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Conservative finite difference schemes for one-dimensional nonlinear thermoelasticity

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Abstract

In this article we give some examples of structure-preserving finite difference schemes for nonlinear thermoelasticity. Here the preserved structure means that the solution for numerical schemes also satisfy the energy conservation law, the momentum conservation law and the law of increasing entropy.

1 Introduction

The dynamics of nonlinear thermoelastic deformation in the one-dimensional space is represented as the following system of partial differential equations:

$$\begin{aligned}&\partial_t^2 u = \frac{\partial^2\varphi}{\partial w^2}(w,\tau)\partial_x^2 u + \frac{\partial^2\varphi}{\partial w\partial\tau}\partial_x\tau,\\ &-\frac{\partial^2\varphi}{\partial\tau^2}\partial_t\tau - \frac{\partial^2\varphi}{\partial w\partial\tau}\partial_t\partial_x u = \frac{\partial_x^2\tau}{\tau}, \qquad x\in\mathbb{X},\ t\in(0,T],\end{aligned}$$

where unknowns u and τ are the displacement and the absolute temperature respectively, w represents a shear strain defined by $w=\partial_x u$ and a given nonlinear function φ means the Helmholtz free energy density. We assume that the domain $\mathbb{X}$, boundary and initial conditions are given suitably as mentioned later. For example, our argument works well in the case $\mathbb{X}=\mathbb{T}$, or bounded domain with the Neumann zero boundary conditions, etc. For the derivation of this model we refer the reader to [6]. We normalize all physical parameters or constants by unity. In the one-dimensional case, it is well-known (see e.g. [6]) that the system can be transformed to the first order system:

$$\partial_t w = \partial_x v,$$
$$\partial_t v = \partial_x \frac{\partial \varphi}{\partial w}(w,\tau),$$
$$-\tau \partial_t \frac{\partial \varphi}{\partial \tau}(w,\tau) = \partial_x^2 \tau.$$

If we set the energy E, the momentum M and the entropy S as follows:

$$E(w,v,\tau) := \frac{1}{2}\int_{\mathbb{X}} |v|^2 dx + \int_{\mathbb{X}} \left\{ \varphi(w,\tau) - \tau \frac{\partial \varphi}{\partial \tau}(w,\tau) \right\} dx,$$
$$M(w) := \int_{\mathbb{X}} w dx, \qquad S(w,\tau) := -\int_{\mathbb{X}} \frac{\partial \varphi}{\partial \tau}(w,\tau) dx,$$

we have

$$\frac{d}{dt}E(w,v,\tau) = \int_{\mathbb{X}} v \partial_t v dx + \int_{\mathbb{X}} \left\{ \partial_t w \frac{\partial \varphi}{\partial w} - \tau \partial_t \frac{\partial \varphi}{\partial \tau} \right\} dx = \left[v \frac{\partial \varphi}{\partial w} + \partial_x \tau \right]_{\partial \mathbb{X}},$$
$$\frac{d}{dt}M(w) = \int_{\mathbb{X}} \partial_x v dx = [v]_{\partial \mathbb{X}},$$
$$\frac{d}{dt}S(w,\tau) = \int_{\mathbb{X}} \frac{\partial_x^2 \tau}{\tau} dx = \int_{\mathbb{X}} \left| \frac{\partial_x^2 \tau}{\tau} \right|^2 dx + \left[\frac{\partial_x \tau}{\tau} \right]_{\mathbb{X}},$$

where $[\cdot]_{\mathbb{X}}$ means a boundary integral. We thus obtain the following energy conservation law, the momentum conservation law and the law of increasing entropy:

$$\frac{d}{dt}M(w) = 0, \qquad \frac{d}{dt}E(w,v,\tau) = 0, \qquad \frac{d}{dt}S(w,\tau) = \int_{\mathbb{X}} \left| \frac{\partial_x^2 \tau}{\tau} \right|^2 dx \geq 0, \tag{1.1}$$

if we assume the boundary integral terms equal to zero and $\theta > 0$. In this article we give some examples of finite difference schemes satisfying these laws in the discrete sense. In [?] and [8], the numerical simulation for this schemes is actually demonstrated.

