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NUMERICAL ANALYSIS FOR A NONLOCAL PHASE FIELD SYSTEM

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Abstract. In this paper, we propose a stable, convergent finite difference scheme to solve numerically a nonlocal phase field system which may model a variety of nonisothermal phase separations in pure materials which can assume two different phases, say solid and liquid, with properties varying in space. The scheme inherits the characteristic property of conservation of internal energy. We also prove that the scheme is uniquely solvable and the numerical solution will approach the true solution in the L^∞- norm.

Key words. Finite difference scheme; Nonisothermal, Long-range interaction.

1. Introduction

In this work, we consider the problem

$$u_t = \int_\Omega J(x-y)u(y)\,dy - \int_\Omega J(x-y)\,dy\; u(x) - f(u) + l\theta, \tag{1.1}$$

$$(\theta + lu)_t = \triangle\theta \tag{1.2}$$

in $(0,T)\times\Omega$, with initial and Neumann boundary conditions

$$u(0,x) = u_0(x),\;\; \theta(0,x) = \theta_0(x), \tag{1.3}$$

$$\left.\frac{\partial\theta}{\partial n}\right|_{\partial\Omega} = 0, \tag{1.4}$$

where $T > 0$ and $\Omega \subset \mathbb{R}^n$ is a bounded domain. Here θ represents temperature, u is an order parameter often used to represent various material phases, l is a latent heat coefficient, the interaction kernel satisfies $J(-x) = J(x)$, and f is bistable.

In order to derive equations (1.1)-(1.2), we begin with the free energy

$$E = \frac{1}{4}\int\int J(x-y)[u(x)-u(y)]^2\,dx\,dy + \int\left[F(u(x)) + \frac{1}{2}\theta^2\right]\,dx, \tag{1.5}$$

where F is a double well function.

We consider the gradient flow associated with (1.5) relative to the order parameter u in L^2 and the internal energy e in $H_0^{-1}(\Omega)$, where by H_0^{-1} we mean the dual space of H^1 with mean value zero. This is done because the total internal energy I, with density denoted by $e = \theta + lu$, should be conserved. We have

$$u_t = -\frac{\partial E(u,e)}{\partial u}, \tag{1.6}$$

$$e_t = -\frac{\partial E(u,e)}{\partial e}, \tag{1.7}$$

where $\frac{\partial E(u,e)}{\partial u}$ is a linear functional on L^2 and $\frac{\partial E(u,e)}{\partial e}$ is a linear functional on H^{-1}.

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If we write $F' = f$, the representative of $\frac{\partial E(u,e)}{\partial u}$ in L^2 is

$$\frac{\partial E(u,e)}{\partial u} = -\int_\Omega J(x-y)u(y)\,dy + \int_\Omega J(x-y)dy\,u(x) + f(u) - l(e-lu), \tag{1.8}$$

and the representative of $\frac{\partial E(u,e)}{\partial e}$ in H^{-1} is

$$\frac{\partial E(u,e)}{\partial e} = -\triangle(e-lu). \tag{1.9}$$

The more familiar Ginzburg-Landau free energy

$$\int \left[\frac{d^2}{2}|\nabla u|^2 + F(u) + \frac{l}{2}\theta^2\right] dx$$

used in [7], [8], and in higher order versions by [6] in deriving phase-field systems, is obtained by approximating the interaction term through a truncated Taylor series. For example, when J is fairly localized, one may hope that

$$\int\int J(x-y)(u(x)-u(y))^2\,dx\,dy$$

is well-approximated by

$$\int \left(\frac{d^2}{2}|\nabla u|^2\right) dx,$$

where $\frac{d^2}{2} = \int J(y)y_i^2 dy$ is assumed to be independent of coordinate, i. Such an approximation was introduced by Van der Waals in [20] in 1893, and has been adopted ever since for ease of analysis.

If $\int_\Omega J(x-y)u(y)dy - \int_\Omega J(x-y)dy\,u(x)$ is replaced by $\triangle u$, the system (1.1)-(1.4) becomes

$$u_t = \triangle u - f(u) + l\theta, \tag{1.10}$$

$$(\theta + lu)_t = \triangle\theta \tag{1.11}$$

in $(0,T)\times\Omega$, with initial and Neumann boundary conditions

$$u(0,x) = u_0(x),\ \theta(0,x) = \theta_0(x),\ \text{and} \tag{1.12}$$

$$\left.\frac{\partial\theta}{\partial n}\right|_{\partial\Omega} = 0. \tag{1.13}$$

The system (1.1)-(1.4) and the system (1.10)-(1.13) were proposed as models for nonisothermal phase separation in pure materials which can assume two different phases, say solid and liquid. The function θ represents the temperature field within the material. The function u is an order parameter that describes the phase of the material, where with appropriate scaling $u = 1$ represents the solid phase and $u = -1$ represents the liquid phase; values of u with $-1 < u < 1$ represent a mixture of the two phases. The results about existence, uniqueness, and the structure of solutions for both systems can be found in references [1,3-5,9-13,15-19].

To the best of our knowledge, there are very few results on the numerical solutions to the system (1.1)-(1.4) and the system (1.10)-(1.13).

When temperature is fixed in both systems, (1.1)-(1.4) is the nonlocal Allen-Cahn equation

$$u_t = \int_\Omega J(x-y)u(y)\,dy - \int_\Omega J(x-y)dy\,u(x) - f(u) \tag{1.14}$$

and the system (1.10)-(1.13) is the Allen-Cahn equation

$$u_t = \triangle u(x) - f(u). \tag{1.15}$$

Numerical analysis related to the nonlocal Allen-Cahn (1.14) and Allen-Cahn (1.15) equations can be found in [2], [14] and the references therein.

In this paper, we develop a finite difference scheme for the system (1.1)-(1.4). The scheme inherits the characteristic property of conservation of internal energy. We also prove that the difference scheme is stable and that the numerical approximation converges to the solution of (1.1)-(1.4).

2. Analysis of the Proposed Scheme

In this section, we consider finite difference approximations of the system (1.1)-(1.4) for $n = 1$ and $n = 2$. We will use $f(u) = u^3 - u$, but the analysis applies to a general smooth bistable function if care is taken in the choice of linearization (see Lemma 2.4).

For $n = 1$ we use the following notation. Setting $\Omega = (-L, L)$, we define

$$\begin{aligned}&\Omega_x = \{x_i |\, x_i = -L + i\triangle x,\, 0 \le i \le M\} \text{ and}\\ &\Omega_t = \{t_k |\, t_k = k\triangle t,\, 0 \le k \le K\},\end{aligned}$$

where $\triangle x = 2L/M$ and $\triangle t = T/K$. Then our choice of difference scheme for the system (1.1)-(1.4) for $n = 1$ is

$$u_i^0 = u_0(x_i) \text{ for } 0 \le i \le M, \texttt{and} \tag{2.1}$$

$$\theta_i^0 = \theta_0(x_i) \text{ for } 0 \le i \le M. \tag{2.2}$$

Then

$$\delta_t u_i^k = (J * u^k)_i - (J * 1)_i u_i^k + \psi(u_i^k, u_i^{k+1}) + l\theta_i^k \tag{2.3}$$

and

$$l\delta_t u_i^k + \delta_t \theta_i^k = \delta_x^2 \theta_i^k, \tag{2.4}$$

both for $0 \le i \le M$ and $0 \le k \le K - 1$. The Neumann boundary condition is expressed by

$$\frac{\theta_1^k - \theta_{-1}^k}{2\triangle x} = 0, \text{ and } \frac{\theta_{M+1}^k - \theta_{M-1}^k}{2\triangle x} = 0 \text{ for } 0 \le k \le K, \tag{2.5}$$

with

$$\delta_t u_i^k = \frac{u_i^{k+1} - u_i^k}{\triangle t}, \quad \delta_x^2 \theta_i^k = \frac{\theta_{i+1}^k - 2\theta_i^k + \theta_{i-1}^k}{\triangle x^2}$$

and

$$(J * u^k)_i = \triangle x \left[\frac{1}{2} J(x_0 - x_i)u_0^k + \sum_{m=1}^{M-1} J(x_m - x_i)u_m^k + \frac{1}{2} J(x_M - x_i)u_M^k\right].$$

Here we use

$$\psi(u_i^k, u_i^{k+1}) = u_i^k - \left(u_i^k\right)^2 u_i^{k+1}$$

for the discretization of f. It will be shown later that this choice of ψ in place of $\psi(u_i^k) = u_i^k - (u_i^k)^3$ is necessary to prove both the convergence and the stability of of the numerical scheme.

