad \text{for 3D}. \end{cases} \quad (2.6)$$
The last two terms in (2.4) and (2.5) are two postulated terms which are not derived by the variational derivative of the total free energy. The function $p(\phi)$ accounts for the generation of latent heat and it is a phenomenological functional taking the form preserving the minima of $\phi$ at $\pm 1$ independently of the local value of $T$. For $p(\phi)$, there are two common choices: $p(\phi) = \frac{1}{5}\phi^5 - \frac{2}{3}\phi^3 + \phi$ and $p'(\phi) = (1 - \phi^2)^2$ (cf. [2, 12]); or $p(\phi) = \phi - \frac{1}{3}\phi^3$ and $p'(\phi) = 1 - \phi^2$ (cf. [45]), that imply the heat only transfers through the interface.

Without the loss of generality, one can adopt the periodic boundary condition or the no-flux homogenous Neumann boundary conditions in order to remove all complexities associated with the boundary integrals in this study, i.e.,

\[(i) \text{ all variables are periodic; or (ii) } \frac{\partial \phi}{\partial n} \bigg|_{\partial \Omega} = \frac{\partial T}{\partial n} \bigg|_{\partial \Omega} = 0, \tag{2.7}\]

where $n$ is the outward normal of the computational domain $\Omega$.

The model equations (2.4)-(2.5) follows the dissipative energy law. By taking the $L^2$ inner product of (2.4) with $\phi_t$, and of (2.5) with $\lambda\epsilon K T$, using the integration by parts and combining the obtained two equalities, we obtain

\[
d\frac{d}{dt} E(\phi, T) = -\| \sqrt{\tau(\phi)\phi_t} \|^2 - \frac{\lambda D}{\epsilon K} \| \nabla T \|^2 \leq 0. \tag{2.8}\]

### 3 Numerical schemes

The aim of this section is to construct decoupled, energy stable schemes to solving the system (2.4)-(2.5). It has been shown that spurious solutions may occur if a numerical scheme does not satisfy the discrete energy dissipation law when the spatial grid and time step sizes are not carefully chosen. In addition, with unconditionally energy stable schemes, one can use relatively large time steps, the size of which is dictated only by accuracy considerations, or a suitable adaptive time stepping. The system (2.4)-(2.5) is a coupled nonlinear model. While it is relatively easy to design some fully implicit schemes with the energy stability, it is very difficult to maintain the unconditional energy stability together with the decoupled feature, that can be seen from our recent paper [46] where we have established a linear and stable, but coupled scheme.

To realize the linear and unconditionally energy stable features, we combine the SAV approach developed in [34] with the stabilization technique to treat the nonlinear gradient potential and the double-well potential. To realize the decoupling feature, we introduce an intermediate temperature that is the combination of the temperature at previous time step and an extra semi-explicit stabilizing term that includes the heat transfer term. As a consequence, the nonlinear heat transfer term in the heat equation vanishes since it is already included in the intermediate temperature. Finally, a decoupled, well-posed linear scheme is obtained and it can be proved to be unconditionally energy stable theoretically and numerically.
We define an auxiliary variable as follows:

\[ u = \sqrt{\int_{\Omega} \left( \frac{1}{2} |\nabla \phi| \nabla \phi|^2 + \frac{1}{4\epsilon^2} F(\phi) \right) \, dx} + B, \tag{3.1} \]

where \( B \) is a constant that can ensure the radicand positive (in all numerical examples, we let \( B = 5 \times 10^4 \) which is the same order of \( \frac{1}{\epsilon^2} \)). Thus the total free energy (2.1) can be rewritten as

\[ E(\phi, U, T) = \int_{\Omega} \frac{\lambda}{2\epsilon K} T^2 \, dx + u^2 - B, \tag{3.2} \]

By taking the time derivative of the new variable \( u \), we then reformulate the system (2.4)-(2.5) as the following equivalent PDE system,

\[ \tau(\phi) \phi_t = -Z(\phi)u - \frac{\lambda}{\epsilon} p'(\phi) T, \tag{3.3} \]
\[ u_t = \frac{1}{2} \int_{\Omega} Z(\phi) \phi_t \, dx, \tag{3.4} \]
\[ T_t = D \Delta T + K p'(\phi) \phi_t, \tag{3.5} \]

where

\[ Z(\phi) = \frac{-\nabla \cdot (\kappa^2 \nabla \phi) \nabla \phi + \kappa (\nabla \phi) |\nabla \phi|^2 H(\phi)) + \frac{1}{\epsilon^2} f(\phi)}{\sqrt{\int_{\Omega} \left( \frac{1}{2} |\nabla \phi| \nabla \phi|^2 + \frac{1}{4\epsilon^2} F(\phi) \right) \, dx} + B}. \tag{3.6} \]