Before discussing our results precisely, we give known related results. For the numerical analysis of nonlinear thermoelasticity, we only find the finite element analysis by S. Jiang [3], [4] and [5]. On the other hand, there seems to be no result by finite difference context. In a choice of special free energy φ the system becomes semilinear PDEs. For example if we choose

$$\varphi = \frac{1}{2}\int |v|^2 dx + \frac{1}{2}\int |\partial_x w|^2 dx + \int \left\{ w^6 - w^4 + (\tau - \tau_0) w^2 \right\} dx + \int (\tau - \tau \log \tau) dx,$$

the derived semilinear system represents a phase transition of shape memory alloys. For the background of this system we refer to [1]. For the system recently in [10],

[11], [12] and [9] the authors propose a new finite difference scheme which satisfies the discrete version of (1.1) and gives existence result of solution, and the error estimate and another existence result of solution are shown by applying the energy method given in [11]. When we consider the numerical scheme of PDEs, structure-preserving property is useful because the numerical stability is often satisfied automatically. There are several popular methods to derive these schemes systematically. For example we refer to [2]. One of advantage using structure-preserving numerical schemes is working the energy method similar to PDEs.

In particular, we remark that the existence of solution for nonlinear thermoelasticity is shown by the energy method (see e.g. [6]) under sufficiently small and smooth initial data and the structural assumptions of nonlinearity as follows:

$$\frac{\partial^2 \varphi}{\partial w^2} \geq c_0 > 0, \qquad \frac{\partial^2 \varphi}{\partial \theta^2} \leq c_1 < 0, \tag{1.2}$$

for some constants c_0 and c_1. The smallness for τ means that the perturbation of temperature from the reference temperature τ_0 is sufficiently small, namely we assume that the temperature difference $\theta = \tau - \tau_0$ is sufficiently small. For the later argument, we rewrite the equations to the one for (w, v, θ) as follows:

$$\partial_t w = \partial_x v, \tag{1.3}$$

$$\partial_t v = \partial_x \frac{\partial \varphi}{\partial w}(w, \theta + \tau_0), \tag{1.4}$$

$$-(\theta + \tau_0)\partial_t \frac{\partial \varphi}{\partial \tau}(w, \theta + \tau_0) = \partial_x^2 \theta. \tag{1.5}$$

Moreover, recently the authors in [14] show that the energy methods given in [13] works successfully also on structure-preserving numerical schemes for some quasilinear PDEs. We thus expect the existence of discrete solution for the numerical scheme and error estimate between the solution and exact solution by the energy method, although we do not mention to such a mathematical treatments here.

2 Preliminaries

We denote by ∂_t and ∂_x partial differential operators with respect to variables t and x, respectively. We split space interval $[0, L]$ into K-th parts and time interval $[0, T]$ into N-th parts, and hence the following relations hold $L = K\Delta x$ and $T = N\Delta t$. For $k = 0, 1, \ldots, K$ and $n = 0, 1, \ldots, N$ we write $w_k^{(n)} = w(k\Delta x, n\Delta t)$, $v_k^{(n)} = v(k\Delta x, n\Delta t)$ and $\theta_k^{(n)} = \theta(k\Delta x, n\Delta t)$, for short. Let $(W_k^{(n)}, V_k^{(n)}, \Theta_k^{(n)})$ be an approximate solution corresponding to the solution $(w_k^{(n)}, v_k^{(n)}, \theta_k^{(n)})$. Let us define difference operators by

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

and δ_n^+, δ_n^-, $\delta_n^{\langle 1\rangle}$ and $\delta_n^{\langle 2\rangle}$ are defined the same manner by replacing the space-variable k and Δx to the time-variable n and Δt. In this article, we approximate an integral by the trapezoidal rule

