Design and analysis of structure-preserving schemes for parabolic partial differential equations with dynamic boundary conditions

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Journal articles

1. M. Okumura, A stable and structure-preserving scheme for a non-local Allen–Cahn equation, Jpn. J. Ind. Appl. Math., **35** (2018), 1245–1281.
2. 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.

Preprint

1. M. Okumura, T. Fukao, D. Furihata, and S. Yoshikawa, A second-order accurate structure-preserving scheme for the Cahn–Hilliard equation with a dynamic boundary condition, preprint arXiv:2007.08355 [math.NA] (2020), 1–32.

Report

1. 奥村 真善美, 体積保存型 Allen–Cahn 方程式に対する離散変分導関数法による非線形及び線形スキーム, 第 39 回発展方程式若手セミナー報告集, 2017 年 11 月, 49–58.

International Conference Presentations

1. M. Okumura, A linear and structure-preserving scheme for a non-local conservative Allen–Cahn equation, The 12th AIMS Conference on Dynamical Systems, Differential Equations and Applications, Taipei (Taiwan), July 2018.
2. M. Okumura, A structure-preserving scheme for the Cahn–Hilliard equation with a dynamic boundary condition, Equadiff 2019, Leiden (Netherlands), July 2019.
3. M. Okumura, Structure-preserving schemes for PDEs with dynamic boundary conditions, 復旦大学数学科学学院 数学総合報告会, Shanghai (China), November 2019.
4. M. Okumura, Recent results on the structure-preserving scheme for the Allen–Cahn equation with a dynamic boundary condition, KAAS seminar, Karlstad (Sweden), June 2020.

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1. 奥村 真善美, 体積保存型 Allen–Cahn 方程式に対する離散変分導関数法による非線形及び線形スキーム, 第 39 回発展方程式若手セミナー, 愛知, 2017 年 9 月.
2. 奥村 真善美, 体積保存型 Allen–Cahn 方程式に対する線形多段階化離散変分導関数法スキームについて, 第 43 回発展方程式研究会, 東京, 2017 年 12 月.
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Design and analysis of structure-preserving schemes for parabolic partial differential equations with dynamic boundary conditions

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Contents

Chapter 1

Introduction

In this thesis, we aim at improving structure-preserving schemes for problems under boundary conditions, including time derivatives, which are called dynamic boundary conditions. Thus, we have worked on the design and the analysis of structure-preserving schemes for the Allen–Cahn equation and the Cahn–Hilliard equation, classified as parabolic partial differential ones. For each target problem, we have designed appropriate structure-preserving schemes and have obtained the theoretical results, i.e., the L^∞-boundedness, the solvability, and the error estimate of the schemes. We have especially obtained the result of improving the spatial accuracy of the structure-preserving schemes for the problems under dynamic boundary conditions.

Recently, initial-boundary-value problems of partial differential equations with dynamic boundary conditions are actively studied mainly by the European research team [9, 12–21, 33–35, 39, 42, 46–49, 54, 55, 58]. It is often difficult to solve complicated partial differential equations describing nonlinear phenomena analytically. Thus, the numerical analysis, which solves them numerically, is important. In the numerical analysis for partial differential equations, we discretize the equations, which are continuous systems, and replace them with discrete systems based on discrete approximations (henceforth called schemes), which are then solved. Although numerical computations for partial differential equations are not simple, structure-preserving numerical methods are expected to be effective for difficult problems to solve numerically, such as the Cahn–Hilliard equation [8], which describes phase separation phenomena. Throughout this thesis, structure-preserving means that the scheme inherits the conservative property such as mass conservation or the dissipative property such as energy dissipation. In fact, Furihata and Matsuo have designed a structure-preserving scheme for the above equation with the Neumann boundary condition using the discrete variational derivative method (DVDM), the structure-preserving numerical method developed by Furihata and Matsuo, and the scheme has realized the fast and stable computation [29–31]. We remark that the history of numerical computation of problems with dynamic boundary conditions is short and that, in particular, there are almost no results of structure-preserving schemes for the problems with dynamic boundary conditions. Actually, in [28], Fukao, Yoshikawa, and Wada proposed a structure-preserving scheme based on DVDM for the following one-dimensional Cahn–Hilliard equation:

$$\begin{cases} \partial_t u = \partial_x^2 p & \text{in } (0, L) \times (0, \infty), \\ p = -\gamma \partial_x^2 u + F'(u) & \text{in } (0, L) \times (0, \infty), \end{cases}$$

under the dynamic boundary condition and the Neumann boundary condition:

$$\begin{cases} \partial_t u(0,t) = \partial_x u(x,t)|_{x=0}, \quad \partial_t u(L,t) = -\,\partial_x u(x,t)|_{x=L} & \text{in } (0,\infty), \\ \partial_x p(x,t)|_{x=0} = \partial_x p(x,t)|_{x=L} = 0 & \text{in } (0,\infty). \end{cases}$$

Their proposed scheme inherits mass conservation law and energy dissipation law from the original problem. However, they use a forward difference as an approximation of an outward normal derivative on the boundary, and as a result, the scheme is only first-order accurate in space. Thus, we aim to improve structure-preserving schemes for the problems with dynamic boundary conditions and start with the Allen–Cahn equation [1] that is easier to handle than the Cahn–Hilliard equation. First, to understand the idea of designing a structure-preserving scheme by DVDM, we have designed a structure-preserving scheme for the Allen–Cahn equation with a non-local term proposed by Rubinstein and Sternberg [56] under the Neumann boundary condition. Next, based on the above idea of designing the structure-preserving scheme, by improving the discretization of energy and a summation-by-parts formula, which are important in DVDM, we have designed structure-preserving schemes for the Allen–Cahn equation and the Cahn–Hilliard equation under dynamic boundary conditions, which approximate the boundary conditions by a standard central difference. Moreover, we have obtained the desired results to improve the spatial accuracy by approximating the boundary conditions with the central difference.

The rest of this thesis proceeds as follows. In Chapter 2, we introduce the basic notations, known facts, commonly used formulas. In Chapters 3–5, we propose structure-preserving schemes for the target problems and obtain the theoretical results, i.e., the L^∞-boundedness, the solvability, and the error estimate for each of the proposed schemes.

In Chapter 3, we study a non-local Allen–Cahn equation [56]. Our proposed scheme inherits the mass conservation and the energy dissipation from the original equation. Furthermore, regarding the error estimate, we did not find any previous studies that gave rigorous proof of this, and related previous studies have only confirmed numerically [41, 43, 69]. On the other hand, we have rigorously proved that our scheme is second-order accurate in space and time, respectively. The contents of this chapter have been published under the title "A stable and structure-preserving scheme for a non-local Allen–Cahn equation" on pages 1245–1281 of volume 35, number 3 of the journal "Japan Journal of Industrial and Applied Mathematics," DOI: 10.1007/s13160-018-0326-8 [51].

In Chapter 4, we study the Allen–Cahn equation with a dynamic boundary condition. By modifying the discretization of energy and the summation-by-parts formula, which are important in DVDM, we design a structure-preserving scheme for the problem and use a central difference as an approximation of an outward normal derivative on the boundary. In the previous results [29, 31], to show the solvability of the discrete variational derivative scheme, Furihata imposed the assumption that we need to take a sufficiently small time mesh size depending on the space mesh size. Whereas, in our study, we show it under only the smallness assumption of the time mesh size without any space mesh size restriction by using the energy method [28, 67, 68]. Besides, we prove that our scheme is second-order accurate in space and time, respectively. The results in this chapter are based on joint research with Daisuke Furihata. Moreover, the contents of this chapter have been published under the title "A structure-preserving scheme for the Allen–Cahn equation with a dynamic boundary condition" on pages 4927–4960 of volume 40, number 8 of the journal "Discrete and Continuous Dynamical Systems," DOI: 10.3934/dcds.2020206 [52]. This is a pre-copy-editing, author-produced PDF of an article accepted for publication in "Discrete and Continuous Dynamical Systems" following peer review. The definitive publisher-authenticated version "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" is available online at: https://www.aimsciences.org/journal/1078-0947/2020/40/8.

In Chapter 5, we study the Cahn–Hilliard equation with a dynamic boundary condition. Similarly to the way of designing the scheme for the Allen–Cahn equation with a dynamic boundary condition, we also design a structure-preserving one, which approximates an outward normal derivative on the boundary by a central difference for the target problem. Although we need to show the regularity of some matrix in the proof of the solvability, Fukao et al. did not even touch it in [28]. In contrast, we show the regularity of the matrix using the fact that we can decompose a quintuple diagonal matrix that constitutes the matrix into a product of two triple diagonal matrices. Moreover, we show that our proposed scheme is second-order accurate in space, although the previous structure-preserving one by Fukao et al. is first-order accurate [28]. This chapter contains the results of the preprint [53]. Moreover, the contents of this chapter have been published under the title "A second-order accurate structure-preserving scheme for the Cahn–Hilliard equation with a dynamic boundary condition" on pages 355–392 of volume 21, number 2 of the journal "Communications on Pure and Applied Analysis," DOI: 10.3934/cpaa.2021181. Also, this is a pre-copy-editing, author-produced PDF of an article accepted for publication in "Communications on Pure and Applied Analysis" following peer review. The definitive publisher-authenticated version "M. Okumura T. Fukao, D. Furihata, and S. Yoshikawa, A second-order accurate structure-preserving scheme for the Cahn–Hilliard equation with a dynamic boundary condition, Commun. Pure Appl. Anal., **21** (2022), 355–392" is available online at: https://www.aimsciences.org/journal/1534-0392/2022/21/2. Additionally, the results in this chapter are based on joint research with Takeshi Fukao, Daisuke Furihata, and Shuji Yoshikawa.

In the last chapter (Chapter 6), we provide a summary of the results obtained in this thesis.

Chapter 2

Preliminaries

In this thesis, we consider problems in the case of one-dimensional space. That is, we consider the domain $[0, L]$, where $L > 0$ be the length of the one-dimensional material. We fix a natural number K. Let Δx be a space mesh size, i.e., $\Delta x := L/K$, and let Δt be a time mesh size. Firstly, we define basic operators to be used from now on.

Definition 2.1 (Shift operators)**.** We define shift operators s_k^+, s_k^- concerning subscript k by

$$s_k^+ f_k := f_{k+1}, \quad s_k^- f_k := f_{k-1}$$

for all $\{f_k\}_{k=-s}^{K+s} \in \mathbb{R}^{K+1+2s}$, where $s \in \mathbb{N} \cup \{0\}$.

Definition 2.2 (Average operators)**.** We define average operators μ_k^+, μ_k^- concerning subscript k by

$$\mu_k^+ f_k := \frac{f_k + f_{k+1}}{2}, \quad \mu_k^- f_k := \frac{f_k + f_{k-1}}{2}$$

for all $\{f_k\}_{k=-s}^{K+s} \in \mathbb{R}^{K+1+2s}$, where $s \in \mathbb{N} \cup \{0\}$.

Definition 2.3 (Difference operators)**.** 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

$$\delta_k^+ f_k := \frac{f_{k+1} - f_k}{\Delta x}, \qquad \delta_k^- f_k := \frac{f_k - f_{k-1}}{\Delta x},$$
$$\delta_k^{\langle 1 \rangle} f_k := \frac{f_{k+1} - f_{k-1}}{2\Delta x}, \qquad \delta_k^{\langle 2 \rangle} f_k := \frac{f_{k+1} - 2f_k + f_{k-1}}{(\Delta x)^2}$$

for all $\{f_k\}_{k=-s}^{K+s} \in \mathbb{R}^{K+1+2s}$, where $s \in \mathbb{N} \cup \{0\}$. Similarly, we define the difference operator δ_n^+ corresponding superscript (n) by

$$\delta_n^+ f^{(n)} := \frac{f^{(n+1)} - f^{(n)}}{\Delta t}.$$

Definition 2.4 (Summation operator)**.** As a discretization of the integral, we define the summation operator $\sum_{k=0}^{K}{}''$: $\mathbb{R}^{K+1+2s} \to \mathbb{R}$ by

$$\sum_{k=0}^{K}{}'' f_k := \frac{1}{2} f_0 + \sum_{k=1}^{K-1} f_k + \frac{1}{2} f_K \quad \text{for all } \{f_k\}_{k=-s}^{K+s} \in \mathbb{R}^{K+1+2s}, \text{ where } s \in \mathbb{N} \cup \{0\}.$$

For later use, we next define the difference quotient.

Definition 2.5 (Difference quotient)**.** Let Ω be a domain in $\mathbb{R}$. For a function $F \in C^1(\Omega)$ and $\xi, \eta \in \Omega$, we define the difference quotient $dF/d(\xi,\eta)$ of F at (ξ,η) by

$$\frac{dF}{d(\xi,\eta)} := \begin{cases} \dfrac{F(\xi)-F(\eta)}{\xi-\eta} & (\xi \neq \eta), \\ F'(\eta) & (\xi = \eta). \end{cases}$$

Definition 2.6. Let Ω be a domain in $\mathbb{R}$. For a function $F \in C^2(\Omega)$, let us define $\bar{F}''$: $\Omega^4 \to \mathbb{R}$ by

$$\bar{F}''(\xi,\tilde{\xi};\eta,\tilde{\eta}) := \begin{cases} \dfrac{1}{\xi-\tilde{\xi}}\left\{\left(\dfrac{dF}{d(\xi,\eta)}+\dfrac{dF}{d(\xi,\tilde{\eta})}\right)-\left(\dfrac{dF}{d(\tilde{\xi},\eta)}+\dfrac{dF}{d(\tilde{\xi},\tilde{\eta})}\right)\right\}, & (\xi \neq \tilde{\xi}), \\ \partial_\xi \left(\dfrac{dF}{d(\xi,\eta)}+\dfrac{dF}{d(\xi,\tilde{\eta})}\right)\Bigg|_{\xi=\tilde{\xi}}, & (\xi = \tilde{\xi}) \end{cases}$$

for all $(\xi,\tilde{\xi},\eta,\tilde{\eta}) \in \Omega^4$.

We also define the discrete Lebesgue norm, the discrete Dirichlet semi-norm, and the discrete Sobolev norm.

Definition 2.7 (Discrete norms)**.** We define the discrete L^∞-norm $\|\cdot\|_{L^\infty_{\mathrm{d}}}$ and the discrete L^2-norm $\|\cdot\|_{L^2_{\mathrm{d}}}$ by

$$\|\boldsymbol{f}\|_{L^\infty_{\mathrm{d}}} := \max_{0\le k\le K} |f_k|, \quad \|\boldsymbol{f}\|_{L^2_{\mathrm{d}}} := \sqrt{\sum_{k=0}^{K}{}'' |f_k|^2 \Delta x}$$

for all $\boldsymbol{f} = \{f_k\}_{k=0}^K \in \mathbb{R}^{K+1}$. Furthermore, for all $\boldsymbol{f} = \{f_k\}_{k=0}^K \in \mathbb{R}^{K+1}$, we define the discrete Dirichlet semi-norm $\|D\boldsymbol{f}\|$ of $\boldsymbol{f}$ by

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

where $D\boldsymbol{f}$ is denoted by $D\boldsymbol{f} := \{\delta_k^+ f_k\}_{k=0}^{K-1} \in \mathbb{R}^K$. Also, define the discrete Sobolev norm $\|\cdot\|_{\tilde{H}^1_{\mathrm{d}}}$ by

$$\|\boldsymbol{f}\|_{\tilde{H}^1_{\mathrm{d}}} := \sqrt{\|\boldsymbol{f}\|_{L^2_{\mathrm{d}}}^2 + \|D\boldsymbol{f}\|^2} \quad \text{for all } \{f_k\}_{k=0}^K \in \mathbb{R}^{K+1}.$$

Moreover, we describe propositions we will frequently use later.

Proposition 2.1. The following equality holds:

$$\frac{1}{2}\left(\sum_{k=0}^{K-1} f_k \Delta x + \sum_{k=1}^{K} f_k \Delta x\right) = \sum_{k=0}^{K}{}'' f_k \Delta x \quad \text{for all } \{f_k\}_{k=0}^K \in \mathbb{R}^{K+1}.$$

Proof. For all $\{f_k\}_{k=0}^K \in \mathbb{R}^{K+1}$, we have from the direct calculation that

$$\frac{1}{2}\left(\sum_{k=0}^{K-1} f_k \Delta x + \sum_{k=1}^{K} f_k \Delta x\right) = \frac{1}{2} f_0 \Delta x + \sum_{k=1}^{K-1} f_k \Delta x + \frac{1}{2} f_K \Delta x = \sum_{k=0}^{K}{}'' f_k \Delta x.$$

□

Since proofs of the following lemmas can be found in [31], we omit them.

Proposition 2.2 (Summation of a difference [31, Propositon 3.1])**.** Let us denote $f_K - f_0$ by $[f_k]_0^K$. The following fundamental formula holds:

$$\sum_{k=0}^{K}{}'' \delta_k^{\langle 2\rangle} f_k \Delta x = \left[\delta_k^{\langle 1\rangle} f_k\right]_0^K \quad \text{for all } \{f_k\}_{k=-1}^{K+1} \in \mathbb{R}^{K+3}.$$

Proposition 2.3 (Second-order summation by parts formula [31, Propositon 3.3])**.** The following summation by parts formula holds:

$$\begin{aligned}\sum_{k=0}^{K}{}'' \frac{\left(\delta_k^+ f_k\right)\left(\delta_k^+ g_k\right) + \left(\delta_k^- f_k\right)\left(\delta_k^- g_k\right)}{2}\Delta x = &-\sum_{k=0}^{K}{}'' \left(\delta_k^{\langle 2\rangle} f_k\right) g_k \Delta x \\ &+ \left[\frac{\left(\delta_k^+ f_k\right)\left(\mu_k^+ g_k\right) + \left(\delta_k^- f_k\right)\left(\mu_k^- g_k\right)}{2}\right]_0^K\end{aligned}$$

for all $\{f_k\}_{k=-1}^{K+1}, \{g_k\}_{k=-1}^{K+1} \in \mathbb{R}^{K+3}$.

Proposition 2.4 (Second-order summation by parts formulas)**.** The following summation by parts formulas hold:

$$\sum_{k=0}^{K-1}(\delta_k^+ f_k)(\delta_k^+ g_k)\Delta x = -\sum_{k=0}^{K-1}(\delta_k^{\langle 2\rangle} f_k) g_k \Delta x + [(\delta_k^- f_k) g_k]_0^K, \tag{2.1}$$

$$\sum_{k=1}^{K}(\delta_k^- f_k)(\delta_k^- g_k)\Delta x = -\sum_{k=1}^{K}(\delta_k^{\langle 2\rangle} f_k) g_k \Delta x + [(\delta_k^+ f_k) g_k]_0^K, \tag{2.2}$$

for all $\{f_k\}_{k=-1}^{K+1}, \{g_k\}_{k=-1}^{K+1} \in \mathbb{R}^{K+3}$.

Remark 2.1. The left-hand side of (2.1) and the left-hand side of (2.2) appear to be different, but they are the same. In fact, by direct calculation, we can see that

$$\sum_{k=1}^{K}\left(\delta_k^- f_k\right)\left(\delta_k^- g_k\right)\Delta x = \sum_{k=1}^{K}\left(\delta_k^+ f_{k-1}\right)\left(\delta_k^+ g_{k-1}\right)\Delta x = \sum_{k=0}^{K-1}\left(\delta_k^+ f_k\right)\left(\delta_k^+ g_k\right)\Delta x. \tag{2.3}$$

Proof. For all $\{f_k\}_{k=-1}^{K+1}, \{g_k\}_{k=-1}^{K+1} \in \mathbb{R}^{K+3}$, we obtain from the direct calculation that

$$\begin{aligned}\sum_{k=0}^{K-1}(\delta_k^+ f_k)(\delta_k^+ g_k)\Delta x &= \sum_{k=0}^{K-1}\frac{f_{k+1}-f_k}{\Delta x}\frac{g_{k+1}-g_k}{\Delta x}\Delta x \\ &= \sum_{k=0}^{K-1}\frac{f_{k+1}-f_k}{(\Delta x)^2} g_{k+1}\Delta x - \sum_{k=0}^{K-1}\frac{f_{k+1}-f_k}{(\Delta x)^2} g_k \Delta x \\ &= \sum_{k=1}^{K}\frac{f_k - f_{k-1}}{(\Delta x)^2} g_k \Delta x - \sum_{k=0}^{K-1}\frac{f_{k+1}-f_k}{(\Delta x)^2} g_k \Delta x \\ &= -\sum_{k=0}^{K-1}\frac{f_{k+1}-2f_k+f_{k-1}}{(\Delta x)^2} g_k \Delta x + \frac{f_K - f_{K-1}}{\Delta x} g_K - \frac{f_0 - f_{-1}}{\Delta x} g_0 \\ &= -\sum_{k=0}^{K-1}(\delta_k^{\langle 2\rangle} f_k) g_k \Delta x + (\delta_k^- f_k\big|_{k=K}) g_K - (\delta_k^- f_k\big|_{k=0}) g_0 \\ &= -\sum_{k=0}^{K-1}(\delta_k^{\langle 2\rangle} f_k) g_k \Delta x + [(\delta_k^- f_k) g_k]_0^K.\end{aligned}$$

In the same way as the above calculation, we have

$$\begin{aligned}
\sum_{k=1}^{K}(\delta_k^- f_k)(\delta_k^- g_k)\Delta x &= \sum_{k=1}^{K}\frac{f_k - f_{k-1}}{\Delta x}\frac{g_k - g_{k-1}}{\Delta x}\Delta x \\
&= \sum_{k=1}^{K}\frac{f_k - f_{k-1}}{(\Delta x)^2}g_k\Delta x - \sum_{k=1}^{K}\frac{f_k - f_{k-1}}{(\Delta x)^2}g_{k-1}\Delta x \\
&= \sum_{k=1}^{K}\frac{f_k - f_{k-1}}{(\Delta x)^2}g_k\Delta x - \sum_{k=0}^{K-1}\frac{f_{k+1} - f_k}{(\Delta x)^2}g_k\Delta x \\
&= -\sum_{k=1}^{K}\frac{f_{k+1} - 2f_k + f_{k-1}}{(\Delta x)^2}g_k\Delta x + \frac{f_{K+1} - f_K}{\Delta x}g_K - \frac{f_1 - f_0}{\Delta x}g_0 \\
&= -\sum_{k=1}^{K}(\delta_k^{\langle 2\rangle} f_k)g_k\Delta x + (\delta_k^+ f_k\big|_{k=K})g_K - (\delta_k^+ f_k\big|_{k=0})g_0 \\
&= -\sum_{k=1}^{K}(\delta_k^{\langle 2\rangle} f_k)g_k\Delta x + [(\delta_k^+ f_k)g_k]_0^K.
\end{aligned}$$

These complete the proof. □

Corollary 2.1 (Second-order summation by parts formula)**.** The summation by parts formula holds as follows:

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

for all $\{f_k\}_{k=-1}^{K+1}, \{g_k\}_{k=-1}^{K+1} \in \mathbb{R}^{K+3}$.

Proof. For all $\{f_k\}_{k=-1}^{K+1}, \{g_k\}_{k=-1}^{K+1} \in \mathbb{R}^{K+3}$, summing (2.1) and (2.2) and dividing by 2, we have

$$\begin{aligned}
&\frac{1}{2}\left\{\sum_{k=0}^{K-1}\left(\delta_k^+ f_k\right)\left(\delta_k^+ g_k\right)\Delta x + \sum_{k=1}^{K}\left(\delta_k^- f_k\right)\left(\delta_k^- g_k\right)\Delta x\right\} \\
&= -\frac{1}{2}\left\{\sum_{k=0}^{K-1}\left(\delta_k^{\langle 2\rangle} f_k\right)g_k\Delta x + \sum_{k=1}^{K}\left(\delta_k^{\langle 2\rangle} f_k\right)g_k\Delta x\right\} + \frac{1}{2}\left\{\left[\left(\delta_k^- f_k\right)g_k\right]_0^K + \left[\left(\delta_k^+ f_k\right)g_k\right]_0^K\right\}.
\end{aligned} \tag{2.4}$$

By (2.3), we transform the left-hand side of (2.4) as follows:

$$\frac{1}{2}\left\{\sum_{k=0}^{K-1}\left(\delta_k^+ f_k\right)\left(\delta_k^+ g_k\right)\Delta x + \sum_{k=1}^{K}\left(\delta_k^- f_k\right)\left(\delta_k^- g_k\right)\Delta x\right\} = \sum_{k=0}^{K-1}\left(\delta_k^+ f_k\right)\left(\delta_k^+ g_k\right)\Delta x.$$

Next, by Proposition 2.1, we transform the right-hand side of (2.4) as follows:

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

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

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

From the above, we obtain

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

This completes the proof. □

Proposition 2.5 (Discrete Sobolev inequality [67, Proposition 2.2])**.** We define a constant $\tilde{C}_L$ as follows:

$$
\tilde{C}_L := \sqrt{\frac{\sqrt{1+4L^2}+1}{2L}}.
$$

Then, the following inequality holds:

$$
\|\boldsymbol{f}\|_{L_{\mathrm{d}}^{\infty}} \leq \tilde{C}_L \|\boldsymbol{f}\|_{\tilde{H}_{\mathrm{d}}^{1}} \quad \text{for all } \{f_k\}_{k=0}^{K} \in \mathbb{R}^{K+1}. \tag{2.5}
$$

Proof. We can obtain (2.5) from the proof by Yoshikawa [67]. □

Proposition 2.6 (Discrete Poincaré–Wirtinger inequality [31, Lemma 3.3])**.** For all $\boldsymbol{f} = \{f_k\}_{k=0}^{K} \in \mathbb{R}^{K+1}$, the following inequality holds:

$$
\left| f_l - \frac{1}{L}\sum_{k=0}^{K}{}'' f_k\Delta x\right|^2 \leq L\|D\boldsymbol{f}\|^2 \quad (l = 0,\ldots,K). \tag{2.6}
$$

Proof. We can obtain the discrete Poincaré–Wirtinger inequality (2.6) from the proof by Furihata and Matsuo [31]. □

Let Ω be a domain in $\mathbb{R}$. We give several lemmas necessary for the proof of the existence and uniqueness of the solution. Since proofs of the following lemmas can be found in [67], we omit them.

Lemma 2.1 ([67, Lemma 2.4])**.** If $F \in C^2(\Omega)$, then $\bar{F}'' \in C(\Omega^4)$. Moreover, we have

$$
\left|\bar{F}''(\xi,\tilde{\xi};\eta,\tilde{\eta})\right| \leq \sup_{\eta,\tilde{\eta}\in\Omega}\sup_{\xi\in\Omega}\left|\partial_\xi\left(\frac{dF}{d(\xi,\eta)} + \frac{dF}{d(\xi,\tilde{\eta})}\right)\right| \leq \sup_{\xi\in\Omega}|F''(\xi)|
$$

for all $(\xi,\tilde{\xi},\eta,\tilde{\eta}) \in \Omega^4$.

Lemma 2.2 ([67, Proposition 2.5])**.** Assume that $F \in C^2(\Omega)$. For any ξ, $\tilde{\xi}$, η, $\tilde{\eta} \in \Omega$, we have

$$
\frac{dF}{d(\xi,\eta)} - \frac{dF}{d(\tilde{\xi},\tilde{\eta})} = \frac{1}{2}\bar{F}''(\xi,\tilde{\xi};\eta,\tilde{\eta})(\xi-\tilde{\xi}) + \frac{1}{2}\bar{F}''(\eta,\tilde{\eta};\xi,\tilde{\xi})(\eta-\tilde{\eta}).
$$

Lemma 2.3 ([67, Lemma 2.3])**.** The following inequality holds:

$$\|D(\boldsymbol{fg})\| \leq \|\boldsymbol{f}\|_{L^\infty_{\mathrm{d}}} \|D\boldsymbol{g}\| + \|\boldsymbol{g}\|_{L^\infty_{\mathrm{d}}} \|D\boldsymbol{f}\|$$

for all $\boldsymbol{f} = \{f_k\}_{k=0}^K, \boldsymbol{g} = \{g_k\}_{k=0}^K \in \mathbb{R}^{K+1}$, where $\boldsymbol{fg} = \{f_k g_k\}_{k=0}^K \in \mathbb{R}^{K+1}$.

The following lemma follows from the same argument as Lemma 2.6 in [67].

Lemma 2.4 ([28, Lemma 3.3 (2)])**.** Assume that $F \in C^3(\Omega)$. For any $\boldsymbol{f}_1 = \{f_{1,k}\}_{k=0}^K$, $\boldsymbol{f}_2 = \{f_{2,k}\}_{k=0}^K$, $\boldsymbol{f}_3 = \{f_{3,k}\}_{k=0}^K$, $\boldsymbol{f}_4 = \{f_{4,k}\}_{k=0}^K \in \mathbb{R}^{K+1}$, all the elements of which are in Ω, we have

$$\left\|D\bar{F}''(\boldsymbol{f}_1, \boldsymbol{f}_2; \boldsymbol{f}_3, \boldsymbol{f}_4)\right\| \leq \frac{1}{6} \sup_{\xi\in\Omega} |F'''(\xi)| \left(2\|D\boldsymbol{f}_1\| + 2\|D\boldsymbol{f}_2\| + \|D\boldsymbol{f}_3\| + \|D\boldsymbol{f}_4\|\right).$$

Chapter 3

A non-local Allen–Cahn equation

In this chapter, as mentioned in Chapter 1, to understand the idea of the discrete variational derivative method (DVDM) [29], we design a structure-preserving finite difference scheme for a non-local Allen–Cahn equation that describes a process of phase separation in a binary mixture based on DVDM. Our proposed scheme inherits characteristic properties, mass conservation, and energy dissipation from the original equation. Besides, we show the stability, the existence, and the uniqueness of the solution to the scheme. We also prove the error estimate for the scheme. Computation examples demonstrate the effectiveness of the proposed scheme.

§1 Introduction

Allen and Cahn introduced the Allen–Cahn equation as a model for antiphase domain coarsening in a binary alloy [1]. It has been applied to various problems, for example, phase transition [1, 10], image analysis [4, 23, 44], and motion by mean curvature [2, 3, 24, 26, 38, 40, 50]. Let $L > 0$ be the length of the one-dimensional material. In this chapter, we study the following initial-boundary value problem for a non-local Allen–Cahn equation introduced by Rubinstein and Sternberg [56]:

$$\begin{cases} \partial_t u = \partial_x^2 u + \dfrac{2u}{\varepsilon^2}(1-u^2) + \lambda^\varepsilon & \text{in } (0,L)\times(0,\infty), \\ \lambda^\varepsilon = -\dfrac{1}{L}\displaystyle\int_0^L \dfrac{2u}{\varepsilon^2}(1-u^2)dx & \text{in } (0,\infty), \end{cases} \tag{3.1}$$

under the Neumann boundary conditions:

$$\partial_x u(x,t)|_{x=0} = \partial_x u(x,t)|_{x=L} = 0 \quad \text{for all } t > 0. \tag{3.2}$$

The unknown function u: $[0,L]\times[0,\infty) \to \mathbb{R}$ is an order parameter, which is the concentration of one of two components in a binary mixture. The parameter $0 < \varepsilon \ll 1$ is related to the thickness of the interface layer, which can develop in parts of the solution with a steep gradient.

Rubinstein and Sternberg introduced the equation (3.1) as a model for a process of phase separation in a binary mixture that conserves the total mass of two species [56]. They introduced the non-local term λ^ε, which is a Lagrange multiplier, to ensure mass conservation (3.6). Here, we remark that the classical Allen–Cahn equation, in which the non-local term λ^ε in (3.1) is absent, does not have mass conservation. Bronsard and Stoth proved that the equation (3.1) converges, as $\varepsilon \to 0$, to the volume-preserving mean curvature flow in a radial symmetry case [7]. Golovaty obtained a similar result to [7] for the Allen–Cahn equation with a different non-local term [36]. Chen et al. [11] obtained the convergence in the general case. Moreover, the equation (3.1) has been studied analytically and numerically [5, 6, 22, 59, 62, 69]. However, compared with the number of studies of the classical Allen–Cahn equation, there are not many numerical results of the non-local Allen–Chan equation.

Brassel and Bretin [6] concluded that the following another non-local Allen–Cahn equation:

$$\begin{cases} \partial_t u = \partial_x^2 u + \dfrac{2u}{\varepsilon^2}(1-u^2) + \dfrac{1}{\varepsilon^2}\tilde{\lambda}^\varepsilon(1-u^2) & \text{in } (0,L)\times(0,\infty), \\ \tilde{\lambda}^\varepsilon = \dfrac{-\displaystyle\int_0^L 2u(1-u^2)dx}{\displaystyle\int_0^L (1-u^2)dx} & \text{in } (0,\infty), \end{cases} \tag{3.3}$$

has better volume-preserving properties than (3.1) in the sense that an error of the conservation of the volume is small. However, as Takasao [60] mentioned, (3.3) does not have the dissipative property (3.7) of energy J. Kim et al. [41] proposed a practically unconditionally stable scheme for (3.3), and yet they did not give the proof of the stability and the error estimate for the scheme. Zhai et al. [69] compared three methods to approximate (3.3), including the Crank–Nicolson (CN) finite difference method, the finite difference operator splitting (OS) method, and the Fourier spectral operator splitting (FSOS) method. They checked that the convergence rates of the CN scheme and the OS scheme approach second as the mesh size becomes small and that the FSOS scheme is second-order accurate in time through numerical computations. Nevertheless, Lee [43] commented that their proposed schemes are not second-order accurate in time and/or do not satisfy mass conservation. In addition, Lee [43] discretized (3.3) by a Fourier spectral method in space and first-, second-, third-order implicit-explicit Runge–Kutta schemes in time. Although he checked the convergence of the schemes, the convergence rate, and that the schemes are first-, second-, third-order accurate in time respectively, through numerical computations, he did not give the proof of them.

Thus, we propose a structure-preserving scheme for (3.1) based on DVDM. Our proposed scheme inherits two characteristic properties, mass conservation (3.6), and energy dissipation (3.7), from the original equation, whereas the DVDM scheme inherits just one property in general. Furthermore, we prove that the solution of the scheme converges to the one of the target equation in the sense of discrete L^2-norm and that the convergence rate is $O((\Delta x)^2+(\Delta t)^2)$. Moreover, we prove the stability of the scheme, the existence and the uniqueness of the solution of the scheme. Also, based on this study, we expect that we can design a structure-preserving scheme for another non-local Allen–Cahn equation, such as (3.3) by using DVDM. Here, we remark that there are not that many results of the application of DVDM to partial differential equations (PDEs) with a non-local term to the best of our knowledge.

In this chapter, as mentioned previously, we design a finite difference scheme for (3.1) based on DVDM so that the scheme inherits the conservative and dissipative properties such as (3.6) and (3.7) from the original equation (3.1) in a discrete sense. Here, let us define the "local energy" G and the "global energy" J, which characterize the equation above (3.1):

$$G(u,\partial_x u) := \frac{|\partial_x u|^2}{2} + \frac{1}{\varepsilon^2}\frac{(1-u^2)^2}{2}, \tag{3.4}$$

$$J(u) := \int_0^L G(u,\partial_x u)dx. \tag{3.5}$$

Then, the equation (3.1) has the following properties:

$$\frac{d}{dt}\int_0^L u dx = 0, \tag{3.6}$$

$$\frac{d}{dt}J(u) \leq 0. \tag{3.7}$$

DVDM is a numerical method for designing numerical schemes for PDEs with conservative and dissipative properties such as (3.6) and (3.7), and the DVDM schemes inherit conservative/dissipative property from the original PDEs in a discrete sense. From the perspective of numerical computation, the properties often lead us to stable computation. Hence, if the designed schemes retain the properties in a discrete sense, they are expected to be stable.

Also, the following property holds for global energy J:

$$\frac{d}{dt}J(u) = \int_0^L \frac{\delta G}{\delta u}\partial_t u dx \tag{3.8}$$

under the boundary conditions (3.2). The notation $\delta G/\delta u$ is the (first) variational derivative of G concerning u. From the integration by parts and the boundary conditions (3.2), we can show

$$\frac{d}{dt}J(u) = \int_0^L \left\{-\partial_x^2 u - \frac{2}{\varepsilon^2}u(1-u^2)\right\}\partial_t u dx.$$

Therefore, we have

$$\frac{\delta G}{\delta u} = -\partial_x^2 u - \frac{2}{\varepsilon^2}u(1-u^2) \tag{3.9}$$

from (3.8). We can rewrite (3.1) as follows by using (3.9):

$$\partial_t u = -\frac{\delta G}{\delta u} + \lambda^\varepsilon \quad \text{in } (0,L)\times(0,\infty). \tag{3.10}$$

Furthermore, we obtain

$$\lambda^\varepsilon = -\frac{1}{L}\int_0^L \left\{-\frac{\delta G}{\delta u} - \partial_x^2 u\right\}dx = \frac{1}{L}\left\{\int_0^L \frac{\delta G}{\delta u}dx + [\partial_x u]_0^L\right\} = \frac{1}{L}\int_0^L \frac{\delta G}{\delta u}dx \quad \text{in } (0,\infty), \tag{3.11}$$

by the boundary conditions (3.2). Namely, we can rewrite (3.1) as

$$\begin{cases} \partial_t u = -\dfrac{\delta G}{\delta u} + \lambda^\varepsilon & \text{in } (0,L)\times(0,\infty), \\ \lambda^\varepsilon = \dfrac{1}{L}\displaystyle\int_0^L \frac{\delta G}{\delta u}dx & \text{in } (0,\infty). \end{cases} \tag{3.12}$$

Therefore, we can apply DVDM and can easily prove the conservative property (3.6) and the dissipative property (3.7). In fact, it holds that

$$\begin{aligned}\frac{d}{dt}\int_0^L u dx = \int_0^L \left(-\frac{\delta G}{\delta u} + \lambda^{\varepsilon}\right) dx &= -\int_0^L \frac{\delta G}{\delta u} dx + \lambda^{\varepsilon} \int_0^L dx \\ &= -\int_0^L \frac{\delta G}{\delta u} dx + \frac{1}{L}\int_0^L \frac{\delta G}{\delta u} dx \cdot L = 0,\end{aligned}$$

where we have used (3.10) in the first equality, and (3.11) in the third equality. Moreover, from (3.8), (3.10), and mass conservation (3.6), we can show

$$\begin{aligned}\frac{d}{dt}J(u) = \int_0^L \frac{\delta G}{\delta u}\partial_t u dx = \int_0^L \left(-\partial_t u + \lambda^{\varepsilon}\right)\partial_t u dx &= -\int_0^L (\partial_t u)^2 dx + \lambda^{\varepsilon}\int_0^L \partial_t u dx \\ &= -\int_0^L (\partial_t u)^2 dx \le 0.\end{aligned}$$

The rest of this chapter proceeds as follows. In section 2, we propose a finite difference scheme for (3.12), whose solution satisfies the discrete versions of the conservation property (3.6) and the dissipative property (3.7). In section 3, we prove that the solution of the proposed scheme satisfies the global boundedness. In section 4, we prove that the scheme has a unique solution under a specific condition. In section 5, we prove the error estimate for the scheme. In section 6, we show that the numerical examples demonstrate the effectiveness of the scheme.

§2 Proposed scheme

In this section, we propose a scheme for (3.12) and show that it has two properties corresponding to (3.6) and (3.7).

We define $U_k^{(n)}$ ($k = -1, 0, 1, \ldots, K, K+1, n = 0, 1, \ldots$) to be the approximation to $u(x,t)$ at location $x = k\Delta x$ and time $t = n\Delta t$, where Δx is a space mesh size, i.e., $\Delta x := L/K$ and Δt is a time mesh size. They are also written in vector as

$$\boldsymbol{U}^{(n)} := (U_{-1}^{(n)}, U_0^{(n)}, \ldots, U_K^{(n)}, U_{K+1}^{(n)})^{\top} \quad \text{or} \quad \boldsymbol{U}^{(n)} := (U_0^{(n)}, U_1^{(n)}, \ldots, U_{K-1}^{(n)}, U_K^{(n)})^{\top}.$$

The superscript (n) is omitted when no confusion occurs. Guess the meaning of $\boldsymbol{U}$ from the context.

Remark 3.1. $U_{-1}^{(n)}$ and $U_{K+1}^{(n)}$ are the artificial quantities and determined by the imposed discrete boundary condition.

The concrete form of the proposed scheme for (3.12) is, for $n = 0, 1, \ldots$,

$$\begin{cases}\dfrac{U_k^{(n+1)} - U_k^{(n)}}{\Delta t} = -\dfrac{\delta G_{\mathrm{d}}}{\delta(\boldsymbol{U}^{(n+1)}, \boldsymbol{U}^{(n)})_k} + \lambda_{\mathrm{d}}^{\varepsilon}\left(\boldsymbol{U}^{(n+1)}, \boldsymbol{U}^{(n)}\right) \quad (k=0,\ldots,K), \\ \lambda_{\mathrm{d}}^{\varepsilon}\left(\boldsymbol{U}^{(n+1)}, \boldsymbol{U}^{(n)}\right) = \dfrac{1}{L}\displaystyle\sum_{k=0}^{K}{}'' \dfrac{\delta G_{\mathrm{d}}}{\delta\left(\boldsymbol{U}^{(n+1)}, \boldsymbol{U}^{(n)}\right)_k}\Delta x,\end{cases} \tag{3.13}$$

where

$$\frac{\delta G_{\mathrm{d}}}{\delta(\boldsymbol{U},\boldsymbol{V})_k} = -\delta_k^{\langle 2\rangle}\left(\frac{U_k+V_k}{2}\right) - \frac{2}{\varepsilon^2}\left(\frac{U_k+V_k}{2}\right)\left(1-\frac{U_k^2+V_k^2}{2}\right) \quad (k=0,\ldots,K). \tag{3.14}$$

The discrete boundary conditions are

$$\delta_k^{\langle 1\rangle} U_k^{(n)} = 0 \quad (k=0,K,\ n=0,1,\ldots). \tag{3.15}$$

Note that these discrete boundary conditions (3.15) mean that

$$U_{-1}^{(n)} = U_1^{(n)}, \quad U_{K+1}^{(n)} = U_{K-1}^{(n)} \quad (n=0,1,\ldots).$$

Let us define a discrete local energy G_{d}: $\mathbb{R}^{K+3} \to \mathbb{R}^{K+1}$ by

$$G_{\mathrm{d},k}(\boldsymbol{U}) := \frac{1}{2}\frac{(\delta_k^+ U_k)^2 + (\delta_k^- U_k)^2}{2} + \frac{(1-U_k^2)^2}{2\varepsilon^2} \quad (k=0,\ldots,K). \tag{3.16}$$

From Proposition 2.3 (second-order summation by parts formula), the relation between G_{d} of (3.16) and $\delta G_{\mathrm{d}}/\delta(\cdot,\cdot)$ of (3.14) is given by

$$\begin{aligned}
&\sum_{k=0}^{K}{}'' G_{\mathrm{d},k}(\boldsymbol{U})\,\Delta x - \sum_{k=0}^{K}{}'' G_{\mathrm{d},k}(\boldsymbol{V})\,\Delta x \\
&= \sum_{k=0}^{K}{}'' \frac{\delta G_{\mathrm{d}}}{\delta(\boldsymbol{U},\boldsymbol{V})_k}(U_k - V_k)\,\Delta x + \left[\frac{\delta_k^+\left(\frac{U_k+V_k}{2}\right)\mu_k^+(U_k-V_k) + \delta_k^-\left(\frac{U_k+V_k}{2}\right)\mu_k^-(U_k-V_k)}{2}\right]_0^K.
\end{aligned}$$

Hence, we have

$$\begin{aligned}
&\sum_{k=0}^{K}{}'' G_{\mathrm{d},k}\left(\boldsymbol{U}^{(n+1)}\right)\Delta x - \sum_{k=0}^{K}{}'' G_{\mathrm{d},k}\left(\boldsymbol{U}^{(n)}\right)\Delta x \\
&= \sum_{k=0}^{K}{}'' \frac{\delta G_{\mathrm{d}}}{\delta(\boldsymbol{U}^{(n+1)},\boldsymbol{U}^{(n)})_k}\left(U_k^{(n+1)} - U_k^{(n)}\right)\Delta x \\
&\quad + \frac{1}{4}\left[\delta_k^+\left(U_k^{(n+1)}+U_k^{(n)}\right)\mu_k^+\left(U_k^{(n+1)}-U_k^{(n)}\right) + \delta_k^-\left(U_k^{(n+1)}+U_k^{(n)}\right)\mu_k^-\left(U_k^{(n+1)}-U_k^{(n)}\right)\right]_0^K
\end{aligned}$$

for $n=0,1,\ldots$. Here, we show the following equality:

$$\begin{aligned}
&\left[\delta_k^+\left(U_k^{(n+1)}+U_k^{(n)}\right)\mu_k^+\left(U_k^{(n+1)}-U_k^{(n)}\right)\right. \\
&\qquad \left. +\delta_k^-\left(U_k^{(n+1)}+U_k^{(n)}\right)\mu_k^-\left(U_k^{(n+1)}-U_k^{(n)}\right)\right]_0^K = 0 \quad (n=0,1,\ldots).
\end{aligned} \tag{3.17}$$

Since it holds from the discrete boundary conditions (3.15) that

$$\left(\frac{\delta_k^+ + \delta_k^-}{2}\right)U_k^{(n)} = \delta_k^{\langle 1\rangle}U_k^{(n)} = 0 \quad (n=0,1,\ldots),$$

we have $\delta_k^+ U_k^{(n)} = -\delta_k^- U_k^{(n)}$ $(n = 0, 1, \ldots)$. Namely, $\delta_k^+(U_k^{(n+1)} + U_k^{(n)}) = -\delta_k^-(U_k^{(n+1)} + U_k^{(n)})$ $(n = 0, 1, \ldots)$. Furthermore, we obtain

$$\left(\frac{\mu_k^+ - \mu_k^-}{\Delta x}\right) U_k^{(n)} = \delta_k^{\langle 1 \rangle} U_k^{(n)} = 0 \quad (n = 0, 1, \ldots),$$

since it holds that

$$\frac{\mu_k^+ - \mu_k^-}{\Delta x} = \frac{1 + s_k^+ - (1 - s_k^-)}{2\Delta x} = \frac{s_k^+ - s_k^-}{2\Delta x} = \delta_k^{\langle 1 \rangle}.$$

That is $\mu_k^+ U_k^{(n)} = \mu_k^- U_k^{(n)}$, i.e., $\mu_k^+(U_k^{(n+1)} + U_k^{(n)}) = \mu_k^-(U_k^{(n+1)} + U_k^{(n)})$ $(n = 0, 1, \ldots)$. Hence, (3.17) holds. Therefore, we have

$$\sum_{k=0}^{K}{}'' G_{\mathrm{d},k}\left(\boldsymbol{U}^{(n+1)}\right)\Delta x - \sum_{k=0}^{K}{}'' G_{\mathrm{d},k}\left(\boldsymbol{U}^{(n)}\right)\Delta x = \sum_{k=0}^{K}{}'' \frac{\delta G_{\mathrm{d}}}{\delta(\boldsymbol{U}^{(n+1)}, \boldsymbol{U}^{(n)})_k}\left(U_k^{(n+1)} - U_k^{(n)}\right)\Delta x$$

for $n = 0, 1, \ldots$. The proposed scheme (3.13) has properties corresponding to (3.6) and (3.7), i.e.,

Theorem 3.1. The solution of the scheme (3.13) under the discrete boundary conditions (3.15) satisfies the following equality and inequality:

$$\sum_{k=0}^{K}{}'' U_k^{(n)}\Delta x = \sum_{k=0}^{K}{}'' U_k^{(0)}\Delta x \quad (n = 0, 1, \ldots), \tag{3.18}$$

$$J_{\mathrm{d}}(\boldsymbol{U}^{(n+1)}) \le J_{\mathrm{d}}(\boldsymbol{U}^{(n)}) \quad (n = 0, 1, \ldots), \tag{3.19}$$

where

$$J_{\mathrm{d}}\left(\boldsymbol{U}^{(n)}\right) := \sum_{k=0}^{K}{}'' G_{\mathrm{d},k}\left(\boldsymbol{U}^{(n)}\right)\Delta x \quad (n = 0, 1, \ldots).$$

We call (3.18) the discrete mass conservation and (3.19) the discrete energy dissipation.

Proof. First, we can show the discrete mass conservation (3.18) from (3.13) as follows:

$$\begin{aligned}
&\frac{1}{\Delta t}\left\{\sum_{k=0}^{K}{}'' U_k^{(n+1)}\Delta x - \sum_{k=0}^{K}{}'' U_k^{(n)}\Delta x\right\} \\
&= \sum_{k=0}^{K}{}'' \left\{-\frac{\delta G_{\mathrm{d}}}{\delta\left(\boldsymbol{U}^{(n+1)}, \boldsymbol{U}^{(n)}\right)_k} + \lambda_{\mathrm{d}}^{\varepsilon}\left(\boldsymbol{U}^{(n+1)}, \boldsymbol{U}^{(n)}\right)\right\}\Delta x \\
&= -\sum_{k=0}^{K}{}'' \frac{\delta G_{\mathrm{d}}}{\delta\left(\boldsymbol{U}^{(n+1)}, \boldsymbol{U}^{(n)}\right)_k}\Delta x + \lambda_{\mathrm{d}}^{\varepsilon}\left(\boldsymbol{U}^{(n+1)}, \boldsymbol{U}^{(n)}\right)\sum_{k=0}^{K}{}''\Delta x \\
&= -\sum_{k=0}^{K}{}'' \frac{\delta G_{\mathrm{d}}}{\delta\left(\boldsymbol{U}^{(n+1)}, \boldsymbol{U}^{(n)}\right)_k}\Delta x + \frac{1}{L}\sum_{k=0}^{K}{}'' \frac{\delta G_{\mathrm{d}}}{\delta\left(\boldsymbol{U}^{(n+1)}, \boldsymbol{U}^{(n)}\right)_k}\Delta x \cdot L = 0 \quad (n = 0, 1, \ldots).
\end{aligned}$$

Next, the discrete energy dissipation (3.19) can be shown as follows:

$$
\begin{aligned}
\frac{J_{\mathrm{d}}(\boldsymbol{U}^{(n+1)})-J_{\mathrm{d}}(\boldsymbol{U}^{(n)})}{\Delta t} &= \frac{1}{\Delta t}\sum_{k=0}^{K}{}'' \left\{G_{\mathrm{d},k}\left(\boldsymbol{U}^{(n+1)}\right) - G_{\mathrm{d},k}\left(\boldsymbol{U}^{(n)}\right)\right\}\Delta x \\
&= \sum_{k=0}^{K}{}'' \frac{\delta G_{\mathrm{d}}}{\delta\left(\boldsymbol{U}^{(n+1)},\boldsymbol{U}^{(n)}\right)_k}\frac{U_k^{(n+1)}-U_k^{(n)}}{\Delta t}\Delta x \\
&= \sum_{k=0}^{K}{}'' \left\{-\frac{U_k^{(n+1)}-U_k^{(n)}}{\Delta t} + \lambda_{\mathrm{d}}^{\varepsilon}\left(\boldsymbol{U}^{(n+1)},\boldsymbol{U}^{(n)}\right)\right\}\frac{U_k^{(n+1)}-U_k^{(n)}}{\Delta t}\Delta x \\
&= -\sum_{k=0}^{K}{}''\left(\frac{U_k^{(n+1)}-U_k^{(n)}}{\Delta t}\right)^2\Delta x + \lambda_{\mathrm{d}}^{\varepsilon}\left(\boldsymbol{U}^{(n+1)},\boldsymbol{U}^{(n)}\right)\sum_{k=0}^{K}{}''\left(\frac{U_k^{(n+1)}-U_k^{(n)}}{\Delta t}\right)\Delta x \\
&= -\sum_{k=0}^{K}{}''\left(\frac{U_k^{(n+1)}-U_k^{(n)}}{\Delta t}\right)^2\Delta x \le 0 \quad (n=0,1,\ldots),
\end{aligned}
$$

where we have used (3.18) in the fifth equality. □

§3 Stability of the proposed scheme

In this section, we show that, if the proposed scheme has a solution, then the discrete L^∞-norm of the solution is bounded.

Lemma 3.1. The solution of the scheme (3.13) under the discrete boundary conditions (3.15) satisfies the following inequality:

$$
\left\|\boldsymbol{U}^{(n)}\right\|_{\tilde{H}_{\mathrm{d}}^1}^2 \le \frac{1}{\min\left\{\frac{2}{\varepsilon^2},\frac{1}{2}\right\}}\left\{\sum_{k=0}^{K}{}''G_{\mathrm{d},k}\left(\boldsymbol{U}^{(0)}\right)\Delta x + \frac{4}{\varepsilon^2}L\right\} \quad (n=0,1,\ldots). \tag{3.20}
$$

Proof. From the discrete energy dissipation (3.19) and the following inequality:

$$
-rY^2 + \frac{1}{2}rY^4 \ge 2rY^2 - \frac{9}{2}r \quad \text{for all } Y\in\mathbb{R},\ r>0,
$$

we can show that

$$
\begin{aligned}
\sum_{k=0}^{K}{}''G_{\mathrm{d},k}\left(\boldsymbol{U}^{(0)}\right)\Delta x &\ge \sum_{k=0}^{K}{}''G_{\mathrm{d},k}\left(\boldsymbol{U}^{(n)}\right)\Delta x \\
&= \sum_{k=0}^{K}{}''\left\{\frac{1}{2\varepsilon^2} - \frac{1}{\varepsilon^2}\left(U_k^{(n)}\right)^2 + \frac{1}{2\varepsilon^2}\left(U_k^{(n)}\right)^4 + \frac{1}{2}\frac{\left(\delta_k^+U_k^{(n)}\right)^2+\left(\delta_k^-U_k^{(n)}\right)^2}{2}\right\}\Delta x \\
&\ge \sum_{k=0}^{K}{}''\left\{\frac{1}{2\varepsilon^2} + \frac{2}{\varepsilon^2}\left(U_k^{(n)}\right)^2 - \frac{9}{2\varepsilon^2} + \frac{1}{2}\frac{\left(\delta_k^+U_k^{(n)}\right)^2+\left(\delta_k^-U_k^{(n)}\right)^2}{2}\right\}\Delta x \\
&\ge \min\left\{\frac{2}{\varepsilon^2},\frac{1}{2}\right\}\sum_{k=0}^{K}{}''\left\{\left(U_k^{(n)}\right)^2 + \frac{\left(\delta_k^+U_k^{(n)}\right)^2+\left(\delta_k^-U_k^{(n)}\right)^2}{2}\right\}\Delta x + \left(\frac{1}{2\varepsilon^2}-\frac{9}{2\varepsilon^2}\right)L \\
&= \min\left\{\frac{2}{\varepsilon^2},\frac{1}{2}\right\}\left\|\boldsymbol{U}^{(n)}\right\|_{\tilde{H}_{\mathrm{d}}^1}^2 - \frac{4}{\varepsilon^2}L \quad (n=0,1,\ldots).
\end{aligned}
$$

In the above calculation, we have also used the following equality:

$$\sum_{k=0}^{K}{}'' \frac{\left(\delta_k^+ U_k^{(n)}\right)^2 + \left(\delta_k^- U_k^{(n)}\right)^2}{2} \Delta x = \sum_{k=0}^{K-1} \left(\delta_k^+ U_k^{(n)}\right)^2 \Delta x. \tag{3.21}$$

In fact, we obtain the above equality (3.21) by using discrete boundary conditions (3.15). Therefore, (3.20) holds. □

Applying Proposition 2.5 (Sobolev type inequality) to (3.20), we can obtain the following inequality:

Theorem 3.2. The solution of the scheme (3.13) under the discrete boundary conditions (3.15) satisfies

$$\left\|\boldsymbol{U}^{(n)}\right\|_{L_{\mathrm{d}}^{\infty}} \leq \tilde{C}_L \left[\frac{1}{\min\left\{\dfrac{2}{\varepsilon^2}, \dfrac{1}{2}\right\}} \left\{ \sum_{k=0}^{K}{}'' G_{\mathrm{d},k}\left(\boldsymbol{U}^{(0)}\right) \Delta x + \frac{4}{\varepsilon^2} L \right\} \right]^{\frac{1}{2}} \quad (n = 0, 1, \ldots).$$

§4 Existence and uniqueness of the solution to the proposed scheme

In this section, we prove that, through the fixed-point theorem for a contraction mapping, the proposed scheme (3.13) has a unique solution under a specific condition on Δt and Δx.

To prove the existence and uniqueness of the solution to the proposed scheme, we rewrite the scheme (3.13) as follows:

$$\begin{aligned}
&\frac{U_k^{(n+1)} - U_k^{(n)}}{\Delta t} \\
&= \delta_k^{\langle 2\rangle}\left(\frac{U_k^{(n+1)} + U_k^{(n)}}{2}\right) + \frac{1}{\varepsilon^2}\left(U_k^{(n+1)} + U_k^{(n)}\right)\left\{1 - \frac{\left(U_k^{(n+1)}\right)^2 + \left(U_k^{(n)}\right)^2}{2}\right\} \\
&\quad - \frac{1}{L}\sum_{k=0}^{K}{}'' \left[\delta_k^{\langle 2\rangle}\left(\frac{U_k^{(n+1)} + U_k^{(n)}}{2}\right) + \frac{1}{\varepsilon^2}\left(U_k^{(n+1)} + U_k^{(n)}\right)\left\{1 - \frac{\left(U_k^{(n+1)}\right)^2 + \left(U_k^{(n)}\right)^2}{2}\right\}\right]\Delta x \\
&= \delta_k^{\langle 2\rangle}\left(\frac{U_k^{(n+1)} + U_k^{(n)}}{2}\right) + \frac{1}{\varepsilon^2}\left(U_k^{(n+1)} + U_k^{(n)}\right)\left\{1 - \frac{\left(U_k^{(n+1)}\right)^2 + \left(U_k^{(n)}\right)^2}{2}\right\} \\
&\quad - \frac{1}{L}\left[\delta_k^{\langle 1\rangle}\left(\frac{U_k^{(n+1)} + U_k^{(n)}}{2}\right)\right]_0^K - \frac{1}{L}\sum_{k=0}^{K}{}'' \left[\frac{1}{\varepsilon^2}\left(U_k^{(n+1)} + U_k^{(n)}\right)\left\{1 - \frac{\left(U_k^{(n+1)}\right)^2 + \left(U_k^{(n)}\right)^2}{2}\right\}\right]\Delta x
\end{aligned}$$

$$
= \delta_k^{\langle 2\rangle}\left(\frac{U_k^{(n+1)}+U_k^{(n)}}{2}\right)+\frac{1}{\varepsilon^2}\left(U_k^{(n+1)}+U_k^{(n)}\right)-\frac{1}{2\varepsilon^2}\left(U_k^{(n+1)}+U_k^{(n)}\right)\left\{\left(U_k^{(n+1)}\right)^2+\left(U_k^{(n)}\right)^2\right\}
$$

$$
-\frac{1}{L}\sum_{k=0}^{K}{}'' \left[\frac{1}{\varepsilon^2}\left(U_k^{(n+1)}+U_k^{(n)}\right)-\frac{1}{2\varepsilon^2}\left(U_k^{(n+1)}+U_k^{(n)}\right)\left\{\left(U_k^{(n+1)}\right)^2+\left(U_k^{(n)}\right)^2\right\}\right]\Delta x,
$$

by using Proposition 2.2 (summation of differences) and the discrete boundary conditions (3.15). Namely, we obtain

$$
\frac{1}{\Delta t}U_k^{(n+1)}-\frac{1}{2}\delta_k^{\langle 2\rangle}U_k^{(n+1)} = \frac{1}{\Delta t}U_k^{(n)}+\frac{1}{2}\delta_k^{\langle 2\rangle}U_k^{(n)}+\frac{1}{\varepsilon^2}U_k^{(n+1)}+\frac{1}{\varepsilon^2}U_k^{(n)}+\left\{F_{\boldsymbol{U}^{(n)}}\boldsymbol{U}^{(n+1)}\right\}_k
$$

$$
-\frac{1}{L\varepsilon^2}\sum_{k=0}^{K}{}''U_k^{(n+1)}\Delta x-\frac{1}{L\varepsilon^2}\sum_{k=0}^{K}{}''U_k^{(n)}\Delta x-\frac{1}{L}\sum_{k=0}^{K}{}''\left\{F_{\boldsymbol{U}^{(n)}}\boldsymbol{U}^{(n+1)}\right\}_k\Delta x,
$$

where the mapping $F_{\boldsymbol{U}^{(n)}}\colon \mathbb{R}^{K+1}\to\mathbb{R}^{K+1}$ is defined by

$$
\{F_{\boldsymbol{U}^{(n)}}\boldsymbol{V}\}_k := -\frac{1}{2\varepsilon^2}\left(V_k+U_k^{(n)}\right)\left\{(V_k)^2+\left(U_k^{(n)}\right)^2\right\} \quad (k=0,\ldots,K),
$$

for all $\boldsymbol{V}=\{V_k\}_{k=0}^K\in\mathbb{R}^{K+1}$. That is, we have

$$
\left(\frac{1}{\Delta t}-\frac{1}{2}\delta_k^{\langle 2\rangle}\right)U_k^{(n+1)} = \left(\frac{1}{\Delta t}+\frac{1}{\varepsilon^2}+\frac{1}{2}\delta_k^{\langle 2\rangle}\right)U_k^{(n)}-\frac{1}{L\varepsilon^2}\sum_{k=0}^{K}{}''U_k^{(n)}\Delta x+\frac{1}{\varepsilon^2}\left(U_k^{(n+1)}-\frac{1}{L}\sum_{k=0}^{K}{}''U_k^{(n+1)}\Delta x\right)
$$

$$
+\left\{F_{\boldsymbol{U}^{(n)}}\boldsymbol{U}^{(n+1)}\right\}_k-\frac{1}{L}\sum_{k=0}^{K}{}''\left\{F_{\boldsymbol{U}^{(n)}}\boldsymbol{U}^{(n+1)}\right\}_k\Delta x. \tag{3.22}
$$

In connection with the scheme (3.22), we define a mapping $\mathcal{T}_{\boldsymbol{U}^{(n)}}\colon \mathbb{R}^{K+1}\to\mathbb{R}^{K+1}$ by using the following equation:

$$
\left(\frac{1}{\Delta t}-\frac{1}{2}\delta_k^{\langle 2\rangle}\right)\{\mathcal{T}_{\boldsymbol{U}^{(n)}}\boldsymbol{V}\}_k
$$

$$
=\left(\frac{1}{\Delta t}+\frac{1}{\varepsilon^2}+\frac{1}{2}\delta_k^{\langle 2\rangle}\right)U_k^{(n)}-\frac{1}{L\varepsilon^2}\sum_{k=0}^{K}{}''U_k^{(n)}\Delta x+\frac{1}{\varepsilon^2}\left(V_k-\frac{1}{L}\sum_{k=0}^{K}{}''V_k\Delta x\right)
$$

$$
+\{F_{\boldsymbol{U}^{(n)}}\boldsymbol{V}\}_k-\frac{1}{L}\sum_{k=0}^{K}{}''\{F_{\boldsymbol{U}^{(n)}}\boldsymbol{V}\}_k\Delta x \quad (k=0,\ldots,K),
$$

for all $\boldsymbol{V}=\{V_k\}_{k=0}^K\in\mathbb{R}^{K+1}$. Here, the operator in the equation above is defined under the discrete boundary conditions (3.15), i.e., $\{\mathcal{T}_{\boldsymbol{U}^{(n)}}\boldsymbol{V}\}_{-1}=\{\mathcal{T}_{\boldsymbol{U}^{(n)}}\boldsymbol{V}\}_1$, $\{\mathcal{T}_{\boldsymbol{U}^{(n)}}\boldsymbol{V}\}_{K+1}=\{\mathcal{T}_{\boldsymbol{U}^{(n)}}\boldsymbol{V}\}_{K-1}$, $U_{-1}^{(n)}=U_1^{(n)}$, and $U_{K+1}^{(n)}=U_{K-1}^{(n)}$. If the mapping $\mathcal{T}_{\boldsymbol{U}^{(n)}}$ has a fixed-point $\boldsymbol{V}^*$, then $\boldsymbol{V}^*$ is the solution $\boldsymbol{U}^{(n+1)}$ of the proposed scheme (3.13) under the discrete boundary conditions (3.15). The matrix expression of $\mathcal{T}_{\boldsymbol{U}^{(n)}}$ is given by

$$
\left(\frac{1}{\Delta t}I-\frac{1}{2}D_2\right)\mathcal{T}_{\boldsymbol{U}^{(n)}}\boldsymbol{V}=\left\{\left(\frac{1}{\Delta t}+\frac{1}{\varepsilon^2}\right)I+\frac{1}{2}D_2\right\}\boldsymbol{U}^{(n)}-\frac{1}{L\varepsilon^2}S\boldsymbol{U}^{(n)}
$$

$$
+\frac{1}{\varepsilon^2}\left(I-\frac{1}{L}S\right)\boldsymbol{V}+\left(I-\frac{1}{L}S\right)F_{\boldsymbol{U}^{(n)}}\boldsymbol{V} \quad \text{for all } \boldsymbol{V}\in\mathbb{R}^{K+1},
$$

where I is the $(K+1)$-dimensional identity matrix, further, S, and D_2 are $(K+1)\times(K+1)$ matrices and defined by

$$S := \Delta x \begin{pmatrix} \frac{1}{2} & 1 & \cdots & 1 & \frac{1}{2} \\ \frac{1}{2} & 1 & \cdots & 1 & \frac{1}{2} \\ \vdots & \vdots & \cdots & \vdots & \vdots \\ \frac{1}{2} & 1 & \cdots & 1 & \frac{1}{2} \\ \frac{1}{2} & 1 & \cdots & 1 & \frac{1}{2} \end{pmatrix}, \quad D_2 := \frac{1}{(\Delta x)^2} \begin{pmatrix} -2 & 2 & & & 0 \\ 1 & -2 & 1 & & \\ & \ddots & \ddots & \ddots & \\ & & 1 & -2 & 1 \\ 0 & & & 2 & -2 \end{pmatrix}.$$

The following lemma implies that the mapping $\mathcal{T}_{\boldsymbol{U}^{(n)}}$ is well-defined for all $\boldsymbol{U}^{(n)} \in \mathbb{R}^{K+1}$.

Lemma 3.2. The $(K+1)\times(K+1)$ matrix $(1/\Delta t)I - (1/2)D_2$ is nonsingular.

Proof. Eigenvalues of D_2 are

$$\lambda_k := \frac{2}{(\Delta x)^2}\left\{\cos\left(\frac{k}{K}\pi\right) - 1\right\} \quad (k = 0, \ldots, K), \tag{3.23}$$

and the eigenvector $\boldsymbol{x}_k$ corresponding to the eigenvalue λ_k is

$$\boldsymbol{x}_k = \left(\cos\left(\frac{0\cdot k}{K}\pi\right), \cos\left(\frac{1\cdot k}{K}\pi\right), \ldots, \cos\left(\frac{K\cdot k}{K}\pi\right)\right)^{\top} \qquad (k = 0, \ldots, K). \tag{3.24}$$

Since it holds that $D_2\boldsymbol{x}_k = \lambda_k \boldsymbol{x}_k$ $(k = 0, \ldots, K)$, we have

$$\left(\frac{1}{\Delta t}I - \frac{1}{2}D_2\right)\boldsymbol{x}_k = \frac{1}{\Delta t}\boldsymbol{x}_k - \frac{1}{2}D_2\boldsymbol{x}_k = \frac{1}{\Delta t}\boldsymbol{x}_k - \frac{1}{2}\lambda_k\boldsymbol{x}_k = \left(\frac{1}{\Delta t} - \frac{1}{2}\lambda_k\right)\boldsymbol{x}_k \quad (k = 0, \ldots, K).$$

Thus, eigenvalues of $(1/\Delta t)I - (1/2)D_2$ are

$$\frac{1}{\Delta t} - \frac{1}{2}\lambda_k = \frac{1}{\Delta t} + \frac{1}{\Delta x^2}\left\{1 - \cos\left(\frac{k}{K}\pi\right)\right\} \geq \frac{1}{\Delta t} > 0 \quad (k = 0, \ldots, K).$$

The positiveness of the eigenvalues implies the nonsingularity of $(1/\Delta t)I - (1/2)D_2$. $\square$

Next, we prove the existence and uniqueness of the solution for the proposed scheme by the fixed-point theorem for a contraction mapping.

