Energy and entropy preserving numerical approximations of thermodynamically consistent crystal growth models

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\textbf{A B S T R A C T}

We present a numerical scheme that preserves the total energy and the entropy production rate, termed the energy and entropy production rate preserving scheme, for a general class of thermodynamically consistent phase field models for dendritic crystal growth derived from the first and second law of thermodynamics. The scheme is second order in time, linear and energy and entropy production rate preserving for any time steps. The scheme is first discretized in time aided by the energy quadratization (EQ) method and then in space using compact finite difference methods. The linear system resulting from the scheme is shown to be uniquely solvable at both the semi-discrete and the fully discrete level. Mesh refinement tests are performed to show the second-order time convergence rate in the scheme. Several numerical examples of dendritic crystal growth are provided to demonstrate the accuracy and efficiency of the scheme. The effects of various model parameters on growth patterns of the crystal are further investigated in details with the numerical solver. The approach to developing the energy and entropy production rate-preserving numerical scheme proposed in this study is so general that it can be applied to a wide range of thermodynamically consistent models not limited to phase field models.

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1. Introduction

Crystal growth is the result of phase changes between at least two distinct phases, one of which is a solid phase. Sharp interface methods were first employed to study the evolution of phase boundaries historically. Recently, phase field or diffuse interface models have been introduced to model crystal growth in some material systems with a remarkable success due to their ease of use in resolving topological transitions. Some phase field models are regularizations of certain sharp-interface models, which converge to the sharp-interface limits as the thickness of the diffuse interface tends to zero [20], while others are developed for multiphase materials from the beginning [1].

A crystal dendrite is a crystal that develops with a typical multi-branching tree-like form. The word “dendrite” came from the Greek word “dendron”, meaning “tree”. Dendritic crystallization usually forms natural fractal microstructure that is commonly observable in nature such as snowflakes or frost patterns on a window. Microstructures formed during solidifica-
tion (freezing) of a molten material play an enormous role in forming the properties of the final solid material. Specifically, during the solidification of an alloy, micro-segregation patterns formed during dendritic solidification of an alloy are of substantial interests to material processing communities.

To understand the process of dendritic crystal growth, researchers have proposed many theoretical models, along with numerical simulations based on these models [13,28,2,27,23,32,17,20,18,36,16,15] to study transport of heat and solute in the vicinity of the dendrite tip and the factors that control the stability of the shape of the dendrite tip, and to determine the tip radius and initial secondary spacing. In a pioneering work [13], a diffuse interface approach was first applied to the solidification problem accounting for the Gibbs–Thomson equation at the solid-liquid interface for solidification problems. Subsequently, the phase field dendritic crystal growth model has been improved quite a bit in the last two decades. In [28,36,16,20], based on the time-dependent Ginzburg–Landau mesoscopic model, the authors developed various phase field models that exhibit great versatility to study dynamics of atomic-scale dendritic crystal growth dependent on temperature and isotropic/anisotropic diffusive time scales. The essential idea of the phase field dendritic growth model is that an order parameter (phase field variable) is employed to define the physical state (liquid or solid) of the system at each point, and a free energy functional is devised by incorporating a specific form of the conformational entropy with anisotropic spatial gradients. Unfortunately, many of these models are not thermodynamically consistent, mainly due to the coupled equation for the temperature. In these models, only when the temperature is fixed, an energy dissipation law can be established [42]. Apparently, these models satisfy neither of the first and the second law of thermodynamics and are therefore named thermodynamically inconsistent.

In a seminal work of Wang et al. [35], a thermodynamically-consistent phase field model for solidification is derived. The proposed model is shown to preserve the total energy and guarantee the property of positive entropy production. This model has since been used to model and simulate crystal growth and solidification processes. However, with only one work [11] in the literature, there has not been adequate accompanying numerical analysis to explore the thermodynamically consistent structure in the model nor to address the preservation of the positive entropy production rate so far. Over the years, many numerical strategies have been developed to design structure-preserving schemes for gradient flow problems, in which the energy dissipation rate or the dissipation property is preserved. These include the convex splitting approach [6,25,34,33,4], stabilizing approach [31], energy quadratization approach [41,40,42,43,3,10], SAV approach [30] and some other classes of structure-preserving discretization [24–26,7,8,37,12].

In this paper, we develop numerical approximations for the thermodynamically consistent phase field model of dendritic crystal growth, aiming at preserving the thermodynamically consistent properties of the model at the discrete level. In particular, we propose an energy and entropy production rate preserving scheme (which preserves the total internal energy and the entropy-production-rate simultaneously), using the newly developed energy quadratization (EQ) approach. Our proposed scheme has several desired physical and numerical properties: 1) it is linear, such that only a linear algebraic system needs to be solved at each time step; 2) the linear system is uniquely solvable at each time step; 3) the proposed scheme preserves the thermodynamical structure of the continuum model at the discrete level, in particular, it preserves the total internal energy and entropy production rate for the phase field dendritic growth model in both the semi-discrete system in time and the fully discrete system in both time and space.

The paper is organized as follows. In §2, we give a systematical derivation of the thermodynamically consistent phase field dendritic crystal growth model. In §3, we formulate it to an equivalent system via the EQ approach and show it is thermodynamically consistent as well. Then, we propose the numerical scheme and prove that it preserves the positive entropy production rate and its solvability in the semi-discrete case. In §4, we present the numerical convergence test result and various numerical simulations of dendritic crystal growth in 2D space to demonstrate the accuracy and usefulness of the new schemes. Finally, some concluding remarks are given in Section 5.

2. Thermodynamically consistent phase-field models for dendritic crystal growth

2.1. Derivation using the Onsager principle

We revisit briefly the derivation of the thermodynamically consistent phase field model for dendritic crystal growth given in [5] and discuss the approximation of the internal energy as a function of temperature. For the two-phase material system, we use a phase-field model to describe the dendritic crystal growth due to phase transition from the liquid phase into the solid phase. We introduce a phase variable \( \phi(x,t) \) to differentiate the solid phase from the liquid phase in the binary material system. We stipulate that

\[
\phi = \begin{cases} 
1, & \text{liquid phase}, \\
0, & \text{solid phase}.
\end{cases}
\] (2.1)

We denote \( e \) the bulk internal energy and \( s \) the bulk entropy. At any nonzero absolute temperature \( T \) and fixed \( \phi \), \( \frac{\partial e}{\partial T} |_{\phi = T} \neq 0 \). Then we assume that there exists a one-to-one correspondence between the bulk internal energy \( e \) and bulk part of the entropy \( s \) at any given value of \( \phi \). When there is no heat source in the system, the first law of thermodynamics (energy conservation) dictates that

\[
\frac{\partial e}{\partial t} + \nabla \cdot \mathbf{q} = 0,
\] (2.2)
where \( q \) is the flux of the internal energy. For a given material volume \( \Omega \), we assume the entropy of the system is given by the functional

\[
S(e, \phi, \nabla \phi) = \int_\Omega [s(e, \phi) + s_1(\nabla \phi)] dx,
\]

where \( s = s(e, \phi) \) is the bulk entropy, \( s_1(\nabla \phi) \) is the conformational entropy. The rate of entropy production in the fixed material volume \( \Omega \) is given by

\[
\frac{dS}{dt} = \int_\Omega [\frac{\partial s}{\partial e} e_t + \frac{\partial s}{\partial \phi} \phi_t + \frac{\partial s_1}{\partial \nabla \phi} \nabla \phi_t] dx,
\]

\[
= \int_\Omega [\nabla \cdot \delta S + q] dx + \int_\partial \Omega \n \cdot (\frac{\partial s_1}{\partial \nabla \phi} \phi_t - \frac{\partial s}{\partial e} q) da
\]

(2.4)

(2.5)

where \( n \) is the unit external normal of the boundary \( \partial \Omega \). By the second law of thermodynamics, the entropy production rate in the bulk should be positive, which leads to the positive entropy production rate

\[
\dot{S}_{\text{gen}} = \frac{dS}{dt} = \int_\Omega \n \cdot q + \int_{\partial \Omega} \n \cdot (\frac{\partial s_1}{\partial \nabla \phi} \phi_t - \frac{\partial s}{\partial e} q) da \geq 0.
\]

(2.6)

We note that \( \dot{S}_{\text{gen}} \) is a function of time and \( \Omega \). We adopt this boundary condition in this study. We note however that other boundary conditions may be applicable when there are nontrivial boundary fluxes, which we will not pursue here.