Now for $n = 2$, meaning a rectangular domain $(-L, L) \times (-W, W) \subset \mathbb{R}^2$, we have

$$\Omega_{x,\,y} = \{(x_i, y_j)|\, x_i = -L + i\triangle x,\, y_j = -W + j\triangle y,\, 0 \le i \le M,\, 0 \le j \le N\}$$

and

$$\Omega_t = \{t_k|\, t_k = k\triangle t,\, 0 \le t \le K\},$$

where $\triangle x = 2L/M$ and $\triangle y = 2W/N$.

Our difference scheme in this case is

$$u^0_{i,\,j} = u_0(x_i, y_j) \text{ for } 0 \le i \le M,\, 0 \le j \le N, \texttt{and} \tag{2.6}$$

$$\theta^0_{i,\,j} = \theta_0(x_i, y_j) \text{ for } 0 \le i \le M,\, 0 \le j \le N, \tag{2.7}$$

with

$$\delta_t u^k_{i,\,j} = (J * u^k)_{i,\,j} - (J * 1)_{i,\,j} u^k_{i,\,j} + \psi(u^k_{i,\,j}, u^{k+1}_{i,\,j}) + l\theta^k_{i,j} \tag{2.8}$$

for $0 \le i \le M$, $0 \le j \le N$, $0 \le k \le K - 1$, and

$$l\delta_t u^k_{i,\,j} + \delta_t \theta^k_{i,j} = \delta^2_x \theta^k_{i,\,j} + \delta^2_y \theta^k_{i,\,j} \tag{2.9}$$

for $0 \le i \le M$, $0 \le j \le N$, $1 \le k \le K$. The Neumann boundary condition yields

$$\begin{aligned} &\frac{\theta^k_{1,j} - \theta^k_{-1,j}}{2\triangle x} = 0,\ \frac{\theta^k_{M+1,j} - \theta^k_{M-1,j}}{2\triangle x} = 0 \ \text{ for } 0 \le j \le N \text{ and} \\ &\frac{\theta^k_{i,1} - \theta^k_{i,-1}}{2\triangle y} = 0,\ \frac{\theta^k_{i,N+1} - \theta^k_{i,N-1}}{2\triangle y} = 0 \ \text{ for } 0 \le i \le M. \end{aligned} \tag{2.10}$$

In (2.8)-(2.9),

$$\begin{aligned} \delta_t u^k_{i,\,j} &= \frac{u^{k+1}_{i,\,j} - u^k_{i,\,j}}{\triangle t}, \\ \delta^2_x \theta^k_{i,\,j} &= \frac{\theta^k_{i+1,\,j} - 2\theta^k_{i,\,j} + \theta^k_{i-1,\,j}}{\triangle x^2}, \\ \delta^2_y \theta^k_{i,\,j} &= \frac{\theta^k_{i,\,j+1} - 2\theta^k_{i,\,j} + \theta^k_{i,\,j-1}}{\triangle y^2}, \end{aligned}$$

$$\begin{aligned} (J * u^k)_{i,\,j} =& \triangle x \triangle y \Bigg[\sum_{m=1}^{M-1} \sum_{n=1}^{N-1} J(x_m - x_i, y_n - y_j) u^k_{m,\,n} \\ &+ \frac{1}{2} \sum_{m=1}^{M-1} \big(J(x_m - x_i, y_0 - y_j) u^k_{m,\,0} + J(x_m - x_i, y_N - y_j) u^k_{m,\,N} \big) \\ &+ \frac{1}{2} \sum_{n=1}^{N-1} \big(J(x_0 - x_i, y_n - y_j) u^k_{0,\,n} + J(x_M - x_i, y_n - y_j) u^k_{M,\,n} \big) \\ &+ \frac{1}{4} \big(J(x_0 - x_i, y_0 - y_j) u^k_{0,\,0} + J(x_M - x_i, y_0 - y_j) u^k_{M,\,0} \\ &+ J(x_0 - x_i, y_N - y_j) u^k_{0,\,N} + J(x_M - x_i, y_N - y_j) u^k_{M,\,N} \big) \Big] \end{aligned}$$

and, as in the $n = 1$ case, we need choose for the discretization of f

$$\psi(u^k_{i,\,j}, u^{k+1}_{i,\,j}) = u^k_{i,\,j} - \left(u^k_{i,\,j}\right)^2 u^{k+1}_{i,\,j}.$$

From (2.6)-(2.10), we have

$$\begin{aligned}\left[1+(u_{i,j}^k)^2\triangle t\right]u_{i,j}^{k+1} &= \\ &\left[(J*u^k)_{i,\,j}-(J*1)_{i,\,j}u_{i,\,j}^k+u_{i,\,j}^k+l\theta_{i,j}^k\right]\triangle t+u_{i,j}^k.\end{aligned}\tag{2.11}$$

If we define $r_x = \frac{\triangle t}{\triangle x^2}$ and $r_y = \frac{\triangle t}{\triangle y^2}$, then (2.9)-(2.10) yield

$$\begin{aligned}\theta_{i,j}^{k+1} &= r_x(\theta_{i+1,j}^k+\theta_{i-1,j}^k)+(1-2r_x-2r_y)\theta_{i,j}^k\\ &+r_y(\theta_{i,j+1}^k+\theta_{i,j-1}^k)-l(u_{i,j}^{k+1}-u_{i,j}^k)\end{aligned}\tag{2.12}$$

for $1\le i\le M-1$ and $1\le j\le N-1$. The boundary conditions give rise to

$$\begin{aligned}\theta_{0,0}^{k+1} &= 2r_x\theta_{1,0}^k+(1-2r_x-2r_y)\theta_{0,0}^k\\ &+2r_y\theta_{0,1}^k-l(u_{0,0}^{k+1}-u_{0,0}^k),\end{aligned}\tag{2.13}$$

$$\begin{aligned}\theta_{0,N}^{k+1} &= 2r_x\theta_{1,N}^k+(1-2r_x-2r_y)\theta_{0,N}^k\\ &+2r_y\theta_{0,N-1}^k-l(u_{0,N}^{k+1}-u_{0,N}^k),\end{aligned}\tag{2.14}$$

$$\begin{aligned}\theta_{M,0}^{k+1} &= 2r_x\theta_{M-1,0}^k+(1-2r_x-2r_y)\theta_{M,0}^k\\ &+2r_y\theta_{M,1}^k-l(u_{M,0}^{k+1}-u_{M,0}^k),\quad\text{and}\end{aligned}\tag{2.15}$$

$$\begin{aligned}\theta_{M,N}^{k+1} &= 2r_x\theta_{M-1,N}^k+(1-2r_x-2r_y)\theta_{M,N}^k\\ &+2r_y\theta_{M,N-1}^k-l(u_{M,N}^{k+1}-u_{M,N}^k),\end{aligned}\tag{2.16}$$

each for $0\le k\le K-1$. For $1\le j\le N-1$,

$$\begin{aligned}\theta_{0,j}^{k+1} &= 2r_x\theta_{1,j}^k+(1-2r_x-2r_y)\theta_{0,j}^k\\ &+r_y(\theta_{0,j+1}^k+\theta_{0,j-1}^k)-l(u_{M,N}^{k+1}-u_{M,N}^k)\end{aligned}\tag{2.17}$$