The initial conditions are given by

\[ \begin{cases} \phi(t=0) = \phi_0, & T(t=0) = T_0, \\ u(t=0) = \sqrt{\int_{\Omega} \left( \frac{1}{2} |\nabla \phi_0| \nabla \phi_0|^2 + \frac{1}{4\epsilon^2} F(\phi_0) \right) \, dx} + B. \end{cases} \tag{3.7} \]

The boundary conditions are still (2.7) that we alluded before.

Next, we will develop a time marching algorithm for solving the transformed system (3.3)-(3.5). Let \( \delta t > 0 \) be a time step size and set \( t^n = n\delta t \) for \( 0 \leq n \leq N \) with \( t_{\max} = N\delta t \). We denote the \( L^2 \) inner product of any two spatial functions \( \psi_1(x) \) and \( \psi_2(x) \) by \( (\psi_1(x), \psi_2(x)) = \int_{\Omega} \psi_1(x) \psi_2(x) \, dx \), and the \( L^2 \) norm of the function \( \psi(x) \) by \( \| \psi \|^2 = (\psi, \psi) \). Let \( \psi^n \) denotes the numerical approximation to \( \psi(\cdot, t)|_{t=t^n} \) for any function \( \psi \).

### 3.1 First order scheme

We construct a first-order time marching scheme for solving the system (3.3)-(3.5) based on the first-order backward formula, shown as follows.
Assuming $\phi^n, u^n, T^n$ are known, we update $\phi^{n+1}, u^{n+1}, T^{n+1}$ by solving the following scheme.

**Step 1:**

\[
\tau(\phi^n) \frac{\phi^{n+1} - \phi^n}{\delta t} + \frac{S_1}{\epsilon^2} (\phi^{n+1} - \phi^n) - S_2 \Delta (\phi^{n+1} - \phi^n) = -Z^n u^{n+1} - \frac{\lambda}{\epsilon} p'(\phi^n) T^n_*, \tag{3.8}
\]

\[
\frac{T^n_* - T^n}{\delta t} = K p'(\phi^n) \frac{\phi^{n+1} - \phi^n}{\delta t}, \tag{3.9}
\]

\[
u^{n+1} - u^n = \frac{1}{2} \int_{\Omega} Z^n (\phi^{n+1} - \phi^n) dx, \tag{3.10}
\]

where $Z^n = Z(\phi^n)$ and $S_i, i = 1, 2$ are two positive stabilizing parameters. The boundary conditions are either periodic or $\frac{\partial \phi^n}{\partial n} \bigg|_{\partial \Omega} = 0$.

**Step 2:**

\[
\frac{T^{n+1} - T^n_*}{\delta t} - D \Delta T^{n+1} = 0. \tag{3.11}
\]

The boundary conditions are either periodic or $\frac{\partial T^{n+1}}{\partial n} \bigg|_{\partial \Omega} = 0$.

**Remark 3.1.** When $S_1 = S_2 = 0$, the above scheme is the SAV type scheme which had been developed in [34]. Note even though the SAV method is formally unconditionally energy stable, the spatial oscillations (shown in Figure 4) caused by the anisotropic coefficient $\kappa(\nabla \phi)$ can still make the scheme blow up while large time steps are used, which are illustrated in Figure 2 and Figure 5(b).

**Remark 3.2.** We introduce a new, intermediate temperature $T^n_*$ that plays a key role to decouple the computations of the phase variable from the temperature equation. (3.9) can be rewritten as the following form

\[
T^n_* = T^n + \delta t K p'(\phi^n) \frac{\phi^{n+1} - \phi^n}{\delta t}, \tag{3.12}
\]

that implies $T^n_*$ is a first-order approximation to $T^n$. Moreover, from (3.12), the heat transfer term is already included in the intermediate temperature $T^n_*$, hence this term vanishes in the heat equation as a result.

