A stable finite difference method for a Cahn-Hilliard type equation with long-range interaction

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Abstract   We propose a stable numerical scheme for a Cahn-Hilliard type equation with long-range interaction describing the micro-phase separation of diblock copolymer melts. The scheme is designed by using the discrete variational derivative method, one of structure preserving numerical methods. The derivation of the discrete variational derivative of a discretized energy functional is simplified by using a suitable discrete L^2 space and fractional powers of a discrete approximation of the Laplace operator. The proposed scheme has the same characteristic properties, mass conservation and energy dissipation, as the original equation does. We also discuss the stability and unique solvability of the scheme.

1   Introduction

In this paper we consider a numerical scheme for the following initial-boundary value problem:

$$\frac{\partial u}{\partial t} = \Delta\left(-\varepsilon^2 \Delta u + W'(u)\right) - \sigma(u - \overline{u}), \quad x \in \Omega,\, t > 0, \tag{1.1}$$

$$\frac{\partial u}{\partial \nu} = \frac{\partial \Delta u}{\partial \nu} = 0, \qquad\qquad x \in \partial\Omega,\, t > 0, \tag{1.2}$$

$$u(0, x) = u_0(x), \qquad\qquad x \in \Omega, \tag{1.3}$$

where Ω is a rectangular domain in $\mathbb{R}^n$, ν is the outward unit normal to $\partial\Omega$, $W(u) = \frac{1}{4}(u^2 - 1)^2$ is a double-well potential with equal well-depth and ε, σ are positive con-

stants.

Problem (1.1)–(1.3) arises in a model of micro-phase separation of diblock copoly-mers where subchains of two different type of monomers are chemically bonded. Repul-sive forces between different monomers induce phase separation. However, macroscopic phase separation does not occur because of the chemical bond and hence microscopic patterns may appear. Ohta and Kawasaki [12] proposed a phenomenological model for the copolymer configuration based on the Landau-type free energy functional incorpo-rated with a Coulomb-type long-range effect. Nishiura and Ohnishi [10] reformulated the energy functional in the following form:

$$J(u) = \int_{\Omega} G(u, \nabla u) dx, \tag{1.4}$$

$$G(u, \nabla u) = \frac{\varepsilon^2}{2} |\nabla u|^2 + W(u) + \frac{\sigma}{2} \left| (-\Delta_N)^{-1/2} (u - \overline{u}) \right|^2, \tag{1.5}$$

where u is a rescaled ratio of the densities of two monomers, $\varepsilon > 0$ is a small param-eter depending on the size and mobility of monomers, $W(u)$ is a double-well potential with global minima at $u = \pm 1$, $\sigma > 0$ is a parameter related to the polymerization in-dex, $(-\Delta_N)^{-1/2}$ is a fractional power of the Laplace operator in Ω under the zero-flux boundary conditions and

$$\overline{u} = \frac{1}{|\Omega|} \int_{\Omega} u \, dx \in [-1, 1]$$

is the average of the rescaled density ratio. The third term of the energy functional de-scribes nonlocal interactions which prevent copolymers forming large blocks of mono-mers. Indeed, the term is computed by using the Green's function $\Gamma(x, y)$ of $-\Delta$ under the zero-flux boundary conditions in the following way:

$$\frac{\sigma}{2} \int_{\Omega} \left| (-\Delta_N)^{-1/2} (u - \overline{u}) \right|^2 dx = \frac{\sigma}{2} \int_{\Omega} |\nabla v|^2 dx,$$

where

$$v(x) = \int_{\Omega} \Gamma(x, y) (u(y) - \overline{u}) dy.$$

Due to the compactness of $(-\Delta_N)^{-1/2}$, the third term prefers rapid oscillation of u around $\overline{u}$ [10].

In order to build a dynamical model for diblock copolymers, we consider a mass-conserved gradient flow of the energy functional with respect to the H^{-1}-norm. The resulting equation is

$$\frac{\partial u}{\partial t} = \Delta \frac{\delta J}{\delta u}, \tag{1.6}$$

where $\delta J / \delta u$ is the (first) functional derivative of J given by

$$\frac{\delta J}{\delta u} = -\varepsilon^2 \Delta u + W'(u) + \sigma (-\Delta_N)^{-1} (u - \overline{u}). \tag{1.7}$$

Thus we obtain equation (1.1). When $\sigma = 0$, equation (1.1) reduces to the well-known Cahn-Hilliard equation, a model of macro-phase separation in binary alloys [2].

From the above derivation we easily see that problem (1.1)–(1.3) has mass conservation and energy dissipation properties as follows:

$$\frac{d}{dt}\int_\Omega u\,dx = \int_\Omega \Delta\frac{\delta J}{\delta u}dx = \int_{\partial\Omega}\frac{\partial}{\partial\nu}\frac{\delta J}{\delta u}dS = 0,$$

$$\frac{d}{dt}J(u) = \int_\Omega \frac{\delta J}{\delta u}\frac{\partial u}{\partial t}dx = -\int_\Omega\left|\nabla\left(\frac{\delta J}{\delta u}\right)\right|^2 dx \le 0.$$

Here we used the fact that the normal derivative of each term of $\delta J/\delta u$ vanishes on $\partial\Omega$ due to the boundary conditions (1.2).

It is experimentally and numerically known that the final asymptotic states in the evolution of the copolymer configuration are periodic patterns such as lamellar, cylindrical, spherical and gyroid structures [1, 9]. However, it is not easy to solve numerically the Cahn-Hilliard-type equation (1.1). One reason is that the right-hand side of (1.1) includes the term $\Delta W'(u) = (3u^2 - 1)\Delta u + 6u|\nabla u|^2$. Since ε is small, (1.1) is nearly backward parabolic where u is close to 0 and its numerical solution is obviously unstable. Another reason is the presence of nonlocal term $\overline{u}$ in (1.1). Since $\overline{u}$ is exactly constant as is seen above, we have to choose a suitable numerical method by which the approximated value of $\overline{u}$ is computable with high accuracy.

The first aim of the present paper is to propose a stable finite difference scheme for the Cahn-Hilliard type equation (1.1) by using the so-called discrete variational derivative method. The method was proposed by Furihata and Mori [6] to give a stable numerical scheme for the Cahn-Hilliard equation, and has been applied to various partial differential equations with variational structure such as energy conservation/dissipation. A standard procedure for constructing the scheme by the discrete variational derivative method is the following (see [5] for details):

Step 1: Define a discrete energy as an approximation of the energy associated with the original problem.

Step 2: Take its discrete variation to obtain the discrete variational derivative.

Step 3: Construct a scheme using the discrete variational derivative.

Usually, a lengthy discrete calculus is required in Step 2 to obtain discrete formulas such as summation by parts. The second aim is to simplify the derivation of discrete variational derivatives by using a suitable discrete L^2 space and fractional powers of a discrete approximation of the Laplace operator.

This paper is organized as follows. In Section 2, we define a discrete energy functional J_d as an approximation of the original energy functional J in (1.4) using fractional

powers of the discrete Laplacian and propose a finite difference scheme for (1.1)–(1.3) in the one-dimensional case by the discrete variational derivative method. In Section 3, we derive a variational formula for the discrete variational derivative of J_d in a suitable discrete L^2 space. Characteristic properties of the proposed scheme, mass-conservation and energy dissipation, are shown in Section 4, while the stability of the scheme is proved in Section 5. Since the proposed scheme is nonlinear, the condition for unique solvability of the scheme is to be determined. In Section 6, we prove that the proposed scheme is uniquely solvable for all time steps under some assumptions on the space and time mesh sizes. We introduce a dissipative scheme for higher dimensional problems in Section 7 and give some numerical examples in Section 8.