$$\begin{aligned}\theta_{M,j}^{k+1} &= 2r_x\theta_{M-1,j}^k+(1-2r_x-2r_y)\theta_{M,j}^k\\ &+r_y(\theta_{M,j+1}^k+\theta_{M,j-1}^k)-l(u_{M,j}^{k+1}-u_{M,j}^k);\end{aligned}\tag{2.18}$$

while for $1\le i\le M-1$, we have

$$\begin{aligned}\theta_{i,0}^{k+1} &= r_x(\theta_{i+1,0}^k+\theta_{i-1,0}^k)+(1-2r_x-2r_y)\theta_{i,0}^k\\ &+2r_y\theta_{i,1}^k-l(u_{i,0}^{k+1}-u_{i,0}^k)\end{aligned}\tag{2.19}$$

and

$$\begin{aligned}\theta_{i,N}^{k+1} &= r_x(\theta_{i+1,N}^k+\theta_{i-1,N}^k)+(1-2r_x-2r_y)\theta_{i,N}^k\\ &+2r_y\theta_{i,N-1}^k-l(u_{i,N}^{k+1}-u_{i,N}^k),\end{aligned}\tag{2.20}$$

where for each equation, $1\le k\le K-1$.

For the sake of conciseness, it will be helpful in the following theorem to make some preliminary definitions. We note that each Λ_i will exist under the assumption of boundedness of $u(0,x,y)$ and $\theta(0,x,y)$. To this end, define

$$\begin{aligned}&\Lambda_1=\sup|u(0,x,y)|,\quad \Lambda_2=\sup|\theta(0,x,y)|,\quad \Lambda_3=\sup\textstyle\int_\Omega|J(x-y)|,\\ &C_1=l\Lambda_1+\Lambda_2+2(2\Lambda_3+1)+2l^2\ \text{and}\ \ C=C_1e^{C_1T},\end{aligned}$$

where $e^{\cdot}$ is the standard exponential function.

Theorem 2.1. *If $u(0,x,y),\theta(0,x,y) \in L^\infty(\Omega)$, there exists a unique solution to the system (2.6)-(2.10), and the internal energy is conserved under this scheme. Furthermore, if $r_x + r_y < 1/2$ and $\triangle t < (l/C)^2$ where C is given above, then*

$$l \max_{i,\,j} |u^k_{i,\,j}| + \max_{i,\,j} |\theta^k_{i,\,j}| \le C \tag{2.21}$$

i.e., the scheme is stable under the maximum norm.

Proof. From equations (2.11)-(2.20), it is clear that the scheme is uniquely solvable.

The internal energy $e = \int_\Omega (\theta + lu)dx$ under this scheme can be represented by defining $e^k = e(k\triangle t)$ as

$$\begin{aligned} e^k =& \triangle x \triangle y \left[\sum_{m=1}^{M-1} \sum_{n=1}^{N-1} (lu^k_{m,n} + \theta^k_{m,n}) \right. \\ &+ \frac{1}{2} \sum_{m=1}^{M-1} \left(lu^k_{m,0} + \theta^k_{m,0} + lu^k_{m,N} + \theta^k_{m,N} \right) \\ &+ \frac{1}{2} \sum_{n=1}^{N-1} \left(lu^k_{0,n} + \theta^k_{0,n} + lu^k_{M,n} + \theta^k_{M,n} \right) \\ &+ \frac{1}{4} \left(lu^k_{0,0} + \theta^k_{0,0} + lu^k_{M,0} + \theta^k_{M,0} \right. \\ &\left.\left. + lu^k_{0,N} + \theta^k_{0,N} + lu^k_{M,N} + \theta^k_{M,N} \right) \right]. \end{aligned} \tag{2.22}$$

For $k \ge 0$, using (2.9) we have

$$\begin{aligned} e^{k+1} - e^k = & \triangle t \triangle x \triangle y \left[\sum_{m=1}^{M-1} \sum_{n=1}^{N-1} (\delta_x^2 \theta^k_{m,\,n} + \delta_y^2 \theta^k_{m,\,n}) \right. \\ &+ \frac{1}{2} \sum_{m=1}^{M-1} \left(\delta_x^2 \theta^k_{m,\,0} + \delta_y^2 \theta^k_{m,\,0} + \delta_x^2 \theta^k_{m,\,N} + \delta_y^2 \theta^k_{m,\,N} \right) \\ &+ \frac{1}{2} \sum_{n=1}^{N-1} \left(\delta_x^2 \theta^k_{0,\,n} + \delta_y^2 \theta^k_{0,\,n} + \delta_x^2 \theta^k_{M,\,n} + \delta_y^2 \theta^k_{M,\,n} \right) \\ &+ \frac{1}{4} \left(\delta_x^2 \theta^k_{0,\,0} + \delta_y^2 \theta^k_{0,\,0} + \delta_x^2 \theta^k_{M,\,0} + \delta_y^2 \theta^k_{M,\,0} \right. \\ &\left.\left. + \delta_x^2 \theta^k_{0,\,N} + \delta_y^2 \theta^k_{0,\,N} + \delta_x^2 \theta^k_{M,\,N} + \delta_y^2 \theta^k_{M,\,N} \right) \right]. \end{aligned} \tag{2.23}$$

Using the definition of the central schems and the summation gives

$$\begin{aligned} &\triangle t \sum_{m=1}^{M-1} \sum_{n=1}^{N-1} (\delta_x^2 \theta^k_{m,\,n} + \delta_y^2 \theta^k_{m,\,n}) \\ &= r_x \sum_{n=1}^{N-1} (\theta^k_{M,\,n} - \theta^k_{M-1,\,n} - \theta^k_{1,\,n} + \theta^k_{0,\,n}) \\ &+ r_y \sum_{m=1}^{M-1} (\theta^k_{m,\,N} - \theta^k_{m,\,N-1} - \theta^k_{m,\,1} + \theta^k_{m,\,0}). \end{aligned} \tag{2.24}$$

Invoking the Neumann boundary condition and the central schemes definition gives

$$\begin{aligned}
&\frac{\triangle t}{2}\sum_{m=1}^{M-1}\left(\delta_x^2\theta_{m,\,0}^k+\delta_y^2\theta_{m,\,0}^k+\delta_x^2\theta_{m,\,N}^k+\delta_y^2\theta_{m,\,N}^k\right)\\
&=r_y\sum_{m=1}^{M-1}(-\theta_{m,\,N}^k+\theta_{m,\,N-1}^k+\theta_{m,\,1}^k-\theta_{m,\,0}^k)\\
&\quad+\frac{1}{2}r_x(\theta_{M,\,0}^k-\theta_{M-1,\,0}^k-\theta_{1,\,0}^k+\theta_{0,\,0}^k)\\
&\quad+\frac{1}{2}r_x(\theta_{M,\,N}^k-\theta_{M-1,\,N}^k-\theta_{1,\,N}^k+\theta_{0,\,N}^k),
\end{aligned}\tag{2.25}$$

$$\begin{aligned}
&\frac{\triangle t}{2}\sum_{n=1}^{N-1}\left(\delta_x^2\theta_{0,\,n}^k+\delta_y^2\theta_{0,\,n}^k+\delta_x^2\theta_{M,\,n}^k+\delta_y^2\theta_{M,\,n}^k\right)\\
&=r_x\sum_{n=1}^{N-1}(-\theta_{M,\,n}^k+\theta_{M-1,\,n}^k+\theta_{1,\,n}^k-\theta_{0,\,n}^k)\\
&\quad+\frac{1}{2}r_y(\theta_{0,\,N}^k-\theta_{0,\,N-1}^k-\theta_{0,\,1}^k+\theta_{0,\,0}^k)\\
&\quad+\frac{1}{2}r_y(\theta_{M,\,N}^k-\theta_{M,\,N-1}^k-\theta_{M,\,1}^k+\theta_{M,\,0}^k),
\end{aligned}\tag{2.26}$$