The scheme (3.8)-(3.11) is a totally decoupled, linear scheme by using the intermediate temperature $T^n_*$ and the implicit-explicit discretization for the nonlinear terms. Meanwhile, the intermediate variable $T^{n+1}_*$ and the new variable $U^{n+1}$ will not bring up any extra computational costs. Indeed, (3.8)-(3.10), and (3.11) are respectively (decoupled) linear elliptic equations for $\phi^{n+1}$ and $T^{n+1}$. This is because we can rewrite (3.11) as follows

\[
u^{n+1} = \frac{1}{2} \int_{\Omega} Z^n \phi^{n+1} dx + A_1, \tag{3.13}
\]
where $A_1 = \frac{1}{2} \int_{\Omega} Z^n \phi^n dx$. Then, by substituting (3.13) and (3.12) to (3.8), the system (3.8)-(3.10) can be rewritten as

$$\mathcal{P} (\phi^{n+1}) + \frac{1}{2} Z^n \int_{\Omega} Z^n \phi^{n+1} dx = f, \quad (3.14)$$

where

$$\mathcal{P}(\psi) = \frac{1}{\delta t} \tau(\phi^n) \psi + \frac{S_1}{\epsilon^2} \psi - S_2 \Delta \psi + \frac{\lambda K}{\epsilon} p'(\phi^n) p'(\phi^n) \psi,$$

$$f = \tau(\phi^n) \frac{\phi^n}{\delta t} + \frac{S_1}{\epsilon^2} \phi^n - S_2 \Delta \phi^n - Z^n A_1 - \frac{\lambda}{\epsilon} p'(\phi^n)(T^n - K p'(\phi^n) \phi^n), \quad (3.15)$$

Apparently, one needs to a nonlocal system (3.14) that might bring up very costly computational cost. Indeed in practice, we can implement it through the following procedure to avoid the nonlocal computations. We define a linear operator $\mathcal{P}^{-1}$, such that for any function $\phi \in L^2(\Omega)$, $\psi = \mathcal{P}^{-1}(\phi)$ is the solution of the following linear system

$$\mathcal{P}(\psi) = \phi, \quad (3.16)$$

with the appropriate boundary conditions specified in (3.8)-(3.10).

By applying the operator $\mathcal{P}^{-1}$ to (3.14), we obtain

$$\phi^{n+1} + \frac{1}{2} \mathcal{P}^{-1}(Z^n) \int_{\Omega} Z^n \phi^{n+1} dx = \mathcal{P}^{-1}(f). \quad (3.17)$$

By taking the $L^2$ inner product of (3.17) with $Z^n$, we derive

$$\int_{\Omega} Z^n \phi^{n+1} dx = \frac{\int_{\Omega} Z^n \mathcal{P}^{-1}(f) dx}{1 + \frac{1}{2} \int_{\Omega} Z^n \mathcal{P}^{-1}(Z^n) dx}. \quad (3.18)$$

It is easy to check $\int_{\Omega} Z^n \mathcal{P}^{-1}(Z^n) dx \geq 0$ is non-zero since the operator $\mathcal{P}^{-1}$ is positive definite. Thus the linear system (3.14) is uniquely solvable.

Furthermore, (3.18) actually provides an explicit formulation for the nonlocal term. Therefore, in computations, we first find

$$\psi_1 = \mathcal{P}^{-1}(Z^n), \quad \psi_2 = \mathcal{P}^{-1}(f), \quad (3.19)$$

that implies to solve the following two decoupled linear equations

$$\frac{1}{\delta t} \tau(\phi^n) \psi_1 + \frac{S_1}{\epsilon^2} \psi_1 - S_2 \Delta \psi_1 + \frac{\lambda K}{\epsilon} p'(\phi^n) p'(\phi^n) \psi_1 = Z^n, \quad (3.20)$$

$$\frac{1}{\delta t} \tau(\phi^n) \psi_2 + \frac{S_1}{\epsilon^2} \psi_2 - S_2 \Delta \psi_2 + \frac{\lambda K}{\epsilon} p'(\phi^n) p'(\phi^n) \psi_2 = f, \quad (3.21)$$

with the appropriate boundary conditions. And then, after by applying (3.18) to obtain $\int_{\Omega} Z^n \phi^{n+1} dx$, we can directly solve $\phi^{n+1}$ from (3.17).