One set of boundary conditions can be chosen to annihilate the boundary contributions to the entropy production rate is listed below

\[
\n \cdot \frac{\partial s_1}{\partial \nabla \phi} = 0, \quad \n \cdot q = 0.
\]

(2.7)

The entropy flux cross the boundary is given by

\[
B_S = \n \cdot \frac{\partial s}{\partial e} e_t - \frac{\partial s}{\partial \phi} \phi_t.
\]

(2.8)

The above boundary conditions annihilate the flux so that there is no entropy fluxes crossing the boundary.

We assume a linear response relation between the generalized flux and force, and apply the Onsager reciprocal relation to arrive at a constitutive equation:

\[
\left( \begin{array}{c} \phi_t \\ q_t \end{array} \right) = M \cdot \left( \begin{array}{c} \frac{\delta S}{\delta e} e_t \\ \frac{\delta S}{\delta \phi} \phi_t \end{array} \right)
\]

(2.9)

where \( M \) is the mobility matrix which is symmetric mandated by the Onsager reciprocal relation [22]. Combining it with the internal energy equation, the governing system of equations for the nonisothermal two-phase material system is given by the following

\[
\left( \begin{array}{c} \phi_t \\ e_t \end{array} \right) = \left( \begin{array}{cc} 1 & 0 \\ 0 & -\nabla \end{array} \right) \cdot M \cdot \left( \begin{array}{c} \frac{\delta S}{\delta e} e_t \\ \frac{\delta S}{\delta \phi} \phi_t \end{array} \right)
\]

(2.10)

The entropy production rate can be rewritten into

\[
\frac{dS}{dt} = \int_{\Omega} (\frac{\delta S}{\delta e} e_t + \nabla \cdot \frac{\delta S}{\delta \phi} \phi_t) dx = \int_{\Omega} \left( \frac{\delta S}{\delta e} e_t + \nabla \cdot (\frac{\delta S}{\delta \phi} \phi_t) \right) d\Omega
\]

(2.11)

The non-negativeness of the entropy production rate implies \( M \geq 0 \). Notice that \( de = T ds + \frac{\partial e}{\partial \phi} d\phi \). So,

\[
\frac{\delta S}{\delta \phi} | e = \frac{\delta S}{\delta \phi} | e + \nabla \cdot (\frac{\delta S}{\delta \phi} \phi_t) = \frac{\delta S}{\delta \phi} | e - \nabla \cdot (\frac{\delta S}{\delta \phi} \phi_t),
\]

(2.12)

This gives a general formulation of the phase field model to describe dynamics of two-phase materials systems under nonisothermal conditions, including the phase transition. To complete the model, we need to specify the form of the entropy functional as well as the mobility matrix. We next present a general model and then focus on two special cases in internal energy approximations.
2.2. A general model for dendritic growth of crystals

We consider a diagonal mobility coefficient matrix \( \mathbf{M} \) in a special form for an anisotropic dendritic growth of crystals and the conformational entropy

\[
\mathbf{M} = \begin{pmatrix}
\frac{1}{\tau} & 0 & 0 \\
0 & D_x & 0 \\
0 & 0 & D_y
\end{pmatrix}, \quad s_1 = -\frac{\epsilon^2}{2} |\kappa \nabla \phi|^2.
\] (2.13)

where \( \epsilon \) is a model parameter, \( D_x = D_y T^2 \), \( D_y > 0 \) is the heat conductivity, \( \tau = \tau(\phi(\theta)) > 0 \) is the mobility coefficient chosen either as a constant by some papers or as a function of the angle \( \theta \) defined as \( \tan(\theta(\theta)) = \frac{\partial \phi}{\partial \theta} \) in 2D [20]. By assuming the conformational entropy coefficient \( \kappa = \kappa(\theta(\phi(\theta))) \) depends on the direction of the outer normal vector \( \mathbf{n} \) at the interface \( \mathbf{n} \sim -\nabla \phi \), the anisotropy is effectively introduced into the system. In 2D, the anisotropy of conformational entropy is usually given by

\[
\kappa = 1 + \epsilon_4 \cos(m(\theta - \theta_0)),
\] (2.14)

where \( m \) is the number of folds in the spatial anisotropy, \( \epsilon_4 \) is a parameter for the strength of anisotropy and \( \theta_0 \) is a constant rotation angle. One can easily derive when \( m = 4 \), the fourfold symmetric anisotropy coefficient is given by the following: in 2D [15,16,21,42]

\[
\kappa = (1 - 3\epsilon_4)(1 + \frac{4\epsilon_4}{1 - 3\epsilon_4} \frac{\phi_4}{|\nabla \phi|^4}),
\] (2.15)

and in 3D [18,42]

\[
\kappa = (1 - 3\epsilon_4)(1 + \frac{4\epsilon_4}{1 - 3\epsilon_4} \frac{\phi_4 + \phi_6}{|\nabla \phi|^4}).
\] (2.16)

In this case, the governing equation for the material system is given by

\[
\begin{align*}
\tau \phi_t &= -\frac{\partial}{\partial x}(\frac{\partial \phi}{\partial x}) + \epsilon^2 \nabla \cdot (\kappa |\nabla \phi|^2 \frac{\partial \phi}{\partial x} + \kappa^2 \nabla \phi), \\
\epsilon_t &= \nabla \cdot (D_u \nabla T),
\end{align*}
\] (2.17)

where \( \kappa' = \frac{\partial}{\partial x}(\frac{\partial \phi}{\partial x}) = (\frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2}) = \frac{1}{|\nabla \phi|^2} (-\phi_y, \phi_x). \) This dynamical system guarantees a positive entropy production.

2.3. Internal energy for two phases

In thermodynamics, the measurable quantities are temperature \( T \) and phase variable \( \phi \). We would like to express the energy balance equation in the measurable quantities \( (T, \phi) \) instead of \( (\epsilon, \phi) \). In general, the bulk internal energy is a function of \( T \) and \( \phi \). As a customary practice, we need to prescribe the internal energy in order to have a closed system for \( (T, \phi) \). Once the internal energy is given, the calculation of entropy follows. In order to do it, we need to consider the bulk Helmholtz free energy density[35,11]

\[
f(\phi, T) = e - TS
\] (2.18)

from thermodynamics. We note that

\[
\frac{\partial f}{\partial \phi} |_T = \frac{\partial e}{\partial \phi} |_T, \quad \frac{\partial T}{\partial \phi} |_T = -\frac{\epsilon}{T^2}.
\] (2.19)

It follows from the second equation

\[
f(\phi, T) = T[-\int_{TM}^{T} \left( \frac{e(\xi, \phi)}{\xi^2} \xi + F(\phi) \right) d\xi],
\] (2.20)

where \( TM \) is a specific temperature and \( F(\phi) \) is a function of \( \phi \) that needs to be determined by additional conditions. The bulk entropy is now calculated by \( s = -\frac{f}{T} \), where both \( e \) and \( f \) are functions of \( (T, \phi) \). So, the bulk entropy is a function of \( (T, \phi) \).