and

(2.27)

$$\begin{aligned}
&\triangle t\frac{1}{4}(\delta_x^2\theta_{0,\,0}^k+\delta_y^2\theta_{0,\,0}^k+\delta_x^2\theta_{M,\,0}^k+\delta_y^2\theta_{M,\,0}^k+\delta_x^2\theta_{0,\,N}^k+\delta_y^2\theta_{0,\,N}^k+\delta_x^2\theta_{M,\,N}^k+\delta_y^2\theta_{M,\,N}^k)\\
&=\frac{1}{2}r_x(-\theta_{M,\,0}^k+\theta_{M-1,\,0}^k+\theta_{1,\,0}^k-\theta_{0,\,0}^k-\theta_{M,\,N}^k+\theta_{M-1,\,N}^k+\theta_{1,\,N}^k-\theta_{0,\,N}^k)\\
&+\frac{1}{2}r_y(-\theta_{0,\,N}^k+\theta_{0,\,N-1}^k+\theta_{0,\,1}^k-\theta_{0,\,0}^k-\theta_{M,\,N}^k+\theta_{M,\,N-1}^k+\theta_{M,\,1}^k-\theta_{M,\,0}^k).
\end{aligned}$$

Using (2.22)-(2.27), we arrive at

$$e^{k+1}=e^k\tag{2.28}$$

for $k\geq 0$. Therefore,

$$e^k=e^0,\tag{2.29}$$

showing that internal energy is conserved.

Finally, we prove statement (2.21) using induction. For $k=0$, using definitions preceding the theorem

$$\max_{i,j}|u_{i,\,j}^0|\leq\Lambda_1\tag{2.30}$$

and

$$\max_{i,j}|\theta_{i,\,j}^0|\leq\Lambda_2,\tag{2.31}$$

so that

$$l\max_{i,j}|u_{i,\,j}^0|+\max_{i,j}|\theta_{i,\,j}^0|\leq l\Lambda_1+\Lambda_2<C,\tag{2.32}$$

where C is defined before the statement of the theorem.

Assuming (2.21) is true for some natural number k, we consider $u_{i,j}^{k+1}$ and $\theta_{i,j}^{k+1}$. Here, (2.11)- (2.12) imply that

(2.33)
$$u_{i,j}^{k+1} = \left((J*u^k)_{i,\,j} - (J*1)_{i,\,j}u_{i,\,j}^k + u_{i,\,j}^k + l\theta_{i,j}^k\right)\frac{\triangle t}{1+(u_{i,j}^k)^2\triangle t} + \frac{1}{1+(u_{i,j}^k)^2\triangle t}u_{i,j}^k$$

and

$$\begin{aligned}\theta_{i,j}^{k+1} &= r_x(\theta_{i+1,j}^k + \theta_{i-1,j}^k) + (1-2r_x-2r_y)\theta_{i,j}^k \\ &\quad + r_y(\theta_{i,j+1}^k + \theta_{i,j-1}^k) - l(u_{i,j}^{k+1} - u_{i,j}^k).\end{aligned} \tag{2.34}$$

Plugging (2.33) into (2.34), we have

(2.35)
$$\begin{aligned}\theta_{i,j}^{k+1} &= r_x(\theta_{i+1,j}^k + \theta_{i-1,j}^k) + (1-2r_x-2r_y)\theta_{i,j}^k + r_y(\theta_{i,j+1}^k + \theta_{i,j-1}^k) \\ &\quad - l\left[\left((J*u^k)_{i,\,j} - (J*1)_{i,\,j}u_{i,\,j}^k + u_{i,\,j}^k + l\theta_{i,j}^k\right)\frac{\triangle t}{1+(u_{i,j}^k)^2\triangle t} - \frac{(u_{i,j}^k)^2\triangle t}{1+(u_{i,j}^k)^2\triangle t}u_{i,j}^k\right].\end{aligned}$$

If we set $|u^k| = \max_{i,j}|u_{i,j}^k|$ and $|\theta^k| = \max_{i,j}|\theta_{i,j}^k|$, and if $r_x + r_y < 1/2$, then invoking Λ_3 defined before the theorem, (2.33)-(2.35) imply

$$|u_{i,j}^{k+1}| \le (2\Lambda_3+1)|u^k|\triangle t + l|\theta^k|\triangle t + \frac{1}{1+(u_{i,j}^k)^2\triangle t}|u_{i,j}^k| \tag{2.36}$$

and

$$|\theta_{i,j}^{k+1}| \le |\theta^k| + l(2\Lambda_3+1)|u^k|\triangle t + l^2|\theta^k|\triangle t + \frac{l(u_{i,j}^k)^2\triangle t}{1+(u_{i,j}^k)^2\triangle t}|u_{i,j}^k|. \tag{2.37}$$

Since $h(x) = \frac{x}{1+x}$ is an increasing function for $x \ge 0$, we have

$$\frac{(u_{i,j}^k)^2\triangle t}{1+(u_{i,j}^k)^2\triangle t}|u_{i,j}^k| \le \frac{|u^k|^2\triangle t}{1+|u^k|^2\triangle t}|u^k|.$$

This inequality together with (2.37) imply

$$|\theta^{k+1}| \le |\theta^k| + l(2\Lambda_3+1)|u^k|\triangle t + l^2|\theta^k|\triangle t + \frac{l|u^k|^2\triangle t}{1+|u^k|^2\triangle t}|u^k| \;\; . \tag{2.38}$$

Since (2.36) is true for all i and j, and because there exist i_0 and j_0 such that $|u^{k+1}| = |u_{i_0,j_0}^{k+1}|$, we arrive at

$$l|u^{k+1}| = l|u_{i_0,j_0}^{k+1}| \le l(2\Lambda_3+1)|u^k|\triangle t + l^2|\theta^k|\triangle t + \frac{l}{1+(u_{i_0,j_0}^k)^2\triangle t}|u_{i_0,j_0}^k|. \tag{2.39}$$

We need the following lemma.

Lemma 2.2. *If $b \ge a > 0$ and $\triangle t \le 1/b^2$, then*

$$\frac{1}{1+a^2\triangle t}a + \frac{b^2\triangle t}{1+b^2\triangle t}b \le b. \tag{2.40}$$

Proof. Since the proof is straightforward, we omit it here. □

Adding (2.38) and (2.39) implies

$$
\begin{aligned}
|\theta^{k+1}| + l|u^{k+1}| \le |\theta^k| &+ 2l(2\Lambda_3+1)|u^k|\triangle t + 2l^2|\theta^k|\triangle t \\
&+ \frac{l|u^k|^2\triangle t}{1+|u^k|^2\triangle t}|u^k| + \frac{l}{1+(u^k_{i_0,j_0})^2\triangle t}|u^k_{i_0,j_0}|.
\end{aligned} \tag{2.41}
$$

We have assumed the statement is true for k, so $l|u^k| + |\theta^k| < C$. Therefore $|u^k| < C/l$. Also by the definition of $|u^k|$, we have $|u^k| \ge |u^k_{i_0,j_0}|$. If $\triangle t < (l/C)^2$, then $\triangle t < 1/|u^k|^2$. Using Lemma 2.2 we have

$$
\frac{l}{1+(u^k_{i_0,j_0})^2\triangle t}|u^k_{i_0,j_0}| + \frac{l|u^k|^2\triangle t}{1+|u^k|^2\triangle t}|u^k| \le l|u^k|. \tag{2.42}
$$

Using (2.41) and (2.42) together with the definiton of C_1 preceding the theorem, we get

$$
\begin{aligned}
|\theta^{k+1}| + l|u^{k+1}| &\le |\theta^k| + l|u^k| + 2l(2\Lambda_3+1)|u^k|\triangle t + 2l^2|\theta^k|\triangle t \\
&\le (1+C_1\triangle t)(|\theta^k| + l|u^k|) \\
&\cdots \\
&\le (1+C_1\triangle t)^{k+1}(|\theta^0| + l|u^0|) \\
&\le e^{C_1T}C_1 = C.
\end{aligned} \tag{2.43}
$$

So the statement is true for $k+1$. Therefore,

$$
\max_{i,\,j,\,k} l|u^k_{i,\,j}| + \max_{i,\,j,\,k} |\theta^k_{i,\,j}| \le C, \tag{2.44}
$$

where C is independent of k and of the spatial mesh size. □

Remark 2.3. *A similar result holds for $n \ge 3$.*

Next we consider error estimates for the proposed scheme. For the solution of (1.1)-(1.4), we have the following lemma.