Now we prove the scheme (3.8)-(3.11) is unconditionally energy stable as follows.
**Theorem 3.1.** The scheme (3.8)-(3.11) is unconditionally energy stable which satisfies the following discrete energy dissipation law,  

\[
\frac{1}{\delta t} (E^{n+1} - E^n) \leq - \| \tau(\phi^n) \frac{\phi^{n+1} - \phi^n}{\delta t} \|^2 - \frac{\lambda D}{\epsilon K} \| \nabla T^{n+1} \|^2 \leq 0, \quad (3.22)
\]

where  

\[
E^{n+1} = \int_{\Omega} \frac{\lambda}{2\epsilon K} |T^{n+1}|^2 dx + (u^{n+1})^2 - B. \quad (3.23)
\]

**Proof.** By taking the \( L^2 \) inner product of (3.8) with \( (\phi^{n+1} - \phi^n) \), and using the following identity,  

\[
2(a - b)a = a^2 - b^2 + (a - b)^2, \quad (3.24)
\]

we obtain  

\[
\delta t \left\| \sqrt{\tau(\phi^n)} \frac{\phi^{n+1} - \phi^n}{\delta t} \right\|^2 + \frac{S_1}{\epsilon^2} \| \phi^{n+1} - \phi^n \|^2 + S_2 \| \nabla (\phi^{n+1} - \phi^n) \|^2 \leq -u^{n+1}(\mathcal{Z}, \phi^{n+1} - \phi^n) - \frac{\lambda}{\epsilon} (p'(\phi^n)(\phi^{n+1} - \phi^n), T^*_n). \quad (3.25)
\]

By taking the \( L^2 \) inner product of (3.9) with \( \frac{\lambda}{\epsilon K} \delta t T^n \), we obtain  

\[
\frac{\lambda}{2\epsilon K} \left( \| T^n \|^2 - \| T^n \|^2 + \| T^n - T^n \|^2 \right) = \frac{\lambda}{\epsilon} (p'(\phi^n)(\phi^{n+1} - \phi^n), T^*_n). \quad (3.26)
\]

By multiplying (3.10) with \( 2u^{n+1} \), we obtain  

\[
(u^{n+1})^2 - (u^n)^2 + (u^{n+1} - u^n)^2 = u^{n+1} \int_{\Omega} \mathcal{Z}^n(\phi^{n+1} - \phi^n) dx. \quad (3.27)
\]

By taking the \( L^2 \) inner product of (3.11) with \( \frac{\lambda}{\epsilon K} \delta t T^{n+1} \), we obtain  

\[
\frac{\lambda}{2\epsilon K} \left( \| T^{n+1} \|^2 - \| T^{n+1} \|^2 + \| T^{n+1} - T^{n+1} \|^2 \right) = \frac{\lambda D}{\epsilon K} \delta t \| \nabla T^{n+1} \|^2. \quad (3.28)
\]

By combining (3.25), (3.26), (3.27), and (3.28), we obtain  

\[
(u^{n+1})^2 - (u^n)^2 + \frac{\lambda}{2\epsilon K} (\| T^{n+1} \|^2 - \| T^n \|^2) \\
+ \frac{\lambda}{2\epsilon K} (\| T^n - T^n \|^2 + \| T^{n+1} - T^n \|^2) + (u^{n+1} - u^n)^2 \\
+ \frac{S_1}{\epsilon^2} \| \phi^{n+1} - \phi^n \|^2 + S_2 \| \nabla (\phi^{n+1} - \phi^n) \|^2 \\
= -\delta t \left\| \sqrt{\tau(\phi^n)} \frac{\phi^{n+1} - \phi^n}{\delta t} \right\|^2 - \frac{\lambda D}{\epsilon K} \delta t \| \nabla T^{n+1} \|^2. \quad (3.29)
\]

Finally, we obtain the desired result after dropping some positive terms. \( \square \)
3.2 Second order scheme

A formally decoupled, second-order scheme can be constructed similar to the first-order scheme, which is based on the backward differentiation formula (BDF2) that reads as follows.

Assuming \( \phi^n, u^n, T^n \) and \( \phi^{n-1}, u^{n-1}, T^{n-1} \) are known, we update \( \phi^{n+1}, u^{n+1}, T^{n+1} \) by solving the following linear decoupled scheme.