Next, we assume the initial energy density is approximated by an interpolated internal energy from the liquid phase to the solid phase as follows:

\[
e(T, \phi) = e_s(T) + p(\phi)L(T) = e_L(T) + (p(\phi) - 1)L(T),
\] (2.21)
where \( e_s(T) \) and \( e_L(T) \) are the classical internal energy density of the solid and the liquid phase, respectively, and \( L(T) = e_L(T) - e_s(T) \) measures the difference, \( p(\phi) \) is an interpolation function that satisfies \( p(0) = 0 \) and \( p(1) = 1 \). We assume that the internal energy in the liquid phase is higher than that in the solid phase, i.e., \( L(T) > 0 \) and denote \( L_0 = L(T_M) \) as the latent heat of fusion (the heat released during solidification). Then, the Helmholtz free energy (2.20) is given by

\[
f(\phi, T) = T[-\int_{T_M}^T \frac{\epsilon(\xi)}{\xi} \, d\xi - (p(\phi) - 1) Q(T) + F(\phi)],
\]

(2.22)

where \( Q(T) = \int_{T_M}^T \frac{\epsilon(\xi)}{\xi} \, d\xi \) is monotonically increasing with respect to \( T \) and \( Q(T_M) = 0 \). It follows that

\[
\frac{\partial s}{\partial \phi} |_{\phi=0} = -\frac{1}{T} \frac{\partial e}{\partial \phi} |_{\phi=0} = \frac{1}{T} \frac{\partial f}{\partial \phi} |_{\phi=0} = Q(T)p'(\phi) - F'(\phi).
\]

(2.23)

For the Helmholtz free energy density \( f \), we require it to have minima with respect to \( \phi \) at \( \phi = 0, 1 \) for all \( T \) in order for it to be able to describe the two stable phases, liquid and solid phase, and \( f \) should be continuous with respect to \( T \) at \( T_M \). The sufficient conditions that satisfy the requirements are

\[
f(0, T_M) = f(1, T_M), \quad \frac{\partial f}{\partial \phi} |_{\phi=0} = 0, \quad \frac{\partial^2 f}{\partial \phi^2} |_{\phi=0} > 0.
\]

(2.24)

This states that the free energy density function is double-well for any \( T > 0 \). These conditions imply that

\[
F(0) = F(1), \quad [F'(\phi) - p'(\phi) Q(T)]|_{\phi=0} = 0, \quad [F''(\phi) - p''(\phi) Q(T)]|_{\phi=0} > 0.
\]

(2.25a, 2.25b, 2.25c)

One choice of \( F \) which satisfies the above conditions is \( F(\phi) = \frac{1}{4} \phi^{2m'}(1 - \phi)^{2m'} \) with \( m' \geq 1 \). With this choice of \( F \), we can choose \( p \) as follows:

\[
p(\phi) = \frac{\int_0^\phi \phi^n(1 - \phi)^m d\phi}{\int_0^1 \phi^n(1 - \phi)^m d\phi}, \quad n \geq 2.
\]

(2.26)

which satisfies required normalization that \( p(0) = 0 \), \( p(1) = 1 \) as well as the conditions in (2.25b) and (2.25c) independent of \( Q(T) \) because \( p'(\phi) = p''(\phi) = 0 \) at \( \phi = 0, 1 \). We remark that in order for the free energy to be bounded below, we need to have \( 2m' \geq n \). In practice, this may not be necessary however. In this study, we adopt the case of \( m' = 1, n = 2 \) in the following.

\[
F(\phi) = \frac{1}{4} \phi^2(1 - \phi)^2, \quad p(\phi) = 30(\frac{\phi^2}{2} - \frac{1}{2} \phi^4 + \frac{1}{2} \phi^3).
\]

(2.27)

2.4. Approximation of the internal energy

We expand the internal energy in the liquid phase near \( T_M \) and propose \( L(T) \) as a quadratic function.

\[
e_L(T) = e_L(T_M) + C_L(T - T_M), \quad L(T) = L_0 + L_1(T - T_M) + L_2(T - T_M)^2,
\]

(2.28)

where \( C_L \) is the specific heat of the liquid phase, \( L_0, L_1, L_2 \) are constants. It follows that

\[
Q(T) = (L_0 - L_1 T_M + L_2 T_M^2)(\frac{1}{T_M} - \frac{1}{T}) + (L_1 - 2L_2 T_M)(\ln T - \ln T_M) + L_2(T - T_M). \quad (2.29)
\]

The internal energy is given by

\[
e = e_L(T_M) + C_L(T - T_M) + (p(\phi) - 1)(L_0 + L_1(T - T_M) + L_2(T - T_M)^2).
\]

(2.30)

The bulk entropy of the system is given by

\[
s(e, \phi) = \frac{e}{\xi} + \int_{T_M}^T \frac{\epsilon(\xi)}{\xi} \, d\xi + (p(\phi) - 1) Q(T) - F(\phi)
\]

\[
= (p(\phi) - 1)(\frac{L_0}{T_M} + L_2(T - T_M)) + ((p(\phi) - 1)(L_1 - 2L_2 T_M) + C_L)(\ln T - \ln T_M)
\]

\[
+ \frac{\epsilon(T_M)}{4eT_M} - \frac{1}{4e}(1 - \phi)^2.
\]

(2.31)

where \( e, e_L(T), \ Q(T), \ p(\phi), \ F(\phi) \) are given by (2.30), (2.28), (2.29), (2.27), respectively.
The specific form of the governing system of equations (2.17) is given by
\[
\begin{align*}
\tau \phi_t &= \left[ (L_0 - L_1T_M + L_2T_M^2)T_M - \frac{1}{T_M} \right] + (L_1 - 2L_2T_M)(\ln T - \ln T_M) \\
&\quad + L_2(T - T_M) p'(\phi) - F'(\phi) + \epsilon^2 \nabla \cdot (\kappa \nabla \phi)^2 \frac{\partial \kappa}{\partial \phi} + \kappa^2 \nabla \phi), \\
\left[ C_{1\lambda} + (p(\phi) - 1)(L_1 + 2L_2(T - T_M)) \right] T_t + p'(\phi) \left[ L_0 + L_1(T - T_M) \right] + L_2(T - T_M)^2 \phi_t &= \nabla \cdot (D_u \nabla T).
\end{align*}
\]
(2.32)

Remark 2.1. Particularly, if we set \( L_0 = L_2T_M^2, L_1 = 2L_2T_M \), then the system reduces to
\[
\begin{align*}
\tau \phi_t &= L_2(T - T_M) p'(\phi) - F'(\phi) + \epsilon^2 \nabla \cdot (\kappa |\nabla \phi|^2 \frac{\partial \kappa}{\partial \phi} + \kappa^2 \nabla \phi), \\
\left[ C_{1\lambda} + 2L_2(p(\phi) - 1)T \right] T_t + L_2T^2 p'(\phi) \phi_t &= \nabla \cdot (D_u \nabla T).
\end{align*}
\]
(2.33)

This equation system is very close to the one used for studying dendritic crystal growth in [21] in its mathematical structure. But, that model does not respect the positive entropy production and there exist some quantitative differences in two coupling terms. Normally, the equation system is applied to the case where \( T \geq T_M \).

3. Entropy-production rate preserving schemes

The thermodynamically consistent dendritic crystal growth model presented above warrants positive entropy production during the phase transition process. We follow the energy quadratization (EQ) approach proposed recently to develop numerical approximations to the model to preserve this important physical property [14,39,38,42]. The scheme so developed will be called the entropy production rate preserving scheme.

We denote the inner product \((\cdot, \cdot)\) and the \(L^2\) norm \(\| \cdot \|\) for functions as follows:
\[
(f, g) = \int_{\Omega} fg dx, \quad \|f\| = \left( \int_{\Omega} f^2 dx \right)^{1/2}, \quad \forall f, g \in L^2(\Omega).
\]
(3.1)

3.1. Model reformulation using EQ

Given that \( S(\epsilon, \phi, \nabla \phi) = \int_{\Omega} \hat{s}(\phi, \nabla \phi, \epsilon) dx \), the phase field model is given by
\[
\begin{align*}
\partial_t \phi &= \lambda \frac{\delta S}{\delta \phi}, \quad \lambda = \frac{1}{2}, \\
\partial_t \epsilon &= -\nabla \cdot (D_\epsilon \nabla \frac{\delta S}{\delta \epsilon} |\phi|).
\end{align*}
\]
(3.2)