Lemma 2.4. *Suppose that J and f satisfy the following assumptions:*

- (A_1) *$M \equiv \sup \int_\Omega |J(x-y)|dy < \infty$ and $f \in C(\mathbb{R})$.*
- (A_2) *There exist $c_1 > 0$, $c_2 > 0$, $c_3 > 0$, $c_4 > 0$ and $r > 2$ such that $f(u)u \ge c_1|u|^r - c_2|u|$, and $|f(u)| \le c_3|u|^{r-1} + c_4$.*

If assumptions $(A_1) - (A_2)$ are satisfied, $u_0 \in L^\infty(\Omega)$ and $\theta_0 \in L^\infty \cap H^1(\Omega)$, then there exists a unique solution $(u,\theta) \in C([0,T], L^\infty(\Omega))$ to the system (1.1)-(1.4) such that $u_t \in L^\infty(Q_T)$, and u_{tt}, θ_t, $\triangle\theta \in L^2(Q_T)$, where $Q_T = [0,T]\times\bar{\Omega}$.

Proof. The proof of the lemma is a similar argument to that in the proof of Theorem 2.3 in [4]; we omit it here. □

We note that although Lemma 2.4 is more general than for $f(u) = u^3 - u$ that we consider here, the conditions in the lemma are satisfied for our choice of f for the nonlinear function in (1.1).

Theorem 2.5. *If the system (1.1)-(1.4) has a solution $(u,\theta) \in C^{1,2}([0,T]\times\bar{\Omega})$, then the solution of the difference scheme converges to this solution uniformly, and the convergence rate is $O(\triangle t + \triangle x^2 + \triangle y^2)$.*

Proof. Let $(U(t,x,y),\, V(t,x,y))$ be the solution of the system (1.1)-(1.4). We use the following notation:

$$\begin{aligned} U^0_{i,\,j} &= u_0(x_i,y_j),\, U^k_{i,\,j} = u(t_k,x_i,y_j), \\ V^0_{i,\,j} &= \theta_0(x_i,y_j),\, V^k_{i,\,j} = \theta(t_k,x_i,y_j). \end{aligned} \tag{2.45}$$

From (1.1)-(1.4), we have for $k \geq 0$,

$$\begin{aligned} \frac{U^{k+1}_{i,\,j} - U^k_{i,\,j}}{\triangle t} &= (J * U^k)_{i,\,j} - (J*1)_{i,\,j} U^k_{i,\,j} \\ &\quad + U^k_{i,\,j} - (U^k_{i,\,j})^3 + l V^k_{i,j} + R_1(\triangle t, \triangle x, \triangle y), \end{aligned} \tag{2.46}$$

where $R_1(\triangle t, \triangle x, \triangle y) = O(\triangle t + \triangle x^2 + \triangle y^2)$.

Then

$$\begin{aligned} l\frac{U^{k+1}_{i,\,j} - U^k_{i,\,j}}{\triangle t} + \frac{V^{k+1}_{i,\,j} - V^k_{i,\,j}}{\triangle t} &= \frac{V^k_{i+1,j} - 2V^k_{i,j} + V^k_{i-1,j}}{\triangle x^2} \\ &\quad + \frac{V^k_{i,j+1} - 2V^k_{i,j} + V^k_{i,j-1}}{\triangle y^2} + R_2(\triangle t, \triangle x, \triangle y), \end{aligned} \tag{2.47}$$

with Neumann boundary condition

$$\begin{aligned} V^k_{1,j} = V^k_{-1,j} + O(\triangle x^2),\, V^k_{M+1,j} = V^k_{M-1,j} + O(\triangle x^2) \quad \text{for } 0 \leq j \leq N, \\ V^k_{i,1} = V^k_{i,-1} + O(\triangle y^2),\, V^k_{i,N+1} = V^k_{i,N-1} + O(\triangle y^2) \quad \text{for } 0 \leq i \leq M, \end{aligned} \tag{2.48}$$

where $R_2(\triangle t, \triangle x, \triangle y) = O(\triangle t + \triangle x^2 + \triangle y^2)$.
We define error terms

$$X^k_{i,\,j} = U^k_{i,\,j} - u^k_{i,\,j} \text{ for } k = 0,\, \ldots, K,\; i = 0,\, \ldots, M,\; j = 0,\, \ldots, N \tag{2.49}$$

and

$$Y^k_{i,\,j} = V^k_{i,\,j} - \theta^k_{i,\,j} \text{ for } k = 0,\, \ldots, K,\; i = 0,\, \ldots, M,\; j = 0,\, \ldots, N. \tag{2.50}$$

From (2.6), (2.7) and (2.45), we have

$$X^0_{i,\,j} = 0,\;\; Y^0_{i,\,j} = 0 \;\text{ for } i = 0, \cdots, M,\; j = 0, \cdots, N. \tag{2.51}$$

Turning now to $k \geq 1$, (2.8) and (2.46) yield

$$\begin{aligned} X^{k+1}_{i,\,j} &= \triangle t[(J * X^k)_{i,\,j} - (J*1)_{i,j} X^k_{i,\,j} + X^k_{i,\,j} \\ &\quad - (U^3(t_k,x_i,y_j) - (u^k_{i,\,j})^2 u^{k+1}_{i,\,j}) + X^k_{i,\,j} + l Y^k_{i,j}] \\ &\quad + X^k_{i,\,j} + \triangle t R_1(\triangle t, \triangle x, \triangle y). \end{aligned} \tag{2.52}$$

Since

$$\begin{aligned} (U^k_{i,j})^3 - (u^k_{i,j})^2 u^{k+1}_{i,j} &= (U^k_{i,j})^2 (U^k_{i,j} - U^{k+1}_{i,j}) \\ &\quad + X^k_{i,j}(U^k_{i,j} + u^k_{i,j}) U^{k+1}_{i,j} \\ &\quad + (u^k_{i,j})^2 X^{k+1}_{i,j}, \end{aligned} \tag{2.53}$$

equation (2.52) implies

$$\begin{aligned}&\left[1+\triangle t(u^k_{i,\,j})^2\right]X^{k+1}_{i,\,j}=\\&\quad\triangle t\left[(J*X^k)_{i,\,j}-(J*1)_{i,j}X^k_{i,\,j}+X^k_{i,\,j}\right.\\&\qquad\left.-(U^k_{i,j})^2(U^k_{i,j}-U^{k+1}_{i,j})-X^k_{i,j}(U^k_{i,j}+u^k_{i,j})U^{k+1}_{i,j}\right]\\&\qquad+X^k_{i,j}+l\triangle tY^k_{i,j}+\triangle t\cdot O(\triangle t+\triangle x^2+\triangle y^2).\end{aligned}\tag{2.54}$$

From Lemma 2.4, u and u_t are bounded in Q_T, so

$$|(U^k_{i,j})^2(U^k_{i,j}-U^{k+1}_{i,j})|\le(\Lambda_2)^2\Lambda_4\triangle t,\tag{2.55}$$

where $\Lambda_2=\max_{i,j,k}|U^k_{i,\,j}|$, $\Lambda_4=\max_{Q_T}|u_t|$.