**Step 1:**

\[
\tau(\phi^n) \frac{3\phi^{n+1} - 4\phi^n + \phi^{n-1}}{2\delta t} + \frac{S_1}{\epsilon^2}(\phi^{n+1} - \phi^{n+1, x}) - S_2 \Delta (\phi^{n+1} - \phi^{n+1, x}) = -Z^{n+1, x} u^{n+1} - \lambda \frac{e}{\epsilon} p'(\phi^{n+1, x}) T^n, \quad (3.30)
\]

\[
\frac{3T^n - 4T^n + T^{n-1}}{2\delta t} = k p'(\phi^{n+1, x}) \frac{3\phi^{n+1} - 4\phi^n + \phi^{n-1}}{2\delta t}, \quad (3.31)
\]

\[
3u^{n+1} - 4u^n + u^{n-1} = \frac{1}{2} \int_\Omega Z^{n+1, x} (3\phi^{n+1} - 4\phi^n + \phi^{n-1}) d\Omega, \quad (3.32)
\]

where \( Z^n = Z(\phi^{n+1, x}), \phi^{n+1, x} = 2\phi^n - \phi^{n-1} \), and \( S_i, i = 1, 2 \) are two positive stabilizing parameters.

**Step 2:**

\[
\frac{3T^{n+1} - 3T^n}{2\delta t} - D\Delta T^{n+1} = 0. \quad (3.33)
\]

Where the boundary conditions and the implementation procedure are the same as the first-order scheme (3.8)-(3.11). However, while it appears possible to prove the energy stability for the second-order scheme, the process will be so technically complicated that we shall not pursue it in this paper.

4 Numerical simulations

In this section, we present various numerical examples to validate the proposed schemes and demonstrate their accuracy, energy stability, and efficiency numerically.

4.1 Accuracy test

We first implement a numerical example with fourfold anisotropy (2.3) in 2D space \( \Omega = [0,h_1] \times [0,h_2] \) to test the convergence rates of the proposed first-order scheme (3.8)-(3.11), denoted by SSAV; and the second-order scheme (3.30)-(3.33), denoted by SSAV-2nd. For comparisons, we also compute the convergence rates by using the non-stabilized version of scheme, i.e., scheme (3.8)-(3.11) but with \( S_1 = S_2 = 0 \), denoted by SAV.
We assume the following two functions
\[
\phi(x,y,t) = \sin(x)\cos(y)\cos(t), \quad T(x,y,t) = \cos(x)\sin(y)\cos(t)
\]  
(4.1)
to be the exact solutions, and impose some suitable force fields such that the given solutions can satisfy the system (2.4)-(2.5). The model parameters are set as follows,
\[
h_1 = h_2 = 2\pi, \quad \tau(\phi) = \tau_0, \quad \epsilon = 0.06, \quad \epsilon_4 = 0.05, \quad D = \lambda = K = 1, \quad S_1 = S_2 = 4.
\]  
(4.2)
Figure 3: The $L^2$ numerical errors for the phase variable $\phi$ and temperature $T$ at $t = 0.2$ with the mobility parameter $\tau_0 = \frac{1}{4}$, that are computed using the second-order scheme SSAV-2nd and various temporal resolutions with the exact solutions given by (4.1).

We discretize the space using $N_x = N_y = 129$ Fourier modes for $x$ and $y$ directions so that the errors from the spatial discretization are negligible compared to the temporal discretization errors.

In Figures 1 and 2, by using the the first-order scheme SSAV and its non-stabilized version SAV scheme, we plot the $L^2$ errors of the phase and temperature variables between the numerical solution and the exact solution at $t = 0.2$ with different time step sizes by varying the parameter $\tau_0$ decreasingly. Some observed features are listed as follows.

- In Figure 1, we set $\tau_0 = \frac{1}{4}$ and plot the errors computed by using the two first-order schemes, SSAV and SAV. We observe these schemes not only present the good convergence rate that almost perfectly matches the first-order accuracy for the time step but also good approximations to the exact solution, regardless of whether they are stabilized or not.

Figure 4: The profile of $\gamma(n_0)$ with $\epsilon_4 = 0.25$ and the initial condition (4.3). The two subfigures are from the different view angle.
Figure 5: (a) The 2D dynamical evolution of the phase variable $\phi$ by using the initial condition (4.3) and the time step $\delta t = 1e^{-2}$ where snapshots of the numerical approximation are taken at $t = 0, 2, 4, 6, 8$. (b)-(c) Time evolution of the free energy functional (2.1) when using three combinations of linear stabilizers where (I) $S_1 = S_2 = 0$; (II) $S_1 = 4, S_2 = 0$; and (III) $S_1 = 4, S_2 = 4$.

