Recent results on the structure-preserving scheme for the Allen–Cahn equation with a dynamic boundary condition

Makoto Okumura

Department of Pure and Applied Mathematics,
Graduate School of Information Science and Technology, Osaka University

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Toy problem

Example 1

We consider the following ODE:

$$\partial_t u = -u^3. \tag{1}$$

Multiplying both sides of (1) by $\partial_t u$, we have

$$|\partial_t u|^2 = -u^3 \partial_t u = -\partial_t \left(\frac{1}{4} u^4 \right)$$

Namely,

$$\partial_t \left(\frac{1}{4} u^4 \right) + |\partial_t u|^2 = 0. \tag{2}$$

Integrating both sides of (2), we obtain

$$\frac{1}{4}|u(t)|^4 + \int_0^t |\partial_t u(s)|^2 ds = \frac{1}{4}|u(0)|^4.$$

Finite difference schemes for the toy problem

Example 1

$$\partial_t u = -u^3 \tag{1}$$

Δt; a time mesh size
$U^{(n)}$; the approximation to $u(n\Delta t)$

For example, we have the following finite difference schemes for (1):

$$\frac{U^{(n+1)} - U^{(n)}}{\Delta t} = -\left(U^{(n)}\right)^3,$$

$$\frac{U^{(n+1)} - U^{(n)}}{\Delta t} = -\left(U^{(n+1)}\right)^3,$$

$$\frac{U^{(n+1)} - U^{(n)}}{\Delta t} = -\frac{\left(U^{(n+1)}\right)^3 + \left(U^{(n+1)}\right)^2 U^{(n)} + U^{(n+1)} \left(U^{(n)}\right)^2 + \left(U^{(n)}\right)^3}{4}. \tag{3}$$

We focus on the scheme (3).

The structure-preserving scheme for the toy problem

$$\partial_t u = -u^3 \quad (\times \partial_t u)$$

$$\Rightarrow \partial_t \left(\frac{1}{4} u^4 \right) + |\partial_t u|^2 = 0$$

$$\Rightarrow \frac{1}{4}|u(t)|^4 + \int_0^t |\partial_t u(s)|^2 ds = \frac{1}{4}|u(0)|^4$$

Δt; a time mesh size
$U^{(n)}$; the approximation to $u(n\Delta t)$

$$\frac{U^{(n+1)} - U^{(n)}}{\Delta t} = -\frac{\left(U^{(n+1)}\right)^3 + \left(U^{(n+1)}\right)^2 U^{(n)} + U^{(n+1)} \left(U^{(n)}\right)^2 + \left(U^{(n)}\right)^3}{4}. \tag{3}$$

Multiplying both sides of (3) by $(U^{(n+1)} - U^{(n)})/\Delta t$, we have

$$\left| \frac{U^{(n+1)} - U^{(n)}}{\Delta t} \right|^2$$

$$= -\frac{\left(U^{(n+1)}\right)^3 + \left(U^{(n+1)}\right)^2 U^{(n)} + U^{(n+1)} \left(U^{(n)}\right)^2 + \left(U^{(n)}\right)^3}{4} \frac{U^{(n+1)} - U^{(n)}}{\Delta t}$$

$$= -\frac{1}{\Delta t} \left\{ \frac{1}{4} \left(U^{(n+1)}\right)^4 - \frac{1}{4} \left(U^{(n)}\right)^4 \right\}.$$

The structure-preserving scheme for the toy problem

$$\partial_t u = -u^3 \quad (\times \partial_t u)$$

$$\Rightarrow \partial_t \left(\frac{1}{4}u^4\right) + |\partial_t u|^2 = 0$$

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Δt; a time mesh size
$U^{(n)}$; the approximation to $u(n\Delta t)$

$$\frac{U^{(n+1)} - U^{(n)}}{\Delta t} = -\frac{\left(U^{(n+1)}\right)^3 + \left(U^{(n+1)}\right)^2 U^{(n)} + U^{(n+1)} \left(U^{(n)}\right)^2 + \left(U^{(n)}\right)^3}{4}. \tag{3}$$

Multiplying both sides of (3) by $(U^{(n+1)} - U^{(n)})/\Delta t$, we have

$$\frac{1}{\Delta t}\left\{\frac{1}{4}\left(U^{(n+1)}\right)^4 - \frac{1}{4}\left(U^{(n)}\right)^4\right\} + \left|\frac{U^{(n+1)} - U^{(n)}}{\Delta t}\right|^2 = 0. \tag{4}$$

Summing both sides of (4) from 0 to $n-1$, we obtain

$$\frac{1}{4}\left(U^{(n)}\right)^4 + \sum_{l=0}^{n-1}\left|\frac{U^{(n+1)} - U^{(n)}}{\Delta t}\right|^2 \Delta t = \frac{1}{4}\left(U^{(0)}\right)^4.$$

The structure-preserving scheme for the toy problem

$$\partial_t u = -u^3 \quad (\times \partial_t u)$$
$$\Rightarrow \partial_t \left(\frac{1}{4} u^4 \right) + |\partial_t u|^2 = 0$$
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A failure case of a numerical computation

We consider the following Cahn–Hilliard equation with the homogeneous Neumann boundary conditions:

$$\begin{cases} \partial_t u = \partial_x^2(-\gamma \partial_x^2 u + u^3 - u), & \text{in } (0, L) \times (0, T], \\ \partial_x u(x,t)\big|_{x=0,L} = \partial_x^3 u(x,t)\big|_{x=0,L} = 0, & \text{in } (0, T]. \end{cases}$$

Figure 1–2 show the numerical results obtained by the Runge–Kutta scheme. The numerical computation by this scheme fails when the time mesh size is coarse.

Fig. 1: $\Delta t = 1/2500$

Fig. 2: $\Delta t = 1/25000$

The dissipative and conservative properties

$$\begin{cases} \partial_t u = \partial_x^2(-\gamma \partial_x^2 u + u^3 - u), & \text{in } (0,L) \times (0,T], \\ \partial_x u(x,t)\big|_{x=0,L} = \partial_x^3 u(x,t)\big|_{x=0,L} = 0, & \text{in } (0,T]. \end{cases}$$

The solution u to the above problem satisfies the following energy dissipation and mass conservation:

$$\frac{d}{dt} J(u(t)) \leq 0, \quad \int_0^L u(x,t)dx = \int_0^L u(x,0)dx,$$

where the the "global energy" J and "local energy" G are defined by

$$J(u) := \int_0^L G(u, \partial_x u)dx, \quad G(u, \partial_x u) := \frac{\gamma}{2} |\partial_x u|^2 + \frac{1}{4}u^4 - \frac{1}{2}u^2.$$

Remark

In generic numerical methods, such as the Runge-Kutta method, **the above essential structure of the equation is highly likely to be destroyed**.

The dissipative and conservative properties

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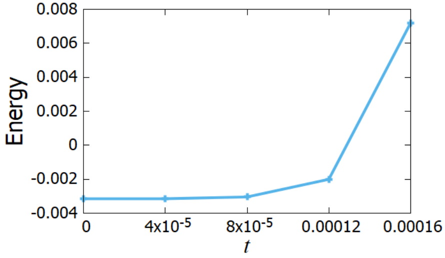
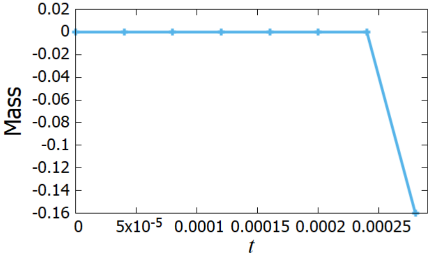
These figures show the time developments of the discrete energy and the discrete mass by the Runge–Kutta scheme, respectively.





The dissipative and conservative properties

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Thus, we use **the discrete variational derivative method (DVDM)**, which is for designing numerical schemes which inherit the above properties from the original equation (Furihata–Matsuo(2010)).

A successful case by DVDM

Figure 3 is the earlier result obtained by the Runge–Kutta scheme. Figure 4 is the one obtained by the discrete variational derivative scheme.

Fig. 3: Runge–Kutta ($\Delta t = 1/25000$)

Fig. 4: DVDM ($\Delta t = 1/1000$)

We can stably obtain the numerical solution by the discrete variational derivative one even when the time mesh size Δt is coarse.

The energy dissipation of the Cahn–Hilliard equation

$$G(u, \partial_x u) = \frac{\gamma}{2} |\partial_x u|^2 + \frac{1}{4}u^4 - \frac{1}{2}u^2, \quad J(u) = \int_0^L G(u, \partial_x u) dx.$$

The Cahn–Hilliard equation can be written as

$$\partial_t u = \partial_x^2 \left(\frac{\delta G}{\delta u} \right),$$

where $\delta G / \delta u = -\gamma \partial_x^2 u + u^3 - u$ is the (first) variational derivative of G.

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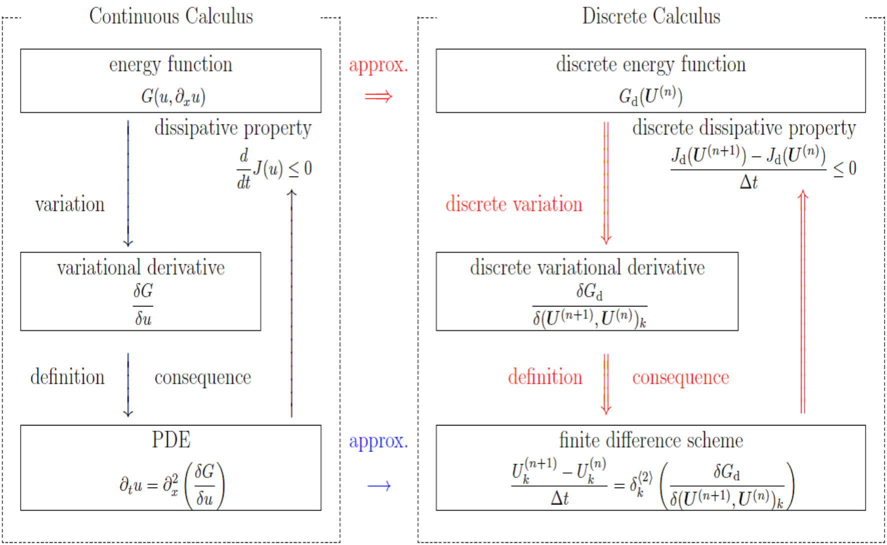
where $\delta G / \delta u = -\gamma \partial_x^2 u + u^3 - u$ is the (first) variational derivative of G.
Then we can show the energy dissipation as follows:

$$\begin{aligned} \frac{d}{dt} J(u) &= \frac{d}{dt} \int_0^L G(u, \partial_x u) dx \\ &= \int_0^L \frac{\delta G}{\delta u} \partial_t u dx + (\text{b.t}) = \int_0^L \frac{\delta G}{\delta u} \left\{ \partial_x^2 \left(\frac{\delta G}{\delta u} \right) \right\} dx + (\text{b.t.}) \\ &= -\int_0^L \left\{ \partial_x \left(\frac{\delta G}{\delta u} \right) \right\}^2 dx + (\text{b.t.}) \leq 0. \end{aligned}$$

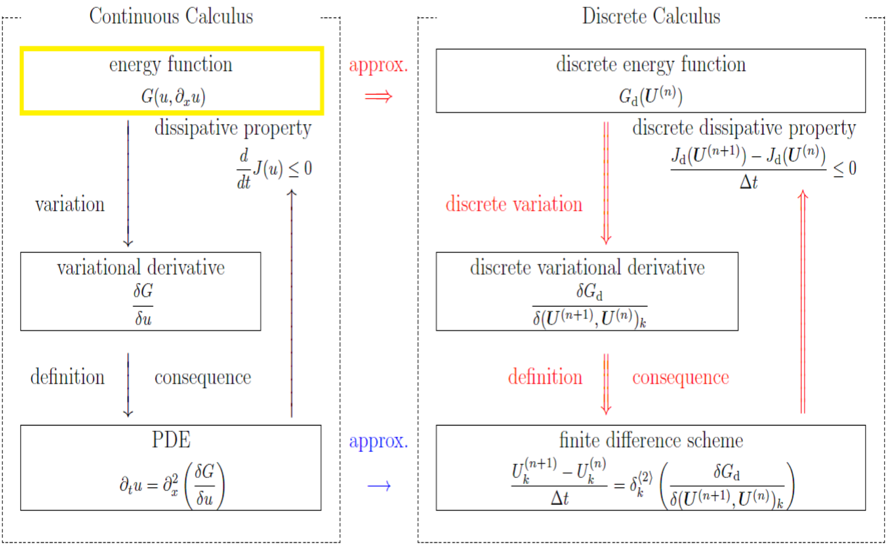
We construct a structure-preserving scheme by retaining the relationship between the equation and the variational derivative in a discrete setting.