2   Finite difference scheme for the one-dimensional case

In this section, we consider the one-dimensional case $\Omega = (0,L)$ for some fixed $L > 0$ to understand the method of deriving a dissipative scheme easily. Let $\triangle x = L/N$ be the space mesh size for uniform spatial discretization of $\overline{\Omega} = [0,L]$, where $N+1$ is the number of spatial grid points including two endpoints 0 and L. Then each vector $U = (U_0,\dots,U_N)^\mathsf{T} \in \mathbb{R}^{N+1}$ denotes an approximation of functions on $[0,L]$.

Let

$$D_2 = \frac{1}{(\triangle x)^2} \begin{pmatrix} -2 & 2 & & & \\ 1 & -2 & 1 & & \\ & \ddots & \ddots & \ddots & \\ & & 1 & -2 & 1 \\ & & & 2 & -2 \end{pmatrix}$$

be an $(N+1) \times (N+1)$ tridiagonal matrix defined as the matrix expression of the second-order central difference $(U_{k+1} - 2U_k + U_{k-1})/(\triangle x)^2$ for $U = (U_0,\dots,U_N)^\mathsf{T}$ associated with the central discretization of homogeneous Neumann boundary conditions $(U_{k+1} - U_{k-1})/(2\triangle x) = 0$ at $k = 0,N$. It is known that eigenvalues and corresponding eigenfunctions of $A = -D_2$ are given by

$$\lambda_k = \frac{2}{(\triangle x)^2} \left(1 - \cos \frac{k}{N}\pi \right), \quad \phi_k = (\phi_{k,0},\dots,\phi_{k,N})^\mathsf{T} \tag{2.1}$$

for $k = 0,\dots,N$, where $\phi_{k,j} = \cos(kj\pi/N)$ for $j = 0,\dots,N$. Note that the matrix A is singular since $\lambda_0 = 0$.

We regard $\mathbb{R}^{N+1}$ as a discrete L^2 space by introducing an inner product on $\mathbb{R}^{N+1}$, which is an analogue of the standard inner product on $L^2(\Omega)$.

Definition 2.1. For $U = (U_0,\dots,U_N)^\mathsf{T}, V = (V_0,\dots,V_N)^\mathsf{T} \in \mathbb{R}^{N+1}$, we define an inner product on $\mathbb{R}^{N+1}$ by

$$\langle U,V \rangle = \sum_{k=0}^{N} {}'' U_k V_k \triangle x, \tag{2.2}$$

where

$$\sum_{k=0}^{N}{}'' a_k = \frac{1}{2}a_0 + \sum_{k=1}^{N-1} a_k + \frac{1}{2}a_N$$

is the trapezoidal rule for numerical integration.

Remark 2.2. Letting $Q = \mathrm{diag}(1/2, 1, \ldots, 1, 1/2)$, we see that

$$\langle U, V \rangle = (QU, V)\triangle x, \tag{2.3}$$

where the symbol $(\cdot, \cdot)$ denotes the standard inner product on $\mathbb{R}^{N+1}$. Hence the positive definiteness of Q implies that (2.2) defines an inner product on $\mathbb{R}^{N+1}$.

Lemma 2.3. *The matrix A is symmetric with respect to the inner product $\langle \cdot, \cdot \rangle$, in other words,*

$$\langle AU, V \rangle = \langle U, AV \rangle \quad \text{for all } U, V \in \mathbb{R}^{N+1}. \tag{2.4}$$

Furthermore, A is positive semi-definite in the sense that

$$\langle AU, U \rangle \geq 0 \quad \text{for all } U \in \mathbb{R}^{N+1}. \tag{2.5}$$

Proof. Since QA is symmetric,

$$\langle AU, V \rangle = (QAU, V)\triangle x = (U, QAV)\triangle x = \langle U, AV \rangle.$$

Furthermore, A satisfies (2.5) since all the eigenvalues of A are nonnegative. $\quad\square$

The above lemma implies that the eigenvectors $\Phi_k = c_k \phi_k$ ($k = 0, \ldots, N$) of A form an orthonormal basis of $\mathbb{R}^{N+1}$ equipped with the inner product $\langle \cdot, \cdot \rangle$, where ϕ_k is defined in (2.1) and

$$c_k = \begin{cases} 1/\sqrt{L}, & k = 0, N, \\ \sqrt{2/L}, & k = 1, \ldots, N-1 \end{cases} \tag{2.6}$$

is a normalization constant satisfying $\langle \Phi_k, \Phi_k \rangle = 1$. In particular, $\Phi_0 = (1/\sqrt{L})\mathbf{1}$ is the eigenvector corresponding to $\lambda_0 = 0$, where $\mathbf{1} = (1, 1, \ldots, 1)^\mathsf{T}$. Furthermore, A has the following spectral decomposition:

$$A = \sum_{k=0}^{N} \lambda_k \langle \cdot, \Phi_k \rangle \Phi_k. \tag{2.7}$$

Since $\lambda_0 = 0$, the equation $AU = V$ has a solution if and only if $\langle V, \Phi_0 \rangle = 0$. Indeed, letting

$$M_0 = \{U \in \mathbb{R}^{N+1} \mid \langle U, \Phi_0 \rangle = 0\},$$

we see that $A_0 := A|_{M_0} : M_0 \to M_0$, the restriction of A to M_0 is bijective and that its inverse is given by

$$A_0^{-1} = \sum_{k=1}^{N} \frac{1}{\lambda_k} \langle \cdot, \Phi_k \rangle \Phi_k.$$

Definition 2.4. For $\alpha > 0$, we define the fractional powers A^α and $A_0^{-\alpha}$ by

$$A^\alpha = \sum_{k=0}^{N} \lambda_k^\alpha \langle \cdot, \Phi_k \rangle \Phi_k,$$

$$A_0^{-\alpha} = \sum_{k=1}^{N} \frac{1}{\lambda_k^\alpha} \langle \cdot, \Phi_k \rangle \Phi_k.$$

The following lemma is derived straightforwardly by simple calculations, so we omit the proof.

Lemma 2.5. *For $\alpha, \beta > 0$, we have the following:*

(i) *A^α and $A_0^{-\alpha}$ are symmetric with respect to $\langle \cdot, \cdot \rangle$.*

(ii) *$A^{\alpha+\beta} = A^\alpha A^\beta$, $A_0^{-(\alpha+\beta)} = A_0^{-\alpha} A_0^{-\beta}$.*

(iii) *$A_0^{-\alpha}$ is the inverse of $A^\alpha|_{M_0}$.*

Definition 2.6. For $U = (U_0, \ldots, U_N)^{\mathsf{T}} \in \mathbb{R}^{N+1}$, we define the average of U by

$$\overline{U} := \overline{U}\mathbf{1} = (\overline{U}, \ldots, \overline{U})^{\mathsf{T}},$$

where

$$\overline{U} = \frac{1}{L} \sum_{k=0}^{N} {}'' U_k \triangle x \left(= \frac{1}{L} \langle U, \mathbf{1} \rangle \right).$$

Remark 2.7. Since $\Phi_0 = (1/\sqrt{L})\mathbf{1}$, we have $\overline{U} \in \mathrm{span}\{\Phi_0\}$ for $U \in \mathbb{R}^{N+1}$. Hence the solvability condition for $-D_2 U = V$ can be expressed as

$$\overline{V} = \frac{1}{L} \sum_{k=0}^{N} {}'' V_k \triangle x = 0.$$

This corresponds to the fact that the problem

$$\begin{cases} -\dfrac{\partial^2 u}{\partial x^2} = v & \text{in } (0, L) \\ \dfrac{\partial u}{\partial x} = 0 & \text{at } x = 0, L \end{cases}$$

has a solution if and only if

$$\overline{v} = \frac{1}{L} \int_0^L v\, dx = 0.$$

Now we are ready to present a finite difference scheme for problem (1.1)–(1.3). For $U \in \mathbb{R}^{N+1}$, we define a discrete energy functional by

$$J_d(U) = \sum_{k=0}^{N} {}'' G_d(U)_k \triangle x \ (= \langle G_d(U), 1 \rangle), \tag{2.8}$$

where $G_d(U)_k$ is the k-th component of the discretized energy density

$$G_d(U) = \frac{\varepsilon^2}{2} \left(A^{1/2} U \right)^2 + W(U) + \frac{\sigma}{2} \left\{ A_0^{-1/2}(U - \overline{U}) \right\}^2. \tag{2.9}$$