- In Figure 2, we set $\tau_0 = \frac{1}{\epsilon}$ and plot the errors computed by using the schemes SSAV and SAV. We observe that the non-stabilized scheme SAV totally loses the accuracy for all tested time steps. On the contrary, the scheme SSAV is stable for all tested time steps and perform good approximations and the first-order accuracy all along. Therefore, through these numerical tests, we conclude that (i) if the mobility parameter $\tau_0$ is large, all schemes can solve the model well; (ii) if the mobility parameter $\tau_0$ is small, the stabilized scheme SSAV overwhelmingly defeats its non-stabilized version SAV from the stability and/or accuracy.

Finally, in Figure 3, we set $\tau_0 = \frac{1}{\epsilon}$ and plot the errors computed by using the second-order scheme SSAV-2nd. We observe the second-order scheme presents perfect convergence rate and good approximations to the exact solution.

4.2 Evolution of a circle

In this subsection, we consider the evolution of a circle driven by the fourfold anisotropy. We set the mobility parameter $\tau_0 = 1$, the anisotropic strength parameter $\epsilon_4 = 0.25$, and still use other model parameters from the previous example. The initial conditions...
The dynamical evolutions of the dendritic crystal growth process with fourfold anisotropy where $K=0.5$ and default parameters of (4.5), computed by using the scheme SAV and the time step $\delta t = 1e^{-2}$. Snapshots of the numerical approximation are taken at $t=0$, 40, 60, 80, and 120.

Figure 6: The dynamical evolutions of the dendritic crystal growth process with fourfold anisotropy where $K=0.5$ and default parameters of (4.5), computed by using the scheme SAV and the time step $\delta t = 1e^{-2}$. Snapshots of the numerical approximation are taken at $t=0$, 40, 60, 80, and 120.

4.3 2D dendrite crystal growth

In this subsection, we investigate the dynamics on how the anisotropic coefficient affects the shape of the dendritic crystal. We initially deposit a single small crystal nucleus in center of the computed domain and observe how it grows heterogeneously. This is a benchmark simulation that had been extensively studied in [2, 12, 14, 15].
The dynamical evolutions of the dendritic crystal growth process with fourfold anisotropy where $K = 0.6$ and default parameters of (4.5), computed by the using the scheme SSAV and the time step $\delta t = 1e^{-2}$. Snapshots of the numerical approximation are taken at $t = 0, 40, 60, 80,$ and $120$.

The initial condition reads as

\[
\begin{align*}
\phi(x,y,t=0) &= \tanh \left( \frac{r_0 - \sqrt{(x-x_0)^2 + (y-y_0)^2}}{\epsilon_0} \right); \\
T(x,y,t=0) &= \begin{cases} 
0, & \phi > 0; \\
T_0, & \text{otherwise},
\end{cases}
\end{align*}
\]

(4.4)

where $(x_0,y_0,r_0,\epsilon_0,T_0) = (\pi,\pi,0.02,0.072,-0.55)$, and the model parameters read as fol-
Figure 9: The dynamical evolutions of the dendritic crystal growth process with fourfold anisotropy where $K = 0.8$ and default parameters of (4.5), computed by the using scheme SSAV and the time step $\delta t = 1e^{-2}$. Snapshots of the numerical approximation are taken at $t = 0, 40, 60, 80,$ and $120$.

We discretize the space using $N_x = N_y = 513$ Fourier modes.

4.3.1 Fourfold anisotropy

We first investigate the fourfold anisotropy case by varying the parameter $K$ and fixing all other parameters from (4.5). We use the first-order scheme SSAV, and the time step $\delta t$ is set to be $0.001$ for better accuracy. In Figure 6(a), we show snapshots of the phase variable at various times with $K = 0.5$. We observe that the tiny nucleus grows up with time and finally evolves to an anisotropic shape with missing orientations at four corners due to the anisotropic effect. In Figure 6(b), snapshots of the temperature variable $T$ are presented. The interfacial contour of the temperature actually agrees well with the phase-field interface since the latent heat transfers only through the interface.