Procedure of DVDM



$\Longrightarrow$ DVDM $\longrightarrow$ standard strategy

Procedure of DVDM



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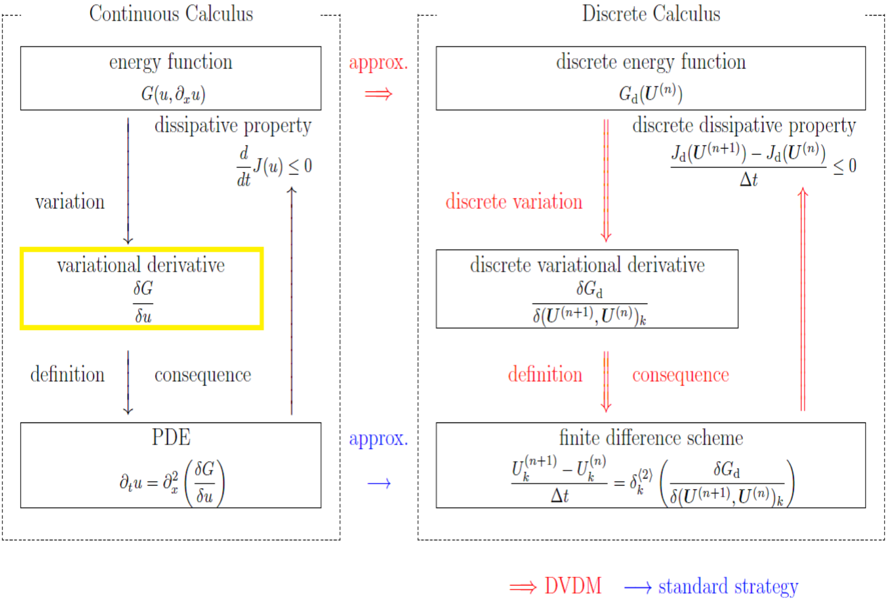

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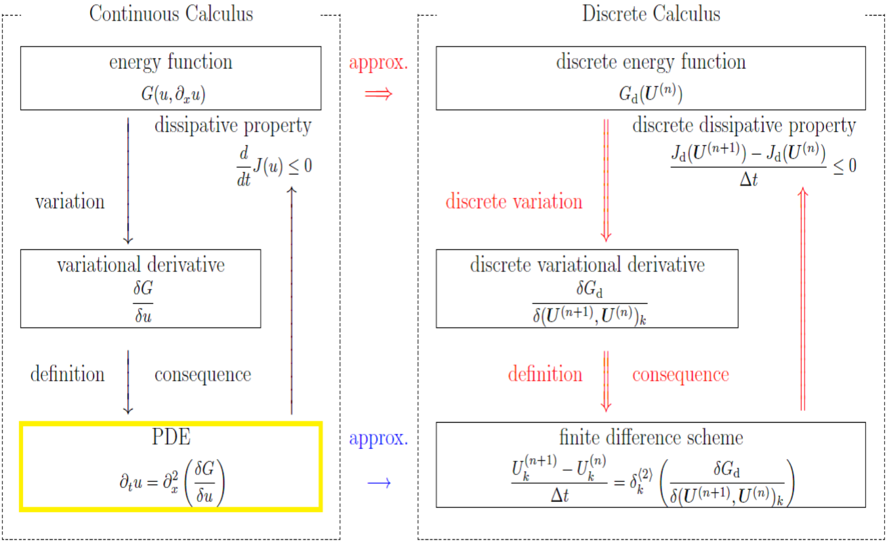

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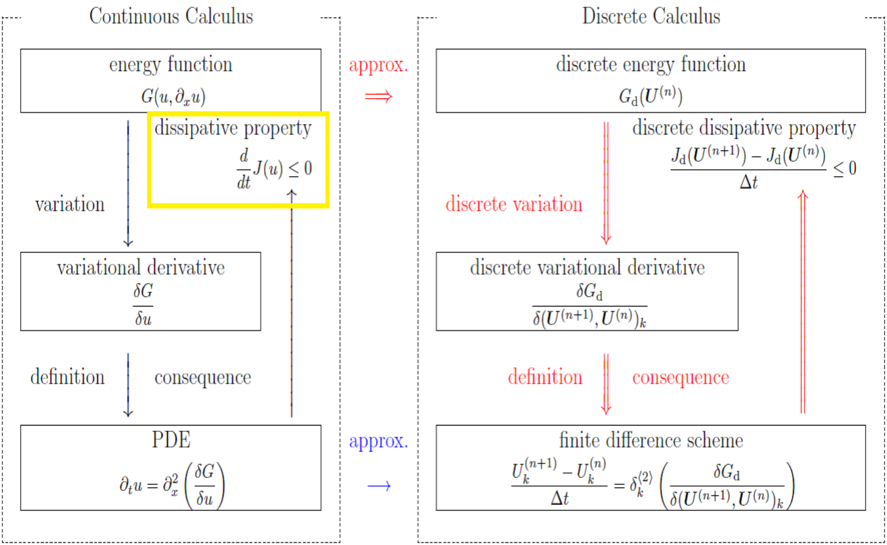

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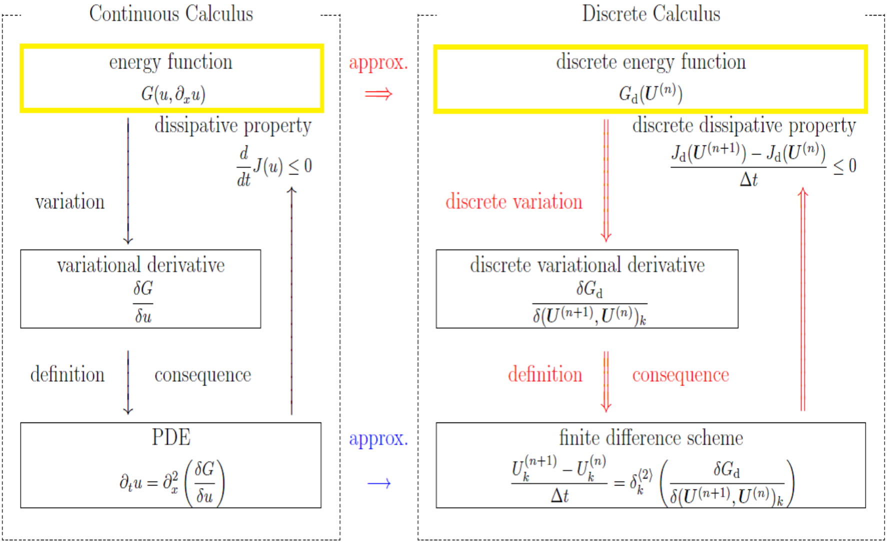

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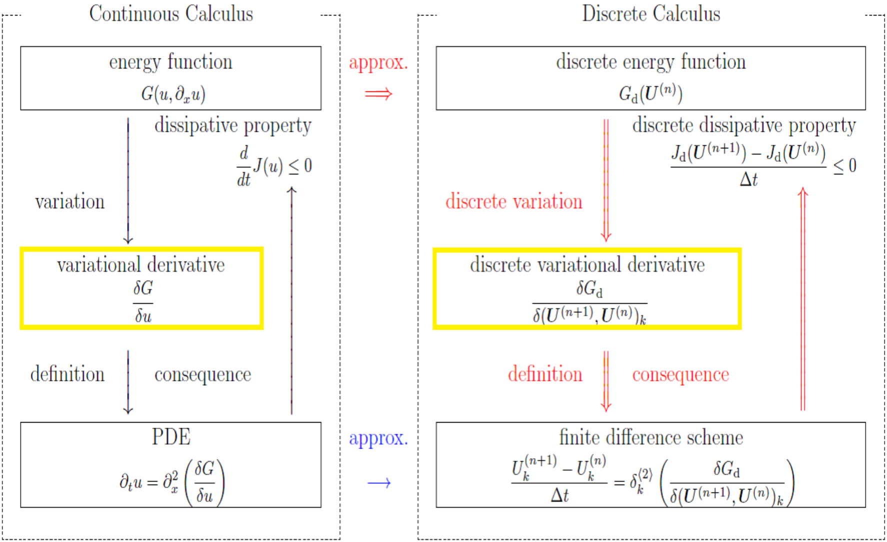

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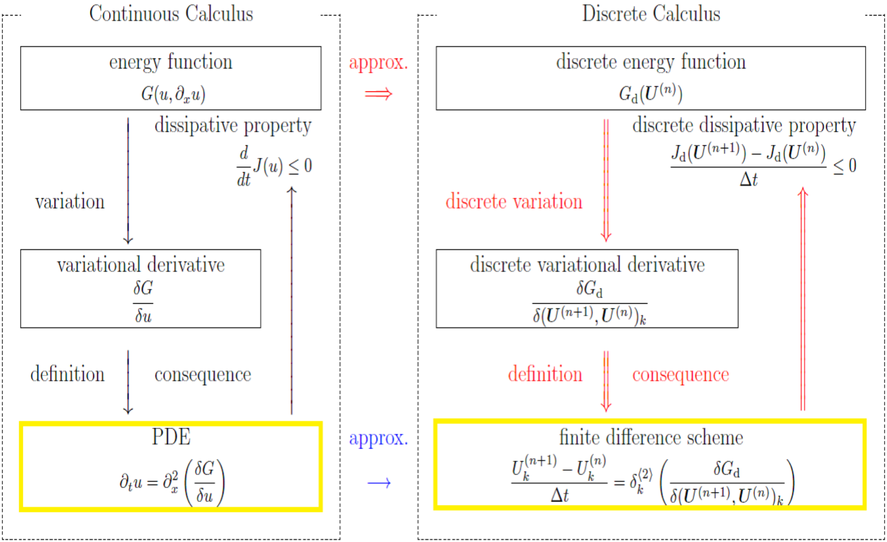