We introduce new variables to transform the entropy functional into a quadratic form. Specifically, we set
\[
\begin{align*}
U &= \sqrt{\varepsilon^2 (k^2 - k_0)} |\nabla \phi|^2 + 2B, \\
\hat{s} &= s - \frac{\varepsilon^2 k_0}{2} |\nabla \phi|^2 - \frac{C_0}{2} |\phi|^2 - C_1 \epsilon^2 - \frac{1}{2} |\nabla \epsilon|^2 + A, \\
q(\phi, \epsilon) &= \sqrt{2 \left( -s - \frac{C_0}{2} |\phi|^2 - C_1 \epsilon^2 + A \right)}.
\end{align*}
\]
(3.3)

such that the entropy density is expressed as follows
\[
\hat{s} = -\frac{\varepsilon^2 k_0}{2} |\nabla \phi|^2 - \frac{C_0}{2} |\phi|^2 - C_1 \epsilon^2 - \frac{1}{2} |\nabla \epsilon|^2 + A + B,
\]
(3.4)

where \( C_0, C_1 \) are two positive constants and \( A, B \geq 0 \) are two positive constants large enough to ensure that \( q \) and \( U \) are real. We reformulate the model into the following extended system
\[
\begin{align*}
\tau \partial_t \phi &= \varepsilon^2 k_0 \Delta \phi + \nabla \cdot \left[ U \mathbf{H} \right] - C_0 \phi - qg, \\
\partial_t \epsilon &= \nabla \cdot \left[ D_\epsilon \nabla \left( C_1 \epsilon + qh \right) \right], \quad D_\epsilon = D_u T^2, \\
\partial_t U &= \mathbf{H} \cdot \nabla \partial_t \phi, \\
\partial_t q &= g \partial_t \phi + h \partial_t \epsilon.
\end{align*}
\]
(3.5)

where
Theorem 3.2. Conditions, method

with periodic boundary conditions and proper initial conditions \( \phi|_{t=0}, e|_{t=0} \) as well as

\[
q(\phi, e)|_{t=0} = \sqrt{2\left(-\frac{C_0}{2} \phi^2 - \frac{C_1}{2} \phi^2 + A\right)} , \quad U|_{t=0} = \sqrt{\epsilon^2 (\kappa^2 - k_0) \frac{\nabla \phi|^{2} + 2B}{\nabla \phi|}} \bigg|_{t=0} .
\]

In this formulation, \( T \) is a function of \( (\phi, e) \) obtained from the quadratic expression of \( e \). It’s solved using the continuation method analytically once \( e \) is solved numerically. Throughout this paper, the results are only used for periodic boundary conditions, while the validity of physical boundary conditions (2.7) or combinations of physical and periodic boundary conditions will be presented in the further work.

3.2. Time discretization

We discretize the reformulated system using a modified Crank–Nicholson method in time to arrive at a second order semi-discrete algorithm in time.

**Scheme 3.1.** First of all, assign the initial conditions of \( \phi^0, e^0, U^0, q^0 \). After obtaining the values of \( \phi^{n-1}, e^{n-1}, U^{n-1}, q^{n-1} \) and \( \phi^n, e^n, U^n, q^n \), we calculate \( \phi^{n+1}, e^{n+1}, U^{n+1}, q^{n+1} \) via the following scheme

\[
\tau^{n+1} \delta_t \phi^n = \epsilon^2 k_0 \Delta \phi^{n+\frac{1}{2}} + \nabla \left[ U^{n+\frac{1}{2}} \phi^{n+\frac{1}{2}} \right] - C_0 \phi^{n+\frac{1}{2}} - q^{n+\frac{1}{2}} \frac{\phi^n + \frac{1}{2} \phi^{n+1}}{2} .
\]

\[
\delta_t e^n = \nabla \cdot \left[ D_e e^n + \frac{1}{2} \nabla \left( C_1 e^{n+\frac{1}{2}} + q^{n+\frac{1}{2}} \frac{\phi^n + \frac{1}{2} \phi^{n+1}}{2} \right) \right] ,
\]

\[
\delta_t U^n = \frac{1}{\tau^{n+\frac{1}{2}}} \nabla \delta_t \phi^n ,
\]

\[
\delta_t q^n = \frac{1}{\tau^{n+\frac{1}{2}}} \delta_t \phi^n + \frac{1}{\tau^{n+\frac{1}{2}}} \delta_t e^n ,
\]

where \( (\bullet)^{n+1/2} = \frac{1}{2} (\bullet^{n+1} + \bullet^n) \) and \( (\bullet)^{(n+1)/2} = \frac{1}{2} (3(\bullet)^n - (\bullet)^{n-1}) \).

We note that this is a linear scheme. A fully nonlinear scheme can also be obtained by not using extrapolations, which will not be pursued in this study. Scheme 3.1 in the new variables form a hybrid partial differential equation (PDE) with spatial derivatives and algebraic system subject to periodic boundary conditions.

**Theorem 3.1.** Scheme 3.1 preserves the positive entropy production rate, i.e.,

\[
S^{n+1} - S^n = \Delta t \int_{\Omega} \left[ \frac{1}{\tau^{n+\frac{1}{2}}} \left( \epsilon^2 k_0 \Delta \phi^{n+\frac{1}{2}} + \nabla \cdot \left( U^{n+\frac{1}{2}} \phi^{n+\frac{1}{2}} \right) - C_0 \phi^{n+\frac{1}{2}} - q^{n+\frac{1}{2}} \frac{\phi^n + \frac{1}{2} \phi^{n+1}}{2} \right)^2 + D_e e^{n+\frac{1}{2}} \left( \nabla \left( C_1 e^{n+\frac{1}{2}} + q^{n+\frac{1}{2}} \frac{\phi^n + \frac{1}{2} \phi^{n+1}}{2} \right) \right) \right] dx \geq 0,
\]

where the entropy expression is given as

\[
S^n(\phi^n, \phi^n, U^n, q^n) = - \int_{\Omega} \left[ \frac{\epsilon^2 k_0}{2} \nabla \phi^n |^2 + \frac{1}{2} |U^n|^2 + \frac{1}{2} |q^n|^2 + C_2 \frac{\phi^n}{2} (\phi^n) \right] dx + (A + B)|\Omega|.
\]
Proof. For simplicity, we denote
\[
\begin{align*}
\frac{\Delta S^{n+\frac{1}{2}}}{\Delta t} &= \varepsilon^2 k_0 \Delta \phi^{n+\frac{1}{2}} + \nabla \cdot \left( U^{n+\frac{1}{2}} \mathbf{H}^{n+\frac{1}{2}} \right) - C_0 \phi^{n+\frac{1}{2}} - q^{n+\frac{1}{2}} g^{n+\frac{1}{2}} \approx \frac{1}{\Delta t}, \\
\frac{\Delta S^{n+\frac{1}{2}}}{\Delta t} &= -C_1 e^{n+\frac{1}{2}} - q^{n+\frac{1}{2}} h^{n+\frac{1}{2}}.
\end{align*}
\]
(3.11)

On one hand, taking inner products of the first two equations in (3.8) with \( \Delta t \frac{\Delta S^{n+\frac{1}{2}}}{\Delta t} \), \( \Delta t \frac{\Delta S^{n+\frac{1}{2}}}{\Delta t} \) respectively and using integration by parts, we have
\[
\begin{align*}
\int \nabla \cdot \left( \frac{\Delta S^{n+\frac{1}{2}}}{\Delta t} \right) = \int \nabla \cdot \left( \frac{\Delta S^{n+\frac{1}{2}}}{\Delta t} \right) + \int \nabla \cdot \left( \frac{\Delta S^{n+\frac{1}{2}}}{\Delta t} \right)
\end{align*}
\]
(3.12)

Combining the two equations in (3.12) and (3.13), we arrive at the desired result. □

We name the scheme that respects the positive entropy production rate as energy stable. The theorem simply states that the new scheme is unconditionally energy stable.

