Numerical Simulation for Nonlinear Partial Differential Equation with Variable Coefficients by Means of The Discrete Variational Method *

Takanori Ide
Product Engineering Department No.1, AISIN AW CO. LTD.
Anjo, Japan. and
Department of Mathematics, Tokyo Metropolitan University
Hachioji, Japan. *E-mail: tide@comp.metro-u.ac.jp*

Masami Okada
Department of Mathematics, Tokyo Metropolitan University
Hachioji, Japan. *E-mail: moka@comp.metro-u.ac.jp*

Abstract

Partial differential equations with variable coefficients involving discontinuous case play an important part in engineering, physics and ecology. In this paper, we will study nonlinear partial differential equations with variable coefficients arised from population models. Generally speaking, it is hard to analyze the behavior of nonlinear partial differential equations, therefore we usually rely on the numerical approximation. Currently, there is an increasing interest in designing numerical schemes that preserve invariants for differential equations. We will design the numerical schemes that preserve energy property and give conjectures for our target equation.

1 Introduction

The main purpose of this paper is to investigate the numerical solutions of nonlinear partial differential equation with variable coefficients arised from population model [1]. The variable coefficients of our equation involve the discontinuous case. Therefore, we think that the behavior of solution rapidly changes around the neighborhood of the discontinuous point. Rannacher has already studied the finite element solution of diffusion problem with irregularities in the initial or boundary data [30].

These days, many works exist concerning for designing of structure preserving numerical schemes for ordinary differential equations [5], [13], [15], [19], [22], [23], [24], [31], [33], [34] (and their references) and partial differential equations [6], [16], [21], [29], [32] (and their references).

Recently, Furihata and Mori proposed *the discrete variational method* which is an exact discretization of the continuous variational method [9], [10], [11]. This method is one procedure for designing finite difference scheme preserving energy properties such as energy dissipation, energy conservation and so on [17]. Matsuo and others expanded the discrete variational method to complex valued problem [25]. They also expanded this method to designing spatially accurate schemes under periodic conditions [26].

In this paper, we will design the finite difference scheme for nonlinear partial differential equation with variable coefficients that Furihata and Matsuo did not consider by means of the discrete variational method.

The contents of this paper are as follows : In section 2, we will define the notation of the discrete symbols and their calculus employed throughout this paper. In section 3, we will describe the relationship between the continuous variational derivative and the discrete variational derivative [9], [10] [11]. In section 4, we

*AMS Subject Classification: 35-04, 35K55, 37K05, 65M06 will show the partial differential equation that we analyze in this paper and its energy property. We will also derive the finite difference scheme for nonlinear partial differential equation with variable coefficients that preserve energy property. In section 5, we will show our target equation. In section 6, we will prove the stability and unique existence of numerical solution that we propose in section 5. Finally, we will demonstrate the numerical simulation. We will also give conjectures of our target equation.

2 Notations and preliminaries

In this section, we define the one-dimensional discrete operators. Let $\Omega = [a, b]$ and the mesh size with respect to x is defined by

$$\Delta x \stackrel{def}{=} \frac{b-a}{N}. \tag{1}$$

We denote by f_k a numerical value supposed to be an approximation of $f(a + k\Delta x)$, $k = 0, 1, \cdots, N$

$$f_k \simeq f(a + k\Delta x), \quad \boldsymbol{f} = \{f_k\}_{k=0}^{N} \in \boldsymbol{R}^{N+1}. \tag{2}$$

Difference operators
We define the difference operators as follows :

$$\delta_k^+ f_k \stackrel{def}{=} \frac{f_{k+1} - f_k}{\Delta x}, \tag{3}$$

$$\delta_k^- f_k \stackrel{def}{=} \frac{f_k - f_{k-1}}{\Delta x}, \tag{4}$$

$$\delta_k^{(1)} f_k \stackrel{def}{=} \frac{f_{k+1} - f_{k-1}}{2\Delta x}, \tag{5}$$

$$\delta_k^{(2)} f_k \stackrel{def}{=} \frac{f_{k+1} - 2f_k + f_{k-1}}{(\Delta x)^2}. \tag{6}$$

2.1 Other discrete operators

We define the shift operators and averaging operators in this subsection.
Shift operators
The shift operators are defined as follows :

$$s_k^+ f_k \stackrel{def}{=} f_{k+1}, \tag{7}$$

$$s_k^- f_k \stackrel{def}{=} f_{k-1}, \tag{8}$$

$$s_k^{(1)} f_k \stackrel{def}{=} \frac{s_k^+ + s_k^-}{2}. \tag{9}$$

Averaging operators
We define the averaging operators by using shift operators as follows :

$$\mu_k^+ \stackrel{def}{=} \frac{1}{2}(s_k^+ + 1), \tag{10}$$

$$\mu_k^- \stackrel{def}{=} \frac{1}{2}(s_k^- + 1), \tag{11}$$

$$\mu_k^{(1)} \stackrel{def}{=} \frac{\mu_k^+ + \mu_k^-}{2} = \frac{1 + s_k^{(1)}}{2}. \tag{12}$$

2.2 Summation

As the discretization of the integral, we adopt the periozoidal rule $\sum_{k=0}^{N}{}''$ that is defined by

$$\sum_{k=0}^{N}{}'' f_k \Delta x \stackrel{def}{=} \left(\frac{1}{2}f_0 + \sum_{k=0}^{N-1} f_k + \frac{1}{2}f_N\right)\Delta x. \tag{13}$$

Summation by parts with periozoidal rule

The following is the discretization of the integral by parts formula in usual calculus for two sequences

$$\sum_{k=0}^{N}{}'' f_k(\delta_k^+ g_k)\Delta x + \sum_{k=0}^{N}{}''(\delta_k^- f_k)g_k\Delta x = \left[\frac{f_k(s_k^+ g_k) + (s_k^- f_k)g_k}{2}\right]_{k=0}^{N} \tag{14}$$

where $\boldsymbol{f} = \{f_k\}_{k=0}^{N}, \boldsymbol{g} = \{g_k\}_{k=0}^{N} \in \boldsymbol{R}^{N+1}$ and g_k is an approximation of $g(a + k\Delta x)$.
Remark : The discrete operators with respect to t are defined in the same manner with f^n corresponding to $f(n\Delta t)$,$n = 0, 1, 2, \cdots$.

3 The discrete variational method

In this section, we give a brief description of our method as it applies to the partial differential equations that concerns us here. The discrete variational method is an exact discretization of the usual continuous variational method. We will summarize the definition of the discrete variational derivative [10].

We will recall the continuous variational method briefly. Firstly, we define the energy as follows

$$J[u] \overset{def}{=} \int_a^b G(u, u_x)dx, \tag{15}$$

where we call $G(u, u_x)$ the energy function in this paper.
By the usual variational argument, we have

$$J[u + \delta u] - J[u] \simeq \int_a^b \frac{\delta G}{\delta u}\delta u dx + \left[\frac{\partial G}{\partial u_x}\delta u\right]_a^b, \tag{16}$$

where $\frac{\delta G}{\delta u}$ is the Euler-Lagrange variational derivative defined by

$$\frac{\delta G}{\delta u} \overset{def}{=} \frac{\partial G}{\partial u} - \frac{\partial}{\partial x}\frac{\partial G}{\partial u_x}. \tag{17}$$

From now on, we will discretize the variational derivative in an exact manner. Firstly, the discrete energy is defined by

$$J_d[\boldsymbol{U}] \quad = \quad \sum_{k=0}^{N}{}'' G_d(U_k)\Delta x, \quad \boldsymbol{U} = \{U_k\}_{k=0}^{N} \in \boldsymbol{R}^{N+1}, \tag{18}$$

where $G_d(U_k)$ corresponds to an approximation to $G(u, u_x)$ at $x = k\Delta x$. $G_d(U_k)$ takes the following form

$$G_d(U_k) = \sum_{l=1}^{m} f_l(U_k)g_l^+(\delta_k^+ U_k)g_l^-(\delta_k^- U_k), \tag{19}$$

where $m \in \mathbf{Z}^+$ and f_l, g_l^+, g_l^- : $\mathbf{R} \to \mathbf{R}$ are differential functions. Secondly, we rewrite U_k and V_k as the discretization for $u + \delta u$ and u as follows

$$\boldsymbol{U} \quad = \quad \{U_k\}_{k=0}^{N} \in \boldsymbol{R}^{N+1}, \tag{20}$$
$$\boldsymbol{V} \quad = \quad \{V_k\}_{k=0}^{N} \in \boldsymbol{R}^{N+1}. \tag{21}$$