Here and in what follows, for any vectors $U = (U_0, \ldots, U_N)^\mathsf{T}, V = (V_0, \ldots, V_N)^\mathsf{T} \in \mathbb{R}^{N+1}$, UV denotes the componentwise product of U and V, namely, $UV = (U_0 V_0, \ldots, U_N V_N)^\mathsf{T}$. Since

$$\langle U - \overline{U}, \Phi_0 \rangle = \frac{1}{\sqrt{L}} \left(\langle U, 1 \rangle - \overline{U} \langle 1, 1 \rangle \right) = \frac{1}{\sqrt{L}} \langle U, 1 \rangle \left(1 - \frac{\langle 1, 1 \rangle}{L} \right) = 0,$$

we have $U - \overline{U} \in M_0$ for $U \in \mathbb{R}^{N+1}$. Therefore, $G_d(U)$ is defined for all $U \in \mathbb{R}^{N+1}$.

Let $\triangle t > 0$ be the (uniform) time step size and define the approximate solution by $U^{(m)} = (U_0^{(m)}, U_1^{(m)}, \ldots, U_N^{(m)})^\mathsf{T}$, where $U_k^{(m)}$ is the approximation to the solution $u(x,t)$ of (1.1)–(1.3) at $(x,t) = (k \triangle x, m \triangle t)$. Our scheme is the following:

Scheme . *Let* $U^{(0)} = (U_0^{(0)}, \ldots, U_N^{(0)})^\mathsf{T}$, $U_k^{(0)} = u_0(k \triangle x) \ (k = 0, \ldots, N)$ *be the initial vector. Then the scheme is given by*

$$\frac{U^{(m+1)} - U^{(m)}}{\triangle t} = -A \frac{\delta J_d}{\delta(U^{(m+1)}, U^{(m)})}, \quad m = 0, 1, \ldots, \tag{2.10}$$

where $\delta J_d / \delta(U, V)$ *is given by*

$$\frac{\delta J_d}{\delta(U, V)} = \varepsilon^2 A \left(\frac{U + V}{2} \right) + f(U, V) + \sigma A_0^{-1} \left(\frac{U + V}{2} - \frac{\overline{U} + \overline{V}}{2} \right), \tag{2.11}$$

and

$$f(u, v) := \frac{W(u) - W(v)}{u - v} = \frac{1}{4}(u + v)(u^2 + v^2) - \frac{1}{2}(u + v). \tag{2.12}$$

We call the vector $\delta J_d / \delta(U, V)$ the discrete variational derivative of J_d. Note that the above scheme is nonlinear. The condition for the unique solvability of (2.10) will be discussed in Section 6.

Remark 2.8. For the Cahn-Hilliard equation ($\sigma = 0$), Furihata [4] used the following discrete energy functional:

$$J_d^{CH}(U) = \sum_{k=0}^{N} {}'' G_d^{CH}(U)_k \triangle x, \tag{2.13}$$

where G_d^{CH} is a discrete local energy density defined by

$$G_d^{CH}(U) = \frac{\varepsilon^2}{2} \left\{ \frac{(D_+U)^2 + (D_-U)^2}{2} \right\} + W(U), \qquad (2.14)$$

and

$$D_+ = \frac{1}{\triangle x} \begin{pmatrix} -1 & 1 & & & \\ 0 & -1 & 1 & & \\ & \ddots & \ddots & \ddots & \\ & & 0 & -1 & 1 \\ & & & 1 & -1 \end{pmatrix}, \quad D_- = \frac{1}{\triangle x} \begin{pmatrix} 1 & -1 & & & \\ -1 & 1 & 0 & & \\ & \ddots & \ddots & \ddots & \\ & & -1 & 1 & 0 \\ & & & -1 & 1 \end{pmatrix}$$

are the matrix expressions of the forward difference $(U_{k+1} - U_k)/\triangle x$ and the backward difference $(U_k - U_{k-1})/\triangle x$ for $U = (U_0, \ldots, U_N)^\mathsf{T}$, respectively, associated with the discretization of homogeneous Neumann boundary conditions $(U_{k+1} - U_{k-1})/(2\triangle x) = 0$ at $k = 0, N$. (The density G_d^{CH} in [3] is not given in a vector form like (2.14), but it is essentially the same as (2.14).) Though the local energy densities G_d with $\sigma = 0$ and G_d^{CH} are different, it can be shown that the corresponding total energies J_d with $\sigma = 0$ and J_d^{CH} are the same. Indeed,

$$\left\langle \frac{(D_+U)^2 + (D_-U)^2}{2}, 1 \right\rangle = \frac{\langle D_+U, D_+U \rangle + \langle D_-U, D_-U \rangle}{2} \qquad (2.15)$$
$$= \left\langle \frac{D_+^* D_+ U + D_-^* D_- U}{2}, U \right\rangle,$$

where $D_\pm^* = Q^{-1} D_\pm^\mathsf{T} Q$ denotes the adjoint matrix of $D_\pm$ with respect to the inner product $\langle \cdot, \cdot \rangle$. On the other hand,

$$\left\langle \left(A^{1/2} U \right)^2, 1 \right\rangle = \left\langle A^{1/2} U, A^{1/2} U \right\rangle = \langle AU, U \rangle. \qquad (2.16)$$

Since we have

$$\frac{D_+^* D_+ + D_-^* D_-}{2} = A$$

by a simple calculation, the left-hand sides of (2.15) and (2.16) coincide and thus the energies J_d with $\sigma = 0$ and J_d^{CH} are the same. Therefore, when $\sigma = 0$, the discrete variational derivative J_d in (2.11) is the same as that of J_d^{CH} and thus our proposed scheme (2.10) coincides with Furihata's.

3 Derivation of a variational formula for the discrete variational derivative

The following is the main result of this section:

Proposition 3.1. The vector $\delta J_d/\delta(U,V)$ defined in (2.11) satisfies

$$J_d(U) - J_d(V) = \sum_{k=0}^{N} {}'' \left(\frac{\delta J_d}{\delta(U,V)} \right)_k (U_k - V_k) \triangle x, \tag{3.1}$$

or equivalently,

$$J_d(U) - J_d(V) = \left\langle \frac{\delta J_d}{\delta(U,V)}, U - V \right\rangle \tag{3.2}$$

for all $U,V \in \mathbb{R}^{N+1}$.

Remark 3.2. The variational formula (3.1) was originally introduced by Furihata and Mori [6] as a discrete formulation of the first variation of a functional $J(u)$:

$$\delta J = \int_\Omega \frac{\delta J}{\delta u} \delta u \, dx.$$

They defined a vector $\delta J_d/\delta(U,V)$ (we use this notation in accordance with the above formula) called the discrete variational derivative for a discrete energy functional J_d associated with a functional J of the form

$$J(u) = \int_0^L G(u,u_x)dx, \quad G(u,u_x) = \sum_{j=1}^{M} f_j(u)g_j(u_x),$$

and proved the formula (3.1) by using summation-by-parts formulas. On the other hand, (3.2) means that the vector $\delta J_d/\delta(U,V)$ is a discrete gradient of J_d with respect to the inner product $\langle \cdot, \cdot \rangle$. Discrete gradients are used to construct a numerical integration algorithms that preserve exactly first integrals of Hamilton systems. See [8] for details.