Next, we examine the solvability of the linear system resulting from the linear unconditionally energy stable scheme. We introduce a new variable \( \mu^{n+1/2} = C_1 e^{n+\frac{1}{2}} + q^{n+\frac{1}{2}} h^{n+\frac{1}{2}} \) to rewrite the scheme as follows
\[
\begin{align*}
\tau^{n+\frac{1}{2}} \delta t \phi^n &= \varepsilon^2 k_0 \Delta \phi^{n+\frac{1}{2}} + \nabla \cdot \left[ U^{n+\frac{1}{2}} \mathbf{H}^{n+\frac{1}{2}} \right] - C_0 \phi^{n+\frac{1}{2}} - q^{n+\frac{1}{2}} g^{n+\frac{1}{2}}, \\
\delta t e^n &= \nabla \cdot \left[ D_e^{n+\frac{1}{2}} \nabla \left( \mu^{n+\frac{1}{2}} \right) \right], \quad D_e = D_u T^2, \\
\mu^{n+\frac{1}{2}} &= C_1 e^{n+\frac{1}{2}} + q^{n+\frac{1}{2}} h^{n+\frac{1}{2}}, \\
\delta t U^n &= \mathbf{H}^{n+\frac{1}{2}}, \quad \nabla \delta t \phi^n, \\
\delta t q^n &= \mathbf{g}^{n+\frac{1}{2}} \delta t \phi^n + \mathbf{h}^{n+\frac{1}{2}} \delta t e^n.
\end{align*}
\]
(3.14)

We define \( V_{\mu,n+\frac{1}{2}} = \frac{1}{|\Omega|} \int \mu^{n+\frac{1}{2}} \, dx \) and introduce \( \tilde{\mu}^{n+\frac{1}{2}} = \mu^{n+\frac{1}{2}} - V_{\mu,n+\frac{1}{2}} \). As it can be readily observed that
\[
\int \Omega e^{n+1} \, dx = \int \Omega e^n \, dx = \ldots = \int \Omega e^0 \, dx.
\]
(3.15)

Hence, the scheme preserves the energy at the semidiscrete level. We further define \( V_e = \frac{1}{|\Omega|} \int \Omega e^0 \, dx \) and introduce \( \tilde{e}^{n+\frac{1}{2}} = e^{n+\frac{1}{2}} - V_e \). Then, \( V_{\mu,n+\frac{1}{2}} = C_1 V_e + \frac{1}{|\Omega|} \int \Omega q^{n+1/2} h^{n+1/2} \, dx \). Linear system (3.14) can be written in an equivalent system as follows
\[
\begin{align*}
\tau^{n+\frac{1}{2}} \delta t \phi^n &= \varepsilon^2 k_0 \Delta \phi^{n+\frac{1}{2}} + \nabla \cdot \left[ U^{n+\frac{1}{2}} \mathbf{H}^{n+\frac{1}{2}} \right] - C_0 \phi^{n+\frac{1}{2}} - q^{n+\frac{1}{2}} g^{n+\frac{1}{2}}, \\
\delta t e^n &= \nabla \cdot \left[ D_e^{n+\frac{1}{2}} \nabla \left( \tilde{\mu}^{n+\frac{1}{2}} + V_{\mu,n+\frac{1}{2}} \right) \right], \quad D_e = D_u T^2, \\
\tilde{\mu}^{n+\frac{1}{2}} + V_{\mu,n+\frac{1}{2}} &= C_1 \tilde{e}^{n+\frac{1}{2}} + q^{n+\frac{1}{2}} h^{n+\frac{1}{2}} + C_1 V_e.
\end{align*}
\]
(3.16)
Theorem 3.2. The weak form given by (3.18) admits a unique solution in $\mathcal{H}$.

Proof. It is straightforward to show that the bilinear form $a(\bullet, \bullet)$ and the linear form $l(\bullet)$ are continuous. Next, we will show that the bilinear form is strongly coercive. We will assume the domain is rectangular and focus on periodic boundary conditions here.

Note that

$$\left(\bar{\Omega}^{n+\frac{1}{2}}, \frac{1}{|\Omega|} \int_\Omega \bar{\Omega}^{n+\frac{1}{2}} q^{n+\frac{1}{2}} d\Omega \right) = \left(\frac{1}{|\Omega|} \int_\Omega \bar{\Omega}^{n+\frac{1}{2}} q^{n+\frac{1}{2}} d\Omega \right) \left(\frac{1}{|\Omega|} \int_\Omega \bar{\Omega}^{n+\frac{1}{2}} q^{n+\frac{1}{2}} d\Omega \right) = 0. \quad (3.21)$$

Then there exists a constant $C_3, C_4 > 0$ such that

$$C_4 \| \Phi \|^2_\mathcal{H} \geq a(\Phi, \Phi) = \left(\frac{2\bar{\Omega}^{n+\frac{1}{2}}}{\Delta t} + C_0\right)(\Phi_1, \Phi_1) + \varepsilon^2 k_0 (\nabla \Phi_1, \nabla \Phi_1)$$

+ $\frac{\varepsilon}{\Delta t} \left(D_e \bar{\Omega}^{n+\frac{1}{2}} \nabla \Phi_2, \nabla \Phi_2\right) + C_1 (\Phi_3, \Phi_3) + (\Phi_4, \Phi_4) + (\Phi_5, \Phi_5)$

$$\geq C_3 \| \Phi \|^2_\mathcal{H}, \quad (3.22)$$

where we use the Pančarev’s inequality for periodic functions with $\frac{1}{|\Omega|} \int_\Omega \Phi_2 d\Omega = 0$ and $D_e \bar{\Omega}^{n+\frac{1}{2}} = D_u \bar{T}_0^{n+\frac{1}{2}} > D_u T_0^2 > 0$, and $T_0$ is a constant.

Then, by the Lax–Milgram theorem, there exists a unique solution $\Phi \in \mathcal{H}$ for the linear system in the weak form given by (3.18). □

3.3. Spatial discretization

In space, we discretize the linear PDE-algebraic system using compact second-order finite difference methods. We consider a 2D domain $\Omega = [0, L_x] \times [0, L_y]$, where $L_x$ and $L_y$ are two positive real numbers. We divide the domain into...
rectangular meshes with mesh sizes $h_x = L_x/N_x$, $h_y = L_y/N_y$, where $N_x$ and $N_y$ are the number of mesh nodes in each direction. Then we define the sets of grid points in 1D as follows

$$
E_x = \{x_i \mid i = 0, 1, \ldots, N_x\}, \quad C_x = \{x_i \mid i = 1, 2, \ldots, N_x\},
E_y = \{y_j \mid j = 0, 1, \ldots, N_y\}, \quad C_y = \{y_j \mid j = 1, 2, \ldots, N_y\},
$$

(3.23)

where $x_i = (l - \frac{1}{2})h_x$ and $y_j = (l - \frac{1}{2})h_y$. The sets $E_x$, $E_y$ are the edge-centered points for the uniform partition, and $C_x$, $C_y$ are the cell-centered points for the uniform partition.

We define the following spaces for periodic functions:

$$
C_{xy} = \{ \phi : C_x \times C_y \rightarrow \mathbb{R} \mid \phi_{0,j} = \phi_{N_x,j}, \phi_{N_x+1,j} = \phi_{1,j} \},
$$

(3.24)

$$
\phi_{i,0} = \phi_{i,N_y}, \phi_{i,N_y+1} = \phi_{i,1}, \quad i = 1, 2, \ldots, N_x; \quad j = 1, 2, \ldots, N_y,
$$

$$
E^{ew}_{xy} = \{ u : E_x \times C_y \rightarrow \mathbb{R} \mid u_{\frac{1}{2},j} = u_{N_x+\frac{1}{2},j} \},
$$

(3.25)

$$
u_{i,0} = \nu_{i,N_y}, \nu_{i,N_y+1} = \nu_{i,1}, \quad i = 1, 2, \ldots, N_x; \quad j = 1, 2, \ldots, N_y,
$$

$$
E^{ns}_{xy} = \{ v : C_x \times E_y \rightarrow \mathbb{R} \mid v_{0,j} = v_{N_y,j}, \; v_{N_y+1,j} = v_{1,j} \},
$$

(3.26)

$$
u_{i,\frac{1}{2}} = \nu_{i,N_y+\frac{1}{2}}, \; i = 1, 2, \ldots, N_x; \; j = 1, 2, \ldots, N_y.
$$

We define the east-west-edge-to-center average and difference operator $a_x, d_x : E^{ew}_{xy} \rightarrow C_{xy}$ as follows:

$$
a_x u_{i,j} = \frac{1}{2} (u_{i+\frac{1}{2},j} + u_{i-\frac{1}{2},j}), \quad d_x u_{i,j} = \frac{1}{h_x} (u_{i+\frac{1}{2},j} - u_{i-\frac{1}{2},j}) \quad \forall u \in E^{ew}_{xy},
$$

(3.27)

and the north–south-edge-to-center average and difference operators $a_y, d_y : E^{ns}_{xy} \rightarrow C_{xy}$:

$$
a_y v_{i,j} = \frac{1}{2} (v_{i,j+\frac{1}{2}} + v_{i,j-\frac{1}{2}}), \quad d_y v_{i,j} = \frac{1}{h_y} (v_{i,j+\frac{1}{2}} - v_{i,j-\frac{1}{2}}) \quad \forall v \in E^{ns}_{xy}.
$$

(3.28)