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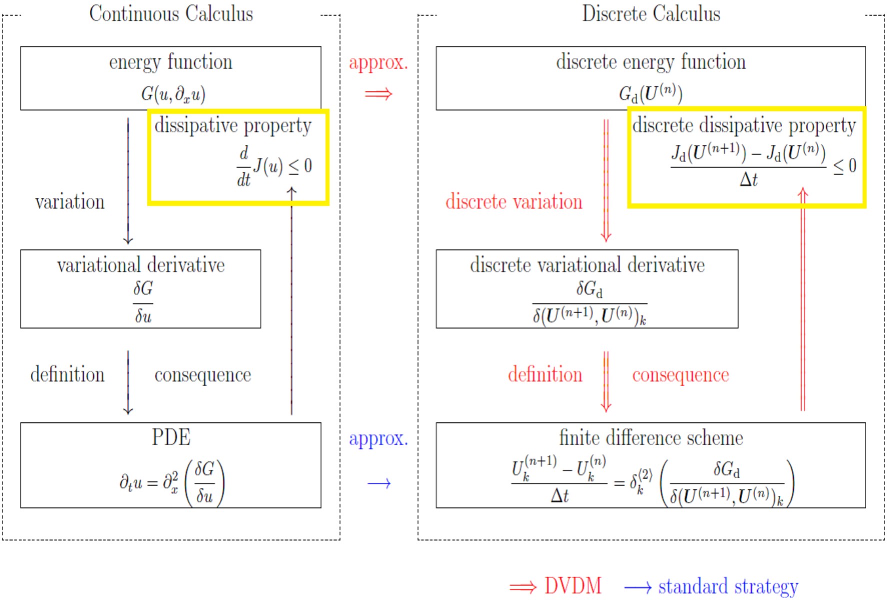


Procedure of DVDM

Continuous Calculus | Discrete Calculus

PDE

$$\partial_t u = \partial_x^2 \left(\frac{\delta G}{\delta u} \right)$$

approx. $\longrightarrow$

finite difference scheme

$$\frac{U_k^{(n+1)} - U_k^{(n)}}{\Delta t} = \delta_k^{\langle 2 \rangle} \left(\frac{\delta G_{\mathrm{d}}}{\delta (\boldsymbol{U}^{(n+1)}, \boldsymbol{U}^{(n)})_k} \right)$$

$\Longrightarrow$ DVDM $\longrightarrow$ standard strategy

Discrete operators

Notation

$$\Delta x := L/K;\ \text{a space mesh size}, \quad \Delta t;\ \text{a time mesh size},$$
$$U_k^{(n)};\ \text{the approximation to } u(k\Delta x, n\Delta t),$$
$$\boldsymbol{U}^{(n)} := \left(U_{-1}^{(n)}, U_0^{(n)}, \ldots, U_K^{(n)}, U_{K+1}^{(n)}\right)^\top.$$

Definition 2

Let us define the difference operators δ_k^+, δ_k^-, $\delta_k^{\langle 1\rangle}$, and $\delta_k^{\langle 2\rangle}$ concerning subscript k by

$$\delta_k^+ f_k := \frac{f_{k+1} - f_k}{\Delta x}, \quad \delta_k^- f_k := \frac{f_k - f_{k-1}}{\Delta x},$$
$$\delta_k^{\langle 1\rangle} f_k := \frac{f_{k+1} - f_{k-1}}{2\Delta x}, \quad \delta_k^{\langle 2\rangle} f_k := \frac{f_{k+1} - 2f_k + f_{k-1}}{(\Delta x)^2} \quad (k = 0, 1, \ldots, K).$$

δ_k^+, δ_k^-, and $\delta_k^{\langle 1\rangle}$ correspond to ∂_x, and $\delta_k^{\langle 2\rangle}$ corresponds to ∂_x^2.

Discrete operator and summation-by-parts formula

Definition 3

We adopt the summation operator $\sum_{k=0}^{K}{}''$ defined by

$$\sum_{k=0}^{K}{}'' f_k \Delta x := \frac{1}{2} f_0 \Delta x + \sum_{k=1}^{K-1} f_k \Delta x + \frac{1}{2} f_K \Delta x \quad \text{for all } \{f_k\}_{k=-1}^{K+1} \in \mathbb{R}^{K+3}.$$

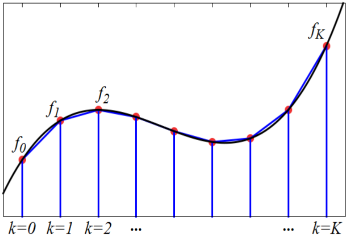
This operator corresponds to the integral:

$$\int_0^L f(x) dx.$$

Summation-by-parts formula

$$\sum_{k=0}^{K}{}'' \frac{(\delta_k^+ f_k)(\delta_k^+ g_k) + (\delta_k^- f_k)(\delta_k^- g_k)}{2} \Delta x$$

$$= \sum_{k=0}^{K}{}'' (\delta_k^{\langle 2 \rangle} f_k) g_k \Delta x + \text{(b.t.)}.$$



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Summation-by-parts formula

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$$= \sum_{k=0}^{K}{}'' (\delta_k^{\langle 2 \rangle} f_k) g_k \Delta x + (\text{b.t.}).$$

Integration-by-parts formula

$$\int_0^L (\partial_x f(x))(\partial_x g(x)) dx$$

$$= \int_0^L (\partial_x^2 f(x)) g(x) dx + (\text{b.t.}).$$

Discretization of the energy

We define the discrete local energy $G_{\mathrm{d},k}$ by

$$G_{\mathrm{d},k}(\boldsymbol{U}) := \frac{\gamma}{2}\frac{(\delta_k^+ U_k)^2 + (\delta_k^- U_k)^2}{2} + \frac{1}{4}U_k^4 - \frac{1}{2}U_k^2 \quad (k = 0, \ldots, K).$$

This G_{d} is a discrete analogue of G:

$$G(u, \partial_x u) = \frac{\gamma}{2}\left|\partial_x u\right|^2 + \frac{1}{4}u^4 - \frac{1}{2}u^2.$$

Accordingly, we define the discrete global energy J_{d} as follows:

$$J_{\mathrm{d}}(\boldsymbol{U}) := \sum_{k=0}^{K}{}'' G_{\mathrm{d},k}(\boldsymbol{U})\Delta x.$$

This J_{d} corresponds to J:

$$J(u) = \int_0^L G(u, \partial_x u)dx.$$

Remark

There are several selections of the discrete energy G_{d}. In general, a different selection will lead us to a different scheme in DVDM.

Discrete variational derivative

Based on DVDM, we calculate the discrete variation $J_{\mathrm{d}}(\boldsymbol{U})-J_{\mathrm{d}}(\boldsymbol{V})$ to get the discrete variational derivative by the summation-by-parts formula.

Remark

The discrete variational derivative $\delta G_{\mathrm{d}}/\delta(\cdot,\cdot)_k$ is defined so that the following identity holds:

$$\sum_{k=0}^{K}{}'' \left(G_{\mathrm{d},k}(\boldsymbol{U})-G_{\mathrm{d},k}(\boldsymbol{V})\right)\Delta x=\sum_{k=0}^{K}{}''\frac{\delta G_{\mathrm{d}}}{\delta(\boldsymbol{U},\boldsymbol{V})_k}(U_k-V_k)\Delta x+\text{(b.t.)}.$$

The above identity is a discrete version of the Gâteaux differentiation:

$$\lim_{\varepsilon\to 0}\int_0^L\frac{G(u+\varepsilon\eta,\partial_x u+\varepsilon\partial_x\eta)-G(u,\partial_x u)}{\varepsilon}dx=\int_0^L\frac{\delta G}{\delta u}\eta dx+\text{(b.t.)},$$

where η: $[0,L]\times[0,T]\to\mathbb{R}$ is a smooth function.

The structure-preserving scheme by DVDM

Thus, we define the scheme with the discrete variational derivative:

$$\frac{U_k^{(n+1)} - U_k^{(n)}}{\Delta t} = \delta_k^{\langle 2 \rangle}\left(\frac{\delta G_{\mathrm{d}}}{\delta(\boldsymbol{U}^{(n+1)}, \boldsymbol{U}^{(n)})_k}\right) \quad (k=0,\ldots,K,\ n=0,1,\ldots),$$

$$\frac{\delta G_{\mathrm{d}}}{\delta(\boldsymbol{U}^{(n+1)}, \boldsymbol{U}^{(n)})_k} = -\gamma\delta_k^{\langle 2 \rangle}\left(\frac{U_k^{(n+1)} + U_k^{(n)}}{2}\right) + \frac{\left(U_k^{(n+1)}\right)^3 + \left(U_k^{(n+1)}\right)^2 U_k^{(n)} + U_k^{(n+1)}\left(U_k^{(n)}\right)^2 + \left(U_k^{(n)}\right)^3}{4} - \frac{U_k^{(n+1)} + U_k^{(n)}}{2} \quad (k=0,\ldots,K,\ n=0,1,\ldots).$$

This scheme corresponds to the Cahn–Hilliard equation:

$$\partial_t u = \partial_x^2\left(\frac{\delta G}{\delta u}\right), \quad \frac{\delta G}{\delta u} = -\gamma\partial_x^2 u + u^3 - u.$$

Discretization of the nonlinear term

Discrete variational derivative

$$\sum_{k=0}^{K}{}'' \left(G_{\mathrm{d},k}(\boldsymbol{U}) - G_{\mathrm{d},k}(\boldsymbol{V}) \right) \Delta x = \sum_{k=0}^{K}{}'' \frac{\delta G_{\mathrm{d}}}{\delta(\boldsymbol{U},\boldsymbol{V})_k} (U_k - V_k) \Delta x + (\text{b.t.}),$$

$$\frac{\delta G_{\mathrm{d}}}{\delta(\boldsymbol{U},\boldsymbol{V})_k} = -\gamma \delta_k^{\langle 2 \rangle} \left(\frac{U_k + V_k}{2} \right) + \frac{U_k^3 + U_k^2 V_k + U_k V_k^2 + V_k^3}{4} - \frac{U_k + V_k}{2}.$$

By the factorization, we can easily obtain the following identity:

$$\sum_{k=0}^{K}{}'' \left\{ \left(\frac{1}{4} U_k^4 - \frac{1}{2} U_k^2 \right) - \left(\frac{1}{4} V_k^4 - \frac{1}{2} V_k^2 \right) \right\} \Delta x$$

$$= \sum_{k=0}^{K}{}'' \left\{ \frac{1}{4} (U_k - V_k)(U_k^3 + U_k^2 V_k + U_k V_k^2 + V_k^3) - \frac{1}{2} (U_k - V_k)(U_k + V_k) \right\} \Delta x$$

$$= \sum_{k=0}^{K}{}'' \left(\frac{U_k^3 + U_k^2 V_k + U_k V_k^2 + V_k^3}{4} - \frac{U_k + V_k}{2} \right) (U_k - V_k) \Delta x.$$

The discrete energy dissipation

$$\frac{d}{dt}J(u) = -\int_0^L \left\{ \partial_x \left(\frac{\delta G}{\delta u} \right) \right\}^2 dx \leq 0.$$

Then we can show the discrete energy dissipation by imposing suitable discrete boundary conditions with which the boundary terms vanish.