We then increase the parameter $K$ to $0.6$, $0.7$, and $0.8$ in Figure 7, Figure 8, and Figure 9, respectively. When $K = 0.6$, in Figure 7, we observe that the tiny nucleus finally grows into a star-shape with four fat branches. When $K = 0.7$ and $0.8$, star-shapes with much sharper tips and thinner branches are formed. To get more detailed evolution of the dendrites, in Fig 10(a), we summarize the contour of the interface $\{ \phi = 0 \}$ every 20 time units from the initial moment for the above four cases. It can be seen that the shape of the dendrites is significantly influenced by the parameter $K$. All these numerical results demonstrate similar features to those obtained in [2, 8, 12, 15]. In Figure 10(b) and (c), for the above four cases, we summarize the evolutions of the logarithm of the total free energy which
Figure 10: (a) The summary of the contour of the interface \( \{ \phi = 0 \} \) every 20 time units from the initial moment for the four different parameter \( K \), where, (a) \( K = 0.5 \), (b) \( K = 0.6 \), (c) \( K = 0.7 \), and (d) \( K = 0.8 \). (b) Time evolutions of the logarithm of the free energy functional. (c) The size of the dendritic crystals changing with time, where the crystal size is measured by an equivalent radius of a circle with the same area.

Figure 11: (a) The summary of the contour of the interface \( \{ \phi = 0 \} \) every 20 time units from the initial moment for the four anisotropic strengths \( \epsilon_4 \) and \( K = 0.8 \), where, (a) \( \epsilon_4 = 0.01 \), (b) \( \epsilon_4 = 0.03 \), (c) \( \epsilon_4 = 0.05 \), and (d) \( \epsilon_4 = 0.07 \). (b) Time evolutions of the logarithm of the free energy functional. (c) The size of the dendritic crystals changing with time, where the crystal size is measured by an equivalent radius of a circle with the same area.
monotonically decays and the radius of the crystal that is measured by an equivalent radius of a circle with the same area. We observe that the decaying speed of the total energy and growing speed of the area become slower when the parameter K is larger.

We further investigate the effects of the anisotropic lengths \( \epsilon_4 \) by fixing \( K = 0.8 \) and all other parameters from (4.5). In Figure 11, we summarize the contour of the interface \( \{ \phi = 0 \} \) every 20 time units from the initial moment for four cases of \( \epsilon_4 = 0.01, \epsilon_4 = 0.03, \epsilon_4 = 0.05, \) and \( \epsilon_4 = 0.07 \), respectively. We observe that the thickness of formed branches are affected by the magnitude of \( \epsilon_4 \), and larger value of it can bring more slender pattern of branches.

We finally show the two developed schemes, the first-order SSAV scheme (3.8)-(3.11),
Figure 14: The dynamical evolutions of the dendritic crystal growth process with sixfold anisotropy where $K = 0.65$ and default parameters of (4.5), computed by the scheme SSAV-2nd and the time step $\delta t = 1e^{-2}$. Snapshots of the numerical approximation are taken at $t = 20, 40, 60, 120, \text{ and } 160$.

(a) The profiles of the phase-field variable $\phi$.

(b) The profiles of the temperature variable $T$.

Figure 15: The dynamical evolutions of the dendritic crystal growth process with sixfold anisotropy where $K = 0.65$ and default parameters of (4.5), computed by the scheme SSAV-2nd and the time step $\delta t = 1e^{-2}$. Snapshots of the numerical approximation are taken at $t = 20, 40, 60, 120, \text{ and } 160$.

(a) The profiles of the phase-field variable $\phi$.

(b) The profiles of the temperature variable $T$.

and the second-order SSAV-2nd (3.30)-(3.33), are unconditionally energy stable numerically. In Figure 12, we plot the evolution curves of the total free energy (2.1) computed by six different time step sizes until $t = 10$ for $\epsilon_4 = 0.05$ and $K = 0.5$. For all tested time steps, the obtained energy curves show the monotonic decays that confirm these two algorithms are unconditionally stable. We also observe that, for the first-order scheme SSAV, when $\delta t \leq 0.00125$, the energy curves coincide very well. But when $\delta t > 0.00125$, the energy curves deviate viewable away from others. This means the adopted time step size for the first-order scheme SSAV should not be larger than 0.00125, in order to get reasonably good accuracy (we set $\delta t = 0.001$ in the computations). For second-order scheme
Figure 16: The dynamical evolutions of the dendritic crystal growth process with sixfold anisotropy where $K=0.75$ and default parameters of (4.5), computed by using the scheme SSAV-2nd and the time step $\delta t = 1e^{-2}$. Snapshots of the numerical approximation are taken at $t=20, 40, 60, 120,$ and $160$.