Then we define the discrete variational derivative $\frac{\delta G_d}{\delta(U_k,V_k)}$ as follows

$$\frac{\delta G_d}{\delta(U_k, V_k)} \overset{def}{=} \sum_{l=1}^{m}\Bigg(\frac{df_l}{d(U_k, V_k)}\frac{g_l^+(\delta_k^+ U_k)g_l^-(\delta_k^- U_k) + g_l^+(\delta_k^+ V_k)g_l^-(\delta_k^- V_k)}{2} - \delta_k^+ W_l^-(U_k, V_k) - \delta_k^- W_l^+(U_k, V_k)\Bigg), \tag{22}$$

where

$$W_l^{\pm}(U_k, V_k) = \left(\frac{f_l(U_k) + f_l(V_k)}{2}\right)\left(\frac{g_l^{\mp}(\delta_k^{\mp} U_k) + g_l^{\mp}(\delta_k^{\mp} V_k)}{2}\right)\frac{dg_l^{\pm}}{d(\delta_k^{\pm} U_k, \delta_k^{\pm} V_k)} \tag{23}$$

and

$$\frac{df}{d(a,b)} \stackrel{def}{=} \begin{cases} \frac{f(b)-f(a)}{b-a} & : \quad a \neq b, \\ \frac{df}{da} & : \quad a = b. \end{cases} \tag{24}$$

We apply the summation by parts formula to the difference $J_d[\boldsymbol{U}] - J_d[\boldsymbol{V}]$ to obtain

$$J_d[\boldsymbol{U}] - J_d[\boldsymbol{V}] = \sum_{k=0}^{N}{}'' \frac{\delta G_d}{\delta(U_k, V_k)}(U_k - V_k)\Delta x + \left[\frac{\partial G_d}{\partial \delta(U_k, V_k)}\right]_0^N, \tag{25}$$

where

$$\begin{aligned} \frac{\partial G_d}{\partial \delta(U_k, V_k)} \stackrel{def}{=} \frac{1}{2}\sum_{l=1}^{m}\Bigg(& W_l^{+}(U_k, V_k)s_k^{+}(U_k - V_k) + W_l^{-}(U_k, V_k)s_k^{-}(U_k - V_k) \\ & + (s_k^{+} W_l^{-}(U_k, V_k) + s_k^{-} W_l^{+}(U_k, V_k))(U_k - V_k)\Bigg). \end{aligned} \tag{26}$$

Therefore, we can regard (25) as a discrete analogue of (16).

Thus we get finite difference scheme that inherits energy properties, such as energy dissipation, energy conservation law and energy non-decreasing property [10], [17], [25].

4 Partial differential equation and its finite difference scheme by means of the discrete variational method

4.1 Partial differential equations and its corresponding the energy property

The purpose of this section is to show the energy properties of partial differential equations. Our target equation is written by the Euler–Lagrange derivative as follows,

$$\begin{cases} \frac{\partial u}{\partial t} & = & -\frac{\delta G}{\delta u} \\ \frac{\delta G}{\delta u} & : & \text{variational derivative} \\ G(u, u_x) & : & \text{energy function.} \end{cases} \tag{27}$$

This partial differential equation (27) has the energy dissipation property. We assume that the partial differential equation satisfies the boundary condition

$$\left[\frac{\partial G}{\partial u_x}\frac{\partial u}{\partial t}\right]_a^b = 0, \tag{28}$$

which is implied e.g. by the Neumann boundary condition.

4.2 Energy dissipation property

We have the following theorem for the partial differential equation (27) under the boundary condition (28).

Theorem 4.1 (Energy dissipation property)
Let u be a solution of (27) *with boundary condition* (28)*. Then the energy $\int_a^b G(u, u_x)dx$ is dissipation with respect to t. Namely,*

$$\frac{d}{dt}\int_a^b G(u, u_x)dx \leq 0. \tag{29}$$

Proof.

$$\begin{aligned}
\frac{d}{dt}\int_a^b G(u,u_x)dx &= \int_a^b \left(\frac{\partial G}{\partial u}\frac{\partial u}{\partial t} + \frac{\partial G}{\partial u_x}\frac{\partial u_x}{\partial t}\right)dx \\
&= \int_a^b \frac{\partial G}{\partial u}\frac{\partial u}{\partial t}dx + \left[\frac{\partial G}{\partial u_x}\frac{\partial u}{\partial t}\right]_a^b - \int_a^b \frac{\partial}{\partial x}\frac{\partial G}{\partial u_x}\frac{\partial u}{\partial t}dx \\
&= \int_a^b \left(\frac{\partial G}{\partial u} - \frac{\partial}{\partial x}\frac{\partial G}{\partial u_x}\right)\frac{\partial u}{\partial t}dx + \left[\frac{\partial G}{\partial u_x}\frac{\partial u}{\partial t}\right]_a^b \\
&= \int_a^b \frac{\delta G}{\delta u}\frac{\partial u}{\partial t}dx \\
&= -\int_a^b \left(\frac{\delta G}{\delta u}\right)^2 dx \le 0.
\end{aligned}$$

4.3 The implicit finite difference scheme and its discrete energy property

For the partial differential equation (27), an implicit scheme is obtained by the discrete variational method as follows

$$\frac{U_k^{(n+1)} - U_k^{(n)}}{\Delta t} = -\frac{\delta G_d}{\delta(U_k^{(n+1)}, U_k^{(n)})}, \quad k = 0, 1, \cdots, N, n = 0, 1, \cdots \tag{30}$$

with the boundary condition

$$\left[\frac{\partial G_d}{\partial \delta(U_k^{(n+1)}, U_k^{(n)})}\right]_0^N = 0. \tag{31}$$

We can prove the discrete energy property for finite difference scheme (30).

Theorem 4.2 (Discrete energy dissipation property)
Let $U_k^{(n)}$ be a solution of (30) *with boundary condition* (31)*. Then the energy $J_d[\boldsymbol{U}^{(n)}]$ is dissipation with respect to the time step n. Namely,*

$$\begin{aligned}
\frac{1}{\Delta t}\{J_d[\boldsymbol{U}^{(n+1)}] - J_d[\boldsymbol{U}^{(n)}]\} &= \frac{1}{\Delta t}\sum_{k=0}^{N}{}'' \{G_d(U_k^{(n+1)}) - G_d(U_k^{(n)})\}\Delta x \le 0, \\
&\qquad \boldsymbol{U}^{(n)} = \{U_k^{(n)}\}_{k=0}^N \in \boldsymbol{R}^{N+1}.
\end{aligned} \tag{32}$$

Proof.

$$\begin{aligned}
\frac{1}{\Delta t}\{J_d[\boldsymbol{U}^{(n+1)}] - J_d[\boldsymbol{U}^{(n)}]\} &= \frac{1}{\Delta t}\sum_{k=0}^{N}{}'' \{G_d(U_k^{(n+1)}) - G_d(U_k^{(n)})\}\Delta x \\
&= \frac{1}{\Delta t}\sum_{k=0}^{N}{}'' \frac{\delta G_d}{\delta(U_k^{(n+1)}, U_k^{(n)})}(U_k^{(n+1)} - U_k^{(n)})\Delta x \\
&= \sum_{k=0}^{N}{}'' \frac{\delta G_d}{\delta(U_k^{(n+1)}, U_k^{(n)})}\frac{(U_k^{(n+1)} - U_k^{(n)})}{\Delta t}\Delta x \\
&= -\sum_{k=0}^{N}{}'' \left(\frac{\delta G_d}{\delta(U_k^{(n+1)}, U_k^{(n)})}\right)^2 \Delta x \le 0 \qquad .
\end{aligned}$$

5 The target equation –Nonlinear partial differential equation with variable coefficients–

In this section, we derive the finite difference scheme of nonlinear partial differential equation with variable coefficients involving discontinuous case which arized from population model of the form $u_t = du_{xx} + u^2(b(x) - u)$, where u represents the population density, d is constant of the diffusion rate and $b(x)$ describes the growth rate of the living being. If the growth rate $b(x)$ is positive, $b(x)$ means favorable habits i.e. $b(x)$ represents the easiness of living of the environment surrounding the living being. If the growth rate $b(x)$ is negative, $b(x)$ means unfavorable habits i.e. $b(x)$ represents the living being is surrounded by a harsh environment. Cantrell and Cosner have already considered the partial differential equation of the form $u_t = du_{xx} + u(b(x) - u)$ analytically [3], but the nonlinear term of this partial differential equation is different from our target equation.

5.1 The partial differential equation with variable coefficient and its energy property

We consider the nonlinear partial differential equation with variable coefficient as the following initial-boundary value problem,

$$\begin{cases} \frac{\partial u}{\partial t} & = & -\frac{\delta G}{\delta u} \quad where \\ \frac{\delta G}{\delta u} & = & d\frac{\partial^2 u}{\partial x^2} + u^2(b(x) - u) \quad in \quad \Omega, \quad t > 0, \\ \frac{\partial u}{\partial x} & = & 0 \quad on \quad \partial\Omega, \quad t > 0, \\ u(x,0) & = & \varphi(x) \geq 0, \end{cases} \tag{33}$$

which corresponds, in our formulation, to the energy function

$$G(u, u_x) = -\frac{1}{2}\left(\frac{\partial u}{\partial x}\right)^2 + \frac{b(x)}{3}u^3. \tag{34}$$

In this paper, we have assumed $\Omega = [a, b]$ and d is small constant and $b(x)$ is bounded. The total energy of this problem is given by

$$J(t) = \int_a^b G(u, u_x)dx. \tag{35}$$

And we prove the following energy property for the total energy of (33).