$$\frac{J_{\mathrm{d}}(\boldsymbol{U}^{(n+1)}) - J_{\mathrm{d}}(\boldsymbol{U}^{(n)})}{\Delta t} = \frac{1}{\Delta t} \sum_{k=0}^{K}{}'' \left(G_{\mathrm{d},k}(\boldsymbol{U}^{(n+1)}) - G_{\mathrm{d},k}(\boldsymbol{U}^{(n)}) \right) \Delta x$$

$$= \sum_{k=0}^{K}{}'' \frac{\delta G_{\mathrm{d}}}{\delta(\boldsymbol{U}^{(n+1)}, \boldsymbol{U}^{(n)})_k} \frac{U_k^{(n+1)} - U_k^{(n)}}{\Delta t} \Delta x + (\mathrm{b.t.})$$

$$= \sum_{k=0}^{K}{}'' \frac{\delta G_{\mathrm{d}}}{\delta(\boldsymbol{U}^{(n+1)}, \boldsymbol{U}^{(n)})_k} \left\{ \delta_k^{\langle 2 \rangle} \left(\frac{\delta G_{\mathrm{d}}}{\delta(\boldsymbol{U}^{(n+1)}, \boldsymbol{U}^{(n)})_k} \right) \right\} \Delta x + (\mathrm{b.t.})$$

$$= -\frac{1}{2} \sum_{k=0}^{K}{}'' \left\{ \left| \delta_k^{+} \left(\frac{\delta G_{\mathrm{d}}}{\delta(\boldsymbol{U}^{(n+1)}, \boldsymbol{U}^{(n)})_k} \right) \right|^2 + \left| \delta_k^{-} \left(\frac{\delta G_{\mathrm{d}}}{\delta(\boldsymbol{U}^{(n+1)}, \boldsymbol{U}^{(n)})_k} \right) \right|^2 \right\} \Delta x + (\mathrm{b.t.})$$

$$\leq 0 \quad (n = 0, 1, \ldots).$$

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$$\frac{d}{dt}J(u) = -\int_0^L \left\{ \partial_x \left(\frac{\delta G}{\delta u} \right) \right\}^2 dx \le 0.$$

Then we can show the discrete energy dissipation by imposing suitable discrete boundary conditions with which the boundary terms vanish.

$$\frac{J_{\mathrm{d}}(\boldsymbol{U}^{(n+1)}) - J_{\mathrm{d}}(\boldsymbol{U}^{(n)})}{\Delta t} = \frac{1}{\Delta t} \sum_{k=0}^{K}{}'' \left(G_{\mathrm{d},k}(\boldsymbol{U}^{(n+1)}) - G_{\mathrm{d},k}(\boldsymbol{U}^{(n)}) \right) \Delta x$$

$$= \sum_{k=0}^{K}{}'' \frac{\delta G_{\mathrm{d}}}{\delta(\boldsymbol{U}^{(n+1)}, \boldsymbol{U}^{(n)})_k} \frac{U_k^{(n+1)} - U_k^{(n)}}{\Delta t} \Delta x + (\text{b.t.})$$

$$= \sum_{k=0}^{K}{}'' \frac{\delta G_{\mathrm{d}}}{\delta(\boldsymbol{U}^{(n+1)}, \boldsymbol{U}^{(n)})_k} \left\{ \delta_k^{\langle 2 \rangle} \left(\frac{\delta G_{\mathrm{d}}}{\delta(\boldsymbol{U}^{(n+1)}, \boldsymbol{U}^{(n)})_k} \right) \right\} \Delta x + (\text{b.t.})$$

$$= -\frac{1}{2} \sum_{k=0}^{K}{}'' \left\{ \left| \delta_k^{+} \left(\frac{\delta G_{\mathrm{d}}}{\delta(\boldsymbol{U}^{(n+1)}, \boldsymbol{U}^{(n)})_k} \right) \right|^2 + \left| \delta_k^{-} \left(\frac{\delta G_{\mathrm{d}}}{\delta(\boldsymbol{U}^{(n+1)}, \boldsymbol{U}^{(n)})_k} \right) \right|^2 \right\} \Delta x + (\text{b.t.})$$

$$\le 0 \quad (n = 0, 1, \ldots).$$

The discrete mass conservation

$$\int_0^L u(x,t)dx = \int_0^L u(x,0)dx.$$

Summing the following equation:

$$\frac{U_k^{(n+1)} - U_k^{(n)}}{\Delta t} = \delta_k^{\langle 2\rangle}\left(\frac{\delta G_{\mathrm{d}}}{\delta(\boldsymbol{U}^{(n+1)}, \boldsymbol{U}^{(n)})_k}\right), \quad (k=0,\ldots,K,\ n=0,1,\ldots)$$

over $k = 0, \ldots, K$ based on the trapezoidal rule, we can also show the discrete mass conservation:

$$\sum_{k=0}^{K}{}'' U_k^{(n)} \Delta x = \sum_{k=0}^{K}{}'' U_k^{(0)} \Delta x \quad (n = 0, 1, \ldots).$$

To summarize, by using DVDM,

1. we can construct a structure-preserving scheme that retains the dissipative and conservative properties in a discrete setting,
2. we can stably obtain the numerical solution.

The Allen–Cahn equation with a dynamic boundary condition

Let $\Omega := (0, L)$. We study the Allen–Cahn equation with a dynamic boundary condition:

$$\begin{cases} \partial_t u = \partial_x^2 u - u^3 + u, \quad \text{in } \Omega \times (0,T], \\ \partial_t u(0,t) = \partial_x u(x,t)|_{x=0} - (u(0,t))^3 + u(0,t), \quad \text{in } (0,T], \\ \partial_t u(L,t) = -\partial_x u(x,t)|_{x=L} - (u(L,t))^3 + u(L,t), \quad \text{in } (0,T], \end{cases}$$

The nonlinear term is the derivative of $W(s) := (1/4)(s^2 - 1)^2$. Then, the solution u of the problem satisfies the following total energy dissipation:

$$\frac{d}{dt}\{J_{AC}(u(t)) + W(u(0,t)) + W(u(L,t))\} = -\int_0^L \left|\frac{\delta G_{AC}}{\delta u}\right|^2 dx - |\partial_t u(0,t)|^2 - |\partial_t u(L,t)|^2 \le 0,$$

where the "local energy" G_{AC} and the "global energy" J_{AC} are defined by

$$G_{AC}(u, \partial_x u) := \frac{|\partial_x u|^2}{2} + W(u), \quad J_{AC}(u) := \int_0^L G_{AC}(u, \partial_x u) dx.$$

Previous study

Difficulty

In the problem with dynamic boundary conditions, it was difficult to find a suitable discrete boundary condition in the conventional way of DVDM.

Thus, Fukao et al. defined another discrete energy and used another summation-by-parts formula:

$$\sum_{k=1}^{K}\left(\delta_k^- f_k\right)\left(\delta_k^- g_k\right)\Delta x = -\sum_{k=1}^{K}\left(\delta_k^{\langle 2\rangle} f_k\right) g_k \Delta x + \left[\left(\delta_k^+ f_k\right) g_k\right]_0^K .$$

As a result, they have to approximate the boundary condition by a forward difference, and their scheme is first-order accurate in space.

∘ T. Fukao, S. Yoshikawa and S. Wada, Structure-preserving finite difference schemes for the Cahn–Hilliard equation with dynamic boundary conditions in the one-dimensional case, Commun. Pure Appl. Anal., **16** (2017), 1915–1938.

Discretization of the energy

Let us define two discrete local energies $G^{\pm}_{AC\mathrm{d},k}$ by

$$G^{+}_{AC\mathrm{d},k}(\boldsymbol{U}) := \frac{(\delta^{+}_{k} U_k)^2}{2} + W(U_k) \quad (k = 0, \ldots, K-1),$$

$$G^{-}_{AC\mathrm{d},k}(\boldsymbol{U}) := \frac{(\delta^{-}_{k} U_k)^2}{2} + W(U_k) \quad (k = 1, \ldots, K).$$

Then we define a discrete global energy $J_{AC\mathrm{d}}$ as follows:

$$J_{AC\mathrm{d}}(\boldsymbol{U}) := \frac{1}{2}\left\{\sum_{k=0}^{K-1} G^{+}_{AC\mathrm{d},k}(\boldsymbol{U})\,\Delta x + \sum_{k=1}^{K} G^{-}_{AC\mathrm{d},k}(\boldsymbol{U})\,\Delta x\right\}$$

$$= \sum_{k=0}^{K-1} \frac{\left(\delta^{+}_{k} U_k\right)^2}{2}\Delta x + \sum_{k=0}^{K}{}'' W(U_k)\,\Delta x.$$

Remark

There are several selections of the discrete energy G_{d}. In general, a different selection will lead us to a different scheme in DVDM.

Discretization of the energy

Let us define two discrete local energies $G^{\pm}_{AC\mathrm{d},k}$ by

$$G^{+}_{AC\mathrm{d},k}(\boldsymbol{U}) := \frac{(\delta_k^{+} U_k)^2}{2} + W\left(U_k\right) \quad (k = 0, \dots, K-1),$$
$$G^{-}_{AC\mathrm{d},k}(\boldsymbol{U}) := \frac{(\delta_k^{-} U_k)^2}{2} + W\left(U_k\right) \quad (k = 1, \dots, K).$$

Then we define a discrete global energy $J_{AC\mathrm{d}}$ as follows:

$$J_{AC\mathrm{d}}(\boldsymbol{U}) := \frac{1}{2}\left\{ \sum_{k=0}^{K-1} G^{+}_{AC\mathrm{d},k}\left(\boldsymbol{U}\right)\Delta x + \sum_{k=1}^{K} G^{-}_{AC\mathrm{d},k}\left(\boldsymbol{U}\right)\Delta x \right\}$$
$$= \sum_{k=0}^{K-1} \frac{\left(\delta_k^{+} U_k\right)^2}{2}\Delta x + \sum_{k=0}^{K}{}'' W\left(U_k\right)\Delta x.$$

Remark

If we follow the way Fukao et al. used, we consequently adopt $\sum_{k=1}^{K} G^{-}_{AC\mathrm{d},k}\left(\boldsymbol{U}\right)\Delta x$ only as a discrete global energy $J_{AC\mathrm{d}}(\boldsymbol{U})$.

Calculation of the discrete variation

Based on DVDM, we calculate $J_{AC\mathrm{d}}(\boldsymbol{U}) - J_{AC\mathrm{d}}(\boldsymbol{V})$ to derive the discrete variational derivative by the following summation-by-parts formula:

$$\sum_{k=0}^{K-1} \left(\delta_k^+ f_k\right)\left(\delta_k^+ g_k\right)\Delta x = -\sum_{k=0}^{K}{}'' \left(\delta_k^{\langle 2\rangle} f_k\right) g_k \Delta x + \left[\left(\delta_k^{\langle 1\rangle} f_k\right) g_k\right]_0^K . \quad (5)$$

Remark

If we follow the method Fukao et al. used, we consequently use the following summation-by-parts formula:

$$\sum_{k=1}^{K} \left(\delta_k^- f_k\right)\left(\delta_k^- g_k\right)\Delta x = -\sum_{k=1}^{K} \left(\delta_k^{\langle 2\rangle} f_k\right) g_k \Delta x + \left[\left(\delta_k^+ f_k\right) g_k\right]_0^K .$$

Remark

By adopting the previously mentioned discrete energy and (5), we can construct a structure-preserving scheme based on DVDM.

Calculation of the discrete variation

Based on DVDM, we calculate $J_{AC\mathrm{d}}(\boldsymbol{U}) - J_{AC\mathrm{d}}(\boldsymbol{V})$ to derive the discrete variational derivative by the following summation-by-parts formula:

$$\sum_{k=0}^{K-1} \left(\delta_k^+ f_k\right) \left(\delta_k^+ g_k\right) \Delta x = -\sum_{k=0}^{K}{}'' \left(\delta_k^{\langle 2\rangle} f_k\right) g_k \Delta x + \left[\left(\delta_k^{\langle 1\rangle} f_k\right) g_k\right]_0^K . \quad (5)$$

Remark

If we follow the method Fukao et al. used, we consequently use the following summation-by-parts formula:

$$\sum_{k=1}^{K} \left(\delta_k^- f_k\right) \left(\delta_k^- g_k\right) \Delta x = -\sum_{k=1}^{K} \left(\delta_k^{\langle 2\rangle} f_k\right) g_k \Delta x + \left[\left(\delta_k^+ f_k\right) g_k\right]_0^K .$$

Remark

By adopting the previously mentioned discrete energy and (5), we can approximate the boundary condition by **a central difference**.