Now equations (2.54) and (2.55) and the boundedness of $|U^k_{i,j}|$ and $|u^k_{i,j}|$ suggest that

$$\begin{aligned}\max_{i,j}|X^{k+1}_{i,\,j}|&\le C(\Lambda_1,\Lambda_2,\Lambda_3)\triangle t\max_{i,j}|X^k_{i,\,j}|\\&\qquad+\max_{i,j}|X^k_{i,\,j}|+l\triangle t\max_{i,j}|Y^k_{i,j}|+|\triangle tR_2|,\end{aligned}\tag{2.56}$$

where $C(\Lambda_1,\Lambda_2,\Lambda_3)$ depends only on $\Lambda_1=\max_{i,j,k}|u^k_{i,\,j}|$, $\Lambda_2=\max_{i,j,k}|U^k_{i,\,j}|$ and $\Lambda_3=\sup\int_\Omega|J(x-y)|dy$, and where $R_2=O(\triangle t+\triangle x^2+\triangle y^2)$. Equations (2.9) and (2.47) together lead to

$$\begin{aligned}&l\frac{X^{k+1}_{i,j}-X^k_{i,j}}{\triangle t}+\frac{Y^{k+1}_{i,j}-Y^k_{i,j}}{\triangle t}\\&=\frac{Y^k_{i+1,j}-2Y^k_{i,j}+Y^k_{i-1,j}}{\triangle x^2}\\&+\frac{Y^k_{i,j+1}-2Y^k_{i,j}+Y^k_{i,j-1}}{\triangle y^2}+R_3(\triangle t,\triangle x,\triangle y),\end{aligned}\tag{2.57}$$

with Neumann boundary condition

$$\begin{aligned}&Y^k_{1,j}=Y^k_{-1,j}+(\triangle x^2),\ Y^k_{M+1,j}=Y^k_{M-1,j}+O(\triangle x^2)\quad\text{for } 0\le j\le N,\\&Y^k_{i,1}=Y^k_{i,-1}+O(\triangle y^2),\ Y^k_{i,N+1}=Y^k_{i,N-1}+O(\triangle y^2)\quad\text{for } 0\le i\le M,\end{aligned}\tag{2.58}$$

where $R_3(\triangle t,\triangle x,\triangle y)=O(\triangle t+\triangle x^2+\triangle y^2)$. Thus

$$\begin{aligned}Y^{k+1}_{i,\,j}&=r_x(Y^k_{i+1,j}+Y^k_{i-1,j})+r_y(Y^k_{i,j+1}+Y^k_{i,j-1})\\&\quad+(1-2r_x-2r_y)Y^k_{i,j}+\\&\quad-l(X^{k+1}_{i,j}-X^k_{i,j})+\triangle tR_3(\triangle t,\triangle x,\triangle y).\end{aligned}\tag{2.59}$$

If $r_x+r_y<1/2$, equation (2.59) gives rise to

$$\begin{aligned}\max_{i,j}|Y^{k+1}_{i,\,j}|&\le\max_{i,j}|Y^k_{i,j}|+l\max_{i,j}|X^{k+1}_{i,j}-X^k_{i,j}|\\&\qquad+\triangle tR_3(\triangle t,\triangle x,\triangle y).\end{aligned}\tag{2.60}$$

Invoking equation (2.52) and the boundedness of $|U^k_{i,j}|$ and $|u^k_{i,j}|$, we have

$$\begin{aligned}l\max_{i,j}|X^{k+1}_{i,j}-X^k_{i,j}|&\le lC(\Lambda_1,\Lambda_2,\Lambda_3)\triangle t\max_{i,j}|X^k_{i,j}|\\&\qquad+l^2\triangle t\max_{i,j}|Y^k_{i,j}|+l\triangle tR_1(\triangle t,\triangle x,\triangle y),\end{aligned}\tag{2.61}$$

where $C(\Lambda_1, \Lambda_2, \Lambda_3)$ and $R_1 = O(\triangle t + \triangle x^2 + \triangle y^2)$ are defined as before. Finally, using equations (2.56), (2.60) and (2.61), we arrive at

$$\begin{aligned}
&\max_{i,j} |X_{i,j}^{k+1}| + \max_{i,j} |Y_{i,j}^{k+1}| \\
&\qquad \le (1 + C(\Lambda_1, \Lambda_2, \Lambda_3, l)\triangle t)(\max_{i,j} |X_{i,j}^{k}| + \max_{i,j} |Y_{i,j}^{k}|) \\
&\qquad\quad + l\triangle t R_4(\triangle t, \triangle x, \triangle y) \\
&\qquad \le (1 + C(\Lambda_1, \Lambda_2, \Lambda_3, l)\triangle t)^2(\max_{i,j} |X_{i,j}^{k-1}| + \max_{i,j} |Y_{i,j}^{k-1}|) \\
&\qquad\quad + 2l\triangle t R_4(\triangle t, \triangle x, \triangle y) \qquad (2.62)\\
&\qquad \vdots \\
&\qquad \le (1 + C(\Lambda_1, \Lambda_2, \Lambda_3, l)\triangle t)^{k+1}(\max_{i,j} |X_{i,j}^{0}| + \max_{i,j} |Y_{i,j}^{0}|) \\
&\qquad\quad + (k+1)\triangle t R_4(\triangle t, \triangle x, \triangle y) \\
&\qquad \le T l R_4(\triangle t, \triangle x, \triangle y) = O(\triangle t + \triangle x^2 + \triangle y^2),
\end{aligned}$$

establishing Theorem 2.5. □

Remark 2.6. *The scheme for the Neumann boundary condition can also be applied to the problem with the Dirichlet boundary condition. However, for the Dirichlet problem, the internal energy is not conserved.*

3. Numerical Results

Having established stability and convergence of the difference scheme, in this section we investigate some numerical approximations of the solution to (1.1)-(1.4). In the graph, we use T as the temperature instead of θ.

For $n = 1$, let $\Omega = (-1, 1)$, $f(u) = u^3 - u$, $J(x) = 10e^{-100x^2}$ and $l = 1$. Figures 1-3 show the numerical results for the phase field system at $t = 0, 10, 20$ and 40 with initial values

$$u_0(x) = 0.8\sin(2\pi x),\ \ \theta_0(x) = 0.5 + 0.1\cos(2\pi x).$$

Figures 4-6 show the numerical results for the phase field system at $t = 0, 10, 20$, and 40 with initial values

$$u_0(x) = 0.8\sin(2\pi x),\ \ \theta_0(x) = 0.5\cos(2\pi x).$$

Figures 7-8 show the numerical results for the phase field system at $t = 0, 10, 20$, and 40 with initial values

$$u_0(x) = 0.8\sin(2\pi x),\ \ \theta_0(x) = -0.5 + 0.1\cos(2\pi x).$$

For $n = 2$, let $\Omega = (0, 1) \times (0, 1)$, $J_\epsilon(x, y) = 10e^{-100(x^2+y^2)}$, $\triangle t = 0.0005$, $\triangle x = 0.05$ and $\triangle y = 0.05$. Figures 10-12 show the numerical results at $t = 2, 4$ and 5 with initial values

$$u_0(x, y) = 0.8\cos(2\pi x) * \cos(2\pi y),\ \theta_0(x, y) = 0.5 + 0.1\cos(2\pi x) * \cos(2\pi y).$$

Figures 13-15 show the numerical results at $t = 2, 4$ and 5 with initial values

$$u_0(x, y) = 0.8\cos(2\pi x) * \cos(2\pi y),\ \theta_0(x, y) = 0.1\cos(2\pi x) * \cos(2\pi y).$$

Figures 16-18 show the numerical results at $t = 2, 4$ and 5 with initial data

$$u_0(x, y) = 0.8\cos(2\pi x) * \cos(2\pi y),\ \theta_0(x, y) = -0.5 + 0.1\cos(2\pi x) * \cos(2\pi y).$$