Theorem 3.3. If Δt satisfies

$$\Delta t < \frac{L\varepsilon^2\Delta x}{\left(L + \sqrt{(K+1)(2K-1)}\Delta x\right)} \min\left\{\frac{1}{9(\Delta x + 65R_{\mathrm{d}}^2)}, \frac{1}{4\,(\Delta x + 209R_{\mathrm{d}}^2)}\right\}, \tag{3.25}$$

then the mapping $\mathcal{T}_{\boldsymbol{U}^{(n)}}$ has a unique fixed-point in the closed ball B, where

$$R_{\mathrm{d}} := \left\|\boldsymbol{U}^{(n)}\right\|_{L_{\mathrm{d}}^2}, \quad B := \left\{\boldsymbol{v} \in \mathbb{R}^{K+1}; \|\boldsymbol{v}\|_{L_{\mathrm{d}}^2} \leq 8R_{\mathrm{d}}\right\},$$

Proof. By the fixed-point theorem for a contraction mapping, it suffices to show that $\mathcal{T}_{\boldsymbol{U}^{(n)}}$ is a contraction mapping on B.

First, we prove that $\mathcal{T}_{\boldsymbol{U}^{(n)}} B \subseteq B$. By Lemma 3.2, we have

$$\mathcal{T}_{\boldsymbol{U}^{(n)}}\boldsymbol{V} = \left(\frac{1}{\Delta t}I - \frac{1}{2}D_2\right)^{-1}\left\{\left(\frac{1}{\Delta t} + \frac{1}{\varepsilon^2}\right)I + \frac{1}{2}D_2\right\}\boldsymbol{U}^{(n)} + \left(\frac{1}{\Delta t}I - \frac{1}{2}D_2\right)^{-1}\left\{-\frac{1}{L\varepsilon^2}S\boldsymbol{U}^{(n)} + \left(I - \frac{1}{L}S\right)\left(\frac{1}{\varepsilon^2}\boldsymbol{V} + F_{\boldsymbol{U}^{(n)}}\boldsymbol{V}\right)\right\} \quad \text{for all } \boldsymbol{V} \in B.$$

We diagonalize the matrix D_2 as follows:

$$D_2 = X\Lambda X^{-1},$$

where X and Λ are $(K+1)\times(K+1)$ matrices defined by

$$X := (\boldsymbol{x}_0, \boldsymbol{x}_1, \ldots, \boldsymbol{x}_K), \quad \Lambda := \mathrm{diag}(\lambda_0, \lambda_1, \ldots, \lambda_K),$$

with $\boldsymbol{x}_k$ given by (3.24) and λ_k given by (3.23). Since it holds that $I = XX^{-1} = XIX^{-1}$, we have

$$\frac{1}{\Delta t}I - \frac{1}{2}D_2 = \frac{1}{\Delta t}XIX^{-1} - \frac{1}{2}X\Lambda X^{-1} = X\left(\frac{1}{\Delta t}I - \frac{1}{2}\Lambda\right)X^{-1}. \tag{3.26}$$

Similarly, we obtain

$$\left(\frac{1}{\Delta t} + \frac{1}{\varepsilon^2}\right)I + \frac{1}{2}D_2 = X\left\{\left(\frac{1}{\Delta t} + \frac{1}{\varepsilon^2}\right)I + \frac{1}{2}\Lambda\right\}X^{-1}.$$

It holds from (3.26) that

$$\left(\frac{1}{\Delta t}I - \frac{1}{2}D_2\right)^{-1} = \left(X^{-1}\right)^{-1}\left(X\left(\frac{1}{\Delta t}I - \frac{1}{2}\Lambda\right)\right)^{-1} = X\left(\frac{1}{\Delta t}I - \frac{1}{2}\Lambda\right)^{-1}X^{-1}.$$

Then, the matrix expression of $\mathcal{T}_{\boldsymbol{U}^{(n)}}$ is given by

$$\mathcal{T}_{\boldsymbol{U}^{(n)}}\boldsymbol{V} = X\left(\frac{1}{\Delta t}I - \frac{1}{2}\Lambda\right)^{-1}\left\{\left(\frac{1}{\Delta t} + \frac{1}{\varepsilon^2}\right)I + \frac{1}{2}\Lambda\right\}X^{-1}\boldsymbol{U}^{(n)} + X\left(\frac{1}{\Delta t}I - \frac{1}{2}\Lambda\right)^{-1}X^{-1}\left\{-\frac{1}{L\varepsilon^2}S\boldsymbol{U}^{(n)} + \left(I - \frac{1}{L}S\right)\left(\frac{1}{\varepsilon^2}\boldsymbol{V} + F_{\boldsymbol{U}^{(n)}}\boldsymbol{V}\right)\right\} \quad \text{for all } \boldsymbol{V} \in B. \tag{3.27}$$

Here, we denote a matrix norm $\|\cdot\|_{L^2_{\mathrm{d}}}$ by

$$\|A\|_{L^2_{\mathrm{d}}} := \sup_{\boldsymbol{x}\neq\boldsymbol{0}} \frac{\|A\boldsymbol{x}\|_{L^2_{\mathrm{d}}}}{\|\boldsymbol{x}\|_{L^2_{\mathrm{d}}}} \quad \text{for all } (K+1)\times(K+1) \text{ matrix } A.$$

By using the following estimates:

$$\|\mathrm{diag}(d_0, d_1, \ldots, d_{K-1}, d_K)\|_{L^2_{\mathrm{d}}} = \max_{0\le k\le K}|d_k|,$$

$$\max_{0\le k\le K}\left|\frac{1}{\frac{1}{\Delta t} - \frac{1}{2}\lambda_k}\right| = \Delta t, \tag{3.28}$$

$$\max_{0\le k\le K}\left|\frac{\dfrac{1}{\Delta t}+\dfrac{1}{\varepsilon^2}+\dfrac{1}{2}\lambda_k}{\dfrac{1}{\Delta t}-\dfrac{1}{2}\lambda_k}\right| \le 1+\frac{1}{\varepsilon^2}\Delta t, \tag{3.29}$$

$$\|S\|_{L^2_{\mathrm{d}}} \le \sqrt{(K+1)(2K-1)}\Delta x, \tag{3.30}$$

$$\left\|I-\frac{1}{L}S\right\|_{L^2_{\mathrm{d}}} \le 1+\frac{1}{L}\sqrt{(K+1)(2K-1)}\Delta x, \tag{3.31}$$

$$\|X\|_{L^2_{\mathrm{d}}} \le 2\sqrt{K}, \tag{3.32}$$

$$\|X^{-1}\|_{L^2_{\mathrm{d}}} \le \frac{2}{\sqrt{K}}, \tag{3.33}$$

$$\|F_{\boldsymbol{U}^{(n)}}\boldsymbol{V}\|_{L^2_{\mathrm{d}}} \le \frac{585}{\varepsilon^2\Delta x}R_{\mathrm{d}}^3, \tag{3.34}$$

we obtain

$$\begin{aligned}
&\|\mathcal{T}_{\boldsymbol{U}^{(n)}}\boldsymbol{V}\|_{L^2_{\mathrm{d}}}\\
&\le \|X\|_{L^2_{\mathrm{d}}}\left\|\left(\frac{1}{\Delta t}I-\frac{1}{2}\Lambda\right)^{-1}\left\{\left(\frac{1}{\Delta t}+\frac{1}{\varepsilon^2}\right)I+\frac{1}{2}\Lambda\right\}\right\|_{L^2_{\mathrm{d}}}\|X^{-1}\|_{L^2_{\mathrm{d}}}\|\boldsymbol{U}^{(n)}\|_{L^2_{\mathrm{d}}}\\
&\quad+\|X\|_{L^2_{\mathrm{d}}}\left\|\left(\frac{1}{\Delta t}I-\frac{1}{2}\Lambda\right)^{-1}\right\|_{L^2_{\mathrm{d}}}\|X^{-1}\|_{L^2_{\mathrm{d}}}\\
&\quad\times\left\{\frac{1}{L\varepsilon^2}\|S\|_{L^2_{\mathrm{d}}}\|\boldsymbol{U}^{(n)}\|_{L^2_{\mathrm{d}}}+\left\|I-\frac{1}{L}S\right\|_{L^2_{\mathrm{d}}}\left(\frac{1}{\varepsilon^2}\|\boldsymbol{V}\|_{L^2_{\mathrm{d}}}+\|F_{\boldsymbol{U}^{(n)}}\boldsymbol{V}\|_{L^2_{\mathrm{d}}}\right)\right\}\\
&\le 4\left(1+\frac{\Delta t}{\varepsilon^2}\right)\|\boldsymbol{U}^{(n)}\|_{L^2_{\mathrm{d}}}+4\Delta t\left\{\frac{1}{L\varepsilon^2}\sqrt{(K+1)(2K-1)}\Delta x\,\|\boldsymbol{U}^{(n)}\|_{L^2_{\mathrm{d}}}\right.\\
&\quad\left.+\left(1+\frac{1}{L}\sqrt{(K+1)(2K-1)}\Delta x\right)\left(\frac{1}{\varepsilon^2}\|\boldsymbol{V}\|_{L^2_{\mathrm{d}}}+\|F_{\boldsymbol{U}^{(n)}}\boldsymbol{V}\|_{L^2_{\mathrm{d}}}\right)\right\}\\
&\le 4\left(1+\frac{\Delta t}{\varepsilon^2}\right)R_{\mathrm{d}}+4\Delta t\left\{\frac{1}{L\varepsilon^2}\sqrt{(K+1)(2K-1)}\Delta x\cdot R_{\mathrm{d}}\right.\\
&\quad\left.+\left(1+\frac{1}{L}\sqrt{(K+1)(2K-1)}\Delta x\right)\left(\frac{8}{\varepsilon^2}R_{\mathrm{d}}+\frac{585}{\varepsilon^2\Delta x}R_{\mathrm{d}}^3\right)\right\}\\
&= 4\left[\left(1+\frac{\Delta t}{\varepsilon^2}\right)+\frac{\Delta t}{\varepsilon^2}\left\{\frac{1}{L}\sqrt{(K+1)(2K-1)}\Delta x\right.\right.\\
&\quad\left.\left.+\left(1+\frac{1}{L}\sqrt{(K+1)(2K-1)}\Delta x\right)\left(8+\frac{585}{\Delta x}R_{\mathrm{d}}^2\right)\right\}\right]R_{\mathrm{d}}\\
&= 4\left[1+\frac{\Delta t}{\varepsilon^2}\left\{1+\frac{1}{L}\sqrt{(K+1)(2K-1)}\Delta x\right.\right.\\
&\quad\left.\left.+\left(1+\frac{1}{L}\sqrt{(K+1)(2K-1)}\Delta x\right)\left(8+\frac{585}{\Delta x}R_{\mathrm{d}}^2\right)\right\}\right]R_{\mathrm{d}}\\
&= 4\left[1+\frac{9\Delta t}{\varepsilon^2}\left(1+\frac{65}{\Delta x}R_{\mathrm{d}}^2\right)\left(1+\frac{1}{L}\sqrt{(K+1)(2K-1)}\Delta x\right)\right]R_{\mathrm{d}}\quad\text{for all }\boldsymbol{V}\in B.
\end{aligned}\tag{3.35}$$

Actually, we show how to obtain the above estimates (3.28)–(3.34). First, we obtain (3.28), since $\lambda_k \le 0$ $(k=0,\dots,K)$, and $\lambda_0 = 0$. In addition, by using (3.28), the estimate (3.29) holds. Next, we show the evaluation of the matrix norm (3.30). From the definition of the matrix S, we have

$$S^\top S = (\Delta x)^2 \begin{pmatrix} \frac{K+1}{4} & \frac{K+1}{2} & \cdots & \frac{K+1}{2} & \frac{K+1}{4} \\ \frac{K+1}{2} & K+1 & \cdots & K+1 & \frac{K+1}{2} \\ \vdots & \vdots & \cdots & \vdots & \vdots \\ \frac{K+1}{2} & K+1 & \cdots & K+1 & \frac{K+1}{2} \\ \frac{K+1}{4} & \frac{K+1}{2} & \cdots & \frac{K+1}{2} & \frac{K+1}{4} \end{pmatrix} = \frac{K+1}{4}(\Delta x)^2 \begin{pmatrix} 1 & 2 & \cdots & 2 & 1 \\ 2 & 4 & \cdots & 4 & 2 \\ \vdots & \vdots & \cdots & \vdots & \vdots \\ 2 & 4 & \cdots & 4 & 2 \\ 1 & 2 & \cdots & 2 & 1 \end{pmatrix}.$$

Let us define a $(K+1) \times (K+1)$ matrix P by

$$P := \begin{pmatrix} 1 & 2 & \cdots & 2 & 1 \\ 2 & 4 & \cdots & 4 & 2 \\ \vdots & \vdots & \cdots & \vdots & \vdots \\ 2 & 4 & \cdots & 4 & 2 \\ 1 & 2 & \cdots & 2 & 1 \end{pmatrix}.$$

Namely, it holds that

$$S^\top S = \frac{K+1}{4}(\Delta x)^2 P.$$

Let μ be an eigenvalue of P. Then, the characteristic polynomial of P is

$$\det(P - \mu I) = (-1)^{K-1}\mu^K(\mu - 4K + 2).$$

Thus, we obtain the eigenvalues $\mu = 0, 4K-2$. Therefore, the largest eigenvalue of $S^\top S$ is

$$\frac{K+1}{4}(\Delta x)^2 \cdot (4K-2) = \frac{(K+1)(2K-1)}{2}(\Delta x)^2$$

from $K \geq 1$. Hence, we have

$$\|S\|_{L^2_{\mathrm{d}}} \leq \sqrt{2}\|S\|_2 = \sqrt{2} \cdot \sqrt{\frac{(K+1)(2-1)}{2}(\Delta x)^2} = \sqrt{(K+1)(2K-1)}\Delta x$$

using the following inequality:

$$\|A\|_{L^2_{\mathrm{d}}} \leq \sqrt{2}\,\|A\|_2 \quad \text{for all } (K+1) \times (K+1) \text{ matrix } A, \tag{3.36}$$

where $\|\cdot\|_2$ is the matrix 2-norm induced by the euclidean vector norm. Moreover, by using the estimate (3.30) and the triangle inequality, we obtain the inequality (3.31). Next, we show the estimates (3.32) and (3.33). Let us define a diagonal matrix Q of order $K+1$ by

$$Q := \begin{pmatrix} \frac{1}{\sqrt{2}} & & & & 0 \\ & 1 & & & \\ & & \ddots & & \\ & & & 1 & \\ 0 & & & & \frac{1}{\sqrt{2}} \end{pmatrix}.$$

Also, let Z be a square matrix of order $K+1$ as

$$Z := \sqrt{\frac{2}{K}} QXQ.$$

Then, Z is an orthogonal matrix, i.e., $Z^{-1} = Z^\top$. In fact, let $Z = (\boldsymbol{z}_0, \ldots, \boldsymbol{z}_K)$, then

$$\boldsymbol{z}_k = \begin{cases} \dfrac{1}{\sqrt{K}} \boldsymbol{y}_k, & (k = 0, K), \\ \sqrt{\dfrac{2}{K}} \boldsymbol{y}_k, & (k = 1, \ldots, K-1), \end{cases}$$

where

$$\boldsymbol{y}_k := \begin{pmatrix} \dfrac{1}{\sqrt{2}} \cos\left(\dfrac{k}{K}\pi \cdot 0\right) \\ \cos\left(\dfrac{k}{K}\pi \cdot 1\right) \\ \vdots \\ \cos\left(\dfrac{k}{K}\pi \cdot (K-1)\right) \\ \dfrac{1}{\sqrt{2}} \cos\left(\dfrac{k}{K}\pi \cdot K\right) \end{pmatrix} \qquad (k = 0, \ldots, K).$$

For all $m, n \in \mathbb{Z}$ such that $0 \leq m, n \leq K$, it holds that

$$\boldsymbol{y}_m^\top \cdot \boldsymbol{y}_n = \sum_{k=0}^{K}{}'' \cos\Big(\frac{m}{K}\pi \cdot k\Big) \cos\Big(\frac{n}{K}\pi \cdot k\Big) = \begin{cases} K, & (m = n = 0, m = n = K), \\ \dfrac{1}{2}K, & (1 \leq m = n \leq K-1), \\ 0 & (m \neq n). \end{cases}$$

That is, $\{z_k\}_{k=0}^K$ is an orthonormal basis of $\mathbb{R}^{K+1}$. Thus, Z is an orthogonal matrix. Hence, it holds from $Z^\top Z = Z^{-1} Z = I$ that $\|Z\|_2 = 1$. Also, we have $\|Q^{-1}\|_2 = \sqrt{2}$. Therefore, by using the inequality (3.36), we obtain

$$\|X\|_{L^2_{\mathrm{d}}} \leq \sqrt{2} \|X\|_2 = \sqrt{2} \cdot \sqrt{\frac{K}{2}} \left\| Q^{-1} Z Q^{-1} \right\|_2 \leq 2\sqrt{K}.$$

Similarly, from $\|Z^\top\|_2 = 1$ and $\|Q\|_2 = 1$, we have

$$\|X^{-1}\|_{L^2_{\mathrm{d}}} \leq \sqrt{2} \|X^{-1}\|_2 = \sqrt{2} \cdot \sqrt{\frac{2}{K}} \left\| Q Z^\top Q \right\|_2 \leq \frac{2}{\sqrt{K}}.$$

Finally, we show the evaluation of the nonlinear term (3.34). By using the following inequality:

$$\sum_{k=0}^{K}{}'' a_k b_k \Delta x \leq \frac{2}{\Delta x} \sum_{k=0}^{K}{}'' a_k \Delta x \sum_{k=0}^{K}{}'' b_k \Delta x$$

for all $\{a_k\}_{k=0}^K, \{b_k\}_{k=0}^K$ such that $a_k, b_k \geq 0$ $(k = 0, \ldots, K)$, we have

$$
\begin{aligned}
\|F_{\boldsymbol{U}^{(n)}}\boldsymbol{V}\|_{L^2_{\mathrm{d}}}^2 &= \left(\frac{1}{2\varepsilon^2}\right)^2 \sum_{k=0}^{K}{}'' \left(V_k + U_k^{(n)}\right)^2 \left\{V_k^2 + \left(U_k^{(n)}\right)^2\right\}^2 \Delta x \\
&\le \left(\frac{1}{2\varepsilon^2}\right)^2 \frac{2}{\Delta x} \sum_{k=0}^{K}{}'' \left(V_k + U_k^{(n)}\right)^2 \Delta x \sum_{k=0}^{K}{}'' \left\{V_k^2 + \left(U_k^{(n)}\right)^2\right\}^2 \Delta x \\
&\le \left(\frac{1}{2\varepsilon^2}\right)^2 \left(\frac{2}{\Delta x}\right)^2 \sum_{k=0}^{K}{}'' \left\{V_k^2 + \left(U_k^{(n)}\right)^2\right\} \Delta x \sum_{k=0}^{K}{}'' \left\{V_k^2 + \left(U_k^{(n)}\right)^2\right\} \Delta x \\
&\quad \times \sum_{k=0}^{K}{}'' \left\{V_k^2 + 2V_k U_k^{(n)} + \left(U_k^{(n)}\right)^2\right\} \Delta x \\
&= \left(\frac{1}{2\varepsilon^2}\right)^2 \left(\frac{2}{\Delta x}\right)^2 \left(\|\boldsymbol{V}\|_{L^2_{\mathrm{d}}}^2 + \left\|\boldsymbol{U}^{(n)}\right\|_{L^2_{\mathrm{d}}}^2\right)^2 \left(\|\boldsymbol{V}\|_{L^2_{\mathrm{d}}}^2 + \left\|\boldsymbol{U}^{(n)}\right\|_{L^2_{\mathrm{d}}}^2 + 2\sum_{k=0}^{K}{}'' V_k U_k^{(n)} \Delta x\right)
\end{aligned}
$$

for all $\boldsymbol{V} \in B$. Moreover, by using Schwarz inequality, we obtain

$$
\left|\sum_{k=0}^{K}{}'' V_k U_k^{(n)} \Delta x\right| \le \sqrt{\sum_{k=0}^{K}{}'' V_k^2 \Delta x} \sqrt{\sum_{k=0}^{K}{}'' \left(U_k^{(n)}\right)^2 \Delta x} = \|\boldsymbol{V}\|_{L^2_{\mathrm{d}}} \left\|\boldsymbol{U}^{(n)}\right\|_{L^2_{\mathrm{d}}} \quad \text{for all } \boldsymbol{V} \in B.
$$

Hence, we have the following estimate:

$$
\begin{aligned}
\|F_{\boldsymbol{U}^{(n)}}\boldsymbol{V}\|_{L^2_{\mathrm{d}}}^2 &\le \left(\frac{1}{2\varepsilon^2}\right)^2 \left(\frac{2}{\Delta x}\right)^2 \left(\|\boldsymbol{V}\|_{L^2_{\mathrm{d}}}^2 + \left\|\boldsymbol{U}^{(n)}\right\|_{L^2_{\mathrm{d}}}^2\right)^2 \left(\|\boldsymbol{V}\|_{L^2_{\mathrm{d}}}^2 + \left\|\boldsymbol{U}^{(n)}\right\|_{L^2_{\mathrm{d}}}^2 + 2\|\boldsymbol{V}\|_{L^2_{\mathrm{d}}} \left\|\boldsymbol{U}^{(n)}\right\|_{L^2_{\mathrm{d}}}\right) \\
&\le \left(\frac{1}{2\varepsilon^2}\right)^2 \left(\frac{2}{\Delta x}\right)^2 \left\{(8R_{\mathrm{d}})^2 + R_{\mathrm{d}}^2\right\}^2 \left\{(8R_{\mathrm{d}})^2 + R_{\mathrm{d}}^2 + 2 \cdot 8R_{\mathrm{d}} \cdot R_{\mathrm{d}}\right\} \\
&= \left(\frac{1}{2\varepsilon^2}\right)^2 \left(\frac{2}{\Delta x}\right)^2 65^2 \cdot 81 \cdot R_{\mathrm{d}}^6.
\end{aligned}
$$

Therefore, we obtain the estimate (3.34). From the assumption (3.25) on Δt, the following inequality holds:

$$
\begin{aligned}
\Delta t &< \frac{L\varepsilon^2 \Delta x}{9\left(\Delta x + 65R_{\mathrm{d}}^2\right)\left(L + \sqrt{(K+1)(2K-1)}\Delta x\right)} \\
&= \frac{\varepsilon^2}{9\left(1 + \dfrac{65}{\Delta x}R_{\mathrm{d}}^2\right)\left\{1 + \dfrac{1}{L}\sqrt{(K+1)(2K-1)}\Delta x\right\}}.
\end{aligned}
$$

Hence, we have

$$
1 + \frac{9\Delta t}{\varepsilon^2}\left(1 + \frac{65}{\Delta x}R_{\mathrm{d}}^2\right)\left\{1 + \frac{1}{L}\sqrt{(K+1)(2K-1)}\Delta x\right\} < 2. \tag{3.37}
$$

From (3.35) and (3.37), we see that $\|\mathcal{T}_{\boldsymbol{U}^{(n)}}\boldsymbol{V}\|_{L^2_{\mathrm{d}}} \le 8R_{\mathrm{d}}$, i.e., $\mathcal{T}_{\boldsymbol{U}^{(n)}}\boldsymbol{V} \in B$. Hence, $\mathcal{T}_{\boldsymbol{U}^{(n)}}B \subseteq B$.

Next, we prove that $\mathcal{T}_{\boldsymbol{U}^{(n)}}$ is contractive. Using (3.27), (3.28), (3.31), (3.32), (3.33), and the following estimate:

$$\|F_{\boldsymbol{U}^{(n)}}\boldsymbol{V} - F_{\boldsymbol{U}^{(n)}}\boldsymbol{V}'\|_{L^2_{\mathrm{d}}} \le \frac{209R_{\mathrm{d}}^2}{\varepsilon^2\Delta x}\|\boldsymbol{V}-\boldsymbol{V}'\|_{L^2_{\mathrm{d}}} \quad \text{for all } \boldsymbol{V},\boldsymbol{V}' \in B, \tag{3.38}$$

we can show that

$$\begin{aligned}
&\|\mathcal{T}_{\boldsymbol{U}^{(n)}}\boldsymbol{V} - \mathcal{T}_{\boldsymbol{U}^{(n)}}\boldsymbol{V}'\|_{L^2_{\mathrm{d}}} \\
&\le \|X\|_{L^2_{\mathrm{d}}}\left\|\left(\frac{1}{\Delta t}I-\frac{1}{2}\Lambda\right)^{-1}\right\|_{L^2_{\mathrm{d}}}\|X^{-1}\|_{L^2_{\mathrm{d}}}\left\|I-\frac{1}{L}S\right\|_{L^2_{\mathrm{d}}}\left(\frac{1}{\varepsilon^2}\|\boldsymbol{V}-\boldsymbol{V}'\|_{L^2_{\mathrm{d}}}+\|F_{\boldsymbol{U}^{(n)}}\boldsymbol{V}-F_{\boldsymbol{U}^{(n)}}\boldsymbol{V}'\|_{L^2_{\mathrm{d}}}\right) \\
&\le 4\Delta t\left(1+\frac{1}{L}\sqrt{(K+1)(2K-1)}\Delta x\right)\left(\frac{1}{\varepsilon^2}\|\boldsymbol{V}-\boldsymbol{V}'\|_{L^2_{\mathrm{d}}}+\|F_{\boldsymbol{U}^{(n)}}\boldsymbol{V}-F_{\boldsymbol{U}^{(n)}}\boldsymbol{V}'\|_{L^2_{\mathrm{d}}}\right) \\
&\le \frac{4\Delta t}{\varepsilon^2}\left(1+\frac{209R_{\mathrm{d}}^2}{\Delta x}\right)\left(1+\frac{1}{L}\sqrt{(K+1)(2K-1)}\Delta x\right)\|\boldsymbol{V}-\boldsymbol{V}'\|_{L^2_{\mathrm{d}}} \quad \text{for all } \boldsymbol{V},\boldsymbol{V}' \in B.
\end{aligned} \tag{3.39}$$

Actually, we show the estimate (3.38). For all $\boldsymbol{V},\boldsymbol{V}' \in B$, we have

$$\begin{aligned}
&\|F_{\boldsymbol{U}^{(n)}}\boldsymbol{V} - F_{\boldsymbol{U}^{(n)}}\boldsymbol{V}'\|_{L^2_{\mathrm{d}}}^2 \\
&= \left(\frac{1}{2\varepsilon^2}\right)^2 \sum_{k=0}^{K}{}'' \left\{V_k^3 + V_k\left(U_k^{(n)}\right)^2 + V_k^2U_k^{(n)} + \left(U_k^{(n)}\right)^3 \right. \\
&\qquad\qquad \left. - (V_k')^3 - V_k'\left(U_k^{(n)}\right)^2 - (V_k')^2U_k^{(n)} - \left(U_k^{(n)}\right)^3\right\}^2 \Delta x \\
&= \left(\frac{1}{2\varepsilon^2}\right)^2 \sum_{k=0}^{K}{}'' \left[\left\{V_k^3-(V_k')^3\right\} + (V_k-V_k')\left(U_k^{(n)}\right)^2 + \left\{V_k^2-(V_k')^2\right\}U_k^{(n)}\right]^2\Delta x \\
&= \left(\frac{1}{2\varepsilon^2}\right)^2 \sum_{k=0}^{K}{}'' \left\{V_k^2+V_kV_k'+(V_k')^2+\left(U_k^{(n)}\right)^2+(V_k+V_k')U_k^{(n)}\right\}^2(V_k-V_k')^2\Delta x.
\end{aligned} \tag{3.40}$$

Moreover, it holds that

$$\max_{0\le k\le K}|V_k| \le \sqrt{\frac{2}{\Delta x}}\sqrt{\sum_{k=0}^{K}{}''V_k^2\Delta x} = \sqrt{\frac{2}{\Delta x}}\|\boldsymbol{V}\|_{L^2_{\mathrm{d}}} \le \sqrt{\frac{2}{\Delta x}}\cdot 8R_{\mathrm{d}} \quad \text{for all } \boldsymbol{V}\in B. \tag{3.41}$$

Similarly, we obtain

$$\max_{0\le k\le K}\left|U_k^{(n)}\right| \le \sqrt{\frac{2}{\Delta x}}R_{\mathrm{d}}. \tag{3.42}$$

Therefore, it follows from (3.40), (3.41), and (3.42) that

$$\begin{aligned}
\|F_{\boldsymbol{U}^{(n)}}\boldsymbol{V} - F_{\boldsymbol{U}^{(n)}}\boldsymbol{V}'\|_{L^2_{\mathrm{d}}}^2 &\le \left(\frac{1}{2\varepsilon^2}\right)^2 \sum_{k=0}^{K}{}''\left\{\frac{2}{\Delta x}\cdot 64R_{\mathrm{d}}^2 + \frac{2}{\Delta x}\cdot 64R_{\mathrm{d}}^2 + \frac{2}{\Delta x}\cdot 64R_{\mathrm{d}}^2 + \frac{2}{\Delta x}R_{\mathrm{d}}^2 \right. \\
&\qquad \left. + \left(\sqrt{\frac{2}{\Delta x}}\cdot 8R_{\mathrm{d}} + \sqrt{\frac{2}{\Delta x}}\cdot 8R_{\mathrm{d}}\right)\sqrt{\frac{2}{\Delta x}}R_{\mathrm{d}}\right\}^2 (V_k-V_k')^2\Delta x \\
&= \left(\frac{1}{2\varepsilon^2}\right)^2 \sum_{k=0}^{K}{}''\left\{\frac{2}{\Delta x}\cdot 192R_{\mathrm{d}}^2 + \frac{2}{\Delta x}R_{\mathrm{d}}^2 + \frac{2}{\Delta x}\cdot 16R_{\mathrm{d}}^2\right\}^2 (V_k-V_k')^2\Delta x \\
&= \left(\frac{209R_{\mathrm{d}}^2}{\varepsilon^2\Delta x}\right)^2\|\boldsymbol{V}-\boldsymbol{V}'\|_{L^2_{\mathrm{d}}}^2 \quad \text{for all } \boldsymbol{V},\boldsymbol{V}'\in B.
\end{aligned}$$

Hence, the estimate (3.38) holds. From the assumption (3.25) on Δt, the following inequality holds:

$$\begin{aligned}\Delta t &< \frac{L\varepsilon^2\Delta x}{4\left(\Delta x + 209R_{\mathrm{d}}^2\right)\left(L+\sqrt{(K+1)(2K-1)}\Delta x\right)}\\ &= \frac{\varepsilon^2}{4\left(1+\dfrac{209R_{\mathrm{d}}^2}{\Delta x}\right)\left(1+\dfrac{1}{L}\sqrt{(K+1)(2K-1)}\Delta x\right)}.\end{aligned}$$

Thus, it holds that

$$0 \le \frac{4\Delta t}{\varepsilon^2}\left(1+\frac{209R_{\mathrm{d}}^2}{\Delta x}\right)\left(1+\frac{1}{L}\sqrt{(K+1)(2K-1)}\Delta x\right) < 1. \tag{3.43}$$

Therefore, from (3.39) and (3.43), $\mathcal{T}_{\boldsymbol{U}^{(n)}}$ is contractive. This completes the proof. □

§5 Error estimate for the proposed scheme

In this section, we show an error estimate of the numerical solution of the proposed scheme. Fix a natural number $N \in \mathbb{N}$. We compute $\boldsymbol{U}^{(n)}$ up to $n = N$ by our proposed scheme (3.13)–(3.15) and estimate the error between it and the solution to the problem (3.2), (3.9), and (3.12) up to $T = N\Delta t$. We define the error by

$$e_k^{(n)} := U_k^{(n)} - u(k\Delta x, n\Delta t). \quad (k = -1, 0, \dots, K, K+1, n = 0, 1, \dots, N),$$

where u is the solution of the target equation (3.12). We define an extension of u by

$$u(x,t) := \begin{cases} u(-x,t) & (-\Delta x \le x < 0),\\ u(2L-x,t) & (L < x \le L+\Delta x),\end{cases} \tag{3.44}$$

for all $t \in [0,T]$. In what follows, we use the following special time-difference and time-averaging operators:

$$\delta_n^{\langle 1\rangle} f^{(n)} := \frac{f^{(n+\frac{1}{2})} - f^{(n-\frac{1}{2})}}{\Delta t}, \quad s_n^{\langle 1\rangle} f^{(n)} := \frac{f^{(n+\frac{1}{2})} + f^{(n-\frac{1}{2})}}{2}.$$

Moreover, for simplicity, we use the following expression $\tilde{u}_k^{(n)} := \tilde{u}(k\Delta x, n\Delta t)$ from now on. Also, $\partial_x f(a)$ means $\partial_x f(x)|_{x=a}$.

Lemma 3.3. For $n = 0, 1, \dots, N-1$, the error $\boldsymbol{e}^{(n)}$ satisfies

$$\begin{aligned}&\frac{1}{\Delta t}\left(\left\|\boldsymbol{e}^{(n+1)}\right\|_{L_{\mathrm{d}}^2}^2 - \left\|\boldsymbol{e}^{(n)}\right\|_{L_{\mathrm{d}}^2}^2\right)\\ &\le \frac{1}{2}\left(\left\|\boldsymbol{e}^{(n+1)}\right\|_{L_{\mathrm{d}}^2}^2 + \left\|\boldsymbol{e}^{(n)}\right\|_{L_{\mathrm{d}}^2}^2\right) + \left\|\boldsymbol{\xi}_1^{(n+\frac{1}{2})}\right\|_{L_{\mathrm{d}}^2}^2 + \left\|\boldsymbol{\xi}_2^{(n+\frac{1}{2})}\right\|_{L_{\mathrm{d}}^2}^2\\ &\quad + 4\left\|\tilde{\phi}(\boldsymbol{U}^{(n+1)},\boldsymbol{U}^{(n)}) - \boldsymbol{\phi}^{(n+\frac{1}{2})}\right\|_{L_{\mathrm{d}}^2}^2 + 4L\left\{\lambda_{\mathrm{d}}^{\varepsilon}(\boldsymbol{U}^{(n+1)},\boldsymbol{U}^{(n)}) - \lambda^{\varepsilon,(n+\frac{1}{2})}\right\}^2.\end{aligned}$$

where

$$\lambda^{\varepsilon,(n+\frac{1}{2})} := \lambda^{\varepsilon}\left(\left(n+\frac{1}{2}\right)\Delta t\right) = -\frac{1}{L}\int_0^L \frac{2}{\varepsilon^2}(u-u^3)dx\Big|_{t=(n+\frac{1}{2})\Delta t},$$

$$\tilde{\phi}(f_k, g_k) := \frac{2}{\varepsilon^2}\left\{\frac{f_k+g_k}{2} - \frac{(f_k)^3+(f_k)^2 g_k + f_k(g_k)^2+(g_k)^3}{4}\right\} \quad (k=0,1,\ldots,K),$$

$$\phi_k^{(n+\frac{1}{2})} := \frac{2}{\varepsilon^2}\left\{u_k^{(n+\frac{1}{2})} - \left(u_k^{(n+\frac{1}{2})}\right)^3\right\} \quad (k=0,1,\ldots,K),$$

$$\xi_{1,k}^{(n+\frac{1}{2})} := 2(\partial_t - \delta_n^{\langle 1\rangle})u_k^{(n+\frac{1}{2})} \quad (k=0,1,\ldots,K),$$

$$\xi_{2,k}^{(n+\frac{1}{2})} := 2(\delta_k^{\langle 2\rangle}s_n^{\langle 1\rangle} - \partial_x^2)u_k^{(n+\frac{1}{2})} \quad (k=0,1,\ldots,K).$$

Proof. For $n=0,1,\ldots,N-1$ and $k=0,1,\ldots,K$, subtracting the following proposed scheme:

$$\delta_n^{\langle 1\rangle}U_k^{(n+\frac{1}{2})} = \delta_k^{\langle 2\rangle}s_n^{\langle 1\rangle}U_k^{(n+\frac{1}{2})} + \tilde{\phi}(U_k^{(n+1)}, U_k^{(n)}) + \lambda_{\mathrm{d}}^{\varepsilon}(\boldsymbol{U}^{(n+1)}, \boldsymbol{U}^{(n)})$$

from the following original equation:

$$\partial_t u_k^{(n+\frac{1}{2})} = \partial_x^2 u_k^{(n+\frac{1}{2})} + \phi_k^{(n+\frac{1}{2})} + \lambda^{\varepsilon,(n+\frac{1}{2})}$$

at $t=(n+1/2)\Delta t$ and $x=k\Delta x$, we obtain

$$\begin{aligned}\delta_n^{\langle 1\rangle}e_k^{(n+\frac{1}{2})} &= \delta_k^{\langle 2\rangle}s_n^{\langle 1\rangle}e_k^{(n+\frac{1}{2})} + \frac{1}{2}\xi_{1,k}^{(n+\frac{1}{2})} + \frac{1}{2}\xi_{2,k}^{(n+\frac{1}{2})} \\ &\quad + \left(\tilde{\phi}(U_k^{(n+1)}, U_k^{(n)}) - \phi_k^{(n+\frac{1}{2})}\right) + \left(\lambda_{\mathrm{d}}^{\varepsilon}(\boldsymbol{U}^{(n+1)}, \boldsymbol{U}^{(n)}) - \lambda^{\varepsilon,(n+\frac{1}{2})}\right). \qquad (3.45)\end{aligned}$$

Hence, we obtain the following equality from (3.45):

$$\begin{aligned}&\frac{1}{\Delta t}\sum_{k=0}^{K}{}''\left\{\left(e_k^{(n+1)}\right)^2 - \left(e_k^{(n)}\right)^2\right\}\Delta x = \sum_{k=0}^{K}{}''\left(\delta_n^{\langle 1\rangle}e_k^{(n+\frac{1}{2})}\right)\left(s_n^{\langle 1\rangle}e_k^{(n+\frac{1}{2})}\right)\Delta x \\ &= \sum_{k=0}^{K}{}''\left(\delta_k^{\langle 2\rangle}s_n^{\langle 1\rangle}e_k^{(n+\frac{1}{2})}\right)\left(s_n^{\langle 1\rangle}e_k^{(n+\frac{1}{2})}\right)\Delta x + \sum_{k=0}^{K}{}''\left(s_n^{\langle 1\rangle}e_k^{(n+\frac{1}{2})}\right) \\ &\quad \times\left\{\frac{1}{2}\xi_{1,k}^{(n+\frac{1}{2})} + \frac{1}{2}\xi_{2,k}^{(n+\frac{1}{2})} + \left(\tilde{\phi}(U_k^{(n+1)}, U_k^{(n)}) - \phi_k^{(n+\frac{1}{2})}\right) + \left(\lambda_{\mathrm{d}}^{\varepsilon}(\boldsymbol{U}^{(n+1)}, \boldsymbol{U}^{(n)}) - \lambda^{\varepsilon,(n+\frac{1}{2})}\right)\right\}\Delta x.\end{aligned}$$

Here, from the discrete boundary conditions (3.15) and the definition of the extension (3.44), we have $\delta_k^{\langle 1\rangle}s_m^{\langle 1\rangle}e_k^{(n+\frac{1}{2})} = 0$ $(k=0,K)$. Therefore, from Proposition 2.3 (second-order summation by parts formula), we obtain the following inequality:

$$\begin{aligned}&\sum_{k=0}^{K}{}''\left(\delta_k^{\langle 2\rangle}s_n^{\langle 1\rangle}e_k^{(n+\frac{1}{2})}\right)\left(s_n^{\langle 1\rangle}e_k^{(n+\frac{1}{2})}\right)\Delta x \\ &= \left[\left(\delta_k^{\langle 1\rangle}s_n^{\langle 1\rangle}e_k^{(n+\frac{1}{2})}\right)\left(s_k^{\langle 1\rangle}s_n^{\langle 1\rangle}e_k^{(n+\frac{1}{2})}\right)\right]_0^K - \frac{1}{2}\sum_{k=0}^{K}{}''\left\{\left(\delta_k^{+}s_n^{\langle 1\rangle}e_k^{(n+\frac{1}{2})}\right)^2 + \left(\delta_k^{-}s_n^{\langle 1\rangle}e_k^{(n+\frac{1}{2})}\right)^2\right\}\Delta x \\ &\leq 0.\end{aligned}$$

From the above, we obtain the following inequality:

$$
\begin{aligned}
&\frac{1}{\Delta t}\sum_{k=0}^{K}{}''\left\{\left(e_k^{(n+1)}\right)^2-\left(e_k^{(n)}\right)^2\right\}\Delta x\\
&\leq \sum_{k=0}^{K}{}''\left(s_n^{\langle 1\rangle}e_k^{(n+\frac{1}{2})}\right)\\
&\quad\times\left\{\frac{1}{2}\xi_{1,k}^{(n+\frac{1}{2})}+\frac{1}{2}\xi_{2,k}^{(n+\frac{1}{2})}+\left(\tilde{\phi}(U_k^{(n+1)},U_k^{(n)})-\phi_k^{(n+\frac{1}{2})}\right)+\left(\lambda_{\mathrm{d}}^{\varepsilon}(\boldsymbol{U}^{(n+1)},\boldsymbol{U}^{(n)})-\lambda^{\varepsilon,(n+\frac{1}{2})}\right)\right\}\Delta x\\
&\leq \frac{1}{2}\sum_{k=0}^{K}{}''\left(s_n^{\langle 1\rangle}e_k^{(n+\frac{1}{2})}\right)^2\Delta x\\
&\quad+\frac{1}{2}\sum_{k=0}^{K}{}''\left\{\frac{1}{2}\xi_{1,k}^{(n+\frac{1}{2})}+\frac{1}{2}\xi_{2,k}^{(n+\frac{1}{2})}+\left(\tilde{\phi}(U_k^{(n+1)},U_k^{(n)})-\phi_k^{(n+\frac{1}{2})}\right)+\left(\lambda_{\mathrm{d}}^{\varepsilon}(\boldsymbol{U}^{(n+1)},\boldsymbol{U}^{(n)})-\lambda^{\varepsilon,(n+\frac{1}{2})}\right)\right\}^2\Delta x\\
&\leq \frac{1}{4}\sum_{k=0}^{K}{}''\left\{\left(e_k^{(n+1)}\right)^2+\left(e_k^{(n)}\right)^2\right\}\Delta x+2\sum_{k=0}^{K}{}''\left\{\frac{1}{4}\left(\xi_{1,k}^{(n+\frac{1}{2})}\right)^2+\frac{1}{4}\left(\xi_{2,k}^{(n+\frac{1}{2})}\right)^2\right.\\
&\quad\left.+\left(\tilde{\phi}(U_k^{(n+1)},U_k^{(n)})-\phi_k^{(n+\frac{1}{2})}\right)^2+\left(\lambda_{\mathrm{d}}^{\varepsilon}(\boldsymbol{U}^{(n+1)},\boldsymbol{U}^{(n)})-\lambda^{\varepsilon,(n+\frac{1}{2})}\right)^2\right\}\Delta x\\
&=\frac{1}{4}\sum_{k=0}^{K}{}''\left(e_k^{(n+1)}\right)^2\Delta x+\frac{1}{4}\sum_{k=0}^{K}{}''\left(e_k^{(n)}\right)^2\Delta x+\frac{1}{2}\sum_{k=0}^{K}{}''\left(\xi_{1,k}^{(n+\frac{1}{2})}\right)^2\Delta x+\frac{1}{2}\sum_{k=0}^{K}{}''\left(\xi_{2,k}^{(n+\frac{1}{2})}\right)^2\Delta x\\
&\quad+2\sum_{k=0}^{K}{}''\left(\tilde{\phi}(U_k^{(n+1)},U_k^{(n)})-\phi_k^{(n+\frac{1}{2})}\right)^2\Delta x+2L\left(\lambda_{\mathrm{d}}^{\varepsilon}(\boldsymbol{U}^{(n+1)},\boldsymbol{U}^{(n)})-\lambda^{\varepsilon,(n+\frac{1}{2})}\right)^2.
\end{aligned}
$$

In the second inequality, we have used the inequality $ab \leq (1/2)(a^2+b^2)$ for all $a, b \in \mathbb{R}$. In the third inequality, we have used the following inequality:

$$
\left(\sum_{i=1}^{n}a_i\right)^2 \leq n\sum_{i=1}^{n}a_i^2 \quad \text{for all } a_1,\ldots,a_n\in\mathbb{R}. \tag{3.46}
$$

This completes the proof. □

Lemma 3.4. The following inequality holds:

$$
\left\{\lambda_{\mathrm{d}}^{\varepsilon}(\boldsymbol{U}^{(n+1)},\boldsymbol{U}^{(n)})-\lambda^{\varepsilon,(n+\frac{1}{2})}\right\}^2 \leq \frac{2}{L}\left\|\tilde{\phi}(\boldsymbol{U}^{(n+1)},\boldsymbol{U}^{(n)})-\boldsymbol{\phi}^{(n+\frac{1}{2})}\right\|_{L_{\mathrm{d}}^2}^2+\frac{C_1^2}{8\varepsilon^4}(\Delta x)^4, \tag{3.47}
$$

where C_1 is a constant defined by

$$
C_1 := \sup_{\substack{0\leq x\leq L\\ 0\leq t\leq T}}\left|\partial_x^2(u-u^3)\right|.
$$

Proof. By using the inequality (3.46), we have

$$
\begin{aligned}
&\left\{\lambda_{\mathrm{d}}^{\varepsilon}(\boldsymbol{U}^{(n+1)},\boldsymbol{U}^{(n)})-\lambda^{\varepsilon,(n+\frac{1}{2})}\right\}^2\\
&=\left\{-\frac{1}{L}\sum_{k=0}^{K}{}''\tilde{\phi}(U_k^{(n+1)},U_k^{(n)})\Delta x+\frac{1}{L}\int_0^L\frac{2}{\varepsilon^2}(u-u^3)dx\bigg|_{t=(n+\frac{1}{2})\Delta t}\right\}^2\\
&=\frac{1}{L^2}\left[\left\{\sum_{k=0}^{K}{}''\left(\tilde{\phi}(U_k^{(n+1)},U_k^{(n)})-\phi_k^{(n+\frac{1}{2})}\right)\Delta x\right\}\right.\\
&\qquad\left.+\left\{\sum_{k=0}^{K}{}''\phi_k^{(n+\frac{1}{2})}\Delta x-\int_0^L\frac{2}{\varepsilon^2}(u-u^3)dx\bigg|_{t=(n+\frac{1}{2})\Delta t}\right\}\right]^2\\
&\le\frac{2}{L^2}\left\{\sum_{k=0}^{K}{}''\left(\tilde{\phi}(U_k^{(n+1)},U_k^{(n)})-\phi_k^{(n+\frac{1}{2})}\right)\Delta x\right\}^2\\
&\quad+\frac{2}{L^2}\left\{\sum_{k=0}^{K}{}''\phi_k^{(n+\frac{1}{2})}\Delta x-\int_0^L\frac{2}{\varepsilon^2}(u-u^3)dx\bigg|_{t=(n+\frac{1}{2})\Delta t}\right\}^2. \qquad (3.48)
\end{aligned}
$$

Using (3.46), we have

$$
\begin{aligned}
\left(\sum_{k=0}^{K}{}''f_k\Delta x\right)^2=\left\{\frac{1}{2}(f_0+f_K)\Delta x+\sum_{k=1}^{K-1}f_k\Delta x\right\}^2&\le K\left\{\frac{1}{4}(f_0+f_K)^2(\Delta x)^2+\sum_{k=1}^{K-1}f_k^2(\Delta x)^2\right\}\\
&\le K\Delta x\left\{\frac{1}{2}(f_0^2+f_K^2)\Delta x+\sum_{k=1}^{K-1}f_k^2\Delta x\right\}\\
&=L\sum_{k=0}^{K}{}''f_k^2\Delta x\quad\text{for all } \{f_k\}_{k=0}^K\in\mathbb{R}^{K+1}.
\end{aligned}
$$

By using this inequality, we obtain

$$
\frac{2}{L^2}\left\{\sum_{k=0}^{K}{}''\left(\tilde{\phi}(U_k^{(n+1)},U_k^{(n)})-\phi_k^{(n+\frac{1}{2})}\right)\Delta x\right\}^2\le\frac{2}{L}\left\|\tilde{\phi}(\boldsymbol{U}^{(n+1)},\boldsymbol{U}^{(n)})-\boldsymbol{\phi}^{(n+\frac{1}{2})}\right\|_{L_{\mathrm{d}}^2}^2. \qquad (3.49)
$$

Let us define

$$
\Phi^{(n+\frac{1}{2})}(x):=u\left(x,\left(n+\frac{1}{2}\right)\Delta t\right)-\left\{u\left(x,\left(n+\frac{1}{2}\right)\Delta t\right)\right\}^3\quad\text{for all } x\in[0,L].
$$

Since $u(\cdot,t)\in C^2([0,L])$ for any fixed $t\in[0,T]$, it holds that $\Phi^{(n+\frac{1}{2})}\in C^2([0,L])$. Therefore, from the Euler–Maclaurin summation formula, we have

$$
\begin{aligned}
\left|\sum_{k=0}^{K}{}''\phi_k^{(n+\frac{1}{2})}\Delta x-\int_0^L\frac{2}{\varepsilon^2}(u-u^3)dx\bigg|_{t=(n+\frac{1}{2})\Delta t}\right|&=\frac{2}{\varepsilon^2}\left|\sum_{k=0}^{K}{}''\Phi^{(n+\frac{1}{2})}(k\Delta x)\Delta x-\int_0^L\Phi^{(n+\frac{1}{2})}(x)dx\right|\\
&\le\frac{2}{\varepsilon^2}\cdot\frac{1}{8}(\Delta x)^2\int_0^L\left|\partial_x^2\Phi^{(n+\frac{1}{2})}(x)\right|dx\\
&=\frac{1}{4\varepsilon^2}(\Delta x)^2\int_0^L\left|\partial_x^2(u-u^3)\big|_{t=(n+\frac{1}{2})\Delta t}\right|dx\\
&\le\frac{C_1L}{4\varepsilon^2}(\Delta x)^2.
\end{aligned}
$$

Thus, we obtain

$$\frac{2}{L^2}\left\{\sum_{k=0}^{K}{}'' \phi_k^{(n+\frac{1}{2})}\Delta x - \int_0^L \frac{2}{\varepsilon^2}(u-u^3)dx\bigg|_{t=(n+\frac{1}{2})\Delta t}\right\}^2 \le \frac{2}{L^2}\cdot\frac{C_1^2L^2}{16\varepsilon^4}(\Delta x)^4 = \frac{C_1^2}{8\varepsilon^4}(\Delta x)^4. \quad (3.50)$$

From (3.48)–(3.50), we have (3.47). □

Lemma 3.5. The following inequality holds:

$$\left\|\tilde{\phi}(\boldsymbol{U}^{(n+1)},\boldsymbol{U}^{(n)}) - \boldsymbol{\phi}^{(n+\frac{1}{2})}\right\|_{L_\mathrm{d}^2}^2 \le \frac{4}{\varepsilon^4}\left(1+3C_2^2\right)^2\left(\left\|\boldsymbol{e}^{(n+1)}\right\|_{L_\mathrm{d}^2}^2 + \left\|\boldsymbol{e}^{(n)}\right\|_{L_\mathrm{d}^2}^2\right) + \frac{1}{12}\left\|\boldsymbol{\xi}_3^{(n+\frac{1}{2})}\right\|_{L_\mathrm{d}^2}^2 + \frac{1}{12}\left\|\boldsymbol{\xi}_4^{(n+\frac{1}{2})}\right\|_{L_\mathrm{d}^2}^2,$$

where C_2, ξ_3, and ξ_4 are defined by

$$C_2 := \max_{0\le l\le N}\left\{\max_{0\le k\le K}\left|U_k^{(l)}\right|, \sup_{x\in[0,L]}|u(x,l\Delta t)|\right\},$$

$$\xi_{3,k}^{(n+\frac{1}{2})} := \frac{2\sqrt{3}}{\varepsilon^2}C_2(u_k^{(n+1)}-u_k^{(n)})^2 \quad (k=0,1,\ldots,K),$$

$$\xi_{4,k}^{(n+\frac{1}{2})} := \frac{8\sqrt{3}}{\varepsilon^2}\left(1+3C_2^2\right)\left\{(s_n^{\langle 1\rangle}-1)u_k^{(n+\frac{1}{2})}\right\} \quad (k=0,1,\ldots,K).$$

Remark 3.2. Note that C_2 is finite since the proposed scheme is numerically stable, and the solution u satisfies $u(\cdot,t)\in C^0([0,L])$ for any fixed $t\in[0,T]$.

Proof. We denote

$$\tilde{\phi}(\boldsymbol{U}^{(n+1)},\boldsymbol{U}^{(n)}) - \boldsymbol{\phi}^{(n+\frac{1}{2})} = \sum_{i=1}^{4}\boldsymbol{I}_i,$$

where $\boldsymbol{I}_i = \{I_{i,k}\}_{k=0}^K$ with

$$I_{1,k} := \tilde{\phi}(U_k^{(n+1)},U_k^{(n)}) - \tilde{\phi}(u_k^{(n+1)},U_k^{(n)}),$$

$$I_{2,k} := \tilde{\phi}(u_k^{(n+1)},U_k^{(n)}) - \tilde{\phi}(u_k^{(n+1)},u_k^{(n)}),$$

$$I_{3,k} := \tilde{\phi}(u_k^{(n+1)},u_k^{(n)}) - \frac{2}{\varepsilon^2}\left\{s_n^{\langle 1\rangle}u_k^{(n+\frac{1}{2})} - \left(s_n^{\langle 1\rangle}u_k^{(n+\frac{1}{2})}\right)^3\right\},$$

$$I_{4,k} := \frac{2}{\varepsilon^2}\left\{s_n^{\langle 1\rangle}u_k^{(n+\frac{1}{2})} - \left(s_n^{\langle 1\rangle}u_k^{(n+\frac{1}{2})}\right)^3\right\} - \phi_k^{(n+\frac{1}{2})}.$$

By direct calculation, we can see that

$$\begin{aligned}
I_{1,k} &= \frac{2}{\varepsilon^2}\left\{\frac{U_k^{(n+1)}+U_k^{(n)}}{2} - \frac{\left(U_k^{(n+1)}\right)^3 + \left(U_k^{(n+1)}\right)^2U_k^{(n)} + U_k^{(n+1)}\left(U_k^{(n)}\right)^2 + \left(U_k^{(n)}\right)^3}{4}\right\} \\
&\quad - \frac{2}{\varepsilon^2}\left\{\frac{u_k^{(n+1)}+U_k^{(n)}}{2} - \frac{\left(u_k^{(n+1)}\right)^3 + \left(u_k^{(n+1)}\right)^2U_k^{(n)} + u_k^{(n+1)}\left(U_k^{(n)}\right)^2 + \left(U_k^{(n)}\right)^3}{4}\right\} \\
&= \frac{1}{\varepsilon^2}\left(U_k^{(n+1)} - u_k^{(n+1)}\right) \\
&\quad - \frac{1}{2\varepsilon^2}\left[\left(U_k^{(n+1)}\right)^3 - \left(u_k^{(n+1)}\right)^3 + \left\{\left(U_k^{(n+1)}\right)^2 - \left(u_k^{(n+1)}\right)^2\right\}U_k^{(n)} + \left(U_k^{(n+1)} - u_k^{(n+1)}\right)\left(U_k^{(n)}\right)^2\right] \\
&= \frac{1}{\varepsilon^2}e_k^{(n+1)}\left[1 - \frac{1}{2}\left\{\left(U_k^{(n+1)}\right)^2 + U_k^{(n+1)}u_k^{(n+1)} + \left(u_k^{(n+1)}\right)^2 + U_k^{(n+1)}U_k^{(n)} + u_k^{(n+1)}U_k^{(n)} + \left(U_k^{(n)}\right)^2\right\}\right]
\end{aligned}$$

for $k = 0, 1, \ldots, K$. Namely, we have

$$
\begin{aligned}
|I_{1,k}| &\le \frac{1}{\varepsilon^2}\left|e_k^{(n+1)}\right|\left\{1 + \frac{1}{2}\left(\left|U_k^{(n+1)}\right|^2 + \left|U_k^{(n+1)}\right|\left|u_k^{(n+1)}\right| + \left|u_k^{(n+1)}\right|^2\right.\right. \\
&\qquad \left.\left. + \left|U_k^{(n+1)}\right|\left|U_k^{(n)}\right| + \left|u_k^{(n+1)}\right|\left|U_k^{(n)}\right| + \left|U_k^{(n)}\right|^2\right)\right\} \\
&\le \frac{1}{\varepsilon^2}\left|e_k^{(n+1)}\right|\left(1 + \frac{1}{2}\cdot 6C_2^2\right) \\
&= \frac{1}{\varepsilon^2}\left(1 + 3C_2^2\right)\left|e_k^{(n+1)}\right| \quad (k = 0, 1, \ldots, K).
\end{aligned}
$$

In the same manner, we obtain

$$
|I_{2,k}| \le \frac{1}{\varepsilon^2}\left(1 + 3C_2^2\right)\left|e_k^{(n)}\right| \quad (k = 0, 1, \ldots, K). \tag{3.51}
$$

Furthermore, it holds from the direct calculation that

$$
\begin{aligned}
I_{4,k} &= \frac{2}{\varepsilon^2}\left\{s_n^{\langle 1\rangle}u_k^{(n+\frac{1}{2})} - \left(s_n^{\langle 1\rangle}u_k^{(n+\frac{1}{2})}\right)^3\right\} - \frac{2}{\varepsilon^2}\left\{u_k^{(n+\frac{1}{2})} - \left(u_k^{(n+\frac{1}{2})}\right)^3\right\} \\
&= \frac{2}{\varepsilon^2}\left\{s_n^{\langle 1\rangle}u_k^{(n+\frac{1}{2})} - u_k^{(n+\frac{1}{2})} - \left(s_n^{\langle 1\rangle}u_k^{(n+\frac{1}{2})}\right)^3 + \left(u_k^{(n+\frac{1}{2})}\right)^3\right\} \\
&= \frac{2}{\varepsilon^2}\left(s_n^{\langle 1\rangle}u_k^{(n+\frac{1}{2})} - u_k^{(n+\frac{1}{2})}\right)\left[1 - \left\{\left(s_n^{\langle 1\rangle}u_k^{(n+\frac{1}{2})}\right)^2 + \left(s_n^{\langle 1\rangle}u_k^{(n+\frac{1}{2})}\right)u_k^{(n+\frac{1}{2})} + \left(u_k^{(n+\frac{1}{2})}\right)^2\right\}\right]
\end{aligned}
$$

for $k = 0, 1, \ldots, K$. That is, we have

$$
\begin{aligned}
|I_{4,k}| &\le \frac{2}{\varepsilon^2}\left|(s_n^{\langle 1\rangle} - 1)u_k^{(n+\frac{1}{2})}\right|\left(1 + \left|s_n^{\langle 1\rangle}u_k^{(n+\frac{1}{2})}\right|^2 + \left|s_n^{\langle 1\rangle}u_k^{(n+\frac{1}{2})}\right|\left|u_k^{(n+\frac{1}{2})}\right| + \left|u_k^{(n+\frac{1}{2})}\right|^2\right) \\
&= \frac{2}{\varepsilon^2}\left|(s_n^{\langle 1\rangle} - 1)u_k^{(n+\frac{1}{2})}\right|\left(1 + \left|\frac{u_k^{(n+1)} + u_k^{(n)}}{2}\right|^2 + \left|\frac{u_k^{(n+1)} + u_k^{(n)}}{2}\right|\left|u_k^{(n+\frac{1}{2})}\right| + \left|u_k^{(n+\frac{1}{2})}\right|^2\right) \\
&\le \frac{2}{\varepsilon^2}\left|(s_n^{\langle 1\rangle} - 1)u_k^{(n+\frac{1}{2})}\right| \\
&\quad \times\left(1 + \frac{\left|u_k^{(n+1)}\right|^2 + \left|u_k^{(n)}\right|^2}{2} + \frac{\left|u_k^{(n+1)}\right|\left|u_k^{(n+\frac{1}{2})}\right| + \left|u_k^{(n)}\right|\left|u_k^{(n+\frac{1}{2})}\right|}{2} + \left|u_k^{(n+\frac{1}{2})}\right|^2\right) \\
&\le \frac{2}{\varepsilon^2}\left|(s_n^{\langle 1\rangle} - 1)u_k^{(n+\frac{1}{2})}\right|\left(1 + \frac{C_2^2 + C_2^2}{2} + \frac{C_2^2 + C_2^2}{2} + C_2^2\right) \\
&= \frac{2}{\varepsilon^2}\left(1 + 3C_2^2\right)\left|(s_n^{\langle 1\rangle} - 1)u_k^{(n+\frac{1}{2})}\right| \quad (k = 0, 1, \ldots, K).
\end{aligned}
$$

By using the following equality:

$$
\frac{a^3 + a^2 b + a b^2 + b^3}{2} - \frac{(a+b)^3}{4} = \frac{(a+b)(a-b)^2}{4} \quad \text{for all } a, b \in \mathbb{R},
$$

we obtain

$$
\begin{aligned}
|I_{3,k}| &= \frac{2}{\varepsilon^2}\left\{\frac{u_k^{(n+1)}+u_k^{(n)}}{2} - \frac{\left(u_k^{(n+1)}\right)^3+\left(u_k^{(n+1)}\right)^2 u_k^{(n)} + u_k^{(n+1)}\left(u_k^{(n)}\right)^2+\left(u_k^{(n)}\right)^3}{4}\right\} \\
&\quad - \frac{2}{\varepsilon^2}\left\{\frac{u_k^{(n+1)}+u_k^{(n)}}{2} - \left(\frac{u_k^{(n+1)}+u_k^{(n)}}{2}\right)^3\right\} \\
&= -\frac{1}{\varepsilon^2}\left\{\frac{\left(u_k^{(n+1)}\right)^3+\left(u_k^{(n+1)}\right)^2 u_k^{(n)} + u_k^{(n+1)}\left(u_k^{(n)}\right)^2+\left(u_k^{(n)}\right)^3}{2} - \frac{\left(u_k^{(n+1)}+u_k^{(n)}\right)^3}{4}\right\} \\
&= -\frac{1}{4\varepsilon^2}\left(u_k^{(n+1)}+u_k^{(n)}\right)\left(u_k^{(n+1)}-u_k^{(n)}\right)^2 \quad (k=0,1,\ldots,K).
\end{aligned}
$$

Thus, we get

$$
|I_{3,k}| \le \frac{1}{4\varepsilon^2}\left(\left|u_k^{(n+1)}\right|+\left|u_k^{(n)}\right|\right)\left(u_k^{(n+1)}-u_k^{(n)}\right)^2 \le \frac{1}{2\varepsilon^2}C_2\left(u_k^{(n+1)}-u_k^{(n)}\right)^2 \quad (k=0,1,\ldots,K).
$$

From the above estimates, we obtain

$$
\begin{aligned}
&\left\|\tilde{\phi}(\boldsymbol{U}^{(n+1)},\boldsymbol{U}^{(n)}) - \boldsymbol{\phi}^{(n+\frac{1}{2})}\right\|_{L^2_{\mathrm{d}}}^2 \le 4\sum_{i=1}^{4}\|\boldsymbol{I}_i\|_{L^2_{\mathrm{d}}}^2 \\
&\le 4\left\{\frac{1}{\varepsilon^4}(1+3C_2^2)^2\left(\left\|\boldsymbol{e}^{(n+1)}\right\|_{L^2_{\mathrm{d}}}^2+\left\|\boldsymbol{e}^{(n)}\right\|_{L^2_{\mathrm{d}}}^2\right)\right. \\
&\qquad\left.+\frac{C_2^2}{4\varepsilon^4}\left\|\left(\boldsymbol{u}^{(n+1)}-\boldsymbol{u}^{(n)}\right)^2\right\|_{L^2_{\mathrm{d}}}^2 + \frac{4}{\varepsilon^4}(1+3C_2^2)^2\left\|(s_n^{\langle 1\rangle}-1)\boldsymbol{u}^{(n+\frac{1}{2})}\right\|_{L^2_{\mathrm{d}}}^2\right\} \\
&= \frac{4}{\varepsilon^4}(1+3C_2^2)^2\left(\left\|\boldsymbol{e}^{(n+1)}\right\|_{L^2_{\mathrm{d}}}^2+\left\|\boldsymbol{e}^{(n)}\right\|_{L^2_{\mathrm{d}}}^2\right) + \frac{1}{12}\left\|\frac{2\sqrt{3}}{\varepsilon^2}C_2\left(\boldsymbol{u}^{(n+1)}-\boldsymbol{u}^{(n)}\right)^2\right\|_{L^2_{\mathrm{d}}}^2 \\
&\qquad+\frac{1}{12}\left\|\frac{8\sqrt{3}}{\varepsilon^2}(1+3C_2^2)(s_n^{\langle 1\rangle}-1)\boldsymbol{u}^{(n+\frac{1}{2})}\right\|_{L^2_{\mathrm{d}}}^2 \\
&= \frac{4}{\varepsilon^4}(1+3C_2^2)^2\left(\left\|\boldsymbol{e}^{(n+1)}\right\|_{L^2_{\mathrm{d}}}^2+\left\|\boldsymbol{e}^{(n)}\right\|_{L^2_{\mathrm{d}}}^2\right)+\frac{1}{12}\left\|\boldsymbol{\xi}_3^{(n+\frac{1}{2})}\right\|_{L^2_{\mathrm{d}}}^2+\frac{1}{12}\left\|\boldsymbol{\xi}_4^{(n+\frac{1}{2})}\right\|_{L^2_{\mathrm{d}}}^2.
\end{aligned}
$$

This completes the proof. □

Lemma 3.6. The following inequality holds:

$$
(1-\Delta t C_3)\left\|\boldsymbol{e}^{(n+1)}\right\|_{L^2_{\mathrm{d}}}^2 \le \left\|\boldsymbol{e}^{(n)}\right\|_{L^2_{\mathrm{d}}}^2 + \Delta t\left\{\left(\sum_{i=1}^{4}\left\|\boldsymbol{\xi}_i^{(n+\frac{1}{2})}\right\|_{L^2_{\mathrm{d}}}^2\right)+\frac{C_1^2 L}{2\varepsilon^4}(\Delta x)^4\right\},
$$

where C_3 is a constant defined by $C_3 := 1+(96/\varepsilon^4)(1+3C_2^2)^2$.

Proof. From Lemma 3.3, Lemma 3.4, and Lemma 3.5, we have

$$\begin{aligned}
&\frac{1}{\Delta t}\left(\left\|\boldsymbol{e}^{(n+1)}\right\|_{L^2_{\mathrm{d}}}^2-\left\|\boldsymbol{e}^{(n)}\right\|_{L^2_{\mathrm{d}}}^2\right)\\
&\le \frac{1}{2}\left(\left\|\boldsymbol{e}^{(n+1)}\right\|_{L^2_{\mathrm{d}}}^2+\left\|\boldsymbol{e}^{(n)}\right\|_{L^2_{\mathrm{d}}}^2\right)+\left\|\boldsymbol{\xi}_1^{(n+\frac{1}{2})}\right\|_{L^2_{\mathrm{d}}}^2+\left\|\boldsymbol{\xi}_2^{(n+\frac{1}{2})}\right\|_{L^2_{\mathrm{d}}}^2\\
&\quad+12\left\|\tilde{\phi}(\boldsymbol{U}^{(n+1)},\boldsymbol{U}^{(n)})-\boldsymbol{\phi}^{(n+\frac{1}{2})}\right\|_{L^2_{\mathrm{d}}}^2+\frac{C_1^2L}{2\varepsilon^4}(\Delta x)^4\\
&\le\left\{\frac{1}{2}+\frac{48}{\varepsilon^4}\left(1+3C_2^2\right)^2\right\}\left(\left\|\boldsymbol{e}^{(n+1)}\right\|_{L^2_{\mathrm{d}}}^2+\left\|\boldsymbol{e}^{(n)}\right\|_{L^2_{\mathrm{d}}}^2\right)+\left(\sum_{i=1}^{4}\left\|\boldsymbol{\xi}_i^{(n+\frac{1}{2})}\right\|_{L^2_{\mathrm{d}}}^2\right)+\frac{C_1^2L}{2\varepsilon^4}(\Delta x)^4.
\end{aligned}$$

Hence, we obtain the following inequality:

$$\begin{aligned}
&\frac{1}{\Delta t}\left(\left\|\boldsymbol{e}^{(n+1)}\right\|_{L^2_{\mathrm{d}}}^2-\left\|\boldsymbol{e}^{(n)}\right\|_{L^2_{\mathrm{d}}}^2\right)\\
&\le\left\{\frac{1}{2}+\frac{48}{\varepsilon^4}\left(1+3C_2^2\right)^2\right\}\cdot 2\left\|\boldsymbol{e}^{(n+1)}\right\|_{L^2_{\mathrm{d}}}^2+\left(\sum_{i=1}^{4}\left\|\boldsymbol{\xi}_i^{(n+\frac{1}{2})}\right\|_{L^2_{\mathrm{d}}}^2\right)+\frac{C_1^2L}{2\varepsilon^4}(\Delta x)^4\\
&=C_3\left\|\boldsymbol{e}^{(n+1)}\right\|_{L^2_{\mathrm{d}}}^2+\left(\sum_{i=1}^{4}\left\|\boldsymbol{\xi}_i^{(n+\frac{1}{2})}\right\|_{L^2_{\mathrm{d}}}^2\right)+\frac{C_1^2L}{2\varepsilon^4}(\Delta x)^4.
\end{aligned}$$

This completes the proof. □

Theorem 3.4. Assume that the target equation (3.12) has a solution u satisfying $u \in C^4([0,L]\times[0,T])$. If Δt satisfies the condition (3.25) and $\Delta t < 1/(2C_3)$, then there exists a constant C_4 such that

$$\left\{\sum_{k=0}^{K}{}''\left(U_k^{(n)}-u(k\Delta x,n\Delta t)\right)^2\Delta x\right\}^{\frac{1}{2}}\le C_4\sqrt{LT}e^{C_3T}((\Delta x)^2+(\Delta t)^2)\quad(n=1,\dots,N).$$

Remark 3.3. This theorem means that the solution of the scheme (3.13) converges to the solution of the target equation (3.12) in the sense of discrete L^2-norm and that the convergence rate is $O((\Delta x)^2+(\Delta t)^2)$.