Our structure-preserving scheme

For $n = 0, 1, \ldots,$

$$\begin{cases} \delta_n^+ U_k^{(n)} = \delta_k^{\langle 2 \rangle} \left(\dfrac{U_k^{(n+1)} + U_k^{(n)}}{2} \right) - \dfrac{dW}{d(U_k^{(n+1)}, U_k^{(n)})}, \quad (k = 0, \ldots, K), \\ \delta_n^+ U_0^{(n)} = \delta_k^{\langle 1 \rangle} \left(\dfrac{U_k^{(n+1)} + U_k^{(n)}}{2} \right) \Bigg|_{k=0} - \dfrac{dW}{d(U_0^{(n+1)}, U_0^{(n)})}, \\ \delta_n^+ U_K^{(n)} = -\delta_k^{\langle 1 \rangle} \left(\dfrac{U_k^{(n+1)} + U_k^{(n)}}{2} \right) \Bigg|_{k=K} - \dfrac{dW}{d(U_K^{(n+1)}, U_K^{(n)})}, \end{cases}$$

where δ_n^+ is the forward difference operator to time index (n). The concrete form of $dW/d(U_k^{(n+1)}, U_k^{(n)})$ is as follows:

$$\frac{dW}{d(U_k^{(n+1)}, U_k^{(n)})} = \frac{\left(U_k^{(n+1)}\right)^3 + \left(U_k^{(n+1)}\right)^2 U_k^{(n)} + U_k^{(n+1)} \left(U_k^{(n)}\right)^2 + \left(U_k^{(n)}\right)^3}{4} - \frac{U_k^{(n+1)} + U_k^{(n)}}{2} \quad (k = 0, \ldots, K).$$

Our structure-preserving scheme

For $n = 0, 1, \ldots,$

$$\begin{cases} \delta_n^+ U_k^{(n)} = \delta_k^{\langle 2 \rangle} \left(\dfrac{U_k^{(n+1)} + U_k^{(n)}}{2} \right) - \dfrac{dW}{d(U_k^{(n+1)}, U_k^{(n)})}, \quad (k = 0, \ldots, K), \\ \delta_n^+ U_0^{(n)} = \delta_k^{\langle 1 \rangle} \left(\dfrac{U_k^{(n+1)} + U_k^{(n)}}{2} \right) \Bigg|_{k=0} - \dfrac{dW}{d(U_0^{(n+1)}, U_0^{(n)})}, \\ \delta_n^+ U_K^{(n)} = - \delta_k^{\langle 1 \rangle} \left(\dfrac{U_k^{(n+1)} + U_k^{(n)}}{2} \right) \Bigg|_{k=K} - \dfrac{dW}{d(U_K^{(n+1)}, U_K^{(n)})}, \end{cases}$$

The solution $\boldsymbol{U}^{(n)}$ of the scheme satisfies the following discrete total energy dissipation:

$$\delta_n^+ \left\{ J_{AC\mathrm{d}}(\boldsymbol{U}^{(n)}) + W(U_0^{(n)}) + W(U_K^{(n)}) \right\}$$

$$= -\sum_{k=0}^{K}{}'' \left| \frac{\delta G_{AC\mathrm{d}}}{\delta \left(\boldsymbol{U}^{(n+1)}, \boldsymbol{U}^{(n)} \right)_k} \right|^2 \Delta x - |\delta_n^+ U_0^{(n)}|^2 - |\delta_n^+ U_K^{(n)}|^2 \leq 0 \quad (n = 0, 1, \ldots).$$

Our structure-preserving scheme

For $n = 0, 1, \ldots,$

$$\begin{cases} \delta_n^+ U_k^{(n)} = \delta_k^{\langle 2 \rangle} \left(\dfrac{U_k^{(n+1)} + U_k^{(n)}}{2} \right) - \dfrac{dW}{d(U_k^{(n+1)}, U_k^{(n)})}, \quad (k = 0, \ldots, K), \\ \delta_n^+ U_0^{(n)} = \delta_k^{\langle 1 \rangle} \left(\dfrac{U_k^{(n+1)} + U_k^{(n)}}{2} \right) \Bigg|_{k=0} - \dfrac{dW}{d(U_0^{(n+1)}, U_0^{(n)})}, \\ \delta_n^+ U_K^{(n)} = - \delta_k^{\langle 1 \rangle} \left(\dfrac{U_k^{(n+1)} + U_k^{(n)}}{2} \right) \Bigg|_{k=K} - \dfrac{dW}{d(U_K^{(n+1)}, U_K^{(n)})}, \end{cases}$$

Also, we have obtained the following mathematical results:

- L^∞-boundedness of the solution of the scheme
- Existence and uniqueness of the solution of the scheme
- Error estimate

Numerical example

As the initial condition, we consider

$$u(x,0) = \exp\{-500(x-0.5)^2\}.$$

Figure 5 shows the time development of the numerical solution. Figure 6 shows the time development of $J_{AC\mathrm{d}}(\boldsymbol{U}^{(n)}) + W(U_0^{(n)}) + W(U_K^{(n)})$.

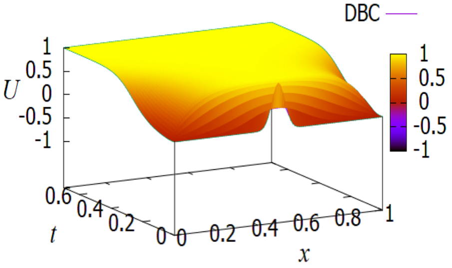


Fig. 5: Numerical solution

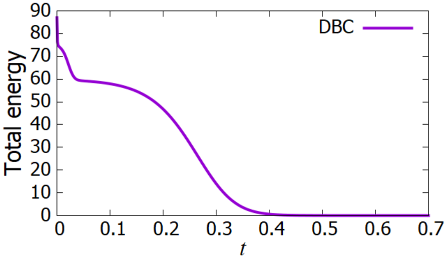


Fig. 6: Total energy

These graphs show that the numerical solution can be stably obtained by our proposed scheme and that the energy decreases numerically.

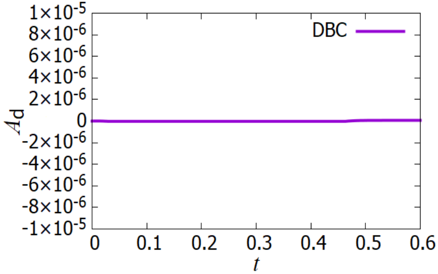
Dissipative property

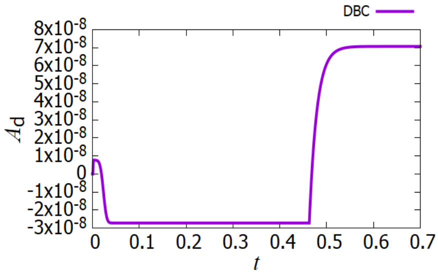
It follows from the discrete energy dissipation that

$$A_{\mathrm{d}}^{(n)} := J_{AC\mathrm{d}}(\boldsymbol{U}^{(n)}) + W(U_0^{(n)}) + W(U_K^{(n)}) + \sum_{l=0}^{n-1} \left\{ \sum_{k=0}^{K}{}'' \left| \frac{\delta G_{AC\mathrm{d}}}{\delta(\boldsymbol{U}^{(l+1)}, \boldsymbol{U}^{(l)})_k} \right|^2 \Delta x + \left| \delta_n^+ U_0^{(l)} \right|^2 + \left| \delta_n^+ U_K^{(l)} \right|^2 \right\} \Delta t = J_{AC\mathrm{d}}(\boldsymbol{U}^{(0)}) + W(U_0^{(0)}) + W(U_K^{(0)}) \quad (n = 1, \ldots, N).$$

These figures show the time development of

$$A_{\mathrm{d}}^{(n)} - (J_{AC\mathrm{d}}(\boldsymbol{U}^{(0)}) + W(U_0^{(0)}) + W(U_K^{(0)})).$$





Comparison between the dynamic boundary condition and the Neumann boundary one

$$u(x,0) = \exp\{-500(x-0.5)^2\}.$$

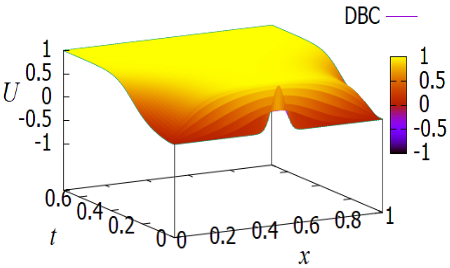


Fig. 7: Dynamic boundary condition: $10\partial_t u = -\partial_\nu u - 100(u^3 - u)$ on $\partial\Omega$.

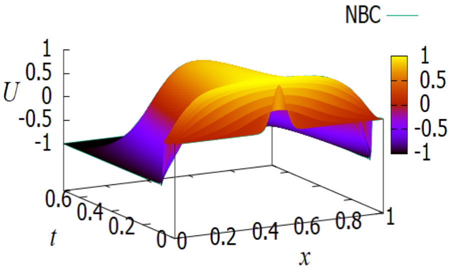


Fig. 8: Neumann boundary condition: $-\partial_\nu u - 100(u^3 - u) = 0$ on $\partial\Omega$.

These solutions arrive at different states from each other, although each stationary problem of the Allen–Cahn equation with the dynamic boundary condition and Neumann boundary one is the same.

Comparison between the dynamic boundary condition and the Neumann boundary one

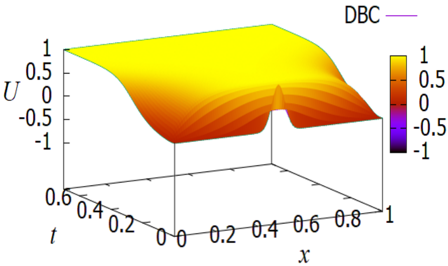


Fig. 11: Dynamic boundary condition: $10\partial_t u = -\partial_\nu u - 100(u^3 - u)$ on $\partial\Omega$.

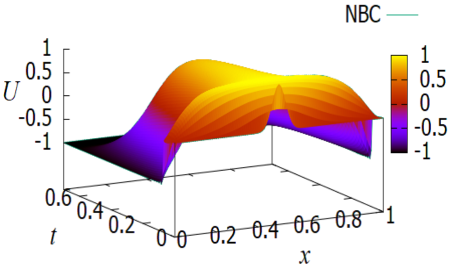


Fig. 12: Neumann boundary condition: $-\partial_\nu u - 100(u^3 - u) = 0$ on $\partial\Omega$.

These solutions arrive at different states from each other, although each stationary problem of the Allen–Cahn equation with the dynamic boundary condition and Neumann boundary one is the same.

Remark

The result assures that the difference in the long-time behavior of the solution occurs.

Comparison between the dynamic boundary condition and the Neumann boundary one

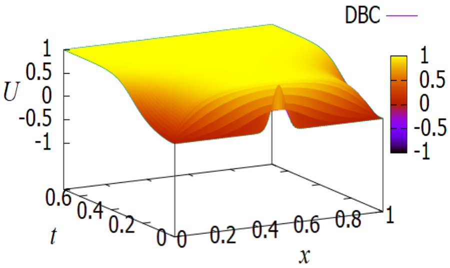


Fig. 11: Dynamic boundary condition: $10\partial_t u = -\partial_\nu u - 100(u^3 - u)$ on $\partial\Omega$.