Similarly, we define the center-to-east–west-edge average and difference operators $A_x, D_x : C_{xy} \rightarrow E^{ew}_{xy}$:

$$
A_x \phi_{i+\frac{1}{2},j} = \frac{1}{2} (\phi_{i+1,j} + \phi_{i,j}), \quad D_x \phi_{i+\frac{1}{2},j} = \frac{1}{h_x} (\phi_{i+1,j} - \phi_{i,j}),
$$

(3.29)

and the center-to-north–south-edge average and difference operators $A_y, D_y : C_{xy} \rightarrow E^{ns}_{xy}$:

$$
A_y \phi_{i,j+\frac{1}{2}} = \frac{1}{2} (\phi_{i,j+1} + \phi_{i,j}), \quad D_y \phi_{i,j+\frac{1}{2}} = \frac{1}{h_y} (\phi_{i,j+1} - \phi_{i,j}).
$$

(3.30)

Denote the full discrete Laplacian operator as

$$
\Delta_h = d_x(D_x \phi) + d_y(D_y \phi).
$$

(3.31)

Then we define the discrete inner product at cell centers as

$$
(f, g)_c = h_x h_y \sum_{i,j} f_{ij} g_{ij},
$$

(3.32)

and the discrete inner product at edges as

$$
(f, g)_{ew} = (a_x(f, g), 1)_c, \quad (f, g)_{ns} = (a_y(f, g), 1)_c.
$$

(3.33)

The corresponding discrete norms defined as

$$
\|f\|_c = (f, f)^{\frac{1}{2}}, \quad \|u\|_{ew} = (u, u)_{ew}^{\frac{1}{2}}, \quad \|v\|_{ns} = (v, v)_{ns}^{\frac{1}{2}}.
$$

(3.34)

With all these notations, we present the full discrete scheme for (3.14) as follows

**Scheme 3.2.** After the solution at the nth level is computed, we use the following to compute the new solution at the $(n+1)$th level:

$$
\begin{align*}
\Phi^{n+\frac{1}{2}} = \Phi^n + \frac{1}{2} \Phi^{n+1} - \frac{1}{2} \Phi^n + \frac{1}{2} \Phi^n \quad &+ d_x(A_x U^{n+\frac{1}{2}} H_x^{n+\frac{1}{2}}) + d_y(A_y U^{n+\frac{1}{2}} H_y^{n+\frac{1}{2}}) - C_0 \phi^{n+\frac{1}{2}} - q^{n+\frac{1}{2}} \phi^{n+\frac{1}{2}} - \frac{1}{2} g^{n+\frac{1}{2}} \phi^{n+\frac{1}{2}}, \\
\delta_t \Phi^n = d_x(A_x U^{n+\frac{1}{2}} D_x \phi^n) + d_y(A_y U^{n+\frac{1}{2}} D_y \phi^n) - C_1 \phi^{n+\frac{1}{2}} - q^{n+\frac{1}{2}} \phi^{n+\frac{1}{2}} - \frac{1}{2} g^{n+\frac{1}{2}} \phi^{n+\frac{1}{2}} - \frac{1}{2} \phi^{n+\frac{1}{2}}, \\
\mu^{n+\frac{1}{2}} = C_1 \phi^{n+\frac{1}{2}} + q^{n+\frac{1}{2}} \phi^{n+\frac{1}{2}} - \frac{1}{2} g^{n+\frac{1}{2}} \phi^{n+\frac{1}{2}}, \\
\delta_t U^n = a_x \left( H_x^{n+\frac{1}{2}} D_x \phi^n \right) + a_y \left( H_y^{n+\frac{1}{2}} D_y \phi^n \right), \\
\delta_t q^n = \frac{1}{2} \delta_t \phi^n + \frac{1}{2} \phi^{n+\frac{1}{2}}.
\end{align*}
$$

(3.35)

where $\phi, u, v, e, i, j, U, u, q, h, q$ are discretized at cell centers, and $(H_x, H_y)_{i,j}$ are discretized at the edge.
One notices that equation (3.35) is a linear system,

\[ A^n \Phi = F^n, \]  

(3.36)

where

\[ A^n = \begin{pmatrix} a_{11} & 0 & 0 & a_{14} & \frac{\phi^{n+1}}{n+\frac{1}{2}} \\ 0 & a_{22} & 1 & 0 & 0 \\ 0 & -1 & C_1 & 0 & \frac{n}{n+\frac{1}{2}} \\ a_{41} & 0 & 0 & 1 & 0 \\ -\frac{n}{n+\frac{1}{2}} & 0 & -\frac{n^2}{n+\frac{1}{2}} & 0 & 1 \end{pmatrix}, \quad \Phi = \begin{pmatrix} \phi^{n+\frac{1}{2}} \\ \mu^{n+\frac{1}{2}} \\ n^{n+\frac{1}{2}} \\ U_{n+\frac{1}{2}} \\ q^{n+\frac{1}{2}} \end{pmatrix}, \]  

(3.37)

with

\begin{align*}
  a_{11} &= \frac{2n^{n+\frac{1}{2}}}{\Delta t} + C_0 - k_0 \varepsilon^2 \Delta h, \\
  a_{14} &= -d_x(A_x \bullet \overline{H}_x^{n+\frac{1}{2}}) - d_y(A_y \bullet \overline{H}_y^{n+\frac{1}{2}}), \\
  a_{22} &= -\frac{n}{2} \rho \Phi(A_x D_{ce}^{n+\frac{1}{2}} D_{x} \bullet \Phi) - \frac{n}{2} \rho \Phi(A_y D_{ce}^{n+\frac{1}{2}} D_{y} \bullet \Phi), \\
  a_{41} &= -\alpha_y(\overline{H}_x^{n+\frac{1}{2}} D_{x} \bullet \Phi) - \alpha_y(\overline{H}_y^{n+\frac{1}{2}} D_{y} \bullet \Phi).
\end{align*}  

(3.38)

Analogous to the semi-discrete scheme, we can show that the entropy production rate is preserved in the fully discrete scheme.

**Theorem 3.3.** Scheme (3.35) preserves the positive entropy production rate, i.e.,

\begin{align*}
  S^{n+1} - S^n &= \Delta t \left( \frac{1}{2} \left( 2d_k \rho \Delta h \Phi^{n+\frac{1}{2}} + d_x(A_x \overline{U}^{n+\frac{1}{2}} \overline{H}_x^{n+\frac{1}{2}}) + d_y(A_y \overline{U}^{n+\frac{1}{2}} \overline{H}_y^{n+\frac{1}{2}}) - C_0 \Phi^{n+\frac{1}{2}} \\ -q^{n+\frac{1}{2}} \Phi^{n+\frac{1}{2}} \right) \right) \\
  &\quad + \frac{1}{2} \rho \Phi^{n+\frac{1}{2}} \left( \overline{A}_x D_{ce}^{n+\frac{1}{2}} D_x (C_1 \Phi^{n+\frac{1}{2}} + q^{n+\frac{1}{2}} \overline{H}_x^{n+\frac{1}{2}}) \right) \\
  &\quad + \frac{1}{2} \rho \Phi^{n+\frac{1}{2}} \left( \overline{A}_y D_{ce}^{n+\frac{1}{2}} D_y (C_1 \Phi^{n+\frac{1}{2}} + q^{n+\frac{1}{2}} \overline{H}_y^{n+\frac{1}{2}}) \right) \geq 0,
\end{align*}  

(3.39)

where the full discrete entropy expression is given by

\begin{align*}
  S^n(e^n, s^n, U^n, q^n) &= -\frac{\varepsilon^2 k_0}{2} \left( \|D_x \Phi^n\|_{ew}^2 + \|D_y \Phi^n\|_{ew}^2 \right) - \frac{1}{2} \|U^n\|_{c}^2 - \frac{1}{2} \|q^n\|_{c}^2 \\
  &\quad - C_{\Phi} \|\Phi^n\|_{c}^2 - C_{q} \|q^n\|_{c}^2 + (A + B)[\Omega].
\end{align*}  

(3.40)

The proof is similar with Theorem 3.1. We thus omit it for simplicity.