Proof. From the regularity assumption of the solution u, applying the Taylor theorem to u, we have

$$\begin{aligned}
\xi_{1,k}^{(n+\frac{1}{2})}&=-\frac{(\Delta t)^2}{12}\,\partial_t^3u\big|_{(x,t)=(k\Delta x,t_1)},\\
\xi_{2,k}^{(n+\frac{1}{2})}&=\frac{(\Delta x)^2}{6}\,\partial_x^4u\big|_{(x,t)=(x_1,(n+\frac{1}{2})\Delta t)}+\frac{(\Delta t)^2}{4}\,\partial_x^2\partial_t^2u\big|_{(x,t)=(x_2,t_2)},\\
\xi_{3,k}^{(n+\frac{1}{2})}&=\frac{2\sqrt{3}}{\varepsilon^2}C_2(\Delta t)^2\left(\partial_tu\big|_{(x,t)=(k\Delta x,t_3)}\right)^2,\\
\xi_{4,k}^{(n+\frac{1}{2})}&=\frac{\sqrt{3}}{\varepsilon^2}(1+3C_2^2)(\Delta t)^2\,\partial_t^2u\big|_{(x,t)=(k\Delta x,t_4)},
\end{aligned}$$

where $t_1,t_2,t_3,t_4\in[n\Delta t,(n+1)\Delta t]$ and $x_1,x_2\in[(k-1)\Delta x,(k+1)\Delta x]$ for $n=0,\dots,N-1$ and $k=0,\dots,K$. From these results, we obtain

$$\sum_{i=1}^{4}\left\|\boldsymbol{\xi}_i^{(n+\frac{1}{2})}\right\|_{L^2_{\mathrm{d}}}^2+\frac{C_1^2L}{2\varepsilon^4}(\Delta x)^4\le 5\tilde{C}_4^2L((\Delta x)^2+(\Delta t)^2)^2\quad(n=0,1,\dots,N-1),\tag{3.52}$$

where $\tilde{C}_4$ is defined by

$$\tilde{C}_4 := \sup_{\substack{0\le x\le L\\ 0\le t\le T}} \max\left\{ \frac{1}{12}\left|\partial_t^3 u\right|, \frac{1}{6}\left|\partial_x^4 u\right|, \frac{1}{4}\left|\partial_t^2\partial_x^2 u\right|, \frac{2\sqrt{3}}{\varepsilon^2}C_2\left|\partial_t u\right|^2, \frac{\sqrt{3}}{\varepsilon^2}(1+3C_2^2)\left|\partial_t^2 u\right|, \right.$$
$$\left. \frac{1}{\sqrt{2}\varepsilon^2}\left|\partial_x^2(u-u^3)\right| \right\}.$$

We remark that $\tilde{C}_4$ is finite from the regularity assumption of the solution u. Let us define a constant C_4 by $C_4 := \sqrt{5}\tilde{C}_4$. From the assumption $\Delta t < 1/(2C_3)$, we have $0 < 1 - 2\Delta t C_3 \le 1 - \Delta t C_3 \le 1$ and

$$\frac{1}{1-\Delta t C_3} \le 1 + 2\Delta t C_3 =: \tilde{C}_3. \tag{3.53}$$

Hence, by using Lemma 3.6, (3.52), and (3.53), we obtain

$$\left\|\boldsymbol{e}^{(n+1)}\right\|_{L^2_{\mathrm{d}}}^2 \le \tilde{C}_3\left\|\boldsymbol{e}^{(n)}\right\|_{L^2_{\mathrm{d}}}^2 + \tilde{C}_3\cdot\Delta t C_4^2 L((\Delta x)^2+(\Delta t)^2)^2 \quad (n=0,1,\ldots,N-1).$$

Therefore, by using this inequality iteratively, we have

$$\begin{aligned}\left\|\boldsymbol{e}^{(n)}\right\|_{L^2_{\mathrm{d}}}^2 &\le \tilde{C}_3\left\|\boldsymbol{e}^{(n-1)}\right\|_{L^2_{\mathrm{d}}}^2 + \tilde{C}_3\cdot\Delta t C_4^2 L((\Delta x)^2+(\Delta t)^2)^2\\ &\le (\tilde{C}_3)^2\left\|\boldsymbol{e}^{(n-2)}\right\|_{L^2_{\mathrm{d}}}^2 + ((\tilde{C}_3)^2+\tilde{C}_3)\cdot\Delta t C_4^2 L((\Delta x)^2+(\Delta t)^2)^2\\ &\le \cdots \quad \cdots \quad \cdots\\ &\le (\tilde{C}_3)^n\left\|\boldsymbol{e}^{(0)}\right\|_{L^2_{\mathrm{d}}}^2 + \Delta t C_4^2 L((\Delta x)^2+(\Delta t)^2)^2\sum_{j=1}^{n}(\tilde{C}_3)^j \quad (n=1,\ldots,N).\end{aligned}$$

It holds from $e_k^{(0)} = 0$ $(k=0,\ldots,K)$ that $\|\boldsymbol{e}^{(0)}\|_{L^2_{\mathrm{d}}}^2 = 0$. Moreover, by using $1+x \le e^x$ for all $x \ge 0$, we obtain

$$\begin{aligned}\sum_{j=1}^{n}(\tilde{C}_3)^j = \sum_{j=1}^{n}(1+2\Delta t C_3)^j \le \sum_{j=1}^{n}\exp(j\cdot 2\Delta t C_3) &\le \exp(N\cdot 2\Delta t C_3)\sum_{j=1}^{N}1\\ &= N\exp\left(N\cdot 2\frac{T}{N}C_3\right)\\ &= N\exp(2C_3T).\end{aligned}$$

Hence, we obtain

$$\left\|\boldsymbol{e}^{(n)}\right\|_{L^2_{\mathrm{d}}}^2 \le \Delta t C_4^2 L((\Delta x)^2+(\Delta t)^2)^2\cdot N e^{2C_3T} = C_4^2 L T e^{2C_3T}((\Delta x)^2+(\Delta t^2))^2 \quad (n=1,\ldots,N).$$

This completes the proof. □

§6 Computation examples

In this section, we demonstrate through numerical computations that the proposed scheme is stable and that the numerical solution of the proposed scheme is efficient.

Moreover, we compare the proposed scheme with the Crank–Nicolson (CN) scheme. The concrete form of the CN scheme for (3.12) is, for $n = 0, 1, \ldots,$

$$\frac{U_k^{(n+1)} - U_k^{(n)}}{\Delta t} = \delta_k^{\langle 2\rangle}\left(\frac{U_k^{(n+1)} + U_k^{(n)}}{2}\right) + \tilde{F}\left(U_k^{(n+1)}, U_k^{(n)}\right) - \frac{1}{L}\sum_{k=0}^{K}{}'' \tilde{F}\left(U_k^{(n+1)}, U_k^{(n)}\right)\Delta x \quad (k=0,\ldots,K),$$

where

$$\tilde{F}\left(U_k^{(n+1)}, U_k^{(n)}\right) := \frac{2}{\varepsilon^2}\left[\left(\frac{U_k^{(n+1)} + U_k^{(n)}}{2}\right) - \left\{\frac{\left(U_k^{(n+1)}\right)^3 + \left(U_k^{(n)}\right)^3}{2}\right\}\right].$$

We perform all our numerical computations by using Julia language.

6.1 Numerical solutions

The left figures show the numerical solution obtained by the proposed scheme. The right ones show that obtained by the CN scheme.

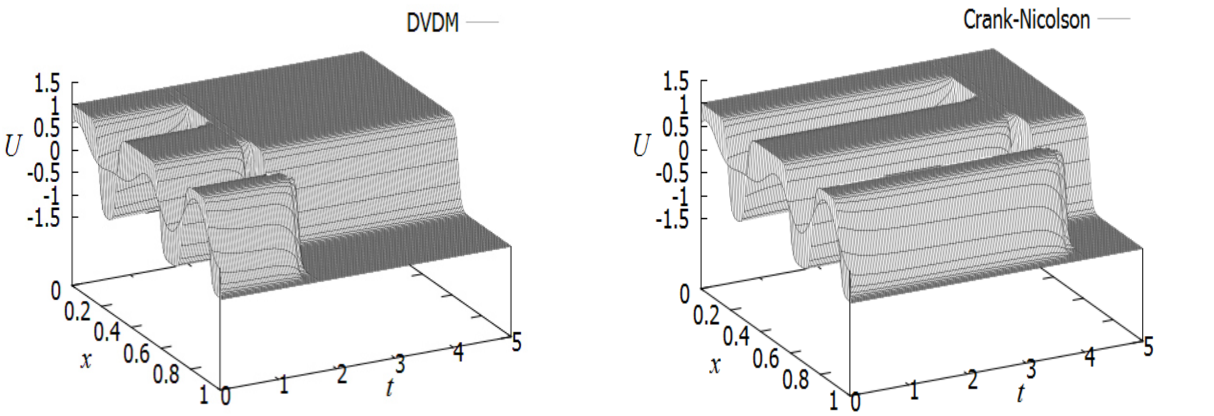

Figure 3.1: Numerical solutions to (3.1) ($\varepsilon = 0.02$) obtained by the proposed scheme and the CN scheme with $\Delta x = 1/100$ and $\Delta t = 1/5000$

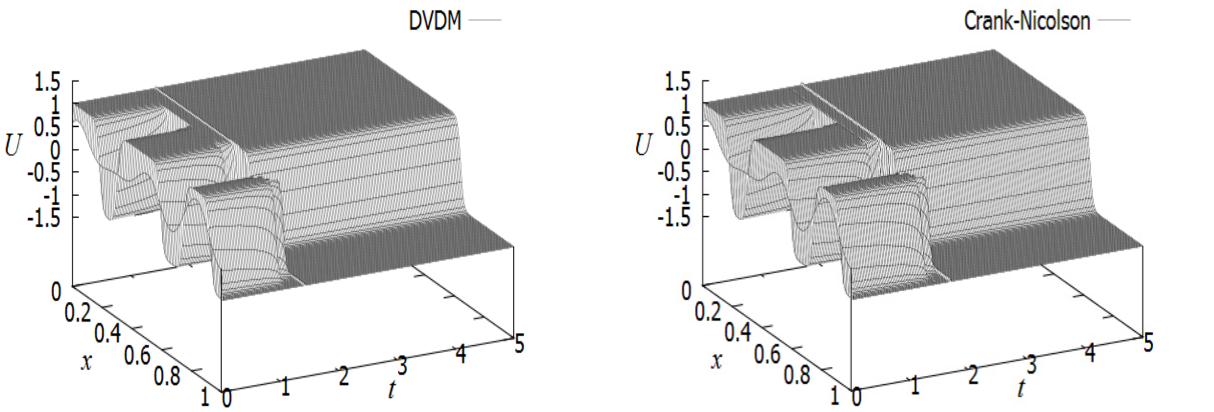

Figure 3.2: Numerical solutions to (3.1) ($\varepsilon = 0.02$) obtained by the proposed scheme and the CN scheme with $\Delta x = 1/200$ and $\Delta t = 1/5000$

• Case 1.

Fig. 3.1 shows numerical results for $\varepsilon = 0.02$ obtained by DVDM and the CN method with $\Delta x = 1/100$ and $\Delta t = 1/5000$. The initial data in Fig. 3.1 is

$$u(x, 0) = 0.26 + 0.07\cos(8\pi x) + 0.41\sin\left(\frac{11}{2}\pi x\right) + 0.24\cos(7\pi x). \tag{3.54}$$

The solution by the proposed scheme arrives at the steady-state around at $t = 1.5$, whereas the one by the CN scheme is stable around at $t = 4$, namely, a little late time. In order to analyze the difference in these results, we refine the space mesh size.

• Case 2.

In Fig. 3.2, we take Δx by half, i.e., $\Delta x = 1/200$. The result of the CN scheme improves. Both solutions arrive at the steady-state around at $t = 1.5$. Furthermore, when we take a smaller space mesh size, both solutions also arrive at the steady-state around at $t = 1.5$. Hence, we expect that the solution by the proposed scheme is more reliable than that by the CN scheme when the space mesh size is coarse.

When we change the initial data into another one, the results are also different from each other. We remark that the direction of the time evolution is reverse to the previous one.

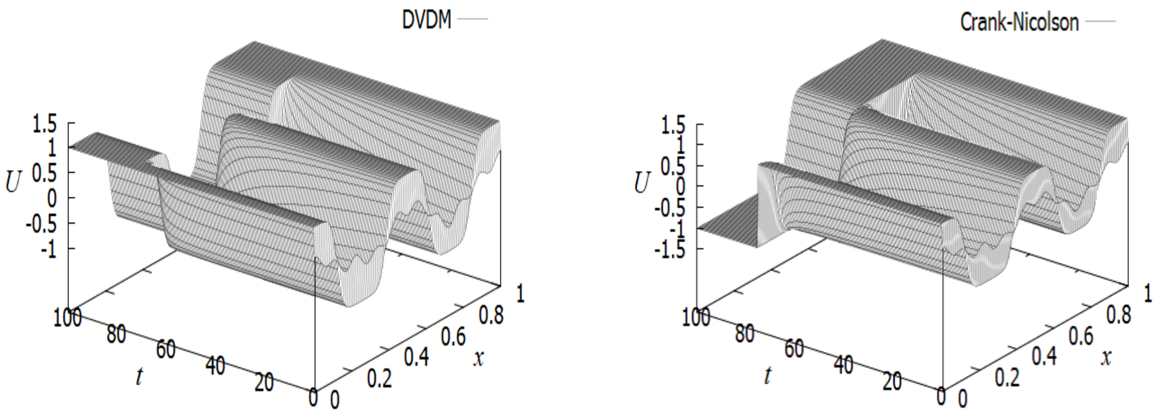

Figure 3.3: Numerical solutions to (3.1) ($\varepsilon = 0.03$) obtained by the proposed scheme and the CN scheme with $\Delta x = 1/100$ and $\Delta t = 1/1000$

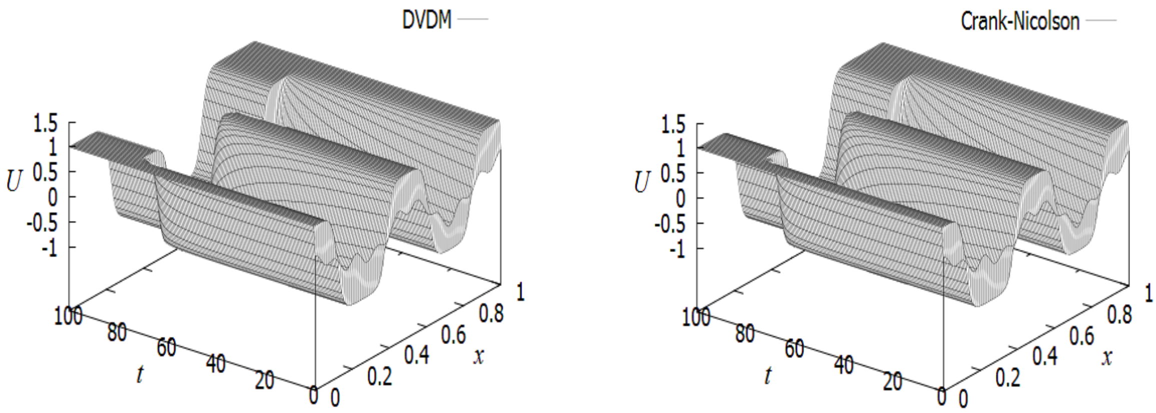

Figure 3.4: Numerical solutions to (3.1) ($\varepsilon = 0.03$) obtained by the proposed scheme and the CN scheme with $\Delta x = 1/100$ and $\Delta t = 1/2000$

• Case 3.

Fig. 3.3 shows numerical results for $\varepsilon = 0.03$ obtained by DVDM and the CN method with $\Delta x = 1/100$ and $\Delta t = 1/1000$. The initial data in Fig. 3.3 is

$$u(x,0) = 0.01 + 0.3\cos(4\pi x) + 0.08\sin\left(\frac{13}{2}\pi x\right)(\cos(4\pi x) - 1) + 0.11\cos(18\pi x). \quad (3.55)$$

Both solutions arrive at the steady-state around at $t = 80$. However, the steady-state of the solution by the CN scheme is different from that by the proposed scheme. As with previous numerical examples, in order to analyze the difference in these results, we refine the time mesh size.

• Case 4.

In Fig. 3.4, we take Δt by half, i.e., $\Delta t = 1/2000$. The result of the CN scheme improves. The steady-state of the solution by the CN scheme coincides with that by the proposed scheme. In addition, when we take a smaller time mesh size, the steady-state of the solution by the CN scheme also coincides with that by the proposed scheme. Therefore, we also expect that the solution by the proposed scheme is more reliable than that by the CN scheme when the time mesh size is coarse.

6.2 Conservative property

Next, we confirm the conservative property. The left figures show the result obtained by the proposed scheme. The right ones show that obtained by the CN scheme.

• Case 1.

Fig. 3.5 shows the following discrepancies:

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

in Fig. 3.1. Theoretically, this value should be conserved. These graphs show that the mass is conserved numerically.

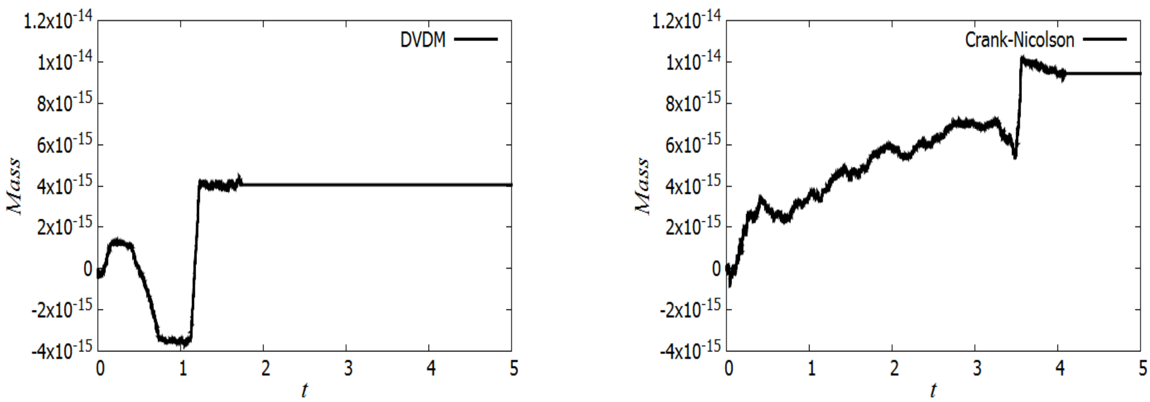

Figure 3.5: The difference between the mass of the numerical solution in Fig. 3.1 and one of the initial data (3.54)

• Case 3.

Fig. 3.6 shows the discrepancies in Fig. 3.3. These graphs also show that the mass is conserved numerically.

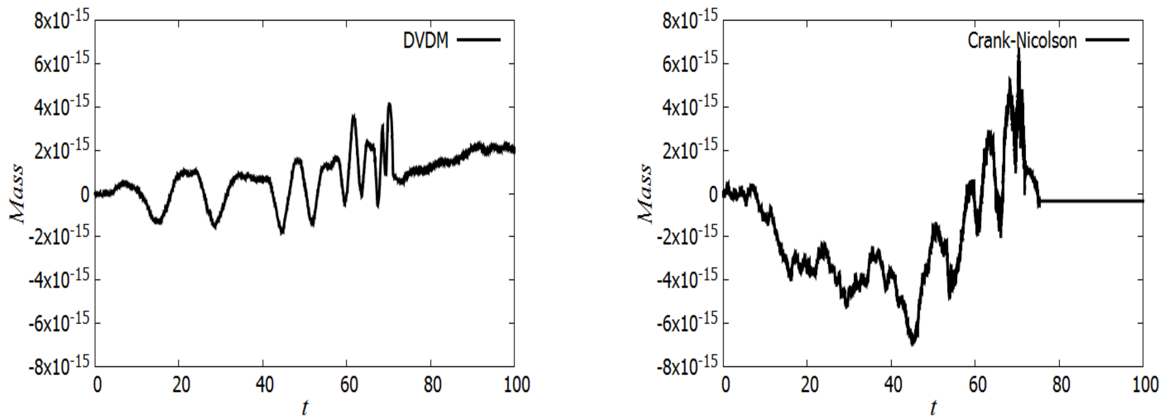

Figure 3.6: The difference between the mass of the numerical solution in Fig. 3.3 and one of the initial data (3.55)

6.3 Dissipative property

Lastly, we confirm the dissipative property of energy. The left figures show the result obtained by the proposed scheme. The right ones show that obtained by the CN scheme.

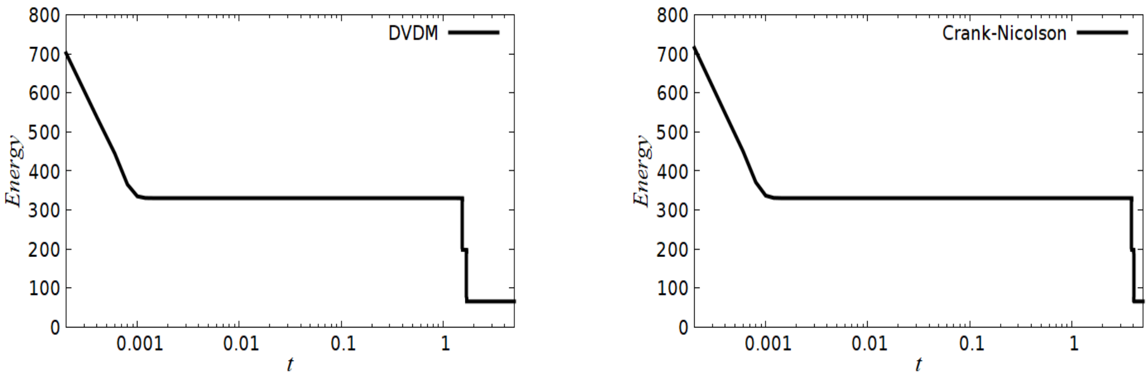

Figure 3.7: The discrete global energy of the numerical solution in Fig. 3.1: The time axis is on the log-scale

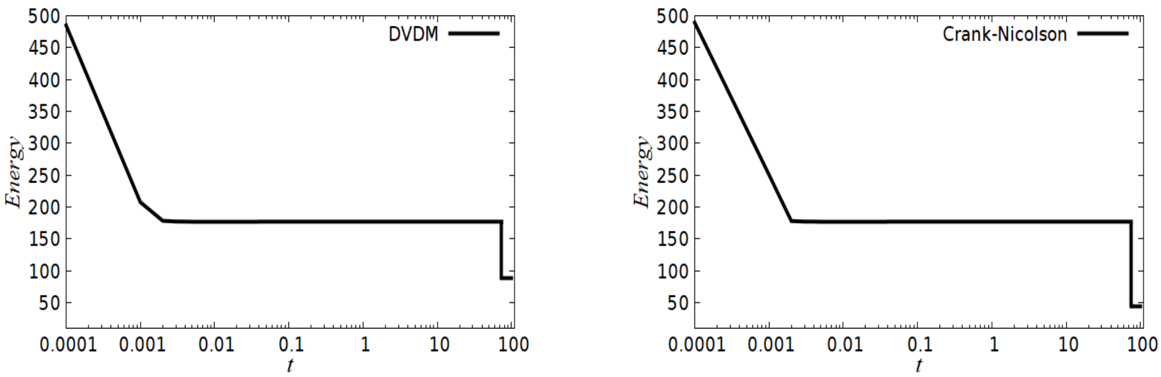

Figure 3.8: The discrete global energy of the numerical solution in Fig. 3.3: The time axis is on the log-scale

• Case 1.

Fig. 3.7 shows the discrete global energies:

$$J_{\mathrm{d}}(\boldsymbol{U}^{(n)}) = \sum_{k=0}^{K}{}'' G_{\mathrm{d},k}(\boldsymbol{U}^{(n)})\Delta x \quad (n = 0, 1, \ldots)$$

in Fig. 3.1. Theoretically, this value should decrease. These graphs show that the decrease in global energy is preserved numerically.

• Case 3.

Fig. 3.8 shows the discrete global energies in Fig. 3.3. In analogy with Case 1, these graphs show that the decrease in global energy is preserved numerically.

From the above, we can obtain the expected results. Additionally, the results of our scheme are better than that of the CN scheme when the mesh size is coarse.

Chapter 4

The Allen–Cahn equation with a dynamic boundary condition

In this chapter, as mentioned in Chapter 1, following the idea of DVDM [29] as understood in Chapter 3, by modifying the discretization of energy from the conventional ones and using the suitable summation-by-parts formula, we propose a structure-preserving finite difference scheme for the Allen–Cahn equation with a dynamic boundary condition. Modifying the conventional manner and using the appropriate summation-by-parts formula, we can use a central difference operator as an approximation of an outward normal derivative on the boundary condition in the scheme. Besides, we show the stability, the existence, and the uniqueness of the solution for the proposed scheme. Also, we give the error estimate for the scheme. Computation examples demonstrate the effectiveness of the proposed scheme. Besides, through computation examples, we confirm that the long-time behavior of the solution under a dynamic boundary condition may differ from the long-time behavior of the solution under the Neumann boundary condition.

§1 Introduction

Let $L > 0$ be the length of the one-dimensional material. In this chapter, we study the following Allen–Cahn equation [1]:

$$\partial_t u = \partial_x^2 u - F'(u) \quad \text{in } (0, L) \times (0, \infty) \tag{4.1}$$

under the following dynamic boundary condition:

$$\partial_t u(0,t) = \partial_x u(x,t)|_{x=0} - F'(u(0,t)) \quad \text{in } (0,\infty), \tag{4.2}$$

$$\partial_t u(L,t) = -\, \partial_x u(x,t)|_{x=L} - F'(u(L,t)) \quad \text{in } (0,\infty). \tag{4.3}$$

The unknown function u: $[0, L] \times [0, \infty) \to \mathbb{R}$ is the order parameter, representing the concentration of one of two components in a binary mixture. Moreover, F: $\mathbb{R} \to \mathbb{R}$ is the potential, and F' is its derivative. For example, F can be a double-well potential, i.e., $F(s) = (1/4)(s^2 - 1)^2$ for all $s \in \mathbb{R}$. In this chapter, we assume that the potential F is in $C^4(\mathbb{R})$ and satisfies the following properties:

$$F'(0) = 0, \quad F(s) \geq \mu s^2 - c \quad \text{for all } s \in \mathbb{R}, \tag{4.4}$$

where μ is a positive constant, and c is a non-negative constant. Let us define the "local energy" G and the "global energy" J, which characterize the equation (4.1) by

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

We remark that the above words "local energy" and "global energy" are ones for space, not for time, and that these "local" and "global" are different from ones of the words "local existence" and "global existence," which appear later. Then, the solution of the equation (4.1) satisfies the following inequality:

$$\frac{d}{dt} \{J(u(t)) + F(u(0,t)) + F(u(L,t))\} \leq 0 \tag{4.5}$$

under the boundary conditions (4.2) and (4.3).

From a mathematical perspective, the above problem (4.1)–(4.3) with an initial value has been studied in [9, 17, 21, 33, 45, 58]. Here, we remark that the original problem was considered in the two-dimensional or three-dimensional case, where the boundary condition (4.2) and (4.3) includes the Laplace–Beltrami operator, which plays the role of diffusion on the boundary. Calatroni and Colli proved the existence and the uniqueness of the solution of the problem (4.1)–(4.3) with an initial value, where the Laplace–Beltrami operator disappears on the boundary [9].

From a numerical point of view, there is a lot of study of a structure-preserving scheme for the Allen–Cahn equation with classical (non-dynamical) boundary conditions, for example, Dirichlet or Neumann boundary conditions (see, for instance, [26,29,37,57]). Also, the results of a structure-preserving scheme for a non-local Allen–Cahn equation with Neumann or periodic boundary conditions can be found in [43, 51, 63, 69]. In [67], Yoshikawa mentioned that the merit of the structure-preserving scheme is that we automatically obtain the stability of numerical solutions. He also mentioned that the advantage of the structure-preserving scheme is that various strategies for the continuous case, such as the energy method, can be applied to the scheme similarly. Actually, Yoshikawa and co-authors applied the energy method to show the existence and the uniqueness of the solution and the error estimate for the scheme (see [28, 65–68]).

Here, we remark that there are few results for the Allen–Cahn equation with dynamic boundary conditions. These conditions are different from the more studied Neumann boundary conditions, and such may give a different long-time behavior of the solution (see Section 6 for an example). In [42], a numerical scheme for semilinear problems with the dynamic boundary condition (4.2) and (4.3) has been considered in a finite element approach, and the error estimate has been obtained. However, there are no results of a structure-preserving scheme for the above problem (4.1)–(4.3) in a finite difference approach to the best of our knowledge. Meanwhile, there are some numerical studies of the Cahn–Hilliard equation with different dynamic boundary conditions (see, for example, [12,13] for the finite element method, [48,49] for the finite volume method, and [28] for the finite difference method). In [28], Fukao, Yoshikawa, and Wada proposed structure-preserving schemes for the Cahn–Hilliard equation with two different dynamic boundary conditions in the one-dimensional case, respectively, based on DVDM. We remark that they use a forward difference operator as an approximation of an outward normal derivative on the discrete boundary condition of the structure-preserving scheme.

The rest of this chapter proceeds as follows. In section 2, we propose a structure-preserving scheme for (4.1)–(4.3), whose solution satisfies the discrete version of the dissipative property (4.5). In section 3, we prove that the solution of the proposed scheme satisfies the global boundedness. In section 4, we prove that the scheme has a unique solution under a specific condition. In section 5, we prove the error estimate for the scheme. In section 6, we show that the computation examples demonstrate the effectiveness of the scheme.

§2 Proposed scheme

In this section, we propose a scheme for (4.1)–(4.3) and show that it has a property corresponding to (4.5).

2.1 Preparation

We define $U_k^{(n)}$ $(k = -1, 0, 1, \ldots, K, K+1, n = 0, 1, \ldots)$ to be the approximation to $u(x,t)$ at location $x = k\Delta x$ and time $t = n\Delta t$, where Δx is a space mesh size, i.e., $\Delta x := L/K$, and Δt is a time mesh size. They are also written in vector as $\boldsymbol{U}^{(n)} := (U_{-1}^{(n)}, U_0^{(n)}, \ldots, U_K^{(n)}, U_{K+1}^{(n)})^\top$ or $\boldsymbol{U}^{(n)} := (U_0^{(n)}, U_1^{(n)}, \ldots, U_{K-1}^{(n)}, U_K^{(n)})^\top$. The superscript (n) is omitted when no confusion occurs. Guess the meaning of $\boldsymbol{U}$ from the context. Let us define two discrete local energies $G_{\mathrm{d},k}^{\pm}$: $\mathbb{R}^{K+3} \to \mathbb{R}^{K+1}$ by

$$
\begin{aligned}
G_{\mathrm{d},k}^{+}(\boldsymbol{U}) &:= \frac{(\delta_k^+ U_k)^2}{2} + F(U_k) \quad (k = 0, \ldots, K), \\
G_{\mathrm{d},k}^{-}(\boldsymbol{U}) &:= \frac{(\delta_k^- U_k)^2}{2} + F(U_k) \quad (k = 0, \ldots, K),
\end{aligned}
$$

for all $\boldsymbol{U} \in \mathbb{R}^{K+3}$. Note that $G_{\mathrm{d},k}^{\pm}(\boldsymbol{U})$ are elements of vectors $G_{\mathrm{d}}^{\pm}(\boldsymbol{U})$, respectively. Furthermore, we define discrete global energy J_{d}: $\mathbb{R}^{K+3} \to \mathbb{R}$ as follows:

$$
J_{\mathrm{d}}(\boldsymbol{U}) := \frac{1}{2}\left\{\sum_{k=0}^{K-1} G_{\mathrm{d},k}^{+}(\boldsymbol{U})\Delta x + \sum_{k=1}^{K} G_{\mathrm{d},k}^{-}(\boldsymbol{U})\Delta x\right\}. \tag{4.6}
$$

From the idea of DVDM [29], we take a discrete variation to derive a structure-preserving scheme for (4.1)–(4.3). That is, we calculate the difference $J_{\mathrm{d}}(\boldsymbol{U}) - J_{\mathrm{d}}(\boldsymbol{V})$ for all $\boldsymbol{U}, \boldsymbol{V} \in \mathbb{R}^{K+3}$. Using Proposition 2.1, we have the following lemma.

Lemma 4.1. The definition (4.6) of J_{d} is rewritten as follows:

$$
J_{\mathrm{d}}(\boldsymbol{U}) = \sum_{k=0}^{K-1} \frac{\left(\delta_k^+ U_k\right)^2}{2}\Delta x + \sum_{k=0}^{K}{}'' F(U_k)\,\Delta x \quad \text{for all } \boldsymbol{U} \in \mathbb{R}^{K+3}.
$$

Proof. It follows from the definitions of $G_{\mathrm{d}}^{\pm}$ and J_{d} and Proposition 2.1 that

$$\begin{aligned}
J_{\mathrm{d}}(\boldsymbol{U}) &= \frac{1}{2}\left[\sum_{k=0}^{K-1}\left\{\frac{\left(\delta_k^{+}U_k\right)^2}{2}+F\left(U_k\right)\right\}\Delta x+\sum_{k=1}^{K}\left\{\frac{\left(\delta_k^{-}U_k\right)^2}{2}+F\left(U_k\right)\right\}\Delta x\right]\\
&= \frac{1}{2}\left\{\sum_{k=0}^{K-1}\frac{\left(\delta_k^{+}U_k\right)^2}{2}\Delta x+\sum_{k=1}^{K}\frac{\left(\delta_k^{-}U_k\right)^2}{2}\Delta x\right\}+\frac{1}{2}\left(\sum_{k=0}^{K-1}F\left(U_k\right)\Delta x+\sum_{k=1}^{K}F\left(U_k\right)\Delta x\right)\\
&= \frac{1}{4}\left\{\sum_{k=0}^{K-1}\left(\delta_k^{+}U_k\right)^2\Delta x+\sum_{k=1}^{K}\left(\delta_k^{+}U_{k-1}\right)^2\Delta x\right\}+\sum_{k=0}^{K}{}''F\left(U_k\right)\Delta x\\
&= \frac{1}{4}\left\{\sum_{k=0}^{K-1}\left(\delta_k^{+}U_k\right)^2\Delta x+\sum_{k=0}^{K-1}\left(\delta_k^{+}U_k\right)^2\Delta x\right\}+\sum_{k=0}^{K}{}''F\left(U_k\right)\Delta x\\
&= \sum_{k=0}^{K-1}\frac{\gamma}{2}\left(\delta_k^{+}U_k\right)^2\Delta x+\sum_{k=0}^{K}{}''F\left(U_k\right)\Delta x \quad \text{for all } \boldsymbol{U}\in\mathbb{R}^{K+3}.
\end{aligned}$$

This completes the proof. □

By using Lemma 4.1 and Corollary 2.1, we have the following lemma.

Lemma 4.2. The following equality holds:

$$\begin{aligned}
J_{\mathrm{d}}(\boldsymbol{U})-J_{\mathrm{d}}(\boldsymbol{V}) &= \sum_{k=0}^{K}{}''\left\{-\delta_k^{\langle 2\rangle}\left(\frac{U_k+V_k}{2}\right)+\frac{dF}{d(U_k,V_k)}\right\}\left(U_k-V_k\right)\Delta x\\
&\quad+\left[\left\{\delta_k^{\langle 1\rangle}\left(\frac{U_k+V_k}{2}\right)\right\}\left(U_k-V_k\right)\right]_0^K \quad \text{for all } \boldsymbol{U},\boldsymbol{V}\in\mathbb{R}^{K+3}. \qquad (4.7)
\end{aligned}$$

Remark 4.1. This equality (4.7) is essential for the discrete dissipation of energy (Theorem 4.1).

Proof. For all $\boldsymbol{U},\boldsymbol{V}\in\mathbb{R}^{K+3}$, by using Corollary 2.1, we have

$$\begin{aligned}
\sum_{k=0}^{K-1}\left\{\frac{(\delta_k^{+}U_k)^2}{2}-\frac{(\delta_k^{+}V_k)^2}{2}\right\}\Delta x &= \sum_{k=0}^{K-1}\left\{\delta_k^{+}\left(\frac{U_k+V_k}{2}\right)\right\}\delta_k^{+}(U_k-V_k)\Delta x\\
&= -\sum_{k=0}^{K-1}\left\{\delta_k^{\langle 2\rangle}\left(\frac{U_k+V_k}{2}\right)\right\}(U_k-V_k)\,\Delta x\\
&\quad+\left[\left\{\delta_k^{\langle 1\rangle}\left(\frac{U_k+V_k}{2}\right)\right\}(U_k-V_k)\right]_0^K.
\end{aligned}$$

Furthermore, it holds from the direct calculation that

$$F(U_k)-F(V_k)=\frac{dF}{d(U_k,V_k)}\left(U_k-V_k\right) \quad (k=0,\dots,K) \qquad (4.8)$$

From the above, we obtain

$$
\begin{aligned}
&J_{\rm d}(\boldsymbol{U}) - J_{\rm d}(\boldsymbol{V}) \\
&= \sum_{k=0}^{K-1} \left\{ \frac{\gamma}{2}(\delta_k^+ U_k)^2 - \frac{\gamma}{2}(\delta_k^+ V_k)^2 \right\} \Delta x + {\sum_{k=0}^{K}}'' \left\{ F(U_k) - F(V_k) \right\} \Delta x \\
&= {\sum_{k=0}^{K}}'' \left\{ -\gamma \delta_k^{\langle 2 \rangle} \left(\frac{U_k + V_k}{2} \right) + \frac{dF}{d(U_k, V_k)} \right\} (U_k - V_k)\, \Delta x + \left[\gamma \left\{ \delta_k^{\langle 1 \rangle} \left(\frac{U_k + V_k}{2} \right) \right\} (U_k - V_k) \right]_0^K .
\end{aligned}
$$

This completes the proof. □

2.2 Proposed scheme

The concrete form of our scheme for (4.1) with (4.2) and (4.3) is, for $n = 0, 1, \ldots,$

$$
\frac{U_k^{(n+1)} - U_k^{(n)}}{\Delta t} = -\frac{\delta G_{\rm d}}{\delta \left(\boldsymbol{U}^{(n+1)}, \boldsymbol{U}^{(n)} \right)_k} \quad (k = 0, \ldots, K), \tag{4.9}
$$

$$
\frac{U_0^{(n+1)} - U_0^{(n)}}{\Delta t} = \delta_k^{\langle 1 \rangle} \left(\frac{U_k^{(n+1)} + U_k^{(n)}}{2} \right) \Bigg|_{k=0} - \frac{dF}{d(U_0^{(n+1)}, U_0^{(n)})}, \tag{4.10}
$$

$$
\frac{U_K^{(n+1)} - U_K^{(n)}}{\Delta t} = -\, \delta_k^{\langle 1 \rangle} \left(\frac{U_k^{(n+1)} + U_k^{(n)}}{2} \right) \Bigg|_{k=K} - \frac{dF}{d(U_K^{(n+1)}, U_K^{(n)})}, \tag{4.11}
$$

where

$$
\frac{\delta G_{\rm d}}{\delta \left(\boldsymbol{U}^{(n+1)}, \boldsymbol{U}^{(n)} \right)_k} = -\delta_k^{\langle 2 \rangle} \left(\frac{U_k^{(n+1)} + U_k^{(n)}}{2} \right) + \frac{dF}{d(U_k^{(n+1)}, U_k^{(n)})} \quad (k = 0, \ldots, K). \tag{4.12}
$$

Then the proposed scheme (4.9)–(4.11) has the following property corresponding to (4.5), i.e.,

Theorem 4.1. The solution to the scheme (4.9)–(4.11) satisfies

$$
\delta_n^+ \left\{ J_{\rm d}(\boldsymbol{U}^{(n)}) + F(U_0^{(n)}) + F(U_K^{(n)}) \right\} \le 0 \quad (n = 0, 1, \ldots). \tag{4.13}
$$

Proof. From Lemma 4.2, we have

$$
\begin{aligned}
\frac{1}{\Delta t} \left\{ J_{\rm d}(\boldsymbol{U}^{(n+1)}) - J_{\rm d}(\boldsymbol{U}^{(n)}) \right\} &= {\sum_{k=0}^{K}}'' \frac{\delta G_{\rm d}}{\delta \left(\boldsymbol{U}^{(n+1)}, \boldsymbol{U}^{(n)} \right)_k} \frac{U_k^{(n+1)} - U_k^{(n)}}{\Delta t} \Delta x \\
&\quad + \left[\left\{ \delta_k^{\langle 1 \rangle} \left(\frac{U_k^{(n+1)} + U_k^{(n)}}{2} \right) \right\} \frac{U_k^{(n+1)} - U_k^{(n)}}{\Delta t} \right]_0^K \quad (n = 0, 1, \ldots).
\end{aligned} \tag{4.14}
$$

Using (4.8), (4.10), and (4.11), we calculate the boundary term on the right-hand side of (4.14) as follows:

$$
\begin{aligned}
&\left[\left\{\delta_k^{\langle 1\rangle}\left(\frac{U_k^{(n+1)}+U_k^{(n)}}{2}\right)\right\}\frac{U_k^{(n+1)}-U_k^{(n)}}{\Delta t}\right]_0^K\\
&=\left\{\delta_k^{\langle 1\rangle}\left(\frac{U_k^{(n+1)}+U_k^{(n)}}{2}\right)\bigg|_{k=K}\right\}\frac{U_K^{(n+1)}-U_K^{(n)}}{\Delta t}-\left\{\delta_k^{\langle 1\rangle}\left(\frac{U_k^{(n+1)}+U_k^{(n)}}{2}\right)\bigg|_{k=0}\right\}\frac{U_0^{(n+1)}-U_0^{(n)}}{\Delta t}\\
&=-(\delta_n^+U_K^{(n)})^2-\frac{dF}{d(U_K^{(n+1)},U_K^{(n)})}\delta_n^+U_K^{(n)}-(\delta_n^+U_0^{(n)})^2-\frac{dF}{d(U_0^{(n+1)},U_0^{(n)})}\delta_n^+U_0^{(n)}\\
&=-(\delta_n^+U_0^{(n)})^2-(\delta_n^+U_K^{(n)})^2-\delta_n^+F(U_0^{(n)})-\delta_n^+F(U_K^{(n)}).
\end{aligned}
\tag{4.15}
$$

Applying (4.9) and (4.15) to (4.14), we obtain

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

Therefore, the inequality (4.13) holds. □

§3 Stability of the proposed scheme

In this section, we show that, if the proposed scheme has a solution, then it satisfies the global boundedness. For the proof of the global boundedness of the numerical solution, we use the following lemma.

Lemma 4.3. The solution to the scheme (4.9)–(4.11) satisfies the following inequality. For $n=0,1,\ldots$, it holds that

$$
\|\boldsymbol{U}^{(n)}\|_{\tilde{H}_{\mathrm{d}}^1}^2+\left|U_0^{(n)}\right|^2+\left|U_K^{(n)}\right|^2\le\frac{1}{\min\left\{\dfrac{1}{2},\mu\right\}}\left\{J_{\mathrm{d}}(\boldsymbol{U}^{(0)})+F(U_0^{(0)})+F(U_K^{(0)})+c(L+2)\right\}.
\tag{4.16}
$$

Proof. From the discrete dissipative property (Theorem 4.1) and the assumption (4.4) for the potential F, we can show

$$
\begin{aligned}
&J_{\mathrm{d}}(\boldsymbol{U}^{(0)})+F(U_0^{(0)})+F(U_K^{(0)})\\
&\ge J_{\mathrm{d}}(\boldsymbol{U}^{(n)})+F(U_0^{(n)})+F(U_K^{(n)})\\
&=\sum_{k=0}^{K-1}\frac{\left|\delta_k^+U_k^{(n)}\right|^2}{2}\Delta x+\sum_{k=0}^{K}{}''F(U_k^{(n)})\Delta x+F(U_0^{(n)})+F(U_K^{(n)})\\
&\ge\frac{1}{2}\sum_{k=0}^{K-1}\left|\delta_k^+U_k^{(n)}\right|^2\Delta x+\sum_{k=0}^{K}{}''\left\{\mu(U_k^{(n)})^2-c\right\}\Delta x+\mu(U_0^{(n)})^2-c+\mu(U_K^{(n)})^2-c\\
&\ge\min\left\{\frac{1}{2},\mu\right\}\left\{\|\boldsymbol{U}^{(n)}\|_{\tilde{H}_{\mathrm{d}}^1}^2+\left|U_0^{(n)}\right|^2+\left|U_K^{(n)}\right|^2\right\}-c(L+2)\quad(n=0,1,\ldots).
\end{aligned}
$$

Therefore, the inequality (4.16) holds. □

Applying Proposition 2.5 (Discrete Sobolev inequality) to (4.16), we can obtain the following global boundedness.

Theorem 4.2 (Global boundedness)**.** The solution of the scheme (4.9) under the discrete boundary conditions (4.10) and (4.11) satisfies the following inequality:

$$\|\boldsymbol{U}^{(n)}\|_{L^\infty_{\mathrm{d}}} \le \tilde{C}_L \left[\frac{1}{\min\left\{\dfrac{1}{2}, \mu\right\}} \left\{ J_{\mathrm{d}}(\boldsymbol{U}^{(0)}) + F(U_0^{(0)}) + F(U_K^{(0)}) + c(L+2) \right\} \right]^{\frac{1}{2}} \quad (n=0,1,\ldots).$$

§4 Existence and uniqueness of the solution to the proposed scheme

In this section, using the energy method in [28, 65–68], we prove that the proposed scheme (4.9)–(4.11) has a unique solution under a specific condition on Δt.

Theorem 4.3 (Local existence and uniqueness)**.** Let

$$R(\rho) := \max\left\{ 5 \max_{|\xi|\le 2\rho} |F''(\xi)|^2, \frac{1}{2} \max_{|\xi|\le 2\rho} |F''(\xi)|^2 + \frac{25}{18}\rho^2 \max_{|\xi|\le 2\rho} |F'''(\xi)|^2 \right\}$$

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

$$(\Delta t)^2 R\left(\tilde{C}_L \sqrt{\|\boldsymbol{U}^{(n)}\|^2_{\tilde{H}^1_{\mathrm{d}}} + \left|U_0^{(n)}\right|^2 + \left|U_K^{(n)}\right|^2} \right) < 1, \tag{4.17}$$

then there exists a unique solution $\{U_k^{(n+1)}\}_{k=-1}^{K+1} \in \mathbb{R}^{K+3}$ satisfying (4.9)–(4.11).

Proof. For any given $\boldsymbol{U}^{(n)} = \{U_k^{(n)}\}_{k=-1}^{K+1} \in \mathbb{R}^{K+3}$, we define the mapping Ψ: $\{U_k\}_{k=0}^{K} \mapsto \{\tilde{U}_k\}_{k=-1}^{K+1}$ by

$$\frac{\tilde{U}_k - U_k^{(n)}}{\Delta t} = \delta_k^{\langle 2\rangle}\left(\frac{\tilde{U}_k + U_k^{(n)}}{2}\right) - \frac{dF}{d(U_k, U_k^{(n)})} \quad (k = 0, \ldots, K), \tag{4.18}$$

$$\frac{\tilde{U}_0 - U_0^{(n)}}{\Delta t} = \delta_k^{\langle 1\rangle}\left(\frac{\tilde{U}_k + U_k^{(n)}}{2}\right)\Bigg|_{k=0} - \frac{dF}{d(U_0, U_0^{(n)})}, \tag{4.19}$$

$$\frac{\tilde{U}_K - U_K^{(n)}}{\Delta t} = -\,\delta_k^{\langle 1\rangle}\left(\frac{\tilde{U}_k + U_k^{(n)}}{2}\right)\Bigg|_{k=K} - \frac{dF}{d(U_K, U_K^{(n)})}. \tag{4.20}$$

Firstly, we show that the mapping Ψ is well-defined. Let $\alpha := \Delta t/(4\Delta x)$ and $\beta := \Delta t/(2(\Delta x)^2)$. For the purpose, we give the following matrix expression of Ψ:

$$A\tilde{\boldsymbol{U}} = f(\boldsymbol{U}, \boldsymbol{U}^{(n)}). \tag{4.21}$$

Here the $(K+3)\times(K+3)$ matrix A is defined by

$$A := \begin{pmatrix} \alpha & 1 & -\alpha & & & & \\ -\beta & 1+2\beta & -\beta & & & & \\ & -\beta & 1+2\beta & -\beta & & & \\ & & \ddots & \ddots & \ddots & & \\ & & & -\beta & 1+2\beta & -\beta & \\ & & & & -\beta & 1+2\beta & -\beta \\ & & & & -\alpha & 1 & \alpha \end{pmatrix}.$$

If the matrix A is nonsingular, then the mapping Ψ is well-defined. We show that A is nonsingular. We calculate the determinant of A as follows:

$$\det A = \begin{vmatrix} \alpha & 1 & -\alpha & & & & \\ -\beta & 1+2\beta & -\beta & & & & \\ & -\beta & 1+2\beta & -\beta & & & \\ & & \ddots & \ddots & \ddots & & \\ & & & -\beta & 1+2\beta & -\beta & \\ & & & & -\beta & 1+2\beta & -\beta \\ & & & & -\alpha & 1 & \alpha \end{vmatrix}$$

$$= \begin{vmatrix} \alpha & 1 & 0 & & & & \\ -\beta & 1+2\beta & -2\beta & & & & \\ & -\beta & 1+2\beta & -\beta & & & \\ & & \ddots & \ddots & \ddots & & \\ & & & -\beta & 1+2\beta & -\beta & \\ & & & & -\beta & 1+2\beta & -\beta \\ & & & & -\alpha & 1 & \alpha \end{vmatrix} \quad \text{(adding the first column to the third column)}$$

$$= \begin{vmatrix} \alpha & 0 & 0 & & & & \\ -\beta & 1+\left(2+\frac{1}{\alpha}\right)\beta & -2\beta & & & & \\ & -\beta & 1+2\beta & -\beta & & & \\ & & \ddots & \ddots & \ddots & & \\ & & & -\beta & 1+2\beta & -\beta & \\ & & & & -\beta & 1+2\beta & -\beta \\ & & & & -\alpha & 1 & \alpha \end{vmatrix} \quad \text{(adding to the second column } -(1/\alpha) \text{ times the first column)}$$

$$= \alpha \begin{vmatrix} 1+\left(2+\frac{1}{\alpha}\right)\beta & -2\beta & & & & \\ -\beta & 1+2\beta & -\beta & & & \\ & \ddots & \ddots & \ddots & & \\ & & -\beta & 1+2\beta & -\beta & \\ & & & -\beta & 1+2\beta & -\beta \\ & & & -\alpha & 1 & \alpha \end{vmatrix} \quad \text{(expanding by the first row)}$$

$$= \alpha \begin{vmatrix} 1+\left(2+\frac{1}{\alpha}\right)\beta & -2\beta & & & & \\ -\beta & 1+2\beta & -\beta & & & \\ & \ddots & \ddots & \ddots & & \\ & & -\beta & 1+2\beta & -\beta & \\ & & & -2\beta & 1+2\beta & -\beta \\ & & & 0 & 1 & \alpha \end{vmatrix} \quad \text{(adding the } (K+2)\text{th column to the } K\text{th column)}$$

$$
=\alpha\begin{vmatrix}
1+\left(2+\frac{1}{\alpha}\right)\beta & -2\beta & & & & & \\
-\beta & 1+2\beta & -\beta & & & & \\
& \ddots & \ddots & \ddots & & & \\
& & -\beta & 1+2\beta & & -\beta & \\
& & & -2\beta & 1+\left(2+\frac{1}{\alpha}\right)\beta & -\beta & \\
& & & 0 & 0 & \alpha &
\end{vmatrix}
$$

(adding to the $(K+1)$th column $-(1/\alpha)$ times the $(K+2)$th column)

$$
=\alpha^2\begin{vmatrix}
1+\left(2+\frac{1}{\alpha}\right)\beta & -2\beta & & & \\
-\beta & 1+2\beta & -\beta & & \\
& \ddots & \ddots & \ddots & \\
& & -\beta & 1+2\beta & -\beta \\
& & & -2\beta & 1+\left(2+\frac{1}{\alpha}\right)\beta
\end{vmatrix}
$$

(expanding by the $(K+2)$th row).

Here, we define $(K+1)\times(K+1)$ matrix B by

$$
B := \begin{pmatrix}
1+\left(2+\frac{1}{\alpha}\right)\beta & -2\beta & & & & & \\
-\beta & 1+2\beta & -\beta & & & & \\
& -\beta & 1+2\beta & -\beta & & & \\
& & \ddots & \ddots & \ddots & & \\
& & & -\beta & 1+2\beta & -\beta & \\
& & & & -\beta & 1+2\beta & -\beta \\
& & & & & -2\beta & 1+\left(2+\frac{1}{\alpha}\right)\beta
\end{pmatrix}.
$$

Namely, $\det A = \alpha^2 \det B$. Since α and β is positive, we have

$$
\left|1+\left(2+\frac{1}{\alpha}\right)\beta\right| > |-2\beta|, \quad |1+2\beta| > |-\beta| + |-\beta|.
$$

Hence, B is a strictly diagonally dominant matrix. Since a strictly diagonally dominant matrix is nonsingular, B is nonsingular, i.e., $\det B \neq 0$. Therefore, we obtain

$$
\det A = \alpha^2 \det B \neq 0.
$$

That is, A is nonsingular.

Next, we prove the existence and uniqueness of the solution to the proposed scheme by the fixed-point theorem for a contraction mapping. From the definition of Ψ (4.19) and (4.20), $\tilde{U}_{-1}$ and $\tilde{U}_{K+1}$ can be explicitly written as

$$
\tilde{U}_{-1} = -U_{-1}^{(n)} + \tilde{U}_1 + U_1^{(n)} - \frac{4\Delta x}{\Delta t}(\tilde{U}_0 - U_0^{(n)}) - 4\Delta x \frac{dF}{d(\tilde{U}_0, U_0^{(n)})},
$$

$$
\tilde{U}_{K+1} = \tilde{U}_{K-1} + U_{K-1}^{(n)} - U_{K+1}^{(n)} - \frac{4\Delta x}{\Delta t}(\tilde{U}_K - U_K^{(n)}) - 4\Delta x \frac{dF}{d(\tilde{U}_K, U_K^{(n)})}.
$$

Hence, it is sufficient to show the existence of a $(K+1)$-dimensional vector $\boldsymbol{U}$ that satisfies $\tilde{U}_k = U_k$ $(k = 0, \ldots, K)$. Here, we define the mapping Φ: $\mathbb{R}^{K+1} \to \mathbb{R}^{K+1}$ by

$$\Phi(\boldsymbol{U}) := \{\tilde{U}_k\}_{k=0}^{K} = \{\Psi_k(\boldsymbol{U})\}_{k=0}^{K} \quad \text{for all } \boldsymbol{U} \in \mathbb{R}^{K+1},$$

where $\Psi_k(\boldsymbol{U})$ is the kth element of $\Psi(\boldsymbol{U})$. Also, let $X := \{\boldsymbol{f} \in \mathbb{R}^{K+1}; \|\boldsymbol{f}\|_X^2 \leq 4M^2\}$, where $M := \|\boldsymbol{U}^{(n)}\|_X$ and $\|\boldsymbol{f}\|_X := \sqrt{\|\boldsymbol{f}\|_{\tilde{H}_{\mathrm{d}}^1}^2 + |f_0|^2 + |f_K|^2}$ for all $\boldsymbol{f} \in \mathbb{R}^{K+1}$. We show that the mapping Φ is a contraction mapping on X. If Φ is a contraction mapping, Φ has a unique fixed-point $\boldsymbol{V}^*$ in the closed ball X from the fixed-point theorem for a contraction mapping. This $\boldsymbol{V}^*$ is the solution $\boldsymbol{U}^{(n+1)}$ to the scheme (4.9)–(4.11). Firstly, we show $\Phi(X) \subset X$. For any fixed $\boldsymbol{U} \in X$, we have

$$
\begin{aligned}
&\frac{1}{2\Delta t}\left(\left\|\tilde{\boldsymbol{U}}\right\|_{L_{\mathrm{d}}^2}^2 - \left\|\boldsymbol{U}^{(n)}\right\|_{L_{\mathrm{d}}^2}^2\right) = \sum_{k=0}^{K}{}'' \frac{\tilde{U}_k - U_k^{(n)}}{\Delta t}\frac{\tilde{U}_k + U_k^{(n)}}{2}\Delta x \\
&= \sum_{k=0}^{K}{}'' \left\{\delta_k^{\langle 2\rangle}\left(\frac{\tilde{U}_k + U_k^{(n)}}{2}\right)\right\}\frac{\tilde{U}_k + U_k^{(n)}}{2}\Delta x - \sum_{k=0}^{K}{}'' \frac{dF}{d(U_k, U_k^{(n)})}\frac{\tilde{U}_k + U_k^{(n)}}{2}\Delta x \\
&= -\left\|D\left(\frac{\tilde{\boldsymbol{U}}+\boldsymbol{U}^{(n)}}{2}\right)\right\|^2 + \left[\left\{\delta_k^{\langle 1\rangle}\left(\frac{\tilde{U}_k+U_k^{(n)}}{2}\right)\right\}\frac{\tilde{U}_k+U_k^{(n)}}{2}\right]_0^K - \sum_{k=0}^{K}{}'' \frac{dF}{d(U_k, U_k^{(n)})}\frac{\tilde{U}_k+U_k^{(n)}}{2}\Delta x \\
&\leq -\frac{|\tilde{U}_K|^2 - \left|U_K^{(n)}\right|^2}{2\Delta t} - \frac{dF}{d(U_K, U_K^{(n)})}\frac{\tilde{U}_K+U_K^{(n)}}{2} - \frac{|\tilde{U}_0|^2 - \left|U_0^{(n)}\right|^2}{2\Delta t} - \frac{dF}{d(U_0, U_0^{(n)})}\frac{\tilde{U}_0+U_0^{(n)}}{2} \\
&\quad - \sum_{k=0}^{K}{}'' \frac{dF}{d(U_k, U_k^{(n)})}\frac{\tilde{U}_k + U_k^{(n)}}{2}\Delta x
\end{aligned}
$$

from Corollary 2.1 (Summation by parts formula), (4.18)–(4.20). Moreover, using the Young inequality: $ab \leq (\varepsilon/2)a^2 + (1/(2\varepsilon))b^2$ and the following inequality: $(a+b)^2 \leq 2(a^2+b^2)$, we obtain

$$
\begin{aligned}
&\frac{1}{2\Delta t}\left(\left\|\tilde{\boldsymbol{U}}\right\|_{L_{\mathrm{d}}^2}^2 - \left\|\boldsymbol{U}^{(n)}\right\|_{L_{\mathrm{d}}^2}^2\right) \\
&\leq -\frac{|\tilde{U}_0|^2 - \left|U_0^{(n)}\right|^2}{2\Delta t} - \frac{|\tilde{U}_K|^2 - \left|U_K^{(n)}\right|^2}{2\Delta t} + \sum_{k=0}^{K}{}'' \left\{\frac{\Delta t}{2}\left|\frac{dF}{d(U_k, U_k^{(n)})}\right|^2 + \frac{1}{2\Delta t}\left|\frac{\tilde{U}_k+U_k^{(n)}}{2}\right|^2\right\}\Delta x \\
&\quad + \frac{\Delta t}{2}\left|\frac{dF}{d(U_0, U_0^{(n)})}\right|^2 + \frac{1}{2\Delta t}\left|\frac{\tilde{U}_0+U_0^{(n)}}{2}\right|^2 + \frac{\Delta t}{2}\left|\frac{dF}{d(U_K, U_K^{(n)})}\right|^2 + \frac{1}{2\Delta t}\left|\frac{\tilde{U}_K+U_K^{(n)}}{2}\right|^2 \\
&\leq -\frac{|\tilde{U}_0|^2 - \left|U_0^{(n)}\right|^2}{2\Delta t} - \frac{|\tilde{U}_K|^2 - \left|U_K^{(n)}\right|^2}{2\Delta t} + \frac{|\tilde{U}_0|^2 + \left|U_0^{(n)}\right|^2}{4\Delta t} + \frac{|\tilde{U}_K|^2 + \left|U_K^{(n)}\right|^2}{4\Delta t} \\
&\quad + \frac{\left\|\tilde{\boldsymbol{U}}\right\|_{L_{\mathrm{d}}^2}^2 + \left\|\boldsymbol{U}^{(n)}\right\|_{L_{\mathrm{d}}^2}^2}{4\Delta t} + \frac{\Delta t}{2}\left\{\left\|\frac{dF}{d(\boldsymbol{U}, \boldsymbol{U}^{(n)})}\right\|_{L_{\mathrm{d}}^2}^2 + \left|\frac{dF}{d(U_0, U_0^{(n)})}\right|^2 + \left|\frac{dF}{d(U_K, U_K^{(n)})}\right|^2\right\}
\end{aligned}
$$

$$= -\frac{1}{4\Delta t}\left(|\tilde{U}_0|^2 + |\tilde{U}_K|^2\right) + \frac{3}{4\Delta t}\left\{\left|U_0^{(n)}\right|^2 + \left|U_K^{(n)}\right|^2\right\} + \frac{1}{4\Delta t}\left\|\tilde{\boldsymbol{U}}\right\|_{L_{\mathrm{d}}^2}^2 + \frac{1}{4\Delta t}\left\|\boldsymbol{U}^{(n)}\right\|_{L_{\mathrm{d}}^2}^2$$
$$+ \frac{\Delta t}{2}\left\{\left\|\frac{dF}{d(\boldsymbol{U},\boldsymbol{U}^{(n)})}\right\|_{L_{\mathrm{d}}^2}^2 + \left|\frac{dF}{d(U_0,U_0^{(n)})}\right|^2 + \left|\frac{dF}{d(U_K,U_K^{(n)})}\right|^2\right\}. \tag{4.22}$$

Therefore, multiplying both sides of (4.22) by $4\Delta t$, we get

$$\left\|\tilde{\boldsymbol{U}}\right\|_{L_{\mathrm{d}}^2}^2 + |\tilde{U}_0|^2 + |\tilde{U}_K|^2 \le 3\left\{\left\|\boldsymbol{U}^{(n)}\right\|_{L_{\mathrm{d}}^2}^2 + \left|U_0^{(n)}\right|^2 + \left|U_K^{(n)}\right|^2\right\}$$
$$+ 2(\Delta t)^2\left\{\left\|\frac{dF}{d(\boldsymbol{U},\boldsymbol{U}^{(n)})}\right\|_{L_{\mathrm{d}}^2}^2 + \left|\frac{dF}{d(U_0,U_0^{(n)})}\right|^2 + \left|\frac{dF}{d(U_K,U_K^{(n)})}\right|^2\right\}. \tag{4.23}$$

Next, using Corollary 2.1 (Summation by parts formula), we have

$$\frac{1}{2\Delta t}\left(\left\|D\tilde{\boldsymbol{U}}\right\|^2 - \left\|D\boldsymbol{U}^{(n)}\right\|^2\right) = \sum_{k=0}^{K-1}\left\{\delta_k^+\left(\frac{\tilde{U}_k + U_k^{(n)}}{2}\right)\right\}\left\{\delta_k^+\left(\frac{\tilde{U}_k - U_k^{(n)}}{\Delta t}\right)\right\}\Delta x$$
$$= -\sum_{k=0}^{K}{}''\left\{\delta_k^{\langle 2\rangle}\left(\frac{\tilde{U}_k + U_k^{(n)}}{2}\right)\right\}\frac{\tilde{U}_k - U_k^{(n)}}{\Delta t}\Delta x + \left[\left\{\delta_k^{\langle 1\rangle}\left(\frac{\tilde{U}_k + U_k^{(n)}}{2}\right)\right\}\frac{\tilde{U}_k - U_k^{(n)}}{\Delta t}\right]_0^K. \tag{4.24}$$

From (4.18), Corollary 2.1 (Summation by parts formula), the Young inequality, and the following inequality: $(a+b)^2 \le 2(a^2+b^2)$, we estimate the first term on the right-hand side of (4.24) as follows:

$$-\sum_{k=0}^{K}{}''\left\{\delta_k^{\langle 2\rangle}\left(\frac{\tilde{U}_k + U_k^{(n)}}{2}\right)\right\}\frac{\tilde{U}_k - U_k^{(n)}}{\Delta t}\Delta x$$
$$= -\sum_{k=0}^{K}{}''\left\{\delta_k^{\langle 2\rangle}\left(\frac{\tilde{U}_k + U_k^{(n)}}{2}\right)\right\}^2\Delta x + \sum_{k=0}^{K}{}''\left\{\delta_k^{\langle 2\rangle}\left(\frac{\tilde{U}_k + U_k^{(n)}}{2}\right)\right\}\frac{dF}{d(U_k,U_k^{(n)})}\Delta x$$
$$\le -\sum_{k=0}^{K-1}\left\{\delta_k^+\left(\frac{\tilde{U}_k + U_k^{(n)}}{2}\right)\right\}\left\{\delta_k^+\left(\frac{dF}{d(U_k,U_k^{(n)})}\right)\right\}\Delta x + \left[\left\{\delta_k^{\langle 1\rangle}\left(\frac{\tilde{U}_k + U_k^{(n)}}{2}\right)\right\}\frac{dF}{d(U_k,U_k^{(n)})}\right]_0^K$$
$$\le \sum_{k=0}^{K-1}\left[\frac{1}{2\Delta t}\left\{\delta_k^+\left(\frac{\tilde{U}_k + U_k^{(n)}}{2}\right)\right\}^2 + \frac{\Delta t}{2}\left\{\delta_k^+\left(\frac{dF}{d(U_k,U_k^{(n)})}\right)\right\}^2\right]\Delta x$$
$$+ \left[\left\{\delta_k^{\langle 1\rangle}\left(\frac{\tilde{U}_k + U_k^{(n)}}{2}\right)\right\}\frac{dF}{d(U_k,U_k^{(n)})}\right]_0^K$$
$$\le \frac{\left\|D\tilde{\boldsymbol{U}}\right\|^2 + \left\|D\boldsymbol{U}^{(n)}\right\|^2}{4\Delta t} + \frac{\Delta t}{2}\left\|D\left(\frac{dF}{d(\boldsymbol{U},\boldsymbol{U}^{(n)})}\right)\right\|^2 + \left[\left\{\delta_k^{\langle 1\rangle}\left(\frac{\tilde{U}_k + U_k^{(n)}}{2}\right)\right\}\frac{dF}{d(U_k,U_k^{(n)})}\right]_0^K.$$

Hence, we obtain

$$\frac{1}{2\Delta t}\left(\left\|D\tilde{\boldsymbol{U}}\right\|^2-\|D\boldsymbol{U}^{(n)}\|^2\right) \le \frac{1}{4\Delta t}\left(\left\|D\tilde{\boldsymbol{U}}\right\|^2+\|D\boldsymbol{U}^{(n)}\|^2\right)+\frac{\Delta t}{2}\left\|D\left(\frac{dF}{d(\boldsymbol{U},\boldsymbol{U}^{(n)})}\right)\right\|^2$$
$$+\left[\left\{\delta_k^{\langle 1\rangle}\left(\frac{\tilde{U}_k+U_k^{(n)}}{2}\right)\right\}\left(\frac{\tilde{U}_k-U_k^{(n)}}{\Delta t}+\frac{dF}{d(U_k,U_k^{(n)})}\right)\right]_0^K.$$

Furthermore, we see from (4.19) and (4.20) that

$$\left[\left\{\delta_k^{\langle 1\rangle}\left(\frac{\tilde{U}_k+U_k^{(n)}}{2}\right)\right\}\left(\frac{\tilde{U}_k-U_k^{(n)}}{\Delta t}+\frac{dF}{d(U_k,U_k^{(n)})}\right)\right]_0^K$$
$$=-\left\{\delta_k^{\langle 1\rangle}\left(\frac{\tilde{U}_k+U_k^{(n)}}{2}\right)\Bigg|_{k=K}\right\}^2-\left\{\delta_k^{\langle 1\rangle}\left(\frac{\tilde{U}_k+U_k^{(n)}}{2}\right)\Bigg|_{k=0}\right\}^2\le 0.$$

Namely, we have

$$\left\|D\tilde{\boldsymbol{U}}\right\|^2 \le 3\left\|D\boldsymbol{U}^{(n)}\right\|^2+2(\Delta t)^2\left\|D\left(\frac{dF}{d(\boldsymbol{U},\boldsymbol{U}^{(n)})}\right)\right\|^2. \tag{4.25}$$

Combining (4.23) and (4.25), we obtain

$$\left\|\tilde{\boldsymbol{U}}\right\|_X^2 \le 3\left\|\boldsymbol{U}^{(n)}\right\|_X^2+2(\Delta t)^2\left\|\frac{dF}{d(\boldsymbol{U},\boldsymbol{U}^{(n)})}\right\|_X^2. \tag{4.26}$$

All that is left to show that the right-hand side of (4.26) is no more than $4M^2$. Using Lemma 2.2 and the assumption (4.4) for F, we get the following equality:

$$\frac{dF}{d(U_k,U_k^{(n)})}=\frac{dF}{d(U_k,U_k^{(n)})}-\frac{dF}{d(0,0)}=\frac{1}{2}\bar{F}''(U_k,0;U_k^{(n)},0)U_k+\frac{1}{2}\bar{F}''(U_k^{(n)},0;U_k,0)U_k^{(n)}$$

for $k=0,\dots,K$. Moreover, from Proposition 2.5 and definitions of X and M, the following inequalities hold:

$$\left\|\boldsymbol{U}^{(n)}\right\|_{L^\infty_{\mathrm{d}}}\le \tilde{C}_L\left\|\boldsymbol{U}^{(n)}\right\|_{\tilde{H}^1_{\mathrm{d}}}\le \tilde{C}_L M,\quad \|\boldsymbol{U}\|_{L^\infty_{\mathrm{d}}}\le \tilde{C}_L\|\boldsymbol{U}\|_{\tilde{H}^1_{\mathrm{d}}}\le 2\tilde{C}_L M.$$

Hence, from Lemma 2.1, we have

$$\left|\bar{F}''(U_k,0;U_k^{(n)},0)\right|\le \max_{|\xi|\le 2\tilde{C}_L M}|F''(\xi)|\quad (k=0,\dots,K),$$
$$\left|\bar{F}''(U_k^{(n)},0;U_k,0)\right|\le \max_{|\xi|\le 2\tilde{C}_L M}|F''(\xi)|\quad (k=0,\dots,K).$$

Therefore, we obtain

$$\left|\frac{dF}{d(U_k,U_k^{(n)})}\right|^2\le 2\left\{\frac{1}{4}\left|\bar{F}''(U_k,0;U_k^{(n)},0)\right|^2|U_k|^2+\frac{1}{4}\left|\bar{F}''(U_k^{(n)},0;U_k,0)\right|^2\left|U_k^{(n)}\right|^2\right\}$$
$$\le\frac{1}{2}\max_{|\xi|\le 2\tilde{C}_L M}|F''(\xi)|^2\left\{|U_k|^2+\left|U_k^{(n)}\right|^2\right\}\quad (k=0,\dots,K). \tag{4.27}$$

Thus, the following inequality holds:

$$\left\|\frac{dF}{d(\boldsymbol{U},\boldsymbol{U}^{(n)})}\right\|_{L^2_{\mathrm{d}}}^2=\sum_{k=0}^{K}{}''\left|\frac{dF}{d(U_k,U_k^{(n)})}\right|^2\Delta x\le\frac{1}{2}\max_{|\xi|\le 2\tilde{C}_LM}|F''(\xi)|^2\left(\|\boldsymbol{U}\|_{L^2_{\mathrm{d}}}^2+\left\|\boldsymbol{U}^{(n)}\right\|_{L^2_{\mathrm{d}}}^2\right).\tag{4.28}$$

From Lemma 2.2, we also have

$$\delta_k^+\left(\frac{dF}{d(U_k,U_k^{(n)})}\right)=\frac{1}{2}\bar{F}''(U_{k+1},U_k;U_{k+1}^{(n)},U_k^{(n)})\delta_k^+U_k+\frac{1}{2}\bar{F}''(U_{k+1}^{(n)},U_k^{(n)};U_{k+1},U_k)\delta_k^+U_k^{(n)}$$

for $k=0,\ldots,K-1$. Hence, it follows from the same argument as (4.27) and (4.28) that

$$\left\|D\left(\frac{dF}{d(\boldsymbol{U},\boldsymbol{U}^{(n)})}\right)\right\|^2\le\frac{1}{2}\max_{|\xi|\le 2\tilde{C}_LM}|F''(\xi)|^2\left(\|D\boldsymbol{U}\|^2+\left\|D\boldsymbol{U}^{(n)}\right\|^2\right).\tag{4.29}$$

Therefore, using (4.27)–(4.29), we obtain the following estimate:

$$\left\|\frac{dF}{d(\boldsymbol{U},\boldsymbol{U}^{(n)})}\right\|_X^2\le\frac{1}{2}\max_{|\xi|\le 2\tilde{C}_LM}|F''(\xi)|^2\left\{\|\boldsymbol{U}\|_X^2+\left\|\boldsymbol{U}^{(n)}\right\|_X^2\right\}\le\frac{5}{2}\max_{|\xi|\le 2\tilde{C}_LM}|F''(\xi)|^2M^2.\tag{4.30}$$

Thus, from (4.26), (4.30), and the assumption (4.17), we conclude that

$$\left\|\tilde{\boldsymbol{U}}\right\|_X^2\le 3M^2+5(\Delta t)^2\max_{|\xi|\le 2\tilde{C}_LM}|F''(\xi)|^2M^2\le\left\{3+(\Delta t)^2R\left(\tilde{C}_LM\right)\right\}M^2\le 4M^2.$$

Namely, it holds that $\Phi(\boldsymbol{U})=\{\tilde{U}_k\}_{k=0}^K\in X$.