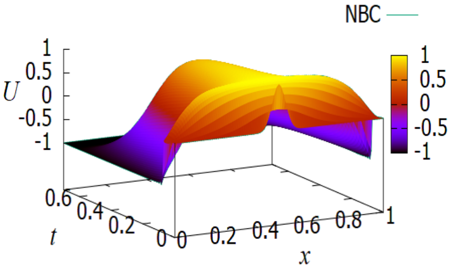


Fig. 12: Neumann boundary condition: $-\partial_\nu u - 100(u^3 - u) = 0$ on $\partial\Omega$.

These solutions arrive at different states from each other, although each stationary problem of the Allen–Cahn equation with the dynamic boundary condition and Neumann boundary one is the same.

Future work

We find initial values that cause differences in the long-time behavior of the solution and classify those that do and do not make the difference.

The discrete norms and the discrete Sobolev type inequality

Definition 4

For all $\boldsymbol{f} = \{f_k\}_{k=0}^{K} \in \mathbb{R}^{K+1}$,we define the discrete L^2-norm, the discrete Dirichlet semi-norm, the discrete Sobolev norm, and the discrete L^∞-norm by

$$\|\boldsymbol{f}\|_{L^2_{\mathrm{d}}} := \sqrt{\sum_{k=0}^{K}{}'' |f_k|^2 \Delta x}, \quad \|D\boldsymbol{f}\| := \sqrt{\sum_{k=0}^{K-1} |\delta_k^+ f_k|^2 \Delta x},$$

$$\|\boldsymbol{f}\|_{\tilde{H}^1_{\mathrm{d}}} := \sqrt{\|\boldsymbol{f}\|_{L^2_{\mathrm{d}}} + \|D\boldsymbol{f}\|^2}, \quad \|\boldsymbol{f}\|_{L^\infty_{\mathrm{d}}} := \max_{0 \le k \le K} |f_k|.$$

Lemma 5 (Discrete Sobolev type inequality, Yoshikawa(2017))

The following inequality holds:

$$\|\boldsymbol{f}\|_{L^\infty_{\mathrm{d}}} \le \tilde{C}_L \|\boldsymbol{f}\|_{\tilde{H}^1_{\mathrm{d}}} \quad \textit{for all } \{f_k\}_{k=0}^{K} \in \mathbb{R}^{K+1},$$

where $\tilde{C}_L$ is a constant depending on L only.

L^∞-boundedness of the solution

The following lemma holds from the discrete total energy dissipation.

Lemma 6

Let us define a constant C_0 independent of k and n by

$$C_0 := 2\left\{ J_{AC\mathrm{d}}(\boldsymbol{U}^{(0)}) + W(U_0^{(0)}) + W(U_K^{(0)}) \right\} + \frac{3}{2}(L+2).$$

Then the solution $\boldsymbol{U}^{(n)}$ of the scheme satisfies the following inequality:

$$\left\| \boldsymbol{U}^{(n)} \right\|_{\tilde{H}^1_\mathrm{d}}^2 + \left| U_0^{(n)} \right|^2 + \left| U_K^{(n)} \right|^2 \le C_0 \quad (n = 0, 1, \ldots).$$

By using Lemma 6 and the discrete Sobolev type inequality, we obtain

Theorem 3.1

The solution $\boldsymbol{U}^{(n)}$ of the scheme satisfies the following inequality:

$$\left\| \boldsymbol{U}^{(n)} \right\|_{L^\infty_\mathrm{d}} \le \tilde{C}_L \sqrt{C_0} \quad (n = 0, 1, \ldots).$$

Existence and uniqueness of the solution

We prove the proposed scheme has a unique solution under a specific condition on Δt.

Theorem 3.2

For any given $\boldsymbol{U}^{(0)} = \{U_k^{(0)}\}_{k=-1}^{K+1} \in \mathbb{R}^{K+3}$, *if* Δt *satisfies*

$$\Delta t^2 \max\left\{ 5 \max_{|\xi| \le 2B_0} \left|W''(\xi)\right|^2, \frac{\max_{|\xi| \le 2B_0} \left|W''(\xi)\right|^2}{2} + \frac{25 \tilde{C}_L^2 B_0^2 \max_{|\xi| \le 2B_0} \left|W'''(\xi)\right|^2}{18} \right\} < 1,$$

where B_0 *is the* L^∞*-bound of the solution, i.e.,* $B_0 := \tilde{C}_L \sqrt{C_0}$, *then there exists a unique solution* $\{U_k^{(n)}\}_{k=-1}^{K+1} \in \mathbb{R}^{K+3}$ $(n \in \mathbb{N})$ *of the scheme.*

Remark

We remark that the assumption is independent of the space mesh size Δx.

Error estimate

Let $\Delta t := T/N$.

Theorem 3.3

Assume that $u \in C^5([0,L] \times [0,T])$. *Also, denote the bounds by*

$$\max_{0\le n\le N}\left\{\left\|D\boldsymbol{U}^{(n)}\right\|, \left\|D\boldsymbol{u}^{(n)}\right\|\right\} \le C_1, \quad \max_{0\le n\le N}\left\{\left\|\boldsymbol{U}^{(n)}\right\|_{L^\infty_{\mathrm{d}}}, \left\|\boldsymbol{u}^{(n)}\right\|_{L^\infty_{\mathrm{d}}}\right\} \le C_2,$$

where C_1 and C_2 are constants independent of n. Let

$$C_W := 2\left\{C_1^2 \tilde{C}_L^2 \max_{|\xi|\le C_2} \left|W'''(\xi)\right|^2 + \max_{|\xi|\le C_2}\left|W''(\xi)\right|^2\right\}.$$

If Δt satisfies $\Delta t < 1/\{3(1+C_W)\}$, then there exists a constant C independent of k and n such that

$$\|(\Pi_{\Delta x,\Delta t}U)(\cdot,t) - u(\cdot,t)\|_{L^\infty(0,L)} \le C\left((\Delta x)^2 + (\Delta t)^2\right) \quad \text{for all } t \in [0,T],$$

where $\Pi_{\Delta x,\Delta t}U$ is the function which interpolates the grid value point $U_k^{(n)}$.

Error estimate

Let $\Delta t := T/N$.

Theorem 3.3

Assume that $u \in C^5([0,L] \times [0,T])$. Also, denote the bounds by

$$\max_{0 \le n \le N} \left\{ \left\| D\boldsymbol{U}^{(n)} \right\|, \left\| D\boldsymbol{u}^{(n)} \right\| \right\} \le C_1, \quad \max_{0 \le n \le N} \left\{ \left\| \boldsymbol{U}^{(n)} \right\|_{L^\infty_{\mathrm{d}}}, \left\| \boldsymbol{u}^{(n)} \right\|_{L^\infty_{\mathrm{d}}} \right\} \le C_2,$$

where C_1 and C_2 are constants independent of n. Let

$$C_W := 2 \left\{ C_1^2 \tilde{C}_L^2 \max_{|\xi| \le C_2} \left| W'''(\xi) \right|^2 + \max_{|\xi| \le C_2} \left| W''(\xi) \right|^2 \right\}.$$

If Δt satisfies $\Delta t < 1/\{3(1 + C_W)\}$, then there exists a constant C independent of k and n such that

$$\|(\Pi_{\Delta x, \Delta t} U)(\cdot, t) - u(\cdot, t)\|_{L^\infty(0,L)} \le C\left((\Delta x)^2 + (\Delta t)^2\right) \quad \textit{for all } t \in [0,T],$$

Remark

This theorem means that our scheme is second-order accurate in space and time, respectively.

Conclusions and future work

- Conclusions
  - We introduced the procedure of constructing a structure-preserving scheme by DVDM.
  - We designed a structure-preserving scheme for the Allen–Cahn equation with a dynamic boundary condition by using DVDM.
  - We can use a central difference as an approximation of an outward normal derivative on the discrete boundary condition of the scheme.
  - We proved the L^∞-boundedness, the existence and the uniqueness of the solution, and the error estimate for our scheme.
- Future work
  - The comparative study of the dynamic and Neumann boundary conditions through the long-time behavior of the solution.

The Cahn–Hilliard equation with a dynamic boundary condition

We study the following Cahn–Hilliard equation with a dynamic boundary condition:

$$\begin{cases} \partial_t u = \partial_x^2 p, & \text{in } \Omega \times (0,T], \\ p = -\gamma \partial_x^2 u + u^3 - u, & \text{in } \Omega \times (0,T], \\ \partial_t u(0,t) = \partial_x u(x,t)\big|_{x=0}, & \text{in } (0,T], \\ \partial_t u(L,t) = -\,\partial_x u(x,t)\big|_{x=L}, & \text{in } (0,T], \\ \partial_x p(x,t)\big|_{x=0} = \partial_x p(x,t)\big|_{x=L} = 0, & \text{in } (0,T], \end{cases}$$

where γ is a positive constant, and the nonlinear term is the derivative of $W(s) := (1/4)s^4 - (1/2)s^2$.

◦ T. Fukao, S. Yoshikawa, and S. Wada, Structure-preserving finite difference schemes for the Cahn–Hilliard equation with dynamic boundary condition in the one-dimensional case, Commun. Pure Appl. Anal., **16** (2017), 1915–1938.

The Cahn–Hilliard equation with a dynamic boundary condition

We study the following Cahn–Hilliard equation with a dynamic boundary condition:

$$\begin{cases} \partial_t u = \partial_x^2 p, & \text{in } \Omega \times (0,T], \\ p = -\gamma \partial_x^2 u + u^3 - u, & \text{in } \Omega \times (0,T], \\ \partial_t u(0,t) = \left. \partial_x u(x,t) \right|_{x=0}, & \text{in } (0,T], \\ \partial_t u(L,t) = - \left. \partial_x u(x,t) \right|_{x=L}, & \text{in } (0,T], \\ \left. \partial_x p(x,t) \right|_{x=0} = \left. \partial_x p(x,t) \right|_{x=L} = 0, & \text{in } (0,T]. \end{cases}$$

The solution u of the problem satisfies the following energy dissipation:

$$\frac{d}{dt} J_{CH}(u(t)) = -\gamma |\partial_t u(0,t)|^2 - \gamma |\partial_t u(L,t)|^2 - \int_0^L |\partial_x p(x,t)|^2 dx \leq 0,$$

where the "local energy" G_{CH} and the "global energy" J_{CH} are defined by

$$G_{CH}(u, \partial_x u) := \frac{\gamma}{2} |\partial_x u|^2 + W(u), \quad J_{CH}(u) := \int_0^L G_{CH}(u, \partial_x u) dx.$$

The Cahn–Hilliard equation with a dynamic boundary condition

We study the following Cahn–Hilliard equation with a dynamic boundary condition:

$$\begin{cases} \partial_t u = \partial_x^2 p, & \text{in } \Omega \times (0,T], \\ p = -\gamma \partial_x^2 u + u^3 - u, & \text{in } \Omega \times (0,T], \\ \partial_t u(0,t) = \left.\partial_x u(x,t)\right|_{x=0}, & \text{in } (0,T], \\ \partial_t u(L,t) = -\left.\partial_x u(x,t)\right|_{x=L}, & \text{in } (0,T], \\ \left.\partial_x p(x,t)\right|_{x=0} = \left.\partial_x p(x,t)\right|_{x=L} = 0, & \text{in } (0,T]. \end{cases}$$

The solution u of the problem satisfies the following energy dissipation:

$$\frac{d}{dt} J_{CH}(u(t)) = -\gamma |\partial_t u(0,t)|^2 - \gamma |\partial_t u(L,t)|^2 - \int_0^L |\partial_x p(x,t)|^2 dx \le 0,$$