**Theorem 3.4.** The linear algebraic system (3.35) admits a unique solution.

**Proof.** We show \( A^n \Phi = 0 \) only has the zero solution. A straightforward calculation leads to

\begin{align*}
  (A^n \Phi, \Phi) &= \left( \frac{2n^{n+\frac{1}{2}}}{\Delta t} + C_0 \right) \|\Phi^{n+\frac{1}{2}}\|_{c}^2 + \varepsilon^2 k_0 \left( \|D_x \Phi\|_{ew}^2 + \|D_y \Phi\|_{ns}^2 \right) \\
  &\quad + (a_{14} (U^{n+\frac{1}{2}}), \Phi^{n+\frac{1}{2}}) + \frac{n}{2} \left( \|A_x D_{ce}^{n+\frac{1}{2}} D_x \Phi\|_{ew}^2 + \|A_y D_{ce}^{n+\frac{1}{2}} D_y \Phi\|_{ns}^2 \right) \\
  &\quad + C_1 (e^{n+\frac{1}{2}}) + \|U^{n+\frac{1}{2}}\|_{c}^2 + (a_{41} (\Phi^{n+\frac{1}{2}}), U^{n+\frac{1}{2}}) + \|q^{n+\frac{1}{2}}\|_{c}^2.
\end{align*}  

(3.41)

Next, we show that

\[ (a_{14} (\Phi^{n+\frac{1}{2}}), U^{n+\frac{1}{2}}) + (a_{41} (U^{n+\frac{1}{2}}), \Phi^{n+\frac{1}{2}}) = 0. \]  

(3.42)

Recall a simple Lemma from [9]

\begin{align*}
  (D_x \Phi, u)_{ew} + (\Phi, d_x u)_{c} &= 0, \quad (A_x \Phi, u)_{ew} = (\Phi, a_x u)_{c}, \\
  (D_y \Phi, v)_{ns} + (\Phi, d_y v)_{c} &= 0, \quad (A_y \Phi, v)_{ns} = (\Phi, a_y v)_{c}.
\end{align*}  

(3.43)

Then we have
Table 4.1

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<td>0.0015625</td>
<td>2.6031e-5</td>
<td>2.08</td>
</tr>
</tbody>
</table>

\[
\begin{align*}
(a_{14}(\phi^{n+1}_c), U^{n+1}_c) + (a_{41}(U^{n+1}_c), \phi^{n+1}_c) &= \\
- (d_x(A_x U^{n+1}_c H_x^{n+1}), \phi^{n+1}_c) - (d_y(A_y U^{n+1}_c H_y^{n+1}), \phi^{n+1}_c) &= \\
- (a_x(H_x^{n+1} D_x \phi^{n+1}_c), U^{n+1}_c) - (a_y(H_y^{n+1} D_y \phi^{n+1}_c), U^{n+1}_c) &= \\
= (A_x U^{n+1}_c H_x^{n+1}, D_x \phi^{n+1}_c) + (A_y U^{n+1}_c H_y^{n+1}, D_y \phi^{n+1}_c) &= \\
= 0. \\
\end{align*}
\]

(3.44)

It follows that

\[
\begin{align*}
(A^T \Phi, \Phi) &= \left(\frac{2\tau_{0.5}}{\Delta t} \right) \| \phi^{n+1}_c \|_C^2 + \epsilon^2 k_0 \left( \| D_x \phi^{n+1}_c \|_e^2 \epsilon + \| D_y \phi^{n+1}_c \|_r^2 \epsilon \right) + \\
+ \frac{\Delta t}{\epsilon} \left[ \| A_x \Delta D^{n+1}_e D_x \mu \|_e^2 \epsilon + \| A_y \Delta D^{n+1}_e D_y \mu \|_r^2 \epsilon \right] + \\
+ C_1 \| \epsilon^{n+1}_c \|_C^2 \epsilon + \| U^{n+1}_c \|_C^2 \epsilon + \| q^{n+1}_c \|_C^2 \epsilon \geq 0. \\
\end{align*}
\]

(3.45)

Hence, $A^T \Psi = 0$ implies $\Psi = 0$. This proves that the linear system has a unique solution.

**Remark 3.1.** In practice of solving the scheme in (3.35), the auxiliary variables $U^{n+1}$ and $q^{n+1}$ could be expressed as

\[
\begin{align*}
U^{n+1} &= U^n + \delta t \left[ a_x \left( H_x^{n+1} D_x \delta \phi^n \right) + a_y \left( H_y^{n+1} D_y \delta \phi^n \right) \right], \\
q^{n+1} &= q^n + \delta t \left[ B \left( H_x^{n+1} D_x \delta \phi^n + H_y^{n+1} D_y \delta \phi^n \right) \right],
\end{align*}
\]

(3.46)

which can be substituted back into the equations for $\phi^{n+1}_c$, $e^{n+1}_c$. Therefore, in each time step, only a linear system for $\phi^{n+1}_c$, $e^{n+1}_c$ need to be solved, and then $U^{n+1}$, $q^{n+1}$ can be updated via (3.46). In other words, the introduction of auxiliary variables does not increase unknowns for the linear algebraic system to be solved in each time step.

4. Numerical results and discussion

In this section, we implement the above algorithm with periodic boundary conditions in a rectangular domain $\Omega = [0, L_x] \times [0, L_y]$ assuming the crystal growth takes place within the computational domain away from the boundary. For the rest of the paper, unless otherwise specified, we use the following default dimensionless parameter values,

\[
\begin{align*}
A &= 10^2, \quad B = 1, \quad \theta_0 = \frac{\pi}{4}, \quad \varepsilon = 10^{-2}, \quad m = 6, \quad \varepsilon_A = \frac{1}{m+1}, \quad \tau = 3, \quad \varepsilon_L(T_M) = 0, \quad k_0 = 1, \quad C_L = 0.6, \quad D_u = 6 \times 10^{-5}, \quad L_1 = L_2 = 0, \quad L_0 = 0.5, \quad T_M = 1, \quad C_0 = 1, \quad C_1 = 1.
\end{align*}
\]

(4.1)

4.1. Mesh refinement test in time

First of all, we verify the second-order convergence rate in time for (3.35) Here, we use $L = L_x = L_y = 18$ and we choose $m = 8$ and $N_x = N_y = 1024$, the initial value $\phi(x, t = 0) = \frac{1}{2} \left( 1 + \tanh \frac{0.3L - \max(|x - 0.5L|, |y - 0.5L|)}{2L} \right)$ and $T(x, t = 0) = 0.5T_M$. The parameter values are given in (4.1). Then we take a linear refinement path $\delta_k = \frac{0.1}{2^k}$, $k = 0, 1, \cdots, 6$ in Table 4.1, where we calculate the rate at which the Cauchy difference (e.g. $\phi^k - \phi^{k-1}$) varies in the $L_2$ norm at time $T = 0.5$, where we observe that the proposed scheme indeed possesses a second order convergence rate in time.

We remark that even though the scheme in (3.35) is shown to be unconditionally energy stable and uniquely solvable, it doesn’t necessarily mean an arbitrarily large time step can be used. Since the proposed scheme is only second-order accurate in time, one can expect the numerical solution may not be accurate when the time step is too large, although it guarantees
an increasing entropy with an arbitrary time step. In other words, the accuracy requirement of numerical solutions, in fact, imposes an upper bound on the step size in practice. To illustrate it, we choose a smooth profile of the solution as \( \phi(x, t = 0) = \frac{1}{2}(1 + \tanh \frac{10 - (x - 0.5L)^2 - (y - 0.5L)^2}{2\delta t}) \) and \( T(x, t = 0) = 0.5T_M \). where \( L = L_x = L_y = 18 \), \( T_M = 10 \). Then we set \( m = 4 \), \( D_x = 0.01 \), \( N_x = N_y = 512 \) and the rest parameters are the same as (4.1). The entropy increment \( S(t) - S(0) \) with different time steps is summarized in Fig. 4.1, where the chosen time steps are \( \delta t = 0.01 \), \( 0.1 \), \( 1 \), \( 2 \), \( 10 \), \( 20 \), \( 100 \), respectively. We observe that the entropy production rate of the numerical solution is always non-negative with any time steps. But when the time step size is too large, it reaches a quasi-steady state immediately, leading to an inaccurate solution. When the time step is getting smaller, the numerical solution converges. This example demonstrates that the numerical scheme guarantees entropy increasing for any time step, but inaccurate results would be produced if the time step is too large.