Next, we show that Φ is contractive. For any fixed $\boldsymbol{U}_1,\boldsymbol{U}_2\in X$, the vector $\{\tilde{U}_{i,k}\}_{k=-1}^{K+1}=\{\Psi_k(\boldsymbol{U}_i)\}_{k=-1}^{K+1}$ satisfies (4.18)–(4.20) ($i=1,2$) from the definition of Ψ. Subtracting these relations, we obtain

$$\frac{\tilde{U}_{1,k}-\tilde{U}_{2,k}}{\Delta t}=\delta_k^{\langle 2\rangle}\left(\frac{\tilde{U}_{1,k}-\tilde{U}_{2,k}}{2}\right)-\left(\frac{dF}{d(U_{1,k},U_k^{(n)})}-\frac{dF}{d(U_{2,k},U_k^{(n)})}\right)\quad(k=0,\ldots,K),\tag{4.31}$$

$$\frac{\tilde{U}_{1,0}-\tilde{U}_{2,0}}{\Delta t}=\delta_k^{\langle 1\rangle}\left(\frac{\tilde{U}_{1,k}-\tilde{U}_{2,k}}{2}\right)\Bigg|_{k=0}-\left(\frac{dF}{d(U_{1,0},U_0^{(n)})}-\frac{dF}{d(U_{2,0},U_0^{(n)})}\right),\tag{4.32}$$

$$\frac{\tilde{U}_{1,K}-\tilde{U}_{2,K}}{\Delta t}=-\delta_k^{\langle 1\rangle}\left(\frac{\tilde{U}_{1,k}-\tilde{U}_{2,k}}{2}\right)\Bigg|_{k=K}-\left(\frac{dF}{d(U_{1,K},U_K^{(n)})}-\frac{dF}{d(U_{2,K},U_K^{(n)})}\right).\tag{4.33}$$

From (4.31), we have

$$\begin{aligned}\frac{1}{\Delta t}\left\|\tilde{\boldsymbol{U}}_1-\tilde{\boldsymbol{U}}_2\right\|_{L^2_{\mathrm{d}}}^2&=\frac{1}{2}\sum_{k=0}^{K}{}''\left\{\delta_k^{\langle 2\rangle}\left(\tilde{U}_{1,k}-\tilde{U}_{2,k}\right)\right\}(\tilde{U}_{1,k}-\tilde{U}_{2,k})\Delta x\\&\quad-\sum_{k=0}^{K}{}''\left(\frac{dF}{d(U_{1,k},U_k^{(n)})}-\frac{dF}{d(U_{2,k},U_k^{(n)})}\right)(\tilde{U}_{1,k}-\tilde{U}_{2,k})\Delta x.\end{aligned}\tag{4.34}$$

Using Corollary 2.1 (Summation by parts formula), (4.32), and (4.33), we estimate the first term on the right-hand side of (4.34) as follows:

$$
\begin{aligned}
&\frac{1}{2}\sum_{k=0}^{K}{}'' \left\{\delta_k^{\langle 2\rangle}\Big(\tilde{U}_{1,k}-\tilde{U}_{2,k}\Big)\right\}(\tilde{U}_{1,k}-\tilde{U}_{2,k})\Delta x \\
&= -\frac{1}{2}\sum_{k=0}^{K-1}\left\{\delta_k^{+}\Big(\tilde{U}_{1,k}-\tilde{U}_{2,k}\Big)\right\}^2\Delta x + \left[\left\{\delta_k^{\langle 1\rangle}\left(\frac{\tilde{U}_{1,k}-\tilde{U}_{2,k}}{2}\right)\right\}(\tilde{U}_{1,k}-\tilde{U}_{2,k})\right]_0^K \\
&\le -\frac{(\tilde{U}_{1,K}-\tilde{U}_{2,K})^2}{\Delta t} - \left(\frac{dF}{d(U_{1,K},U_K^{(n)})}-\frac{dF}{d(U_{2,K},U_K^{(n)})}\right)(\tilde{U}_{1,K}-\tilde{U}_{2,K}) \\
&\quad -\frac{(\tilde{U}_{1,0}-\tilde{U}_{2,0})^2}{\Delta t} - \left(\frac{dF}{d(U_{1,0},U_0^{(n)})}-\frac{dF}{d(U_{2,0},U_0^{(n)})}\right)(\tilde{U}_{1,0}-\tilde{U}_{2,0}).
\end{aligned}
$$

Hence, using the Young inequality, we obtain

$$
\begin{aligned}
\frac{1}{\Delta t}\left\|\tilde{\boldsymbol{U}}_1-\tilde{\boldsymbol{U}}_2\right\|_{L^2_{\mathrm{d}}}^2 &\le -\frac{(\tilde{U}_{1,0}-\tilde{U}_{2,0})^2}{\Delta t} - \left(\frac{dF}{d(U_{1,0},U_0^{(n)})}-\frac{dF}{d(U_{2,0},U_0^{(n)})}\right)(\tilde{U}_{1,0}-\tilde{U}_{2,0}) \\
&\quad -\frac{(\tilde{U}_{1,K}-\tilde{U}_{2,K})^2}{\Delta t} - \left(\frac{dF}{d(U_{1,K},U_K^{(n)})}-\frac{dF}{d(U_{2,K},U_K^{(n)})}\right)(\tilde{U}_{1,K}-\tilde{U}_{2,K}) \\
&\quad -\sum_{k=0}^{K}{}''\left(\frac{dF}{d(U_{1,k},U_k^{(n)})}-\frac{dF}{d(U_{2,k},U_k^{(n)})}\right)(\tilde{U}_{1,k}-\tilde{U}_{2,k})\Delta x \\
&\le -\frac{(\tilde{U}_{1,0}-\tilde{U}_{2,0})^2}{2\Delta t} + \frac{\Delta t}{2}\left|\frac{dF}{d(U_{1,0},U_0^{(n)})}-\frac{dF}{d(U_{2,0},U_0^{(n)})}\right|^2 \\
&\quad -\frac{(\tilde{U}_{1,K}-\tilde{U}_{2,K})^2}{2\Delta t} + \frac{\Delta t}{2}\left|\frac{dF}{d(U_{1,K},U_K^{(n)})}-\frac{dF}{d(U_{2,K},U_K^{(n)})}\right|^2 \\
&\quad +\frac{1}{2\Delta t}\left\|\tilde{\boldsymbol{U}}_1-\tilde{\boldsymbol{U}}_2\right\|_{L^2_{\mathrm{d}}}^2 + \frac{\Delta t}{2}\left\|\frac{dF}{d(\boldsymbol{U}_1,\boldsymbol{U}^{(n)})}-\frac{dF}{d(\boldsymbol{U}_2,\boldsymbol{U}^{(n)})}\right\|_{L^2_{\mathrm{d}}}^2. \qquad (4.35)
\end{aligned}
$$

Therefore, multiplying both sides of (4.35) by $2\Delta t$, we get

$$
\begin{aligned}
&\left\|\tilde{\boldsymbol{U}}_1-\tilde{\boldsymbol{U}}_2\right\|_{L^2_{\mathrm{d}}}^2 + (\tilde{U}_{1,0}-\tilde{U}_{2,0})^2 + (\tilde{U}_{1,K}-\tilde{U}_{2,K})^2 \\
&\le (\Delta t)^2\left\{\left\|\frac{dF}{d(\boldsymbol{U}_1,\boldsymbol{U}^{(n)})}-\frac{dF}{d(\boldsymbol{U}_2,\boldsymbol{U}^{(n)})}\right\|_{L^2_{\mathrm{d}}}^2\right. \\
&\quad \left.+\left|\frac{dF}{d(U_{1,0},U_0^{(n)})}-\frac{dF}{d(U_{2,0},U_0^{(n)})}\right|^2 + \left|\frac{dF}{d(U_{1,K},U_K^{(n)})}-\frac{dF}{d(U_{2,K},U_K^{(n)})}\right|^2\right\}. \qquad (4.36)
\end{aligned}
$$

Next, from Corollary 2.1 (Summation by parts formula), we have

$$
\begin{aligned}
\frac{1}{\Delta t}\left\|D(\tilde{\boldsymbol{U}}_1-\tilde{\boldsymbol{U}}_2)\right\|^2 &= -\sum_{k=0}^{K}{}''\left\{\delta_k^{\langle 2\rangle}(\tilde{U}_{1,k}-\tilde{U}_{2,k})\right\}\frac{\tilde{U}_{1,k}-\tilde{U}_{2,k}}{\Delta t}\Delta x \\
&\quad +\left[\left\{\delta_k^{\langle 1\rangle}(\tilde{U}_{1,k}-\tilde{U}_{2,k})\right\}\frac{\tilde{U}_{1,k}-\tilde{U}_{2,k}}{\Delta t}\right]_0^K. \qquad (4.37)
\end{aligned}
$$

Using (4.31), Corollary 2.1 (Summation by parts formula), and the Young inequality, we estimate the first term on the right-hand side of (4.37) as follows:

$$
\begin{aligned}
&-\sum_{k=0}^{K}{}'' \left\{\delta_k^{\langle 2\rangle}(\tilde{U}_{1,k}-\tilde{U}_{2,k})\right\} \frac{\tilde{U}_{1,k}-\tilde{U}_{2,k}}{\Delta t}\Delta x \\
&\leq \sum_{k=0}^{K}{}'' \left\{\delta_k^{\langle 2\rangle}(\tilde{U}_{1,k}-\tilde{U}_{2,k})\right\} \left(\frac{dF}{d(U_{1,k},U_k^{(n)})}-\frac{dF}{d(U_{2,k},U_k^{(n)})}\right)\Delta x \\
&\leq -\sum_{k=0}^{K-1} \left\{\delta_k^{+}(\tilde{U}_{1,k}-\tilde{U}_{2,k})\right\} \left\{\delta_k^{+}\left(\frac{dF}{d(U_{1,k},U_k^{(n)})}-\frac{dF}{d(U_{2,k},U_k^{(n)})}\right)\right\}\Delta x \\
&\quad + \left[\left\{\delta_k^{\langle 1\rangle}(\tilde{U}_{1,k}-\tilde{U}_{2,k})\right\}\left(\frac{dF}{d(U_{1,k},U_k^{(n)})}-\frac{dF}{d(U_{2,k},U_k^{(n)})}\right)\right]_0^K \\
&\leq \frac{1}{2\Delta t}\left\|D(\tilde{\boldsymbol{U}}_1-\tilde{\boldsymbol{U}}_2)\right\|^2+\frac{\Delta t}{2}\left\|D\left(\frac{dF}{d(\boldsymbol{U}_1,\boldsymbol{U}^{(n)})}-\frac{dF}{d(\boldsymbol{U}_2,\boldsymbol{U}^{(n)})}\right)\right\|^2 \\
&\quad + \left[\left\{\delta_k^{\langle 1\rangle}(\tilde{U}_{1,k}-\tilde{U}_{2,k})\right\}\left(\frac{dF}{d(U_{1,k},U_k^{(n)})}-\frac{dF}{d(U_{2,k},U_k^{(n)})}\right)\right]_0^K .
\end{aligned}
$$

Thus, from (4.32) and (4.33), we have

$$
\begin{aligned}
\frac{1}{\Delta t}\left\|D(\tilde{\boldsymbol{U}}_1-\tilde{\boldsymbol{U}}_2)\right\|^2 &\leq \frac{1}{2\Delta t}\left\|D(\tilde{\boldsymbol{U}}_1-\tilde{\boldsymbol{U}}_2)\right\|^2+\frac{\Delta t}{2}\left\|D\left(\frac{dF}{d(\boldsymbol{U}_1,\boldsymbol{U}^{(n)})}-\frac{dF}{d(\boldsymbol{U}_2,\boldsymbol{U}^{(n)})}\right)\right\|^2 \\
&\quad + \left[\left\{\delta_k^{\langle 1\rangle}(\tilde{U}_{1,k}-\tilde{U}_{2,k})\right\}\left\{\frac{\tilde{U}_{1,k}-\tilde{U}_{2,k}}{\Delta t}+\left(\frac{dF}{d(U_{1,k},U_k^{(n)})}-\frac{dF}{d(U_{2,k},U_k^{(n)})}\right)\right\}\right]_0^K \\
&= \frac{1}{2\Delta t}\left\|D(\tilde{\boldsymbol{U}}_1-\tilde{\boldsymbol{U}}_2)\right\|^2+\frac{\Delta t}{2}\left\|D\left(\frac{dF}{d(\boldsymbol{U}_1,\boldsymbol{U}^{(n)})}-\frac{dF}{d(\boldsymbol{U}_2,\boldsymbol{U}^{(n)})}\right)\right\|^2 \\
&\quad -\frac{1}{2}\left\{\delta_k^{\langle 1\rangle}(\tilde{U}_{1,k}-\tilde{U}_{2,k})\Big|_{k=K}\right\}^2-\frac{1}{2}\left\{\delta_k^{\langle 1\rangle}(\tilde{U}_{1,k}-\tilde{U}_{2,k})\Big|_{k=0}\right\}^2 \\
&\leq \frac{1}{2\Delta t}\left\|D(\tilde{\boldsymbol{U}}_1-\tilde{\boldsymbol{U}}_2)\right\|^2+\frac{\Delta t}{2}\left\|D\left(\frac{dF}{d(\boldsymbol{U}_1,\boldsymbol{U}^{(n)})}-\frac{dF}{d(\boldsymbol{U}_2,\boldsymbol{U}^{(n)})}\right)\right\|^2 .
\end{aligned}
$$

That is,

$$
\left\|D(\tilde{\boldsymbol{U}}_1-\tilde{\boldsymbol{U}}_2)\right\|^2 \leq (\Delta t)^2\left\|D\left(\frac{dF}{d(\boldsymbol{U}_1,\boldsymbol{U}^{(n)})}-\frac{dF}{d(\boldsymbol{U}_2,\boldsymbol{U}^{(n)})}\right)\right\|^2 . \tag{4.38}
$$

Therefore, using (4.36) and (4.38), we obtain

$$
\left\|\tilde{\boldsymbol{U}}_1-\tilde{\boldsymbol{U}}_2\right\|_X^2 \leq (\Delta t)^2\left\|\frac{dF}{d(\boldsymbol{U}_1,\boldsymbol{U}^{(n)})}-\frac{dF}{d(\boldsymbol{U}_2,\boldsymbol{U}^{(n)})}\right\|_X^2 . \tag{4.39}
$$

Using Lemma 2.2, we get the following equality:

$$
\frac{dF}{d(U_{1,k},U_k^{(n)})}-\frac{dF}{d(U_{2,k},U_k^{(n)})}=\frac{1}{2}\bar{F}''(U_{1,k},U_{2,k};U_k^{(n)},U_k^{(n)})(U_{1,k}-U_{2,k}) \quad (k=0,\ldots,K). \tag{4.40}
$$

Since it holds from Proposition 2.5 and the definition of X that

$$\|\boldsymbol{U}_i\|_{L^\infty_{\mathrm{d}}} \le \tilde{C}_L \|\boldsymbol{U}_i\|_{\tilde{H}^1_{\mathrm{d}}} \le 2\tilde{C}_L M \quad (i=1,2),$$

by using Lemma 2.1, we get

$$\left|\bar{F}''(U_{1,k}, U_{2,k}; U_k^{(n)}, U_k^{(n)})\right| \le \max_{|\xi|\le 2\tilde{C}_L M} |F''(\xi)| \quad (k=0,\ldots,K). \tag{4.41}$$

From (4.40) and (4.41), we obtain

$$\left|\frac{dF}{d(U_{1,k}, U_k^{(n)})} - \frac{dF}{d(U_{2,k}, U_k^{(n)})}\right|^2 \le \frac{1}{4} \max_{|\xi|\le 2\tilde{C}_L M} |F''(\xi)|^2 \, |U_{1,k} - U_{2,k}|^2 \quad (k=0,\ldots,K). \tag{4.42}$$

Hence, the following inequality holds:

$$\left\|\frac{dF}{d(\boldsymbol{U}_1, \boldsymbol{U}^{(n)})} - \frac{dF}{d(\boldsymbol{U}_2, \boldsymbol{U}^{(n)})}\right\|^2_{L^2_{\mathrm{d}}} \le \frac{1}{4} \max_{|\xi|\le 2\tilde{C}_L M} |F''(\xi)|^2 \, \|\boldsymbol{U}_1 - \boldsymbol{U}_2\|^2_{L^2_{\mathrm{d}}}. \tag{4.43}$$

Furthermore, using (4.40), (4.41), Proposition 2.5, Lemma 2.3, and Lemma 2.4, we have

$$\begin{aligned}
&\left\|D\left(\frac{dF}{d(\boldsymbol{U}_1, \boldsymbol{U}^{(n)})} - \frac{dF}{d(\boldsymbol{U}_2, \boldsymbol{U}^{(n)})}\right)\right\|^2 \\
&\le \frac{1}{4}\left\{\left\|\bar{F}''(\boldsymbol{U}_1, \boldsymbol{U}_2; \boldsymbol{U}^{(n)}, \boldsymbol{U}^{(n)})\right\|_{L^\infty_{\mathrm{d}}} \|D(\boldsymbol{U}_1 - \boldsymbol{U}_2)\| \right.\\
&\quad \left. + \|\boldsymbol{U}_1 - \boldsymbol{U}_2\|_{L^\infty_{\mathrm{d}}} \left\|D\bar{F}''(\boldsymbol{U}_1, \boldsymbol{U}_2; \boldsymbol{U}^{(n)}, \boldsymbol{U}^{(n)})\right\|\right\}^2 \\
&\le \frac{1}{2} \max_{|\xi|\le 2\tilde{C}_L M} |F''(\xi)|^2 \|D(\boldsymbol{U}_1 - \boldsymbol{U}_2)\|^2 + \frac{\tilde{C}_L^2}{2} \|\boldsymbol{U}_1 - \boldsymbol{U}_2\|^2_{\tilde{H}^1_{\mathrm{d}}} \left\|D\bar{F}''(\boldsymbol{U}_1, \boldsymbol{U}_2; \boldsymbol{U}^{(n)}, \boldsymbol{U}^{(n)})\right\|^2 \\
&\le \frac{1}{2} \max_{|\xi|\le 2\tilde{C}_L M} |F''(\xi)|^2 \|D(\boldsymbol{U}_1 - \boldsymbol{U}_2)\|^2 \\
&\quad + \frac{\tilde{C}_L^2}{18} \max_{|\xi|\le 2\tilde{C}_L M} |F'''(\xi)|^2 \left(\|D\boldsymbol{U}_1\| + \|D\boldsymbol{U}_2\| + \left\|D\boldsymbol{U}^{(n)}\right\|\right)^2 \|\boldsymbol{U}_1 - \boldsymbol{U}_2\|^2_X \\
&\le \frac{1}{2} \max_{|\xi|\le 2\tilde{C}_L M} |F''(\xi)|^2 \|D(\boldsymbol{U}_1 - \boldsymbol{U}_2)\|^2 + \frac{25}{18}\tilde{C}_L^2 M^2 \max_{|\xi|\le 2\tilde{C}_L M} |F'''(\xi)|^2 \|\boldsymbol{U}_1 - \boldsymbol{U}_2\|^2_X.
\end{aligned} \tag{4.44}$$

Thus, from (4.42)–(4.44), we obtain

$$\begin{aligned}
\left\|\frac{dF}{d(\boldsymbol{U}_1, \boldsymbol{U}^{(n)})} - \frac{dF}{d(\boldsymbol{U}_2, \boldsymbol{U}^{(n)})}\right\|^2_X &\le \left\{\frac{1}{2} \max_{|\xi|\le 2\tilde{C}_L M} |F''(\xi)|^2 + \frac{25}{18}\tilde{C}_L^2 M^2 \max_{|\xi|\le 2\tilde{C}_L M} |F'''(\xi)|^2\right\} \\
&\quad \times \|\boldsymbol{U}_1 - \boldsymbol{U}_2\|^2_X.
\end{aligned} \tag{4.45}$$

Applying (4.45) to (4.39), we conclude that

$$\|\Phi(\boldsymbol{U}_1) - \Phi(\boldsymbol{U}_2)\|^2_X = \left\|\tilde{\boldsymbol{U}}_1 - \tilde{\boldsymbol{U}}_2\right\|^2_X \le (\Delta t)^2 R\left(\tilde{C}_L M\right) \|\boldsymbol{U}_1 - \boldsymbol{U}_2\|^2_X.$$

Since it holds that from the assumption (4.17) on Δt that

$$0 \le (\Delta t)^2 R\left(\tilde{C}_L M\right) < 1,$$

the mapping Φ is contraction into X. This completes the proof. □

Theorem 4.4 (Global existence and uniqueness)**.** Let C_0 be the square root of the right-hand side of (4.16), i.e.,

$$C_0 := \left[\frac{1}{\min\left\{\dfrac{1}{2}, \mu\right\}} \left\{ J_{\mathrm{d}}(\boldsymbol{U}^{(0)}) + F(U_0^{(0)}) + F(U_K^{(0)}) + c(L+2) \right\} \right]^{\frac{1}{2}}.$$

If Δt satisfies $(\Delta t)^2 R(\tilde{C}_L C_0) < 1$, then there exists a unique solution $\{U_k^{(n)}\}_{k=-1}^{K+1}$ $(n \in \mathbb{N})$ satisfying (4.9) with (4.10) and (4.11).

Proof. Since $\{\|\boldsymbol{U}^{(0)}\|_{\tilde{H}_{\mathrm{d}}^1}^2 + |U_0^{(0)}|^2 + |U_K^{(0)}|^2\}^{1/2} \le C_0$ from Lemma 4.3, there exists a unique solution $\boldsymbol{U}^{(1)}$ satisfying $\{\|\boldsymbol{U}^{(1)}\|_{\tilde{H}_{\mathrm{d}}^1}^2 + |U_0^{(1)}|^2 + |U_K^{(1)}|^2\}^{1/2} \le C_0$. Repeating the procedure, we have completed the proof. □

§5 Error estimate

In this section, we show an error estimate. We also use the energy method in [28,65–68]. Fix a natural number $N \in \mathbb{N}$. We compute $\boldsymbol{U}^{(n)}$ up to $n = N$ by our proposed scheme (4.9)–(4.11) and estimate the error between it and the solution to the problem (4.1)–(4.3) up to $T = N\Delta t$. Let u be the solution to the problem (4.1)–(4.3) with an initial value satisfying $u \in C^3([0,L] \times [0,T])$. Then, we extend the solution u in $[0,L] \times [0,T]$ to $\tilde{u}$ in $(-\Delta x, L + \Delta x) \times [0,T]$ as follows:

$$\tilde{u}(x,t) := \begin{cases} u(-x,t) + 2x\partial_x u(0,t) + \dfrac{x^3}{3}\partial_x^3 u(0,t), & (-\Delta x \le x < 0), \\ u(x,t), & (0 \le x \le L), \\ u(2L - x, t) + 2(x-L)\partial_x u(L,t) + \dfrac{(x-L)^3}{3}\partial_x^3 u(L,t), & (L < x \le L + \Delta x) \end{cases}$$

for $t \in [0,T]$, where $\partial_x f(a)$ means $\partial_x f(x)|_{x=a}$. From the direct calculation, we can check $\tilde{u} \in C^3((-L,2L) \times [0,T])$. Furthermore, we can also check that if $u \in C^4([0,L] \times [0,T])$, then $\tilde{u} \in C^4([-\Delta x, L + \Delta x] \times [0,T])$. Moreover, we define the error by

$$e_k^{(n)} := U_k^{(n)} - \tilde{u}(k\Delta x, n\Delta t) \quad (k = -1, 0, \ldots, K, K+1, n = 0, 1, \ldots, N).$$

For the sake of simplicity, let us use the expression $\tilde{u}_k^{(n)} := \tilde{u}(k\Delta x, n\Delta t)$ from now on. Also, the expression $\delta_k^* f_l$ means $\delta_k^* f_k|_{k=l}$, where the symbol $*$ denotes $+$, $\langle 1 \rangle$, or $\langle 2 \rangle$. Then, the following lemma and theorem hold:

Lemma 4.4. Let u be the solution to the problem (4.1)–(4.3) with an initial value satisfying $u \in C^3([0,L] \times [0,T])$. Then, we obtain the following equations on the error:

$$\begin{aligned} \frac{e_k^{(n+1)} - e_k^{(n)}}{\Delta t} &= \delta_k^{\langle 2 \rangle}\left(\frac{e_k^{(n+1)} + e_k^{(n)}}{2}\right) - \left(\frac{dF}{d(U_k^{(n+1)}, U_k^{(n)})} - \frac{dF}{d(u_k^{(n+1)}, u_k^{(n)})}\right) \\ &\quad + \xi_{1,k}^{(n+\frac{1}{2})} + \xi_{2,k}^{(n+\frac{1}{2})} + \xi_{3,k}^{(n+\frac{1}{2})} \quad (k = 0, \ldots, K), \end{aligned} \tag{4.46}$$

$$
\begin{aligned}
\frac{e_0^{(n+1)}-e_0^{(n)}}{\Delta t} &= \delta_k^{\langle 1\rangle}\left(\frac{e_0^{(n+1)}+e_0^{(n)}}{2}\right)-\left(\frac{dF}{d(U_0^{(n+1)},U_0^{(n)})}-\frac{dF}{d(u_0^{(n+1)},u_0^{(n)})}\right) \\
&\quad + \xi_{1,0}^{\left(n+\frac{1}{2}\right)} + \xi_{3,0}^{\left(n+\frac{1}{2}\right)} + \xi_{4,0}^{\left(n+\frac{1}{2}\right)},
\end{aligned}
\tag{4.47}
$$

$$
\begin{aligned}
\frac{e_K^{(n+1)}-e_K^{(n)}}{\Delta t} &= -\delta_k^{\langle 1\rangle}\left(\frac{e_K^{(n+1)}+e_K^{(n)}}{2}\right)-\left(\frac{dF}{d(U_K^{(n+1)},U_K^{(n)})}-\frac{dF}{d(u_K^{(n+1)},u_K^{(n)})}\right) \\
&\quad + \xi_{1,K}^{\left(n+\frac{1}{2}\right)} + \xi_{3,K}^{\left(n+\frac{1}{2}\right)} - \xi_{4,K}^{\left(n+\frac{1}{2}\right)}
\end{aligned}
\tag{4.48}
$$

for $n = 0, 1, \ldots, N-1$, where ξ_1, ξ_2, ξ_3, and ξ_4 are defined as follows:

$$
\begin{aligned}
\xi_{1,k}^{\left(n+\frac{1}{2}\right)} &:= \partial_t u_k^{\left(n+\frac{1}{2}\right)} - \frac{u_k^{(n+1)}-u_k^{(n)}}{\Delta t} \quad (k = 0, \ldots, K), \\
\xi_{2,k}^{\left(n+\frac{1}{2}\right)} &:= \delta_k^{\langle 2\rangle}\left(\frac{\tilde{u}_k^{(n+1)}+\tilde{u}_k^{(n)}}{2}\right) - \partial_x^2 u_k^{\left(n+\frac{1}{2}\right)} \quad (k = 0, \ldots, K), \\
\xi_{3,k}^{\left(n+\frac{1}{2}\right)} &:= F'(u_k^{\left(n+\frac{1}{2}\right)}) - \frac{dF}{d(u_k^{(n+1)},u_k^{(n)})} \quad (k = 0, \ldots, K), \\
\xi_{4,k}^{\left(n+\frac{1}{2}\right)} &:= \delta_k^{\langle 1\rangle}\left(\frac{\tilde{u}_k^{(n+1)}+\tilde{u}_k^{(n)}}{2}\right) - \partial_x u_k^{\left(n+\frac{1}{2}\right)} \quad (k = 0, K).
\end{aligned}
$$

Proof. For any fixed $n = 0, 1, \ldots, N-1$, from the definition of $\boldsymbol{e}$, (4.1), (4.9), and (4.12), we have

$$
\begin{aligned}
\frac{e_k^{(n+1)}-e_k^{(n)}}{\Delta t} &= \frac{U_k^{(n+1)}-U_k^{(n)}}{\Delta t} - \partial_t u_k^{\left(n+\frac{1}{2}\right)} + \partial_t u_k^{\left(n+\frac{1}{2}\right)} - \frac{u_k^{(n+1)}-u_k^{(n)}}{\Delta t} \\
&= \delta_k^{\langle 2\rangle}\left(\frac{U_k^{(n+1)}+U_k^{(n)}}{2}\right) - \frac{dF}{d(U_k^{(n+1)},U_k^{(n)})} - \partial_x^2 u_k^{\left(n+\frac{1}{2}\right)} + F'(u_k^{\left(n+\frac{1}{2}\right)}) + \xi_{1,k}^{\left(n+\frac{1}{2}\right)} \\
&= \delta_k^{\langle 2\rangle}\left(\frac{U_k^{(n+1)}+U_k^{(n)}}{2}\right) - \delta_k^{\langle 2\rangle}\left(\frac{u_k^{(n+1)}+u_k^{(n)}}{2}\right) + \delta_k^{\langle 2\rangle}\left(\frac{u_k^{(n+1)}+u_k^{(n)}}{2}\right) - \partial_x^2 u_k^{\left(n+\frac{1}{2}\right)} \\
&\quad - \frac{dF}{d(U_k^{(n+1)},U_k^{(n)})} + \frac{dF}{d(u_k^{(n+1)},u_k^{(n)})} - \frac{dF}{d(u_k^{(n+1)},u_k^{(n)})} + F'(u_k^{\left(n+\frac{1}{2}\right)}) + \xi_{1,k}^{\left(n+\frac{1}{2}\right)} \\
&= \delta_k^{\langle 2\rangle}\left(\frac{e_k^{(n+1)}+e_k^{(n)}}{2}\right) - \left(\frac{dF}{d(U_k^{(n+1)},U_k^{(n)})} - \frac{dF}{d(u_k^{(n+1)},u_k^{(n)})}\right) \\
&\quad + \xi_{1,k}^{\left(n+\frac{1}{2}\right)} + \xi_{2,k}^{\left(n+\frac{1}{2}\right)} + \xi_{3,k}^{\left(n+\frac{1}{2}\right)} \quad (k = 1, \ldots, K-1).
\end{aligned}
\tag{4.49}
$$

We show that the above equality (4.49) holds at $k = 0, K$. We remark that the equation (4.1) holds in the interior of the domain $(0, L)$ only. Hence, we cannot apply the equation (4.1) directly in the calculation of (4.49) on the boundary. Therefore, we consider points slightly inside from the boundary of the domain, and we take the limit of them to show that (4.49) holds at $k = 0, K$. For any $\varepsilon \in (0, 1)$, let

$$
e_{0,\varepsilon}^{(n)} := U_0^{(n)} - u(\varepsilon\Delta x, n\Delta t), \quad e_{K,-\varepsilon}^{(n)} := U_K^{(n)} - u((K-\varepsilon)\Delta x, n\Delta t) \quad (n = 0, 1, \ldots, N).
$$

Furthermore, for $n = 0, 1, \ldots, N-1$, let

$$\xi_{1,\varepsilon}^{\left(n+\frac{1}{2}\right)} := \partial_t u_\varepsilon^{\left(n+\frac{1}{2}\right)} - \frac{u_\varepsilon^{(n+1)} - u_\varepsilon^{(n)}}{\Delta t}, \quad \xi_{1,K-\varepsilon}^{\left(n+\frac{1}{2}\right)} := \partial_t u_{K-\varepsilon}^{\left(n+\frac{1}{2}\right)} - \frac{u_{K-\varepsilon}^{(n+1)} - u_{K-\varepsilon}^{(n)}}{\Delta t},$$

$$\xi_{2,\varepsilon}^{\left(n+\frac{1}{2}\right)} := \delta_k^{\langle 2\rangle}\left(\frac{\tilde{u}_\varepsilon^{(n+1)} + \tilde{u}_\varepsilon^{(n)}}{2}\right) - \partial_x^2 u_\varepsilon^{\left(n+\frac{1}{2}\right)}, \quad \xi_{2,K-\varepsilon}^{\left(n+\frac{1}{2}\right)} := \delta_k^{\langle 2\rangle}\left(\frac{\tilde{u}_{K-\varepsilon}^{(n+1)} + \tilde{u}_{K-\varepsilon}^{(n)}}{2}\right) - \partial_x^2 u_{K-\varepsilon}^{\left(n+\frac{1}{2}\right)},$$

$$\xi_{3,\varepsilon}^{\left(n+\frac{1}{2}\right)} := F'(u_\varepsilon^{\left(n+\frac{1}{2}\right)}) - \frac{dF}{d(u_\varepsilon^{(n+1)}, u_\varepsilon^{(n)})}, \quad \xi_{3,K-\varepsilon}^{\left(n+\frac{1}{2}\right)} := F'(u_{K-\varepsilon}^{\left(n+\frac{1}{2}\right)}) - \frac{dF}{d(u_{K-\varepsilon}^{(n+1)}, u_{K-\varepsilon}^{(n)})}.$$

In the same manner, as (4.49), we have

$$\begin{aligned} \frac{e_{0,\varepsilon}^{(n+1)} - e_{0,\varepsilon}^{(n)}}{\Delta t} &= \delta_k^{\langle 2\rangle}\left(\frac{e_{0,\varepsilon}^{(n+1)} + e_{0,\varepsilon}^{(n)}}{2}\right) - \left(\frac{dF}{d(U_0^{(n+1)}, U_0^{(n)})} - \frac{dF}{d(u_\varepsilon^{(n+1)}, u_\varepsilon^{(n)})}\right) \\ &\quad + \xi_{1,\varepsilon}^{\left(n+\frac{1}{2}\right)} + \xi_{2,\varepsilon}^{\left(n+\frac{1}{2}\right)} + \xi_{3,\varepsilon}^{\left(n+\frac{1}{2}\right)}, \end{aligned} \tag{4.50}$$

$$\begin{aligned} \frac{e_{K,-\varepsilon}^{(n+1)} - e_{K,-\varepsilon}^{(n)}}{\Delta t} &= \delta_k^{\langle 2\rangle}\left(\frac{e_{K,-\varepsilon}^{(n+1)} + e_{K,-\varepsilon}^{(n)}}{2}\right) - \left(\frac{dF}{d(U_K^{(n+1)}, U_K^{(n)})} - \frac{dF}{d(u_{K-\varepsilon}^{(n+1)}, u_{K-\varepsilon}^{(n)})}\right) \\ &\quad + \xi_{1,K-\varepsilon}^{\left(n+\frac{1}{2}\right)} + \xi_{2,K-\varepsilon}^{\left(n+\frac{1}{2}\right)} + \xi_{3,K-\varepsilon}^{\left(n+\frac{1}{2}\right)}. \end{aligned} \tag{4.51}$$

From the smoothness assumption of u, letting ε tend to 0 in (4.50) and (4.51), we have

$$\begin{aligned} \frac{e_k^{(n+1)} - e_k^{(n)}}{\Delta t} &= \delta_k^{\langle 2\rangle}\left(\frac{e_k^{(n+1)} + e_k^{(n)}}{2}\right) - \left(\frac{dF}{d(U_k^{(n+1)}, U_k^{(n)})} - \frac{dF}{d(u_k^{(n+1)}, u_k^{(n)})}\right) \\ &\quad + \xi_{1,k}^{\left(n+\frac{1}{2}\right)} + \xi_{2,k}^{\left(n+\frac{1}{2}\right)} + \xi_{3,k}^{\left(n+\frac{1}{2}\right)} \quad (k = 0, K). \end{aligned}$$

Next, from (4.2) and (4.10), we obtain

$$\begin{aligned} \frac{e_0^{(n+1)} - e_0^{(n)}}{\Delta t} &= \frac{U_0^{(n+1)} - U_0^{(n)}}{\Delta t} - \partial_t u_0^{\left(n+\frac{1}{2}\right)} + \partial_t u_0^{\left(n+\frac{1}{2}\right)} - \frac{u_0^{(n+1)} - u_0^{(n)}}{\Delta t} \\ &= \delta_k^{\langle 1\rangle}\left(\frac{U_0^{(n+1)} + U_0^{(n)}}{2}\right) - \frac{dF}{d(U_0^{(n+1)}, U_0^{(n)})} - \partial_x u_0^{\left(n+\frac{1}{2}\right)} + F'(u_0^{\left(n+\frac{1}{2}\right)}) + \xi_{1,0}^{\left(n+\frac{1}{2}\right)} \\ &= \delta_k^{\langle 1\rangle}\left(\frac{U_0^{(n+1)} + U_0^{(n)}}{2}\right) - \delta_k^{\langle 1\rangle}\left(\frac{\tilde{u}_0^{(n+1)} + \tilde{u}_0^{(n)}}{2}\right) + \delta_k^{\langle 1\rangle}\left(\frac{\tilde{u}_0^{(n+1)} + \tilde{u}_0^{(n)}}{2}\right) - \partial_x u_0^{\left(n+\frac{1}{2}\right)} \\ &\quad - \frac{dF}{d(U_0^{(n+1)}, U_0^{(n)})} + \frac{dF}{d(u_0^{(n+1)}, u_0^{(n)})} - \frac{dF}{d(u_0^{(n+1)}, u_0^{(n)})} + F'(u_0^{\left(n+\frac{1}{2}\right)}) + \xi_{1,0}^{\left(n+\frac{1}{2}\right)} \\ &= \delta_k^{\langle 1\rangle}\left(\frac{e_0^{(n+1)} + e_0^{(n)}}{2}\right) - \left(\frac{dF}{d(U_0^{(n+1)}, U_0^{(n)})} - \frac{dF}{d(u_0^{(n+1)}, u_0^{(n)})}\right) \\ &\quad + \xi_{1,0}^{\left(n+\frac{1}{2}\right)} + \xi_{3,0}^{\left(n+\frac{1}{2}\right)} + \xi_{4,0}^{\left(n+\frac{1}{2}\right)}. \end{aligned}$$

Similarly, from (4.3) and (4.11), we have

$$\begin{aligned} \frac{e_K^{(n+1)} - e_K^{(n)}}{\Delta t} &= -\delta_k^{\langle 1\rangle}\left(\frac{e_K^{(n+1)} + e_K^{(n)}}{2}\right) - \left(\frac{dF}{d(U_K^{(n+1)}, U_K^{(n)})} - \frac{dF}{d(u_K^{(n+1)}, u_K^{(n)})}\right) \\ &\quad + \xi_{1,K}^{\left(n+\frac{1}{2}\right)} + \xi_{3,K}^{\left(n+\frac{1}{2}\right)} - \xi_{4,K}^{\left(n+\frac{1}{2}\right)}. \end{aligned}$$

Therefore, (4.46)–(4.48) holds. □

Theorem 4.5. Assume that the problem (4.1)–(4.3) with an initial value has a smooth solution u that satisfies $u \in C^3([0,L]\times[0,T])$. Denote the bounds by

$$\max_{0\le n\le N}\left\{\left\|D\boldsymbol{U}^{(n)}\right\|,\left\|D\boldsymbol{u}^{(n)}\right\|\right\}\le C_1,\quad \max_{0\le n\le N}\left\{\left\|\boldsymbol{U}^{(n)}\right\|_{L^\infty_{\mathrm{d}}},\left\|\boldsymbol{u}^{(n)}\right\|_{L^\infty_{\mathrm{d}}}\right\}\le C_2. \tag{4.52}$$

Also, let

$$C_F := 2\left\{C_1^2\tilde{C}_L^2\max_{|\xi|\le C_2}|F'''(\xi)|^2+\max_{|\xi|\le C_2}|F''(\xi)|^2\right\}. \tag{4.53}$$

Then, the following inequality holds:

$$\begin{aligned}&\{1-(1+C_F)\Delta t\}\left\{\left\|\boldsymbol{e}^{(n+1)}\right\|^2_{\tilde{H}^1_{\mathrm{d}}}+\left|e_0^{(n+1)}\right|^2+\left|e_K^{(n+1)}\right|^2\right\}\\&\le\{1+(1+C_F)\Delta t\}\left\{\left\|\boldsymbol{e}^{(n)}\right\|^2_{\tilde{H}^1_{\mathrm{d}}}+\left|e_0^{(n)}\right|^2+\left|e_K^{(n)}\right|^2\right\}+2\Delta t\xi^{\left(n+\frac{1}{2}\right)}\quad(n=0,1,\ldots,N-1),\end{aligned}$$

where

$$\begin{aligned}\xi^{\left(n+\frac{1}{2}\right)}:=&\left\{\left\|\boldsymbol{\xi}_1^{\left(n+\frac{1}{2}\right)}\right\|^2_{\tilde{H}^1_{\mathrm{d}}}+\left|\xi_{1,0}^{\left(n+\frac{1}{2}\right)}\right|^2+\left|\xi_{1,K}^{\left(n+\frac{1}{2}\right)}\right|^2\right\}+\left\{\left\|\boldsymbol{\xi}_2^{\left(n+\frac{1}{2}\right)}\right\|^2_{\tilde{H}^1_{\mathrm{d}}}+\left|\xi_{2,0}^{\left(n+\frac{1}{2}\right)}\right|^2+\left|\xi_{2,K}^{\left(n+\frac{1}{2}\right)}\right|^2\right\}\\&+\left\{\left\|\boldsymbol{\xi}_3^{\left(n+\frac{1}{2}\right)}\right\|^2_{\tilde{H}^1_{\mathrm{d}}}+\left|\xi_{3,0}^{\left(n+\frac{1}{2}\right)}\right|^2+\left|\xi_{3,K}^{\left(n+\frac{1}{2}\right)}\right|^2\right\}+2\left\{\left|\xi_{4,0}^{\left(n+\frac{1}{2}\right)}\right|^2+\left|\xi_{4,K}^{\left(n+\frac{1}{2}\right)}\right|^2\right\}.\end{aligned} \tag{4.54}$$

Proof. For any fixed $n=0,1,\ldots,N-1$, using (4.46), we obtain

$$\begin{aligned}&\frac{1}{2\Delta t}\left(\left\|\boldsymbol{e}^{(n+1)}\right\|^2_{L^2_{\mathrm{d}}}-\left\|\boldsymbol{e}^{(n)}\right\|^2_{L^2_{\mathrm{d}}}\right)\\&=\sum_{k=0}^{K}{}''\frac{e_k^{(n+1)}-e_k^{(n)}}{\Delta t}\frac{e_k^{(n+1)}+e_k^{(n)}}{2}\Delta x\\&=\sum_{k=0}^{K}{}''\left\{\delta_k^{\langle 2\rangle}\left(\frac{e_k^{(n+1)}+e_k^{(n)}}{2}\right)\right\}\frac{e_k^{(n+1)}+e_k^{(n)}}{2}\Delta x\\&\quad+\sum_{k=0}^{K}{}''\frac{e_k^{(n+1)}+e_k^{(n)}}{2}\left\{-\left(\frac{dF}{d(U_k^{(n+1)},U_k^{(n)})}-\frac{dF}{d(u_k^{(n+1)},u_k^{(n)})}\right)+\xi_{1,k}^{\left(n+\frac{1}{2}\right)}+\xi_{2,k}^{\left(n+\frac{1}{2}\right)}+\xi_{3,k}^{\left(n+\frac{1}{2}\right)}\right\}\Delta x.\end{aligned} \tag{4.55}$$

From Corollary 2.1 (Summation by parts formula), we calculate the first term on the right-hand side of (4.55) as follows:

$$\begin{aligned}\sum_{k=0}^{K}{}''\left\{\delta_k^{\langle 2\rangle}\left(\frac{e_k^{(n+1)}+e_k^{(n)}}{2}\right)\right\}\frac{e_k^{(n+1)}+e_k^{(n)}}{2}\Delta x=&-\left\|D\left(\frac{\boldsymbol{e}^{(n+1)}+\boldsymbol{e}^{(n)}}{2}\right)\right\|^2\\&+\left[\left\{\delta_k^{\langle 1\rangle}\left(\frac{e_k^{(n+1)}+e_k^{(n)}}{2}\right)\right\}\frac{e_k^{(n+1)}+e_k^{(n)}}{2}\right]_0^K.\end{aligned} \tag{4.56}$$

From (4.47), (4.48), the Young inequality, and the inequality: $(\sum_{i=1}^{n} a_i)^2 \leq n \sum_{i=1}^{n} a_i^2$, we estimate the boundary term on the right-hand side of (4.56) as follows:

$$
\begin{aligned}
&\left[\left\{\delta_k^{\langle 1\rangle}\left(\frac{e_k^{(n+1)}+e_k^{(n)}}{2}\right)\right\}\frac{e_k^{(n+1)}+e_k^{(n)}}{2}\right]_0^K \\
&= -\frac{\left|e_K^{(n+1)}\right|^2-\left|e_K^{(n)}\right|^2}{2\Delta t} - \frac{e_K^{(n+1)}+e_K^{(n)}}{2}\left\{\left(\frac{dF}{d(U_K^{(n+1)},U_K^{(n)})}-\frac{dF}{d(u_K^{(n+1)},u_K^{(n)})}\right)-\xi_{1,K}^{\left(n+\frac{1}{2}\right)}-\xi_{3,K}^{\left(n+\frac{1}{2}\right)}+\xi_{4,K}^{\left(n+\frac{1}{2}\right)}\right\} \\
&\quad -\frac{\left|e_0^{(n+1)}\right|^2-\left|e_0^{(n)}\right|^2}{2\Delta t} - \frac{e_0^{(n+1)}+e_0^{(n)}}{2}\left\{\left(\frac{dF}{d(U_0^{(n+1)},U_0^{(n)})}-\frac{dF}{d(u_0^{(n+1)},u_0^{(n)})}\right)-\xi_{1,0}^{\left(n+\frac{1}{2}\right)}-\xi_{3,0}^{\left(n+\frac{1}{2}\right)}-\xi_{4,0}^{\left(n+\frac{1}{2}\right)}\right\} \\
&\leq -\frac{\left|e_0^{(n+1)}\right|^2-\left|e_0^{(n)}\right|^2}{2\Delta t} - \frac{\left|e_K^{(n+1)}\right|^2-\left|e_K^{(n)}\right|^2}{2\Delta t} \\
&\quad + \left(\frac{e_0^{(n+1)}+e_0^{(n)}}{2}\right)^2 + \frac{1}{4}\left\{\left(\frac{dF}{d(U_0^{(n+1)},U_0^{(n)})}-\frac{dF}{d(u_0^{(n+1)},u_0^{(n)})}\right)-\xi_{1,0}^{\left(n+\frac{1}{2}\right)}-\xi_{3,0}^{\left(n+\frac{1}{2}\right)}-\xi_{4,0}^{\left(n+\frac{1}{2}\right)}\right\}^2 \\
&\quad + \left(\frac{e_K^{(n+1)}+e_K^{(n)}}{2}\right)^2 + \frac{1}{4}\left\{\left(\frac{dF}{d(U_K^{(n+1)},U_K^{(n)})}-\frac{dF}{d(u_K^{(n+1)},u_K^{(n)})}\right)-\xi_{1,K}^{\left(n+\frac{1}{2}\right)}-\xi_{3,K}^{\left(n+\frac{1}{2}\right)}+\xi_{4,K}^{\left(n+\frac{1}{2}\right)}\right\}^2 \\
&\leq -\frac{\left|e_0^{(n+1)}\right|^2-\left|e_0^{(n)}\right|^2}{2\Delta t} - \frac{\left|e_K^{(n+1)}\right|^2-\left|e_K^{(n)}\right|^2}{2\Delta t} + \frac{\left|e_0^{(n+1)}\right|^2+\left|e_0^{(n)}\right|^2}{2} + \frac{\left|e_K^{(n+1)}\right|^2+\left|e_K^{(n)}\right|^2}{2} \\
&\quad + \left|\frac{dF}{d(U_0^{(n+1)},U_0^{(n)})}-\frac{dF}{d(u_0^{(n+1)},u_0^{(n)})}\right|^2 + \left|\xi_{1,0}^{\left(n+\frac{1}{2}\right)}\right|^2 + \left|\xi_{3,0}^{\left(n+\frac{1}{2}\right)}\right|^2 + \left|\xi_{4,0}^{\left(n+\frac{1}{2}\right)}\right|^2 \\
&\quad + \left|\frac{dF}{d(U_K^{(n+1)},U_K^{(n)})}-\frac{dF}{d(u_K^{(n+1)},u_K^{(n)})}\right|^2 + \left|\xi_{1,K}^{\left(n+\frac{1}{2}\right)}\right|^2 + \left|\xi_{3,K}^{\left(n+\frac{1}{2}\right)}\right|^2 + \left|\xi_{4,K}^{\left(n+\frac{1}{2}\right)}\right|^2. \qquad (4.57)
\end{aligned}
$$

Similarly, we also estimate the second term on the right-hand side of (4.55) as follows:

$$
\begin{aligned}
&\sum_{k=0}^{K}{}'' \frac{e_k^{(n+1)}+e_k^{(n)}}{2}\left\{-\left(\frac{dF}{d(U_k^{(n+1)},U_k^{(n)})}-\frac{dF}{d(u_k^{(n+1)},u_k^{(n)})}\right)+\xi_{1,k}^{\left(n+\frac{1}{2}\right)}+\xi_{2,k}^{\left(n+\frac{1}{2}\right)}+\xi_{3,k}^{\left(n+\frac{1}{2}\right)}\right\}\Delta x \\
&\leq \sum_{k=0}^{K}{}'' \left(\frac{e_k^{(n+1)}+e_k^{(n)}}{2}\right)^2 \Delta x \\
&\quad + \frac{1}{4}\sum_{k=0}^{K}{}'' \left\{-\left(\frac{dF}{d(U_k^{(n+1)},U_k^{(n)})}-\frac{dF}{d(u_k^{(n+1)},u_k^{(n)})}\right)+\xi_{1,k}^{\left(n+\frac{1}{2}\right)}+\xi_{2,k}^{\left(n+\frac{1}{2}\right)}+\xi_{3,k}^{\left(n+\frac{1}{2}\right)}\right\}^2 \Delta x \\
&\leq \frac{\left\|\boldsymbol{e}^{(n+1)}\right\|_{L_{\mathrm{d}}^2}^2+\left\|\boldsymbol{e}^{(n)}\right\|_{L_{\mathrm{d}}^2}^2}{2} + \left\|\frac{dF}{d(\boldsymbol{U}^{(n+1)},\boldsymbol{U}^{(n)})}-\frac{dF}{d(\boldsymbol{u}^{(n+1)},\boldsymbol{u}^{(n)})}\right\|_{L_{\mathrm{d}}^2}^2 \\
&\quad + \left\|\boldsymbol{\xi}_1^{\left(n+\frac{1}{2}\right)}\right\|_{L_{\mathrm{d}}^2}^2 + \left\|\boldsymbol{\xi}_2^{\left(n+\frac{1}{2}\right)}\right\|_{L_{\mathrm{d}}^2}^2 + \left\|\boldsymbol{\xi}_3^{\left(n+\frac{1}{2}\right)}\right\|_{L_{\mathrm{d}}^2}^2. \qquad (4.58)
\end{aligned}
$$

Therefore, we see from (4.55)–(4.58) that

$$\begin{aligned}
&\frac{1}{2\Delta t}\left(\|\boldsymbol{e}^{(n+1)}\|_{L^2_\mathrm{d}}^2-\|\boldsymbol{e}^{(n)}\|_{L^2_\mathrm{d}}^2\right)\\
&\le -\left\|D\left(\frac{\boldsymbol{e}^{(n+1)}+\boldsymbol{e}^{(n)}}{2}\right)\right\|^2-\frac{\left|e_0^{(n+1)}\right|^2-\left|e_0^{(n)}\right|^2}{2\Delta t}-\frac{\left|e_K^{(n+1)}\right|^2-\left|e_K^{(n)}\right|^2}{2\Delta t}\\
&\quad+\frac{1}{2}\left\{\|\boldsymbol{e}^{(n+1)}\|_{L^2_\mathrm{d}}^2+\left|e_0^{(n+1)}\right|^2+\left|e_K^{(n+1)}\right|^2\right\}+\frac{1}{2}\left\{\|\boldsymbol{e}^{(n)}\|_{L^2_\mathrm{d}}^2+\left|e_0^{(n)}\right|^2+\left|e_K^{(n)}\right|^2\right\}\\
&\quad+\left\{\left\|\frac{dF}{d(\boldsymbol{U}^{(n+1)},\boldsymbol{U}^{(n)})}-\frac{dF}{d(\boldsymbol{u}^{(n+1)},\boldsymbol{u}^{(n)})}\right\|_{L^2_\mathrm{d}}^2+\left|\frac{dF}{d(U_0^{(n+1)},U_0^{(n)})}-\frac{dF}{d(u_0^{(n+1)},u_0^{(n)})}\right|^2\right.\\
&\quad\left.+\left|\frac{dF}{d(U_K^{(n+1)},U_K^{(n)})}-\frac{dF}{d(u_K^{(n+1)},u_K^{(n)})}\right|^2\right\}+\left\{\left\|\boldsymbol{\xi}_1^{(n+\frac{1}{2})}\right\|_{L^2_\mathrm{d}}^2+\left|\xi_{1,0}^{(n+\frac{1}{2})}\right|^2+\left|\xi_{1,K}^{(n+\frac{1}{2})}\right|^2\right\}\\
&\quad+\left\|\boldsymbol{\xi}_2^{(n+\frac{1}{2})}\right\|_{L^2_\mathrm{d}}^2+\left\{\left\|\boldsymbol{\xi}_3^{(n+\frac{1}{2})}\right\|_{L^2_\mathrm{d}}^2+\left|\xi_{3,0}^{(n+\frac{1}{2})}\right|^2+\left|\xi_{3,K}^{(n+\frac{1}{2})}\right|^2\right\}+\left\{\left|\xi_{4,0}^{(n+\frac{1}{2})}\right|^2+\left|\xi_{4,K}^{(n+\frac{1}{2})}\right|^2\right\}.
\end{aligned}\tag{4.59}$$

Next, using Corollary 2.1 (Summation by parts formula), we have

$$\begin{aligned}
&\frac{1}{2\Delta t}\left(\|D\boldsymbol{e}^{(n+1)}\|^2-\|D\boldsymbol{e}^{(n)}\|^2\right)\\
&=\sum_{k=0}^{K-1}\left\{\delta_k^+\left(\frac{e_k^{(n+1)}+e_k^{(n)}}{2}\right)\right\}\left\{\delta_k^+\left(\frac{e_k^{(n+1)}-e_k^{(n)}}{\Delta t}\right)\right\}\Delta x\\
&=-\sum_{k=0}^{K}{}''\left\{\delta_k^{\langle 2\rangle}\left(\frac{e_k^{(n+1)}+e_k^{(n)}}{2}\right)\right\}\frac{e_k^{(n+1)}-e_k^{(n)}}{\Delta t}\Delta x+\left[\left\{\delta_k^{\langle 1\rangle}\left(\frac{e_k^{(n+1)}+e_k^{(n)}}{2}\right)\right\}\frac{e_k^{(n+1)}-e_k^{(n)}}{\Delta t}\right]_0^K.
\end{aligned}\tag{4.60}$$

Applying (4.46) and Corollary 2.1 (Summation by parts formula) to the first term on the right-hand side of (4.60), we obtain

$$\begin{aligned}
&-\sum_{k=0}^{K}{}''\left\{\delta_k^{\langle 2\rangle}\left(\frac{e_k^{(n+1)}+e_k^{(n)}}{2}\right)\right\}\frac{e_k^{(n+1)}-e_k^{(n)}}{\Delta t}\Delta x\\
&\le\sum_{k=0}^{K}{}''\left\{\delta_k^{\langle 2\rangle}\left(\frac{e_k^{(n+1)}+e_k^{(n)}}{2}\right)\right\}\left\{\left(\frac{dF}{d(U_k^{(n+1)},U_k^{(n)})}-\frac{dF}{d(u_k^{(n+1)},u_k^{(n)})}\right)-\xi_{1,k}^{(n+\frac{1}{2})}-\xi_{2,k}^{(n+\frac{1}{2})}-\xi_{3,k}^{(n+\frac{1}{2})}\right\}\Delta x\\
&=-\sum_{k=0}^{K-1}\left\{\delta_k^+\left(\frac{e_k^{(n+1)}+e_k^{(n)}}{2}\right)\right\}\left[\delta_k^+\left\{\left(\frac{dF}{d(U_k^{(n+1)},U_k^{(n)})}-\frac{dF}{d(u_k^{(n+1)},u_k^{(n)})}\right)-\xi_{1,k}^{(n+\frac{1}{2})}-\xi_{2,k}^{(n+\frac{1}{2})}-\xi_{3,k}^{(n+\frac{1}{2})}\right\}\right]\Delta x\\
&\quad+\left[\left\{\delta_k^{\langle 1\rangle}\left(\frac{e_k^{(n+1)}+e_k^{(n)}}{2}\right)\right\}\left\{\left(\frac{dF}{d(U_k^{(n+1)},U_k^{(n)})}-\frac{dF}{d(u_k^{(n+1)},u_k^{(n)})}\right)-\xi_{1,k}^{(n+\frac{1}{2})}-\xi_{2,k}^{(n+\frac{1}{2})}-\xi_{3,k}^{(n+\frac{1}{2})}\right\}\right]_0^K.
\end{aligned}\tag{4.61}$$

Using (4.61), the Young inequality, and the inequality: $(\sum_{i=1}^{n} a_i)^2 \le n \sum_{i=1}^{n} a_i^2$, we get

$$
\begin{aligned}
&-\sum_{k=0}^{K}{}'' \left\{ \delta_k^{\langle 2 \rangle} \left(\frac{e_k^{(n+1)} + e_k^{(n)}}{2} \right) \right\} \frac{e_k^{(n+1)} - e_k^{(n)}}{\Delta t} \Delta x \\
&\le \sum_{k=0}^{K-1} \left\{ \delta_k^{+} \left(\frac{e_k^{(n+1)} + e_k^{(n)}}{2} \right) \right\}^2 \Delta x \\
&\quad + \frac{1}{4} \sum_{k=0}^{K-1} \left[\delta_k^{+} \left\{ \left(\frac{dF}{d(U_k^{(n+1)}, U_k^{(n)})} - \frac{dF}{d(u_k^{(n+1)}, u_k^{(n)})} \right) - \xi_{1,k}^{\left(n+\frac{1}{2}\right)} - \xi_{2,k}^{\left(n+\frac{1}{2}\right)} - \xi_{3,k}^{\left(n+\frac{1}{2}\right)} \right\} \right]^2 \Delta x \\
&\quad + \left[\left\{ \delta_k^{\langle 1 \rangle} \left(\frac{e_k^{(n+1)} + e_k^{(n)}}{2} \right) \right\} \left\{ \left(\frac{dF}{d(U_k^{(n+1)}, U_k^{(n)})} - \frac{dF}{d(u_k^{(n+1)}, u_k^{(n)})} \right) - \xi_{1,k}^{\left(n+\frac{1}{2}\right)} - \xi_{2,k}^{\left(n+\frac{1}{2}\right)} - \xi_{3,k}^{\left(n+\frac{1}{2}\right)} \right\} \right]_0^K \\
&\le \left\| D \left(\frac{\boldsymbol{e}^{(n+1)} + \boldsymbol{e}^{(n)}}{2} \right) \right\|^2 + \left\| D \left(\frac{dF}{d(\boldsymbol{U}^{(n+1)}, \boldsymbol{U}^{(n)})} - \frac{dF}{d(\boldsymbol{u}^{(n+1)}, \boldsymbol{u}^{(n)})} \right) \right\|^2 \\
&\quad + \left\| D \boldsymbol{\xi}_1^{\left(n+\frac{1}{2}\right)} \right\|^2 + \left\| D \boldsymbol{\xi}_2^{\left(n+\frac{1}{2}\right)} \right\|^2 + \left\| D \boldsymbol{\xi}_3^{\left(n+\frac{1}{2}\right)} \right\|^2 \\
&\quad + \left[\left\{ \delta_k^{\langle 1 \rangle} \left(\frac{e_k^{(n+1)} + e_k^{(n)}}{2} \right) \right\} \left\{ \left(\frac{dF}{d(U_k^{(n+1)}, U_k^{(n)})} - \frac{dF}{d(u_k^{(n+1)}, u_k^{(n)})} \right) - \xi_{1,k}^{\left(n+\frac{1}{2}\right)} - \xi_{2,k}^{\left(n+\frac{1}{2}\right)} - \xi_{3,k}^{\left(n+\frac{1}{2}\right)} \right\} \right]_0^K .
\end{aligned}
$$

Thus, we have

$$
\begin{aligned}
&\frac{1}{2\Delta t} \left(\left\| D \boldsymbol{e}^{(n+1)} \right\|^2 - \left\| D \boldsymbol{e}^{(n)} \right\|^2 \right) \\
&\le \left\| D \left(\frac{\boldsymbol{e}^{(n+1)} + \boldsymbol{e}^{(n)}}{2} \right) \right\|^2 + \left\| D \left(\frac{dF}{d(\boldsymbol{U}^{(n+1)}, \boldsymbol{U}^{(n)})} - \frac{dF}{d(\boldsymbol{u}^{(n+1)}, \boldsymbol{u}^{(n)})} \right) \right\|^2 \\
&\quad + \left\| D \boldsymbol{\xi}_1^{\left(n+\frac{1}{2}\right)} \right\|^2 + \left\| D \boldsymbol{\xi}_2^{\left(n+\frac{1}{2}\right)} \right\|^2 + \left\| D \boldsymbol{\xi}_3^{\left(n+\frac{1}{2}\right)} \right\|^2 + \left[\left\{ \delta_k^{\langle 1 \rangle} \left(\frac{e_k^{(n+1)} + e_k^{(n)}}{2} \right) \right\} \right. \\
&\quad \left. \times \left\{ \frac{e_k^{(n+1)} - e_k^{(n)}}{\Delta t} + \left(\frac{dF}{d(U_k^{(n+1)}, U_k^{(n)})} - \frac{dF}{d(u_k^{(n+1)}, u_k^{(n)})} \right) - \xi_{1,k}^{\left(n+\frac{1}{2}\right)} - \xi_{2,k}^{\left(n+\frac{1}{2}\right)} - \xi_{3,k}^{\left(n+\frac{1}{2}\right)} \right\} \right]_0^K .
\end{aligned}
$$