Theorem 5.1 (Energy dissipation property)
Let u be the solution of (33). *Then we have the following inequality which indicates the dissipation property of total energy. Namely,*

$$\frac{d}{dt}J(t) \leq 0 \tag{36}$$

5.2 The implicit finite difference scheme for target equation and its discrete energy property

5.2.1 A derivation of discrete variational derivative

In this subsection, we will calculate the discrete variational derivative for (33). We compute the solution $U_k^{(n)}$ to a discretized equation of (33), which is expected to approximate the solution $u(x,t)$ to (33) at points $(k\Delta x, n\Delta t)$,

$$U_k^{(n)} \simeq u(k\Delta x, n\Delta t), \quad k = 0, 1, \cdots, N, \quad n = 0, 1, 2, \cdots, \tag{37}$$

and b_k is expected to approximate $b(x)$ at point $k\Delta x$

$$b_k \simeq b(k\Delta x), \quad k = 0, 1, \cdots, N. \tag{38}$$

And also, we assume that b_k is bounded. We define c as

$$c \stackrel{def}{=} \max_k |b_k|, \quad k = 0, 1, \cdots, N. \tag{39}$$

A natural discretization of the energy function is

$$G_d(U_k^{(n)}) = \frac{1}{2}\frac{\left(\delta_k^+ U_k^{(n)}\right)^2 + \left(\delta_k^- U_k^{(n)}\right)^2}{2} - \frac{1}{3}b_k\left(U_k^{(n)}\right)^3 + \frac{1}{4}\left(U_k^{(n)}\right)^4, \quad \boldsymbol{U} = \{U_k\}_{k=0}^N \in \boldsymbol{R}^{N+1}. \tag{40}$$

Then the discretization of total energy is given as follows

$$J_d[\boldsymbol{U}^{(n)}] \quad = \quad \sum_{k=0}^{N}{}'' G_d\left(U_k^{(n)}\right)\Delta x, \quad \boldsymbol{U}^{(n)} = \{U_k^{(n)}\}_{k=0}^N \in \boldsymbol{R}^{N+1}. \tag{41}$$

Then the discrete variational derivative is calculated as in the following proposition.

5.1 Proposition (The discrete variational derivative method for the target equation)
We calculate the discrete variational derivative for the target equation by means of the discrete variational method under the discrete Neumann condition. Then we have

$$\begin{aligned}\frac{\delta G_d}{\delta(U_k^{(n+1)}, U_k^{(n)})} = {} & \frac{1}{2}\delta_k^{(2)}(U_k^{(n+1)} + U_k^{(n)}) - \frac{1}{3}b_k\{(U_k^{(n+1)})^2 + U_k^{(n+1)}U_k^{(n)} + (U_k^{(n)})^2\} \\ & + \frac{1}{4}\{(U_k^{(n+1)})^3 + (U_k^{(n+1)})^2 U_k^{(n)} + U_k^{(n+1)}(U_k^{(n)})^2 + (U_k^{(n)})^3\}.\end{aligned} \tag{42}$$

Proof. We can easily verify this calculation.

Therefore we get the discrete variational derivative (42).

5.2.2 An implicit scheme for target equation

From Proposition 5.1, we get the implicit finite difference scheme for (33).

$$\left\{\begin{array}{lcl} \frac{U_k^{(n+1)} - U_k^{(n)}}{\Delta t} & = & -\frac{\delta G_d}{\delta(U_k^{(n+1)}, U_k^{(n)})} \quad where \\ \frac{\delta G_d}{\delta(U_k^{(n+1)}, U_k^{(n)})} & = & \frac{d}{2}\delta_k^{(2)}\left(U_k^{(n+1)} + U_k^{(n)}\right) + \frac{1}{3}b_k\left\{\left(U_k^{(n+1)}\right)^2 + U_k^{(n+1)}U_k^{(n)} + \left(U_k^{(n)}\right)^2\right\} \\ & & \quad -\frac{1}{4}\left\{\left(U_k^{(n+1)}\right)^3 + \left(U_k^{(n+1)}\right)^2 U_k^{(n)} + U_k^{(n+1)}\left(U_k^{(n)}\right)^2 + \left(U_k^{(n)}\right)^3\right\}, \\ & & \qquad k = 0, \cdots, N, \\ \delta_k^{(1)} U_k^{(n)} & = & 0, \quad k = 0, N, \\ U_k^{(0)} & = & \varphi_k \geq 0, \quad k = 0, \cdots, N. \end{array}\right. \tag{43}$$

The next theorem is the energy dissipation property for the discretized energy function.

Theorem 5.2 (Discrete energy dissipation property)
Let $U_k^{(n)}$ be a solution of (43). *Then the total energy $J_d(U_k^{(n)})$ is dissapation with respect to the time step n. Namely,*

$$\begin{aligned}\frac{1}{\Delta t}\{J_d[\boldsymbol{U}^{(n+1)}] - J_d[\boldsymbol{U}^{(n)}]\} \quad = \quad & \frac{1}{\Delta t}\sum_{k=0}^{N}{}''\{G_d(U_k^{(n+1)}) - G_d(U_k^{(n)})\}\Delta x \leq 0, \\ & \boldsymbol{U}^{(n)} = \{U_k^{(n)}\}_{k=0}^N \in \boldsymbol{R}^{N+1}.\end{aligned} \tag{44}$$

6 Stability and the uniqueness existence of the solution for the implicit finite difference scheme

In this section, we discuss the stability and the unique existence of the solution for the implicit finite difference scheme (43).

6.1 Stability of the implicit finite difference scheme

We prove the stability for the implicit finite difference scheme (43) by the discrete Sobolev Lemma. We define the discrete Sobolev–norm as

$$\|f\|_{d-(1,2)}^2 \stackrel{def}{=} \sum_{k=0}^{N}{}''(f_k)^2\Delta x + \sum_{k=0}^{N}{}''\frac{(\delta_k^+ f_k)^2 + (\delta_k^- f_k)^2}{2}\Delta x, \quad f = (f_k)_{k=-l}^{N+1+2l} \in \boldsymbol{R}^{N+1+2l}; \quad 0 \le l. \tag{45}$$

Then we have following lemma [11].

6.1 Lemma (Discrete Sobolev Lemma)

$$\max_{0\le k\le N} \mid f_k \mid \le 2\max\left(\frac{1}{\sqrt{L}}, \sqrt{L}\right)\|f\|_{d-(1,2)}. \tag{46}$$

where $L \stackrel{def}{=} b-a$.

We recall the discrete energy dissipation property for the implicit finite difference scheme (43). The discrete dissipation property is as follows (44),

$$\sum_{k=0}^{N}{}''G_d\big(U_k^{(n+1)}\big)\Delta x - \sum_{k=0}^{N}{}''G_d\big(U_k^{(n)}\big)\Delta x \le 0.$$

6.2 Lemma *We have the following inequality for the finite difference scheme* (43).

$$\|U^{(n)}\|_{d-(1,2)} \le \sqrt{\frac{1}{\min\big(1,\frac{d}{2}\big)}\left[\sum_{k=0}^{N}{}''G_d(U_k^{(0)})\Delta x + L + \frac{1}{24}\sum_{k=0}^{N}{}''\left\{b_k^4 + 12b_k^2 + b_k(b_k^2+8)\sqrt{b_k^2+8)}\right\}\Delta x\right]}. \tag{47}$$

Proof. We have to prove under three cases.

1. $\min_k b_k \ge 0$.
2. $\min_k b_k < 0$ and $\max_k b_k < 0$.
3. $\min_k b_k < 0$ and $\max_k b_k \ge 0$.

In this paper, we prove the case 1. Similarly, we can prove 2 and 3.
From the energy dissipation property (44), we have the following inequality.

$$\begin{aligned}
\sum_{k=0}^{N}{}''G_d(U_k^{(0)})\Delta x &\ge \sum_{k=0}^{N}{}''G_d(U_k^{(n)})\Delta x \\
&\ge \sum_{k=0}^{N}{}''\left\{-\frac{b_k}{3}(U_k^{(n)})^3 + \frac{1}{4}(U_k^{(n)})^4 + \frac{d}{2}\frac{(\delta_k^+U_k^{(n)})^2 + (\delta_k^-U_k^{(n)})^2}{2}\right\}\Delta x \\
&\ge \sum_{k=0}^{N}{}''\left\{(U_k^{(n)})^2 + \frac{d}{2}\frac{(\delta_k^+U_k^{(n)})^2 + (\delta_k^-U_k^{(n)})^2}{2} - \frac{1}{24}\{b_k^4 + 12b_k^2 + 24 + b_k(b_k^2+8)\sqrt{b_k^2+8}\}\right\}\Delta x
\end{aligned}$$

$$\left(\text{since}\quad \frac{1}{4}x^4 - \frac{p}{3}x^3 \geq x^2 - \frac{1}{24}\left\{p^4 + 12p^2 + 24 + p(p^2+8)\sqrt{p^2+8}\right\},\quad p \geq 0\right)$$

$$\geq \quad \min\left(1, \frac{d}{2}\right)\|U^{(n)}\|^2_{d-(1,2)} - \sum_{k=0}^{N}{}'' \frac{1}{24}\left\{b_k^4 + 12b_k^2 + 24 + b_k(b_k^2+8)\sqrt{b_k^2+8}\right\}\Delta x$$

Then we have following inequality.

$$\|U^{(n)}\|^2_{d-(1,2)} \leq \frac{1}{\min(1,\frac{d}{2})}\left[\sum_{k=0}^{N}{}'' G_d(U_k^{(0)})\Delta x + L + \sum_{k=0}^{N}{}'' \frac{1}{24}\left\{b_k^4 + 12b_k^2 + 24 + b_k(b_k^2+8)\sqrt{b_k^2+8}\right\}\right].$$

From these two lemmas, we have the following theorem.