(a) $K=0.6$.  
(b) $K=0.65$.  
(c) $K=0.7$.  
(d) $K=0.75$.

Figure 17: (a) The summary of the contour of the interface $\{\phi=0\}$ every 20 time units from the initial moment for the sixfold anisotropy by using the four different parameter $K$, where, (a) $K=0.6$, (b) $K=0.65$, (c) $K=0.7$, and (d) $K=0.75$.  (b) Time evolutions of the logarithm of the free energy functional.  (c) The size of the dendritic crystals changing with time, where the crystal size is measured by an equivalent radius of a circle with the same area.
4.3.2 Sixfold anisotropy

In this subsection, we consider the sixfold anisotropy by setting $m = 6$ in (2.2). To compare with the fourfold case, we vary the parameter $K$ with the same initial condition (4.4) and order parameters from (4.5). We use the second-order scheme SSAV-2nd, and the time step $\delta t$ is set to be 0.01 for better accuracy.

We set the latent heat parameter $K$ to be 0.6, 0.7, 0.75, and 0.8 in Figure 13–16, respectively. In Figure 13 with $K = 0.6$, the circular nucleus initially grows into the regular hexagon shape, and then it becomes a snowflake shape, but with few subtle microstructures. When $K = 0.65$, in Figure 14, the obtained snowflake pattern is filled with numerous subtle microstructures which are formed due to the anisotropy in the heat transfer process. When we further increase the parameter $K$ in Figure 15 and Figure 16 with $K = 0.7$ and $K = 0.75$, respectively, we observe the less subtle microstructures and sub-branches. These simulations are qualitatively consistent with [2] where a slightly different model was used. To get more detailed evolution of the dendrites, in Figure 17(a), we summarize the contour of the interface $\{ \phi = 0 \}$ every 20 time units from the initial moment for the above four cases, and present the evolutions of the logarithm of the total free energy and the radius of the crystal in Figure 17(b) and (c), respectively.

Finally, in Figure 18, three tiny nuclei are randomly deposited initially in the computed domain with the sixfold anisotropy and $K = 0.75$. We observe that three dendrites are finally formed but with plenty of squeezed branches during the formation process. In the last subfigure of each figure, we show the corresponding temperature field $T$. 
4.4 Spinodal decomposition

In this example, we study the phase separation dynamics that is called spinodal decomposition using the developed second-order scheme SSAV-2nd. By considering a homogeneous binary mixture, the spontaneous growth of the concentration fluctuations can lead the system from the homogeneous to the two-phase state.

We set the initial condition as the randomly perturbed concentration field as follows,

$$\phi(x,y,t=0) = 0.2 + 0.001 \text{rand}(x,y), \quad T(x,y,t=0) = 0.55,$$

(4.6)

where the \text{rand}(x,y) is the random number in \([-1,1]\) that follows the normal distribution. We set the time step \(\delta t = 0.001\) for better accuracy, and discretize the space using \(N_x = N_y = 257\) Fourier modes. The model parameters are set as follows,

$$h_1 = h_2 = 2\pi, \tau(\phi) = 1, \epsilon = 0.03, \epsilon_4 = 0.25, D = 1, \lambda = 800, K = 0.7, S_1 = S_2 = 4.$$ (4.7)

In Figure 19, Figure 20, Figure 21, and Figure 22, we set \(m = 0, 3, 4,\) and \(5,\) respectively, and present the profiles of the phase field variable \(\phi.\) From the shapes of each case, we conclude that the number of sides of the obtained polygons is determined by \(m\) exclusively. In Figure 23, we present the evolution of the total free energy functional (2.1) for these cases together.

5 Concluding remarks

In this paper, we have developed two totally decoupled, linear, and unconditionally energy stable schemes for solving the anisotropic dendritic phase-field model. The schemes are developed by combining the stabilized-SAV approach and a novel decoupling technique. We add two linear stabilization terms that can suppress high-frequency
oscillations caused by the anisotropic coefficient efficiently, and also introduce an intermediate temperature that help to realize the total decoupling. Compared to the existed schemes for the anisotropic model, the proposed decoupled schemes (i) conquer the inconvenience from nonlinearities by linearizing the nonlinear terms in a new way, (ii) possess advantages of easy implementations and lower computational cost, (iii) are provably and/or numerically unconditionally energy stable, and thus (iv) allow for large time steps in computations. We further numerically verify the accuracy in time and present numerous numerical results for some benchmark numerical simulations.

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