From (4.47), (4.48), and the Young inequality, we estimate the above boundary term as follows:

$$
\begin{aligned}
&\left[\left\{ \delta_k^{\langle 1 \rangle} \left(\frac{e_k^{(n+1)} + e_k^{(n)}}{2} \right) \right\} \left\{ \frac{e_k^{(n+1)} - e_k^{(n)}}{\Delta t} + \left(\frac{dF}{d(U_k^{(n+1)}, U_k^{(n)})} - \frac{dF}{d(u_k^{(n+1)}, u_k^{(n)})} \right) - \xi_{1,k}^{\left(n+\frac{1}{2}\right)} - \xi_{2,k}^{\left(n+\frac{1}{2}\right)} - \xi_{3,k}^{\left(n+\frac{1}{2}\right)} \right\} \right]_0^K \\
&= - \left\{ \delta_k^{\langle 1 \rangle} \left(\frac{e_K^{(n+1)} + e_K^{(n)}}{2} \right) \right\}^2 - \left\{ \delta_k^{\langle 1 \rangle} \left(\frac{e_K^{(n+1)} + e_K^{(n)}}{2} \right) \right\} \left(\xi_{4,K}^{\left(n+\frac{1}{2}\right)} + \xi_{2,K}^{\left(n+\frac{1}{2}\right)} \right) \\
&\quad - \left\{ \delta_k^{\langle 1 \rangle} \left(\frac{e_0^{(n+1)} + e_0^{(n)}}{2} \right) \right\}^2 - \left\{ \delta_k^{\langle 1 \rangle} \left(\frac{e_0^{(n+1)} + e_0^{(n)}}{2} \right) \right\} \left(\xi_{4,0}^{\left(n+\frac{1}{2}\right)} - \xi_{2,0}^{\left(n+\frac{1}{2}\right)} \right) \\
&\le \left| \xi_{2,0}^{\left(n+\frac{1}{2}\right)} \right|^2 + \left| \xi_{2,K}^{\left(n+\frac{1}{2}\right)} \right|^2 + \left| \xi_{4,0}^{\left(n+\frac{1}{2}\right)} \right|^2 + \left| \xi_{4,K}^{\left(n+\frac{1}{2}\right)} \right|^2 .
\end{aligned}
$$

Namely, we have

$$\begin{aligned}
&\frac{1}{2\Delta t}\left(\left\|D\boldsymbol{e}^{(n+1)}\right\|^2-\left\|D\boldsymbol{e}^{(n)}\right\|^2\right)\\
&\le\left\|D\left(\frac{\boldsymbol{e}^{(n+1)}+\boldsymbol{e}^{(n)}}{2}\right)\right\|^2+\left\|D\left(\frac{dF}{d(\boldsymbol{U}^{(n+1)},\boldsymbol{U}^{(n)})}-\frac{dF}{d(\boldsymbol{u}^{(n+1)},\boldsymbol{u}^{(n)})}\right)\right\|^2+\left\|D\boldsymbol{\xi}_1^{\left(n+\frac{1}{2}\right)}\right\|^2\\
&\quad+\left\|D\boldsymbol{\xi}_2^{\left(n+\frac{1}{2}\right)}\right\|^2+\left\|D\boldsymbol{\xi}_3^{\left(n+\frac{1}{2}\right)}\right\|^2+\left|\xi_{2,0}^{\left(n+\frac{1}{2}\right)}\right|^2+\left|\xi_{2,K}^{\left(n+\frac{1}{2}\right)}\right|^2+\left|\xi_{4,0}^{\left(n+\frac{1}{2}\right)}\right|^2+\left|\xi_{4,K}^{\left(n+\frac{1}{2}\right)}\right|^2. \qquad (4.62)
\end{aligned}$$

Combining (4.59) and (4.62), we obtain

$$\begin{aligned}
&\frac{1}{2\Delta t}\left(\left\|\boldsymbol{e}^{(n+1)}\right\|_{\tilde{H}^1_{\mathrm{d}}}^2-\left\|\boldsymbol{e}^{(n)}\right\|_{\tilde{H}^1_{\mathrm{d}}}^2\right)\\
&\le-\frac{\left|e_0^{(n+1)}\right|^2-\left|e_0^{(n)}\right|^2}{2\Delta t}-\frac{\left|e_K^{(n+1)}\right|^2-\left|e_K^{(n)}\right|^2}{2\Delta t}\\
&\quad+\frac{1}{2}\left\{\left\|\boldsymbol{e}^{(n+1)}\right\|_{\tilde{H}^1_{\mathrm{d}}}^2+\left|e_0^{(n+1)}\right|^2+\left|e_K^{(n+1)}\right|^2\right\}+\frac{1}{2}\left\{\left\|\boldsymbol{e}^{(n)}\right\|_{\tilde{H}^1_{\mathrm{d}}}^2+\left|e_0^{(n)}\right|^2+\left|e_K^{(n)}\right|^2\right\}\\
&\quad+\left\{\left\|\frac{dF}{d(\boldsymbol{U}^{(n+1)},\boldsymbol{U}^{(n)})}-\frac{dF}{d(\boldsymbol{u}^{(n+1)},\boldsymbol{u}^{(n)})}\right\|_{\tilde{H}^1_{\mathrm{d}}}^2+\left|\frac{dF}{d(U_0^{(n+1)},U_0^{(n)})}-\frac{dF}{d(u_0^{(n+1)},u_0^{(n)})}\right|^2\right.\\
&\quad\left.+\left|\frac{dF}{d(U_K^{(n+1)},U_K^{(n)})}-\frac{dF}{d(u_K^{(n+1)},u_K^{(n)})}\right|^2\right\}+\xi^{\left(n+\frac{1}{2}\right)}. \qquad (4.63)
\end{aligned}$$

Multiplying both sides of (4.63) by $2\Delta t$, we get

$$\begin{aligned}
&(1-\Delta t)\left\{\left\|\boldsymbol{e}^{(n+1)}\right\|_{\tilde{H}^1_{\mathrm{d}}}^2+\left|e_0^{(n+1)}\right|^2+\left|e_K^{(n+1)}\right|^2\right\}\\
&\le(1+\Delta t)\left\{\left\|\boldsymbol{e}^{(n)}\right\|_{\tilde{H}^1_{\mathrm{d}}}^2+\left|e_0^{(n)}\right|^2+\left|e_K^{(n)}\right|^2\right\}\\
&\quad+2\Delta t\left\{\left\|\frac{dF}{d(\boldsymbol{U}^{(n+1)},\boldsymbol{U}^{(n)})}-\frac{dF}{d(\boldsymbol{u}^{(n+1)},\boldsymbol{u}^{(n)})}\right\|_{\tilde{H}^1_{\mathrm{d}}}^2+\left|\frac{dF}{d(U_0^{(n+1)},U_0^{(n)})}-\frac{dF}{d(u_0^{(n+1)},u_0^{(n)})}\right|^2\right.\\
&\quad\left.+\left|\frac{dF}{d(U_K^{(n+1)},U_K^{(n)})}-\frac{dF}{d(u_K^{(n+1)},u_K^{(n)})}\right|^2\right\}+2\Delta t\xi^{\left(n+\frac{1}{2}\right)}. \qquad (4.64)
\end{aligned}$$

Next, it follows from Lemma 2.2 that

$$\begin{aligned}
\frac{dF}{d(U_k^{(n+1)},U_k^{(n)})}-\frac{dF}{d(u_k^{(n+1)},u_k^{(n)})}&=\frac{1}{2}\bar{F}''\left(U_k^{(n+1)},u_k^{(n+1)};U_k^{(n)},u_k^{(n)}\right)e_k^{(n+1)}\\
&\quad+\frac{1}{2}\bar{F}''\left(U_k^{(n)},u_k^{(n)};U_k^{(n+1)},u_k^{(n+1)}\right)e_k^{(n)} \quad (k=0,\dots,K).
\end{aligned} \qquad (4.65)$$

From the assumption (4.52), using Lemma 2.1, we have

$$\left\|\bar{F}''\left(\boldsymbol{U}^{(n+1)},\boldsymbol{u}^{(n+1)};\boldsymbol{U}^{(n)},\boldsymbol{u}^{(n)}\right)\right\|_{L^\infty_{\mathrm{d}}}\le C_{F,2},\quad \left\|\bar{F}''\left(\boldsymbol{U}^{(n)},\boldsymbol{u}^{(n)};\boldsymbol{U}^{(n+1)},\boldsymbol{u}^{(n+1)}\right)\right\|_{L^\infty_{\mathrm{d}}}\le C_{F,2}, \qquad (4.66)$$

where $C_{F,i}$ $(i=2,3)$ is defined by

$$C_{F,i} := \max_{|\xi|\le C_2} \left|F^{(i)}(\xi)\right| \quad (i=2,3).$$

Hence, we obtain

$$\left|\frac{dF}{d(U_k^{(n+1)},U_k^{(n)})} - \frac{dF}{d(u_k^{(n+1)},u_k^{(n)})}\right|^2 \le \frac{C_{F,2}^2}{2}\left(\left|e_k^{(n+1)}\right|^2 + \left|e_k^{(n)}\right|^2\right) \quad (k=0,\dots,K). \quad (4.67)$$

Thus, we have

$$\left\|\frac{dF}{d\left(\boldsymbol{U}^{(n+1)},\boldsymbol{U}^{(n)}\right)} - \frac{dF}{d\left(\boldsymbol{u}^{(n+1)},\boldsymbol{u}^{(n)}\right)}\right\|_{L_{\mathrm{d}}^2}^2 \le \frac{C_{F,2}^2}{2}\left(\left\|\boldsymbol{e}^{(n+1)}\right\|_{L_{\mathrm{d}}^2}^2 + \left\|\boldsymbol{e}^{(n)}\right\|_{L_{\mathrm{d}}^2}^2\right). \quad (4.68)$$

Next, using (4.65) and Lemma 2.3, we obtain

$$\begin{aligned}\left\|D\left(\frac{dF}{d\left(\boldsymbol{U}^{(n+1)},\boldsymbol{U}^{(n)}\right)} - \frac{dF}{d\left(\boldsymbol{u}^{(n+1)},\boldsymbol{u}^{(n)}\right)}\right)\right\| &\le \frac{1}{2}\left\|D\left(\bar{F}''\left(\boldsymbol{U}^{(n+1)},\boldsymbol{u}^{(n+1)};\boldsymbol{U}^{(n)},\boldsymbol{u}^{(n)}\right)\boldsymbol{e}^{(n+1)}\right)\right\| \\ &\quad + \frac{1}{2}\left\|D\left(\bar{F}''\left(\boldsymbol{U}^{(n)},\boldsymbol{u}^{(n)};\boldsymbol{U}^{(n+1)},\boldsymbol{u}^{(n+1)}\right)\boldsymbol{e}^{(n)}\right)\right\| \\ &\le \frac{1}{2}\left\|D\bar{F}''\left(\boldsymbol{U}^{(n+1)},\boldsymbol{u}^{(n+1)};\boldsymbol{U}^{(n)},\boldsymbol{u}^{(n)}\right)\right\|\left\|\boldsymbol{e}^{(n+1)}\right\|_{L_{\mathrm{d}}^\infty} \\ &\quad + \frac{1}{2}\left\|\bar{F}''\left(\boldsymbol{U}^{(n+1)},\boldsymbol{u}^{(n+1)};\boldsymbol{U}^{(n)},\boldsymbol{u}^{(n)}\right)\right\|_{L_{\mathrm{d}}^\infty}\left\|D\boldsymbol{e}^{(n+1)}\right\| \\ &\quad + \frac{1}{2}\left\|D\bar{F}''\left(\boldsymbol{U}^{(n)},\boldsymbol{u}^{(n)};\boldsymbol{U}^{(n+1)},\boldsymbol{u}^{(n+1)}\right)\right\|\left\|\boldsymbol{e}^{(n)}\right\|_{L_{\mathrm{d}}^\infty} \\ &\quad + \frac{1}{2}\left\|\bar{F}''\left(\boldsymbol{U}^{(n)},\boldsymbol{u}^{(n)};\boldsymbol{U}^{(n+1)},\boldsymbol{u}^{(n+1)}\right)\right\|_{L_{\mathrm{d}}^\infty}\left\|D\boldsymbol{e}^{(n)}\right\|.\end{aligned} \quad (4.69)$$

From the assumption (4.52), using Lemma 2.4, we get

$$\left\|D\bar{F}''\left(\boldsymbol{U}^{(n+1)},\boldsymbol{u}^{(n+1)};\boldsymbol{U}^{(n)},\boldsymbol{u}^{(n)}\right)\right\| \le \frac{C_{F,3}}{6}\left(2C_1+2C_1+C_1+C_1\right) = C_1C_{F,3}. \quad (4.70)$$

Similarly, it holds that

$$\left\|D\bar{F}''\left(\boldsymbol{U}^{(n)},\boldsymbol{u}^{(n)};\boldsymbol{U}^{(n+1)},\boldsymbol{u}^{(n+1)}\right)\right\| \le C_1C_{F,3}. \quad (4.71)$$

Therefore, applying (4.66), (4.70), and (4.71) to (4.69), we obtain

$$\begin{aligned}\left\|D\left(\frac{dF}{d\left(\boldsymbol{U}^{(n+1)},\boldsymbol{U}^{(n)}\right)} - \frac{dF}{d\left(\boldsymbol{u}^{(n+1)},\boldsymbol{u}^{(n)}\right)}\right)\right\|^2 &\le C_1^2C_{F,3}^2\left(\left\|\boldsymbol{e}^{(n+1)}\right\|_{L_{\mathrm{d}}^\infty}^2 + \left\|\boldsymbol{e}^{(n)}\right\|_{L_{\mathrm{d}}^\infty}^2\right) \\ &\quad + C_{F,2}^2\left(\left\|D\boldsymbol{e}^{(n+1)}\right\|^2 + \left\|D\boldsymbol{e}^{(n)}\right\|^2\right).\end{aligned} \quad (4.72)$$

Combining (4.68) and (4.72), we have

$$\begin{aligned}\left\|\frac{dF}{d\left(\boldsymbol{U}^{(n+1)},\boldsymbol{U}^{(n)}\right)} - \frac{dF}{d\left(\boldsymbol{u}^{(n+1)},\boldsymbol{u}^{(n)}\right)}\right\|_{\tilde{H}_{\mathrm{d}}^1}^2 &\le C_1^2C_{F,3}^2\left(\left\|\boldsymbol{e}^{(n+1)}\right\|_{L_{\mathrm{d}}^\infty}^2 + \left\|\boldsymbol{e}^{(n)}\right\|_{L_{\mathrm{d}}^\infty}^2\right) \\ &\quad + C_{F,2}^2\left(\left\|\boldsymbol{e}^{(n+1)}\right\|_{\tilde{H}_{\mathrm{d}}^1}^2 + \left\|\boldsymbol{e}^{(n)}\right\|_{\tilde{H}_{\mathrm{d}}^1}^2\right).\end{aligned}$$

Furthermore, using Proposition 2.5, we get the following estimate:

$$C_1^2 C_{F,3}^2 \left(\|\boldsymbol{e}^{(n+1)}\|_{L_{\rm d}^\infty}^2 + \|\boldsymbol{e}^{(n)}\|_{L_{\rm d}^\infty}^2\right) \le C_1^2 \tilde{C}_L^2 C_{F,3}^2 \left(\|\boldsymbol{e}^{(n+1)}\|_{\tilde{H}_{\rm d}^1}^2 + \|\boldsymbol{e}^{(n)}\|_{\tilde{H}_{\rm d}^1}^2\right).$$

Thus, we have

$$\left\| \frac{dF}{d\left(\boldsymbol{U}^{(n+1)}, \boldsymbol{U}^{(n)}\right)} - \frac{dF}{d\left(\boldsymbol{u}^{(n+1)}, \boldsymbol{u}^{(n)}\right)} \right\|_{\tilde{H}_{\rm d}^1}^2 \le \frac{C_F}{2} \left(\|\boldsymbol{e}^{(n+1)}\|_{\tilde{H}_{\rm d}^1}^2 + \|\boldsymbol{e}^{(n)}\|_{\tilde{H}_{\rm d}^1}^2\right). \tag{4.73}$$

Therefore, using (4.67) and (4.73), we obtain

$$\begin{aligned} &\left\| \frac{dF}{d(\boldsymbol{U}^{(n+1)}, \boldsymbol{U}^{(n)})} - \frac{dF}{d(\boldsymbol{u}^{(n+1)}, \boldsymbol{u}^{(n)})} \right\|_{\tilde{H}_{\rm d}^1}^2 + \left| \frac{dF}{d(U_0^{(n+1)}, U_0^{(n)})} - \frac{dF}{d(u_0^{(n+1)}, u_0^{(n)})} \right|^2 \\ &+ \left| \frac{dF}{d(U_K^{(n+1)}, U_K^{(n)})} - \frac{dF}{d(u_K^{(n+1)}, u_K^{(n)})} \right|^2 \\ &\le \frac{C_F}{2} \left\{ \left(\|\boldsymbol{e}^{(n+1)}\|_{\tilde{H}_{\rm d}^1}^2 + \left|e_0^{(n+1)}\right|^2 + \left|e_K^{(n+1)}\right|^2 \right) + \left(\|\boldsymbol{e}^{(n)}\|_{\tilde{H}_{\rm d}^1}^2 + \left|e_0^{(n)}\right|^2 + \left|e_K^{(n)}\right|^2 \right) \right\}. \end{aligned} \tag{4.74}$$

Applying (4.74) to (4.64), we obtain

$$\begin{aligned} &\{1 - (1 + C_F)\Delta t\} \left\{ \|\boldsymbol{e}^{(n+1)}\|_{\tilde{H}_{\rm d}^1}^2 + \left|e_0^{(n+1)}\right|^2 + \left|e_K^{(n+1)}\right|^2 \right\} \\ &\le \{1 + (1 + C_F)\Delta t\} \left\{ \|\boldsymbol{e}^{(n)}\|_{\tilde{H}_{\rm d}^1}^2 + \left|e_0^{(n)}\right|^2 + \left|e_K^{(n)}\right|^2 \right\} + 2\Delta t \xi^{\left(n+\frac{1}{2}\right)}. \end{aligned}$$

This completes the proof. □

Corollary 4.1. Assume that the problem (4.1)–(4.3) with an initial value has a smooth solution u that satisfies $u \in C^5([0, L] \times [0, T])$. In the same manner, as Theorem 4.5, denote the bounds by (4.52). If Δt satisfies

$$\Delta t < \frac{1}{3(1 + C_F)}, \tag{4.75}$$

then there exists a constant C independent of k and m such that

$$\|\boldsymbol{e}^{(n)}\|_{L_{\rm d}^\infty} \le C\left((\Delta x)^2 + (\Delta t)^2\right) \quad (n = 1, \ldots, N).$$

Proof. If $0 < \Delta t \le 1/(3a)$ for all $a > 0$, then two following inequalities hold:

$$\frac{1 + a\Delta t}{1 - a\Delta t} \le 1 + 3a\Delta t, \quad \frac{1}{1 - a\Delta t} \le \frac{3}{2}. \tag{4.76}$$

From (4.75), using Theorem 4.5 and (4.76), we obtain

$$\begin{aligned} \|\boldsymbol{e}^{(n+1)}\|_{\tilde{H}_{\rm d}^1}^2 + \left|e_0^{(n+1)}\right|^2 + \left|e_K^{(n+1)}\right|^2 &\le \{1 + 3(1 + C_F)\Delta t\} \left\{ \|\boldsymbol{e}^{(n)}\|_{\tilde{H}_{\rm d}^1}^2 + \left|e_0^{(n)}\right|^2 + \left|e_K^{(n)}\right|^2 \right\} \\ &\quad + 3\Delta t \xi^{\left(n+\frac{1}{2}\right)} \quad (n = 0, 1, \ldots, N-1). \end{aligned} \tag{4.77}$$

Let $C_3 := 1 + 3(1 + C_F)\Delta t$, and by using (4.77) repeatedly, we obtain

$$\begin{aligned}
&\|\boldsymbol{e}^{(n)}\|_{\tilde{H}^1_{\mathrm{d}}}^2 + \left|e_0^{(n)}\right|^2 + \left|e_K^{(n)}\right|^2 \\
&\le C_3 \left\{ \|\boldsymbol{e}^{(n-1)}\|_{\tilde{H}^1_{\mathrm{d}}}^2 + \left|e_0^{(n-1)}\right|^2 + \left|e_K^{(n-1)}\right|^2 \right\} + 3\Delta t \xi^{\left(n-1+\frac{1}{2}\right)} \\
&\le C_3^2 \left\{ \|\boldsymbol{e}^{(n-2)}\|_{\tilde{H}^1_{\mathrm{d}}}^2 + \left|e_0^{(n-2)}\right|^2 + \left|e_K^{(n-2)}\right|^2 \right\} + 3\Delta t C_3 \xi^{\left(n-2+\frac{1}{2}\right)} + 3\Delta t \xi^{\left(n-1+\frac{1}{2}\right)} \\
&\le \cdots \\
&\le C_3^n \left\{ \|\boldsymbol{e}^{(0)}\|_{\tilde{H}^1_{\mathrm{d}}}^2 + \left|e_0^{(0)}\right|^2 + \left|e_K^{(0)}\right|^2 \right\} + 3\Delta t \sum_{j=1}^{n} C_3^{j-1} \xi^{\left(n-j+\frac{1}{2}\right)} \\
&= 3\Delta t \sum_{j=1}^{n} C_3^{j-1} \xi^{\left(n-j+\frac{1}{2}\right)} \quad (n = 1, \ldots, N),
\end{aligned}$$

where the last equality holds from $\boldsymbol{e}^{(0)} = \mathbf{0}$. Since it holds that $1 \le C_3$, using the following inequality: $1 + x \le \exp(x)$ for all $x > 0$, we get

$$C_3^{j-1} \le C_3^N = \{1 + 3(1 + C_F)\Delta t\}^N \le \exp\left\{ N \cdot 3(1 + C_F) \frac{T}{N} \right\} = \exp\{3(1 + C_F)T\}$$

for $j = 1, \ldots, N$. Therefore, we obtain

$$\|\boldsymbol{e}^{(n)}\|_{\tilde{H}^1_{\mathrm{d}}}^2 + \left|e_0^{(n)}\right|^2 + \left|e_K^{(n)}\right|^2 \le 3\Delta t \exp\{3(1 + C_F)T\} \sum_{j=1}^{n} \xi^{\left(n-j+\frac{1}{2}\right)} \quad (n = 1, \ldots, N). \tag{4.78}$$

Next, we estimate ξ. Let us define

$$M_{i,j}(v) := \max\left\{ \left| \frac{\partial^{i+j} v}{\partial x^i \partial t^j} \right| ; (x,t) \in [0,L] \times [0,T] \right\} \quad \text{for all } i, j \in \mathbb{Z}.$$

Firstly, we consider $\boldsymbol{\xi}_4$. For any $x \in [0, L]$, applying the Taylor theorem to $\tilde{u}$, there exists $\theta_1 \in (0, 1)$ such that

$$\begin{aligned}
&\frac{\tilde{u}(x, (n+1)\Delta t) + \tilde{u}(x, n\Delta t)}{2} \\
&= \tilde{u}\left(x, \left(n + \frac{1}{2}\right)\Delta t\right) + \frac{(\Delta t)^2}{16} \left\{ \partial_t^2 \tilde{u}\left(x, \left(n + \frac{1+\theta_1}{2}\right)\Delta t\right) + \partial_t^2 \tilde{u}\left(x, \left(n + \frac{1-\theta_1}{2}\right)\Delta t\right) \right\}.
\end{aligned} \tag{4.79}$$

Substituting $k\Delta x$ ($k = 0, K$) into x in (4.79), we obtain

$$\begin{aligned}
&\left| \delta_k^{\langle 1 \rangle} \left(\frac{\tilde{u}_k^{(n+1)} + \tilde{u}_k^{(n)}}{2} \right) - \partial_x u_k^{\left(n+\frac{1}{2}\right)} \right| \\
&= \left| \delta_k^{\langle 1 \rangle} \tilde{u}_k^{\left(n+\frac{1}{2}\right)} + \frac{(\Delta t)^2}{16} \delta_k^{\langle 1 \rangle} \left(\partial_t^2 \tilde{u}_k^{\left(n+\frac{1+\theta_1}{2}\right)} + \partial_t^2 \tilde{u}_k^{\left(n+\frac{1-\theta_1}{2}\right)} \right) - \partial_x u_k^{\left(n+\frac{1}{2}\right)} \right| \\
&\le \left| \delta_k^{\langle 1 \rangle} \tilde{u}_k^{\left(n+\frac{1}{2}\right)} - \partial_x u_k^{\left(n+\frac{1}{2}\right)} \right| + \frac{(\Delta t)^2}{16} \left(\left| \delta_k^{\langle 1 \rangle} \left(\partial_t^2 \tilde{u}_k^{\left(n+\frac{1+\theta_1}{2}\right)} \right) \right| + \left| \delta_k^{\langle 1 \rangle} \left(\partial_t^2 \tilde{u}_k^{\left(n+\frac{1-\theta_1}{2}\right)} \right) \right| \right) \quad (k = 0, K).
\end{aligned}$$

Here, we consider the case of $k = 0$. For any $t \in [0, T]$, from the definition of $\tilde{u}$, we have

$$\tilde{u}(-\Delta x, t) = u(\Delta x, t) - 2\Delta x \partial_x u(0, t) - \frac{(\Delta x)^3}{3} \partial_x^3 u(0, t). \tag{4.80}$$

Hence, substituting $(n + 1/2)\Delta t$ into t in (4.80), we get

$$\begin{aligned}
\left| \delta_k^{\langle 1 \rangle} \tilde{u}_0^{\left(n+\frac{1}{2}\right)} - \partial_x u_0^{\left(n+\frac{1}{2}\right)} \right| &= \left| \frac{\tilde{u}_1^{\left(n+\frac{1}{2}\right)} - \tilde{u}_{-1}^{\left(n+\frac{1}{2}\right)}}{2\Delta x} - \partial_x u_0^{\left(n+\frac{1}{2}\right)} \right| \\
&= \left| \frac{u_1^{\left(n+\frac{1}{2}\right)} - u_1^{\left(n+\frac{1}{2}\right)} + 2\Delta x \partial_x u_0^{\left(n+\frac{1}{2}\right)} + \frac{(\Delta x)^3}{3} \partial_x^3 u_0^{\left(n+\frac{1}{2}\right)}}{2\Delta x} - \partial_x u_0^{\left(n+\frac{1}{2}\right)} \right| \\
&\leq \frac{(\Delta x)^2}{6} M_{3,0}(u).
\end{aligned}$$

Also, for any $t \in [0, T]$, using the definition of $\tilde{u}$ again, the following equality holds:

$$\partial_t^2 \tilde{u}(-\Delta x, t) = \partial_t^2 u(\Delta x, t) - 2\Delta x \partial_t^2 \partial_x u(0, t) - \frac{(\Delta x)^3}{3} \partial_t^2 \partial_x^3 u(0, t). \tag{4.81}$$

Hence, substituting $(n + (1 \pm \theta_1)/2)\Delta t$ into t in (4.81), we obtain

$$\delta_k^{\langle 1 \rangle} \left(\partial_t^2 \tilde{u}_0^{\left(n+\frac{1\pm\theta_1}{2}\right)} \right) = \frac{\partial_t^2 \tilde{u}_1^{\left(n+\frac{1\pm\theta_1}{2}\right)} - \partial_t^2 \tilde{u}_{-1}^{\left(n+\frac{1\pm\theta_1}{2}\right)}}{2\Delta x} = \partial_t^2 \partial_x u_0^{\left(n+\frac{1\pm\theta_1}{2}\right)} + \frac{(\Delta x)^2}{6} \partial_t^2 \partial_x^3 u_0^{\left(n+\frac{1\pm\theta_1}{2}\right)}.$$

Therefore, we get

$$\left| \delta_k^{\langle 1 \rangle} \left(\partial_t^2 \tilde{u}_0^{\left(n+\frac{1\pm\theta_1}{2}\right)} \right) \right| \leq M_{1,2}(u) + \frac{(\Delta x)^2}{6} M_{3,2}(u).$$

Hence, we conclude that

$$\left| \delta_k^{\langle 1 \rangle} \left(\frac{\tilde{u}_k^{(n+1)} + \tilde{u}_k^{(n)}}{2} \right) - \partial_x u_k^{\left(n+\frac{1}{2}\right)} \right| \leq \frac{(\Delta x)^2}{6} M_{3,0}(u) + \frac{(\Delta t)^2}{8} M_{1,2}(u) + \frac{(\Delta t)^2 (\Delta x)^2}{48} M_{3,2}(u)$$

for $k = 0$. In the same manner, the above equality holds in the case of $k = K$, too. From the assumption (4.75) for Δt and the following inequality: $1 + C_F \geq 1$, we get

$$\Delta t < \frac{1}{3(1 + C_F)} \leq \frac{1}{3} < 1. \tag{4.82}$$

Thus, we obtain the following estimate:

$$\begin{aligned}
\left| \xi_{4,k}^{\left(n+\frac{1}{2}\right)} \right| &= \left| \delta_k^{\langle 1 \rangle} \left(\frac{\tilde{u}_k^{(n+1)} + \tilde{u}_k^{(n)}}{2} \right) - \partial_x u_k^{\left(n+\frac{1}{2}\right)} \right| \\
&\leq (\Delta x)^2 \left(\frac{1}{6} M_{3,0}(u) + \frac{1}{48} M_{3,2}(u) \right) + \frac{(\Delta t)^2}{8} M_{1,2}(u) \quad (k = 0, K).
\end{aligned}$$

Next, we consider $\boldsymbol{\xi}_2$. Substituting $k\Delta x$ $(k=0,\dots,K)$ into x in (4.79), we obtain

$$\delta_k^{\langle 2\rangle}\left(\frac{\tilde{u}_k^{(n+1)}+\tilde{u}_k^{(n)}}{2}\right)-\partial_x^2 u_k^{\left(n+\frac{1}{2}\right)}$$
$$=\delta_k^{\langle 2\rangle}\tilde{u}_k^{\left(n+\frac{1}{2}\right)}-\partial_x^2 u_k^{\left(n+\frac{1}{2}\right)}+\frac{(\Delta t)^2}{16}\left\{\delta_k^{\langle 2\rangle}\left(\partial_t^2\tilde{u}_k^{\left(n+\frac{1+\theta_1}{2}\right)}\right)+\delta_k^{\langle 2\rangle}\left(\partial_t^2\tilde{u}_k^{\left(n+\frac{1-\theta_1}{2}\right)}\right)\right\}\quad (k=0,\dots,K). \tag{4.83}$$

For any $t\in[0,T]$ and $k=0,\dots,K$, applying the Taylor theorem to $\tilde{u}$, there exists $\theta_2\in(0,1)$ such that

$$\frac{\tilde{u}((k+1)\Delta x,t)-2\tilde{u}(k\Delta x,t)+\tilde{u}((k-1)\Delta x,t)}{(\Delta x)^2}-\partial_x^2\tilde{u}(k\Delta x,t)$$
$$=\frac{(\Delta x)^2}{24}\left\{\partial_x^4\tilde{u}((k+\theta_2)\Delta x,t)+\partial_x^4\tilde{u}((k-\theta_2)\Delta x,t)\right\}. \tag{4.84}$$

It holds from the definition of $\tilde{u}$ that $\partial_x^4\tilde{u}(x,t)=\partial_x^4 u(-x,t)$ for all $x\in[-\Delta x,0)$. Hence, we have $\partial_x^4\tilde{u}(-\theta_2\Delta x,t)=\partial_x^4 u(\theta_2\Delta x,t)$. Similarly, we obtain $\partial_x^4\tilde{u}((K+\theta_2)\Delta x,t)=\partial_x^4\tilde{u}((K-\theta_2)\Delta x,t)$. Namely, substituting $(n+1/2)\Delta t$ into t in (4.84), we get

$$\delta_k^{\langle 2\rangle}\tilde{u}_k^{\left(n+\frac{1}{2}\right)}-\partial_x^2 u_k^{\left(n+\frac{1}{2}\right)}=\begin{cases}\dfrac{(\Delta x)^2}{12}\partial_x^4 u_{\theta_2}^{\left(n+\frac{1}{2}\right)}, & (k=0),\\ \dfrac{(\Delta x)^4}{24}\left(\partial_x^4 u_{k+\theta_2}^{\left(n+\frac{1}{2}\right)}+\partial_x^4 u_{k-\theta_2}^{\left(m+\frac{1}{2}\right)}\right), & (k=1,\dots,K-1),\\ \dfrac{(\Delta x)^2}{12}\partial_x^4 u_{K-\theta_2}^{\left(n+\frac{1}{2}\right)}, & (k=K).\end{cases}$$

Hence, we conclude that

$$\left|\delta_k^{\langle 2\rangle}\tilde{u}_k^{\left(n+\frac{1}{2}\right)}-\partial_x^2 u_k^{\left(n+\frac{1}{2}\right)}\right|\le\frac{(\Delta x)^2}{12}M_{4,0}(u)\quad (k=0,\dots,K).$$

In the same manner, as described above, we have

$$\left|\delta_k^{\langle 2\rangle}\left(\partial_t^2\tilde{u}_k^{\left(n+\frac{1\pm\theta_1}{2}\right)}\right)\right|\le M_{2,2}(u)+\Delta x M_{3,2}(u)\quad (k=0,\dots,K). \tag{4.85}$$

In fact, for any $t\in[0,T]$ and $k=0,\dots,K$, applying the Taylor theorem to $\partial_t^2\tilde{u}$, there exists $\theta_3\in(0,1)$ such that

$$\frac{\partial_t^2\tilde{u}((k+1)\Delta x,t)-2\partial_t^2\tilde{u}(k\Delta x,t)+\partial_t^2\tilde{u}((k-1)\Delta x,t)}{(\Delta x)^2}$$
$$=\frac{1}{2}\left\{\partial_x^2\partial_t^2\tilde{u}((k+\theta_3)\Delta x,t)+\partial_x^2\partial_t^2\tilde{u}((k-\theta_3)\Delta x,t)\right\}. \tag{4.86}$$

It holds from the definition of $\tilde{u}$ that $\partial_x^2\partial_t^2\tilde{u}(x,t)=\partial_x^2\partial_t^2 u(-x,t)+2x\partial_t^2\partial_x^3 u(0,t)$ for all $x\in[-\Delta x,0)$. Hence, we have

$$\partial_x^2\partial_t^2\tilde{u}(-\theta_3\Delta x,t)=\partial_x^2\partial_t^2 u(\theta_3\Delta x,t)-2\theta_3\Delta x\partial_t^2\partial_x^3 u(0,t).$$

In the same manner, we obtain

$$\partial_x^2\partial_t^2\tilde{u}((K+\theta_3)\Delta x,t)=\partial_x^2\partial_t^2 u((K-\theta_3)\Delta x,t)+2\theta_3\Delta x\partial_t^2\partial_x^3 u(K\Delta x,t).$$

Namely, substituting $(n+(1\pm\theta_1)/2)\Delta t$ into t in (4.86), we get

$$\delta_k^{\langle 2\rangle}\left(\partial_t^2\tilde{u}_k^{\left(n+\frac{1\pm\theta_1}{2}\right)}\right)=\begin{cases}\partial_x^2\partial_t^2 u_{\theta_3}^{\left(n+\frac{1\pm\theta_1}{2}\right)}-\theta_3\Delta x\partial_t^2\partial_x^3 u_0^{\left(n+\frac{1\pm\theta_1}{2}\right)}, & (k=0),\\ \dfrac{1}{2}\left(\partial_x^2\partial_t^2 u_{k+\theta_3}^{\left(n+\frac{1\pm\theta_1}{2}\right)}+\partial_x^2\partial_t^2 u_{k-\theta_3}^{\left(n+\frac{1\pm\theta_1}{2}\right)}\right), & (k=1,\ldots,K-1),\\ \partial_x^2\partial_t^2 u_{K-\theta_3}^{\left(n+\frac{1\pm\theta_1}{2}\right)}+\theta_3\Delta x\partial_t^2\partial_x^3 u_K^{\left(n+\frac{1\pm\theta_1}{2}\right)}, & (k=K).\end{cases}$$

Therefore, we conclude that

$$\left|\delta_k^{\langle 2\rangle}\left(\partial_t^2\tilde{u}_k^{\left(n+\frac{1\pm\theta_1}{2}\right)}\right)\right|\le M_{2,2}(u)\le M_{2,2}(u)+\Delta x M_{3,2}(u)\quad(k=1,\ldots,K-1),$$
$$\left|\delta_k^{\langle 2\rangle}\left(\partial_t^2\tilde{u}_k^{\left(n+\frac{1\pm\theta_1}{2}\right)}\right)\right|\le M_{2,2}(u)+\Delta x M_{3,2}(u)\quad(k=0,K).$$

Thus, we have (4.85). Hence, using the Young inequality and the following inequality: $(\Delta t)^4<(\Delta t)^2$ obtained by (4.82), we obtain

$$\begin{aligned}\left|\xi_{2,k}^{\left(n+\frac{1}{2}\right)}\right|&\le\left|\delta_k^{\langle 2\rangle}\tilde{u}_k^{\left(n+\frac{1}{2}\right)}-\partial_x^2 u_k^{\left(n+\frac{1}{2}\right)}\right|+\frac{(\Delta t)^2}{16}\left\{\left|\delta_k^{\langle 2\rangle}\left(\partial_t^2\tilde{u}_k^{\left(n+\frac{1+\theta_1}{2}\right)}\right)\right|+\left|\delta_k^{\langle 2\rangle}\left(\partial_t^2\tilde{u}_k^{\left(n+\frac{1-\theta_1}{2}\right)}\right)\right|\right\}\\&\le\frac{(\Delta x)^2}{12}M_{4,0}(u)+\frac{(\Delta t)^2}{8}M_{2,2}(u)+\frac{\Delta x(\Delta t)^2}{8}M_{3,2}(u)\\&\le\frac{(\Delta x)^2}{12}M_{4,0}(u)+\frac{(\Delta t)^2}{8}M_{2,2}(u)+\frac{(\Delta x)^2}{16}M_{3,2}(u)+\frac{(\Delta t)^4}{16}M_{3,2}(u)\\&\le(\Delta x)^2\left(\frac{1}{12}M_{4,0}(u)+\frac{1}{16}M_{3,2}(u)\right)+(\Delta t)^2\left(\frac{1}{8}M_{2,2}(u)+\frac{1}{16}M_{3,2}(u)\right).\end{aligned}$$

Similarly, we see from the Taylor theorem that

$$\left|\xi_{1,k}^{\left(n+\frac{1}{2}\right)}\right|\le CM_{0,3}(u)(\Delta t)^2\quad(k=0,\ldots,K),$$
$$\left|\xi_{3,k}^{\left(n+\frac{1}{2}\right)}\right|\le C\left\{C_{F,2}M_{0,2}(u)+C_{F,3}\left(M_{0,1}(u)\right)^2\right\}(\Delta t)^2\quad(k=0,\ldots,K).$$

As a remark, throughout this proof, we need the reader to keep in mind that the meaning of C changes from line to line, whereas C always denotes those constants. From the regularity assumption of the solution u and the potential F, we see that $C_{F,i}$ $(i=2,3)$ and $M_{i,j}(u)$ $(i,j\in\mathbb{Z},0\le i+j\le 5)$ are bounded. Thus, we obtain following estimates:

$$\left|\xi_{i,k}^{\left(n+\frac{1}{2}\right)}\right|\le C_4((\Delta x)^2+(\Delta t)^2)\quad(k=0,\ldots,K,\ i=1,2,3),\tag{4.87}$$
$$\left|\xi_{4,k}^{\left(n+\frac{1}{2}\right)}\right|\le C_4((\Delta x)^2+(\Delta t)^2)\quad(k=0,K),\tag{4.88}$$

where C_4 is a constant. In the same manner, we obtain

$$\left|\delta_k^+ \xi_{i,k}^{\left(n+\frac{1}{2}\right)}\right| \leq C_4((\Delta x)^2 + (\Delta t)^2) \quad (k = 0, \dots, K-1,\ i = 1, 2, 3). \tag{4.89}$$

Therefore, using (4.87) and (4.89), we have

$$\left\|\boldsymbol{\xi}_i^{\left(n+\frac{1}{2}\right)}\right\|_{\tilde{H}_{\mathrm{d}}^1}^2 = \sum_{k=0}^{K}{}'' \left|\xi_{i,k}^{\left(n+\frac{1}{2}\right)}\right|^2 \Delta x + \sum_{k=0}^{K-1} \left|\delta_k^+ \xi_{i,k}^{\left(n+\frac{1}{2}\right)}\right|^2 \Delta x \leq 2C_4^2 L((\Delta x)^2 + (\Delta t)^2)^2 \quad (i = 1, 2, 3). \tag{4.90}$$

From the above estimates (4.87), (4.88), and (4.90), we have

$$\begin{aligned} \xi^{\left(n+\frac{1}{2}\right)} &\leq 3 \cdot 2C_4^2 (L+1)((\Delta x)^2 + (\Delta t)^2)^2 + 2 \cdot 2C_4^2((\Delta x)^2 + (\Delta t)^2)^2 \\ &\leq 10C_4^2(L+1)((\Delta x)^2 + (\Delta t)^2)^2 \quad (n = 0, 1, \dots, N-1). \end{aligned}$$

Therefore, from (4.78), we obtain

$$\begin{aligned} \|\boldsymbol{e}^{(n)}\|_{\tilde{H}_{\mathrm{d}}^1}^2 + \left|e_0^{(n)}\right|^2 + \left|e_K^{(n)}\right|^2 &\leq 3\Delta t [\exp\{3(1 + C_F)T\}] \cdot 10C_4^2(L+1)((\Delta x)^2 + (\Delta t)^2)^2 \sum_{j=1}^{n} 1 \\ &\leq 30C_4^2(L+1)[\exp\{3(1 + C_F)T\}]((\Delta x)^2 + (\Delta t)^2)^2 \cdot \frac{T}{N} \cdot N \\ &= 30C_4^2(L+1)T[\exp\{3(1 + C_F)T\}]((\Delta x)^2 + (\Delta t)^2)^2 \end{aligned}$$

for $n = 1, \dots, N$. That is,

$$\sqrt{\|\boldsymbol{e}^{(n)}\|_{\tilde{H}_{\mathrm{d}}^1}^2 + \left|e_0^{(n)}\right|^2 + \left|e_K^{(n)}\right|^2} \leq C_4\sqrt{30(L+1)T}\left[\exp\left\{\frac{3}{2}(1 + C_F)T\right\}\right]((\Delta x)^2 + (\Delta t)^2).$$

Here, let us define a constant C by

$$C := \tilde{C}_L C_4 \sqrt{30(L+1)T}\left[\exp\left\{\frac{3}{2}(1 + C_F)T\right\}\right].$$

Hence, we conclude from Proposition 2.5 that

$$\left\|\boldsymbol{e}^{(n)}\right\|_{L_{\mathrm{d}}^\infty} \leq \tilde{C}_L \left\|\boldsymbol{e}^{(n)}\right\|_{\tilde{H}_{\mathrm{d}}^1} \leq C((\Delta x)^2 + (\Delta t)^2) \quad (n = 1, \dots, N).$$

This completes the proof. □

§6 Computational examples

In this section, we demonstrate through computation examples that the numerical solution of the proposed scheme is efficient and that the scheme inherits the dissipative property from the original problem in a discrete sense. We consider the following dynamic boundary condition:

$$\begin{cases} \varepsilon_{\mathrm{ex}}\partial_t u(0,t) = \partial_x u(x,t)|_{x=0} - F'(u(0,t)), \\ \varepsilon_{\mathrm{ex}}\partial_t u(L,t) = -\ \partial_x u(x,t)|_{x=L} - F'(u(L,t)), \quad \text{in } (0,T], \end{cases} \tag{4.91}$$

where $\varepsilon_{\mathrm{ex}}$ is a positive constant. We choose $K = 100$ and fix $L = 1$ so that $\Delta x = 1/100$. On the other hand, we choose T and Δt depending on the situation. We fix the parameter $\varepsilon_{\mathrm{ex}} = 10$. Also, we consider the nonlinear function $F(s) = (\gamma/4)(s^2 - 1)^2$, where we fix the parameter $\gamma = 100$.

6.1 Computation example 1

As the initial value, we consider

$$u(x,0) = a_0 + a_1\cos(5\pi x) + a_2\sin(8\pi x) + a_3\cos(2\pi x),$$

where we choose $a_0 = 0.02$, $a_1 = -0.05$, $a_2 = -0.008$, and $a_3 = 0.01$. Also, we choose $N = 6000$ and fix $T = 0.6$ so that $\Delta t = 1/10000$. Figure 4.1 shows the time development of the solution to (4.1) with (4.91) obtained from our scheme. Figure 4.2 shows the time development of $J_{\mathrm{d}}(\boldsymbol{U}^{(n)}) + F(U_0^{(n)}) + F(U_K^{(n)})$. We call $J_{\mathrm{d}}(\boldsymbol{U}^{(n)}) + F(U_0^{(n)}) + F(U_K^{(n)})$ "total energy" from now on. This graph shows that the energy decreases numerically.

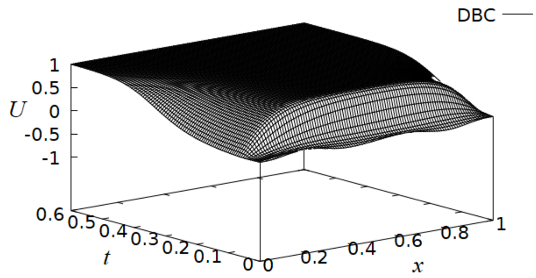

Figure 4.1: Numerical solution of (4.1) with (4.91) obtained by our scheme

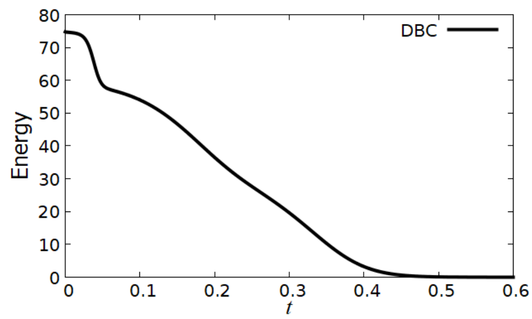

Figure 4.2: Time development of total energy

6.2 Computation example 2

As the initial value, we choose

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

Also, we choose $N = 700$ and fix $T = 0.7$ so that $\Delta t = 1/1000$. Figure 4.3 shows the time development of the solution to (4.1) with (4.91) obtained from our scheme. Figure 4.4 shows the time development of total energy. This graph shows that the energy decreases numerically.

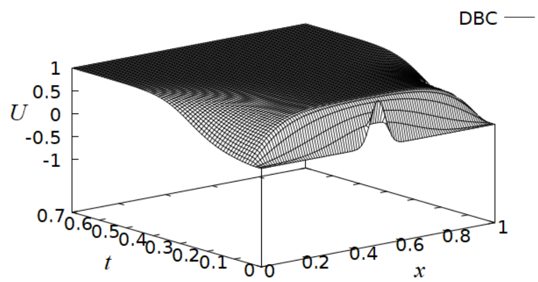

Figure 4.3: Numerical solution of (4.1) with (4.91) obtained by our scheme

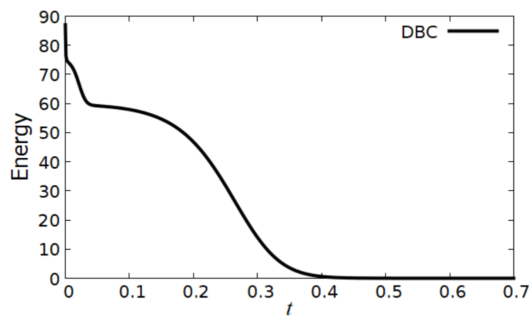

Figure 4.4: Time development of total energy

As stated in the Introduction, our study for the dynamic boundary condition differs from previous studies for non-dynamical boundary conditions such as the Neumann boundary condition. Since there is a term of the time derivative on the boundary in (4.1) with (4.91), it is natural that the long-time behavior of the solution may differ from that to (4.1) with the Neumann boundary condition. In order to assure that the difference occurs, we present the numerical examples of our structure-preserving scheme for (4.1) with the Neumann boundary condition (see next subsection for details).

6.3 Computation example 3 (Numerical results for the Neumann boundary condition)

In order to verify that the difference in the long-time behavior of the solution occurs, we present the numerical examples for (4.1) with the following inhomogeneous Neumann boundary condition:

$$\begin{cases} \partial_x u(x,t)|_{x=0} - F'(u(0,t)) = 0, \\ -\partial_x u(x,t)|_{x=L} - F'(u(L,t)) = 0, \quad \text{in } (0,T], \end{cases} \tag{4.92}$$

in the same setting as Subsections 6.1 and 6.2. We remark that the solution to (4.1) with (4.92) also satisfies the dissipative property (4.5). Since there are no results of the numerical computation in the same setting as the previous subsections in previous studies, we carry out the numerical computation by the following structure-preserving scheme. The concrete form of our structure-preserving scheme for (4.1) with (4.92) is as follows: for $n = 0, 1, \ldots,$

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

$$\delta_k^{\langle 1 \rangle}\left(\frac{U_k^{(n+1)} + U_k^{(n)}}{2}\right)\Bigg|_{k=0} - \frac{dF}{d(U_0^{(n+1)}, U_0^{(n)})} = 0,$$

$$-\delta_k^{\langle 1 \rangle}\left(\frac{U_k^{(n+1)} + U_k^{(n)}}{2}\right)\Bigg|_{k=K} - \frac{dF}{d(U_K^{(n+1)}, U_K^{(n)})} = 0.$$

Figure 4.5 shows the time development of the solution to (4.1) with (4.92) obtained from our scheme. Figure 4.6 shows the time development of total energy. This graph also shows that the energy decreases numerically.

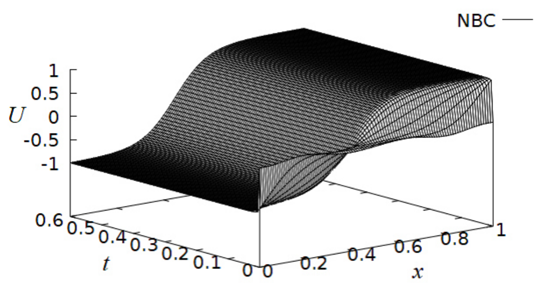

Figure 4.5: Numerical solution of (4.1) with (4.92) obtained by our scheme

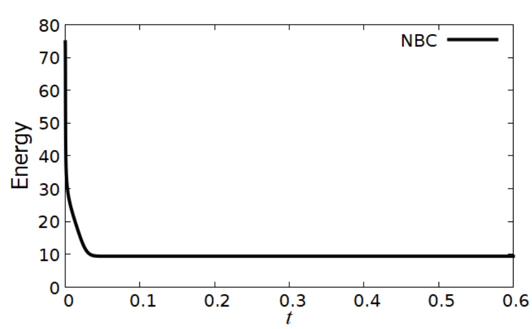

Figure 4.6: Time development of total energy

6.4 Computation example 4 (Numerical results for the Neumann boundary condition)

The setting is the same as Computation example 2. Figure 4.7 shows the time development of the solution to (4.1) with (4.92) from our scheme. Figure 4.8 shows the time development of total energy. This graph also shows that the energy decreases numerically.

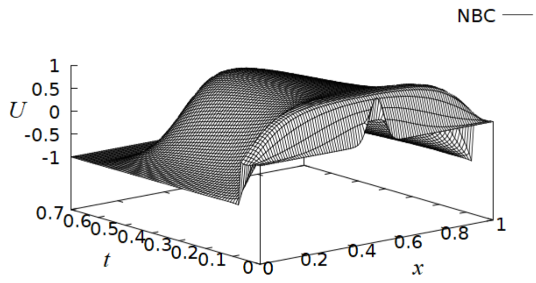

Figure 4.7: Numerical solution of (4.1) with (4.92) obtained by our scheme

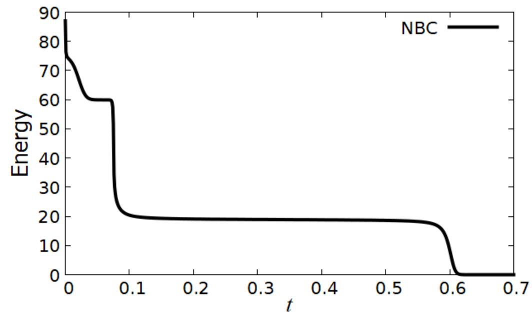

Figure 4.8: Time development of total energy

As can be seen from Figure 4.1, Figure 4.3, Figure 4.5, and Figure 4.7, the solution to (4.1) with (4.92) arrives at a different state from that to (4.1) with (4.91). Thus, the results assure that the difference in the long-time behavior of the solution occurs.

Chapter 5

The Cahn–Hilliard equation with a dynamic boundary condition

In this chapter, as mentioned in Chapter 1, similarly to designing a structure-preserving scheme for the Allen–Cahn equation with a dynamic boundary condition in Chapter 4, we propose a new structure-preserving finite difference scheme for the Cahn–Hilliard equation with a dynamic boundary condition based on DVDM [29]. As in the case of the Allen–Cahn equation, by modifying the discretization of energy and using an appropriate summation-by-parts formula, we can use a central difference operator as an approximation of an outward normal derivative on the discrete boundary condition of the scheme. In addition, we show that our proposed scheme is second-order accurate in space, although the previous structure-preserving scheme proposed by Fukao–Yoshikawa–Wada [28] is first-order accurate in space. Also, we show the stability, the existence, and the uniqueness of the solution for our proposed scheme. Computation examples demonstrate the effectiveness of our proposed scheme. Especially through computation examples, we confirm that the solution obtained by our proposed scheme is more reliable than that by the Fukao–Yoshikawa–Wada scheme when the space mesh size is coarse.

§1 Introduction

Let $L > 0$ be the length of the one-dimensional material. In this chapter, we study the following Cahn–Hilliard equation [8]:

$$\begin{cases} \partial_t u = \partial_x^2 p & \text{in } (0,L)\times(0,\infty), & (5.1)\\ p = -\gamma\partial_x^2 u + F'(u) & \text{in } (0,L)\times(0,\infty), & (5.2)\end{cases}$$

under the dynamic boundary condition and the homogeneous Neumann boundary condition:

$$\begin{cases} \partial_t u(0,t) = \partial_x u(x,t)|_{x=0} & \text{in } (0,\infty), & (5.3)\\ \partial_t u(L,t) = -\left.\partial_x u(x,t)\right|_{x=L} & \text{in } (0,\infty), & (5.4)\\ \partial_x p(x,t)|_{x=0} = \partial_x p(x,t)|_{x=L} = 0 & \text{in } (0,\infty). & (5.5)\end{cases}$$

The unknown functions u: $[0,L]\times[0,\infty)\to\mathbb{R}$ and p: $[0,L]\times[0,\infty)\to\mathbb{R}$ are the order parameter and the chemical potential, respectively. Moreover, γ is a positive constant. Furthermore, F: $\mathbb{R}\to\mathbb{R}$ is a potential, and F' is its derivative. For example, F can be a double-well potential, i.e.,

$$F(s) = \frac{q}{4}s^4 - \frac{r}{2}s^2 \quad \text{for all } s \in \mathbb{R},$$

where q and r are positive constants. Throughout this chapter, we assume that the potential F is bounded from below. Let us define the "local energy" G and the "global energy" J, which characterize the equations (5.1)–(5.2), as follows:

$$G(u, \partial_x u) := \frac{\gamma}{2} |\partial_x u|^2 + F(u), \tag{5.6}$$

$$J(u) := \int_0^L G(u, \partial_x u) dx. \tag{5.7}$$

Also, let us define the "mass" M as follows:

$$M(u) := \int_0^L u dx. \tag{5.8}$$

Then, the solution of the equations (5.1)–(5.2) satisfies the following properties:

$$\frac{d}{dt} M(u(t)) = 0, \tag{5.9}$$

$$\frac{d}{dt} J(u(t)) = -\gamma |\partial_t u(0,t)|^2 - \gamma |\partial_t u(L,t)|^2 - \int_0^L |\partial_x p(x,t)|^2 dx \leq 0, \tag{5.10}$$

under boundary conditions (5.3)–(5.5). In this chapter, we design a structure-preserving finite difference scheme for (5.1)–(5.5) based on DVDM. As mentioned in Chapter 4, in [67, 68], Yoshikawa has mentioned that the merits of the structure-preserving scheme are that we often obtain the stability of numerical solutions automatically and that various strategies for the continuous case, such as the energy method, can be applied to the scheme similarly. Actually, Yoshikawa and co-authors have applied the energy method to show the existence and the uniqueness of the solution and the error estimate for the numerical scheme (see [28, 65–68]).

From a mathematical perspective, the problem (5.1)–(5.5) with initial conditions has been studied in [14–16, 18–20, 32, 34, 35, 46, 47, 54, 55, 64]. First, in the case of $F(s) = (q/4)s^4 - (r/2)s^2$, Racke and Zheng [55] have proved the global existence and uniqueness of the solution to the problem, and Prüss et al. [54] have obtained the result on the maximal L^p-regularity and proved the existence of a global attractor. Also, Wu and Zheng [64] and Chill et al. [15] have proved the convergence of the solution of the problem to equilibrium as time goes to infinity. Moreover, various results of the existence, the uniqueness, and the regularity of the solution, the existence of a global attractor, the convergence to steady states, and the optimal control have been obtained under more general assumptions on the nonlinearities in [14, 16, 18–20, 34, 35, 46, 47]. Especially, Gal [32] has compared the problem under other dynamic boundary conditions with that under our target dynamic boundary conditions. Here, we remark that in these papers, the problem is considered in the multi-dimensional case, where the boundary conditions (5.3) and (5.4) include the Laplace–Beltrami operator, which plays the role of diffusion on the boundary.

From a numerical point of view, there are some numerical studies of the Cahn–Hilliard equation with dynamic boundary conditions (see, for example, [12–14, 28, 39, 48, 49]). In [12, 39], Cherfils et al. and Israel et al. have considered the finite element space semi-discretizations of the problem in the two-dimensional or three-dimensional case and proved the error estimate. Moreover, the results of the unconditional stability of fully discrete schemes based on the backward Euler scheme for the time discretization, and the convergence of the solution to a steady-state have been obtained. See also [14] for other numerical results. Besides, Cherfils and Petcu have obtained the results of the problem with other dynamic boundary conditions by a finite element approach [13]. In addition, Nabet has performed an interesting analysis of the problem in the two-dimensional case using the finite-volume method and proved the convergence of the numerical solution [48]. She also has given the error estimate in [49]. More specifically, she has proved the first-order convergence in the sense of the H^1-norms. In [28], Fukao et al. have already proposed a structure-preserving scheme for (5.1)–(5.5) based on DVDM in the one-dimensional case. We remark that they use a forward difference operator as an approximation of an outward normal derivative on the discrete boundary condition of their scheme and that their scheme is first-order accurate in space. In DVDM, it is essential how to discretize the energy which characterizes the equation. Modifying the conventional manner and using an appropriate summation-by-parts formula, we can use a central difference operator as an approximation of an outward normal derivative on the boundary. Moreover, we show that our proposed scheme is second-order in space.

The rest of this chapter proceeds as follows. In Section 2, we propose a structure-preserving scheme for (5.1)–(5.5), whose solution satisfies the discrete version of the conservative property (5.9) and the dissipative property (5.10). In Section 3, we prove that the solution of the proposed scheme satisfies the global boundedness. In Section 4, we prove that the scheme has a unique solution under a specific condition. In Section 5, we prove the error estimate for the scheme. In Section 6, we show that computation examples demonstrate the effectiveness of the scheme. We also mention the suggestion on comparison of long-time behaviors between the dynamic boundary condition and the Neumann boundary one.

§2 Proposed scheme

In this section, we propose a structure-preserving scheme for (5.1)–(5.5) and show that it has two properties corresponding to (5.9) and (5.10).

2.1 Preparation

Let K be a natural number. We define $U_k^{(n)}$ $(k = -1, 0, 1, \ldots, K, K+1, n = 0, 1, \ldots)$ to be the approximation to $u(x,t)$ at location $x = k\Delta x$ and time $t = n\Delta t$, where Δx is a space mesh size, i.e., $\Delta x := L/K$, and Δt is a time mesh size. They are also written in vector as $\boldsymbol{U}^{(n)} := (U_0^{(n)}, \ldots, U_K^{(n)})^\top$ or $\boldsymbol{U}^{(n)} := (U_{-1}^{(n)}, U_0^{(n)}, \ldots, U_K^{(n)}, U_{K+1}^{(n)})^\top$. The superscript (n) is omitted when no confusion occurs. Guess the meaning of $\boldsymbol{U}$ from the context. Let us define two discrete local energies $G_{\mathrm{d}}^{\pm}\colon \mathbb{R}^{K+3} \to \mathbb{R}^{K+1}$ by

$$
\begin{aligned}
G_{\mathrm{d},k}^{+}(\boldsymbol{U}) &:= \frac{\gamma}{2}(\delta_k^{+} U_k)^2 + F(U_k) \quad (k = 0, \ldots, K),\\
G_{\mathrm{d},k}^{-}(\boldsymbol{U}) &:= \frac{\gamma}{2}(\delta_k^{-} U_k)^2 + F(U_k) \quad (k = 0, \ldots, K),
\end{aligned}
$$

for all $\boldsymbol{U} \in \mathbb{R}^{K+3}$. Note that $G_{\mathrm{d},k}^{\pm}(\boldsymbol{U})$ are elements of vectors $G_{\mathrm{d}}^{\pm}(\boldsymbol{U})$, respectively. Furthermore, we define discrete global energy J_{d}: $\mathbb{R}^{K+3} \to \mathbb{R}$ as follows:

$$J_{\mathrm{d}}(\boldsymbol{U}) := \frac{1}{2}\left\{\sum_{k=0}^{K-1} G_{\mathrm{d},k}^{+}(\boldsymbol{U})\Delta x + \sum_{k=1}^{K} G_{\mathrm{d},k}^{-}(\boldsymbol{U})\Delta x\right\}. \tag{5.11}$$

Also, we define a discrete mass M_{d}: $\mathbb{R}^{K+1+2s} \to \mathbb{R}$ by

$$M_{\mathrm{d}}(\boldsymbol{U}) := \sum_{k=0}^{K}{}'' U_k \Delta x \quad \text{for all } \boldsymbol{U} \in \mathbb{R}^{K+1+2s}, \text{ where } s = 0, 1.$$

Remark 5.1. We remark that we construct a structure-preserving scheme for (5.1)–(5.5), which we can use a central difference operator as an approximation of an outward normal derivative on the boundary conditions by adopting the above discrete global energy J_{d} and using another summation-by-parts formula (Corollary 2.1).

From the idea of DVDM [31], we take a discrete variation to derive a structure-preserving scheme for (5.1)–(5.5). That is, we calculate the difference $J_{\mathrm{d}}(\boldsymbol{U}) - J_{\mathrm{d}}(\boldsymbol{V})$ for all $\boldsymbol{U}, \boldsymbol{V} \in \mathbb{R}^{K+3}$. For the purpose, we use the following lemmas. All the proofs can be found in Lemma 4.1 and Lemma 4.2 and here omitted.

Lemma 5.1. The definition (4.6) of J_{d} is rewritten as follows:

$$J_{\mathrm{d}}(\boldsymbol{U}) = \sum_{k=0}^{K-1} \frac{\gamma}{2}\left(\delta_k^{+} U_k\right)^2 \Delta x + \sum_{k=0}^{K}{}'' F\left(U_k\right)\Delta x \quad \text{for all } \boldsymbol{U} \in \mathbb{R}^{K+3}.$$

Lemma 5.2. The following equality holds:

$$\begin{aligned} J_{\mathrm{d}}(\boldsymbol{U}) - J_{\mathrm{d}}(\boldsymbol{V}) &= \sum_{k=0}^{K}{}'' \left\{-\gamma\delta_k^{\langle 2\rangle}\left(\frac{U_k + V_k}{2}\right) + \frac{dF}{d(U_k, V_k)}\right\}\left(U_k - V_k\right)\Delta x \\ &\quad + \left[\gamma\left\{\delta_k^{\langle 1\rangle}\left(\frac{U_k + V_k}{2}\right)\right\}\left(U_k - V_k\right)\right]_0^K \quad \text{for all } \boldsymbol{U}, \boldsymbol{V} \in \mathbb{R}^{K+3}. \end{aligned} \tag{5.12}$$

Remark 5.2. This equality (5.12) is essential for the discrete energy dissipation (Theorem 5.1).

2.2 Proposed scheme

The concrete form of our scheme for (5.1)–(5.5) is, for $n = 0, 1, \ldots$,

$$\frac{U_k^{(n+1)} - U_k^{(n)}}{\Delta t} = \delta_k^{\langle 2\rangle} P_k^{(n)} \quad (k = 0, \ldots, K), \tag{5.13}$$

$$P_k^{(n)} = -\gamma\delta_k^{\langle 2\rangle}\left(\frac{U_k^{(n+1)} + U_k^{(n)}}{2}\right) + \frac{dF}{d(U_k^{(n+1)}, U_k^{(n)})} \quad (k = 0, \ldots, K), \tag{5.14}$$

$$\frac{U_0^{(n+1)} - U_0^{(n)}}{\Delta t} = \delta_k^{\langle 1\rangle}\left(\frac{U_k^{(n+1)} + U_k^{(n)}}{2}\right)\Bigg|_{k=0}, \tag{5.15}$$

$$\frac{U_K^{(n+1)} - U_K^{(n)}}{\Delta t} = -\,\delta_k^{\langle 1\rangle}\left(\frac{U_k^{(n+1)} + U_k^{(n)}}{2}\right)\Bigg|_{k=K}, \tag{5.16}$$

$$\delta_k^{\langle 1\rangle} P_k^{(n)} = 0 \quad (k = 0, K). \tag{5.17}$$

Remark 5.3. In the previous result [28], Fukao et al. constructed another structure-preserving scheme. They used a forward difference operator as an approximation of an outward normal derivative on the boundary conditions. On the other hand, we have constructed a structure-preserving scheme in which we used a central difference operator as an approximation of an outward normal derivative. This is the difference with their previous scheme.