In the rest of this paper, we conduct several numerical studies on this thermodynamically consistent dendritic growth model. Unless specified otherwise, we use \( L_x = L_y = 18 \) with \( N_x = N_y = 1024 \).

4.2. Effect of the anisotropy fold parameter \( m \)

In the first example, we study how the anisotropy fold parameter \( m \) affects dynamics in dendritic growth. Here we choose \( D_u = 10^{-4} \) with the rest of parameter values given in (4.1). The initial condition is chosen as follows:

\[
\phi(x, t = 0) = \begin{cases} 
1, & (x - 0.5L)^2 + (y - 0.5L)^2 > 0.018, \\
0, & \text{otherwise};
\end{cases} \\
T(x, t = 0) = 0.5T_M.
\] (4.2)

In the simulation, we use \( m = 4, 5, 6, 8 \) respectively. The corresponding crystal growth patterns at different times are shown in Fig. 4.2. We observe that the fold number \( m \) exactly controls the number of branches in the dendritic patterns, and the tip of dendritic crystals with a large fold number grows more slowly. These observations are consistent with previous study with a different model (which is not thermodynamically consistent) \[19,42\].

In addition, we show the temperature at \( t = 5000 \) for each case in Fig. 4.3. We observe that the temperature is higher in the newly formed crystal region than in the liquid region, which is due to the release of latent heat during the solidification process. The temperature reaches approximately constant in the crystallized phase. At the tip of the dendritic crystals, there exists a higher temperature gradient, and the crystal with a larger fold number \( m \) grows more slowly. The entropy evolution with time is shown in Fig. 4.4, where we observe that the entropy with a larger fold number \( m \) increases slower than the one with a smaller fold number \( m \).

4.3. Effect of latent heat \( L_0 \) on the dendritic growth patterns

Next, we consider the role of latent heat parameter \( L_0 \) on dynamics of dendritic crystal growth. In particular, we are interested in how \( L_0 \) correlates with the dendrite patterns during their growth. Here we use the default parameter values given in (4.1) and initial conditions given in (4.2). One simulation result is shown in Fig. 4.5, where we use \( L_0 = \frac{4}{16}, \frac{5}{16}, \frac{6}{16}, \frac{7}{16} \) and \( m = 4, 6, 8 \), respectively. We observe that a larger \( L_0 \) would make the corner sharper and the branches thinner. In other words, a smaller \( L_0 \) value would smooth out the dendritic pattern. This indicates that a quick release of heat during the solidification process would produce a sharper interface than a slow release does.

The temperature profiles for each case of \( L_0 = \frac{4}{16}, \frac{5}{16}, \frac{6}{16}, \frac{7}{16} \) with \( m = 6 \) at time \( t = 4000 \) are depicted in Fig. 4.6. We observe that temperature patterns match the profile of the crystal shape with higher temperature inside the crystals and lower temperature in the liquid. In addition, the temperature gradient at the liquid-solid interface steepens as the latent heat.
Fig. 4.2. Effect of anisotropic fold number \( m \) on dynamics of dendritic crystal growth. Here blue represents \( \phi = 0 \) (the solid), and red represents \( \phi = 1 \) (the liquid). The dendritic crystal patterns with respect to \( m = 4, 5, 6, 8 \) at different times (\( t = 500, 1000, 2500, 5000 \)) are plotted.

Fig. 4.3. Temperature at \( t = 5000 \) with respect to \( m = 4, 5, 6, 8 \) of the examples in Fig. 4.2.
Fig. 4.4. Time evolution of entropies corresponding to \( m = 4, 5, 6, 8 \) of the examples in Fig. 4.2, respectively. The entropy reduces as the number of folds increases.

![Time evolution of entropies](image)

Fig. 4.5. Effect of latent heat parameter \( L_0 \) on dynamics of dendritic crystal growth. Here we choose \( L_0 = \frac{4}{16}, \frac{5}{16}, \frac{6}{16}, \frac{7}{16} \), respectively. The patterns of \( \phi \) at time \( t = 4000 \) are shown.

![Effect of latent heat parameter](image)

Heat parameter \( L_0 \) increases. In addition, the entropy evolution for \( m = 4, 5, 6, 8 \) is shown in Fig. 4.7, where we observe that entropy increases with time as \( L_0 \) increases and the increase saturates beyond a critical \( L_0 \).

4.4. Effects of anisotropic parameter \( \varepsilon_4 \) on dendritic growth patterns

Here we investigate how the anisotropic parameter \( \varepsilon_4 \) affects the dendritic patterns. Analogous to the previous examples, we choose the same set of default parameter values given in (4.1) except \( m = 8 \), and the initial conditions are given in (4.2). A set of numerical experiments with varying \( \varepsilon_4 \) are carried out. The simulation results are summarized in Fig. 4.8. Here we use \( \varepsilon_4 = 0.005, 0.01, 0.02, 0.03, 0.04, 0.06 \), respectively, and plot the crystal patterns at time \( t = 4000 \). We observe that \( \varepsilon_4 \) affects the details of the dendritic patterns in a subtle way.
Fig. 4.6. Effect of $L_0$ on the dendritic crystal patterns. Here we choose $L_0 = \frac{4}{16}, \frac{5}{16}, \frac{6}{16}, \frac{7}{16}$ and $m = 4, 6, 8$ respectively. The temperature profiles $T$ at time $t = 4000$ are shown.

Fig. 4.7. Entropies with respect to $m = 6$ and $L_0 = \frac{4}{16}, \frac{5}{16}, \frac{6}{16}, \frac{7}{16}$ for the examples in Fig. 4.5 are depicted as functions of time. The entropy decreases while $L_0$ increases.

Fig. 4.8. Effect of $\varepsilon_4$ on the dendritic crystal patterns. Here we show the crystal patterns at time $t = 4000$, with $\varepsilon_4 = 0.005, 0.01, 0.02, 0.03, 0.04, 0.06$, respectively. We observe that the larger $\varepsilon_4$ is, the more refined patterns form.

4.5. Multi-crystal growth

In the last example, we consider a situation where multiple dendritic grow simultaneously with seeds from different locations. In particular, we use the following initial profile

$$
\phi(x, t = 0) = \min \left( \phi_a(x), \phi_b(x), \phi_c(x) \right).
$$

(4.3)
where \( \phi_0, \phi_b \) and \( \phi_c \) are defined as

\[
\phi_0 (\mathbf{x}) = \begin{cases} 
1, & (x - \frac{L_x}{4})^2 + (y - \frac{L_y}{4})^2 > 0.018, \\
0, & \text{otherwise}, 
\end{cases}
\]

\[
\phi_b (\mathbf{x}) = \begin{cases} 
1, & (x - \frac{3L_x}{4})^2 + (y - \frac{L_y}{4})^2 > 0.018, \\
0, & \text{otherwise}, 
\end{cases}
\]

\[
\phi_c (\mathbf{x}) = \begin{cases} 
1, & (x - \frac{2L_x}{3})^2 + (y - \frac{3L_y}{4})^2 > 0.018, \\
0, & \text{otherwise}. 
\end{cases}
\]

This simulation represents multiple crystal growth with three distinct initial solidification seeds. We use the default parameter values given in (4.1) except \( m = 8 \). The dendritic crystal growth dynamics is shown in Fig. 4.9, where the patterns at different times are shown. At the early stage of crystal growth, since the three crystal growing regions are far away, they grow independently into three similar dendritic crystals. Later, when crystals are large enough, they grow into each other. Eventually, the tips of three growing crystal regions change directions once they are to collide to form a liquid boundary layer. These boundary layers become thinner and thinner in certain parts of the domain over times.

5. Conclusion

In this paper, we reformulate a thermodynamically consistent crystal growth model into an equivalent form with a quadratic entropy functional. Based on the new formulation, we develop an energy conserving as well as entropy-production rate preserving scheme. The scheme is linear, second order and uniquely solvable. Its second-order convergence in time is verified through a series of mesh refinement tests. Several numerical examples/simulations are conducted to illustrate the accuracy and usefulness of the proposed numerical schemes in resolving fine details in dendritic crystal growth. The idea presented here on formulating and/or reformulating thermodynamically consistent models, developing entropy production rate preserving schemes is rather general, which can be readily applied to many other classes of thermodynamically consistent models.

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