Theorem 6.1 (Stability of the finite difference scheme (43))
We have the following inequality which indicates the stability to the finite difference scheme (43).

$$\max_{0\leq k\leq N}|U_k^{(n)}| \leq 2\sqrt{\frac{\max(L,\frac{1}{L})}{\min(1,\frac{d}{2})}\left[\sum_{k=0}^{N}{}'' G_d(U_k^{(0)})\Delta x + L + \sum_{k=0}^{N}{}'' \frac{1}{24}\left\{b_k^4 + 12b_k^2 + 24 + b_k(b_k^2+8)\sqrt{b_k^2+8}\right\}\right]} \tag{48}$$

6.2 Unique existence of the solution for the implicit finite difference scheme

The purpose of this subsection is to show the existence of the solution for the proposed scheme (43) by Brower fixed–point theorem. And we can also prove the uniqueness of the solution through the contraction mapping argument [11].

The existence of the solution for the finite difference scheme means that we can compute successively n–th solution $U_k^{(n)}$ for $n = 1, 2, \cdots$ for given initial value $\{U_k^{(0)}; k = 0, 1, \cdots, N\}$. Therefore it suffices to show the existence of the sequence $\{U_k^{(n+1)}; k = 0, 1, \cdots, N\}$ satisfying (43).

We rewrite the finite difference scheme. Firstly, we put

$$v_k \stackrel{def}{=} U_k^{(n)} \tag{49}$$

Then (43) is reduced to

$$\frac{1}{\Delta t}\left(U_k^{(n+1)} - v_k\right) = \frac{d}{2}\delta_k^{(2)}(U_k^{(n+1)} + v_k) + Q_d(U_k^{(n+1)}, v_k) \tag{50}$$

where

$$\begin{aligned} Q_d(U_k^{(n+1)}, v_k) \quad \stackrel{def}{=} \quad & \frac{b_k}{3}\{(U_k^{(n+1)})^2 + U_k^{(n+1)}v_k + (v_k)^2\} \\ & - \frac{1}{4}\{(U_k^{(n+1)})^3 + (U_k^{(n+1)})^2 v_k + U_k^{(n+1)}v_k^2 + v_k^3\}. \end{aligned} \tag{51}$$

In order to prove the existence of the solution, we rewrite (50) as follows

$$\left(\frac{1}{\Delta t} - \frac{d}{2}\delta_k^{(2)}\right)U_k^{(n+1)} = \left(\frac{1}{\Delta t} + \frac{d}{2}\delta_k^{(2)}\right)v_k + Q_d(U_k^{(n+1)}, v_k). \tag{52}$$

Remark : Obviously, this is an implicit finite difference scheme.

Note that (52) is expressed as follows,

$$\left(\frac{1}{\Delta t}I - \frac{d}{2}D_2\right)\boldsymbol{U} = \left(\frac{1}{\Delta t}I + \frac{d}{2}D_2\right)\boldsymbol{v} + \boldsymbol{Q}_d(\boldsymbol{U}, \boldsymbol{v}), \tag{53}$$

where $\boldsymbol{U}, \boldsymbol{v} \in \boldsymbol{R}^{N+1}$ are defined by

$$\begin{aligned} \boldsymbol{U} &= (U_0, U_1, \cdots, U_N) && (54)\\ \boldsymbol{v} &= (v_0, v_1, \cdots, v_N) && (55)\end{aligned}$$

and $I \in \boldsymbol{R}^{N+1}$ is the unit matrix and D_2 is

$$D_2 = \frac{1}{(\Delta x)^2}\begin{pmatrix} -2 & 2 & 0 & & & 0 \\ 1 & -2 & 1 & 0 & & \\ 0 & 1 & -2 & 1 & & \\ & \ddots & \ddots & \ddots & \ddots & \\ & & 0 & 1 & -2 & 1 \\ 0 & & & 0 & 2 & -2 \end{pmatrix}, \tag{56}$$

under the boundary condition as in (43).
In (53), we replace the right hand side of $U_k^{(n+1)}$ by u_k $(k = 0, 1, \cdots, N)$. Then we obtain

$$\left(\frac{1}{\Delta t}I - \frac{d}{2}D_2\right)\boldsymbol{U} = \left(\frac{1}{\Delta t}I + \frac{d}{2}D_2\right)\boldsymbol{v} + \boldsymbol{Q}_d(\boldsymbol{u}, \boldsymbol{v}), \tag{57}$$

where $\boldsymbol{u} \in \boldsymbol{R}^{N+1}$ denotes

$$\boldsymbol{u} = (u_0, u_1, \cdots, u_N) \tag{58}$$

Now let $\mathcal{T}_v : \boldsymbol{u} \mapsto \boldsymbol{U}$ be a mapping defined by $\boldsymbol{U} = (\frac{1}{\Delta t}I - \frac{1}{2}D_2)^{-1}\{(\frac{1}{\Delta t}I + \frac{1}{2}D_2)\boldsymbol{v} + Q_d(\boldsymbol{u}, \boldsymbol{v})\}$. Our problem is thus reduced to show $\mathcal{T}_v$ has a unique fixed point, i.e. solution of (53). For that we use the well–known Brouwer fixed point theorem and contraction mapping principle.

We can prove the following theorems for the finite difference scheme (43). Let $\mathcal{K}$ be defined by

$$\mathcal{K} \stackrel{def}{=} \{\boldsymbol{u} \in \boldsymbol{R}^{N+1} \mid \|\boldsymbol{u}\|_2 \leq 4M\}, \tag{59}$$

where

$$\begin{aligned} M &\stackrel{def}{=} \|\boldsymbol{v}\|_2, && (60)\\ \|\boldsymbol{v}\|_2 &\stackrel{def}{=} \sqrt{\sum_{k=0}^{N}(v_k)^2}. && (61)\end{aligned}$$

Then we have the following theorem.

Theorem 6.2 (Unique existence of the solution to the proposed scheme (43))
If

$$\Delta t \leq \frac{1}{M\left(\frac{17}{2}c + \sqrt{\frac{3097}{2}M}\right)}, \tag{62}$$

then the mapping $\mathcal{T}_v : \mathcal{K} \longrightarrow \mathcal{K}$ where $\mathcal{T}_v$ is defined above has unique fixed–point in the closed ball $\mathcal{K}$.

Remark: (62) is independent of Δx.

Proof. We have to show that $\mathcal{T}_v$ has a fixed point under these two conditions.

1. $\mathcal{T}_v$ is *well–defined* for any $\boldsymbol{v}$.

2. $\mathcal{T}_v$ satisfies three conditions of Brouwer fixed–point theorem.
   (B1) $\mathcal{K}(\subset \boldsymbol{R}^{N+1})$ is a bounded convex set.
   (B2) $\mathcal{T}_v$ is mapping $\mathcal{K} \mapsto \mathcal{K}$.
   (B3) $\mathcal{T}_v$ is continuous.

Firstly, we prove 1. The matrix expression of mapping $\mathcal{T}_v$ is

$$\Big(\frac{1}{\Delta t}I - \frac{1}{2}D_2\Big)\boldsymbol{U} = \Big(\frac{1}{\Delta t}I + \frac{1}{2}D_2\Big)\boldsymbol{v} + \boldsymbol{Q}_d(\boldsymbol{u},\boldsymbol{v}),$$

where matrix D_2 is denoted by (56), whose eigenvectors are

$$\boldsymbol{x}_k \overset{def}{=} \begin{pmatrix} \cos(\frac{k}{N}\pi\cdot 0) \\ \cos(\frac{k}{N}\pi\cdot 1) \\ \cos(\frac{k}{N}\pi\cdot 2) \\ \vdots \\ \cos(\frac{k}{N}\pi\cdot (N-1)) \\ \cos(\frac{k}{N}\pi\cdot (N)) \end{pmatrix} \tag{63}$$

where corresponding eigenvalues are

$$\lambda_k \overset{def}{=} \frac{2}{(\Delta x)^2}\big\{\cos(\frac{k}{N}\pi) - 1\big\}, \tag{64}$$

i.e.

$$D_2\boldsymbol{x}_k = \lambda_k\boldsymbol{x}_k, k = 0, 1, \cdots, N. \tag{65}$$