Then, the proposed scheme (5.13)–(5.17) has the following property corresponding to (5.10), i.e.,

Theorem 5.1. The solution to the scheme (5.13)–(5.17) satisfies

$$\delta_n^+ J_{\mathrm{d}}(\boldsymbol{U}^{(n)}) = -\gamma \left|\delta_n^+ U_0^{(n)}\right|^2 - \gamma \left|\delta_n^+ U_K^{(n)}\right|^2 - \sum_{k=0}^{K-1} \left|\delta_k^+ P_k^{(n)}\right|^2 \Delta x \le 0 \quad (n = 0, 1, \ldots). \tag{5.18}$$

Proof. Using Corollary 2.1, Lemma 5.2, (5.13)–(5.17), we have

$$\begin{aligned}
\delta_n^+ J_{\mathrm{d}}(\boldsymbol{U}^{(n)}) &= \frac{J_{\mathrm{d}}\left(\boldsymbol{U}^{(n+1)}\right) - J_{\mathrm{d}}\left(\boldsymbol{U}^{(n)}\right)}{\Delta t} \\
&= \sum_{k=0}^{K}{}'' \left\{ -\gamma \delta_k^{\langle 2\rangle} \left(\frac{U_k^{(n+1)} + U_k^{(n)}}{2} \right) + \frac{dF}{d(U_k^{(n+1)}, U_k^{(n)})} \right\} \frac{U_k^{(n+1)} - U_k^{(n)}}{\Delta t} \Delta x \\
&\quad + \left[\gamma \left\{ \delta_k^{\langle 1\rangle} \left(\frac{U_k^{(n+1)} + U_k^{(n)}}{2} \right) \right\} \frac{U_k^{(n+1)} - U_k^{(n)}}{\Delta t} \right]_0^K \\
&= \sum_{k=0}^{K}{}'' P_k^{(n)} \left(\delta_k^{\langle 2\rangle} P_k^{(n)} \right) \Delta x - \gamma \left|\delta_n^+ U_0^{(n)}\right|^2 - \gamma \left|\delta_n^+ U_K^{(n)}\right|^2 \\
&= \left[\left(\delta_k^{\langle 1\rangle} P_k^{(n)} \right) P_k^{(n)} \right]_0^K - \sum_{k=0}^{K-1} \left|\delta_k^+ P_k^{(n)}\right|^2 \Delta x - \gamma \left|\delta_n^+ U_0^{(n)}\right|^2 - \gamma \left|\delta_n^+ U_K^{(n)}\right|^2 \\
&= -\sum_{k=0}^{K-1} \left|\delta_k^+ P_k^{(n)}\right|^2 \Delta x - \gamma \left|\delta_n^+ U_0^{(n)}\right|^2 - \gamma \left|\delta_n^+ U_K^{(n)}\right|^2 \quad (n = 0, 1, \ldots).
\end{aligned}$$

This completes the proof. □

Furthermore, the proposed scheme (5.13)–(5.17) has the following property corresponding to (5.9), i.e.,

Theorem 5.2. The solution to the scheme (5.13)–(5.17) satisfies the following equality:

$$\delta_n^+ M_{\mathrm{d}}(\boldsymbol{U}^{(n)}) = 0 \quad (n = 0, 1, \ldots).$$

Proof. Using (5.13), (5.17), and Proposition 2.2, we obtain

$$\delta_n^+ M_{\mathrm{d}}(\boldsymbol{U}^{(n)}) = \sum_{k=0}^{K}{}'' \frac{U_k^{(n+1)} - U_k^{(n)}}{\Delta t} \Delta x = \sum_{k=0}^{K}{}'' \delta_k^{\langle 2\rangle} P_k^{(n)} \Delta x = \left[\delta_k^{\langle 1\rangle} P_k^{(n)} \right]_0^K = 0 \quad (n = 0, 1, \ldots).$$

This completes the proof. □

§3 Stability of the proposed scheme

In this section, we show that, if the proposed scheme has a solution, then it satisfies the global boundedness.

For the proof of the global boundedness of the numerical solution, we use the following lemma.

Lemma 5.3. The solution to the scheme (5.13)–(5.17) satisfies the following inequality:

$$\left\|D\boldsymbol{U}^{(n)}\right\| \le \left\{\frac{2}{\gamma}\left(J_{\mathrm{d}}(\boldsymbol{U}^{(0)}) + L\left|\min\left\{\inf_{\xi\in\mathbb{R}} F(\xi), 0\right\}\right|\right)\right\}^{\frac{1}{2}} \quad (n = 0, 1, \ldots). \tag{5.19}$$

Proof. From the dissipative property (Theorem 5.1) and the assumption on the potential F, we obtain

$$\begin{aligned} J_{\mathrm{d}}(\boldsymbol{U}^{(0)}) \ge J_{\mathrm{d}}(\boldsymbol{U}^{(n)}) &= \frac{\gamma}{2}\sum_{k=0}^{K-1}\left|\delta_k^+ U_k^{(n)}\right|^2 \Delta x + \sum_{k=0}^{K}{}'' F\left(U_k^{(n)}\right)\Delta x \\ &\ge \frac{\gamma}{2}\left\|D\boldsymbol{U}^{(n)}\right\|^2 + \min\left\{\inf_{\xi\in\mathbb{R}} F(\xi), 0\right\}\sum_{k=0}^{K}{}''\Delta x \\ &= \frac{\gamma}{2}\left\|D\boldsymbol{U}^{(n)}\right\|^2 + \min\left\{\inf_{\xi\in\mathbb{R}} F(\xi), 0\right\} L \quad (n = 0, 1, \ldots). \end{aligned}$$

Namely, we have

$$\begin{aligned} \frac{\gamma}{2}\left\|D\boldsymbol{U}^{(n)}\right\|^2 &\le J_{\mathrm{d}}(\boldsymbol{U}^{(0)}) - L\min\left\{\inf_{\xi\in\mathbb{R}} F(\xi), 0\right\} \\ &\le J_{\mathrm{d}}(\boldsymbol{U}^{(0)}) + L\left|\min\left\{\inf_{\xi\in\mathbb{R}} F(\xi), 0\right\}\right| \quad (n = 0, 1, \ldots). \end{aligned}$$

Therefore, the inequality (5.19) holds. □

From Lemma 5.3 and Proposition 2.6, we can obtain the following global boundedness:

Theorem 5.3 (Global boundedness)**.** The solution to the scheme (5.13)–(5.17) satisfies the following inequality:

$$\left\|\boldsymbol{U}^{(n)}\right\|_{L_{\mathrm{d}}^\infty} \le \frac{1}{L}\left|M_{\mathrm{d}}(\boldsymbol{U}^{(0)})\right| + \left\{\frac{2L}{\gamma}\left(J_{\mathrm{d}}(\boldsymbol{U}^{(0)}) + L\left|\min\left\{\inf_{\xi\in\mathbb{R}} F(\xi), 0\right\}\right|\right)\right\}^{\frac{1}{2}} \quad (n = 0, 1, \ldots). \tag{5.20}$$

Proof. From Proposition 2.6 (Discrete Poincaré–Wirtinger inequality) and Theorem 5.2, we have

$$\begin{aligned} \left\|\boldsymbol{U}^{(n)}\right\|_{L_{\mathrm{d}}^\infty} &\le \frac{1}{L}\left|M_{\mathrm{d}}(\boldsymbol{U}^{(n)})\right| + L^{\frac{1}{2}}\left\|D\boldsymbol{U}^{(n)}\right\| \\ &= \frac{1}{L}\left|M_{\mathrm{d}}(\boldsymbol{U}^{(0)})\right| + L^{\frac{1}{2}}\left\|D\boldsymbol{U}^{(n)}\right\| \quad (n = 0, 1, \ldots). \end{aligned} \tag{5.21}$$

By applying Lemma 5.3 to (5.21), we can obtain (5.20). □

Remark 5.4. Theorem 5.3 means that our proposed scheme is numerically stable for any time step n. We can obtain a more precise evaluation by evaluating errors of the discrete quantities if the initial data is sufficiently smooth.

Lemma 5.4. If $U_k^{(0)} = u_0(k\Delta x)$ $(k = 0, \ldots, K)$ for a function $u_0 \in C^3([0, L])$, then there exist constants $C_J, C_M > 0$ independent of Δx and Δt such that

$$\left|J_{\mathrm{d}}(\boldsymbol{U}^{(0)}) - J(u_0)\right| \leq C_J, \quad \left|M_{\mathrm{d}}(\boldsymbol{U}^{(0)}) - M(u_0)\right| \leq C_M.$$

Proof. From the triangle inequality, we see that

$$\begin{aligned}
&\left|J_{\mathrm{d}}(\boldsymbol{U}^{(0)}) - J(u_0)\right| \\
&= \left|\frac{1}{2}\left(\sum_{k=0}^{K-1} G^{+}_{\mathrm{d},k}(\boldsymbol{U}^{(0)})\Delta x + \sum_{k=1}^{K} G^{-}_{\mathrm{d},k}(\boldsymbol{U}^{(0)})\Delta x\right) - \int_0^L G(u_0, \partial_x u_0)dx\right| \\
&\leq \left|\frac{1}{2}\left(\sum_{k=0}^{K-1} G^{+}_{\mathrm{d},k}(\boldsymbol{U}^{(0)})\Delta x + \sum_{k=1}^{K} G^{-}_{\mathrm{d},k}(\boldsymbol{U}^{(0)})\Delta x\right) - \sum_{k=0}^{K}{}'' G(u_0(k\Delta x), \partial_x u_0(k\Delta x))\Delta x\right| \\
&\quad + \left|\sum_{k=0}^{K}{}'' G(u_0(k\Delta x), \partial_x u_0(k\Delta x))\Delta x - \int_0^L G(u_0, \partial_x u_0)dx\right|. \qquad (5.22)
\end{aligned}$$

Since $G(u_0, \partial_x u_0) \in C^2([0, L])$ from the assumption $u_0 \in C^3([0, L])$, by using the Euler–Maclaurin summation formula and $\Delta x \leq L$, we estimate the second term on the right-hand side of (5.22) as follows:

$$\begin{aligned}
\left|\sum_{k=0}^{K}{}'' G(u_0(k\Delta x), \partial_x u_0(k\Delta x))\Delta x - \int_0^L G(u_0, \partial_x u_0)dx\right| &\leq \frac{(\Delta x)^2}{8}\int_0^L \left|\partial_x^2 G(u_0, \partial_x u_0)\right| dx \\
&\leq \frac{L^2}{8}\int_0^L \left|\partial_x^2 G(u_0, \partial_x u_0)\right| dx. \qquad (5.23)
\end{aligned}$$

Next, we estimate the first term on the right-hand side of (5.22). By using Proposition 2.1, we have

$$\begin{aligned}
&\left|\frac{1}{2}\left(\sum_{k=0}^{K-1} G^{+}_{\mathrm{d},k}(\boldsymbol{U}^{(0)})\Delta x + \sum_{k=1}^{K} G^{-}_{\mathrm{d},k}(\boldsymbol{U}^{(0)})\Delta x\right) - \sum_{k=0}^{K}{}'' G(u_0(k\Delta x), \partial_x u_0(k\Delta x))\Delta x\right| \\
&\leq \frac{1}{2}\left(\sum_{k=0}^{K-1} \left|G^{+}_{\mathrm{d},k}(\boldsymbol{U}^{(0)}) - G(u_0(k\Delta x), \partial_x u_0(k\Delta x))\right| \Delta x\right. \\
&\quad \left. + \sum_{k=1}^{K} \left|G^{-}_{\mathrm{d},k}(\boldsymbol{U}^{(0)}) - G(u_0(k\Delta x), \partial_x u_0(k\Delta x))\right| \Delta x\right).
\end{aligned}$$

From the assumption $U_k^{(0)} = u_0(k\Delta x)$ $(k = 0, \ldots, K)$, we obtain

$$G^{+}_{\mathrm{d},k}(\boldsymbol{U}^{(0)}) - G(u_0(k\Delta x), \partial_x u_0(k\Delta x)) = \frac{\gamma}{2}\left(\left|\delta_k^{+} u_0(k\Delta x)\right|^2 - \left|\partial_x u_0(k\Delta x)\right|^2\right)$$

for $k = 0, \dots, K-1$. Similarly, we have

$$G^-_{\mathrm{d},k}(\boldsymbol{U}^{(0)}) - G(u_0(k\Delta x), \partial_x u_0(k\Delta x)) = \frac{\gamma}{2}\left(\left|\delta^-_k u_0(k\Delta x)\right|^2 - |\partial_x u_0(k\Delta x)|^2\right)$$

for $k = 1, \dots, K$. For $k = 0, \dots, K-1$, applying the Taylor theorem to u_0, there exists $\zeta_1 \in (0,1)$ such that

$$\frac{u_0((k+1)\Delta x) - u_0(k\Delta x)}{\Delta x} = \partial_x u_0(k\Delta x) + \frac{\Delta x}{2}\partial_x^2 u_0((k+\zeta_1)\Delta x).$$

Similarly, for $1, \dots, K$, there exists $\zeta_2 \in (0,1)$ such that

$$\frac{u_0(k\Delta x) - u_0((k-1)\Delta x)}{\Delta x} = \partial_x u_0(k\Delta x) - \frac{\Delta x}{2}\partial_x^2 u_0((k-\zeta_2)\Delta x).$$

Hence, we have

$$\begin{aligned}
&G^+_{\mathrm{d},k}(\boldsymbol{U}^{(0)}) - G(u_0(k\Delta x), \partial_x u_0(k\Delta x)) \\
&= \frac{\gamma}{2}\left\{\Delta x \partial_x u_0(k\Delta x)\partial_x^2 u_0((k+\zeta_1)\Delta x) + \frac{(\Delta x)^2}{4}\left(\partial_x^2 u_0((k+\zeta_1)\Delta x)\right)^2\right\} \quad (k=0,\dots,K-1), \\
&G^-_{\mathrm{d},k}(\boldsymbol{U}^{(0)}) - G(u_0(k\Delta x), \partial_x u_0(k\Delta x)) \\
&= -\frac{\gamma}{2}\left\{\Delta x \partial_x u_0(k\Delta x)\partial_x^2 u_0((k-\zeta_2)\Delta x) - \frac{(\Delta x)^2}{4}\left(\partial_x^2 u_0((k-\zeta_2)\Delta x)\right)^2\right\} \quad (k=1,\dots,K).
\end{aligned}$$

Therefore, from $\Delta x \leq L$ and $K\Delta x = L$, we obtain

$$\begin{aligned}
&\sum_{k=0}^{K-1}\left|G^+_{\mathrm{d},k}(\boldsymbol{U}^{(0)}) - G(u_0(k\Delta x), \partial_x u_0(k\Delta x))\right|\Delta x \\
&\leq \frac{\gamma}{2}\left\{\Delta x \sum_{k=0}^{K-1}\left|\partial_x u_0(k\Delta x)\partial_x^2 u_0((k+\zeta_1)\Delta x)\right|\Delta x + \frac{(\Delta x)^2}{4}\sum_{k=0}^{K-1}\left|\partial_x^2 u_0((k+\zeta_1)\Delta x)\right|^2\Delta x\right\} \\
&\leq \frac{\gamma L^2}{2}\left(A_1 A_2 + \frac{L}{4}A_2^2\right),
\end{aligned}$$

where $A_i := \max_{x\in[0,L]}\left|\partial_x^i u_0(x)\right|$ $(i = 1,2)$. Similarly, we have

$$\sum_{k=1}^{K}\left|G^-_{\mathrm{d},k}(\boldsymbol{U}^{(0)}) - G(u_0(k\Delta x), \partial_x u_0(k\Delta x))\right|\Delta x \leq \frac{\gamma L^2}{2}\left(A_1 A_2 + \frac{L}{4}A_2^2\right).$$

Thus, we see that

$$\begin{aligned}
&\left|\frac{1}{2}\left(\sum_{k=0}^{K-1} G^+_{\mathrm{d},k}(\boldsymbol{U}^{(0)})\Delta x + \sum_{k=1}^{K} G^-_{\mathrm{d},k}(\boldsymbol{U}^{(0)})\Delta x\right) - {\sum_{k=0}^{K}}'' G(u_0(k\Delta x), \partial_x u_0(k\Delta x))\Delta x\right| \\
&\leq \frac{\gamma L^2}{2}\left(A_1 A_2 + \frac{L}{4}A_2^2\right).
\end{aligned} \tag{5.24}$$

From (5.22), (5.23), and (5.24), we conclude that

$$\left|J_{\mathrm{d}}(\boldsymbol{U}^{(0)}) - J(u_0)\right| \leq \frac{L^2}{8}\int_0^L \left|\partial_x^2 G(u_0, \partial_x u_0)\right| dx + \frac{\gamma L^2}{2}\left(A_1 A_2 + \frac{L}{4}A_2^2\right). \tag{5.25}$$

Also, from the Euler–Maclaurin summation formula, we obtain

$$\left|M_{\mathrm{d}}(\boldsymbol{U}^{(0)}) - M(u_0)\right| = \left|\sum_{k=0}^{K}{}'' u_0(k\Delta x)\Delta x - \int_0^L u_0 dx\right| \le \frac{L^2}{8}\int_0^L \left|\partial_x^2 u_0\right| dx. \tag{5.26}$$

The right-hand sides of (5.25) and (5.26) are the desired constants C_J and C_M, respectively. □

From Theorem 5.3 and Lemma 5.4, we have the following corollary:

Corollary 5.1. If $U_k^{(0)} = u_0(k\Delta x)$ $(k = 0, \ldots, K)$ for a function $u_0 \in C^3([0, L])$, then the solution of the scheme (5.13)–(5.17) satisfies the following inequality:

$$\left\|\boldsymbol{U}^{(n)}\right\|_{L_{\mathrm{d}}^\infty} \le \frac{1}{L}(|M(u_0)|+C_M)+\left\{\frac{2L}{\gamma}\left(J(u_0)+C_J+L\left|\min\left\{\inf_{\xi\in\mathbb{R}} F(\xi), 0\right\}\right|\right)\right\}^{\frac{1}{2}} \quad (n=0,1,\ldots), \tag{5.27}$$

where

$$C_J := L^2\left\{\frac{1}{8}\int_0^L \left|\partial_x^2 G(u_0, \partial_x u_0)\right| dx + \frac{\gamma}{2}\left(A_1 A_2 + \frac{L}{4}A_2^2\right)\right\},$$

$$A_i := \max_{x\in[0,L]}\left|\partial_x^i u_0(x)\right| \quad (i = 1, 2), \quad C_M := \frac{L^2}{8}\int_0^L \left|\partial_x^2 u_0\right| dx.$$

§4 Existence and uniqueness of the solution to the proposed scheme

In this section, using the energy method in [28, 52, 65–68], we prove that the proposed scheme (5.13)–(5.17) has a unique solution under a specific condition on Δt.

Theorem 5.4. Assume that the potential function F is in C^3. For any given $\boldsymbol{U}^{(0)} = \{U_k^{(0)}\}_{k=-1}^{K+1} \in \mathbb{R}^{K+3}$, let us define B_0 and $\tilde{B}_0$ by

$$B_0 := \left\{\frac{2}{\gamma}\left(J_{\mathrm{d}}(\boldsymbol{U}^{(0)}) + L\left|\min\left\{\inf_{\xi\in\mathbb{R}} F(\xi), 0\right\}\right|\right)\right\}^{\frac{1}{2}}, \quad \tilde{B}_0 := \frac{1}{L}\left|M_{\mathrm{d}}(\boldsymbol{U}^{(0)})\right| + L^{\frac{1}{2}} B_0.$$

If Δt satisfies

$$\max\left\{\frac{3}{2}\max_{|\xi|\le 2\tilde{B}_0}|F''(\xi)|,\ \frac{1}{2}\max_{|\xi|\le 2\tilde{B}_0}|F''(\xi)| + \frac{5L^{\frac{1}{2}}B_0}{6}\max_{|\xi|\le 2\tilde{B}_0}|F'''(\xi)|\right\}\sqrt{\frac{\Delta t}{2\gamma}} < 1, \tag{5.28}$$

then there exists a unique solution $\{U_k^{(n)}\}_{k=-1}^{K+1} \in \mathbb{R}^{K+3}$ $(n = 1, 2, \ldots)$ satisfying (5.13)–(5.17).

Remark 5.5. The assumption (5.28) is independent of the space mesh size Δx. Also, it is one of the advantages of the numerical method we apply that the condition on Δt can be derived explicitly as above.

For the proof, we use the following lemmas. Since proofs of these lemmas can be found in [61, 70], we omit them.

Lemma 5.5 ([70, Theorem 2.8])**.** Let A and B be $n \times n$ complex matrices. Then, AB and BA have the same eigenvalues, counting multiplicity.

In the following lemmas, we denote the Hermitian conjugate or adjoint of a $n \times n$ matrix A by A^*.

Lemma 5.6 (Sylvester's law of inertia [70, Theorem 8.3])**.** Let A and B be $n \times n$ Hermitian matrices. Then, there exists a nonsingular $n \times n$ matrix S such that $B = S^* AS$ if and only if A and B have the same inertia, i.e.,

$$\mathrm{In}(A) = \mathrm{In}(B),$$

where the inertia $\mathrm{In}(A)$ of A is defined to be the ordered triple $(i_+(A), i_-(A), i_0(A))$, that is,

$$\mathrm{In}(A) := (i_+(A), i_-(A), i_0(A)),$$

and $i_+(A)$, $i_-(A)$, and $i_0(A)$ are the numbers of positive, negative, and zero eigenvalues of A, respectively (including multiplicities).

Lemma 5.7 (Cholesky factorization [61, Theorem 23.1])**.** For any $n \times n$ Hermitian positive definite matrix A, there exists a unique $n \times n$ upper-triangular matrix R whose diagonal components are all positive such that

$$A = R^* R.$$

Using the above lemmas, we obtain the following lemma:

Lemma 5.8. Let A be an arbitrary $n \times n$ Hermitian positive semi-definite matrix and let B be an arbitrary $n \times n$ Hermitian positive definite matrix. Then, the eigenvalues of AB are all real and nonnegative.

Proof. Applying Lemma 5.7 to the Hermitian positive definite matrix B, there exists a unique $n \times n$ upper-triangular matrix R such that

$$B = R^* R, \quad r_{ii} > 0 \quad (i = 1, \ldots, n),$$

where r_{ii} $(i = 1, \ldots, n)$ are diagonal components of R. Hence, we have

$$AB = A(R^* R) = (AR^*)R. \tag{5.29}$$

It holds from $r_{ii} > 0$ $(i = 1, \ldots, n)$ that $\det R^* = r_{11} \cdots r_{nn} > 0$. That is, R^* is nonsingular. Therefore, using Lemma 5.6, we obtain

$$\mathrm{In}(A) = \mathrm{In}((R^*)^* AR^*) = \mathrm{In}(RAR^*). \tag{5.30}$$

Since $(AR^*)R$ and $R(AR^*)$ have the same eigenvalues from Lemma 5.5, by using (5.29) and (5.30), we obtain

$$\mathrm{In}(A) = \mathrm{In}(RAR^*) = \mathrm{In}((AR^*)R) = \mathrm{In}(AB).$$

Since A is positive semi-definite, the eigenvalues of A are all real and nonnegative. Namely, the eigenvalues of AB are all real and nonnegative, too. □

Proof of Theorem 5.4. We show the existence of a $(K+3)$-vector $\boldsymbol{U}^{(n+1)}=\{U_k^{(n+1)}\}_{k=-1}^{K+1}$ $\in \mathbb{R}^{K+3}$ for a given $\boldsymbol{U}^{(n)} = \{U_k^{(n)}\}_{k=-1}^{K+1} \in \mathbb{R}^{K+3}$ that satisfies (5.13)–(5.17). For the purpose, we define the nonlinear mapping Ψ: $\{U_k\}_{k=0}^{K} \mapsto \{\tilde{U}_k\}_{k=-1}^{K+1}$ by

$$\frac{\tilde{U}_k - U_k^{(n)}}{\Delta t} = \delta_k^{\langle 2\rangle} \tilde{P}_k^{(n)} \quad (k = 0,\dots,K), \tag{5.31}$$

$$\tilde{P}_k^{(n)} = -\gamma\delta_k^{\langle 2\rangle}\left(\frac{\tilde{U}_k + U_k^{(n)}}{2}\right) + \frac{dF}{d(U_k, U_k^{(n)})} \quad (k = 0,\dots,K), \tag{5.32}$$

$$\frac{\tilde{U}_0 - U_0^{(n)}}{\Delta t} = \delta_k^{\langle 1\rangle}\left(\frac{\tilde{U}_k+U_k^{(n)}}{2}\right)\Bigg|_{k=0}, \tag{5.33}$$

$$\frac{\tilde{U}_K - U_K^{(n)}}{\Delta t} = -\,\delta_k^{\langle 1\rangle}\left(\frac{\tilde{U}_k + U_k^{(n)}}{2}\right)\Bigg|_{k=K}, \tag{5.34}$$

$$\delta_k^{\langle 1\rangle} \tilde{P}_k^{(n)} = 0 \quad (k = 0, K). \tag{5.35}$$

Firstly, we show that the mapping Ψ is well-defined. For any fixed $\boldsymbol{U} = \{U_k\}_{k=0}^{K} \in \mathbb{R}^{K+1}$, from (5.33) and (5.34), $\tilde{U}_{-1}$ and $\tilde{U}_{K+1}$ can be explicitly written as

$$\tilde{U}_{-1} = -U_{-1}^{(n)} + \tilde{U}_1 + U_1^{(n)} - \frac{4\Delta x}{\Delta t}\left(\tilde{U}_0 - U_0^{(n)}\right), \tag{5.36}$$

$$\tilde{U}_{K+1} = -U_{K+1}^{(n)} + \tilde{U}_{K-1} + U_{K-1}^{(n)} - \frac{4\Delta x}{\Delta t}\left(\tilde{U}_K - U_K^{(n)}\right). \tag{5.37}$$

Thus, it is sufficient to show that $\tilde{U}_k$ $(k = 0,\dots,K)$ can be explicitly written by given $\boldsymbol{U}$ and $\boldsymbol{U}^{(n)}$. Using (5.35)–(5.37), we eliminate terms at $k = -1, K+1$ in (5.31) and (5.32). Thus, we have

$$\frac{\tilde{U}_0 - U_0^{(n)}}{\Delta t} = \frac{2}{(\Delta x)^2}\left(\tilde{P}_1^{(n)} - \tilde{P}_0^{(n)}\right), \tag{5.38}$$

$$\frac{\tilde{U}_k - U_k^{(n)}}{\Delta t} = \delta_k^{\langle 2\rangle} \tilde{P}_k^{(n)} \quad (k = 1,\dots,K-1), \tag{5.39}$$

$$\frac{\tilde{U}_K - U_K^{(n)}}{\Delta t} = \frac{2}{(\Delta x)^2}\left(\tilde{P}_{K-1}^{(n)} - \tilde{P}_K^{(n)}\right), \tag{5.40}$$

$$\tilde{P}_0^{(n)} = -\frac{2\gamma}{(\Delta x)^2}\left\{\left(\frac{\tilde{U}_1+U_1^{(n)}}{2}\right)-\left(\frac{\tilde{U}_0+U_0^{(n)}}{2}\right)\right\}+\frac{2\gamma}{\Delta x\Delta t}\left(\tilde{U}_0 - U_0^{(n)}\right)+\frac{dF}{d(U_0, U_0^{(n)})}, \tag{5.41}$$

$$\tilde{P}_k^{(n)} = -\gamma\delta_k^{\langle 2\rangle}\left(\frac{\tilde{U}_k + U_k^{(n)}}{2}\right) + \frac{dF}{d(U_k, U_k^{(n)})} \quad (k = 1,\dots,K-1), \tag{5.42}$$

$$\tilde{P}_K^{(n)} = -\frac{2\gamma}{(\Delta x)^2}\left\{\left(\frac{\tilde{U}_{K-1}+U_{K-1}^{(n)}}{2}\right)-\left(\frac{\tilde{U}_K+U_K^{(n)}}{2}\right)\right\} + \frac{2\gamma}{\Delta x\Delta t}\left(\tilde{U}_K - U_K^{(n)}\right) + \frac{dF}{d(U_K, U_K^{(n)})}. \tag{5.43}$$

Here, we give the following matrix expression of Ψ:

$$A\tilde{\boldsymbol{U}} = f(\boldsymbol{U}, \boldsymbol{U}^{(n)}).$$

By using (5.41)–(5.43), we eliminate $\tilde{P}_k^{(n)}$ in (5.38)–(5.40). Then, the $(K+1)\times(K+1)$ matrix A is defined by

$$A := I + \beta \begin{pmatrix} 6+\frac{2}{\alpha} & -8 & 2 & & & & & & \\ -4-\frac{1}{\alpha} & 7 & -4 & 1 & & & & & \\ 1 & -4 & 6 & -4 & 1 & & & & \\ & 1 & -4 & 6 & -4 & 1 & & & \\ & & \ddots & \ddots & \ddots & \ddots & \ddots & & \\ & & & 1 & -4 & 6 & -4 & 1 & \\ & & & & 1 & -4 & 6 & -4 & 1 \\ & & & & & 1 & -4 & 7 & -4-\frac{1}{\alpha} \\ & & & & & & 2 & -8 & 6+\frac{2}{\alpha} \end{pmatrix}, \tag{5.44}$$

where I is the $(K+1)$-dimensional identity matrix. Besides, α and β are defined by $\alpha := \Delta t/(4\Delta x)$ and $\beta := \gamma\Delta t/(2(\Delta x)^4)$, respectively. If the matrix A is nonsingular, then the mapping Ψ is well-defined. In fact, we show that A is nonsingular. For the purpose, we show that the determinant of A is positive. Firstly, let us define the $(K+1)\times(K+1)$ matrices D_2 and $\tilde{D}_2$ by

$$D_2 := \begin{pmatrix} -2 & 2 & & & \\ 1 & -2 & 1 & & \\ & \ddots & \ddots & \ddots & \\ & & 1 & -2 & 1 \\ & & & 2 & -2 \end{pmatrix}, \quad \tilde{D}_2 := \begin{pmatrix} -2-\frac{1}{\alpha} & 2 & & & \\ 1 & -2 & 1 & & \\ & \ddots & \ddots & \ddots & \\ & & 1 & -2 & 1 \\ & & & 2 & -2-\frac{1}{\alpha} \end{pmatrix}.$$

Then, we obtain

$$D_2\tilde{D}_2 = \begin{pmatrix} 6+\frac{2}{\alpha} & -8 & 2 & & & & & & \\ -4-\frac{1}{\alpha} & 7 & -4 & 1 & & & & & \\ 1 & -4 & 6 & -4 & 1 & & & & \\ & 1 & -4 & 6 & -4 & 1 & & & \\ & & \ddots & \ddots & \ddots & \ddots & \ddots & & \\ & & & 1 & -4 & 6 & -4 & 1 & \\ & & & & 1 & -4 & 6 & -4 & 1 \\ & & & & & 1 & -4 & 7 & -4-\frac{1}{\alpha} \\ & & & & & & 2 & -8 & 6+\frac{2}{\alpha} \end{pmatrix}.$$

Namely, $A = I + \beta D_2\tilde{D}_2$. We remark that D_2 and $\tilde{D}_2$ are not symmetric. Accordingly, following the procedure of the proof for Lemma 0.1.1 in [25], we show that D_2 and $\tilde{D}_2$ are similar to some symmetric tridiagonal matrices, respectively. Let us define $b_1 := 2$,

$b_i := 1$ $(i = 2, \ldots, K)$, $c_i := 1$ $(i = 1, \ldots, K-1)$, and $c_K := 2$. Then, D_2 and $\tilde{D}_2$ are expressed as follows:

$$D_2 = \begin{pmatrix} -2 & b_1 & & & \\ c_1 & -2 & b_2 & & \\ & \ddots & \ddots & \ddots & \\ & & c_{K-1} & -2 & b_K \\ & & & c_K & -2 \end{pmatrix}, \quad \tilde{D}_2 = \begin{pmatrix} -2 - \dfrac{1}{\alpha} & b_1 & & & \\ c_1 & -2 & b_2 & & \\ & \ddots & \ddots & \ddots & \\ & & c_{K-1} & -2 & b_K \\ & & & c_K & -2 - \dfrac{1}{\alpha} \end{pmatrix}.$$

Moreover, let $v_{11} := 1$ and $v_{ii} := \sqrt{(b_1 b_2 \cdots b_{i-1})/(c_1 c_2 \cdots c_{i-1})}$ $(i = 2, \ldots, K+1)$. Then, we have

$$v_{ii} = \sqrt{\frac{2 \cdot 1 \cdots 1}{1 \cdot 1 \cdots 1}} = \sqrt{2} \quad (i = 2, \ldots, K), \quad v_{K+1K+1} = \sqrt{\frac{2 \cdot 1 \cdots 1 \cdot 1}{1 \cdot 1 \cdots 1 \cdot 2}} = 1.$$

Furthermore, let us define the $(K+1) \times (K+1)$ matrix V by

$$V := \operatorname*{diag}_{1 \le i \le K+1} v_{ii} = \begin{pmatrix} v_{11} & & & & \\ & v_{22} & & & \\ & & \ddots & & \\ & & & v_{KK} & \\ & & & & v_{K+1K+1} \end{pmatrix} = \begin{pmatrix} 1 & & & & \\ & \sqrt{2} & & & \\ & & \ddots & & \\ & & & \sqrt{2} & \\ & & & & 1 \end{pmatrix}.$$

Then, we have

$$V D_2 V^{-1} = \begin{pmatrix} 1 & & & & \\ & \sqrt{2} & & & \\ & & \ddots & & \\ & & & \sqrt{2} & \\ & & & & 1 \end{pmatrix} \begin{pmatrix} -2 & 2 & & & \\ 1 & -2 & 1 & & \\ & \ddots & \ddots & \ddots & \\ & & 1 & -2 & 1 \\ & & & 2 & -2 \end{pmatrix} \begin{pmatrix} 1 & & & & \\ & \frac{1}{\sqrt{2}} & & & \\ & & \ddots & & \\ & & & \frac{1}{\sqrt{2}} & \\ & & & & 1 \end{pmatrix}$$

$$= \begin{pmatrix} -2 & 2 & & & \\ \sqrt{2} & -2\sqrt{2} & \sqrt{2} & & \\ & \ddots & \ddots & \ddots & \\ & & \sqrt{2} & -2\sqrt{2} & \sqrt{2} \\ & & & 2 & -2 \end{pmatrix} \begin{pmatrix} 1 & & & & \\ & \frac{1}{\sqrt{2}} & & & \\ & & \ddots & & \\ & & & \frac{1}{\sqrt{2}} & \\ & & & & 1 \end{pmatrix}$$

$$= \begin{pmatrix} -2 & \sqrt{2} & & & & & \\ \sqrt{2} & -2 & 1 & & & & \\ & 1 & -2 & 1 & & & \\ & & \ddots & \ddots & \ddots & & \\ & & & 1 & -2 & 1 & \\ & & & & 1 & -2 & \sqrt{2} \\ & & & & & \sqrt{2} & -2 \end{pmatrix}.$$

Similarly, we obtain

$$V\tilde{D}_2V^{-1} = \begin{pmatrix} -2-\dfrac{1}{\alpha} & \sqrt{2} & & & & & \\ \sqrt{2} & -2 & 1 & & & & \\ & 1 & -2 & 1 & & & \\ & & \ddots & \ddots & \ddots & & \\ & & & 1 & -2 & 1 & \\ & & & & 1 & -2 & \sqrt{2} \\ & & & & & \sqrt{2} & -2-\dfrac{1}{\alpha} \end{pmatrix}.$$

Here, let us define the $(K+1)\times(K+1)$ matrices X and Y by $X := VD_2V^{-1}$ and $Y := V\tilde{D}_2V^{-1}$. Then, X and Y are $(K+1)\times(K+1)$ symmetric matrices. Furthermore, it holds that $XY = VD_2V^{-1}V\tilde{D}_2V^{-1} = VD_2\tilde{D}_2V^{-1}$. That is, $D_2\tilde{D}_2$ is similar to XY. Hence, $D_2\tilde{D}_2$ and XY have the same eigenvalues. Moreover, $-X$ is positive semi-definite, and $-Y$ is positive definite. Actually, for any non-zero vector $\boldsymbol{x} = (x_1, x_2, \ldots, x_{K+1})^\top \in \mathbb{R}^{K+1}$, it holds that

$$(-Y)\boldsymbol{x} = \begin{pmatrix} \left(2+\dfrac{1}{\alpha}\right)x_1 - \sqrt{2}x_2 \\ -\sqrt{2}x_1 + 2x_2 - x_3 \\ -x_2 + 2x_3 - x_4 \\ \vdots \\ -x_{K-2} + 2x_{K-1} - x_K \\ -x_{K-1} + 2x_K - \sqrt{2}x_{K+1} \\ -\sqrt{2}x_K + \left(2+\dfrac{1}{\alpha}\right)x_{K+1} \end{pmatrix}.$$

Thus, we have

$$\begin{aligned} &\boldsymbol{x}^\top(-Y)\boldsymbol{x} \\ &= \left(2+\frac{1}{\alpha}\right)x_1^2 - \sqrt{2}x_1x_2 - \sqrt{2}x_1x_2 + 2x_2^2 - x_2x_3 - x_2x_3 + 2x_3^2 - \cdots \\ &\quad \cdots + 2x_{K-1}^2 - x_{K-1}x_K - x_{K-1}x_K + 2x_K^2 - \sqrt{2}x_Kx_{K+1} - \sqrt{2}x_Kx_{K+1} + \left(2+\frac{1}{\alpha}\right)x_{K+1}^2 \\ &= \frac{1}{\alpha}x_1^2 + 2\left(x_1 - \frac{\sqrt{2}}{2}x_2\right)^2 + (x_2-x_3)^2 + \cdots + (x_{K-1}-x_K)^2 + 2\left(x_{K+1} - \frac{\sqrt{2}}{2}x_K\right)^2 + \frac{1}{\alpha}x_{K+1}^2 \geq 0. \end{aligned}$$

Suppose that $\boldsymbol{x}^\top(-Y)\boldsymbol{x} = 0$. Then, we get $x_1 = \cdots = x_{K+1} = 0$. This is contradictory to $\boldsymbol{x} \neq \boldsymbol{0}$. Namely, $-Y$ is positive definite. Similarly, by direct calculation, we can see that $\boldsymbol{x}^\top(-X)\boldsymbol{x} \geq 0$ for any non-zero vector $\boldsymbol{x} = (x_1, x_2, \ldots, x_{K+1})^\top \in \mathbb{R}^{K+1}$. That is, $-X$ is positive semi-definite. Therefore, from Lemma 5.8, eigenvalues of $XY = (-X)(-Y)$ are all real and nonnegative. Hence, eigenvalues of A are all positive from two facts that eigenvalues of $D_2\tilde{D}_2$ are all real and nonnegative and that β is positive. From the above, $\det A > 0$, i.e., A is nonsingular.

Next, we prove the existence and uniqueness of the solution to the proposed scheme by the fixed-point theorem for a contraction mapping. From (5.36) and (5.37), it is sufficient to show the existence of a $(K+1)$-dimensional vector $\boldsymbol{U} = \{U_k\}_{k=0}^K \in \mathbb{R}^{K+1}$ satisfying $\tilde{U}_k = U_k$ $(k = 0, \ldots, K)$. For the purpose, we define the mapping $\Theta : \mathbb{R}^{K+1} \to \mathbb{R}^{K+1}$ by

$$\Theta(\boldsymbol{V}) := \boldsymbol{V} + \frac{1}{L}M_{\mathrm{d}}(\boldsymbol{U}^{(0)})\boldsymbol{1} \quad \text{for all } \boldsymbol{V} \in \mathbb{R}^{K+1}, \tag{5.45}$$

where $\mathbf{1} := (1, 1, \dots, 1)^\top \in \mathbb{R}^{K+1}$. Then, its inverse mapping Θ^{-1} is written as

$$\Theta^{-1}(\boldsymbol{V}) = \boldsymbol{V} - \frac{1}{L} M_{\mathrm{d}}(\boldsymbol{U}^{(0)})\mathbf{1} \quad \text{for all } \boldsymbol{V} \in \mathbb{R}^{K+1}. \tag{5.46}$$

Let us define the mapping $\Phi : \mathbb{R}^{K+1} \to \mathbb{R}^{K+1}$ by

$$\Phi(\boldsymbol{V}) := \Theta^{-1}\left(\{\Psi_k(\Theta(\boldsymbol{V}))\}_{k=0}^{K}\right) \quad \text{for all } \boldsymbol{V} \in \mathbb{R}^{K+1}, \tag{5.47}$$

where $\Psi_k(\Theta(\boldsymbol{V}))$ is the kth element of the vector $(\Psi \circ \Theta)(\boldsymbol{V}) = \Psi(\Theta(\boldsymbol{V}))$. Moreover, let

$$X_0 := \left\{\boldsymbol{f} \in \mathbb{R}^{K+1}; \|D\boldsymbol{f}\| \leq 2B_0,\ M_{\mathrm{d}}(\boldsymbol{f}) = 0\right\}.$$

We show that Φ is a contraction mapping on X_0 under the assumption (5.28) for Δt. If Φ is a contraction mapping, Φ has a unique fixed-point $\boldsymbol{V}^*$ in the closed ball X_0 from the Banach fixed point theorem. That is, $\boldsymbol{V}^*$ satisfies $\Phi(\boldsymbol{V}^*) = \boldsymbol{V}^*$. From (5.46) and (5.47), we have

$$\Phi(\boldsymbol{V}^*) = \Theta^{-1}\left(\{\Psi_k(\Theta(\boldsymbol{V}^*))\}_{k=0}^{K}\right) = \{\Psi_k(\Theta(\boldsymbol{V}^*))\}_{k=0}^{K} - \frac{1}{L} M_{\mathrm{d}}(\boldsymbol{U}^{(0)})\mathbf{1}. \tag{5.48}$$

Furthermore, from (5.45), we obtain

$$\boldsymbol{V}^* = \Theta(\boldsymbol{V}^*) - \frac{1}{L} M_{\mathrm{d}}(\boldsymbol{U}^{(0)})\mathbf{1}. \tag{5.49}$$

Hence, it holds from (5.48) and (5.49) that $\{\Psi_k(\Theta(\boldsymbol{V}^*))\}_{k=0}^{K} = \Theta(\boldsymbol{V}^*)$. Namely, $\Theta(\boldsymbol{V}^*)$ is the solution $\boldsymbol{U}^{(n+1)}$ to the scheme (5.13)–(5.17). Firstly, we show $\Phi(X_0) \subset X_0$. For the purpose, we check $\|D(\Phi(\boldsymbol{V}))\| \leq 2B_0$ and $M_{\mathrm{d}}(\Phi(\boldsymbol{V})) = 0$ for any fixed $\boldsymbol{V} \in X_0$. Let $\boldsymbol{U} := \Theta(\boldsymbol{V})$. Then, from (5.45), we have

$$U_k = V_k + \frac{1}{L} M_{\mathrm{d}}(\boldsymbol{U}^{(0)}) \quad (k = 0, \dots, K). \tag{5.50}$$

Hence, it holds that

$$\delta_k^+ U_k = \delta_k^+\left(V_k + \frac{1}{L} M_{\mathrm{d}}(\boldsymbol{U}^{(0)})\right) = \delta_k^+ V_k \quad (k = 0, \dots, K-1). \tag{5.51}$$

Let us define $\tilde{\boldsymbol{U}} := \Psi(\boldsymbol{U})$ and $\tilde{\boldsymbol{V}} := \Phi(\boldsymbol{V}) = \Theta^{-1}(\{\tilde{U}_k\}_{k=0}^{K})$. Then, from (5.46), we obtain

$$\tilde{V}_k = \tilde{U}_k - \frac{1}{L} M_{\mathrm{d}}(\boldsymbol{U}^{(0)}) \quad (k = 0, \dots, K). \tag{5.52}$$

Hence, we have

$$\delta_k^+ \tilde{V}_k = \delta_k^+\left(\tilde{U}_k - \frac{1}{L} M_{\mathrm{d}}(\boldsymbol{U}^{(0)})\right) = \delta_k^+ \tilde{U}_k \quad (k = 0, \dots, K-1). \tag{5.53}$$

In addition, it follows from (5.31), (5.35), Proposition 2.2, and Theorem 5.2 that

$$\begin{aligned} M_{\mathrm{d}}(\tilde{\boldsymbol{U}}) = \sum_{k=0}^{K}{}'' \tilde{U}_k \Delta x = \sum_{k=0}^{K}{}'' U_k^{(n)} \Delta x + \Delta t \sum_{k=0}^{K}{}'' \delta_k^{\langle 2 \rangle} \tilde{P}_k^{(n)} \Delta x &= M_{\mathrm{d}}(\boldsymbol{U}^{(n)}) + \Delta t \left[\delta_k^{\langle 1 \rangle} \tilde{P}_k^{(n)}\right]_0^K \\ &= M_{\mathrm{d}}(\boldsymbol{U}^{(0)}). \end{aligned}$$

Thus, it holds from (5.52) and this inequality that

$$
\begin{aligned}
M_{\mathrm{d}}(\tilde{\boldsymbol{V}}) = \sum_{k=0}^{K}{}'' \tilde{V}_k \Delta x = \sum_{k=0}^{K}{}'' \left(\tilde{U}_k - \frac{1}{L} M_{\mathrm{d}}(\boldsymbol{U}^{(0)}) \right) \Delta x &= M_{\mathrm{d}}(\tilde{\boldsymbol{U}}) - M_{\mathrm{d}}(\boldsymbol{U}^{(0)}) \\
&= M_{\mathrm{d}}(\boldsymbol{U}^{(0)}) - M_{\mathrm{d}}(\boldsymbol{U}^{(0)}) \\
&= 0.
\end{aligned}
$$

Therefore, all that is left is to show $\|D\tilde{\boldsymbol{V}}\| \leq 2B_0$. From Corollary 2.1 and (5.31)–(5.34), we have

$$
\begin{aligned}
&\frac{1}{\Delta t}\left(\left\| D\tilde{\boldsymbol{U}} \right\|^2 - \| D\boldsymbol{U}^{(n)} \|^2 \right) = 2\sum_{k=0}^{K-1} \left\{ \delta_k^+ \left(\frac{\tilde{U}_k + U_k^{(n)}}{2} \right) \right\} \left\{ \delta_k^+ \left(\frac{\tilde{U}_k - U_k^{(n)}}{\Delta t} \right) \right\} \Delta x \\
&= -2\sum_{k=0}^{K}{}'' \left\{ \delta_k^{\langle 2 \rangle} \left(\frac{\tilde{U}_k + U_k^{(n)}}{2} \right) \right\} \frac{\tilde{U}_k - U_k^{(n)}}{\Delta t} \Delta x + 2\left[\left\{ \delta_k^{\langle 1 \rangle} \left(\frac{\tilde{U}_k + U_k^{(n)}}{2} \right) \right\} \frac{\tilde{U}_k - U_k^{(n)}}{\Delta t} \right]_0^K \\
&= -2\sum_{k=0}^{K}{}'' \left\{ -\frac{1}{\gamma}\tilde{P}_k^{(n)} + \frac{1}{\gamma}\frac{dF}{d(U_k, U_k^{(n)})} \right\} \left(\delta_k^{\langle 2 \rangle} \tilde{P}_k^{(n)} \right) \Delta x - 2\left(\frac{\tilde{U}_K - U_K^{(n)}}{\Delta t} \right)^2 - 2\left(\frac{\tilde{U}_0 - U_0^{(n)}}{\Delta t} \right)^2 \\
&\leq \frac{2}{\gamma}\sum_{k=0}^{K}{}'' \tilde{P}_k^{(n)} \left(\delta_k^{\langle 2 \rangle} \tilde{P}_k^{(n)} \right) \Delta x - \frac{2}{\gamma}\sum_{k=0}^{K}{}'' \frac{dF}{d(U_k, U_k^{(n)})} \left(\delta_k^{\langle 2 \rangle} \tilde{P}_k^{(n)} \right) \Delta x.
\end{aligned}
$$

Now, it holds from Corollary 2.1 and (5.35) that

$$
\frac{2}{\gamma}\sum_{k=0}^{K}{}'' \tilde{P}_k^{(n)} \left(\delta_k^{\langle 2 \rangle} \tilde{P}_k^{(n)} \right) \Delta x = -\frac{2}{\gamma}\sum_{k=0}^{K-1} \left(\delta_k^+ \tilde{P}_k^{(n)} \right)^2 \Delta x + \frac{2}{\gamma}\left[\left(\delta_k^{\langle 1 \rangle} \tilde{P}_k^{(n)} \right) \tilde{P}_k^{(n)} \right]_0^K = -\frac{2}{\gamma}\left\| D\tilde{\boldsymbol{P}}^{(n)} \right\|^2.
$$

Furthermore, from Corollary 2.1, (5.35), and the Young inequality: $ab \leq (\varepsilon/2)a^2 + (1/(2\varepsilon))b^2$ for all $a, b \in \mathbb{R}$, and $\varepsilon > 0$, we obtain

$$
\begin{aligned}
-\frac{2}{\gamma}\sum_{k=0}^{K}{}'' \frac{dF}{d(U_k, U_k^{(n)})} \left(\delta_k^{\langle 2 \rangle} \tilde{P}_k^{(n)} \right) \Delta x &= \frac{2}{\gamma}\sum_{k=0}^{K-1} \left(\delta_k^+ \tilde{P}_k^{(n)} \right) \left\{ \delta_k^+ \left(\frac{dF}{d(U_k, U_k^{(n)})} \right) \right\} \Delta x \\
&\quad - \frac{2}{\gamma}\left[\left(\delta_k^{\langle 1 \rangle} \tilde{P}_k^{(n)} \right) \frac{dF}{d(U_k, U_k^{(n)})} \right]_0^K \\
&\leq \frac{2}{\gamma}\sum_{k=0}^{K-1} \left[\left(\delta_k^+ \tilde{P}_k^{(n)} \right)^2 + \frac{1}{4}\left\{ \delta_k^+ \left(\frac{dF}{d(U_k, U_k^{(n)})} \right) \right\}^2 \right] \Delta x \\
&= \frac{2}{\gamma}\left\| D\tilde{\boldsymbol{P}}^{(n)} \right\|^2 + \frac{1}{2\gamma}\left\| D\left(\frac{dF}{d\left(\boldsymbol{U}, \boldsymbol{U}^{(n)}\right)} \right) \right\|^2.
\end{aligned}
$$

From the above, we have

$$
\frac{1}{\Delta t}\left(\left\| D\tilde{\boldsymbol{U}} \right\|^2 - \| D\boldsymbol{U}^{(n)} \|^2 \right) \leq \frac{1}{2\gamma}\left\| D\left(\frac{dF}{d\left(\boldsymbol{U}, \boldsymbol{U}^{(n)}\right)} \right) \right\|^2.
$$

Consequently, using the triangle inequality: $\sqrt{a^2+b^2} \le |a|+|b|$ for all $a, b \in \mathbb{R}$, we get

$$\left\| D\tilde{\boldsymbol{U}} \right\| \le \|D\boldsymbol{U}^{(n)}\| + \sqrt{\frac{\Delta t}{2\gamma}} \left\| D\left(\frac{dF}{d\left(\boldsymbol{U}, \boldsymbol{U}^{(n)}\right)} \right) \right\|. \tag{5.54}$$

Thus, from (5.53) and (5.54), it is sufficient to show that the right-hand side of (5.54) is not greater than $2B_0$. For $k = 0, \ldots, K-1$, using Lemma 2.2, we have

$$\delta_k^+ \left(\frac{dF}{d(U_k, U_k^{(n)})} \right) = \frac{1}{2} \bar{F}''(U_{k+1}, U_k; U_{k+1}^{(n)}, U_k^{(n)}) \delta_k^+ U_k + \frac{1}{2} \bar{F}''(U_{k+1}^{(n)}, U_k^{(n)}; U_{k+1}, U_k) \delta_k^+ U_k^{(n)}. \tag{5.55}$$

Hence, using (5.55) and the Minkowski inequality, we obtain

$$\begin{aligned}
&\left\| D\left(\frac{dF}{d\left(\boldsymbol{U}, \boldsymbol{U}^{(n)}\right)} \right) \right\| \\
&= \left\{ \sum_{k=0}^{K-1} \left| \frac{1}{2} \bar{F}''(U_{k+1}, U_k; U_{k+1}^{(n)}, U_k^{(n)}) \delta_k^+ U_k + \frac{1}{2} \bar{F}''(U_{k+1}^{(n)}, U_k^{(n)}; U_{k+1}, U_k) \delta_k^+ U_k^{(n)} \right|^2 \Delta x \right\}^{\frac{1}{2}} \\
&\le \left\{ \sum_{k=0}^{K-1} \left| \frac{1}{2} \bar{F}''(U_{k+1}, U_k; U_{k+1}^{(n)}, U_k^{(n)}) \delta_k^+ U_k \right|^2 \Delta x \right\}^{\frac{1}{2}} \\
&\quad + \left\{ \sum_{k=0}^{K-1} \left| \frac{1}{2} \bar{F}''(U_{k+1}^{(n)}, U_k^{(n)}; U_{k+1}, U_k) \delta_k^+ U_k^{(n)} \right|^2 \Delta x \right\}^{\frac{1}{2}} \\
&\le \frac{1}{2} \max_{0 \le k \le K-1} \left| \bar{F}''(U_{k+1}, U_k; U_{k+1}^{(n)}, U_k^{(n)}) \right| \|D\boldsymbol{U}\| \\
&\quad + \frac{1}{2} \max_{0 \le k \le K-1} \left| \bar{F}''(U_{k+1}^{(n)}, U_k^{(n)}; U_{k+1}, U_k) \right| \left\| D\boldsymbol{U}^{(n)} \right\|.
\end{aligned}$$

Next, we consider $|\bar{F}''(U_{k+1}, U_k; U_{k+1}^{(n)}, U_k^{(n)})|$ and $|\bar{F}''(U_{k+1}^{(n)}, U_k^{(n)}; U_{k+1}, U_k)|$. It follows from Proposition 2.6 that

$$\|\boldsymbol{U}\|_{L_{\mathrm{d}}^\infty} \le \frac{1}{L} |M_{\mathrm{d}}(\boldsymbol{U})| + L^{\frac{1}{2}} \|D\boldsymbol{U}\|.$$

We get $M_{\mathrm{d}}(\boldsymbol{V}) = 0$ from $\boldsymbol{V} \in X_0$. Hence, by (5.50), we have

$$M_{\mathrm{d}}(\boldsymbol{U}) = \sum_{k=0}^{K}{}'' U_k \Delta x = M_{\mathrm{d}}(\boldsymbol{V}) + M_{\mathrm{d}}(\boldsymbol{U}^{(0)}) = M_{\mathrm{d}}(\boldsymbol{U}^{(0)}).$$

Since it holds from $\boldsymbol{V} \in X_0$ and (5.51) that $\|D\boldsymbol{U}\| = \|D\boldsymbol{V}\| \le 2B_0$, we obtain

$$\|\boldsymbol{U}\|_{L_{\mathrm{d}}^\infty} \le \frac{1}{L} |M_{\mathrm{d}}(\boldsymbol{U})| + 2L^{\frac{1}{2}} B_0 = \frac{1}{L} \left| M_{\mathrm{d}}(\boldsymbol{U}^{(0)}) \right| + 2L^{\frac{1}{2}} B_0 \le 2\tilde{B}_0.$$

Also, using Theorem 5.3, we get $\|\boldsymbol{U}^{(n)}\|_{L_{\mathrm{d}}^\infty} \le \tilde{B}_0$. Therefore, from Lemma 2.1, we obtain

$$\left| \bar{F}''(U_{k+1}, U_k; U_{k+1}^{(n)}, U_k^{(n)}) \right| \le \max_{|\xi| \le 2\tilde{B}_0} |F''(\xi)|, \quad \left| \bar{F}''(U_{k+1}^{(n)}, U_k^{(n)}; U_{k+1}, U_k) \right| \le \max_{|\xi| \le 2\tilde{B}_0} |F''(\xi)|$$

for $k=0,\dots,K-1$. Hence, it holds that

$$\left\| D\left(\frac{dF}{d(\boldsymbol{U},\boldsymbol{U}^{(n)})}\right)\right\| \leq \frac{1}{2}\max_{|\xi|\leq 2\tilde{B}_0}|F''(\xi)|\left(\|D\boldsymbol{U}\|+\|D\boldsymbol{U}^{(n)}\|\right). \tag{5.56}$$

Consequently, using (5.54), (5.56), and Lemma 5.3, the following estimate holds:

$$\begin{aligned}\left\|D\tilde{\boldsymbol{U}}\right\| &\leq \|D\boldsymbol{U}^{(n)}\| + \sqrt{\frac{\Delta t}{2\gamma}}\cdot\frac{1}{2}\max_{|\xi|\leq 2\tilde{B}_0}|F''(\xi)|\left(\|D\boldsymbol{U}\|+\|D\boldsymbol{U}^{(n)}\|\right)\\ &\leq B_0 + \frac{3\max_{|\xi|\leq 2\tilde{B}_0}|F''(\xi)|}{2}\sqrt{\frac{\Delta t}{2\gamma}}B_0.\end{aligned}$$

Now, from (5.53) and the assumption (5.28), we have $\|D\tilde{\boldsymbol{V}}\| = \|D\tilde{\boldsymbol{U}}\| \leq 2B_0$. From the above, it holds that $\Phi(\boldsymbol{V}) = \tilde{\boldsymbol{V}} \in X_0$, i.e., $\Phi(X_0)\subset X_0$. Next, we prove that Φ is contractive. For any $\boldsymbol{V}_1,\boldsymbol{V}_2\in X_0$, let $\boldsymbol{U}_1 := \Theta(\boldsymbol{V}_1)$ and $\boldsymbol{U}_2 := \Theta(\boldsymbol{V}_2)$. From (5.45), it holds that

$$U_{i,k} = V_{i,k} + \frac{1}{L}M_{\mathrm{d}}(\boldsymbol{U}^{(0)}) \quad (k=0,\dots,K,\ i=1,2). \tag{5.57}$$

It follows from (5.57) that

$$\delta_k^+ U_{i,k} = \delta_k^+\left(V_{i,k}+\frac{1}{L}M_{\mathrm{d}}(\boldsymbol{U}^{(0)})\right) = \delta_k^+ V_{i,k} \quad (k=0,\dots,K-1,\ i=1,2). \tag{5.58}$$

Furthermore, from (5.57) and $\boldsymbol{V}_i\in X_0$ $(i=1,2)$, we have

$$M_{\mathrm{d}}(\boldsymbol{U}_i) = \sum_{k=0}^{K}{}'' U_{i,k}\Delta x = M_{\mathrm{d}}(\boldsymbol{V}_i) + M_{\mathrm{d}}(\boldsymbol{U}^{(0)}) = M_{\mathrm{d}}(\boldsymbol{U}^{(0)}) \quad (i=1,2). \tag{5.59}$$

Moreover, it follows from $U_{1,k}-U_{2,k} = V_{1,k}-V_{2,k}$ $(k=0,\dots,K)$ that $\|D(\boldsymbol{U}_1-\boldsymbol{U}_2)\| = \|D(\boldsymbol{V}_1-\boldsymbol{V}_2)\|$. Now, let us define $\tilde{\boldsymbol{U}}_i := \Psi(\boldsymbol{U}_i)$ and $\tilde{\boldsymbol{V}}_i := \Phi(\boldsymbol{V}_i) = \Theta^{-1}(\{\tilde{U}_{i,k}\}_{k=0}^{K})$ $(i=1,2)$. Then, from (5.46), we have

$$\tilde{V}_{i,k} = \tilde{U}_{i,k} - \frac{1}{L}M_{\mathrm{d}}(\boldsymbol{U}^{(0)}) \quad (k=0,\dots,K,\ i=1,2).$$

Hence, it holds that $\tilde{V}_{1,k}-\tilde{V}_{2,k} = \tilde{U}_{1,k}-\tilde{U}_{2,k}$ $(k=0,\dots,K)$. Namely, $\|D(\tilde{\boldsymbol{V}}_1-\tilde{\boldsymbol{V}}_2)\| = \|D(\tilde{\boldsymbol{U}}_1-\tilde{\boldsymbol{U}}_2)\|$. Now, from the definition of Ψ, the vector $\{\tilde{U}_{i,k}\}_{k=-1}^{K+1} = \{\Psi_k(\boldsymbol{U}_i)\}_{k=-1}^{K+1}$ satisfies (5.31)–(5.35) $(i=1,2)$. Subtracting these relations, we obtain

$$\frac{\tilde{U}_{1,k}-\tilde{U}_{2,k}}{\Delta t} = \delta_k^{\langle 2\rangle}\left(\tilde{P}_{1,k}^{(n)}-\tilde{P}_{2,k}^{(n)}\right) \quad (k=0,\dots,K), \tag{5.60}$$

$$\delta_k^{\langle 2\rangle}\left(\tilde{U}_{1,k}-\tilde{U}_{2,k}\right) = \frac{2}{\gamma}\left\{-\left(\tilde{P}_{1,k}^{(n)}-\tilde{P}_{2,k}^{(n)}\right)+\left(\frac{dF}{d(U_{1,k},U_k^{(n)})}-\frac{dF}{d(U_{2,k},U_k^{(n)})}\right)\right\} \quad (k=0,\dots,K), \tag{5.61}$$

$$\frac{\tilde{U}_{1,0}-\tilde{U}_{2,0}}{\Delta t} = \delta_k^{\langle 1\rangle}\left(\frac{\tilde{U}_{1,k}-\tilde{U}_{2,k}}{2}\right)\Bigg|_{k=0}, \tag{5.62}$$

$$\frac{\tilde{U}_{1,K}-\tilde{U}_{2,K}}{\Delta t} = -\,\delta_k^{\langle 1\rangle}\left(\frac{\tilde{U}_{1,k}-\tilde{U}_{2,k}}{2}\right)\Bigg|_{k=K}, \tag{5.63}$$

$$\delta_k^{\langle 1\rangle}\left(\tilde{P}_{1,k}^{(n)}-\tilde{P}_{2,k}^{(n)}\right) = 0 \quad (k=0,K). \tag{5.64}$$

From Corollary 2.1, (5.60)–(5.64), and the Young inequality, we have

$$
\begin{aligned}
\left\| D(\tilde{\boldsymbol{U}}_1 - \tilde{\boldsymbol{U}}_2) \right\|^2 &= \sum_{k=0}^{K}{}'' \left\{ \delta_k^+ (\tilde{U}_{1,k} - \tilde{U}_{2,k}) \right\}^2 \Delta x \\
&= -\sum_{k=0}^{K}{}'' \left\{ \delta_k^{\langle 2 \rangle} \Big(\tilde{U}_{1,k} - \tilde{U}_{2,k} \Big) \right\} \Big(\tilde{U}_{1,k} - \tilde{U}_{2,k} \Big) \Delta x + \left[\left\{ \delta_k^{\langle 1 \rangle} \Big(\tilde{U}_{1,k} - \tilde{U}_{2,k} \Big) \right\} \Big(\tilde{U}_{1,k} - \tilde{U}_{2,k} \Big) \right]_0^K \\
&= \frac{2\Delta t}{\gamma} \sum_{k=0}^{K}{}'' \Big(\tilde{P}_{1,k}^{(n)} - \tilde{P}_{2,k}^{(n)} \Big) \left\{ \delta_k^{\langle 2 \rangle} \Big(\tilde{P}_{1,k}^{(n)} - \tilde{P}_{2,k}^{(n)} \Big) \right\} \Delta x - \frac{2\Delta t}{\gamma} \sum_{k=0}^{K}{}'' \left(\frac{dF}{d(U_{1,k}, U_{1,k}^{(n)})} - \frac{dF}{d(U_{2,k}, U_{2,k}^{(n)})} \right) \\
&\quad \times \left\{ \delta_k^{\langle 2 \rangle} \Big(\tilde{P}_{1,k}^{(n)} - \tilde{P}_{2,k}^{(n)} \Big) \right\} \Delta x - \frac{2}{\Delta t} \Big(\tilde{U}_{1,K} - \tilde{U}_{2,K} \Big)^2 - \frac{2}{\Delta t} \Big(\tilde{U}_{1,0} - \tilde{U}_{2,0} \Big)^2 \\
&\leq -\frac{2\Delta t}{\gamma} \sum_{k=0}^{K-1} \left\{ \delta_k^+ \Big(\tilde{P}_{1,k}^{(n)} - \tilde{P}_{2,k}^{(n)} \Big) \right\}^2 \Delta x + \frac{2\Delta t}{\gamma} \left[\left\{ \delta_k^{\langle 1 \rangle} \Big(\tilde{P}_{1,k}^{(n)} - \tilde{P}_{2,k}^{(n)} \Big) \right\} \Big(\tilde{P}_{1,k}^{(n)} - \tilde{P}_{2,k}^{(n)} \Big) \right]_0^K \\
&\quad + \frac{2\Delta t}{\gamma} \sum_{k=0}^{K-1} \left\{ \delta_k^+ \left(\frac{dF}{d(U_{1,k}, U_{1,k}^{(n)})} - \frac{dF}{d(U_{2,k}, U_{2,k}^{(n)})} \right) \right\} \left\{ \delta_k^+ \Big(\tilde{P}_{1,k}^{(n)} - \tilde{P}_{2,k}^{(n)} \Big) \right\} \Delta x \\
&\quad - \frac{2\Delta t}{\gamma} \left[\left\{ \delta_k^{\langle 1 \rangle} \Big(\tilde{P}_{1,k}^{(n)} - \tilde{P}_{2,k}^{(n)} \Big) \right\} \left(\frac{dF}{d(U_{1,k}, U_{1,k}^{(n)})} - \frac{dF}{d(U_{2,k}, U_{2,k}^{(n)})} \right) \right]_0^K \\
&\leq -\frac{2\Delta t}{\gamma} \left\| D \left(\tilde{\boldsymbol{P}}_1^{(n)} - \tilde{\boldsymbol{P}}_2^{(n)} \right) \right\|^2 \\
&\quad + \frac{2\Delta t}{\gamma} \sum_{k=0}^{K-1} \left[\frac{1}{4} \left\{ \delta_k^+ \left(\frac{dF}{d(U_{1,k}, U_{1,k}^{(n)})} - \frac{dF}{d(U_{2,k}, U_{2,k}^{(n)})} \right) \right\}^2 + \left\{ \delta_k^+ \Big(\tilde{P}_{1,k}^{(n)} - \tilde{P}_{2,k}^{(n)} \Big) \right\}^2 \right] \Delta x \\
&= \frac{\Delta t}{2\gamma} \left\| D \left(\frac{dF}{d(\boldsymbol{U}_1, \boldsymbol{U}_1^{(n)})} - \frac{dF}{d(\boldsymbol{U}_2, \boldsymbol{U}_2^{(n)})} \right) \right\|^2 .
\end{aligned}
$$

Namely,

$$
\left\| D(\tilde{\boldsymbol{U}}_1 - \tilde{\boldsymbol{U}}_2) \right\| \leq \sqrt{\frac{\Delta t}{2\gamma}} \left\| D \left(\frac{dF}{d(\boldsymbol{U}_1, \boldsymbol{U}_1^{(n)})} - \frac{dF}{d(\boldsymbol{U}_2, \boldsymbol{U}_2^{(n)})} \right) \right\| . \tag{5.65}
$$

Using Lemma 2.2, we get

$$
\frac{dF}{d(U_{1,k}, U_k^{(n)})} - \frac{dF}{d(U_{2,k}, U_k^{(n)})} = \frac{1}{2} \bar{F}''(U_{1,k}, U_{2,k}; U_k^{(n)}, U_k^{(n)})(U_{1,k} - U_{2,k}) \quad (k = 0, \dots, K).
$$

Hence, it follows from Lemma 2.3 that

$$
\begin{aligned}
\left\| D \left(\frac{dF}{d(\boldsymbol{U}_1, \boldsymbol{U}^{(n)})} - \frac{dF}{d(\boldsymbol{U}_2, \boldsymbol{U}^{(n)})} \right) \right\| &= \frac{1}{2} \left\| D \left\{ \bar{F}''(\boldsymbol{U}_1, \boldsymbol{U}_2; \boldsymbol{U}^{(n)}, \boldsymbol{U}^{(n)})(\boldsymbol{U}_1 - \boldsymbol{U}_2) \right\} \right\| \\
&\leq \frac{1}{2} \left\| \bar{F}''(\boldsymbol{U}_1, \boldsymbol{U}_2; \boldsymbol{U}^{(n)}, \boldsymbol{U}^{(n)}) \right\|_{L_{\mathrm{d}}^\infty} \| D(\boldsymbol{U}_1 - \boldsymbol{U}_2) \| \\
&\quad + \frac{1}{2} \| \boldsymbol{U}_1 - \boldsymbol{U}_2 \|_{L_{\mathrm{d}}^\infty} \left\| D\bar{F}''(\boldsymbol{U}_1, \boldsymbol{U}_2; \boldsymbol{U}^{(n)}, \boldsymbol{U}^{(n)}) \right\| .
\end{aligned} \tag{5.66}
$$

We consider $\|\bar{F}''(\boldsymbol{U}_1,\boldsymbol{U}_2;\boldsymbol{U}^{(n)},\boldsymbol{U}^{(n)})\|_{L^\infty_{\mathrm{d}}}$ and $\|D\bar{F}''(\boldsymbol{U}_1,\boldsymbol{U}_2;\boldsymbol{U}^{(n)},\boldsymbol{U}^{(n)})\|$. From $\boldsymbol{V}_i \in X_0$ $(i=1,2)$ and (5.58), we have $\|D\boldsymbol{U}_i\| = \|D\boldsymbol{V}_i\| \le 2B_0$ $(i=1,2)$. Therefore, using Proposition 2.6 and (5.59), we obtain

$$\|\boldsymbol{U}_i\|_{L^\infty_{\mathrm{d}}} \le \frac{1}{L}\left|M_{\mathrm{d}}(\boldsymbol{U}_i)\right| + L^{\frac{1}{2}}\left\|D\boldsymbol{U}_i\right\| \le \frac{1}{L}\left|M_{\mathrm{d}}(\boldsymbol{U}^{(0)})\right| + 2L^{\frac{1}{2}}B_0 \le 2\tilde{B}_0 \quad (i=1,2).$$

Hence, using Theorem 5.3 and Lemma 2.1, we get

$$\left\|\bar{F}''(\boldsymbol{U}_1,\boldsymbol{U}_2;\boldsymbol{U}^{(n)},\boldsymbol{U}^{(n)})\right\|_{L^\infty_{\mathrm{d}}} \le \max_{|\xi|\le 2\tilde{B}_0}\left|F''(\xi)\right|. \tag{5.67}$$

Furthermore, from Lemma 5.3 and Lemma 2.4, the following estimate holds:

$$\begin{aligned}\left\|D\bar{F}''(\boldsymbol{U}_1,\boldsymbol{U}_2;\boldsymbol{U}^{(n)},\boldsymbol{U}^{(n)})\right\| &\le \frac{1}{3}\max_{|\xi|\le 2\tilde{B}_0}\left|F'''(\xi)\right|\left(\|D\boldsymbol{U}_1\| + \|D\boldsymbol{U}_2\| + \left\|D\boldsymbol{U}^{(n)}\right\|\right)\\ &\le \frac{5B_0}{3}\max_{|\xi|\le 2\tilde{B}_0}\left|F'''(\xi)\right|. \end{aligned}\tag{5.68}$$

Now, it follows from $U_{1,k} - U_{2,k} = V_{1,k} - V_{2,k}$ $(k=0,\dots,K)$ and $\boldsymbol{V}_i \in X_0$ $(i=1,2)$ that

$$M_{\mathrm{d}}(\boldsymbol{U}_1 - \boldsymbol{U}_2) = M_{\mathrm{d}}(\boldsymbol{V}_1 - \boldsymbol{V}_2) = M_{\mathrm{d}}(\boldsymbol{V}_1) - M_{\mathrm{d}}(\boldsymbol{V}_2) = 0.$$

Hence, from Proposition 2.6, we have

$$\|\boldsymbol{U}_1 - \boldsymbol{U}_2\|_{L^\infty_{\mathrm{d}}} \le \frac{1}{L}\left|M_{\mathrm{d}}(\boldsymbol{U}_1 - \boldsymbol{U}_2)\right| + L^{\frac{1}{2}}\left\|D\left(\boldsymbol{U}_1 - \boldsymbol{U}_2\right)\right\| = L^{\frac{1}{2}}\left\|D\left(\boldsymbol{U}_1 - \boldsymbol{U}_2\right)\right\|. \tag{5.69}$$

Thus, using (5.66)–(5.69), we get the following estimate:

$$\begin{aligned}\left\|D\left(\frac{dF}{d(\boldsymbol{U}_1,\boldsymbol{U}^{(n)})} - \frac{dF}{d(\boldsymbol{U}_2,\boldsymbol{U}^{(n)})}\right)\right\| &\le \left(\frac{\max\limits_{|\xi|\le 2\tilde{B}_0}\left|F''(\xi)\right|}{2} + \frac{5L^{\frac{1}{2}}B_0\max\limits_{|\xi|\le 2\tilde{B}_0}\left|F'''(\xi)\right|}{6}\right)\\ &\quad\times\left\|D\left(\boldsymbol{U}_1 - \boldsymbol{U}_2\right)\right\|. \end{aligned}\tag{5.70}$$

Consequently, from (5.65) and (5.70), we obtain

$$\begin{aligned}\left\|D(\tilde{\boldsymbol{V}}_1 - \tilde{\boldsymbol{V}}_2)\right\| &= \left\|D(\tilde{\boldsymbol{U}}_1 - \tilde{\boldsymbol{U}}_2)\right\|\\ &\le \left(\frac{\max\limits_{|\xi|\le 2\tilde{B}_0}\left|F''(\xi)\right|}{2} + \frac{5L^{\frac{1}{2}}B_0\max\limits_{|\xi|\le 2\tilde{B}_0}\left|F'''(\xi)\right|}{6}\right)\sqrt{\frac{\Delta t}{2\gamma}}\left\|D\left(\boldsymbol{U}_1 - \boldsymbol{U}_2\right)\right\|\\ &= \left(\frac{\max\limits_{|\xi|\le 2\tilde{B}_0}\left|F''(\xi)\right|}{2} + \frac{5L^{\frac{1}{2}}B_0\max\limits_{|\xi|\le 2\tilde{B}_0}\left|F'''(\xi)\right|}{6}\right)\sqrt{\frac{\Delta t}{2\gamma}}\left\|D\left(\boldsymbol{V}_1 - \boldsymbol{V}_2\right)\right\|. \end{aligned}$$

Since it holds from the assumption (5.28) on Δt that

$$\left(\frac{\max\limits_{|\xi|\le 2\tilde{B}_0}\left|F''(\xi)\right|}{2} + \frac{5L^{\frac{1}{2}}B_0\max\limits_{|\xi|\le 2\tilde{B}_0}\left|F'''(\xi)\right|}{6}\right)\sqrt{\frac{\Delta t}{2\gamma}} < 1,$$

the mapping Φ is contraction into X_0. This completes the proof. □

The following corollary holds from the same argument as Corollary 3.3 in [67].