The following lemma is useful for proving Proposition 3.1:

Lemma 3.3. *For $\alpha > 0$, let A^α and $A_0^{-\alpha}$ be fractional powers of A and A_0 in Definition 2.4. Then,*

$$\langle A^\alpha U, U \rangle - \langle A^\alpha V, V \rangle = \langle A^\alpha(U+V), U-V \rangle \quad \text{for } U,V \in \mathbb{R}^{N+1}, \tag{3.3}$$

$$\langle A_0^{-\alpha} U, U \rangle - \langle A_0^{-\alpha} V, V \rangle = \langle A_0^{-\alpha}(U+V), U-V \rangle \quad \text{for } U,V \in M_0. \tag{3.4}$$

We omit the proof of this lemma since it is easily shown by the symmetry of A^α and $A_0^{-\alpha}$ with respect to $\langle \cdot, \cdot \rangle$.

Proof of Proposition 3.1. For $U,V \in \mathbb{R}^{N+1}$,

$$J_d(U) - J_d(V) = \langle G_d(U), 1 \rangle - \langle G_d(V), 1 \rangle$$
$$= \frac{\varepsilon^2}{2}I_1 + I_2 + \frac{\sigma}{2}I_3,$$

where

$$I_1 = \left\langle \left\{ A^{1/2} U \right\}^2, 1 \right\rangle - \left\langle \left\{ A^{1/2} V \right\}^2, 1 \right\rangle,$$

$$I_2 = \langle W(U) - W(V), 1 \rangle,$$

$$I_3 = \left\langle \left\{ A_0^{-1/2}(U - \overline{U}) \right\}^2, 1 \right\rangle - \left\langle \left\{ A_0^{-1/2}(V - \overline{V}) \right\}^2, 1 \right\rangle.$$

By Lemmas 2.5 and 3.3,

$$I_1 = \left\langle A^{1/2} U, A^{1/2} U \right\rangle - \left\langle A^{1/2} V, A^{1/2} V \right\rangle$$

$$= \langle AU, U \rangle - \langle AV, V \rangle = \langle A(U + V), U - V \rangle.$$

Similarly,

$$I_3 = \left\langle A_0^{-1/2}(U - \overline{U}), A_0^{-1/2}(U - \overline{U}) \right\rangle - \left\langle A_0^{-1/2}(V - \overline{V}), A_0^{-1/2}(V - \overline{V}) \right\rangle$$

$$= \left\langle A_0^{-1}(U - \overline{U}), U - \overline{U} \right\rangle - \left\langle A_0^{-1}(V - \overline{V}), V - \overline{V} \right\rangle$$

$$= \left\langle A_0^{-1}(U + V - \overline{U} - \overline{V}), U - V - (\overline{U} - \overline{V}) \right\rangle$$

$$= \left\langle A_0^{-1}(U + V - \overline{U} - \overline{V}), U - V \right\rangle.$$

Here the last equality follows from the fact that $A_0^{-1}(U + V - \overline{U} - \overline{V}) \in M_0$ and $\overline{U} - \overline{V} = \overline{U - V} \in \mathrm{span}\{\Phi_0\}$. On the other hand, by (2.12),

$$I_2 = \langle f(U, V)(U - V), 1 \rangle = \langle f(U, V), U - V \rangle,$$

where f is the function defined in (2.12) and the product of two vectors in $\mathbb{R}^{N+1}$ is defined by componentwise operation.

Consequently, the vector $\delta J_d / \delta(U, V)$ defined by

$$\frac{\delta J_d}{\delta(U, V)} = \frac{\varepsilon^2}{2} A(U + V) + f(U, V) + \frac{\sigma}{2} A_0^{-1}(U + V - \overline{U} - \overline{V})$$

satisfies (3.2) and thus the proposition is proved.   □

4   Mass conservation and energy dissipation properties of the scheme

In this section we show that the proposed scheme (2.10) has the same characteristic properties, mass conservation and energy dissipation, as the original problem (1.1)–(1.3) has.

Definition 4.1. The total mass of $U = (U_0, \ldots, U_N)^\mathsf{T} \in \mathbb{R}^{N+1}$ is defined by

$$M_d(U) := \sum_{k=0}^{N} {}'' U_k \triangle x = \langle U, 1 \rangle.$$

Theorem 4.2. *The scheme* (2.10) *has mass-conservation and energy-dissipation proper-ties in the sense that for all* $m = 0, 1, \ldots$,

$$M_d(U^{(m+1)}) = M_d(U^{(m)}), \tag{4.1}$$

$$J_d(U^{(m+1)}) \leq J_d(U^{(m)}). \tag{4.2}$$

Proof. By (2.10) and Lemma 2.3,

$$\frac{M_d(U^{(m+1)}) - M_d(U^{(m)})}{\triangle t} = \left\langle \frac{U^{(m+1)} - U^{(m)}}{\triangle t}, 1 \right\rangle = \left\langle -A \frac{\delta J_d}{\delta(U^{(m+1)}, U^{(m)})}, 1 \right\rangle$$

$$= \left\langle -\frac{\delta J_d}{\delta(U^{(m+1)}, U^{(m)})}, A1 \right\rangle = 0.$$

The last equality follows from the fact that $\Phi_0 = (1/\sqrt{L})1$ is an eigenvector of A with eigenvalue 0. Thus we obtain (4.1).

Next we show (4.2). By (3.2) and (2.10),

$$\frac{J_d(U^{(m+1)}) - J_d(U^{(m)})}{\triangle t} = \left\langle \frac{\delta J_d}{\delta(U^{(m+1)}, U^{(m)})}, \frac{U^{(m+1)} - U^{(m)}}{\triangle t} \right\rangle$$

$$= \left\langle \frac{\delta J_d}{\delta(U^{(m+1)}, U^{(m)})}, -A \frac{\delta J_d}{\delta(U^{(m+1)}, U^{(m)})} \right\rangle$$

$$\leq 0.$$

The last inequality follows from the positive semi-definiteness of A. The theorem is proved. $\qquad\square$

5   Stability of the proposed scheme

In this paper, we use the following norms on $\mathbb{R}^{N+1}$ induced by the inner product $\langle \cdot, \cdot \rangle$.

$$\|U\|_{L_d^2} := \left(\sum_{k=0}^{N}{}'' |U_k|^2 \triangle x \right)^{1/2} = \langle U, U \rangle^{1/2},$$

$$\|U\|_{L_d^\infty} := \max_{0 \leq k \leq N} |U_k|,$$

$$\|U\|_{H_d^1} := \left(\langle U, U \rangle + \frac{1}{2}(\langle D_+U, D_+U \rangle + \langle D_-U, D_-U \rangle) \right)^{1/2}$$

$$= \left(\langle U, U \rangle + \left\langle A^{1/2}U, A^{1/2}U \right\rangle \right)^{1/2}.$$

The following lemma gives relations between above norms:

Lemma 5.1.

$$\frac{1}{\sqrt{L}}\|U\|_{L_d^2} \leq \|U\|_{L_d^\infty} \leq \max\left\{\sqrt{\frac{3}{L}}, \sqrt{\frac{3L}{2}}\right\}\|U\|_{H_d^1}.$$

Proof. Since $N\triangle x = L$,

$$\|U\|_{L_d^2} \leq \|U\|_{L_d^\infty}\left(\sum_{k=0}^{N}{}''\triangle x\right)^{1/2} = \sqrt{L}\|U\|_{L_d^\infty}.$$

This proves the first inequality.