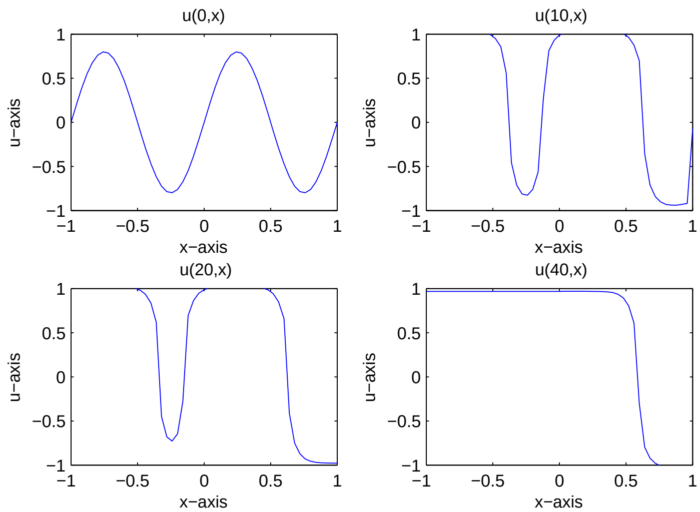

FIGURE 1. The order parameter u in the phase field system for $n = 1$ with $u_0(x) = 0.8\sin(2\pi x),\ \theta_0(x) = 0.5 + 0.1\cos(2\pi x), \triangle t = 0.0001, \triangle x = 0.002$.

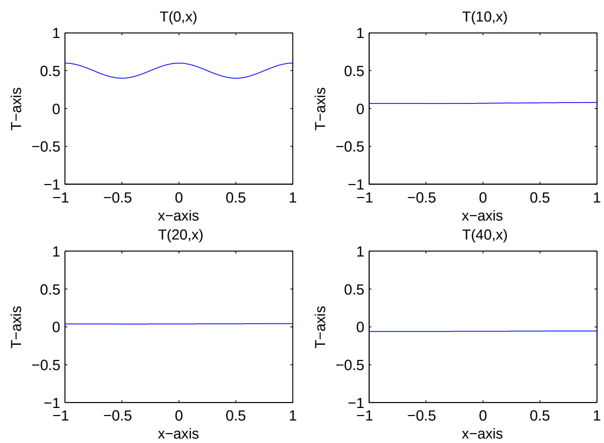

FIGURE 2. The temperature T in the phase field system for $n = 1$ with $u_0(x) = 0.8\sin(2\pi x),\ \theta_0(x) = 0.5 + 0.1\cos(2\pi x), \triangle t = 0.0001, \triangle x = 0.002$.

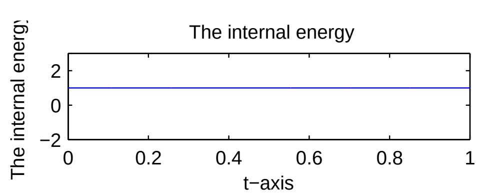

FIGURE 3. The internal energy in the phase field system for $n = 1$ with $u_0(x) = 0.8\sin(2\pi x),\ \theta_0(x) = 0.5 + 0.1\cos(2\pi x), \triangle t = 0.0001, \triangle x = 0.002$.

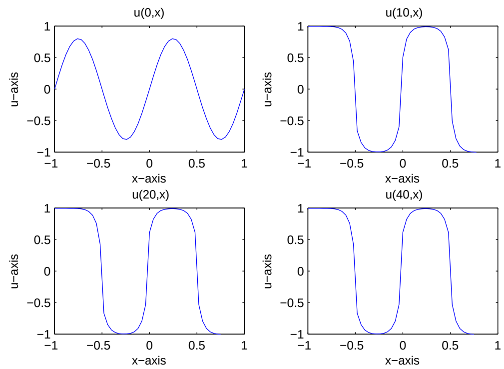

FIGURE 4. The order parameter u in the phase field system for $n = 1$ with $u_0(x) = 0.8\sin(2\pi x),\ \theta_0(x) = 0.5\cos(2\pi x), \triangle t = 0.0001, \triangle x = 0.002$.

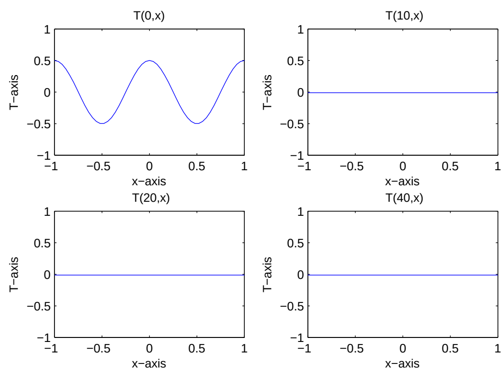

FIGURE 5. The temperature T in the phase field system for $n = 1$.

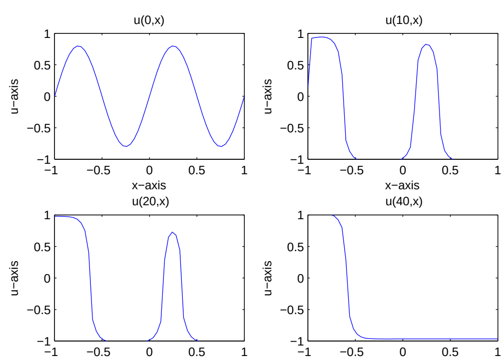

FIGURE 6. The order parameter u in the phase field system for $n = 1$ with $u_0(x) = 0.8\sin(2\pi x),\ \theta_0(x) = -0.5 + 0.1\cos(2\pi x), \triangle t = 0.0001, \triangle x = 0.002$.

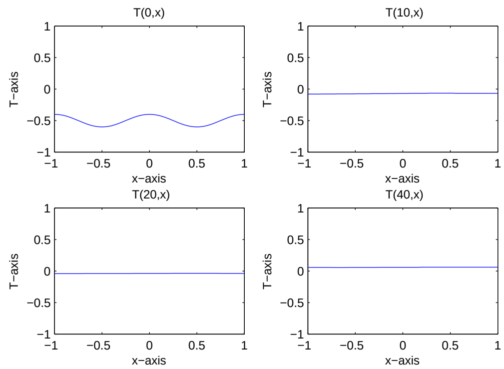

FIGURE 7. The temperature T in the phase field system for $n = 1$ with $u_0(x) = 0.8\sin(2\pi x)$, $\theta_0(x) = -0.5 + 0.1\cos(2\pi x), \triangle t = 0.0001, \triangle x = 0.002$.

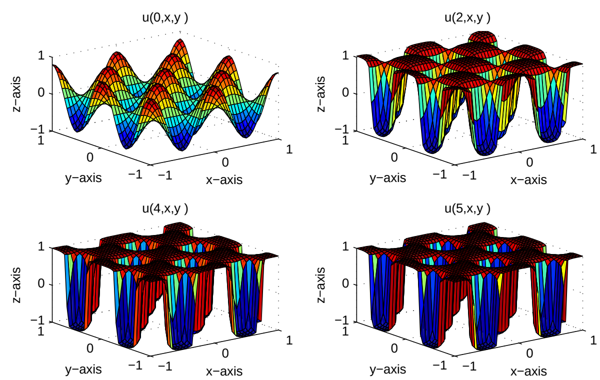

FIGURE 8. The order parameter u in the phase field system for $n = 2$ with $u_0(x, y) = 0.8\cos(2\pi x) * \cos(2\pi y)$, $\theta_0(x, y) = 0.5 + 0.1\cos(2\pi x) * \cos(2\pi y), \triangle t = 0.0005, \triangle x = 0.05, \triangle y = 0.05$.