Corollary 5.2. Assume that $F(s) = (q/4)s^4 - (r/2)s^2$ for all $s \in \mathbb{R}$, where q and r are positive constants. If Δt satisfies

$$\max\left\{\frac{3r}{2},\ \frac{17q}{2}\tilde{B}_0^2 + \frac{r}{2},\ \frac{51q}{4}\tilde{B}_0^2 - \frac{r}{2}\right\}\sqrt{\frac{\Delta t}{2\gamma}} < 1,$$

then there exists a unique solution $\{U_k^{(n)}\}_{k=-1}^{K+1} \in \mathbb{R}^{K+3}$ $(n = 1, 2, \ldots)$ satisfying (5.13)–(5.17).

§5 Error estimate

In this section, we show the error estimate. We also use the energy method in [28, 52, 65–68]. Fix a natural number $N \in \mathbb{N}$. We compute $\boldsymbol{U}^{(n)}$ up to $n = N$ by our proposed scheme (5.13)–(5.17) and estimate the error between it and the solution to the problem (5.1)–(5.5) up to $T = N\Delta t$. Let u and p be the solutions to the problem (5.1)–(5.5) with an initial condition. Besides, assume that $u \in C^4([0, L] \times [0, T])$. Also, we assume that the potential F is sufficiently smooth. Moreover, we extend the solutions u and p in $[0, L] \times [0, T]$ to $\tilde{u}$ and $\tilde{p}$ in $[-\Delta x, L + \Delta x] \times [0, T]$, respectively, as follows:

$$\tilde{u}(x,t) := \begin{cases} u(-x,t) + 2x\partial_x u(0,t) + \dfrac{x^3}{3}\partial_x^3 u(0,t) & (-\Delta x \le x < 0), \\ u(x,t) & (0 \le x \le L), \\ u(2L-x,t) + 2(x-L)\partial_x u(L,t) + \dfrac{(x-L)^3}{3}\partial_x^3 u(L,t) & (L < x \le L + \Delta x), \end{cases} \tag{5.71}$$

$$\tilde{p}(x,t) := \begin{cases} p(-x,t) + \dfrac{\partial_x^3 p(0,t)}{3}\left\{1 + \dfrac{x^3}{(\Delta x)^3}\right\}x^3 + \dfrac{\partial_x^5 p(0,t)}{60}\left(1 + \dfrac{x}{\Delta x}\right)x^5, \quad (-\Delta x \le x < 0), \\ p(x,t), \quad (0 \le x \le L), \\ p(2L-x,t) + \dfrac{\partial_x^3 p(L,t)}{3}\left\{1 - \dfrac{(x-L)^3}{(\Delta x)^3}\right\}(x-L)^3 + \dfrac{\partial_x^5 p(L,t)}{60}\left(1 - \dfrac{x-L}{\Delta x}\right)(x-L)^5, \\ \qquad (L < x \le L + \Delta x), \end{cases}$$

for all $t \in [0, T]$, where $\partial_x f(a)$ means $\partial_x f(x)|_{x=a}$. By direct calculation, we can check that $\tilde{u} \in C^4([-\Delta x, L + \Delta x] \times [0, T])$. We can also check that $\partial_x^5 \tilde{p}$ exists and is continuous on $[-\Delta x, L + \Delta x] \times [0, T]$ and that the following property holds:

$$\tilde{p}(-\Delta x, t) = \tilde{p}(\Delta x, t), \quad \tilde{p}(L + \Delta x, t) = \tilde{p}(L - \Delta x, t), \quad \text{for all } t \in [0, T]. \tag{5.72}$$

Let $U_k^{(0)} = \tilde{u}(k\Delta x, 0)$ $(k = -1, 0, \ldots, K, K+1)$. In addition, we define errors $e_{u,k}^{(n)}$ and $e_{p,k}^{(n)}$ by

$$e_{u,k}^{(n)} := U_k^{(n)} - \tilde{u}(k\Delta x, n\Delta t) \quad (k = -1, 0, \ldots, K, K+1,\ n = 0, 1, \ldots, N),$$

$$e_{p,k}^{(n)} := P_k^{(n)} - \tilde{p}\left(k\Delta x, \left(n + \frac{1}{2}\right)\Delta t\right) \quad (k = -1, 0, \ldots, K, K+1,\ n = 0, 1, \ldots, N-1).$$

For simplicity, we use the expression $\tilde{u}_k^{(n)} := \tilde{u}(k\Delta x, n\Delta t)$ from now on. Also, the expression $\delta_k^* f_l$ means $\delta_k^* f_k|_{k=l}$, where the symbol "$*$" denotes $+$, $\langle 1 \rangle$, or $\langle 2 \rangle$. Then, the following lemmas hold:

Lemma 5.9. Assume that $u \in C^4([0,L]\times[0,T])$. Then, we obtain the following equations on the errors:

$$\frac{e_{u,k}^{(n+1)} - e_{u,k}^{(n)}}{\Delta t} = \delta_k^{\langle 2\rangle} e_{p,k}^{(n)} + \xi_{1,k}^{\left(n+\frac{1}{2}\right)} \quad (k = 0,\ldots,K), \tag{5.73}$$

$$e_{p,k}^{(n)} = -\gamma\delta_k^{\langle 2\rangle}\left(\frac{e_{u,k}^{(n+1)} + e_{u,k}^{(n)}}{2}\right) + \left(\frac{dF}{d(U_k^{(n+1)}, U_k^{(n)})} - \frac{dF}{d(u_k^{(n+1)}, u_k^{(n)})}\right) + \xi_{2,k}^{\left(n+\frac{1}{2}\right)} \quad (k = 0,\ldots,K), \tag{5.74}$$

$$\frac{e_{u,0}^{(n+1)} - e_{u,0}^{(n)}}{\Delta t} = \delta_k^{\langle 1\rangle}\left(\frac{e_{u,0}^{(n+1)} + e_{u,0}^{(n)}}{2}\right) + \xi_{3,0}^{\left(n+\frac{1}{2}\right)}, \tag{5.75}$$

$$\frac{e_{u,K}^{(n+1)} - e_{u,K}^{(n)}}{\Delta t} = -\delta_k^{\langle 1\rangle}\left(\frac{e_{u,K}^{(n+1)} + e_{u,K}^{(n)}}{2}\right) + \xi_{3,K}^{\left(n+\frac{1}{2}\right)}, \tag{5.76}$$

$$\delta_k^{\langle 1\rangle} e_{p,k}^{(n)} = 0 \quad (k = 0, K) \tag{5.77}$$

for $n = 0, 1, \ldots, N-1$, where ξ_1, ξ_2, and ξ_3 are defined as follows:

$$\xi_{1,k}^{\left(n+\frac{1}{2}\right)} := \partial_t u_k^{\left(n+\frac{1}{2}\right)} - \frac{u_k^{(n+1)} - u_k^{(n)}}{\Delta t} + \delta_k^{\langle 2\rangle}\tilde{p}_k^{\left(n+\frac{1}{2}\right)} - \partial_x^2 p_k^{\left(n+\frac{1}{2}\right)} \quad (k = 0,\ldots,K),$$

$$\xi_{2,k}^{\left(n+\frac{1}{2}\right)} := \gamma\left\{\partial_x^2 u_k^{\left(n+\frac{1}{2}\right)} - \delta_k^{\langle 2\rangle}\left(\frac{\tilde{u}_k^{(n+1)} + \tilde{u}_k^{(n)}}{2}\right)\right\} + \frac{dF}{d(u_k^{(n+1)}, u_k^{(n)})} - F'(u_k^{\left(n+\frac{1}{2}\right)}) \quad (k = 0,\ldots,K),$$

$$\xi_{3,0}^{\left(n+\frac{1}{2}\right)} := \partial_t u_0^{\left(n+\frac{1}{2}\right)} - \frac{u_0^{(n+1)} - u_0^{(n)}}{\Delta t} + \delta_k^{\langle 1\rangle}\left(\frac{\tilde{u}_0^{(n+1)} + \tilde{u}_0^{(n)}}{2}\right) - \partial_x u_0^{\left(n+\frac{1}{2}\right)},$$

$$\xi_{3,K}^{\left(n+\frac{1}{2}\right)} := \partial_t u_K^{\left(n+\frac{1}{2}\right)} - \frac{u_K^{(n+1)} - u_K^{(n)}}{\Delta t} + \partial_x u_K^{\left(n+\frac{1}{2}\right)} - \delta_k^{\langle 1\rangle}\left(\frac{\tilde{u}_K^{(n+1)} + \tilde{u}_K^{(n)}}{2}\right).$$

Proof. For any fixed $n = 0, 1, \ldots, N-1$, from the definition of $\boldsymbol{e}_u$, (5.1), and (5.13), we have

$$\begin{aligned}
\frac{e_{u,k}^{(n+1)} - e_{u,k}^{(n)}}{\Delta t} &= \frac{U_k^{(n+1)} - U_k^{(n)}}{\Delta t} - \frac{u_k^{(n+1)} - u_k^{(n)}}{\Delta t} \\
&= \frac{U_k^{(n+1)} - U_k^{(n)}}{\Delta t} - \partial_t u_k^{\left(n+\frac{1}{2}\right)} + \partial_t u_k^{\left(n+\frac{1}{2}\right)} - \frac{u_k^{(n+1)} - u_k^{(n)}}{\Delta t} \\
&= \delta_k^{\langle 2\rangle} P_k^{(n)} - \partial_x^2 p_k^{\left(n+\frac{1}{2}\right)} + \partial_t u_k^{\left(n+\frac{1}{2}\right)} - \frac{u_k^{(n+1)} - u_k^{(n)}}{\Delta t} \\
&= \delta_k^{\langle 2\rangle} P_k^{(n)} - \delta_k^{\langle 2\rangle} p_k^{\left(n+\frac{1}{2}\right)} + \delta_k^{\langle 2\rangle} p_k^{\left(n+\frac{1}{2}\right)} - \partial_x^2 p_k^{\left(n+\frac{1}{2}\right)} + \partial_t u_k^{\left(n+\frac{1}{2}\right)} - \frac{u_k^{(n+1)} - u_k^{(n)}}{\Delta t} \\
&= \delta_k^{\langle 2\rangle} e_{p,k}^{(n)} + \xi_{1,k}^{\left(n+\frac{1}{2}\right)} \quad (k = 1,\ldots,K-1).
\end{aligned} \tag{5.78}$$

Similarly, from (5.2), (5.14), and the definitions of $\boldsymbol{e}_u$ and $\boldsymbol{e}_p$, we obtain

$$e_{p,k}^{(n)} = -\gamma\delta_k^{\langle 2\rangle}\left(\frac{U_k^{(n+1)} + U_k^{(n)}}{2}\right) + \frac{dF}{d(U_k^{(n+1)}, U_k^{(n)})} + \gamma\partial_x^2 u_k^{\left(n+\frac{1}{2}\right)} - F'(u_k^{\left(n+\frac{1}{2}\right)})$$

$$
\begin{aligned}
&= -\gamma\delta_k^{\langle 2\rangle}\left(\frac{e_{u,k}^{(n+1)} + u_k^{(n+1)} + e_{u,k}^{(n)} + u_k^{(n)}}{2}\right) + \gamma\partial_x^2 u_k^{\left(n+\frac{1}{2}\right)} \\
&\quad + \frac{dF}{d(U_k^{(n+1)}, U_k^{(n)})} - \frac{dF}{d(u_k^{(n+1)}, u_k^{(n)})} + \frac{dF}{d(u_k^{(n+1)}, u_k^{(n)})} - F'(u_k^{\left(n+\frac{1}{2}\right)}) \\
&= -\gamma\delta_k^{\langle 2\rangle}\left(\frac{e_{u,k}^{(n+1)} + e_{u,k}^{(n)}}{2}\right) + \gamma\left\{\partial_x^2 u_k^{\left(n+\frac{1}{2}\right)} - \delta_k^{\langle 2\rangle}\left(\frac{u_k^{(n+1)} + u_k^{(n)}}{2}\right)\right\} \\
&\quad + \left(\frac{dF}{d(U_k^{(n+1)}, U_k^{(n)})} - \frac{dF}{d(u_k^{(n+1)}, u_k^{(n)})}\right) + \left(\frac{dF}{d(u_k^{(n+1)}, u_k^{(n)})} - F'(u_k^{\left(n+\frac{1}{2}\right)})\right) \\
&= -\gamma\delta_k^{\langle 2\rangle}\left(\frac{e_{u,k}^{(n+1)} + e_{u,k}^{(n)}}{2}\right) + \left(\frac{dF}{d(U_k^{(n+1)}, U_k^{(n)})} - \frac{dF}{d(u_k^{(n+1)}, u_k^{(n)})}\right) + \xi_{2,k}^{\left(n+\frac{1}{2}\right)} \quad (k=1,\ldots,K-1).
\end{aligned}
\tag{5.79}
$$

We show that (5.78) and (5.79) hold at $k = 0, K$. We remark that the equations (5.1)–(5.2) hold in the interior of the domain $(0, L)$ only. Hence, we cannot apply the equations (5.1)–(5.2) directly in the calculation of (5.78) and (5.79) on the boundary. Therefore, we consider points slightly inside from the boundary of the domain, and we take the limit of them to show that (5.78) and (5.79) hold at $k = 0, K$. For any $\varepsilon \in (0, 1)$, let

$$
\begin{aligned}
e_{u,0,\varepsilon}^{(n)} &:= U_0^{(n)} - u(\varepsilon\Delta x, n\Delta t), \quad e_{u,K,-\varepsilon}^{(n)} := U_K^{(n)} - u((K-\varepsilon)\Delta x, n\Delta t) \quad (n = 0, 1, \ldots, N), \\
e_{p,0,\varepsilon}^{(n)} &:= P_0^{(n)} - p\left(\varepsilon\Delta x, \left(n + \frac{1}{2}\right)\Delta t\right) \quad (n = 0, 1, \ldots, N-1), \\
e_{p,K,-\varepsilon}^{(n)} &:= P_K^{(n)} - p\left((K-\varepsilon)\Delta x, \left(n + \frac{1}{2}\right)\Delta t\right) \quad (n = 0, 1, \ldots, N-1).
\end{aligned}
$$

Furthermore, for $n = 0, 1, \ldots, N-1$, let

$$
\begin{aligned}
\xi_{1,\varepsilon}^{\left(n+\frac{1}{2}\right)} &:= \partial_t u_\varepsilon^{\left(n+\frac{1}{2}\right)} - \frac{u_\varepsilon^{(n+1)} - u_\varepsilon^{(n)}}{\Delta t} + \delta_k^{\langle 2\rangle}\tilde{p}_\varepsilon^{\left(n+\frac{1}{2}\right)} - \partial_x^2 p_\varepsilon^{\left(n+\frac{1}{2}\right)}, \\
\xi_{1,K-\varepsilon}^{\left(n+\frac{1}{2}\right)} &:= \partial_t u_{K-\varepsilon}^{\left(n+\frac{1}{2}\right)} - \frac{u_{K-\varepsilon}^{(n+1)} - u_{K-\varepsilon}^{(n)}}{\Delta t} + \delta_k^{\langle 2\rangle}\tilde{p}_{K-\varepsilon}^{\left(n+\frac{1}{2}\right)} - \partial_x^2 p_{K-\varepsilon}^{\left(n+\frac{1}{2}\right)}, \\
\xi_{2,\varepsilon}^{\left(n+\frac{1}{2}\right)} &:= \gamma\left\{\partial_x^2 u_\varepsilon^{\left(n+\frac{1}{2}\right)} - \delta_k^{\langle 2\rangle}\left(\frac{\tilde{u}_\varepsilon^{(n+1)} + \tilde{u}_\varepsilon^{(n)}}{2}\right)\right\} + \frac{dF}{d(u_\varepsilon^{(n+1)}, u_\varepsilon^{(n)})} - F'(u_\varepsilon^{\left(n+\frac{1}{2}\right)}), \\
\xi_{2,K-\varepsilon}^{\left(n+\frac{1}{2}\right)} &:= \gamma\left\{\partial_x^2 u_{K-\varepsilon}^{\left(n+\frac{1}{2}\right)} - \delta_k^{\langle 2\rangle}\left(\frac{\tilde{u}_{K-\varepsilon}^{(n+1)} + \tilde{u}_{K-\varepsilon}^{(n)}}{2}\right)\right\} + \frac{dF}{d(u_{K-\varepsilon}^{(n+1)}, u_{K-\varepsilon}^{(n)})} - F'(u_{K-\varepsilon}^{\left(n+\frac{1}{2}\right)}).
\end{aligned}
$$

In a similar way as (5.78), we have

$$
\frac{e_{u,0,\varepsilon}^{(n+1)} - e_{u,0,\varepsilon}^{(n)}}{\Delta t} = \delta_k^{\langle 2\rangle} e_{p,0,\varepsilon}^{(n)} + \xi_{1,\varepsilon}^{\left(n+\frac{1}{2}\right)}, \quad \frac{e_{u,K,-\varepsilon}^{(n+1)} - e_{u,K,-\varepsilon}^{(n)}}{\Delta t} = \delta_k^{\langle 2\rangle} e_{p,K,-\varepsilon}^{(n)} + \xi_{1,K-\varepsilon}^{\left(n+\frac{1}{2}\right)}. \tag{5.80}
$$

From the smoothness assumption of u, letting ε tend to 0 in (5.80), we obtain

$$
\frac{e_{u,0}^{(n+1)} - e_{u,0}^{(n)}}{\Delta t} = \delta_k^{\langle 2\rangle} e_{p,0}^{(n)} + \xi_{1,0}^{\left(n+\frac{1}{2}\right)}, \quad \frac{e_{u,K}^{(n+1)} - e_{u,K}^{(n)}}{\Delta t} = \delta_k^{\langle 2\rangle} e_{p,K}^{(n)} + \xi_{1,K}^{\left(n+\frac{1}{2}\right)} \quad (n = 0, 1, \ldots, N-1).
$$

In a similar way as (5.79), we get

$$e_{p,0,\varepsilon}^{(n)} = -\gamma\delta_k^{\langle 2\rangle}\left(\frac{e_{u,0,\varepsilon}^{(n+1)} + e_{u,0,\varepsilon}^{(n)}}{2}\right) + \left(\frac{dF}{d(U_0^{(n+1)}, U_0^{(n)})} - \frac{dF}{d(u_\varepsilon^{(n+1)}, u_\varepsilon^{(n)})}\right) + \xi_{2,\varepsilon}^{\left(n+\frac{1}{2}\right)}, \quad (5.81)$$

$$e_{p,K,-\varepsilon}^{(n)} = -\gamma\delta_k^{\langle 2\rangle}\left(\frac{e_{u,K,-\varepsilon}^{(n+1)} + e_{u,K,-\varepsilon}^{(n)}}{2}\right) + \left(\frac{dF}{d(U_K^{(n+1)}, U_K^{(n)})} - \frac{dF}{d(u_{K-\varepsilon}^{(n+1)}, u_{K-\varepsilon}^{(n)})}\right) + \xi_{2,K-\varepsilon}^{\left(n+\frac{1}{2}\right)}. \quad (5.82)$$

From the smoothness assumptions of u and F, letting ε tend to zero in (5.81) and (5.82), we obtain

$$e_{p,0}^{(n)} = -\gamma\delta_k^{\langle 2\rangle}\left(\frac{e_{u,0}^{(n+1)} + e_{u,0}^{(n)}}{2}\right) + \left(\frac{dF}{d(U_0^{(n+1)}, U_0^{(n)})} - \frac{dF}{d(u_0^{(n+1)}, u_0^{(n)})}\right) + \xi_{2,0}^{\left(n+\frac{1}{2}\right)},$$

$$e_{p,K}^{(n)} = -\gamma\delta_k^{\langle 2\rangle}\left(\frac{e_{u,K}^{(n+1)} + e_{u,K}^{(n)}}{2}\right) + \left(\frac{dF}{d(U_K^{(n+1)}, U_K^{(n)})} - \frac{dF}{d(u_K^{(n+1)}, u_K^{(n)})}\right) + \xi_{2,K}^{\left(n+\frac{1}{2}\right)}$$

for $n = 0, 1, \ldots, N-1$. Next, from the definition of $\boldsymbol{e}_u$, (5.3), and (5.15), we have

$$\begin{aligned}
\frac{e_{u,0}^{(n+1)} - e_{u,0}^{(n)}}{\Delta t} &= \frac{U_0^{(n+1)} - U_0^{(n)}}{\Delta t} - \partial_t u_0^{\left(n+\frac{1}{2}\right)} + \partial_t u_0^{\left(n+\frac{1}{2}\right)} - \frac{u_0^{(n+1)} - u_0^{(n)}}{\Delta t} \\
&= \delta_k^{\langle 1\rangle}\left(\frac{U_0^{(n+1)} + U_0^{(n)}}{2}\right) - \partial_x u_0^{\left(n+\frac{1}{2}\right)} + \partial_t u_0^{\left(n+\frac{1}{2}\right)} - \frac{u_0^{(n+1)} - u_0^{(n)}}{\Delta t} \\
&= \delta_k^{\langle 1\rangle}\left(\frac{U_0^{(n+1)} + U_0^{(n)}}{2}\right) - \delta_k^{\langle 1\rangle}\left(\frac{\tilde{u}_0^{(n+1)} + \tilde{u}_0^{(n)}}{2}\right) + \delta_k^{\langle 1\rangle}\left(\frac{\tilde{u}_0^{(n+1)} + \tilde{u}_0^{(n)}}{2}\right) - \partial_x u_0^{\left(n+\frac{1}{2}\right)} \\
&\quad + \partial_t u_0^{\left(n+\frac{1}{2}\right)} - \frac{u_0^{(n+1)} - u_0^{(n)}}{\Delta t} \\
&= \delta_k^{\langle 1\rangle}\left(\frac{e_{u,0}^{(n+1)} + e_{u,0}^{(n)}}{2}\right) + \xi_{3,0}^{\left(n+\frac{1}{2}\right)} \quad (n = 0, 1, \ldots, N-1).
\end{aligned}$$

Similarly, from the definition of $\boldsymbol{e}_u$, (5.4), and (5.16), we get

$$\frac{e_{u,K}^{(n+1)} - e_{u,K}^{(n)}}{\Delta t} = -\delta_k^{\langle 1\rangle}\left(\frac{e_{u,K}^{(n+1)} + e_{u,K}^{(n)}}{2}\right) + \xi_{3,K}^{\left(n+\frac{1}{2}\right)} \quad (n = 0, 1, \ldots, N-1).$$

Lastly, it holds from the definition of $\boldsymbol{e}_p$, (5.17), and (5.72) that

$$0 = \delta_k^{\langle 1\rangle} P_k^{(n)} = \delta_k^{\langle 1\rangle} e_{p,k}^{(n)} + \delta_k^{\langle 1\rangle} \tilde{p}_k^{\left(n+\frac{1}{2}\right)} = \delta_k^{\langle 1\rangle} e_{p,k}^{(n)} \quad (k = 0, K,\ n = 0, 1, \ldots, N-1).$$

From the above, equations (5.73)–(5.77) on the errors $\boldsymbol{e}_u$ and $\boldsymbol{e}_p$ hold. □

Lemma 5.10. Assume that $u \in C^4([0, L] \times [0, T])$. Furthermore, we suppose that the potential function F is in C^3. Denote the bounds by

$$\max_{0 \le n \le N}\left\{\left\|D\boldsymbol{U}^{(n)}\right\|, \left\|D\boldsymbol{u}^{(n)}\right\|\right\} \le C_1, \quad \max_{0 \le n \le N}\left\{\left\|\boldsymbol{U}^{(n)}\right\|_{L_{\mathrm{d}}^\infty}, \left\|\boldsymbol{u}^{(n)}\right\|_{L_{\mathrm{d}}^\infty}\right\} \le C_2. \quad (5.83)$$

Also, let

$$C_3 := \frac{C_1 L^{\frac{1}{2}} \max_{|\xi|\le C_2} |F'''(\xi)| + \max_{|\xi|\le C_2} |F''(\xi)|}{2}.$$

Then, for any fixed $\varepsilon > 0$, the following inequality holds:

$$\left\{1 - \Delta t\left(\frac{C_3^2}{\gamma} + \varepsilon\right)\right\} \left\|D\boldsymbol{e}_u^{(n+1)}\right\|^2 \le \left\{1 + \Delta t\left(\frac{C_3^2}{\gamma} + \varepsilon\right)\right\} \left\|D\boldsymbol{e}_u^{(n)}\right\|^2 + \Delta t R^{\left(n+\frac{1}{2}\right)}$$

for $n = 0, 1, \ldots, N-1$, where

$$R^{\left(n+\frac{1}{2}\right)} := \frac{1}{2\gamma}\left(1 + \frac{2C_3^2}{\varepsilon\gamma}\right)\left(\Delta t C_1 \max_{|\xi|\le C_2}|F'''(\xi)| \sum_{j=0}^{n} \left\|\boldsymbol{\xi}_1^{\left(j+\frac{1}{2}\right)}\right\|_{L_{\mathrm{d}}^{\infty}} + \left\|D\boldsymbol{\xi}_2^{\left(n+\frac{1}{2}\right)}\right\|\right)^2$$
$$+ \frac{1}{\varepsilon}\left\|D\boldsymbol{\xi}_1^{\left(n+\frac{1}{2}\right)}\right\|^2 + \left|\xi_{1,0}^{\left(n+\frac{1}{2}\right)}\right|^2 + \left|\xi_{1,K}^{\left(n+\frac{1}{2}\right)}\right|^2 + \left|\xi_{3,0}^{\left(n+\frac{1}{2}\right)}\right|^2 + \left|\xi_{3,K}^{\left(n+\frac{1}{2}\right)}\right|^2. \tag{5.84}$$

Proof. For any fixed $n = 0, 1, \ldots, N-1$, using Corollary 2.1, we have

$$\frac{1}{2\Delta t}\left(\left\|D\boldsymbol{e}_u^{(n+1)}\right\|^2 - \left\|D\boldsymbol{e}_u^{(n)}\right\|^2\right) = \sum_{k=0}^{K-1}\left\{\delta_k^+\left(\frac{e_{u,k}^{(n+1)} - e_{u,k}^{(n)}}{\Delta t}\right)\right\}\left\{\delta_k^+\left(\frac{e_{u,k}^{(n+1)} + e_{u,k}^{(n)}}{2}\right)\right\}\Delta x$$
$$= -\sum_{k=0}^{K}{}'' \frac{e_{u,k}^{(n+1)} - e_{u,k}^{(n)}}{\Delta t}\delta_k^{\langle 2\rangle}\left(\frac{e_{u,k}^{(n+1)} + e_{u,k}^{(n)}}{2}\right)\Delta x + \left[\frac{e_{u,k}^{(n+1)} - e_{u,k}^{(n)}}{\Delta t}\delta_k^{\langle 1\rangle}\left(\frac{e_{u,k}^{(n+1)} + e_{u,k}^{(n)}}{2}\right)\right]_0^K. \tag{5.85}$$

Firstly, we consider the first term on the right-hand side of (5.85). From (5.73), (5.74), (5.77), Corollary 2.1, and the Hölder inequality, we obtain

$$-\sum_{k=0}^{K}{}'' \frac{e_{u,k}^{(n+1)} - e_{u,k}^{(n)}}{\Delta t}\delta_k^{\langle 2\rangle}\left(\frac{e_{u,k}^{(n+1)} + e_{u,k}^{(n)}}{2}\right)\Delta x$$
$$= -\sum_{k=0}^{K}{}''\left(\delta_k^{\langle 2\rangle} e_{p,k}^{(n)}\right)\delta_k^{\langle 2\rangle}\left(\frac{e_{u,k}^{(n+1)} + e_{u,k}^{(n)}}{2}\right)\Delta x - \sum_{k=0}^{K}{}''\xi_{1,k}^{\left(n+\frac{1}{2}\right)}\delta_k^{\langle 2\rangle}\left(\frac{e_{u,k}^{(n+1)} + e_{u,k}^{(n)}}{2}\right)\Delta x$$
$$= \frac{1}{\gamma}\sum_{k=0}^{K}{}''\left(\delta_k^{\langle 2\rangle} e_{p,k}^{(n)}\right) e_{p,k}^{(n)}\Delta x - \frac{1}{\gamma}\sum_{k=0}^{K}{}''\left(\delta_k^{\langle 2\rangle} e_{p,k}^{(n)}\right)$$
$$\times\left\{\left(\frac{dF}{d(U_k^{(n+1)}, U_k^{(n)})} - \frac{dF}{d(u_k^{(n+1)}, u_k^{(n)})}\right) + \xi_{2,k}^{\left(n+\frac{1}{2}\right)}\right\}\Delta x - \sum_{k=0}^{K}{}''\xi_{1,k}^{\left(n+\frac{1}{2}\right)}\delta_k^{\langle 2\rangle}\left(\frac{e_{u,k}^{(n+1)} + e_{u,k}^{(n)}}{2}\right)\Delta x$$
$$= -\frac{1}{\gamma}\sum_{k=0}^{K-1}\left(\delta_k^+ e_{p,k}^{(n)}\right)^2\Delta x + \frac{1}{\gamma}\left[\left(\delta_k^{\langle 1\rangle} e_{p,k}^{(n)}\right) e_{p,k}^{(n)}\right]_0^K$$
$$+ \frac{1}{\gamma}\sum_{k=0}^{K-1}\left(\delta_k^+ e_{p,k}^{(n)}\right)\left\{\delta_k^+\left(\frac{dF}{d(U_k^{(n+1)}, U_k^{(n)})} - \frac{dF}{d(u_k^{(n+1)}, u_k^{(n)})} + \xi_{2,k}^{\left(n+\frac{1}{2}\right)}\right)\right\}\Delta x$$
$$- \frac{1}{\gamma}\left[\left(\delta_k^{\langle 1\rangle} e_{p,k}^{(n)}\right)\left(\frac{dF}{d(U_k^{(n+1)}, U_k^{(n)})} - \frac{dF}{d(u_k^{(n+1)}, u_k^{(n)})} + \xi_{2,k}^{\left(n+\frac{1}{2}\right)}\right)\right]_0^K$$
$$+ \sum_{k=0}^{K-1}\left(\delta_k^+\xi_{1,k}^{\left(n+\frac{1}{2}\right)}\right)\left\{\delta_k^+\left(\frac{e_{u,k}^{(n+1)} + e_{u,k}^{(n)}}{2}\right)\right\}\Delta x - \left[\xi_{1,k}^{\left(n+\frac{1}{2}\right)}\delta_k^{\langle 1\rangle}\left(\frac{e_{u,k}^{(n+1)} + e_{u,k}^{(n)}}{2}\right)\right]_0^K$$

$$\leq -\frac{1}{\gamma}\left\|D\boldsymbol{e}_p^{(n)}\right\|^2 + \frac{1}{\gamma}\left\|D\boldsymbol{e}_p^{(n)}\right\|\left\|D\left(\frac{dF}{d\left(\boldsymbol{U}^{(n+1)},\boldsymbol{U}^{(n)}\right)} - \frac{dF}{d\left(\boldsymbol{u}^{(n+1)},\boldsymbol{u}^{(n)}\right)} + \boldsymbol{\xi}_2^{\left(n+\frac{1}{2}\right)}\right)\right\|$$
$$+ \left\|D\boldsymbol{\xi}_1^{\left(n+\frac{1}{2}\right)}\right\|\left\|D\left(\frac{\boldsymbol{e}_u^{(n+1)}+\boldsymbol{e}_u^{(n)}}{2}\right)\right\| - \left[\xi_{1,k}^{\left(n+\frac{1}{2}\right)}\delta_k^{\langle 1\rangle}\left(\frac{e_{u,k}^{(n+1)}+e_{u,k}^{(n)}}{2}\right)\right]_0^K.$$

Next, we consider the second term on the right-hand side of (5.85). It follows from (5.75) and (5.76) that

$$\left[\frac{e_{u,k}^{(n+1)}-e_{u,k}^{(n)}}{\Delta t}\delta_k^{\langle 1\rangle}\left(\frac{e_{u,k}^{(n+1)}+e_{u,k}^{(n)}}{2}\right)\right]_0^K = -\left\{\delta_k^{\langle 1\rangle}\left(\frac{e_{u,K}^{(n+1)}+e_{u,K}^{(n)}}{2}\right)\right\}^2 - \left\{\delta_k^{\langle 1\rangle}\left(\frac{e_{u,0}^{(n+1)}+e_{u,0}^{(n)}}{2}\right)\right\}^2$$
$$+ \xi_{3,K}^{\left(n+\frac{1}{2}\right)}\delta_k^{\langle 1\rangle}\left(\frac{e_{u,K}^{(n+1)}+e_{u,K}^{(n)}}{2}\right) - \xi_{3,0}^{\left(n+\frac{1}{2}\right)}\delta_k^{\langle 1\rangle}\left(\frac{e_{u,0}^{(n+1)}+e_{u,0}^{(n)}}{2}\right).$$

From the above, we obtain

$$\frac{1}{2\Delta t}\left(\left\|D\boldsymbol{e}_u^{(n+1)}\right\|^2 - \left\|D\boldsymbol{e}_u^{(n)}\right\|^2\right)$$
$$\leq -\frac{1}{\gamma}\left\|D\boldsymbol{e}_p^{(n)}\right\|^2 + \frac{1}{\gamma}\left\|D\boldsymbol{e}_p^{(n)}\right\|\left\|D\left(\frac{dF}{d\left(\boldsymbol{U}^{(n+1)},\boldsymbol{U}^{(n)}\right)} - \frac{dF}{d\left(\boldsymbol{u}^{(n+1)},\boldsymbol{u}^{(n)}\right)} + \boldsymbol{\xi}_2^{\left(n+\frac{1}{2}\right)}\right)\right\|$$
$$+ \left\|D\boldsymbol{\xi}_1^{\left(n+\frac{1}{2}\right)}\right\|\left\|D\left(\frac{\boldsymbol{e}_u^{(n+1)}+\boldsymbol{e}_u^{(n)}}{2}\right)\right\| - \left\{\delta_k^{\langle 1\rangle}\left(\frac{e_{u,K}^{(n+1)}+e_{u,K}^{(n)}}{2}\right)\right\}^2 - \left\{\delta_k^{\langle 1\rangle}\left(\frac{e_{u,0}^{(n+1)}+e_{u,0}^{(n)}}{2}\right)\right\}^2$$
$$+ \left(-\xi_{1,K}^{\left(n+\frac{1}{2}\right)} + \xi_{3,K}^{\left(n+\frac{1}{2}\right)}\right)\delta_k^{\langle 1\rangle}\left(\frac{e_{u,K}^{(n+1)}+e_{u,K}^{(n)}}{2}\right) + \left(\xi_{1,0}^{\left(n+\frac{1}{2}\right)} - \xi_{3,0}^{\left(n+\frac{1}{2}\right)}\right)\delta_k^{\langle 1\rangle}\left(\frac{e_{u,0}^{(n+1)}+e_{u,0}^{(n)}}{2}\right).$$

From the above inequality, the Young inequality, and the inequality: $(a+b)^2 \leq 2(a^2+b^2)$ for all $a, b \in \mathbb{R}$, we have

$$\frac{1}{2\Delta t}\left(\left\|D\boldsymbol{e}_u^{(n+1)}\right\|^2 - \left\|D\boldsymbol{e}_u^{(n)}\right\|^2\right) + \frac{1}{\gamma}\left\|D\boldsymbol{e}_p^{(n)}\right\|^2 + \left\{\delta_k^{\langle 1\rangle}\left(\frac{e_{u,K}^{(n+1)}+e_{u,K}^{(n)}}{2}\right)\right\}^2 + \left\{\delta_k^{\langle 1\rangle}\left(\frac{e_{u,0}^{(n+1)}+e_{u,0}^{(n)}}{2}\right)\right\}^2$$
$$\leq \frac{1}{\gamma}\left\|D\boldsymbol{e}_p^{(n)}\right\|\left\|D\left(\frac{dF}{d\left(\boldsymbol{U}^{(n+1)},\boldsymbol{U}^{(n)}\right)} - \frac{dF}{d\left(\boldsymbol{u}^{(n+1)},\boldsymbol{u}^{(n)}\right)} + \boldsymbol{\xi}_2^{\left(n+\frac{1}{2}\right)}\right)\right\|$$
$$+ \left\|D\boldsymbol{\xi}_1^{\left(n+\frac{1}{2}\right)}\right\|\left\|D\left(\frac{\boldsymbol{e}_u^{(n+1)}+\boldsymbol{e}_u^{(n)}}{2}\right)\right\| + \left(-\xi_{1,K}^{\left(n+\frac{1}{2}\right)} + \xi_{3,K}^{\left(n+\frac{1}{2}\right)}\right)\delta_k^{\langle 1\rangle}\left(\frac{e_{u,K}^{(n+1)}+e_{u,K}^{(n)}}{2}\right)$$
$$+ \left(\xi_{1,0}^{\left(n+\frac{1}{2}\right)} - \xi_{3,0}^{\left(n+\frac{1}{2}\right)}\right)\delta_k^{\langle 1\rangle}\left(\frac{e_{u,0}^{(n+1)}+e_{u,0}^{(n)}}{2}\right)$$
$$\leq \frac{1}{\gamma}\left\|D\boldsymbol{e}_p^{(n)}\right\|^2 + \frac{1}{4\gamma}\left\|D\left(\frac{dF}{d\left(\boldsymbol{U}^{(n+1)},\boldsymbol{U}^{(n)}\right)} - \frac{dF}{d(\boldsymbol{u}^{(n+1)},\boldsymbol{u}^{(n)})} + \boldsymbol{\xi}_2^{\left(n+\frac{1}{2}\right)}\right)\right\|^2$$
$$+ \left\|D\boldsymbol{\xi}_1^{\left(n+\frac{1}{2}\right)}\right\|\left\|D\left(\frac{\boldsymbol{e}_u^{(n+1)}+\boldsymbol{e}_u^{(n)}}{2}\right)\right\| + \frac{1}{2}\left\{\left|\xi_{1,K}^{\left(n+\frac{1}{2}\right)}\right|^2 + \left|\xi_{3,K}^{\left(n+\frac{1}{2}\right)}\right|^2\right\} + \left\{\delta_k^{\langle 1\rangle}\left(\frac{e_{u,K}^{(n+1)}+e_{u,K}^{(n)}}{2}\right)\right\}^2$$
$$+ \frac{1}{2}\left\{\left|\xi_{1,0}^{\left(n+\frac{1}{2}\right)}\right|^2 + \left|\xi_{3,0}^{\left(n+\frac{1}{2}\right)}\right|^2\right\} + \left\{\delta_k^{\langle 1\rangle}\left(\frac{e_{u,0}^{(n+1)}+e_{u,0}^{(n)}}{2}\right)\right\}^2.$$

Namely,

$$\frac{1}{2\Delta t}\left(\left\|D\boldsymbol{e}_u^{(n+1)}\right\|^2-\left\|D\boldsymbol{e}_u^{(n)}\right\|^2\right)$$
$$\le \frac{1}{4\gamma}\left\|D\left(\frac{dF}{d\left(\boldsymbol{U}^{(n+1)},\boldsymbol{U}^{(n)}\right)}-\frac{dF}{d\left(\boldsymbol{u}^{(n+1)},\boldsymbol{u}^{(n)}\right)}+\boldsymbol{\xi}_2^{\left(n+\frac{1}{2}\right)}\right)\right\|^2$$
$$+\left\|D\boldsymbol{\xi}_1^{\left(n+\frac{1}{2}\right)}\right\|\left\|D\left(\frac{\boldsymbol{e}_u^{(n+1)}+\boldsymbol{e}_u^{(n)}}{2}\right)\right\|+\frac{1}{2}\left\{\left|\xi_{1,0}^{\left(n+\frac{1}{2}\right)}\right|^2+\left|\xi_{1,K}^{\left(n+\frac{1}{2}\right)}\right|^2+\left|\xi_{3,0}^{\left(n+\frac{1}{2}\right)}\right|^2+\left|\xi_{3,K}^{\left(n+\frac{1}{2}\right)}\right|^2\right\}. \tag{5.86}$$

We consider the difference quotient of F. Using Lemma 2.2, we have

$$\frac{dF}{d(U_k^{(n+1)},U_k^{(n)})}-\frac{dF}{d(u_k^{(n+1)},u_k^{(n)})}=\frac{1}{2}\bar{F}''\Big(U_k^{(n+1)},u_k^{(n+1)};U_k^{(n)},u_k^{(n)}\Big)e_{u,k}^{(n+1)}$$
$$+\frac{1}{2}\bar{F}''\Big(U_k^{(n)},u_k^{(n)};U_k^{(n+1)},u_k^{(n+1)}\Big)e_{u,k}^{(n)}\quad(k=0,\dots,K).$$

Hence, it follows from Lemma 2.3 that

$$\left\|D\left(\frac{dF}{d\left(\boldsymbol{U}^{(n+1)},\boldsymbol{U}^{(n)}\right)}-\frac{dF}{d\left(\boldsymbol{u}^{(n+1)},\boldsymbol{u}^{(n)}\right)}\right)\right\|$$
$$\le\frac{1}{2}\left\|D\big(\bar{F}''\big(\boldsymbol{U}^{(n+1)},\boldsymbol{u}^{(n+1)};\boldsymbol{U}^{(n)},\boldsymbol{u}^{(n)}\big)\boldsymbol{e}_u^{(n+1)}\big)\right\|+\frac{1}{2}\left\|D\big(\bar{F}''\big(\boldsymbol{U}^{(n)},\boldsymbol{u}^{(n)};\boldsymbol{U}^{(n+1)},\boldsymbol{u}^{(n+1)}\big)\boldsymbol{e}_u^{(n)}\big)\right\|$$
$$\le\frac{1}{2}\left\|D\bar{F}''\big(\boldsymbol{U}^{(n+1)},\boldsymbol{u}^{(n+1)};\boldsymbol{U}^{(n)},\boldsymbol{u}^{(n)}\big)\right\|\left\|\boldsymbol{e}_u^{(n+1)}\right\|_{L^\infty_{\mathrm{d}}}$$
$$+\frac{1}{2}\left\|\bar{F}''\big(\boldsymbol{U}^{(n+1)},\boldsymbol{u}^{(n+1)};\boldsymbol{U}^{(n)},\boldsymbol{u}^{(n)}\big)\right\|_{L^\infty_{\mathrm{d}}}\left\|D\boldsymbol{e}_u^{(n+1)}\right\|$$
$$+\frac{1}{2}\left\|D\bar{F}''\big(\boldsymbol{U}^{(n)},\boldsymbol{u}^{(n)};\boldsymbol{U}^{(n+1)},\boldsymbol{u}^{(n+1)}\big)\right\|\left\|\boldsymbol{e}_u^{(n)}\right\|_{L^\infty_{\mathrm{d}}}$$
$$+\frac{1}{2}\left\|\bar{F}''\big(\boldsymbol{U}^{(n)},\boldsymbol{u}^{(n)};\boldsymbol{U}^{(n+1)},\boldsymbol{u}^{(n+1)}\big)\right\|_{L^\infty_{\mathrm{d}}}\left\|D\boldsymbol{e}_u^{(n)}\right\|.$$

Let us define $C_{F,i}$ $(i=2,3,4)$ by

$$C_{F,i}:=\max_{|\eta|\le C_2}\left|F^{(i)}(\eta)\right|\quad(i=2,3,4).$$

From (5.83) and Lemma 2.1, we have

$$\left\|\bar{F}''\big(\boldsymbol{U}^{(n+1)},\boldsymbol{u}^{(n+1)};\boldsymbol{U}^{(n)},\boldsymbol{u}^{(n)}\big)\right\|_{L^\infty_{\mathrm{d}}}\le C_{F,2},\quad\left\|\bar{F}''\big(\boldsymbol{U}^{(n)},\boldsymbol{u}^{(n)};\boldsymbol{U}^{(n+1)},\boldsymbol{u}^{(n+1)}\big)\right\|_{L^\infty_{\mathrm{d}}}\le C_{F,2},$$

Moreover, from (5.83) and Lemma 2.4, we obtain

$$\left\|D\bar{F}''\left(\boldsymbol{U}^{(n+1)},\boldsymbol{u}^{(n+1)};\boldsymbol{U}^{(n)},\boldsymbol{u}^{(n)}\right)\right\|\le\frac{C_{F,3}}{6}\left(2C_1+2C_1+C_1+C_1\right)=C_1C_{F,3},$$
$$\left\|D\bar{F}''\left(\boldsymbol{U}^{(n)},\boldsymbol{u}^{(n)};\boldsymbol{U}^{(n+1)},\boldsymbol{u}^{(n+1)}\right)\right\|\le\frac{C_{F,3}}{6}\left(2C_1+2C_1+C_1+C_1\right)=C_1C_{F,3}.$$

From the above, it holds that

$$\left\|D\left(\frac{dF}{d\left(\boldsymbol{U}^{(n+1)},\boldsymbol{U}^{(n)}\right)}-\frac{dF}{d\left(\boldsymbol{u}^{(n+1)},\boldsymbol{u}^{(n)}\right)}\right)\right\|\le\frac{C_1C_{F,3}}{2}\left(\left\|\boldsymbol{e}_u^{(n+1)}\right\|_{L^\infty_{\mathrm{d}}}+\left\|\boldsymbol{e}_u^{(n)}\right\|_{L^\infty_{\mathrm{d}}}\right)$$
$$+\frac{C_{F,2}}{2}\left(\left\|D\boldsymbol{e}_u^{(n+1)}\right\|+\left\|D\boldsymbol{e}_u^{(n)}\right\|\right). \tag{5.87}$$

Next, we consider $\|\boldsymbol{e}_u^{(n+1)}\|_{L_{\mathrm{d}}^\infty}$ and $\|\boldsymbol{e}_u^{(n)}\|_{L_{\mathrm{d}}^\infty}$. Now, using (5.73), (5.77), and Proposition 2.2, we have

$$\delta_n^+\left(\sum_{k=0}^{K}{}'' e_{u,k}^{(n)}\Delta x\right)=\sum_{k=0}^{K}{}''\delta_k^{\langle 2\rangle}e_{p,k}^{(n)}\Delta x+\sum_{k=0}^{K}{}''\xi_{1,k}^{\left(n+\frac{1}{2}\right)}\Delta x=\left[\delta_k^{\langle 1\rangle}e_{p,k}^{(n)}\right]_0^K+\sum_{k=0}^{K}{}''\xi_{1,k}^{\left(n+\frac{1}{2}\right)}\Delta x$$
$$=\sum_{k=0}^{K}{}''\xi_{1,k}^{\left(n+\frac{1}{2}\right)}\Delta x\quad(n=0,1,\ldots,N-1).$$

That is,

$$\sum_{k=0}^{K}{}'' e_{u,k}^{(n+1)}\Delta x=\sum_{k=0}^{K}{}'' e_{u,k}^{(n)}\Delta x+\Delta t\sum_{k=0}^{K}{}''\xi_{1,k}^{\left(n+\frac{1}{2}\right)}\Delta x\quad(n=0,1,\ldots,N-1).$$

Using this equality iteratively, we obtain

$$\begin{aligned}\sum_{k=0}^{K}{}'' e_{u,k}^{(n)}\Delta x&=\sum_{k=0}^{K}{}'' e_{u,k}^{(n-1)}\Delta x+\Delta t\sum_{k=0}^{K}{}''\xi_{1,k}^{\left(n-1+\frac{1}{2}\right)}\Delta x\\&=\sum_{k=0}^{K}{}'' e_{u,k}^{(n-2)}\Delta x+\Delta t\sum_{k=0}^{K}{}''\xi_{1,k}^{\left(n-2+\frac{1}{2}\right)}\Delta x+\Delta t\sum_{k=0}^{K}{}''\xi_{1,k}^{\left(n-1+\frac{1}{2}\right)}\Delta x\\&=\cdots\\&=\sum_{k=0}^{K}{}'' e_{u,k}^{(0)}\Delta x+\sum_{j=0}^{n-1}\sum_{k=0}^{K}{}''\xi_{1,k}^{\left(j+\frac{1}{2}\right)}\Delta x\Delta t\\&=\sum_{j=0}^{n-1}\sum_{k=0}^{K}{}''\xi_{1,k}^{\left(j+\frac{1}{2}\right)}\Delta x\Delta t\quad(n=1,\ldots,N),\end{aligned}$$

where the last equality holds from $\boldsymbol{e}_u^{(0)}=\mathbf{0}$. Hence, from Proposition 2.6 and the above equality, we have

$$\begin{aligned}\left\|\boldsymbol{e}_u^{(n)}\right\|_{L_{\mathrm{d}}^\infty}\le\frac{1}{L}\left|\sum_{k=0}^{K}{}'' e_{u,k}^{(n)}\Delta x\right|+L^{\frac{1}{2}}\left\|D\boldsymbol{e}_u^{(n)}\right\|&=\frac{1}{L}\left|\sum_{j=0}^{n-1}\sum_{k=0}^{K}{}''\xi_{1,k}^{\left(j+\frac{1}{2}\right)}\Delta x\Delta t\right|+L^{\frac{1}{2}}\left\|D\boldsymbol{e}_u^{(n)}\right\|\\&\le\frac{1}{L}\sum_{j=0}^{n-1}\sum_{k=0}^{K}{}''\left|\xi_{1,k}^{\left(j+\frac{1}{2}\right)}\right|\Delta x\Delta t+L^{\frac{1}{2}}\left\|D\boldsymbol{e}_u^{(n)}\right\|\\&\le\frac{1}{L}\sum_{j=0}^{n-1}\max_{0\le k\le K}\left|\xi_{1,k}^{\left(j+\frac{1}{2}\right)}\right|\sum_{k=0}^{K}{}''\Delta x\Delta t+L^{\frac{1}{2}}\left\|D\boldsymbol{e}_u^{(n)}\right\|\\&=\Delta t\sum_{j=0}^{n-1}\left\|\boldsymbol{\xi}_1^{\left(j+\frac{1}{2}\right)}\right\|_{L_{\mathrm{d}}^\infty}+L^{\frac{1}{2}}\left\|D\boldsymbol{e}_u^{(n)}\right\|\quad(n=1,\ldots,N).\end{aligned}\tag{5.88}$$

Applying (5.88) to (5.87), we obtain

$$\left\|D\left(\frac{dF}{d\left(\boldsymbol{U}^{(n+1)},\boldsymbol{U}^{(n)}\right)}-\frac{dF}{d\left(\boldsymbol{u}^{(n+1)},\boldsymbol{u}^{(n)}\right)}\right)\right\|\le C_3\left(\left\|D\boldsymbol{e}_u^{(n+1)}\right\|+\left\|D\boldsymbol{e}_u^{(n)}\right\|\right)$$
$$+\Delta tC_1C_{F,3}\sum_{j=0}^{n}\left\|\boldsymbol{\xi}_1^{\left(j+\frac{1}{2}\right)}\right\|_{L_{\mathrm{d}}^\infty}$$

for $n = 0, 1, \ldots, N-1$. Therefore, we have

$$
\begin{aligned}
&\frac{1}{4\gamma} \left\| D \left(\frac{dF}{d\left(\boldsymbol{U}^{(n+1)}, \boldsymbol{U}^{(n)}\right)} - \frac{dF}{d\left(\boldsymbol{u}^{(n+1)}, \boldsymbol{u}^{(n)}\right)} + \boldsymbol{\xi}_2^{\left(n+\frac{1}{2}\right)} \right) \right\|^2 \\
&\leq \frac{1}{4\gamma} \left(\left\| D \left(\frac{dF}{d\left(\boldsymbol{U}^{(n+1)}, \boldsymbol{U}^{(n)}\right)} - \frac{dF}{d\left(\boldsymbol{u}^{(n+1)}, \boldsymbol{u}^{(n)}\right)} \right) \right\| + \left\| D\boldsymbol{\xi}_2^{\left(n+\frac{1}{2}\right)} \right\| \right)^2 \\
&\leq \frac{1}{4\gamma} \left\{ C_3 \left(\left\| D\boldsymbol{e}_u^{(n+1)} \right\| + \left\| D\boldsymbol{e}_u^{(n)} \right\| \right) + \left(\Delta t C_1 C_{F,3} \sum_{j=0}^{n} \left\| \boldsymbol{\xi}_1^{\left(j+\frac{1}{2}\right)} \right\|_{L_{\mathrm{d}}^\infty} + \left\| D\boldsymbol{\xi}_2^{\left(n+\frac{1}{2}\right)} \right\| \right) \right\}^2 .
\end{aligned}
\tag{5.89}
$$

for $n = 0, 1, \ldots, N-1$. For simplicity, let

$$
R_1^{(n)} := \Delta t C_1 C_{F,3} \sum_{j=0}^{n} \left\| \boldsymbol{\xi}_1^{\left(j+\frac{1}{2}\right)} \right\|_{L_{\mathrm{d}}^\infty} + \left\| D\boldsymbol{\xi}_2^{\left(n+\frac{1}{2}\right)} \right\| \quad (n = 0, 1, \ldots, N-1).
$$

Let $\varepsilon > 0$ be an arbitrarily fixed number. From (5.89) and the inequality: $(a+b+c)^2 \leq 2(a^2+b^2) + (\tilde{\varepsilon}/2)(a^2+b^2) + (1+(4/\tilde{\varepsilon}))c^2$ for all $a, b, c \in \mathbb{R}$, and $\tilde{\varepsilon} > 0$, we obtain

$$
\begin{aligned}
&\frac{1}{4\gamma} \left\| D \left(\frac{dF}{d\left(\boldsymbol{U}^{(n+1)}, \boldsymbol{U}^{(n)}\right)} - \frac{dF}{d\left(\boldsymbol{u}^{(n+1)}, \boldsymbol{u}^{(n)}\right)} + \boldsymbol{\xi}_2^{\left(n+\frac{1}{2}\right)} \right) \right\|^2 \\
&\leq \frac{1}{4\gamma} \left(C_3 \left\| D\boldsymbol{e}_u^{(n+1)} \right\| + C_3 \left\| D\boldsymbol{e}_u^{(n)} \right\| + R_1^{(n)} \right)^2 \\
&\leq \frac{1}{4\gamma} \left\{ 2 \left(C_3^2 \left\| D\boldsymbol{e}_u^{(n+1)} \right\|^2 + C_3^2 \left\| D\boldsymbol{e}_u^{(n)} \right\|^2 \right) \right. \\
&\quad \left. + \frac{\varepsilon\gamma}{C_3^2} \left(C_3^2 \left\| D\boldsymbol{e}_u^{(n+1)} \right\|^2 + C_3^2 \left\| D\boldsymbol{e}_u^{(n)} \right\|^2 \right) + \left(1 + \frac{2C_3^2}{\varepsilon\gamma} \right) \left(R_1^{(n)} \right)^2 \right\} \\
&= \frac{C_3^2}{2\gamma} \left(\left\| D\boldsymbol{e}_u^{(n+1)} \right\|^2 + \left\| D\boldsymbol{e}_u^{(n)} \right\|^2 \right) + \frac{\varepsilon}{4} \left(\left\| D\boldsymbol{e}_u^{(n+1)} \right\|^2 + \left\| D\boldsymbol{e}_u^{(n)} \right\|^2 \right) + \frac{1}{4\gamma} \left(1 + \frac{2C_3^2}{\varepsilon\gamma} \right) \left(R_1^{(n)} \right)^2 .
\end{aligned}
\tag{5.90}
$$

In addition, it follows from the Young inequality and the inequality: $(a+b)^2 \leq 2(a^2+b^2)$ for all $a, b \in \mathbb{R}$ that

$$
\begin{aligned}
\left\| D\boldsymbol{\xi}_1^{\left(n+\frac{1}{2}\right)} \right\| \left\| D \left(\frac{\boldsymbol{e}_u^{(n+1)} + \boldsymbol{e}_u^{(n)}}{2} \right) \right\| &\leq \frac{1}{2} \left\| D\boldsymbol{\xi}_1^{\left(n+\frac{1}{2}\right)} \right\| \left(\left\| D\boldsymbol{e}_u^{(n+1)} \right\| + \left\| D\boldsymbol{e}_u^{(n)} \right\| \right) \\
&\leq \frac{1}{2} \left\{ \frac{\varepsilon}{4} \left(\left\| D\boldsymbol{e}_u^{(n+1)} \right\| + \left\| D\boldsymbol{e}_u^{(n)} \right\| \right)^2 + \frac{1}{\varepsilon} \left\| D\boldsymbol{\xi}_1^{\left(n+\frac{1}{2}\right)} \right\|^2 \right\} \\
&\leq \frac{\varepsilon}{4} \left(\left\| D\boldsymbol{e}_u^{(n+1)} \right\|^2 + \left\| D\boldsymbol{e}_u^{(n)} \right\|^2 \right) + \frac{1}{2\varepsilon} \left\| D\boldsymbol{\xi}_1^{\left(n+\frac{1}{2}\right)} \right\|^2 .
\end{aligned}
\tag{5.91}
$$

Consequently, using (5.86), (5.90), and (5.91), we obtain

$$
\begin{aligned}
&\frac{1}{2\Delta t}\left(\left\|D\boldsymbol{e}_u^{(n+1)}\right\|^2-\left\|D\boldsymbol{e}_u^{(n)}\right\|^2\right)\\
&\le \frac{C_3^2}{2\gamma}\left(\left\|D\boldsymbol{e}_u^{(n+1)}\right\|^2+\left\|D\boldsymbol{e}_u^{(n)}\right\|^2\right)+\frac{\varepsilon}{4}\left(\left\|D\boldsymbol{e}_u^{(n+1)}\right\|^2+\left\|D\boldsymbol{e}_u^{(n)}\right\|^2\right)+\frac{1}{4\gamma}\left(1+\frac{2C_3^2}{\varepsilon\gamma}\right)\left(R_1^{(n)}\right)^2\\
&\quad+\frac{\varepsilon}{4}\left(\left\|D\boldsymbol{e}_u^{(n+1)}\right\|^2+\left\|D\boldsymbol{e}_u^{(n)}\right\|^2\right)+\frac{1}{2\varepsilon}\left\|D\boldsymbol{\xi}_1^{(n+\frac{1}{2})}\right\|^2\\
&\quad+\frac{1}{2}\left\{\left|\xi_{1,0}^{(n+\frac{1}{2})}\right|^2+\left|\xi_{1,K}^{(n+\frac{1}{2})}\right|^2+\left|\xi_{3,0}^{(n+\frac{1}{2})}\right|^2+\left|\xi_{3,K}^{(n+\frac{1}{2})}\right|^2\right\}\\
&=\frac{C_3^2}{2\gamma}\left(\left\|D\boldsymbol{e}_u^{(n+1)}\right\|^2+\left\|D\boldsymbol{e}_u^{(n)}\right\|^2\right)+\frac{\varepsilon}{2}\left(\left\|D\boldsymbol{e}_u^{(n+1)}\right\|^2+\left\|D\boldsymbol{e}_u^{(n)}\right\|^2\right)+\frac{1}{2}R^{(n)}.
\end{aligned}
$$

Multiplying both sides of the above inequality by $2\Delta t$, we conclude that

$$
\left\{1-\left(\frac{C_3^2}{\gamma}+\varepsilon\right)\Delta t\right\}\left\|D\boldsymbol{e}_u^{(n+1)}\right\|^2\le\left\{1+\left(\frac{C_3^2}{\gamma}+\varepsilon\right)\Delta t\right\}\left\|D\boldsymbol{e}_u^{(n)}\right\|^2+\Delta t R^{(n)}
$$

for $n=0,1,\ldots,N-1$. □

Theorem 5.5. Assume that $u\in C^5([0,L]\times[0,T])$. Furthermore, we suppose that the potential function F is in C^4. In the same manner, as Lemma 5.10, denote the bounds by (5.83). Fix $B\in(0,(\gamma/C_3^2))$. If Δt satisfies

$$
\Delta t<B\left(<\frac{\gamma}{C_3^2}\right), \tag{5.92}
$$

then there exists a constant $C:=C(B)$ dependent on B and independent of k and n such that

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

where $\mathit{\Pi}_{\Delta x,\Delta t}U$ is the function that interpolates the grid value point $U_k^{(n)}$ and is defined by

$$
\begin{aligned}
(\mathit{\Pi}_{\Delta x,\Delta t}U)(x,t)&:=\left(\mathit{\Pi}_{\Delta x}(\mathit{\Pi}_{\Delta t}U_k)\right)(x,t)\\
&=\left(\mathit{\Pi}_{\Delta t}(\mathit{\Pi}_{\Delta x}U^{(n)})\right)(x,t)\\
&=\left(k+1-\frac{x}{\Delta x}\right)\left(n+1-\frac{t}{\Delta t}\right)U_k^{(n)}+\left(k+1-\frac{x}{\Delta x}\right)\left(\frac{t}{\Delta t}-n\right)U_k^{(n+1)}\\
&\quad+\left(\frac{x}{\Delta x}-k\right)\left(n+1-\frac{t}{\Delta t}\right)U_{k+1}^{(n)}+\left(\frac{x}{\Delta x}-k\right)\left(\frac{t}{\Delta t}-n\right)U_{k+1}^{(n+1)}
\end{aligned}
$$

for $(x,t)\in[k\Delta x,(k+1)\Delta x]\times[n\Delta t,(n+1)\Delta t],\ k=0,1,\ldots,K-1,\ n=0,1,\ldots,N-1.$ Also, $\mathit{\Pi}_{\Delta x}$ is the function that interpolates the grid value point f_k and is defined as follows:

$$
\begin{aligned}
(\mathit{\Pi}_{\Delta x}f)(x)&:=f_k+\frac{f_{k+1}-f_k}{\Delta x}(x-k\Delta x)\\
&=\left(k+1-\frac{x}{\Delta x}\right)f_k+\left(\frac{x}{\Delta x}-k\right)f_{k+1}\quad\text{for } x\in[k\Delta x,(k+1)\Delta x],\quad k=0,\ldots,K-1.
\end{aligned}
$$

Besides, $\Pi_{\Delta t}$ is the function that interpolates the grid value point $f^{(n)}$ and is defined as follows:

$$\begin{aligned}(\Pi_{\Delta t}f)(t) &:= f^{(n)} + \frac{f^{(n+1)} - f^{(n)}}{\Delta t}(t - n\Delta t)\\ &= \left(n+1-\frac{t}{\Delta t}\right) f^{(n)} + \left(\frac{t}{\Delta t}-n\right) f^{(n+1)} \quad \text{for } t \in [n\Delta t, (n+1)\Delta t], \quad n=0,\ldots,N-1.\end{aligned}$$

Proof. Step1. Let ε be an arbitrarily fixed positive number satisfying

$$\varepsilon < \frac{1}{B}\left(1 - \frac{C_3^2}{\gamma}B\right).$$

In other words, we have $B < 1/C_4$ for $C_4 := (C_3^2/\gamma) + \varepsilon$. Let $\tilde{C}_4 := (2C_4)/(1 - C_4B)$. Then, it follows from (5.92) that

$$\frac{1 + C_4\Delta t}{1 - C_4\Delta t} < 1 + \tilde{C}_4\Delta t < \exp(\tilde{C}_4\Delta t). \tag{5.93}$$

Actually, since C_4 is positive, it holds from (5.92) that $1 - C_4\Delta t > 1 - C_4B$. Also, from the definition of $\tilde{C}_4$, we obtain $\tilde{C}_4(1 - C_4B) = 2C_4$. Thus, we have

$$(1+\tilde{C}_4\Delta t)(1-C_4\Delta t) = 1-C_4\Delta t+\tilde{C}_4\Delta t(1-C_4\Delta t) > 1-C_4\Delta t+\tilde{C}_4\Delta t(1-C_4B) = 1+C_4\Delta t.$$