Also, the solution u satisfies the following mass conservation:

$$\frac{d}{dt} \int_0^L u(x,t) dx = 0.$$

Our structure-preserving scheme

For $n = 0, 1, \ldots,$

$$\begin{cases} \delta_n^+ U_k^{(n)} = \delta_k^{\langle 2 \rangle} P_k^{(n)}, \quad (k = 0, \ldots, K), \\ P_k^{(n)} = -\gamma \delta_k^{\langle 2 \rangle} \left(\frac{U_k^{(n+1)} + U_k^{(n)}}{2} \right) + \frac{dW}{d(U_k^{(n+1)}, U_k^{(n)})}, \quad (k=0, \ldots, K), \\ \delta_n^+ U_0^{(n)} = \delta_k^{\langle 1 \rangle} \left(\frac{U_k^{(n+1)} + U_k^{(n)}}{2} \right) \Bigg|_{k=0}, \\ \delta_n^+ U_K^{(n)} = - \delta_k^{\langle 1 \rangle} \left(\frac{U_k^{(n+1)} + U_k^{(n)}}{2} \right) \Bigg|_{k=K}, \\ \delta_k^{\langle 1 \rangle} P_k^{(n)} = 0 \quad (k = 0, K), \end{cases}$$

The solution of the scheme satisfies the following discrete energy dissipation: for $n = 0, 1, \ldots,$

$$\delta_n^+ J_{CH\mathrm{d}}(\boldsymbol{U}^{(n)}) = -\gamma \left| \delta_n^+ U_0^{(n)} \right|^2 - \gamma \left| \delta_n^+ U_K^{(n)} \right|^2 - \sum_{k=0}^{K-1} \left| \delta_k^+ P_k^{(n)} \right|^2 \Delta x \leq 0,$$

where $J_{CH\mathrm{d}}(\boldsymbol{U}) := \sum_{k=0}^{K-1} (\gamma/2)(\delta_k^+ U_k)^2 \Delta x + \sum_{k=0}^{K}{}'' W(U_k) \Delta x.$

Our structure-preserving scheme

For $n = 0, 1, \ldots,$

$$\begin{cases} \delta_n^+ U_k^{(n)} = \delta_k^{\langle 2 \rangle} P_k^{(n)}, \quad (k = 0, \ldots, K), \\ P_k^{(n)} = -\gamma \delta_k^{\langle 2 \rangle} \left(\frac{U_k^{(n+1)} + U_k^{(n)}}{2} \right) + \frac{dW}{d(U_k^{(n+1)}, U_k^{(n)})}, \quad (k = 0, \ldots, K), \\ \delta_n^+ U_0^{(n)} = \delta_k^{\langle 1 \rangle} \left(\frac{U_k^{(n+1)} + U_k^{(n)}}{2} \right) \Bigg|_{k=0}, \\ \delta_n^+ U_K^{(n)} = - \delta_k^{\langle 1 \rangle} \left(\frac{U_k^{(n+1)} + U_k^{(n)}}{2} \right) \Bigg|_{k=K}, \\ \delta_k^{\langle 1 \rangle} P_k^{(n)} = 0 \quad (k = 0, K), \end{cases}$$

The solution of the scheme satisfies the following discrete mass conservation: for $n = 0, 1, \ldots,$

$$\delta_n^+ M_{\mathrm{d}}(\boldsymbol{U}^{(n)}) = 0,$$

where M_{d} is the discrete mass and defined by $M_{\mathrm{d}}(\boldsymbol{U}) := \sum_{k=0}^{K}{}'' U_k \Delta x$.

Our structure-preserving scheme

For $n = 0, 1, \ldots,$

$$\begin{cases} \delta_n^+ U_k^{(n)} = \delta_k^{\langle 2\rangle} P_k^{(n)}, \quad (k = 0, \ldots, K), \\ P_k^{(n)} = -\gamma \delta_k^{\langle 2\rangle} \left(\dfrac{U_k^{(n+1)} + U_k^{(n)}}{2} \right) + \dfrac{dW}{d(U_k^{(n+1)}, U_k^{(n)})}, \quad (k=0, \ldots, K), \\ \delta_n^+ U_0^{(n)} = \delta_k^{\langle 1\rangle} \left(\dfrac{U_k^{(n+1)} + U_k^{(n)}}{2} \right) \Bigg|_{k=0}, \\ \delta_n^+ U_K^{(n)} = -\delta_k^{\langle 1\rangle} \left(\dfrac{U_k^{(n+1)} + U_k^{(n)}}{2} \right) \Bigg|_{k=K}, \\ \delta_k^{\langle 1\rangle} P_k^{(n)} = 0 \quad (k = 0, K), \end{cases}$$

Remark

We use **a central difference** as an approximation of an outward normal derivative on the boundary, although Fukao, Yoshikawa, and Wada use a forward difference in their structure-preserving scheme's boundary conditions (Fukao–Yoshikawa–Wada(2017)).

Our structure-preserving scheme

For $n = 0, 1, \ldots,$

$$
\begin{cases}
\delta_n^+ U_k^{(n)} = \delta_k^{\langle 2 \rangle} P_k^{(n)}, \quad (k = 0, \ldots, K), \\
P_k^{(n)} = -\gamma \delta_k^{\langle 2 \rangle} \left(\dfrac{U_k^{(n+1)} + U_k^{(n)}}{2} \right) + \dfrac{dW}{d(U_k^{(n+1)}, U_k^{(n)})}, \quad (k = 0, \ldots, K), \\
\delta_n^+ U_0^{(n)} = \delta_k^{\langle 1 \rangle} \left(\dfrac{U_k^{(n+1)} + U_k^{(n)}}{2} \right) \Bigg|_{k=0}, \\
\delta_n^+ U_K^{(n)} = - \delta_k^{\langle 1 \rangle} \left(\dfrac{U_k^{(n+1)} + U_k^{(n)}}{2} \right) \Bigg|_{k=K}, \\
\delta_k^{\langle 1 \rangle} P_k^{(n)} = 0 \quad (k = 0, K),
\end{cases}
$$

Also, we have obtained the following mathematical results:

- L^∞-boundedness of the solution of the scheme
- Existence and uniqueness of the solution of the scheme
- Error estimate

Note that our scheme is second-order accurate in space, although the previous scheme by Fukao–Yoshikawa–Wada(2017) is first-order accurate.

GMS model

We study the following GMS model:

$$\begin{cases} \partial_t u = \partial_x^2 p, \quad \text{in } \Omega \times (0,T] \\ p = -\gamma \partial_x^2 u + u^3 - u, \quad \text{in } \Omega \times (0,T], \\ \partial_t u(0,t) = \partial_x p(x,t)|_{x=0}, \quad \partial_t u(L,t) = -\partial_x p(x,t)|_{x=L}, \quad \text{in } (0,T], \\ p(0,t) = -\gamma \partial_x u(x,t)|_{x=0} + (u(0,t))^3 - u(0,t), \quad \text{in } (0,T], \\ p(L,t) = \gamma \partial_x u(x,t)|_{x=L} + (u(L,t))^3 - u(L,t), \quad \text{in } (0,T]. \end{cases}$$

Then, the solution u of the problem satisfies the following total energy dissipation:

$$\frac{d}{dt}\{J_{CH}(u(t)) + W(u(0,t)) + W(u(L,t))\} \leq 0.$$

Also, the solution u satisfies the following total mass conservation:

$$\frac{d}{dt}\left\{\int_0^L u(x,t)dx + u(0,t) + u(L,t)\right\} = 0.$$

◦ G. R. Goldstein, A. Miranville and G. Schimperna, A Cahn–Hilliard model in a domain with non-permeable walls, Physica D, **240** (2011), 754–766.

Our structure-preserving scheme

For $n = 0, 1, \dots,$

$$\begin{cases} \delta_n^+ U_k^{(n)} = \delta_k^{\langle 2 \rangle} P_k^{(n)}, \quad (k = 0, \dots, K), \\ P_k^{(n)} = -\gamma \delta_k^{\langle 2 \rangle} \left(\dfrac{U_k^{(n+1)} + U_k^{(n)}}{2} \right) + \dfrac{dW}{d(U_k^{(n+1)}, U_k^{(n)})}, \quad (k=0, \dots, K), \\ \delta_n^+ U_0^{(n)} = \left. \delta_k^{\langle 1 \rangle} P_k^{(n)} \right|_{k=0}, \quad \delta_n^+ U_K^{(n)} = - \left. \delta_k^{\langle 1 \rangle} P_k^{(n)} \right|_{k=K}, \\ P_0^{(n)} = -\gamma \left. \delta_k^{\langle 1 \rangle} \left(\dfrac{U_k^{(n+1)} + U_k^{(n)}}{2} \right) \right|_{k=0} + \dfrac{dW}{d(U_0^{(n+1)}, U_0^{(n)})}, \\ P_K^{(n)} = \gamma \left. \delta_k^{\langle 1 \rangle} \left(\dfrac{U_k^{(n+1)} + U_k^{(n)}}{2} \right) \right|_{k=K} + \dfrac{dW}{d(U_K^{(n+1)}, U_K^{(n)})}. \end{cases}$$

The solution of the scheme satisfies the following discrete total energy dissipation and discrete total mass conservation:

$$\delta_n^+ \left\{ J_{CH\mathrm{d}}(\boldsymbol{U}^{(n)}) + W(U_0^{(n)}) + W(U_K^{(n)}) \right\} \leq 0 \quad (n = 0, 1, \dots),$$

$$\delta_n^+ \left\{ M_{\mathrm{d}}(\boldsymbol{U}^{(n)}) + U_0^{(n)} + U_K^{(n)} \right\} = 0 \quad (n = 0, 1, \dots).$$

Our structure-preserving scheme

For $n = 0, 1, \ldots,$

$$
\begin{cases}
\delta_n^+ U_k^{(n)} = \delta_k^{\langle 2 \rangle} P_k^{(n)}, \quad (k = 0, \ldots, K), \\
P_k^{(n)} = -\gamma \delta_k^{\langle 2 \rangle} \left(\dfrac{U_k^{(n+1)} + U_k^{(n)}}{2} \right) + \dfrac{dW}{d(U_k^{(n+1)}, U_k^{(n)})}, \quad (k = 0, \ldots, K), \\
\delta_n^+ U_0^{(n)} = \delta_k^{\langle 1 \rangle} P_k^{(n)} \Big|_{k=0}, \quad \delta_n^+ U_K^{(n)} = -\delta_k^{\langle 1 \rangle} P_k^{(n)} \Big|_{k=K}, \\
P_0^{(n)} = -\gamma \delta_k^{\langle 1 \rangle} \left(\dfrac{U_k^{(n+1)} + U_k^{(n)}}{2} \right) \Bigg|_{k=0} + \dfrac{dW}{d(U_0^{(n+1)}, U_0^{(n)})}, \\
P_K^{(n)} = \gamma \delta_k^{\langle 1 \rangle} \left(\dfrac{U_k^{(n+1)} + U_k^{(n)}}{2} \right) \Bigg|_{k=K} + \dfrac{dW}{d(U_K^{(n+1)}, U_K^{(n)})}.
\end{cases}
$$

Remark

Fukao, Yoshikawa, and Wada use a forward difference in their scheme's boundary conditions (Fukao–Yoshikawa–Wada(2017)).

Also, we have obtained the following mathematical results.

- L^∞-boundedness of the solution of the scheme
- Existence and uniqueness of the solution of the scheme

References

[1] T. Fukao, S. Yoshikawa, and S. Wada, Structure-preserving finite difference schemes for the Cahn–Hilliard equation with dynamic boundary conditions in the one-dimensional case, Commun. Pure Appl. Anal., **16** (2017), 1915–1938.

[2] D. Furihata and T. Matsuo, *Discrete variational derivative method: A structure-preserving numerical method for partial differential equations*, CRC Press, 2010.