Let $K \in \{0,\dots,N\}$ be such that $|U_K| = \min_{0\leq k\leq N}|U_k|$. Then, arguing as above, we obtain

$$|U_K| \leq \frac{1}{\sqrt{L}}\langle U,U\rangle^{1/2}.$$

Since

$$U_j - U_K = \begin{cases} \displaystyle\sum_{k=K}^{j-1}(U_{k+1}-U_k), & j > K, \\ \displaystyle-\sum_{k=j}^{K-1}(U_{k+1}-U_k), & j < K, \end{cases}$$

we have for $j = 0,\dots,N$,

$$|U_j| \leq |U_K| + \sum_{k=0}^{N-1}\left|\frac{U_{k+1}-U_k}{\triangle x}\right|\triangle x$$

$$\leq |U_K| + \left(\sum_{k=0}^{N-1}\left(\frac{U_{k+1}-U_k}{\triangle x}\right)^2\triangle x\right)^{1/2}\left(\sum_{k=0}^{N-1}\triangle x\right)^{1/2}$$

$$\leq \frac{1}{\sqrt{L}}\langle U,U\rangle^{1/2} + \sqrt{L}\langle D_+U,D_+U\rangle^{1/2}.$$

We also have

$$|U_j| \leq \frac{1}{\sqrt{L}}\langle U,U\rangle^{1/2} + \sqrt{L}\langle D_-U,D_-U\rangle^{1/2}$$

for $j = 0,\dots,N$ in a similar manner. Combining these inequalities, we obtain

$$\|U\|_{L_d^\infty} \leq \frac{1}{\sqrt{L}}\langle U,U\rangle^{1/2} + \frac{\sqrt{L}}{2}\left(\langle D_+U,D_+U\rangle^{1/2} + \langle D_-U,D_-U\rangle^{1/2}\right)$$

$$\leq C\left(\langle U,U\rangle + \left\langle A^{1/2}U,A^{1/2}U\right\rangle\right)^{1/2}$$

with $C = \max\{\sqrt{3/L}, \sqrt{3L/2}\}$. Here the last inequality follows from the inequality $\sqrt{a}+\sqrt{b}+\sqrt{c} \leq \sqrt{3(a+b+c)}$ for $a,b,c > 0$. The lemma is proved. $\quad\square$

The following result yields that the proposed scheme is numerically stable for any time step:

Theorem 5.2. *The numerical solutions $U^{(m)}$ $(m = 0, 1, \dots)$ obtained by the proposed scheme (2.10) satisfy for all $m \geq 0$,*

$$\|U^{(m)}\|_{L_d^2} \leq \left\{ J_d(U^{(0)}) + 2L \right\}^{1/2}, \tag{5.1}$$

$$\|U^{(m)}\|_{L_d^\infty} \leq C \left\{ \frac{2}{\varepsilon^2} J_d(U^{(0)}) + \frac{L}{2}(\varepsilon^2 + 2) \right\}^{1/2} \tag{5.2}$$

with $C = \max\{\sqrt{3/L}, \sqrt{3L/2}\}$.

Proof. Since

$$W(u) = \frac{1}{4}(u^2 - 1)^2 \geq au^2 - a(a+1)$$

for $a \in \mathbb{R}$, we have

$$\left\langle W(U^{(m)}), 1 \right\rangle \geq \left\langle a(U^{(m)})^2 - a(a+1)1, 1 \right\rangle = a \left\langle U^{(m)}, U^{(m)} \right\rangle - a(a+1)L. \tag{5.3}$$

Therefore, Theorem 4.2 implies that for $m \geq 0$,

$$J_d(U^{(0)}) \geq J_d(U^{(m)}) \geq \left\langle W(U^{(m)}), 1 \right\rangle \geq \left\langle U^{(m)}, U^{(m)} \right\rangle - 2L.$$

Here we take $a = 1$ in (5.3). Thus we obtain (5.1).

Similarly, taking $a = \varepsilon^2/2$ in (5.3), we have for $m \geq 0$,

$$
\begin{aligned}
J_d(U^{(0)}) \geq J_d(U^{(m)}) &\geq \frac{\varepsilon^2}{2} \left\langle A^{1/2} U^{(m)}, A^{1/2} U^{(m)} \right\rangle + \left\langle W(U^{(m)}), 1 \right\rangle \\
&\geq \frac{\varepsilon^2}{2} \left(\left\langle A^{1/2} U^{(m)}, A^{1/2} U^{(m)} \right\rangle + \left\langle U^{(m)}, U^{(m)} \right\rangle \right) - \frac{\varepsilon^2}{4}(\varepsilon^2 + 2) \left\langle 1, 1 \right\rangle \\
&= \frac{\varepsilon^2}{2} \|U^{(m)}\|_{H_d^1}^2 - \frac{\varepsilon^2}{4}(\varepsilon^2 + 2)L.
\end{aligned}
$$

Combining this with Lemma 5.1, we obtain

$$\|U^{(m)}\|_{L_d^\infty}^2 \leq C^2 \left\{ \frac{2}{\varepsilon^2} J_d(U^{(0)}) + \frac{L}{2}(\varepsilon^2 + 2) \right\}$$

with $C = \max\{\sqrt{3/L}, \sqrt{3L/2}\}$. The theorem is proved. $\qquad\square$

6 Unique solvability of the scheme

In this section, we prove that the proposed scheme (2.10) has a unique solution $U^{(m+1)}$.

Let $\mathscr{T} : \mathbb{R}^{N+1} \times \mathbb{R}^{N+1} \to \mathbb{R}^{N+1}$ be a map defined by

$$\mathscr{T}(U, V) := U - \frac{\triangle t}{2} A \left\{ \varepsilon^2 AV + g(U, V) - V \right\} - \frac{\triangle t}{2} \sigma(V - \overline{V}), \tag{6.1}$$

where $g(u, v) := u^2 v - 2uv^2 + 2v^3$ is a cubic function. Then, if $\mathscr{T}(U^{(m)}, \cdot) : \mathbb{R}^{N+1} \to \mathbb{R}^{N+1}$ has a fixed point V^*, then $U^{(m+1)} := 2V^* - U^{(m)}$ is a solution of (2.10).

Proposition 6.1. Let $R > 0$ be a constant satisfying $\|U\|_{L^2_d} \leq R$. Then $\mathscr{T}(U, \cdot) : \mathbb{R}^{N+1} \to \mathbb{R}^{N+1}$ has a unique fixed point in $B := \{V \in \mathbb{R}^{N+1} \mid \|V\|_{L^2_d} \leq 2R\}$ if

$$\triangle t \left\{ \frac{16\varepsilon^2}{(\triangle x)^4} + \frac{132R^2}{(\triangle x)^3} + \frac{4}{(\triangle x)^2} + \frac{\sigma}{2} \right\} \leq 1. \tag{6.2}$$

Proof. In this proof we drop the subscript L^2_d of $\|\cdot\|_{L^2_d}$ for brevity. By the spectral decomposition (2.7) of A,

$$\|AU\|^2 = \sum_{k=0}^{N} \lambda_k^2 \langle U, \Phi_k \rangle^2 \leq \lambda_N^2 \|U\|^2,$$

where $\lambda_N = 4/(\triangle x)^2$ is the largest eigenvalue of A. Hence we have

$$\|\mathscr{T}(U,V)\| \leq \|U\| + \frac{\triangle t}{2} \left\{ \varepsilon^2 \|A^2 V\| + \|Ag(U,V)\| + \|AV\| + \sigma \|V - \overline{V}\| \right\}$$

$$\leq \|U\| + \frac{\triangle t}{2} \left\{ \varepsilon^2 \lambda_N^2 \|V\| + \lambda_N \|g(U,V)\| + \lambda_N \|V\| + \sigma \|V\| \right\}.$$

Here we used the fact that $\|V - \overline{V}\| \leq \|V\|$ since $V - \overline{V}$ is the orthogonal projection of V onto M_0 with respect to the inner product $\langle \cdot, \cdot \rangle$. Furthermore, since

$$\|UV\| \leq \sqrt{\frac{2}{\triangle x}} \|U\| \|V\|,$$

we have

$$\|g(U,V)\| \leq \frac{2}{\triangle x} \left(\|U\|^2 \|V\| + 2\|U\| \|V\|^2 + 2\|V\|^3 \right),$$

and hence, if $\|U\| \leq R$ and $\|V\| \leq 2R$,

$$\|\mathscr{T}(U,V)\| \leq R \left[1 + \triangle t \left\{ \frac{16\varepsilon^2}{(\triangle x)^4} + \frac{104R^2}{(\triangle x)^3} + \frac{4}{(\triangle x)^2} + \frac{\sigma}{2} \right\} \right].$$