From this inequality, the first inequality in (4.76) holds. The second inequality in (4.76) holds from the following inequality: $1 + x < \exp(x)$ for all $x > 0$. Using Lemma 5.10, (5.92), and (5.93), we obtain

$$\begin{aligned}\left\|D\boldsymbol{e}_u^{(n+1)}\right\|^2 &\le \frac{1+C_4\Delta t}{1-C_4\Delta t}\left\|D\boldsymbol{e}_u^{(n)}\right\|^2 + \frac{\Delta t}{1-C_4\Delta t}R^{\left(n+\frac{1}{2}\right)}\\ &\le \exp(\tilde{C}_4\Delta t)\left\|D\boldsymbol{e}_u^{(n)}\right\|^2 + \frac{\Delta t}{1-C_4B}R^{\left(n+\frac{1}{2}\right)} \quad (n = 0, 1, \ldots, N-1).\end{aligned} \tag{5.94}$$

Using (5.94) repeatedly, we have

$$\begin{aligned}\left\|D\boldsymbol{e}_u^{(n)}\right\|^2 &\le \exp(\tilde{C}_4\Delta t)\left\|D\boldsymbol{e}_u^{(n-1)}\right\|^2 + \frac{\Delta t}{1 - C_4B}R^{\left(n-1+\frac{1}{2}\right)}\\ &\le \exp(2\tilde{C}_4\Delta t)\left\|D\boldsymbol{e}_u^{(n-2)}\right\|^2 + \frac{\Delta t}{1 - C_4B}\left[\left\{\exp(\tilde{C}_4\Delta t)\right\}R^{\left(n-2+\frac{1}{2}\right)} + R^{\left(n-1+\frac{1}{2}\right)}\right]\\ &\le \cdots\\ &\le \exp(n\tilde{C}_4\Delta t)\left\|D\boldsymbol{e}_u^{(0)}\right\|^2 + \frac{\Delta t}{1 - C_4B}\sum_{j=1}^{n}\left[\exp\{(j-1)\tilde{C}_4\Delta t\}\right]R^{\left(n-j+\frac{1}{2}\right)}\\ &= \frac{\Delta t}{1 - C_4B}\sum_{j=1}^{n}\left[\exp\{\tilde{C}_4(j-1)\Delta t\}\right]R^{\left(n-j+\frac{1}{2}\right)} \quad (n = 1, \ldots, N),\end{aligned}$$

where the last equality holds from $\boldsymbol{e}_u^{(0)} = \boldsymbol{0}$. For any $j = 1, 2, \ldots, n$, it holds from $j - 1 \le n - 1 < N$ that

$$\exp\{\tilde{C}_4(j-1)\Delta t\} < \exp(\tilde{C}_4N\Delta t) = \exp\left(\tilde{C}_4N\cdot\frac{T}{N}\right) = \exp(\tilde{C}_4T).$$

Therefore, we obtain

$$\left\|D\boldsymbol{e}_u^{(n)}\right\|^2 \le \frac{\exp(\tilde{C}_4 T)}{1 - C_4 B}\Delta t \sum_{j=1}^{n} R^{\left(n-j+\frac{1}{2}\right)} \quad (n = 1, \ldots, N). \tag{5.95}$$

Hence, from (5.88) in the proof of Lemma 5.10, and (5.95), we have

$$\begin{aligned}\left\|\boldsymbol{e}_u^{(n)}\right\|_{L_{\mathrm{d}}^\infty} &\le \Delta t \sum_{j=0}^{n-1} \left\|\boldsymbol{\xi}_1^{\left(j+\frac{1}{2}\right)}\right\|_{L_{\mathrm{d}}^\infty} + L^{\frac{1}{2}} \left\|D\boldsymbol{e}_u^{(n)}\right\| \\ &\le \Delta t \sum_{j=0}^{n-1} \left\|\boldsymbol{\xi}_1^{\left(j+\frac{1}{2}\right)}\right\|_{L_{\mathrm{d}}^\infty} + \left\{\frac{L\exp(\tilde{C}_4 T)}{1 - C_4 B}\Delta t \sum_{j=1}^{n} R^{\left(n-j+\frac{1}{2}\right)}\right\}^{\frac{1}{2}} \quad (n = 1, \ldots, N).\end{aligned} \tag{5.96}$$

Next, we estimate $\boldsymbol{\xi}_i^{(n+1/2)}$ $(i = 1, 2)$ and $\xi_{3,k}^{(n+1/2)}$ $(k = 0, K)$. Let us define

$$\begin{aligned} M_{i,j}(v) &:= \max\left\{\left|\frac{\partial^{i+j} v}{\partial x^i \partial t^j}\right|; (x,t) \in [0,L] \times [0,T]\right\} \quad \text{for all } i, j \in \mathbb{Z}, \\ \tilde{M}_{i,j}(\tilde{v}) &:= \max\left\{\left|\frac{\partial^{i+j} \tilde{v}}{\partial x^i \partial t^j}\right|; (x,t) \in [-\Delta x, L + \Delta x] \times [0,T]\right\} \quad \text{for all } i, j \in \mathbb{Z}. \end{aligned}$$

Firstly, we consider $\xi_{3,0}$ and $\xi_{3,K}$. Applying the Taylor theorem to $\tilde{u}$ and using (5.71), we obtain the following estimate (for details, see the proof of Corollary 4.1):

$$\left|\delta_k^{\langle 1\rangle}\left(\frac{\tilde{u}_k^{(n+1)} + \tilde{u}_k^{(n)}}{2}\right) - \partial_x u_k^{\left(n+\frac{1}{2}\right)}\right| \le C\left\{(\Delta x)^2 M_{3,0}(u) + (\Delta t)^2 M_{1,2}(u) + (\Delta t)^2 (\Delta x)^2 M_{3,2}(u)\right\}$$

for $k = 0, K$. As a remark, throughout this proof, we need the reader to keep in mind that the meaning of C changes from line to line, whereas C always denote those constants. From the assumption (5.92) on Δt, we obtain the following estimate:

$$\left|\delta_k^{\langle 1\rangle}\left(\frac{\tilde{u}_k^{(n+1)} + \tilde{u}_k^{(n)}}{2}\right) - \partial_x u_k^{\left(n+\frac{1}{2}\right)}\right| \le C\left\{(\Delta x)^2\left(M_{3,0}(u) + \frac{\gamma^2}{C_3^4} M_{3,2}(u)\right) + (\Delta t)^2 M_{1,2}(u)\right\}$$

for $k = 0, K$. Furthermore, using the Taylor theorem, we have the following estimate:

$$\left|\partial_t u_k^{\left(n+\frac{1}{2}\right)} - \frac{u_k^{(n+1)} - u_k^{(n)}}{\Delta t}\right| \le C M_{0,3}(u)(\Delta t)^2 \quad (k = 0, \ldots, K). \tag{5.97}$$

From the above, we estimate $\xi_{3,0}$ and $\xi_{3,K}$ as follows:

$$\begin{aligned}\left|\xi_{3,k}^{\left(n+\frac{1}{2}\right)}\right| &\le \left|\partial_t u_k^{\left(n+\frac{1}{2}\right)} - \frac{u_k^{(n+1)} - u_k^{(n)}}{\Delta t}\right| + \left|\delta_k^{\langle 1\rangle}\left(\frac{\tilde{u}_k^{(n+1)} + \tilde{u}_k^{(n)}}{2}\right) - \partial_x u_k^{\left(n+\frac{1}{2}\right)}\right| \\ &\le C(\Delta x)^2\left(M_{3,0}(u) + \frac{\gamma^2}{C_3^4} M_{3,2}(u)\right) + C(\Delta t)^2\left(M_{0,3}(u) + M_{1,2}(u)\right) \quad (k = 0, K).\end{aligned}$$

Next, we consider $\boldsymbol{\xi}_1$. For any $t \in [0,T]$ and $k = 0, \ldots, K$, applying the Taylor theorem to $\tilde{p}$, there exists $\theta_1 \in (0,1)$ such that

$$\begin{aligned} &\frac{\tilde{p}((k+1)\Delta x, t) - 2\tilde{p}(k\Delta x, t) + \tilde{p}((k-1)\Delta x, t)}{(\Delta x)^2} \\ &= \partial_x^2 \tilde{p}(k\Delta x, t) + \frac{(\Delta x)^2}{24} \left\{ \partial_x^4 \tilde{p}((k+\theta_1)\Delta x, t) + \partial_x^4 \tilde{p}((k-\theta_1)\Delta x, t) \right\}. \end{aligned} \tag{5.98}$$

Substituting $(n+1/2)\Delta t$ into t in (5.98), we obtain

$$\delta_k^{\langle 2 \rangle} \tilde{p}_k^{\left(n+\frac{1}{2}\right)} - \partial_x^2 p_k^{\left(n+\frac{1}{2}\right)} = \delta_k^{\langle 2 \rangle} \tilde{p}_k^{\left(n+\frac{1}{2}\right)} - \partial_x^2 \tilde{p}_k^{\left(n+\frac{1}{2}\right)} = \frac{(\Delta x)^2}{24} \left(\partial_x^4 \tilde{p}_{k+\theta_1}^{\left(n+\frac{1}{2}\right)} + \partial_x^4 \tilde{p}_{k-\theta_1}^{\left(n+\frac{1}{2}\right)} \right) \quad (k=0, \ldots, K). \tag{5.99}$$

Therefore, we have

$$\left| \delta_k^{\langle 2 \rangle} \tilde{p}_k^{\left(n+\frac{1}{2}\right)} - \partial_x^2 p_k^{\left(n+\frac{1}{2}\right)} \right| \le \frac{(\Delta x)^2}{12} \tilde{M}_{4,0}(\tilde{p}) \quad (k = 0, \ldots, K). \tag{5.100}$$

Hence, using (5.97) and (5.100), the following estimate holds:

$$\begin{aligned} \left| \xi_{1,k}^{\left(n+\frac{1}{2}\right)} \right| &\le \left| \partial_t u_k^{\left(n+\frac{1}{2}\right)} - \frac{u_k^{(n+1)} - u_k^{(n)}}{\Delta t} \right| + \left| \delta_k^{\langle 2 \rangle} \tilde{p}_k^{\left(n+\frac{1}{2}\right)} - \partial_x^2 p_k^{\left(n+\frac{1}{2}\right)} \right| \\ &\le C M_{0,3}(u) (\Delta t)^2 + \frac{(\Delta x)^2}{12} \tilde{M}_{4,0}(\tilde{p}) \quad (k = 0, \ldots, K). \end{aligned}$$

Next, for $k = 0, \ldots, K-1$, from (5.99), we have

$$\begin{aligned} &\delta_k^+ \left(\delta_k^{\langle 2 \rangle} \tilde{p}_k^{\left(n+\frac{1}{2}\right)} - \partial_x^2 p_k^{\left(n+\frac{1}{2}\right)} \right) \\ &= \frac{1}{\Delta x} \left\{ \left(\delta_k^{\langle 2 \rangle} \tilde{p}_{k+1}^{\left(n+\frac{1}{2}\right)} - \partial_x^2 p_{k+1}^{\left(n+\frac{1}{2}\right)} \right) - \left(\delta_k^{\langle 2 \rangle} \tilde{p}_k^{\left(n+\frac{1}{2}\right)} - \partial_x^2 p_k^{\left(n+\frac{1}{2}\right)} \right) \right\} \\ &= \frac{1}{\Delta x} \left\{ \frac{(\Delta x)^2}{24} \left(\partial_x^4 \tilde{p}_{k+1+\theta_1}^{\left(n+\frac{1}{2}\right)} + \partial_x^4 \tilde{p}_{k+1-\theta_1}^{\left(n+\frac{1}{2}\right)} \right) - \frac{(\Delta x)^2}{24} \left(\partial_x^4 \tilde{p}_{k+\theta_1}^{\left(n+\frac{1}{2}\right)} + \partial_x^4 \tilde{p}_{k-\theta_1}^{\left(n+\frac{1}{2}\right)} \right) \right\} \\ &= \frac{(\Delta x)^2}{24} \frac{\partial_x^4 \tilde{p}_{k+1+\theta_1}^{\left(n+\frac{1}{2}\right)} - \partial_x^4 \tilde{p}_{k+\theta_1}^{\left(n+\frac{1}{2}\right)}}{\Delta x} + \frac{(\Delta x)^2}{24} \frac{\partial_x^4 \tilde{p}_{k+1-\theta_1}^{\left(n+\frac{1}{2}\right)} - \partial_x^4 \tilde{p}_{k-\theta_1}^{\left(n+\frac{1}{2}\right)}}{\Delta x}. \end{aligned} \tag{5.101}$$

Since $\tilde{p}$ satisfies $\tilde{p}(\cdot, t) \in C^5([0,L])$ for any fixed $t \in [0,T]$, applying the mean value theorem to $\partial_x^4 \tilde{p}(\cdot, t)$ and using (5.101), we obtain

$$\left| \delta_k^+ \left(\delta_k^{\langle 2 \rangle} \tilde{p}_k^{\left(n+\frac{1}{2}\right)} - \partial_x^2 p_k^{\left(n+\frac{1}{2}\right)} \right) \right| \le \frac{(\Delta x)^2}{12} \tilde{M}_{5,0}(\tilde{p}) \quad (k = 0, \ldots, K-1).$$

Besides, applying the Taylor theorem to u and using the mean value theorem, we have

$$\left| \delta_k^+ \left(\partial_t u_k^{\left(n+\frac{1}{2}\right)} - \frac{u_k^{(n+1)} - u_k^{(n)}}{\Delta t} \right) \right| \le C M_{1,3}(u) (\Delta t)^2 \quad (k = 0, \ldots, K-1).$$

Hence, we have the following estimate:

$$\begin{aligned}\left|\delta_k^+\xi_{1,k}^{\left(n+\frac{1}{2}\right)}\right| &\le \left|\delta_k^+\left(\partial_t u_k^{\left(n+\frac{1}{2}\right)} - \frac{u_k^{(n+1)} - u_k^{(n)}}{\Delta t}\right)\right| + \left|\delta_k^+\left(\delta_k^{\langle 2\rangle}\tilde{p}_k^{\left(n+\frac{1}{2}\right)} - \partial_x^2 p_k^{\left(n+\frac{1}{2}\right)}\right)\right| \\ &\le CM_{1,3}(u)(\Delta t)^2 + \frac{(\Delta x)^2}{12}\tilde{M}_{5,0}(\tilde{p}) \quad (k = 0, \dots, K-1).\end{aligned}$$

Next, we consider $\boldsymbol{\xi}_2$. For any $x \in [0, L]$, applying the Taylor theorem to $\tilde{u}$, there exists $\theta_2 \in (0, 1)$ such that

$$\begin{aligned}&\frac{\tilde{u}(x,(n+1)\Delta t) + \tilde{u}(x, n\Delta t)}{2} \\ &= \tilde{u}\left(x, \left(n + \frac{1}{2}\right)\Delta t\right) + \frac{(\Delta t)^2}{16}\left\{\partial_t^2\tilde{u}\left(x, \left(n+\frac{1+\theta_2}{2}\right)\Delta t\right) + \partial_t^2\tilde{u}\left(x, \left(n+\frac{1-\theta_2}{2}\right)\Delta t\right)\right\}.\end{aligned} \tag{5.102}$$

Substituting $k\Delta x$ $(k = 0, \dots, K)$ into x in (5.102), we obtain

$$\begin{aligned}\delta_k^{\langle 2\rangle}\left(\frac{\tilde{u}_k^{(n+1)} + \tilde{u}_k^{(n)}}{2}\right) - \partial_x^2 u_k^{\left(n+\frac{1}{2}\right)} &= \delta_k^{\langle 2\rangle}\tilde{u}_k^{\left(n+\frac{1}{2}\right)} - \partial_x^2 u_k^{\left(n+\frac{1}{2}\right)} \\ &\quad + \frac{(\Delta t)^2}{16}\left\{\delta_k^{\langle 2\rangle}\left(\partial_t^2\tilde{u}_k^{\left(n+\frac{1+\theta_2}{2}\right)}\right) + \delta_k^{\langle 2\rangle}\left(\partial_t^2\tilde{u}_k^{\left(n+\frac{1-\theta_2}{2}\right)}\right)\right\}\end{aligned} \tag{5.103}$$

for $k = 0, \dots, K$. Also, for $k = 0, \dots, K$, applying the Taylor theorem to $\tilde{u}$ and using (5.71), there exists $\theta_3 \in (0, 1)$ such that

$$\delta_k^{\langle 2\rangle}\tilde{u}_k^{\left(n+\frac{1}{2}\right)} - \partial_x^2 u_k^{\left(n+\frac{1}{2}\right)} = \begin{cases}\dfrac{(\Delta x)^2}{12}\partial_x^4 u_{\theta_3}^{\left(n+\frac{1}{2}\right)} & (k = 0), \\ \dfrac{(\Delta x)^4}{24}\left(\partial_x^4 u_{k+\theta_3}^{\left(n+\frac{1}{2}\right)} + \partial_x^4 u_{k-\theta_3}^{\left(n+\frac{1}{2}\right)}\right) & (k = 1, \dots, K-1), \\ \dfrac{(\Delta x)^2}{12}\partial_x^4 u_{K-\theta_3}^{\left(n+\frac{1}{2}\right)} & (k = K).\end{cases} \tag{5.104}$$

For details, see the proof of Corollary 4.1. Since u satisfies $u \in C^5([0, L] \times [0, T])$ from the regularity assumption of u, applying the mean value theorem to $\partial_x^4 u$ and using (5.104), we obtain

$$\left|\delta_k^+\left(\delta_k^{\langle 2\rangle}\tilde{u}_k^{\left(n+\frac{1}{2}\right)} - \partial_x^2 u_k^{\left(n+\frac{1}{2}\right)}\right)\right| \le \frac{(\Delta x)^2}{12}M_{5,0}(u) \quad (k = 0, \dots, K-1). \tag{5.105}$$

Similarly, for $k = 0, \dots, K$, applying the Taylor theorem to $\partial_t^2\tilde{u}$ and using (5.71), there exists $\theta_4 \in (0, 1)$ such that

$$\delta_k^{\langle 2\rangle}\left(\partial_t^2\tilde{u}_k^{\left(n+\frac{1\pm\theta_2}{2}\right)}\right) = \begin{cases}\partial_x^2\partial_t^2 u_{\theta_4}^{\left(n+\frac{1\pm\theta_2}{2}\right)} - \theta_4\Delta x\partial_t^2\partial_x^3 u_0^{\left(n+\frac{1\pm\theta_2}{2}\right)} & (k=0), \\ \dfrac{1}{2}\left(\partial_x^2\partial_t^2 u_{k+\theta_4}^{\left(n+\frac{1\pm\theta_2}{2}\right)} + \partial_x^2\partial_t^2 u_{k-\theta_4}^{\left(n+\frac{1\pm\theta_2}{2}\right)}\right) & (k=1, \dots, K-1), \\ \partial_x^2\partial_t^2 u_{K-\theta_4}^{\left(n+\frac{1\pm\theta_2}{2}\right)} + \theta_4\Delta x\partial_t^2\partial_x^3 u_K^{\left(n+\frac{1\pm\theta_2}{2}\right)} & (k=K).\end{cases} \tag{5.106}$$

Applying the mean value theorem to $\partial_x^2\partial_t^2 u$ and using (5.106), we obtain

$$\left|\delta_k^+\left\{\delta_k^{\langle 2\rangle}\left(\partial_t^2\tilde{u}_k^{\left(n+\frac{1\pm\theta_2}{2}\right)}\right)\right\}\right| \le M_{3,2}(u) \quad (k=1,\ldots,K-2), \tag{5.107}$$

$$\left|\delta_k^+\left\{\delta_k^{\langle 2\rangle}\left(\partial_t^2\tilde{u}_k^{\left(n+\frac{1\pm\theta_2}{2}\right)}\right)\right\}\right| \le M_{3,2}(u)+\theta_4 M_{3,2}(u) \le 2M_{3,2}(u) \quad (k=0,K-1). \tag{5.108}$$

Hence, from (5.103), (5.105), (5.107), and (5.108), we conclude that

$$\begin{aligned}
&\left|\delta_k^+\left\{\partial_x^2 u_k^{\left(n+\frac{1}{2}\right)} - \delta_k^{\langle 2\rangle}\left(\frac{\tilde{u}_k^{(n+1)}+\tilde{u}_k^{(n)}}{2}\right)\right\}\right| \\
&\le \left|\delta_k^+\left(\partial_x^2 u_k^{\left(n+\frac{1}{2}\right)} - \delta_k^{\langle 2\rangle}\tilde{u}_k^{\left(n+\frac{1}{2}\right)}\right)\right| \\
&\quad + \frac{(\Delta t)^2}{16}\left(\left|\delta_k^+\left\{\delta_k^{\langle 2\rangle}\left(\partial_t^2\tilde{u}_k^{\left(n+\frac{1+\theta_2}{2}\right)}\right)\right\}\right| + \left|\delta_k^+\left\{\delta_k^{\langle 2\rangle}\left(\partial_t^2\tilde{u}_k^{\left(n+\frac{1-\theta_2}{2}\right)}\right)\right\}\right|\right) \\
&\le \frac{(\Delta x)^2}{12}M_{5,0}(u) + \frac{(\Delta t)^2}{4}M_{3,2}(u) \quad (k=0,\ldots,K-1).
\end{aligned}$$

Similarly, from the Taylor theorem and the mean value theorem, we see that

$$\begin{aligned}
&\left|\delta_k^+\left(\frac{dF}{d(u_k^{(n+1)},u_k^{(n)})} - F'(u_k^{\left(n+\frac{1}{2}\right)})\right)\right| \\
&\le C\left\{C_{F,2}M_{1,2}(u)+C_{F,3}\left(M_{1,1}(u)M_{0,1}(u)+M_{0,2}(u)M_{1,0}(u)\right)+C_{F,4}M_{1,0}(u)(M_{0,1}(u))^2\right\}(\Delta t)^2
\end{aligned}$$

for $k=0,\ldots,K-1$. From the regularity assumption of the solution u and the potential F, we see that $C_{F,i}$ $(i=2,3,4)$, $M_{i,j}(u)$ $(i,j\in\mathbb{Z}, 0\le i+j\le 5)$, and $\tilde{M}_{i,0}(\tilde{p})$ $(i=4,5)$ are bounded. Thus, we obtain the following estimates:

$$\begin{aligned}
\left|\xi_{1,k}^{\left(n+\frac{1}{2}\right)}\right| &\le C_5((\Delta x)^2+(\Delta t)^2) \quad (k=0,\ldots,K), \\
\left|\xi_{3,k}^{\left(n+\frac{1}{2}\right)}\right| &\le C_5((\Delta x)^2+(\Delta t)^2) \quad (k=0,K), \\
\left|\delta_k^+\xi_{i,k}^{\left(n+\frac{1}{2}\right)}\right| &\le C_5((\Delta x)^2+(\Delta t)^2) \quad (k=0,\ldots,K-1,\ i=1,2),
\end{aligned} \tag{5.109}$$

where C_5 is a constant independent of Δx and Δt. Therefore, the following estimates hold:

$$\left\|\boldsymbol{\xi}_1^{\left(n+\frac{1}{2}\right)}\right\|_{L_{\mathrm{d}}^\infty} \le C_5((\Delta x)^2+(\Delta t)^2), \tag{5.110}$$

$$\begin{aligned}
\left\|D\boldsymbol{\xi}_i^{\left(n+\frac{1}{2}\right)}\right\|^2 = \sum_{k=0}^{K-1}\left|\delta_k^+\xi_{i,k}^{\left(n+\frac{1}{2}\right)}\right|^2\Delta x &\le C_5^2((\Delta x)^2+(\Delta t)^2)^2\sum_{k=0}^{K-1}\Delta x \\
&= LC_5^2((\Delta x)^2+(\Delta t)^2)^2 \quad (i=1,2).
\end{aligned} \tag{5.111}$$

Furthermore, using (5.110), we obtain

$$\Delta t\sum_{j=0}^{n-1}\left\|\boldsymbol{\xi}_1^{\left(j+\frac{1}{2}\right)}\right\|_{L_{\mathrm{d}}^\infty} \le C_5((\Delta x)^2+(\Delta t)^2)n\Delta t \le C_5 T((\Delta x)^2+(\Delta t)^2) \quad (n=1,\ldots,N). \tag{5.112}$$

Hence, from (5.84), (5.109)–(5.112), it holds that

$$
\begin{aligned}
R^{\left(n+\frac{1}{2}\right)} &= \frac{1}{2\gamma}\left(1+\frac{2C_3^2}{\varepsilon\gamma}\right)\left(C_1C_{F,3}\Delta t\sum_{j=0}^{n}\left\|\boldsymbol{\xi}_1^{\left(j+\frac{1}{2}\right)}\right\|_{L^\infty_{\mathrm{d}}}+\left\|D\boldsymbol{\xi}_2^{\left(n+\frac{1}{2}\right)}\right\|\right)^2+\frac{1}{\varepsilon}\left\|D\boldsymbol{\xi}_1^{\left(n+\frac{1}{2}\right)}\right\|^2 \\
&\quad +\left|\xi_{1,0}^{\left(n+\frac{1}{2}\right)}\right|^2+\left|\xi_{1,K}^{\left(n+\frac{1}{2}\right)}\right|^2+\left|\xi_{3,0}^{\left(n+\frac{1}{2}\right)}\right|^2+\left|\xi_{3,K}^{\left(n+\frac{1}{2}\right)}\right|^2 \\
&\leq \frac{1}{2\gamma}\left(1+\frac{2C_3^2}{\varepsilon\gamma}\right)\left\{(C_1C_{F,3}C_5T)\left((\Delta x)^2+(\Delta t)^2\right)+L^{\frac{1}{2}}C_5((\Delta x)^2+(\Delta t)^2)\right\}^2 \\
&\quad +\frac{C_5^2L}{\varepsilon}((\Delta x)^2+(\Delta t)^2)^2+4C_5^2((\Delta x)^2+(\Delta t)^2)^2 \\
&\leq C_5^2\left\{\frac{1}{2\gamma}\left(1+\frac{2C_3^2}{\varepsilon\gamma}\right)\left(C_1C_{F,3}T+L^{\frac{1}{2}}\right)^2+\frac{L}{\varepsilon}+4\right\}((\Delta x)^2+(\Delta t)^2)^2
\end{aligned}
$$

for $n=0,\dots,N-1$. Now, let us define the constant C_6 as follows:

$$
C_6 := C_5^2\left\{\frac{1}{2\gamma}\left(1+\frac{2C_3^2}{\varepsilon\gamma}\right)\left(C_1C_{F,3}T+L^{\frac{1}{2}}\right)^2+\frac{L}{\varepsilon}+4\right\}.
$$

Then, we obtain

$$
\begin{aligned}
\frac{L\exp(\tilde{C}_4T)}{1-C_4B}\Delta t\sum_{j=1}^{n}R^{\left(n-j+\frac{1}{2}\right)} &\leq \frac{C_6L\exp(\tilde{C}_4T)}{1-C_4B}n\Delta t((\Delta x)^2+(\Delta t)^2)^2 \\
&\leq \frac{C_6LT\exp(\tilde{C}_4T)}{1-C_4B}((\Delta x)^2+(\Delta t)^2)^2 \qquad (5.113)
\end{aligned}
$$

for $n=1,\dots,N$. From the above, using (5.96), (5.112), and (5.113), we conclude that

$$
\begin{aligned}
\left\|\boldsymbol{e}_u^{(n)}\right\|_{L^\infty_{\mathrm{d}}} &\leq C_5T((\Delta x)^2+(\Delta t)^2)+\left\{\frac{C_6LT\exp(\tilde{C}_4T)}{1-C_4B}\right\}^{\frac{1}{2}}((\Delta x)^2+(\Delta t)^2) \\
&= C_7((\Delta x)^2+(\Delta t)^2) \quad (n=1,\dots,N), \qquad (5.114)
\end{aligned}
$$

where the constant C_7 is defined by

$$
C_7 := C_7(B) := C_5T+\left\{\frac{C_6LT\exp(\tilde{C}_4T)}{1-C_4B}\right\}^{\frac{1}{2}}.
$$

Step2. It holds from the triangle inequality that

$$
\begin{aligned}
\|(\Pi_{\Delta x,\Delta t}U)(\cdot,t)-u(\cdot,t)\|_{L^\infty(0,L)} &\leq \|(\Pi_{\Delta x,\Delta t}U)(\cdot,t)-(\Pi_{\Delta x,\Delta t}u)(\cdot,t)\|_{L^\infty(0,L)} \\
&\quad +\|(\Pi_{\Delta x,\Delta t}u)(\cdot,t)-u(\cdot,t)\|_{L^\infty(0,L)} \quad \text{for all } t\in[0,T]. \qquad (5.115)
\end{aligned}
$$

Firstly, we estimate the first term on the right-hand side of (5.115). For $t\in[n\Delta t,(n+1)\Delta t]$, $n=0,1,\dots,N-1$, there exists $\eta\in[0,1]$ satisfying $t=(n+\eta)\Delta t$. Hence, using

(5.114) and the following inequality $\|\mathit{\Pi}_{\Delta x} f\|_{L^\infty(0,L)} \le \|\boldsymbol{f}\|_{L^\infty_{\mathrm{d}}}$ for all $\{f_k\}_{k=0}^K \in \mathbb{R}^{K+1}$, we obtain

$$
\begin{aligned}
&\|(\mathit{\Pi}_{\Delta x,\Delta t} U)(\cdot,t) - (\mathit{\Pi}_{\Delta x,\Delta t} u)(\cdot,t)\|_{L^\infty(0,L)} \\
&= \left\| \left\{ \left(n+1-\frac{(n+\eta)\Delta t}{\Delta t} \right) \left(\mathit{\Pi}_{\Delta x} U^{(n)}\right) + \left(\frac{(n+\eta)\Delta t}{\Delta t} - n \right) \left(\mathit{\Pi}_{\Delta x} U^{(n+1)}\right) \right\} \right. \\
&\quad \left. - \left\{ \left(n+1-\frac{(n+\eta)\Delta t}{\Delta t} \right) \left(\mathit{\Pi}_{\Delta x} u^{(n)}\right) + \left(\frac{(n+\eta)\Delta t}{\Delta t} - n \right) \left(\mathit{\Pi}_{\Delta x} u^{(n+1)}\right) \right\} \right\|_{L^\infty(0,L)} \\
&= \left\| (1-\eta) \left\{ \left(\mathit{\Pi}_{\Delta x} U^{(n)}\right) - \left(\mathit{\Pi}_{\Delta x} u^{(n)}\right) \right\} + \eta \left\{ \left(\mathit{\Pi}_{\Delta x} U^{(n+1)}\right) - \left(\mathit{\Pi}_{\Delta x} u^{(n+1)}\right) \right\} \right\|_{L^\infty(0,L)} \\
&\le (1-\eta) \left\| \mathit{\Pi}_{\Delta x} \left(U^{(n)} - u^{(n)} \right) \right\|_{L^\infty(0,L)} + \eta \left\| \mathit{\Pi}_{\Delta x} \left(U^{(n+1)} - u^{(n+1)} \right) \right\|_{L^\infty(0,L)} \\
&\le (1-\eta) \left\| \boldsymbol{U}^{(n)} - \boldsymbol{u}^{(n)} \right\|_{L^\infty_{\mathrm{d}}} + \eta \left\| \boldsymbol{U}^{(n+1)} - \boldsymbol{u}^{(n+1)} \right\|_{L^\infty_{\mathrm{d}}} \\
&\le C_7 \left((\Delta x)^2 + (\Delta t)^2 \right). \qquad (5.116)
\end{aligned}
$$

Next, we estimate the second term on the right-hand side of (5.115). For any fixed $(x,t) \in [0,L]\times[0,T]$, there exists $k_0 \in \{0,1,\dots,K-1\}$ satisfying $x \in [k_0\Delta x, (k_0+1)\Delta x]$, and there exists $n_0 \in \{0,1,\dots,N-1\}$ satisfying $t \in [n_0\Delta t, (n_0+1)\Delta t]$. Hence, we have

$$
\begin{aligned}
(\mathit{\Pi}_{\Delta x,\Delta t} u)(x,t) - u(x,t) &= \left(k_0+1-\frac{x}{\Delta x} \right) \left(n_0+1-\frac{t}{\Delta t} \right) \{u(k_0\Delta x, n_0\Delta t) - u(x,t)\} \\
&\quad + \left(k_0+1-\frac{x}{\Delta x} \right) \left(\frac{t}{\Delta t} - n_0 \right) \{u(k_0\Delta x, (n_0+1)\Delta t) - u(x,t)\} \\
&\quad + \left(\frac{x}{\Delta x} - k_0 \right) \left(n_0+1-\frac{t}{\Delta t} \right) \{u((k_0+1)\Delta x, n_0\Delta t) - u(x,t)\} \\
&\quad + \left(\frac{x}{\Delta x} - k_0 \right) \left(\frac{t}{\Delta t} - n_0 \right) \{u((k_0+1)\Delta x, (n_0+1)\Delta t) - u(x,t)\}.
\end{aligned}
$$

Let $C_8 := (1/8)(M_{2,0}(u) + M_{0,2}(u))$. Then, using the Taylor theorem, we obtain

$$
|(\mathit{\Pi}_{\Delta x,\Delta t} u)(x,t) - u(x,t)| \le C_8((\Delta x)^2 + (\Delta t)^2).
$$

Therefore, we estimate the second term on the right-hand side of (5.115) as follows:

$$
\|(\mathit{\Pi}_{\Delta x,\Delta t} u)(\cdot,t) - u(\cdot,t)\|_{L^\infty(0,L)} \le C_8((\Delta x)^2 + (\Delta t)^2) \quad \text{for all } t \in [0,T]. \qquad (5.117)
$$

Hence using (5.115)–(5.117), we conclude that

$$
\|(\mathit{\Pi}_{\Delta x,\Delta t} U)(\cdot,t) - u(\cdot,t)\|_{L^\infty(0,L)} \le (C_7 + C_8)((\Delta x)^2 + (\Delta t)^2) \quad \text{for all } t \in [0,T].
$$

This completes the proof. □

§6 Computation examples

In this section, we demonstrate through computation examples that the numerical solution of our proposed scheme is efficient and that the scheme inherits the conservative property and the dissipative property from the original problem in a discrete sense. Also, we compare our scheme with the previous structure-preserving scheme proposed by Fukao–Yoshikawa–Wada [28]. Throughout the computation examples, we consider the double-well potential $F(s) = (1/4)s^4 - (1/2)s^2$. In the same manner as Section 5, we use the following notation $T = N\Delta t$.

6.1 Computation example 1

As the initial condition, we consider

$$u(x, 0) = u_0(x) = 0.01 \cos\left(\frac{\pi}{2} x\right).$$

We choose $N = 20000$ and fix $T = 400$ so that $\Delta t = 1/50$. Also, we choose $K = 40$ and fix $L = 20$ so that $\Delta x = 1/2$. Besides, we fix the parameter $\gamma = 2.0$. Figure 5.1 shows the time development of the solution obtained by our proposed structure-preserving scheme. Figure 5.2 shows the one by the previous structure-preserving scheme proposed by Fukao–Yoshikawa–Wada.

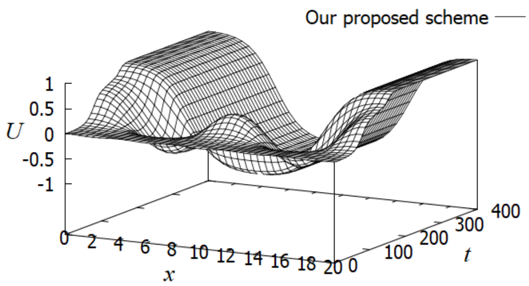

Figure 5.1: Numerical solution by our scheme with $\Delta x = 1/2$

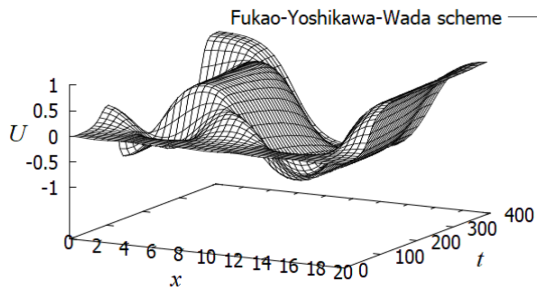

Figure 5.2: Numerical solution by Fukao–Yoshikawa–Wada scheme with $\Delta x = 1/2$

The behavior of the solution obtained by our proposed scheme is different from the one by the Fukao–Yoshikawa–Wada scheme. In order to analyze the difference in these results, we refine the space mesh size. Specifically, in the following results, we choose $K = 800$ so that $\Delta x = 1/40$. In this case, the result of the Fukao–Yoshikawa–Wada scheme improves. Figure 5.3 shows the time development of the solution obtained by our proposed scheme. Also, Figure 5.4 shows the one by the Fukao–Yoshikawa–Wada scheme. Both results are similar to the result obtained by our scheme with $\Delta x = 1/2$. Note that we can obtain a valid numerical solution by our proposed scheme even when the space mesh size Δx is coarse.

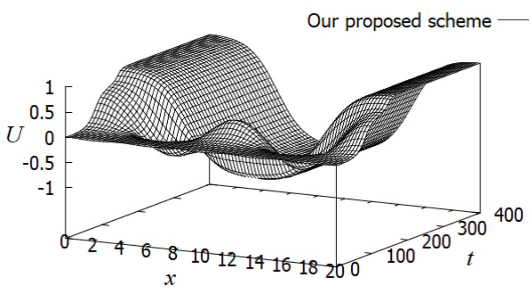

Figure 5.3: Numerical solution by our scheme with $\Delta x = 1/40$

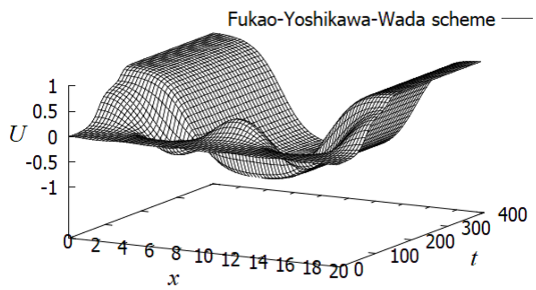

Figure 5.4: Numerical solution by Fukao–Yoshikawa–Wada scheme with $\Delta x = 1/40$

Next, we confirm the conservative property and the dissipative property. Figure 5.5 shows the time development of $M_{\rm d}(\boldsymbol{U}^{(n)})$ obtained by our scheme with $\Delta x = 1/40$. Figure 5.6 shows the time development of $E_{\rm d}^{(n)} - J_{\rm d}(\boldsymbol{U}^{(0)})$ obtained by our scheme with $\Delta x = 1/40$, where

$$E_{\rm d}^{(n)} := J_{\rm d}(\boldsymbol{U}^{(n)}) + \sum_{l=0}^{n-1} \left\{ \gamma \left| \delta_n^+ U_0^{(l)} \right|^2 + \gamma \left| \delta_n^+ U_K^{(l)} \right|^2 + \sum_{k=0}^{K-1} \left| \delta_k^+ P_k^{(l)} \right|^2 \Delta x \right\} \Delta t \quad (n = 1, 2, \ldots).$$

We remark that the following equality holds from Theorem 5.1 (the discrete dissipative property):

$$E_{\rm d}^{(n)} = J_{\rm d}(\boldsymbol{U}^{(0)}) \quad (n = 1, 2, \ldots).$$

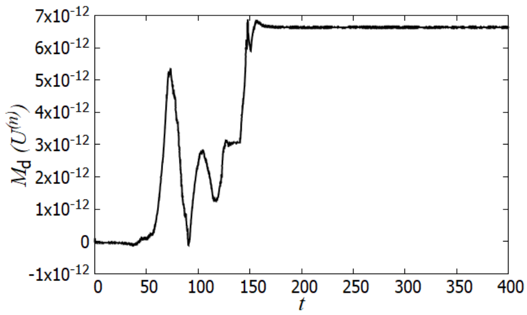

Figure 5.5: Time development of $M_{\rm d}(\boldsymbol{U}^{(n)})$ obtained by our scheme with $\Delta x = 1/40$: $M_{\rm d}(\boldsymbol{U}^{(n)})$ does not change by about 11 orders of magnitude

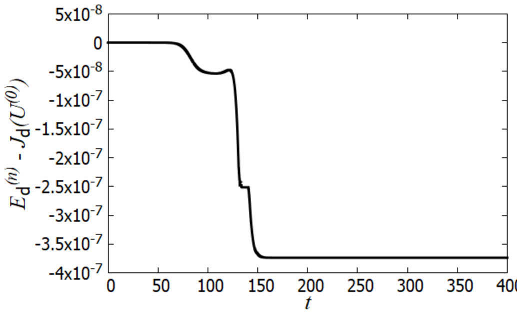

Figure 5.6: Time development of $E_{\rm d}^{(n)} - J_{\rm d}(\boldsymbol{U}^{(0)})$ obtained by our scheme with $\Delta x = 1/40$: $E_{\rm d}^{(n)}$ does not change by about 6 orders of magnitude

These graphs show that the quantities $M_{\rm d}(\boldsymbol{U}^{(n)})$ and $E_{\rm d}^{(n)}$ are conserved numerically. More precisely, $M_{\rm d}(\boldsymbol{U}^{(n)})$ does not change by about 11 orders of magnitude, and $E_{\rm d}^{(n)}$ does not change by about 6 orders of magnitude.

6.2 Computation example 2

As the initial condition, we consider

$$u(x, 0) = u_0(x) = 0.01 \sin(2\pi x) + 0.001 \cos(4\pi x) + 0.006 \sin(4\pi x) + 0.002 \cos(10\pi x).$$

We choose $N = 50000$ and fix $T = 1000$ so that $\Delta t = 1/50$. Also, we choose $K = 250$ and fix $L = 10$ so that $\Delta x = 1/25$. In addition, we fix the parameter $\gamma = 1.0$. Figure 5.7 shows the time development of the solution obtained by our proposed scheme. Figure 5.8 shows the one by the Fukao–Yoshikawa–Wada scheme.

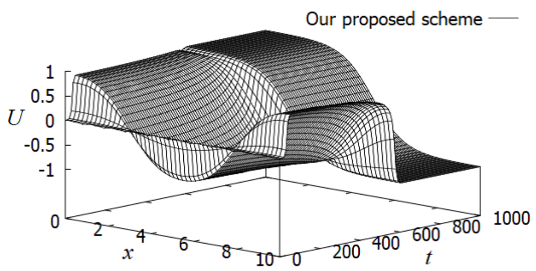

Figure 5.7: Numerical solution by our scheme with $\Delta x = 1/25$

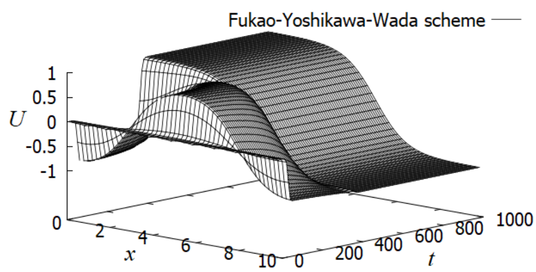

Figure 5.8: Numerical solution by Fukao–Yoshikawa–Wada scheme with $\Delta x = 1/25$

The behavior of the solution obtained by our scheme ranging from $t = 0$ to $t = 600$ is different from the one by the Fukao–Yoshikawa–Wada scheme. In order to analyze the difference in these results, we refine the space mesh size. To be specific, in the following results, we choose $K = 500$ so that $\Delta x = 1/50$. Even in this case, the result of the Fukao–Yoshikawa–Wada scheme improves. Also, we remark that we can obtain a valid numerical solution by our proposed scheme even when the space mesh size Δx is coarse.

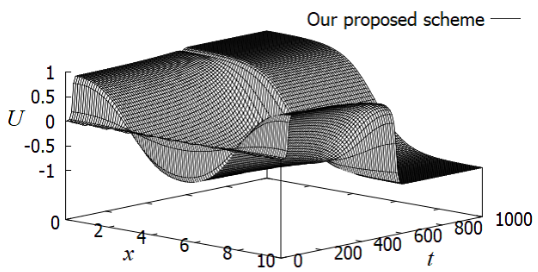

Figure 5.9: Numerical solution by our scheme with $\Delta x = 1/50$

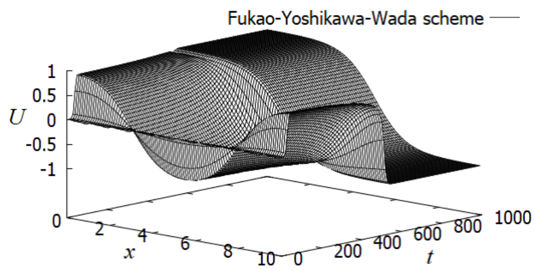

Figure 5.10: Numerical solution by Fukao–Yoshikawa–Wada scheme with $\Delta x = 1/50$

Figure 5.9 shows the time development of the solution obtained by our proposed scheme. Also, Figure 5.10 shows the one by the Fukao–Yoshikawa–Wada scheme. Both results are similar to the result obtained by our scheme with $\Delta x = 1/25$. Hence, as can be seen from Figures 5.1–5.4 and Figures 5.7–5.10, we expect that the solution obtained by our proposed scheme is more reliable than that by the Fukao–Yoshikawa–Wada scheme when the space mesh size is coarse.

Next, we confirm the conservative property and the dissipative property. Figure 5.11 shows the time development of $M_{\mathrm{d}}(\boldsymbol{U}^{(n)})$ obtained by our scheme with $\Delta x = 1/50$. Figure 5.12 shows the time development of $E_{\mathrm{d}}^{(n)} - J_{\mathrm{d}}(\boldsymbol{U}^{(0)})$ obtained by our scheme with $\Delta x = 1/50$.

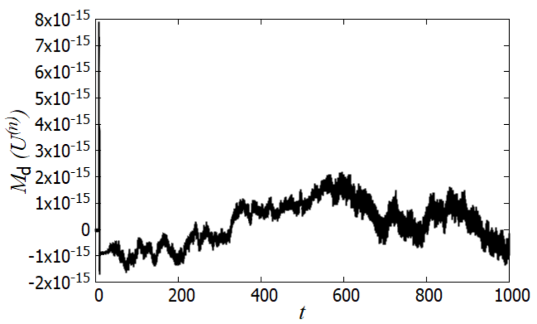

Figure 5.11: Time development of $M_{\mathrm{d}}(\boldsymbol{U}^{(n)})$ obtained by our scheme with $\Delta x = 1/50$: $M_{\mathrm{d}}(\boldsymbol{U}^{(n)})$ does not change by about 14 orders of magnitude

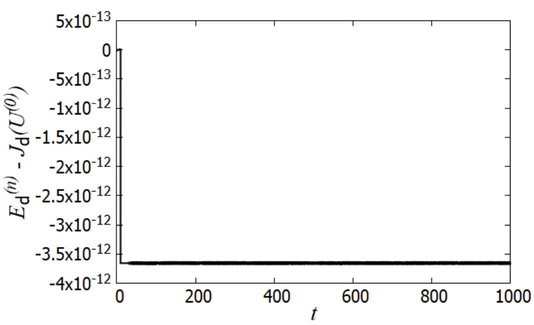

Figure 5.12: Time development of $E_{\mathrm{d}}^{(n)} - J_{\mathrm{d}}(\boldsymbol{U}^{(0)})$ obtained by our scheme with $\Delta x = 1/50$: $E_{\mathrm{d}}^{(n)}$ does not change by about 11 orders of magnitude

These graphs show that the quantities $M_{\mathrm{d}}(\boldsymbol{U}^{(n)})$ and $E_{\mathrm{d}}^{(n)}$ are conserved numerically. More precisely, $M_{\mathrm{d}}(\boldsymbol{U}^{(n)})$ does not change by about 14 orders of magnitude, and $E_{\mathrm{d}}^{(n)}$ does not change by about 11 orders of magnitude.

6.3 Computation example 3

We consider the following dynamic boundary condition for the order parameter u:

$$\begin{cases} \varepsilon_{\rm ex}\partial_t u(0,t) = \partial_x u(x,t)|_{x=0} & \text{in } (0,\infty), \\ \varepsilon_{\rm ex}\partial_t u(L,t) = -\,\partial_x u(x,t)|_{x=L} & \text{in } (0,\infty), \end{cases} \tag{5.118}$$

where $\varepsilon_{\rm ex}$ is a positive constant. For the chemical potential p, we consider the same homogeneous Neumann boundary condition as before. In this computation example, we fix $\varepsilon_{\rm ex} = 1000$. We consider

$$u(x,0) = u_0(x) = 0.05\sin(2\pi x)$$

as the initial condition. We choose $K = 50$ and fix $L = 1$ so that $\Delta x = 1/50$. Also, we choose $N = 500000$ and fix $T = 1000$ so that $\Delta t = 1/500$. Besides, we fix the parameter $\gamma = 0.001$. Figure 5.13 shows the time development of the solution obtained by our proposed scheme.

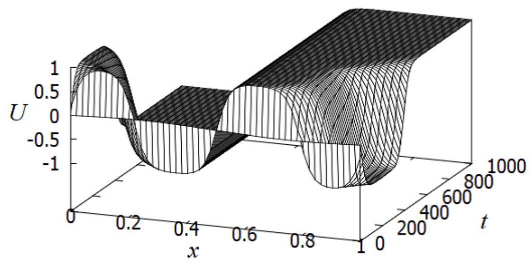

Figure 5.13: Numerical solution to (5.1)–(5.2) with (5.5) and (5.118) obtained by our scheme

As stated in the Introduction, our study for the dynamic boundary condition differs from previous studies for non-dynamical boundary conditions such as the Neumann boundary condition. Since there is a term of the time derivative on the boundary, it is natural that the long-time behavior of the solution to (5.1)–(5.2) with (5.5) and (5.118) may differ from that to (5.1)–(5.2) with the homogeneous Neumann boundary conditions for the order parameter and the chemical potential. In order to assure that the difference occurs, we present the computation example of our structure-preserving scheme for (5.1)–(5.2) with the Neumann boundary conditions (see next subsection for details).

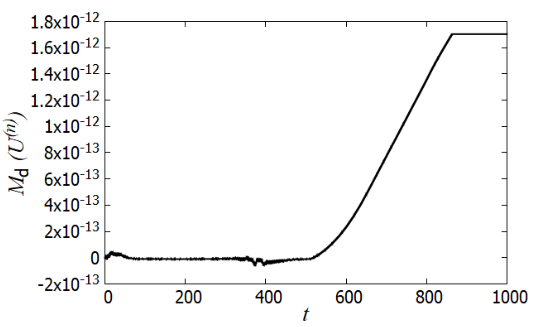

Figure 5.14: Time development of $M_{\rm d}(\boldsymbol{U}^{(n)})$ obtained by our scheme: $M_{\rm d}(\boldsymbol{U}^{(n)})$ does not change by about 11 orders of magnitude

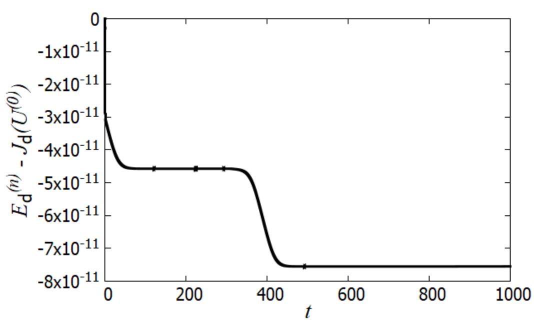

Figure 5.15: Time development of $E_{\rm d}^{(n)} - J_{\rm d}(\boldsymbol{U}^{(0)})$ obtained by our scheme: $E_{\rm d}^{(n)}$ does not change by about 10 orders of magnitude

Next, we confirm the conservative property and the dissipative property. Figure 5.14 shows the time development of $M_{\mathrm{d}}(\boldsymbol{U}^{(n)})$ obtained by our scheme. Figure 5.15 shows the time development of $E_{\mathrm{d}}^{(n)} - J_{\mathrm{d}}(\boldsymbol{U}^{(0)})$ obtained by our scheme. These graphs show that the quantities $M_{\mathrm{d}}(\boldsymbol{U}^{(n)})$ and $E_{\mathrm{d}}^{(n)}$ are conserved numerically. More precisely, $M_{\mathrm{d}}(\boldsymbol{U}^{(n)})$ does not change by about 11 orders of magnitude, and $E_{\mathrm{d}}^{(n)}$ does not change by about 10 orders of magnitude. From the above, we can obtain the expected results.

6.4 Computation example 4 (Numerical results for the Neumann boundary condition)

In order to verify that the difference in the long-time behavior of the solution occurs, we present the computation example for (5.1)–(5.2) with the following homogeneous Neumann boundary conditions:

$$\begin{cases} \partial_x u(x,t)|_{x=0} = \partial_x u(x,t)|_{x=L} = 0 & \text{in } (0,\infty), \\ \partial_x p(x,t)|_{x=0} = \partial_x p(x,t)|_{x=L} = 0 & \text{in } (0,\infty), \end{cases} \tag{5.119}$$

in the same setting as Computation example 3. We remark that the solution of (5.1)–(5.2) with (5.119) also satisfies the conservative property (5.9) and the dissipative property. However, in this case, the dissipative property is slightly different from (5.10). More precisely, the solution of (5.1)–(5.2) with (5.119) satisfies the following dissipative property:

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

Since there is no result in the same setting as Computation example 3 in previous studies, we carry out the numerical computation by the following structure-preserving scheme. By using DVDM (see [31]), the scheme is derived as follows:

$$\begin{aligned} \frac{U_k^{(n+1)} - U_k^{(n)}}{\Delta t} &= \delta_k^{\langle 2\rangle} P_k^{(n)} \quad (k = 0,\ldots,K,\ n = 0,1,\ldots), \\ P_k^{(n)} &= -\gamma \delta_k^{\langle 2\rangle}\left(\frac{U_k^{(n+1)} + U_k^{(n)}}{2}\right) + \frac{dF}{d(U_k^{(n+1)}, U_k^{(n)})} \quad (k = 0,\ldots,K,\ n = 0,1,\ldots), \\ \delta_k^{\langle 1\rangle} U_k^{(n)} &= 0 \quad (k = 0, K,\ n = 0,1,\ldots), \\ \delta_k^{\langle 1\rangle} P_k^{(n)} &= 0 \quad (k = 0, K,\ n = 0,1,\ldots). \end{aligned}$$

Figure 5.16 shows the time development of the solution obtained by the above scheme.

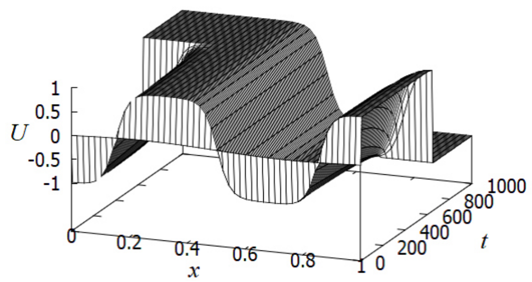

Figure 5.16: Numerical solution to (5.1)–(5.2) with (5.119) obtained by the discrete variational derivative scheme

As shown in Figure 5.13 and Figure 5.16, the solution to (5.1)–(5.2) with (5.119) arrives at a different state from that to (5.1)–(5.2) with (5.5) and (5.118). Thus, the results assure that the difference in the long-time behavior of the solution occurs.

Next, Figure 5.17 shows the time development of $M_{\mathrm{d}}(\boldsymbol{U}^{(n)})$ obtained by the above scheme. Figure 5.18 shows the time development of $A_{\mathrm{d}}^{(n)} - \bar{J}_{\mathrm{d}}(\boldsymbol{U}^{(0)})$ obtained by the above scheme, where

$$A_{\mathrm{d}}^{(n)} := \bar{J}_{\mathrm{d}}(\boldsymbol{U}^{(n)}) + \sum_{l=0}^{n-1} \sum_{k=0}^{K}{}'' \frac{\left|\delta_k^+ P_k^{(l)}\right|^2 + \left|\delta_k^- P_k^{(l)}\right|^2}{2} \Delta x \Delta t \quad (n = 1, 2, \ldots),$$

$$\bar{J}_{\mathrm{d}}(\boldsymbol{U}^{(n)}) := \sum_{k=0}^{K}{}'' \left\{ \frac{\gamma}{2} \frac{\left|\delta_k^+ U_k^{(n)}\right|^2 + \left|\delta_k^- U_k^{(n)}\right|^2}{2} + F(U_k^{(n)}) \right\} \Delta x \quad (n = 0, 1, \ldots).$$

Remark 5.6. For any $\{f_k\}_{k=-1}^{K+1} \in \mathbb{R}^{K+3}$ satisfying the discrete homogeneous Neumann boundary condition $\delta_k^{\langle 1 \rangle} f_k = 0$ $(k = 0, K)$, the following equality holds:

$$\sum_{k=0}^{K}{}'' \frac{|\delta_k^+ f_k|^2 + |\delta_k^- f_k|^2}{2} \Delta x = \sum_{k=0}^{K-1} |\delta_k^+ f_k|^2 \Delta x.$$

From this equality, we obtain $\bar{J}_{\mathrm{d}}(\boldsymbol{U}^{(n)}) = J_{\mathrm{d}}(\boldsymbol{U}^{(n)})$ $(n = 0, 1, \ldots)$.

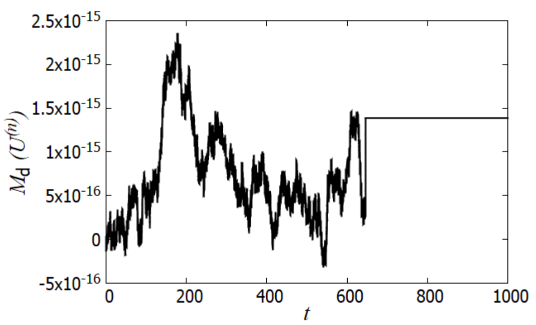

Figure 5.17: Time development of $M_{\mathrm{d}}(\boldsymbol{U}^{(n)})$ obtained by the discrete variational derivative scheme: $M_{\mathrm{d}}(\boldsymbol{U}^{(n)})$ does not change by about 14 orders of magnitude

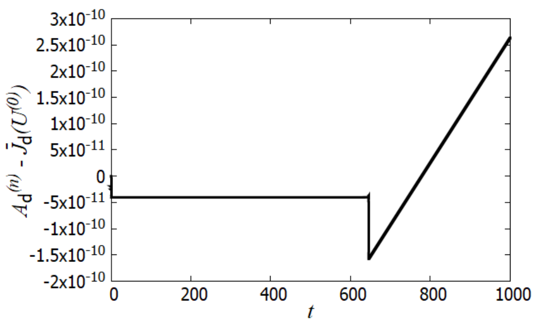

Figure 5.18: Time development of $A_{\mathrm{d}}^{(n)} - \bar{J}_{\mathrm{d}}(\boldsymbol{U}^{(0)})$ obtained by the discrete variational derivative scheme: $A_{\mathrm{d}}^{(n)}$ does not change by about 9 orders of magnitude

These graphs show that the quantities $M_{\mathrm{d}}(\boldsymbol{U}^{(n)})$ and $A_{\mathrm{d}}^{(n)}$ are conserved numerically. More precisely, $M_{\mathrm{d}}(\boldsymbol{U}^{(n)})$ does not change by about 14 orders of magnitude, and $A_{\mathrm{d}}^{(n)}$ does not change by about 9 orders of magnitude.

Chapter 6

Summary

We have designed structure-preserving schemes for the Allen–Cahn equation and the Cahn–Hilliard equation by the discrete variational derivative method and then have analyzed schemes.

First, we have proposed a structure-preserving scheme for a non-local Allen–Cahn equation. Our proposed scheme retains the mass conservation and the energy dissipation in a discrete sense. Additionally, we have obtained the results of the stability, the solvability, and the error estimate for the scheme. In particular, we have rigorously proved that our scheme is second-order accurate in space and time, respectively, in the sense of the discrete L^2-norm. Also, through computational examples, we confirm that the solution obtained by our proposed scheme is more reliable than that by the Crank–Nicolson scheme when the time mesh size is coarse.

Next, by modifying the discretization of energy from the conventional ones and using the suitable summation-by-parts formula, we have designed a structure-preserving scheme for the Allen–Cahn equation under a dynamic boundary condition, where the boundary condition is approximated by a standard central difference. Moreover, we have obtained the results of the stability, the solvability, and the error estimate for the scheme. Especially, we show the solvability of our proposed scheme under only the smallness assumption of the time mesh size without any space mesh size restriction by using the energy method. Furthermore, we prove that our scheme is second-order accurate in space and time, respectively, in the sense of the discrete L^∞-norm. Besides, through numerical computations, we confirm that the long-time behavior of the solution under a dynamic boundary condition may differ from that under the Neumann boundary condition.

Lastly, in the same manner, as the design of the scheme for the Allen–Cahn equation with a dynamic boundary condition, we have proposed a structure-preserving difference scheme for the Cahn–Hilliard equation with a dynamic boundary condition. Moreover, even in this case, we have shown the stability, the solvability, and the error estimate for the scheme. Especially, we have shown that our proposed scheme is second-order accurate in space, although the previous structure-preserving scheme by Fukao–Yoshikawa–Wada is first-order accurate in space. Also, through computation examples, we have confirmed that we can obtain a valid numerical solution by our proposed scheme even when the space mesh size is coarse. Additionally, as in the case of the Allen–Cahn equation, we confirm that the long-time behavior of the solution under a dynamic boundary condition may differ from that under the Neumann boundary condition through computation examples.

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Appendix A

Program codes

In this appendix, we note down three program codes for solving proposed structure-preserving schemes in this thesis. The first is an algorithm for solving the scheme for the Allen–Cahn equation with a non-local term. The second is an algorithm for solving the scheme for the Allen–Cahn equation under a dynamic boundary condition. The third is an algorithm for solving the scheme for the Cahn–Hilliard equation with a dynamic boundary condition. The computer language used is Julia (Version 1.4.1). We use the package "NLsolve" in Julia to obtain the next time-step for the numerical solutions to the schemes.

§1 A structure-preserving scheme for a non-local Allen–Cahn equation

```
const L = 1.0
const K = 100
const \Delta x = L/K
const \Delta t = 2.0e-4
const \varepsilon =0.02

function u0(x)
    A0 = 8; A1 = 7;
    B0 = 11;
    C0 = 0.26; C1 = 0.07; C2 = 0.41; C3 = 0.24
    return C0 + C1*cos(A0*\pi*x) + C2*sin((B0/2)*\pi*x) + C3*cos(
        A1*\pi*x)
end

function d2(u)
    v = similar(u)
    v[1] = ( 2*(u[2] - u[1]) )/(\Delta x^2)

    for k in 2:K
        v[k] = (u[k+1] -2*u[k] + u[k-1])/(\Delta x^2)
    end

    v[K+1] = ( 2*(u[K] - u[K+1]) )/(\Delta x^2)

    return v
end

function S(u)
    S = sum(u)
    S = S - 0.5*(u[1] + u[K+1])
    return \Delta x*S
end

function \delta G(up,u::Array{Float64,1})
   return -\varepsilon*d2( (up + u)/2 ) - (2/\varepsilon)*( (up +
        u)/2 ) + (2/\varepsilon)*( ( (up.^3) + ((up.^2).*u) + (up
       .*(u.^2)) + (u.^3) )/4 )
end

function \lambda (up,u::Array{Float64,1})
    I_1 = S( \delta G(up,u) )
    return ( 1/(\varepsilon *L) )*I_1
end

function scheme(vp,v)
    return vp - v + (\Delta t/\varepsilon)*\delta G(vp,v) - \
        Delta t*\lambda(vp,v)
end

using NLsolve
function nls(func, params...; ini = [0.0])
    if typeof(ini) <: Number
        r = nlsolve((vout,vin)->vout[1]=func(vin[1],params...), [
            ini])
        v = r.zero[1]
    else
        r = nlsolve((vout,vin)->vout .= func(vin,params...), ini)
        v = r.zero
    end
    return v, r.f_converged
end

u = zeros(K+1)
for k in 1:K+1
    u[k]=u0((k-1)*\Delta x)
end
u_sq = u

using ProgressMeter
@showprogress for n in 1:10000
    global u, u_sq
    u = nls(scheme,u,ini=u)[1]
    u_sq = hcat(u_sq,u)
end
```

§2 A structure-preserving scheme for the Allen–Cahn equation with a dynamic boundary condition

```
const L = 1.0
const K = 100
const \Delta x = L/K
const \Delta t = 1.0/10000
const \varepsilon_ex = 10
const \gamma = 100

A0 = 5
A1 = 8
A2 = 2
B0 = 0.02
B1 = -0.05
B2 = -0.008
B3 = 0.01

function u0(x)
    return B0 + B1*cos(A0*\pi*x) + B2*sin(A1*\pi*x) + B3*cos(A2*\
        pi*x)
end

function d2(u)
    v = similar(u[2:K+2])
    for k in 2:K+2
        v[k-1] = (u[k+1] - 2*u[k] + u[k-1])/(\Delta x^2)
    end
    return v
end

function dF(U,V)
    return \gamma*(- 0.5*(U + V) + 0.25*( (U.^3) + (U.^2).*V + U
        .*(V.^2) + (V.^3) ) )
end

function \delta G(up,u)
    return -d2( (up + u)/2 ) + dF(up[2:K+2],u[2:K+2])
end

function scheme(up, u)
    r = similar(up)

    r[1] = \varepsilon_ex*(up[2] - u[2]) + 0.25*\Delta t*(- (1/\
        Delta x) )*(up[3] + u[3] - up[1] - u[1]) + dF(up[2],u[2]))
    r[2:K+2] = up[2:K+2] - u[2:K+2] + \Delta t*\delta G(up,u)

    r[K+3] = \varepsilon_ex*(up[K+2] - u[K+2]) + 0.25*\Delta t*(
        1/\Delta x )*(up[K+3] + u[K+3] - up[K+1] - u[K+1]) + dF(up
        [K+2],u[K+2]))

    return r
end

using NLsolve
function nls(func, params...; ini = [0.0])
    if typeof(ini) <: Number
        r = nlsolve((vout,vin)->vout[1]=func(vin[1],params...), [
            ini])
        v = r.zero[1]
    else
        r = nlsolve((vout,vin)->vout .= func(vin,params...), ini)
        v = r.zero
    end
    return v, r.f_converged
end

u = zeros(K+3)
for k in 1:K+3
    u[k] = u0((k-2)*\Delta x)
end
u_sq = u

using ProgressMeter
@showprogress for n in 1:6000
    global u, u_sq
    u = nls(scheme,u,ini=u)[1]
    u_sq = hcat(u_sq,u)
end
```

§3 A structure-preserving scheme for the Cahn–Hilliard equation with a dynamic boundary condition

```
const L = 20
const K = 40
const \Delta x = L/K
const N = 20000
const T = 400
const \Delta t = T/N
const \gamma = 2.0

function u0(x)
    return 0.01*cos(0.5*\pi*x)
end

function d2(u)
    v = similar(u)
    v[1] = 2*(u[2] - u[1])/(\Delta x^2)
    for k in 2:K
        v[k] = (u[k+1] - 2*u[k] + u[k-1])/(\Delta x^2)
    end
    v[K+1] = 2*(u[K] - u[K+1])/(\Delta x^2)
    return v
end

function dF(U,V)
    return - 0.5*(U + V) + 0.25*( (U.^3) + (U.^2).*V + U.*(V.^2)
        + (V.^3) )
end

function P(up,u)
    v = similar(up)
    v = -\gamma*d2( (up + u)/2 ) + dF(up,u)
    v[1] += ( (2*\gamma)/(\Delta x*\Delta t) )*(up[1] - u[1])
    v[K+1] += ( (2*\gamma)/(\Delta x*\Delta t) )*(up[K+1] - u[K
        +1])
    return v
end

function scheme(up, u)
    return up - u - \Delta t*d2( P(up,u) )
end

using NLsolve
function nls(func, params...; ini = [0.0])
    if typeof(ini) <: Number
        r = nlsolve((vout,vin)->vout[1]=func(vin[1],params...), [
            ini])
        v = r.zero[1]
    else
        r = nlsolve((vout,vin)->vout .= func(vin,params...), ini)
        v = r.zero
    end
    return v, r.f_converged
end

u = zeros(K+1)
for k in 1:K+1
    u[k] = u0((k - 1)*\Delta x)
end
u_sq = u

using ProgressMeter
@showprogress for n in 1:N
    global u, u_sq
    u = nls(scheme,u,ini=u)[1]
    u_sq = hcat(u_sq,u)
end
```