Therefore, we get the inequality for the eigenvalues of $\frac{1}{\Delta t}I - \frac{1}{2}D_2$,

$$\frac{1}{\Delta t} - \frac{1}{2}\frac{2}{(\Delta x)^2}\big\{\cos(\frac{k}{N}\pi) - 1\big\} \geq \frac{1}{\Delta t} \tag{66}$$

which implies that $\frac{1}{\Delta t}I - \frac{1}{2}D_2$ is invertible. Therefore the mapping $\mathcal{T}_v$ is well-defined.
Secondly, we prove 2.
(B1) is tririal. Let us prove (B2).
We diagonalize the matrix D_2 by using eigenvectors of (63). Then

$$D_2 = X\Lambda X^{-1}, \tag{67}$$

where

$$X = (\boldsymbol{x}_0, \boldsymbol{x}_1, \cdots, \boldsymbol{x}_N), \tag{68}$$

$$\Lambda = \mathrm{diag}(\lambda_k). \tag{69}$$

Then the matrix expression of proposed scheme is given by

$$\begin{aligned}\boldsymbol{U} &= X\Big(\frac{1}{\Delta t}I - \frac{1}{2}\Lambda\Big)^{-1}\Big(\frac{1}{\Delta t}I + \frac{1}{2}\Lambda\Big)X^{-1}\boldsymbol{v} \\ &\quad + X\Big(\frac{1}{\Delta t}I - \frac{1}{2}\Lambda\Big)^{-1}X^{-1}\boldsymbol{Q}_d(\boldsymbol{u},\boldsymbol{v}),\end{aligned} \tag{70}$$

from which follows

$$\begin{aligned}\|\boldsymbol{U}\|_2 &\leq \|X\|_2 \cdot \Big\|\Big(\frac{1}{\Delta t}I - \frac{1}{2}\Lambda\Big)^{-1}\Big(\frac{1}{\Delta t}I + \frac{1}{2}\Lambda\Big)\Big\|_2 \cdot \|X^{-1}\|_2 \cdot \|\boldsymbol{v}\|_2 \\ &\quad + \|X\|_2 \cdot \Big\|\Big(\frac{1}{\Delta t}I - \frac{1}{2}\Lambda\Big)^{-1}\Big\|_2 \cdot \|X^{-1}\|_2 \cdot \|\boldsymbol{Q}_d(\boldsymbol{u},\boldsymbol{v})\|_2,\end{aligned} \tag{71}$$

where the matrix norm is defined by

$$\|A\|_2 = \sup_{\boldsymbol{x}\neq 0}\frac{\|A\boldsymbol{x}\|_2}{\|\boldsymbol{x}\|_2}, \quad \boldsymbol{x} \in \boldsymbol{R}^{N+1}, \tag{72}$$

and thus

$$\|\mathrm{diag}(\lambda_k)\|_2 = \max_k |\lambda_k|. \tag{73}$$

By using (73), we can estimate (71) as follows

$$\begin{aligned} \|\boldsymbol{U}\|_2 \quad \leq \quad & \|X\|_2 \cdot \max_k \left| \frac{\frac{1}{\Delta t} + \frac{1}{2}\lambda_k}{\frac{1}{\Delta t} - \frac{1}{2}\lambda_k} \right| \cdot \|X^{-1}\|_2 \cdot \|\boldsymbol{v}\|_2 \\ & + \|X\|_2 \cdot \max_k \left| \frac{1}{\frac{1}{\Delta t} - \frac{1}{2}\lambda_k} \right| \cdot \|X^{-1}\|_2 \cdot \|\boldsymbol{Q}_d(\boldsymbol{u}, \boldsymbol{v})\|_2. \end{aligned} \tag{74}$$

Here we note that

$$\max_k \left| \frac{\frac{1}{\Delta t} + \frac{1}{2}\lambda_k}{\frac{1}{\Delta t} - \frac{1}{2}\lambda_k} \right| \quad \leq \quad 1, \tag{75}$$

$$\max_k \left| \frac{1}{\frac{1}{\Delta t} - \frac{1}{2}\lambda_k} \right| \quad \leq \quad \Delta t. \tag{76}$$

Making use of these two inequalities (75) and (76), we have (77),

$$\|\boldsymbol{U}\|_2 \leq \|X\|_2 \cdot \|X^{-1}\|_2 \cdot \|\boldsymbol{v}\|_2 + \|X\|_2 \cdot \Delta t \cdot \|X^{-1}\|_2 \cdot \|\boldsymbol{Q}_d(\boldsymbol{u}, \boldsymbol{v})\|_2. \tag{77}$$

From the assumption (60), we obtain

$$\|\boldsymbol{U}\|_2 \leq \|X\|_2 \cdot \|X^{-1}\|_2 \cdot M + \|X\|_2 \cdot \Delta t \cdot \|X^{-1}\|_2 \cdot \|\boldsymbol{Q}_d(\boldsymbol{u}, \boldsymbol{v})\|_2. \tag{78}$$

Now we can estimate $\|Q_d(\boldsymbol{u}, \boldsymbol{v})\|_2$ by the assumption (59). We divide into $\|Q_d(\boldsymbol{u}, \boldsymbol{v})\|_2$ as follows,

$$Q_d(\boldsymbol{u}, \boldsymbol{v}) = Q_{d1}(\boldsymbol{u}, \boldsymbol{v}) + Q_{d2}(\boldsymbol{u}, \boldsymbol{v}), \tag{79}$$

where we define $Q_{d1}(\boldsymbol{u}, \boldsymbol{v})$ and $Q_{d2}(\boldsymbol{u}, \boldsymbol{v})$ as

$$Q_{d1}(\boldsymbol{u}, \boldsymbol{v}) \quad = \quad \frac{b_k}{3}(u_k^2 + u_k v_k + v_k^2), \tag{80}$$

$$Q_{d2}(\boldsymbol{u}, \boldsymbol{v}) \quad = \quad -\frac{1}{4}(u_k^3 + u_k^2 v_k + u_k v_k^2 + u_k^3). \tag{81}$$

We can estimate $\|\boldsymbol{Q}_{d1}(\boldsymbol{u}, \boldsymbol{v})\|_2^2$ as follows,

$$\begin{aligned} \|\boldsymbol{Q}_{d1}(\boldsymbol{u}, \boldsymbol{v})\|_2^2 \quad &= \quad \sum_{k=0}^{N} \left\{ \frac{b_k}{3}(u_k^2 + u_k v_k + v_k^2) \right\}^2 \\ &\leq \quad \sum_{k=0}^{N} \left\{ \frac{b_k}{3}\left(u_k^2 + \frac{u_k^2 + v_k^2}{2} + v_k^2\right) \right\}^2 \\ &= \quad \sum_{k=0}^{N} \left\{ \frac{b_k}{2}(u_k^2 + v_k^2) \right\}^2 \\ &\leq \quad \sum_{k=0}^{N} \left(\frac{b_k}{2} \right)^2 \left\{ (u_k^2 + v_k^2) \right\} \cdot \sum_{l=0}^{N} \left\{ (u_l^2 + v_l^2) \right\} \\ &\leq \quad \left(\frac{c}{2} \right)^2 \{(4M)^2 + M^2\}^2 \\ &= \quad \left(c\frac{17M^2}{2} \right)^2. \end{aligned}$$

Therefore we obtain

$$\|\boldsymbol{Q}_{d1}(\boldsymbol{u},\boldsymbol{v})\|_2 \leq \frac{17M^2}{2}c. \tag{82}$$

And we can estimate $\boldsymbol{Q}_{d2}(\boldsymbol{u},\boldsymbol{v})$ as follows,

$$\begin{aligned}
\|\boldsymbol{Q}_{d2}(\boldsymbol{u},\boldsymbol{v})\|_2^2 &= \sum_{k=0}^{N}\left\{\left(-\frac{1}{4}\right)(u_k^3+u_k^2v_k+u_kv_k^2+v_k^3)\right\}^2 \\
&= \left(\frac{1}{4}\right)^2\sum_{k=0}^{N}\{(u_k^2+v_k^2)(u_k+v_k)\}^2 \\
&\leq \left(\frac{1}{4}\right)^2\sum_{k=0}^{N}\left(\frac{4^2u_k^6+4^2v_k^6}{2}\right) \\
&\leq \frac{1}{2}\{\big(\sum_{k=0}^{N}u_k^2\big)^3+\big(\sum_{k=0}^{N}v_k^2\big)^3\} \\
&\leq \frac{1}{2}[\{(4M)^2\}^3+(M^2)^3] \\
&= \frac{3097}{2}M^6.
\end{aligned}$$

Therefore we obtain

$$\|\boldsymbol{Q}_{d2}(\boldsymbol{u},\boldsymbol{v})\|_2 \leq \sqrt{\frac{3097}{2}}M^3. \tag{83}$$

From (82) and (83),

$$\begin{aligned}
\|\boldsymbol{Q}_{d}(\boldsymbol{u},\boldsymbol{v})\|_2 &\leq \|\boldsymbol{Q}_{d1}(\boldsymbol{u},\boldsymbol{v})\|_2+\|\boldsymbol{Q}_{d2}(\boldsymbol{u},\boldsymbol{v})\|_2 \\
&\leq M^2\left(\frac{17}{2}c+\sqrt{\frac{3097}{2}}M\right).
\end{aligned} \tag{84}$$

We substitute (84) into (78). Then we have

$$\|\boldsymbol{U}\|_2 \leq \|X\|_2\cdot\|X^{-1}\|_2\cdot M+\|X\|_2\cdot\Delta t\cdot\|X^{-1}\|_2\cdot M^2\left(\frac{17}{2}c+\sqrt{\frac{3097}{2}}M\right). \tag{85}$$