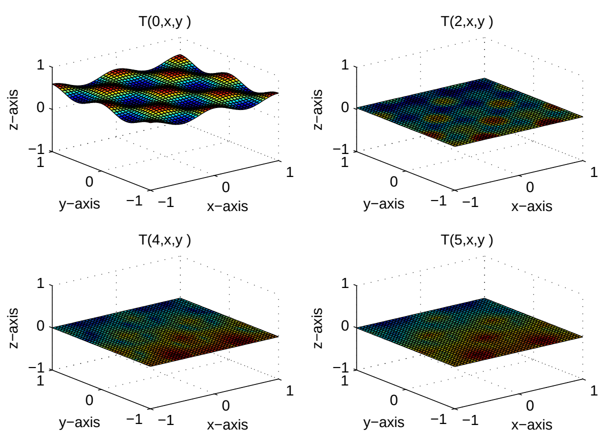

FIGURE 9. The temperature T in the phase field system for $n = 2$.

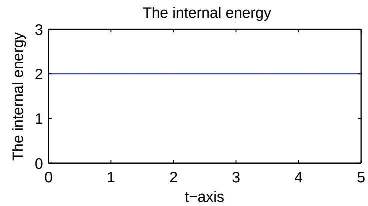

FIGURE 10. The internal energy in the phase field system for $n = 2$ with $u_0(x, y) = 0.8\cos(2\pi x) * \cos(2\pi y)$, $\theta_0(x, y) = 0.5 + 0.1\cos(2\pi x) * \cos(2\pi y)$, $\triangle t = 0.0005$, $\triangle x = 0.05$, $\triangle y = 0.05$.

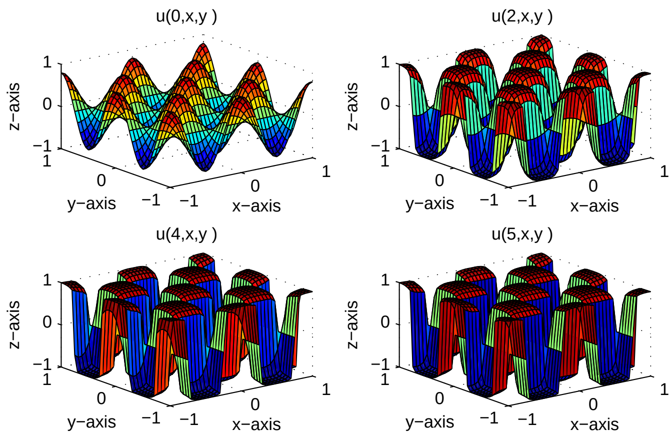

FIGURE 11. The order parameter u in the phase field system for $n = 2$ with $u_0(x, y) = 0.8\cos(2\pi x) * \cos(2\pi y)$, $\theta_0(x, y) = 0.1\cos(2\pi x) * \cos(2\pi y)$, $\triangle t = 0.0005$, $\triangle x = 0.05$, $\triangle y = 0.05$.

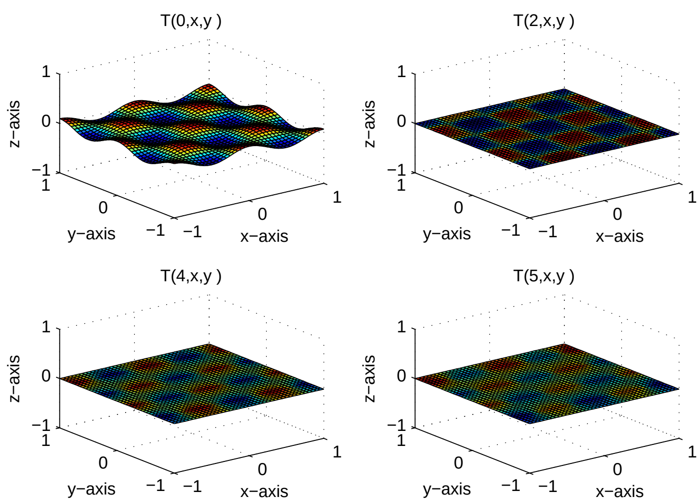

FIGURE 12. The temperature T in the phase field system for $n = 2$ with $u_0(x, y) = 0.8\cos(2\pi x) * \cos(2\pi y)$, $\theta_0(x, y) = 0.1\cos(2\pi x) * \cos(2\pi y)$, $\triangle t = 0.0005$, $\triangle x = 0.05$, $\triangle y = 0.05$.

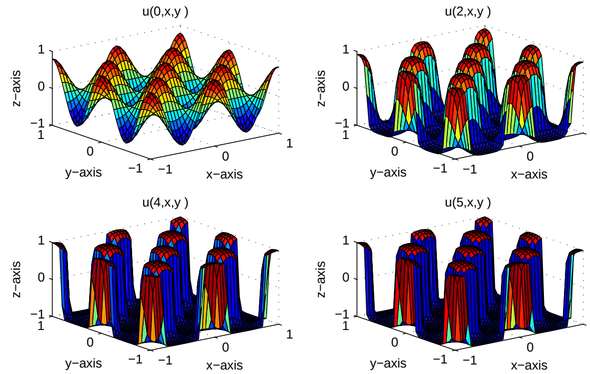

FIGURE 13. The order parameter u in the phase field system for $n = 2$ with $u_0(x, y) = 0.8\cos(2\pi x) * \cos(2\pi y)$, $\theta_0(x, y) = -0.5 + 0.1\cos(2\pi x) * \cos(2\pi y), \triangle t = 0.0005, \triangle x = 0.05, \triangle y = 0.05$.

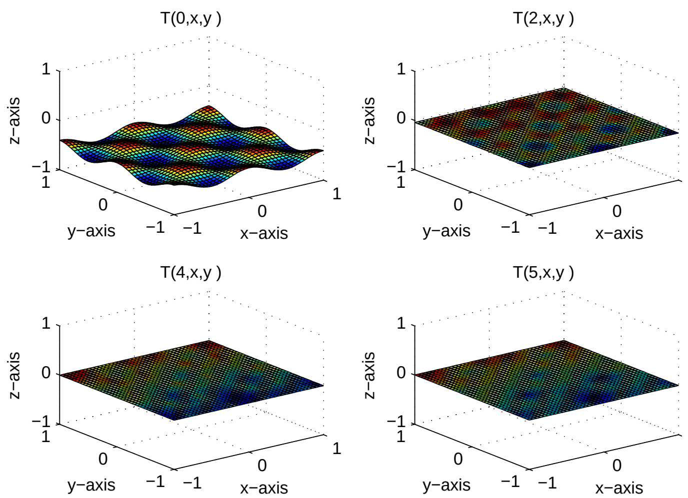

FIGURE 14. The temperature T in the phase field system for $n = 2$ with $u_0(x, y) = 0.8\cos(2\pi x) * \cos(2\pi y)$, $\theta_0(x, y) = -0.5 + 0.1\cos(2\pi x) * \cos(2\pi y), \triangle t = 0.0005, \triangle x = 0.05, \triangle y = 0.05$.

In Figures 1-3 and Figures 10-12, we see that when the initial temperature is greater than zero, θ will decrease to a negative constant and u will approach a piecewise defined constant function which will approach 1 in the greater portion of the region. During this process, the internal energy is conserved as predicted by Theorem 2.1.

Figures 4-5 and Figures 11-12 suggest that when the initial temperature oscillates about zero, θ will approach zero while u approaches a piecewise defined constant function. Both are also steady state solutions for the phase-field system. During this process, we have checked that the internal energy is also conserved as expected.

The graphs in figures 6-7 and Figures 13-14 demonstrate the reasonable result that over time and with the negative, nonconstant initial temperature, θ will increase to a positive constant on Ω, while u approaches a piecewise-constant function that is represented by state value of -1 in the greater portion of Ω. The theoretical analysis for this steady state solution will be investigated in a future paper.

Remark 3.1. *We also checked the numerical result with discontinuous but bounded functions used as initial conditions functions. The numerical results show behavior similar to that obtained with smooth initial functions agreeing with the finding that they need only be bounded functions.*

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