Therefore, $\mathscr{T}(U, \cdot)$ is a mapping from B to B, if

$$\triangle t \left\{ \frac{16\varepsilon^2}{(\triangle x)^4} + \frac{104R^2}{(\triangle x)^3} + \frac{4}{(\triangle x)^2} + \frac{\sigma}{2} \right\} \leq 1. \tag{6.3}$$

Next we prove that $\mathscr{T}(U, \cdot)$ is a contraction. In the same way as above,

$$\|\mathscr{T}(U,V) - T(U,V')\|$$
$$\leq \frac{\triangle t}{2} \left\{ (\varepsilon^2 \lambda_N^2 + \lambda_N + \sigma) \|V - V'\| + \lambda_N \|g(U,V) - g(U,V')\| \right\}.$$

Since

$$\|g(U,V) - g(U,V')\| \leq \frac{66R^2}{\triangle x} \|V - V'\|,$$

we have

$$\|\mathscr{T}(U,V) - T(U,V')\| \leq \triangle t \left\{ \frac{8\varepsilon^2}{(\triangle x)^4} + \frac{132R^2}{(\triangle x)^3} + \frac{2}{(\triangle x)^2} + \frac{\sigma}{2} \right\} \|V - V'\|.$$

Therefore, $\mathscr{T}(U,\cdot)$ is a contraction, if

$$\triangle t \left\{ \frac{8\varepsilon^2}{(\triangle x)^4} + \frac{132R^2}{(\triangle x)^3} + \frac{2}{(\triangle x)^2} + \frac{\sigma}{2} \right\} < 1. \tag{6.4}$$

Hence, if $\triangle t$ satisfies (6.2), there exists a unique fixed point $V^* \in B$. $\qquad\square$

Theorem 6.2. *If $\triangle t$ satisfies* (6.2) *with $R = \{J_d(U^{(0)}) + 2L\}^{1/2}$, then the proposed scheme* (2.10) *has a unique solution $U^{(m+1)}$ for all $m \geq 0$. Furthermore, the numerical solutions $U^{(m)}$ by the scheme* (2.10) *satisfy $\|U^{(m)}\|_{L^2_d} \leq R$ for $m \geq 0$.*

Proof. Arguing as in the proof of Theorem 5.2, we have $\|U^{(0)}\| \leq R$. Hence Proposition 6.1 yields that $\mathscr{T}(U^{(0)},\cdot)$ has a unique fixed point $V^{(0)}$ satisfying $\|V^{(0)}\|_{L^2_d} \leq 2R$. Consequently, $U^{(1)} := 2V^{(0)} - U^{(0)}$ is a solution of (2.10) for $m = 0$. Furthermore, by Theorem 5.2, we have $\|U^{(1)}\|_{L^2_d} \leq R$.

If U' is another solution of (2.10) for $m = 0$, then $\|U'\|_{L^2_d} \leq R$ by Theorem 5.2 and hence $V' := (U^{(0)} + U')/2$ is another fixed point of $\mathscr{T}(U^{(0)},\cdot)$ with $\|V'\|_{L^2_d} \leq R$. Therefore, V' must coincide with $V^{(0)}$ and thus the uniqueness of $U^{(1)}$ is proved.

Arguing inductively, we obtain the conclusion. $\qquad\square$

Remark 6.3. The above theorem implies that taking

$$\triangle t = O\left(\varepsilon^{-2}(\triangle x)^4 + (\triangle x)^3 \right) \tag{6.5}$$

guarantees the unique solvability of the scheme. On the other hand, Furihata [4] used a map different from $\mathscr{T}$ to obtain the solvability of a numerical scheme for the Cahn-Hilliard equation ($\sigma = 0$). Applying his argument to our scheme, we see that the solvability condition is given by

$$\triangle t = O(\varepsilon^2(\triangle x)^2). \tag{6.6}$$

See [5, Theorem 4.3] for details. However, the parameter ε represents the interfacial thickness at the bonding point and is assumed to be sufficiently small. Therefore, in order to track the interface accurately, the spatial mesh size $\triangle x$ is empirically chosen to satisfy $C_1\varepsilon \leq \triangle x \leq C_2\varepsilon$ for some positive constants C_1 and C_2. Hence (6.5) becomes $\triangle t = O((\triangle x)^3)$ in this setting, while (6.6) is $\triangle t = O((\triangle x)^4)$.

7 Numerical scheme for higher dimensional problems

By a similar argument to the one-dimensional case, we can construct a dissipative scheme for (1.1)–(1.3) in higher dimensional rectangular domains.

Let $\Omega = (0, L_x) \times (0, L_y)$ be a two-dimensional rectangular domain and let $\triangle x = L_x/N_x$ and $\triangle y = L_y/N_y$ be spatial meshes in x- and y-direction, respectively. Then each element $U = (U_{i,j})_{0 \leq i \leq N_x, 0 \leq j \leq N_y} \in \mathbb{R}^{N_x+1} \times \mathbb{R}^{N_y+1}$ denotes an approximation of functions defined on $\overline{\Omega}$.

Let $D_2^{\langle 2 \rangle}$ be a linear mapping on $\mathbb{R}^{N_x+1} \times \mathbb{R}^{N_y+1}$ defined by the second-order central difference

$$(D_2 U)_{i,j} = \frac{U_{i+1,j} - 2U_{i,j} + U_{i-1,j}}{(\triangle x)^2} + \frac{U_{i,j+1} - 2U_{i,j} + U_{i,j-1}}{(\triangle y)^2}$$

under the following boundary conditions:

$$U_{-1,j} = U_{1.j}, \ \ U_{N_x+1,j} = U_{N_x-1,j} \quad (j = 0, \ldots, N_y),$$
$$U_{i,-1} = U_{i,1}, \ \ U_{i,N_y+1} = U_{i,N_y-1} \quad (i = 0, \ldots, N_x).$$

We also introduce an inner product on $\mathbb{R}^{N_x+1} \times \mathbb{R}^{N_y+1}$ approximating the standard inner product on $L^2(\Omega)$ by the trapezoidal rule

$$\langle\langle U, V \rangle\rangle = \sum_{i=0}^{N_x} \sum_{j=0}^{N_y} \alpha_{i,j} U_{i,j} V_{i,j} \triangle x \triangle y \tag{7.1}$$

for $U = (U_{i,j})$ and $V = (V_{i,j})$, where $\alpha_{i,j}$ is a positive constant defined by

$$\alpha_{i,j} = \begin{cases} 1/4, & \text{if } (i, j) = (0,0), (N_x, 0), (0, N_y), (N_x, N_y) \\ 1, & \text{if } 1 \leq i \leq N_x - 1, 1 \leq j \leq N_y - 1, \\ 1/2, & \text{otherwise.} \end{cases}$$

Then, similar to the one-dimensional problem, we can show that $A^{\langle 2 \rangle} = -D_2^{\langle 2 \rangle}$ is symmetric with respect to the inner product (7.1) and that 1, the element of $\mathbb{R}^{N_x+1} \times \mathbb{R}^{N_y+1}$ whose components are all 1, is an eigenvalue of $A^{\langle 2 \rangle}$ corresponding to the zero eigenvalue. We define $A_0^{\langle 2 \rangle}$ as the restriction of $A^{\langle 2 \rangle}$ to $\{U \mid \langle\langle U, 1 \rangle\rangle = 0\}$.