Now we use the following estimates for $\|X\|_2$, $\|X^{-1}\|_2$ ([8],pp36)

$$\|X\|_2 \leq \sqrt{2N}, \tag{86}$$

$$\|X^{-1}\|_2 \leq \sqrt{\frac{2}{N}}. \tag{87}$$

Making use of these two inequalities (86) and (87), we can compute

$$\begin{aligned}
\|\boldsymbol{U}\|_2 &\leq 2M+2\Delta tM^2\left(\frac{17}{2}c+\sqrt{\frac{3097}{2}}M\right) \\
&= \left\{1+\Delta tM\left(\frac{17}{2}c+\sqrt{\frac{3097}{2}}M\right)\right\}2M.
\end{aligned} \tag{88}$$

Therefore we see that $\mathcal{T}_v$ is a mapping $\mathcal{K}\to\mathcal{K}$, if Δt satisfies

$$\Delta t \leq \frac{1}{M\left(\frac{17}{2}c+\sqrt{\frac{3097}{2}}M\right)}, \tag{89}$$

because of the definition of $\mathcal{K}$ (59). And thus we have proved the property (B2).
Thirdly, we prove the continuity of the mapping $\mathcal{T}_v$. This is the property of (B3).
We put $U = \mathcal{T}_v u$, $U' = \mathcal{T}_v u'$ for two vectors $\boldsymbol{u}$ and $\boldsymbol{u}'$ whose components are given respectively by

$$\begin{aligned} \boldsymbol{U} &= (U_0, U_1, \cdots, U_N), && (90) \\ \boldsymbol{U}' &= (U'_0, U'_1, \cdots, U'_N), && (91) \\ \boldsymbol{u} &= (u_0, u_1, \cdots, u_N), && (92) \\ \boldsymbol{u}' &= (u'_0, u'_1, \cdots, u'_N). && (93) \end{aligned}$$

Similarly to the estimate for (B2), we have

$$\begin{aligned} \|\boldsymbol{U} - \boldsymbol{U}'\|_2 &\leq 2\Delta t \|\boldsymbol{Q}_d(\boldsymbol{u}, \boldsymbol{v}) - \boldsymbol{Q}_d(\boldsymbol{u}', \boldsymbol{v})\|_2 \\ &\leq 2\Delta t (\|\boldsymbol{Q}_{d1}(\boldsymbol{u}, \boldsymbol{v}) - \boldsymbol{Q}_{d1}(\boldsymbol{u}', \boldsymbol{v})\|_2 + \|\boldsymbol{Q}_{d2}(\boldsymbol{u}, \boldsymbol{v}) - \boldsymbol{Q}_{d2}(\boldsymbol{u}', \boldsymbol{v})\|_2). \qquad (94) \end{aligned}$$

We can estimate $\|\boldsymbol{Q}_{d1}(\boldsymbol{u}, \boldsymbol{v}) - \boldsymbol{Q}_{d1}(\boldsymbol{u}', \boldsymbol{v})\|_2$ as follows.

$$\begin{aligned} \|\boldsymbol{Q}_{d1}(\boldsymbol{u}, \boldsymbol{v}) - \boldsymbol{Q}_{d1}(\boldsymbol{u}', \boldsymbol{v})\|_2^2 &= \sum_{k=0}^{N} \left\{ \frac{b_k}{3}(u_k - u'_k)(u_k + v_k + u'_k) \right\}^2 \\ &\leq \sum_{k=0}^{N} \left\{ \frac{c}{3}(u_k - u'_k)(u_k + v_k + u'_k) \right\}^2 \\ &\leq \sum_{k=0}^{N} \left\{ \frac{c}{3}(u_k - u'_k)(\max_k |u_k| + \max_k |v_k| + \max_k |u'_k|) \right\}^2 \\ &\leq \sum_{k=0}^{N} \left\{ \frac{c}{3}(u_k - u'_k)(4M + M + 4M) \right\}^2 \\ &= \sum_{k=0}^{N} \left(\frac{c}{3} \right)^2 (9M)^2 (u_k - u'_k)^2 \\ &= (3cM)^2 \|\boldsymbol{u} - \boldsymbol{u}'\|_2^2 \end{aligned}$$

Then we obtain

$$\|\boldsymbol{Q}_{d1}(\boldsymbol{u}, \boldsymbol{v}) - \boldsymbol{Q}_{d1}(\boldsymbol{u}', \boldsymbol{v})\|_2 \leq 3cM \|\boldsymbol{u} - \boldsymbol{u}'\|_2. \qquad (95)$$

And we can also estimate $\|\boldsymbol{Q}_{d2}(\boldsymbol{u}, \boldsymbol{v}) - \boldsymbol{Q}_{d2}(\boldsymbol{u}', \boldsymbol{v})\|_2$ as follows.

$$\begin{aligned} \|\boldsymbol{Q}_{d1}(\boldsymbol{u}, \boldsymbol{v}) - \boldsymbol{Q}_{d1}(\boldsymbol{u}', \boldsymbol{v})\|_2^2 &= \sum_{k=0}^{N} \left\{ \left(-\frac{1}{4} \right)(u_k - u'_k)\{u_k^2 + u_k u'_k + (u'_k)^2 + v_k(u_k + u'_k) + v_k^2\} \right\}^2 \\ &= \left(\frac{1}{4} \right)^2 \sum_{k=0}^{N} \left\{ (u_k - u'_k)\{u_k^2 + u_k u'_k + (u'_k)^2 + v_k(u_k + u'_k) + v_k^2\} \right\}^2 \\ &\leq \left(\frac{1}{4} \right)^2 \sum_{k=0}^{N} \left\{ (u_k - u'_k)\{(\max_k |u_k|)^2 + (\max_k |u_k|)(\max_k |u'_k|) \right. \\ &\qquad \left. + (\max_k |u'_k|)^2 + (\max_k |v_k|)(\max_k |u_k| + \max_k |u'_k|) + (\max_k |v_k|)^2\} \right\}^2 \\ &\leq \left(\frac{1}{4} \right)^2 \sum_{k=0}^{N} (u_k - u'_k)^2 \{16M^2 + 16M^2 + 16M^2 + M(8M) + M^2\}^2 \\ &\leq \left(\frac{1}{4} \right)^2 \sum_{k=0}^{N} (u_k - u'_k)^2 (57M^2)^2 \end{aligned}$$

$$= \left(\frac{57M^2}{4}\right)^2 \sum_{k=0}^{N} (u_k - u_k')^2$$
$$= \left(\frac{57M^2}{4}\right)^2 \|\boldsymbol{u} - \boldsymbol{u}'\|_2^2$$

Then we obtain

$$\|\boldsymbol{Q}_{d2}(\boldsymbol{u}, \boldsymbol{v}) - \boldsymbol{Q}_{d2}(\boldsymbol{u}', \boldsymbol{v})\|_2 \leq \frac{57M^2}{4} \|\boldsymbol{u} - \boldsymbol{u}'\|_2. \tag{96}$$

From these inequalities (95) and (96), we obtain

$$\begin{aligned}
\|\boldsymbol{U} - \boldsymbol{U}'\|_2 &\leq 2\Delta t \|\boldsymbol{Q}_d(\boldsymbol{u}, \boldsymbol{v}) - \boldsymbol{Q}_d(\boldsymbol{u}', \boldsymbol{v})\|_2 \\
&\leq 2\Delta t (\|\boldsymbol{Q}_{d1}(\boldsymbol{u}, \boldsymbol{v}) - \boldsymbol{Q}_{d1}(\boldsymbol{u}', \boldsymbol{v})\|_2 + \|\boldsymbol{Q}_{d2}(\boldsymbol{u}, \boldsymbol{v}) - \boldsymbol{Q}_{d2}(\boldsymbol{u}', \boldsymbol{v})\|_2) \\
&\leq 2\Delta t (3cM + \frac{57}{4} M^2) \|\boldsymbol{u} - \boldsymbol{u}'\|_2 \\
&= 6M\left(c + \frac{19}{4} M\right) \Delta t \|\boldsymbol{u} - \boldsymbol{u}'\|_2,
\end{aligned} \tag{97}$$

which means the mapping $\mathcal{T}_v$ is continuous. We have proved the property of (B3).
Finally, we prove the uniqueness of the solution of proposed implicit scheme.
In fact, the estimate (97) gives us condition of contraction mapping,

$$\begin{aligned}
& 6M\left(c + \frac{19}{4} M\right) \Delta t < 1 \\
\Longleftrightarrow \quad & \Delta t < \frac{1}{6M\left(c + \frac{19}{4} M\right)}.
\end{aligned} \tag{98}$$

Comparing (89) and (98), we have arrived the conclusion.

7 Numerical simulation and discussion

The purpose of this section is to show the numerical experiments and to discuss about the stable numerical solutions of our proposed scheme (43).