[3] G. R. Goldstein, A. Miranville, and G. Schimperna, A Cahn–Hilliard model in a domain with non-permeable walls, Physica D, **240** (2011), 754–766.

[4] M. Okumura and D. Furihata, A structure-preserving scheme for the Allen-Cahn equation with a dynamic boundary condition, Discrete Contin. Dyn. Syst., **40** (2020), 4927–4960.

[5] S. Yoshikawa, Energy method for structure-preserving finite difference schemes and some properties of difference quotient, J. Comput. Appl. Math., **311** (2017), 394–413.

[6] S. Yoshikawa, Remarks on energy methods for structure-preserving finite difference schemes – Small data global existence and unconditional error estimate, Appl. Math. Comput., **341** (2019), 80–92.

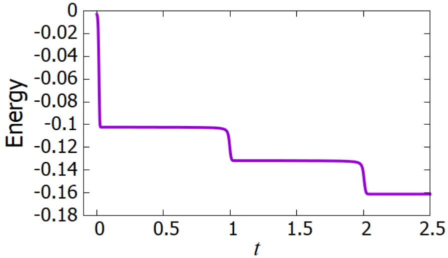
The dissipative and conservative properties

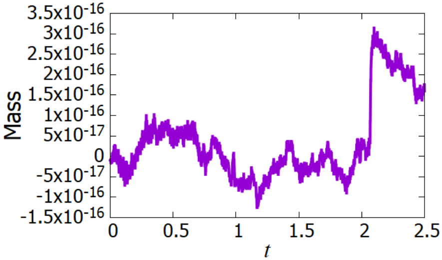
$$\begin{cases} \partial_t u = \partial_x^2(-\gamma \partial_x^2 u + u^3 - u), & \text{in } (0,L)\times(0,T], \\ \partial_x u(x,t)\big|_{x=0,L} = \partial_x^3 u(x,t)\big|_{x=0,L} = 0, & \text{in } (0,T]. \end{cases}$$

The solution u to the above problem satisfies the following energy dissipation and mass conservation:

$$\frac{d}{dt}J(u(t)) \le 0, \quad \int_0^L u(x,t)dx = \int_0^L u(x,0)dx,$$

These figures show the time developments of the discrete energy and the discrete mass by the discrete variational derivative scheme, respectively.





Calculation of the discrete variation

First, using the summation-by-parts formula:

$$\sum_{k=0}^{K}{}'' \frac{(\delta_k^+ f_k)(\delta_k^+ g_k) + (\delta_k^- f_k)(\delta_k^- g_k)}{2} \Delta x = \sum_{k=0}^{K}{}'' (\delta_k^{\langle 2\rangle} f_k) g_k \Delta x + (\text{b.t.}),$$

we have the following identity:

$$\sum_{k=0}^{K}{}'' \left\{ \frac{\gamma}{2} \frac{(\delta_k^+ U_k)^2 + (\delta_k^- U_k)^2}{2} - \frac{\gamma}{2} \frac{(\delta_k^+ V_k)^2 + (\delta_k^- V_k)^2}{2} \right\} \Delta x$$

$$= \frac{\gamma}{2} \sum_{k=0}^{K}{}'' \left[\left\{ \delta_k^+ \left(\frac{U_k + V_k}{2} \right) \right\} \left\{ \delta_k^+ (U_k - V_k) \right\} + \left\{ \delta_k^- \left(\frac{U_k + V_k}{2} \right) \right\} \left\{ \delta_k^- (U_k - V_k) \right\} \right] \Delta x$$

$$= \sum_{k=0}^{K}{}'' \left\{ -\gamma \delta_k^{\langle 2\rangle} \left(\frac{U_k + V_k}{2} \right) \right\} (U_k - V_k) \Delta x + (\text{b.t.}).$$

The discrete mass conservation

Summing the following equation:

$$\frac{U_k^{(n+1)} - U_k^{(n)}}{\Delta t} = \delta_k^{\langle 2 \rangle}\left(\frac{\delta G_{\mathrm{d}}}{\delta(\boldsymbol{U}^{(n+1)}, \boldsymbol{U}^{(n)})_k}\right), \quad (k=0,\ldots,K,\ n=0,1,\ldots)$$

over $k = 0, \ldots, K$ based on the trapezoidal rule, we can also show the discrete mass conservation:

$$\frac{1}{\Delta t}\left(\sum_{k=0}^{K}{}'' U_k^{(n+1)}\Delta x - \sum_{k=0}^{K}{}'' U_k^{(n)}\Delta x\right) = \sum_{k=0}^{K}{}'' \frac{U_k^{(n+1)} - U_k^{(n)}}{\Delta t}\Delta x$$

$$= \sum_{k=0}^{K}{}'' \delta_k^{\langle 2 \rangle}\left(\frac{\delta G_{\mathrm{d}}}{\delta(\boldsymbol{U}^{(n+1)}, \boldsymbol{U}^{(n)})_k}\right)\Delta x = \left[\delta_k^{\langle 1 \rangle}\left(\frac{\delta G_{\mathrm{d}}}{\delta(\boldsymbol{U}^{(n+1)}, \boldsymbol{U}^{(n)})_k}\right)\right]_0^K$$

$$= 0 \quad (n = 0, 1, \ldots).$$

under the suitable discrete boundary condition. For example, we impose the following discrete Neumann boundary conditions:

$$\delta_k^{\langle 1 \rangle} U_k^{(n)} = \delta_k^{\langle 1 \rangle}\left(\frac{\delta G_{\mathrm{d}}}{\delta(\boldsymbol{U}^{(n+1)}, \boldsymbol{U}^{(n)})_k}\right) = 0 \quad (k = 0, K,\ n = 0, 1, \ldots).$$

Calculation of the discrete variation

Based on DVDM, we calculate $J_{AC\mathrm{d}}(\boldsymbol{U}) - J_{AC\mathrm{d}}(\boldsymbol{V})$ to derive the discrete variational derivative by the following summation-by-parts formula:

$$\sum_{k=0}^{K-1} \left(\delta_k^+ f_k\right)\left(\delta_k^+ g_k\right)\Delta x = -\sum_{k=0}^{K}{}'' \left(\delta_k^{\langle 2\rangle} f_k\right) g_k \Delta x + \left[\left(\delta_k^{\langle 1\rangle} f_k\right) g_k\right]_0^K .$$

Property

For all $\boldsymbol{U} = \{U_k\}_{k=-1}^{K+1}, \boldsymbol{V} = \{V_k\}_{k=-1}^{K+1} \in \mathbb{R}^{K+3}$, it holds that

$$J_{AC\mathrm{d}}(\boldsymbol{U}) - J_{AC\mathrm{d}}(\boldsymbol{V}) = \sum_{k=0}^{K}{}'' \left\{ -\delta_k^{\langle 2\rangle}\left(\frac{U_k+V_k}{2}\right) + \frac{dW}{d(U_k,V_k)} \right\}(U_k - V_k)\,\Delta x + \left[\left\{\delta_k^{\langle 1\rangle}\left(\frac{U_k+V_k}{2}\right)\right\}(U_k - V_k)\right]_0^K ,$$

where

$$\frac{dW}{d(U_k,V_k)} = \frac{U_k^3 + U_k^2 V_k + U_k V_k^2 + V_k^3}{4} - \frac{U_k + V_k}{2}$$

Numerical example 2

As the initial condition, we consider

$$u(x,0) = 0.02 - 0.05\cos(5\pi x) - 0.008\sin(8\pi x) + 0.01\cos(2\pi x).$$

Figure 13 shows the time development of the numerical solution. Figure 14 shows the time development of $J_{AC\mathrm{d}}(\boldsymbol{U}^{(n)}) + W(U_0^{(n)}) + W(U_K^{(n)})$.

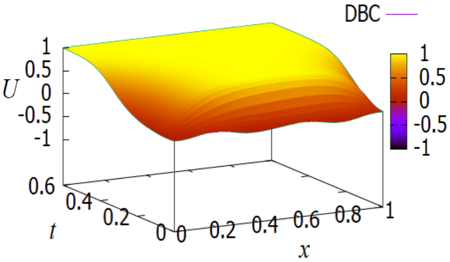


Fig. 13: Numerical solution

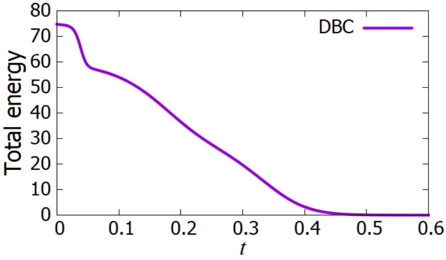


Fig. 14: Total energy

These graphs show that the numerical solution can be stably obtained by our proposed scheme and that the energy decreases numerically.

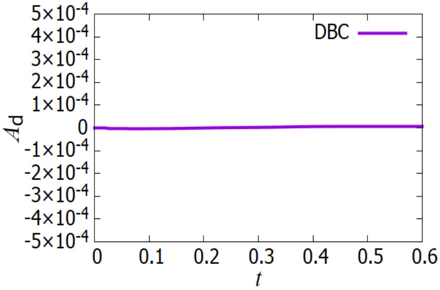
Dissipative property

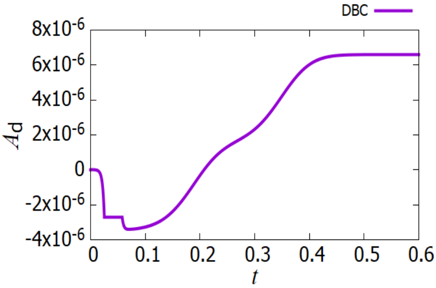
It follows from the discrete energy dissipation that

$$A_{\mathrm{d}}^{(n)} = J_{AC\mathrm{d}}(\boldsymbol{U}^{(0)}) + W(U_0^{(0)}) + W(U_K^{(0)}) \quad (n = 1, \dots, N).$$

These figures show the time development of

$$A_{\mathrm{d}}^{(n)} - (J_{AC\mathrm{d}}(\boldsymbol{U}^{(0)}) + W(U_0^{(0)}) + W(U_K^{(0)})).$$





These graphs show that $A_{\mathrm{d}}^{(n)}$ is conserved numerically.

Comparison between the dynamic boundary condition and the Neumann boundary one

$$u(x,0) = 0.02 - 0.05\cos(5\pi x) - 0.008\sin(8\pi x) + 0.01\cos(2\pi x).$$

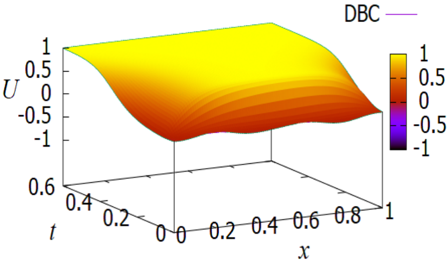


Fig. 15: Dynamic boundary condition: $10\partial_t u = -\partial_\nu u - 100(u^3 - u)$ on $\partial\Omega$.

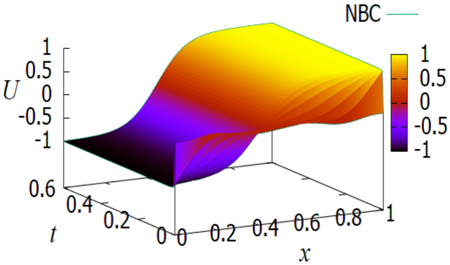


Fig. 16: Neumann boundary condition: $-\partial_\nu u - 100(u^3 - u) = 0$ on $\partial\Omega$.

These solutions arrive at different states from each other, although each stationary problem of the Allen–Cahn equation with the dynamic boundary condition and Neumann boundary one is the same.