In the same way as in Section 2, we define a discrete energy functional by

$$J_d(U) = \langle\langle G_d(U), 1 \rangle\rangle,$$

where G_d is defined by (2.9) with $A = A^{\langle 2 \rangle}$, $A_0 = A_0^{\langle 2 \rangle}$ and $\overline{U} = \langle\langle U, 1 \rangle\rangle / (L_x L_y)$.

We define the approximate solution by $U^{(m)} = (U_{i,j}^{(m)})_{0 \leq i \leq N_x, 0 \leq j \leq N_y}$, where $U_{i,j}^{(m)} \simeq u(i \triangle x, j \triangle y, m \triangle t)$. Then our proposed scheme is

$$\frac{U^{(m+1)} - U^{(m)}}{\triangle t} = -A^{\langle 2 \rangle} \frac{\delta J_d}{\delta(U^{(m+1)}, U^{(m)})}, \quad m = 0, 1, \ldots,$$

where the discrete variational derivative of J_d is given by (2.11) with $A = A^{\langle 2 \rangle}$ and $A_0 = A_0^{\langle 2 \rangle}$. As in Section 4, the scheme has mass-conservation and energy-dissipation properties.

We can also extend the above argument to higher dimensional problems in a similar manner. We omit the details.

8 Numerical examples

In this section, we give some numerical examples of the proposed scheme.

Figure 1 shows numerical results for $\sigma = 0$ (the Cahn-Hilliard equation) and $\sigma = 50$ in the one-dimensional case by the proposed scheme (2.10) with $\Omega = (0,1)$, $\varepsilon = 10^{-3/2} \approx 0.0316$, $\triangle x = 0.005$ and $\triangle t = 10^{-8}$. Since the principal term of the period of the global minimizer of J is $O((\varepsilon/\sigma)^{1/3}))$ [11], the larger σ is, the finer the spatial pattern becomes.

Figure 2 shows a comparison between numerical solutions by the explicit Euler scheme and the proposed scheme with $\Omega = (0,1)$, $\sigma = 5$, $\varepsilon = 10^{-3/2} \approx 0.0316$, $\triangle x = 0.01$ and $\triangle t = 1.25 \times 10^{-6}$. Figure 3 shows the time evolution of the energy (top) and that of the mass (middle) for the numerical solutions. For the explicit Euler case, the energy of the numerical solution is dissipative, but the mass is not preserved; while for the proposed scheme (2.10), the numerical solution has both mass-conservation and energy-dissipation properties.

Figure 4 shows a numerical solution with random initial data for two-dimensional problem by the scheme in Section 7. The numerical computation proceeds quite stably and a fine structure (a micro-phase separation) is observed as expected.

9 Conclusion

The discrete variational derivative method has been widely used to obtain some special numerical schemes that have the same conservation/dissipation properties in a discrete sense. Using a suitable discrete L^2 inner product and fractional powers of a discretization of the Laplace operator, we have given a new method in deriving a variational formula for the discrete variational derivative and have proposed a finite-difference scheme for a Cahn-Hilliard type equation with a nonlocal term. The scheme has the same characteristic properties, mass conservation and energy dissipation, as the original equation does. The stability and unique solvability of the scheme are also obtained.

Since our method is not based on discrete calculus, it applies easily to higher dimensional problems where discrete calculus is much more difficult and complicated.

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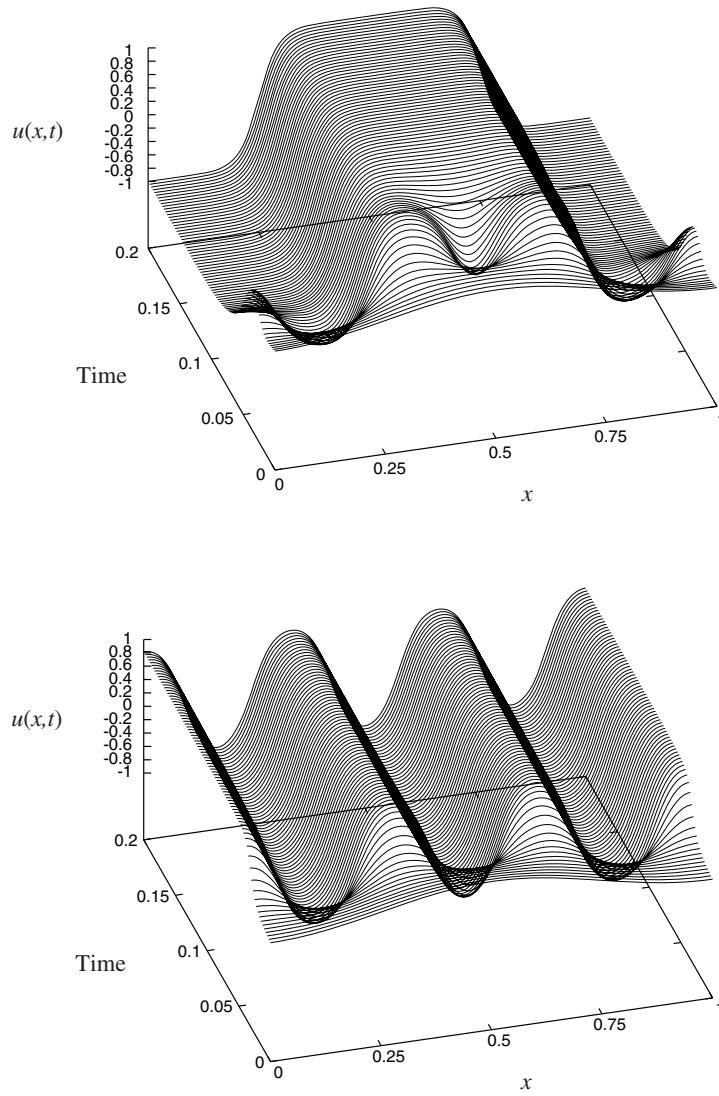
Figure 1: Numerical solutions of one-dimensional problem by the scheme (2.10): (upper) $\sigma = 0$, (lower) $\sigma = 50$.
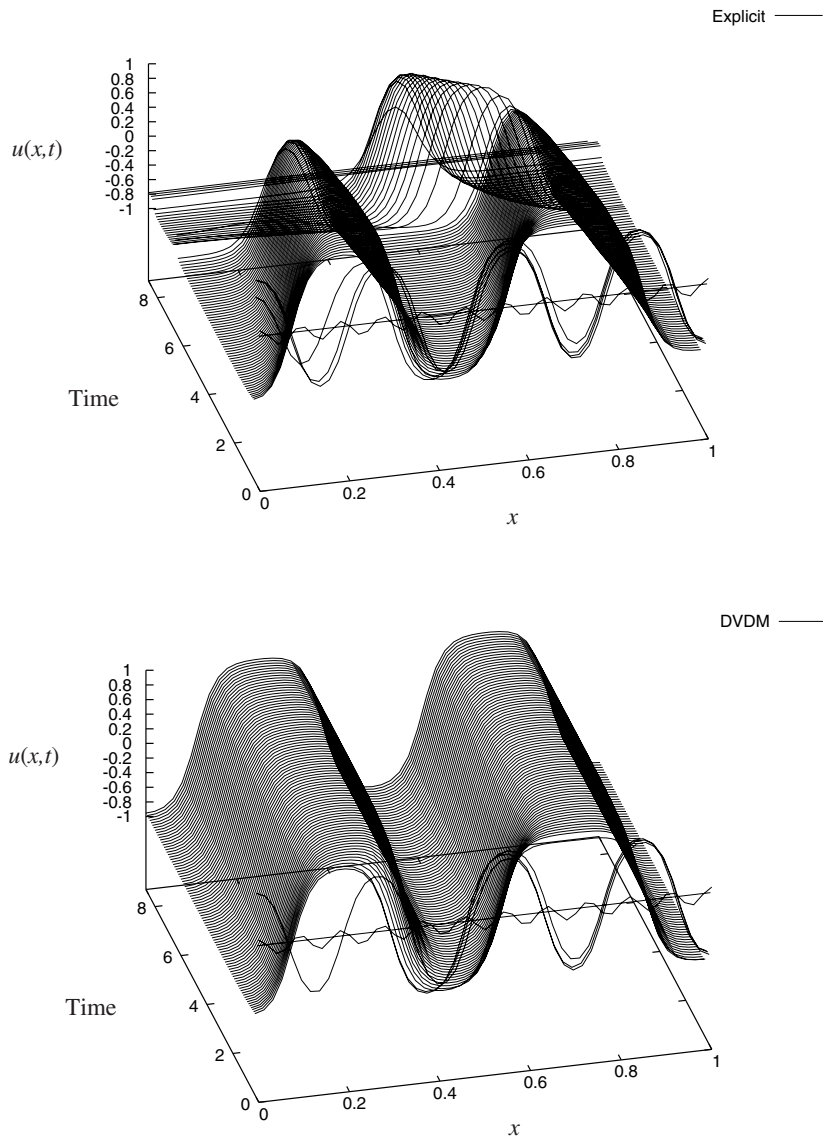
Explicit ——