7.1 Numerical simulation

Let us show the numerical experiments of finite difference scheme (43). In the numerical experiments, we compute solutions to the finite difference scheme in the domain $\{(x,t) | 0 \leq x \leq 1, 0 \leq t \leq 0.015\}$ under the diffusion coefficient $d = 0.0001$.
In this paper, we consider two cases of variable coefficients of $b(x)$ and three different initial values.
Case 1.

$$b(x) = \begin{cases} 1, & 0 \leq x \leq \frac{20}{60}, \\ -1, & \frac{20}{60} \leq x \leq \frac{40}{60}, \\ 1, & \frac{40}{60} \leq x \leq 1. \end{cases} \tag{99}$$

1.
$$\varphi(x) = 0.5(1.0 - \cos(6\pi x))/2. \tag{100}$$

2.
$$\varphi(x) = \begin{cases} 0.4, & 0 \leq x \leq \frac{10}{60}, \\ 0, & \frac{11}{60} \leq x \leq 1. \end{cases} \tag{101}$$

3.

$$\varphi(x) = \begin{cases} 0, & 0 \le x \le \frac{49}{60}, \\ 0.4, & \frac{50}{60} \le x \le 1. \end{cases} \tag{102}$$

Case 2.

$$b(x) = \begin{cases} 1, & 0 \le x \le \frac{10}{60}, \\ -1, & \frac{10}{60} \le x \le \frac{50}{60}, \\ 1, & \frac{50}{60} \le x \le 1. \end{cases} \tag{103}$$

1.

$$\varphi(x) = 0.5(1.0 - \cos(6\pi x))/2. \tag{104}$$

2.

$$\varphi(x) = \begin{cases} 0.4, & 0 \le x \le \frac{6}{60}, \\ 0, & \frac{7}{60} \le x \le 1. \end{cases} \tag{105}$$

3.

$$\varphi(x) = \begin{cases} 0, & 0 \le x \le \frac{53}{60}, \\ 0.4, & \frac{54}{60} \le x \le 1. \end{cases} \tag{106}$$

7.2 Discussion

From these numerical experiments, we consider that the stable solution of partial differential equation (33) depend on variable coefficients and initial values. We assume that the variable coefficients

$$b(x) = \begin{cases} 1, & [a, \alpha] \cup [\beta, b], \\ -1, & [\alpha, \beta]. \end{cases} \tag{107}$$

Then we have conjectures as follows :

1. If $[\alpha, \beta]$ is sufficiently smaller than $[a, \alpha] \cup [\beta, b]$, then the nontrivial stable solution of (33) is

$$u \sim 1, \quad x \in [a, \alpha] \cup [\beta, b], \tag{108}$$
$$u \sim 0, \quad x \in [\alpha, \beta]. \tag{109}$$

2. If $[\alpha, \beta]$ is sufficiently longer than $[a, \alpha] \cup [\beta, b]$, then nontrivial stable solutions of (33) are

$$u \sim 1, \quad x \in [a, \alpha], \tag{110}$$
$$u \sim 0, \quad x \in [\alpha, \beta], \tag{111}$$
$$u \sim 1, \quad x \in [\beta, b] \tag{112}$$

and

$$u \sim 1, \quad x \in [a, \alpha], \tag{113}$$
$$u \sim 0, \quad x \in [\alpha, \beta], \tag{114}$$
$$u \sim 0, \quad x \in [\beta, b] \tag{115}$$

and

$$u \sim 0, \quad x \in [a, \alpha], \tag{116}$$
$$u \sim 0, \quad x \in [\alpha, \beta], \tag{117}$$
$$u \sim 1, \quad x \in [\beta, b]. \tag{118}$$

8 Conclusion

We have proposed the implicit finite difference scheme preserving energy dissipation property by means of the discrete variational method. This finite difference scheme is also stable for the sake of the discrete energy dissipation property. And this finite difference scheme has unique solution. We did not show the convergence rate of our scheme because it is hard to analyze the regularity of our target equation. We will study regularity of our target equation and the convergence rate of our finite difference scheme. In the last section, we gave conjectures of analytical stable solution of our target equation. Our conjectures state that the stable solution depends on initial values and variable coefficients. We will investigate about these conjectures analytically soon.

9 Acknowledgement

The authors would like to thank to Professors Rolf Rannacher, Daisuke Furihata, Takayasu Matsuo and Tetsuya Ishiwata for their helpful suggestions and valuable advice. And the authors also would like to thank for Professor Kazuhiro Kurata for giving this problem and Kazunaga Tanaka for simulating discussion. The first author also gives thanks to Professors Peter J. Olver, Robert I. McLachlan, Brynjulf Owren, Hans Munthe–Kaas, Elena Celledoni and AISIN AW CO., LTD.

References

[1] D.G.Aronson and H.F.Weinberger, Nonlinear diffusion in Population Genetics, Combustion, and nerve Pulse Propagation, *Partial Differential Equations and Related Topics*, Lecture Note in Mathematics 446, 5–49.

[2] R.Becker, H.Kapp and R.Rannacher, Adaptive finite element methods for optimal control of partial differential equations: basic concept. *SIAM J. Control Optim.* 39 (2000), no.1, 113–132

[3] R.S.Cantrell and C.Conser, Diffusive logistic equations with indefinite weights : population model in disrupted environments, *Proc.Roy.Soc.Edinburgh* Sect.A 112 (1989), no.3-4, 293–318.

[4] R.S.Cantrell, C.Conser and V.Hutson, Ecological models, permanence and spatial heterogenety, *Rocky Mountain J.Math.* 26.No.1.1–35. 1996.

[5] A.J.Chorin, M.F.McCracken, T.J.R.Hughes and J.E.Marsden, Product formulas and numerical algorithms. *Comm. Pure Appl. Math.* 31(1978), no.2, 205–256.

[6] Z.Fei and L.Vázquez, Two energy conserving numerical schemes for the sine-Gordon equation, *Appl.Math.Comput.*, 45(1991), 17–31.

[7] K.O.Friedrichs, Symmetric hyperbolic linear differential equations, *Comm. Pure Appl.Math.*, **7** (1954) no.1, 345–392.

[8] D.Furihata, *General Derivation of Finite Difference Schemes by Means of a Discrete Variation* (in Japanese), Doctoral Thesis(1997),University of Tokyo.

[9] D.Furihata and M.Mori, General derivation of finite difference schemes by means of a discrete variation (in Japanese), *Trans.Japan.Soc.Indust.Appl.Math.*, 8(1998) 317-340.

[10] D.Furihata, Finite difference schemes for $\frac{\partial u}{\partial t} = \left(\frac{\partial}{\partial x}\right)^{\alpha} \frac{\delta G}{\delta u}$ that inherit energy conservation or dissipation property, *J.Comput.Phys.*, 156(1999), 181–205.

[11] D.Furihata, A stable and conservative finite difference scheme for the Cahn-Hilliard equation, *Numer.Math.*, 87(2001), 675–699.

[12] I.M.Gelfand and S.V.Fomin, *Calculus of Variations*, Prentice-Hall N.J.,1963.(Dover,2000)

[13] D.Greenspan, Conservative numerical methods for $\ddot{x} = f(x)$, *J.Comput.Phys.*, 41(1984) 28–41.

[14] J. Hadamard, Sur l'intégrale résiduelle, *Bull.Soc.Math.France*, **28** (1900), 69–90.

[15] E.Hairer, C.Lubich and G.Wanner, *Geometric Numerical Integration – Structure–Preserving Algorithms for Ordinary Differential Equations –*, Springer Verlag. (2002).

[16] C.Hirota, T.ide, M.Okada and N.Fukuoka, Generalized energy integrals and energy conserving numerical schemes for partial differential equations, *to appear*

[17] T.Ide, C.Hirota and M.Okada, Generalized energy integral for $\frac{\partial u}{\partial t} = \frac{\delta G}{\delta u}$, its finite difference schemes by means of the discrete variational method and an application to Fujita problem, *to appear in Adv.Math.Sci.Appl.*

[18] T.Ide, Error estimates for the implicit finite difference scheme for the Fujita problem by means of the discrete variational method, *to appear in Far East J.Appl.Math.*

[19] Y.Ishimori, Explicit energy conservative difference schemes for nonlinear dynamical systems with at most quartic potentials, *Phys.Lett.* A191(1994), no.5-6, 373–378.

[20] T.Itoh and K.Abe, Hamiltonian–conserving discrete canonical equations based on variational difference quotients, *J.Comput.Phys.***77**(1988), 85–102.

[21] S.Li and Vu-Quoc, Finite difference calculus invariant structure of a class of algorithms for the nonlinear Klein-Gordon equation, *SIAM J.Numer.Anal.*, 32(1995), 1839–1875.

[22] S.Maeda, Symplectic Runge-Kutta methods from the viewpoint of symmetry, *J.Math.Tokushima Univ.* 34.(2000)15–22.

[23] R.I.McLachlan, G.R.W.Quispel and N.Robidoux, Geometric integration using discrete gradients, *Phil.Trans.R.Soc.Lond.* A (1999) **357**, 1027–1045.

[24] R.I.McLachlan and G.R.W.Quispel, Splitting methods, *Acta.Numerica*.11(2002), 341-434.

[25] T.Matsuo and D.Furihata, Dissipative or conservative finite difference schemes for complex-valued nonlinear partial differential equations, *J.Comput.Phys.*, 171 (2001), 425-447.