DVDM ——

Figure 2: Numerical solutions of one-dimensional problem:
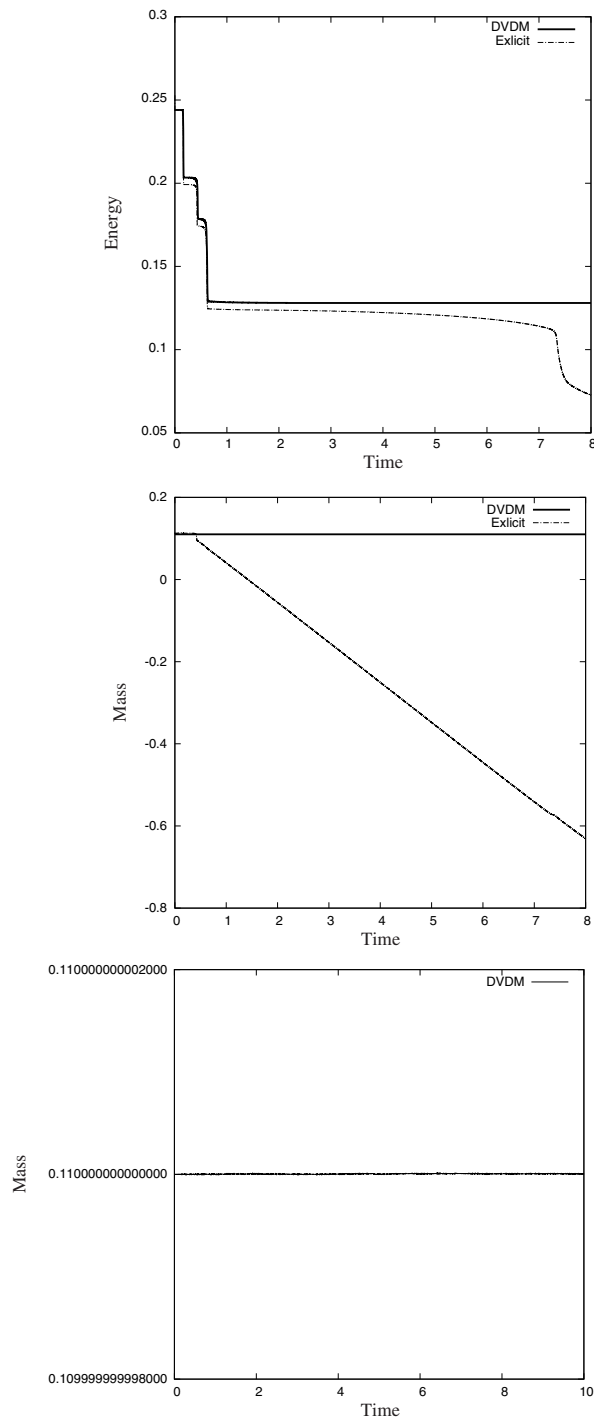(upper) the explicit Euler scheme, (lower) Scheme (2.10).

Figure 3: Numerical solutions of one-dimensional problem:
(top) time evolution of energy, (middle) time evolution of mass,
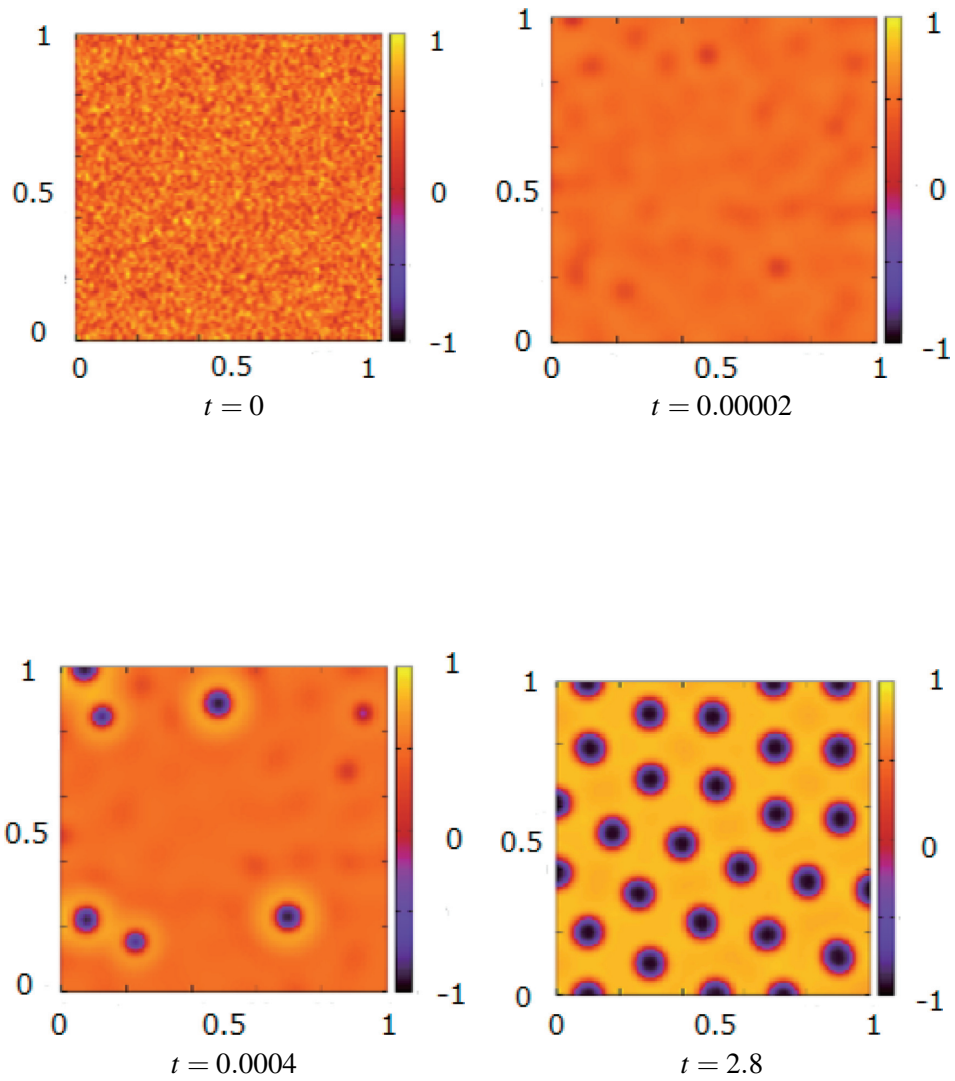(bottom) time evolution of mass by Scheme (2.10).

Figure 4: Numerical solutions of two-dimensional problem by the scheme (2.10).