[26] T.Matsuo, D.Furihata, M.Sugihara and M.Mori, Spatially accurate dissipative or conservative finite difference schemes derived by the discrete variational method, *to appear*.

[27] K.W.Morton and D.F.Mayers, *Numerical Solution of Partial Differential Equations*, Cambridge University Press. (1994)

[28] P.J.Olver, *Application of Lie groups to Differential equations*, Second Edition, Graduate Texts in Mathematics, vol.107, Springer Verlag, New York, 1993.

[29] P.J.Olver, Geometric foundations of numerical algorithms and symmetry, *Appl.Alg.Engin. Comp.Commun.*11 (2001) 417–436.

[30] R.Rannacher, Finite element solution of diffusion problems with irregular data, *Numer.Math.* 43, (1984), 309–327.

[31] J.M.Sanz–Serna and M.P.Calvo, *Numerical Hamiltonian Problems*, Chapman and Hall, London 1994.

[32] W.Strauss and L.Vázquez, Numerical solution of nonlinear Klein-Gordon equation, *J.Comput.Phys.*, 28(1978), 271–278.

[33] J.M.Wendlandt and J.E.Marsden, Mechanical integrators derived from a discrete variational principle, *Physica D.*, 106(1997), 223–246.

[34] H.Yoshida, Constructioin of higher order symplectic numerical scheme, *Phys.Lett.***A**, 87(1990), 675–699.

Illustrations of numerical experiments of Case 1

Initial value 1.

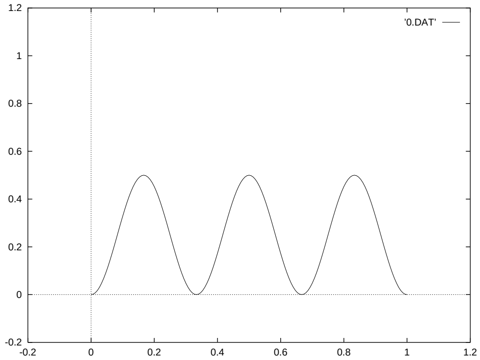

Figure 1: Initial data

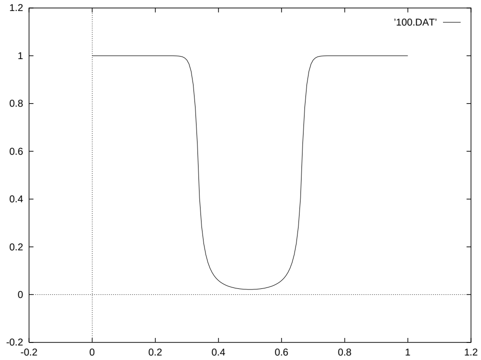

Figure 2: Stable solution

Initial value 2.

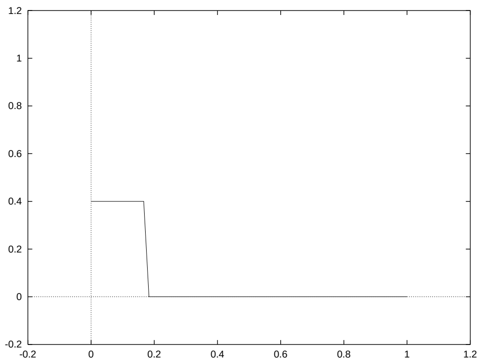

Figure 3: Initial data

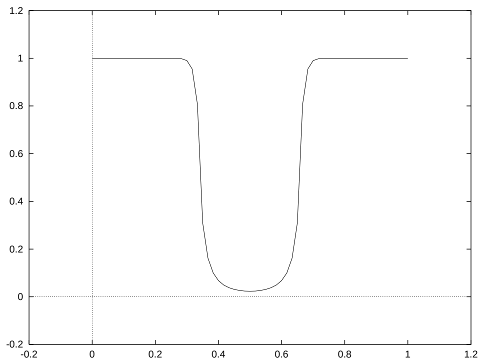

Figure 4: Stable solution

Initial value 3.

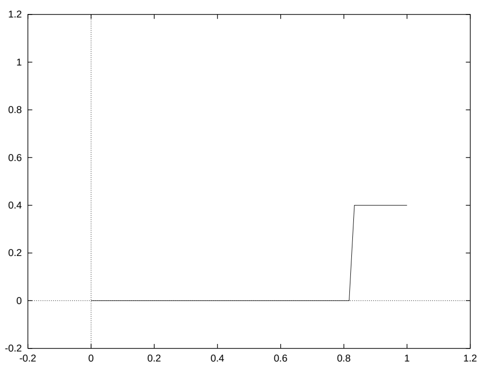

Figure 5: Initial data

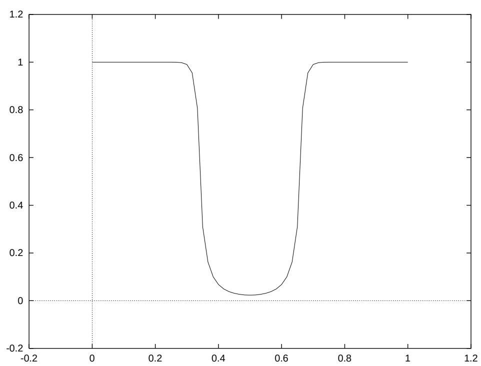

Figure 6: Stable solution

Illustrations of numerical experiments of Case 2

Initial value 1.

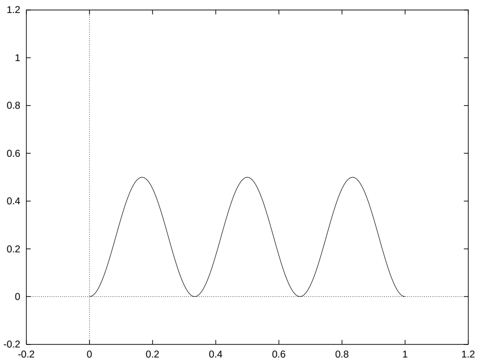

Figure 7: Initial data

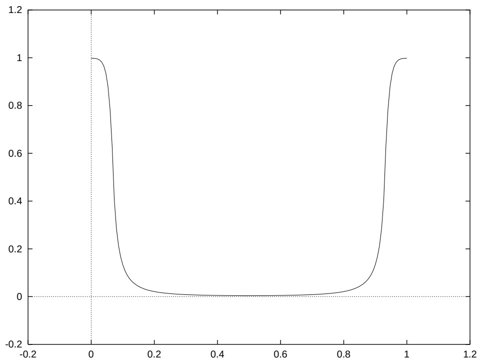

Figure 8: Stable solution

Initial value 2.

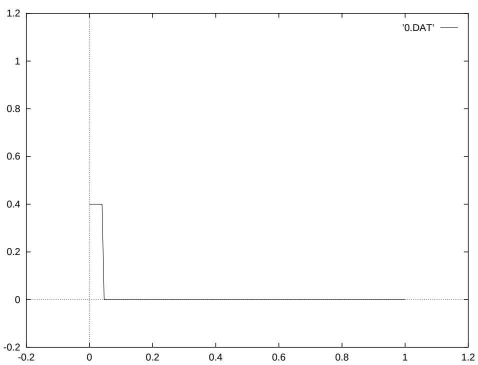

Figure 9: Initial data

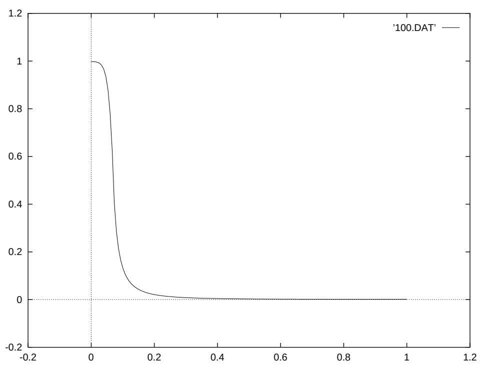

Figure 10: Stable solution

Initial value 3.

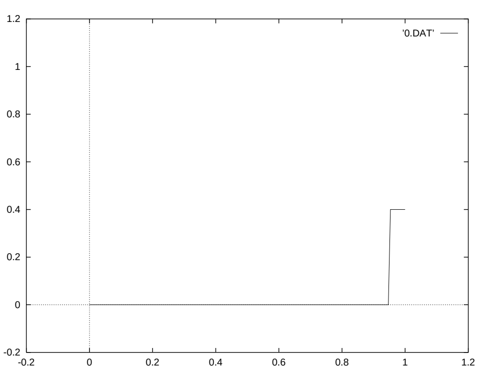

Figure 11: Initial data

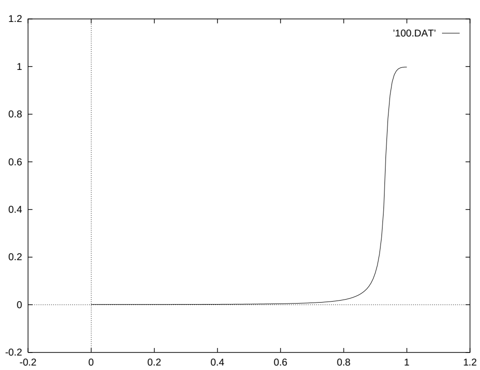

Figure 12: Stable solution