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

Let us introduce the discrete version of *integration by parts.*

Lemma 2.1 (Summation by parts [2, Propositions 3.2 and 3.3])**.** *For any vectors* $\{f_k\}_{k=-1}^{K+1}$ *and* $\{g_k\}_{k=-1}^{K+1}$ *it holds that*

$$\begin{aligned} &\sum_{k=0}^{K}{}'' f_k \cdot \delta_k^{\langle 1\rangle} g_k \Delta x + \sum_{k=0}^{K}{}'' \delta_k^{\langle 1\rangle} f_k \cdot g_k \Delta x \\ &\qquad = \left[\frac{f_k \cdot (g_{k+1} + g_{k-1}) + (f_{k+1} + f_{k-1}) \cdot g_k}{4} \right]_{k=0}^{K}, \end{aligned} \tag{2.1}$$

$$\sum_{k=0}^{K}{}'' f_k \cdot \delta_k^{+} g_k \Delta x + \sum_{k=0}^{K}{}'' \delta_k^{-} f_k \cdot g_k \Delta x = \left[\frac{f_k \cdot g_{k+1} + f_{k-1} \cdot g_k}{2} \right]_{k=0}^{K}, \tag{2.2}$$

$$\begin{aligned} &\sum_{k=0}^{K}{}'' \frac{\delta_k^{+} f_k \cdot \delta_k^{+} g_k + \delta_k^{-} f_k \cdot \delta_k^{-} g_k}{2} \Delta x + \sum_{k=0}^{K}{}'' \delta_k^{\langle 2\rangle} f_k \cdot g_k \Delta x \\ &\qquad = \left[\frac{\delta_k^{+} f_k \cdot (g_{k+1} + g_k) + \delta_k^{-} f_k \cdot (g_k + g_{k-1})}{4} \right]_{k=0}^{K}. \end{aligned} \tag{2.3}$$

It is easily seen that the above formulas correspond to

$$\int_{\mathbb{X}} f \cdot \partial_x g dx + \int_{\mathbb{X}} \partial_x f \cdot g dx = [fg]_{\partial \mathbb{X}},$$
$$\int_{\mathbb{X}} \partial_x f \cdot \partial_x g dx + \int_{\mathbb{X}} \partial_x^2 f \cdot g dx = [\partial_x f \cdot g]_{\partial \mathbb{X}}.$$

By setting $g_k = 1$ $(k = -1, 0, 1, \ldots, K, K+1)$ in (2.1) and (2.3), we also obtain the following formulas

$$\sum_{k=0}^{K}{}'' \delta_k^{\langle 1\rangle} f_k \Delta x = \left[\frac{f_{k+1} + 2f_k + f_{k-1}}{4} \right]_{k=0}^{K}, \tag{2.4}$$

$$\sum_{k=0}^{K}{}'' \delta_k^{\langle 2\rangle} f_k \Delta x = \left[\delta_k^{\langle 1\rangle} f_k \right]_{k=0}^{K}, \tag{2.5}$$

which correspond to *fundamental theorem of calculus*:

$$\int_{\mathbb{X}} \partial_x f dx = [f]_{\partial\mathbb{X}}, \qquad \int_{\mathbb{X}} \partial_x^2 f dx = [\partial_x f]_{\partial\mathbb{X}}.$$

We assume the case of $\mathbb{X} = \mathbb{T}$ is represented as $f_{k+K} = f_k$ for any $k = -1, 0, 1, \ldots, K$. Observe that in the case the trapezoidal rule is equivalent to the rectangle rule;

$$\sum_{k=0}^{K}{}'' f_k \Delta x = \sum_{k=0}^{K-1} f_k \Delta x,$$

and all the boundary integral terms of (2.1)–(2.5) vanish.

Next, if we regard $\mathbb{X}$ as a standard bounded interval $[0, L]$ $(L < \infty)$ with the Neumann boundary condition, we assume that the discrete boundary conditions are given as

$$\delta_k^{\langle 1 \rangle} f_0 = \delta_k^{\langle 1 \rangle} f_K = \delta_k^{\langle 1 \rangle} g_0 = \delta_k^{\langle 1 \rangle} g_K = 0.$$

In the case the boundary integral terms of (2.1), (2.3), (2.4) and (2.5) vanish, but the one of (2.2) remains. The most important problem of the finite difference method is which difference operators we should choose. This argument implies how to choose the difference operators according to the boundary conditions. From now on, we give the argument under the assumption $\mathbb{X} = \mathbb{T}$, for simplicity.

For a smooth function $F = F(u, v)$, the *partial difference quotients* $\partial F(\cdot, V)/\partial(U, \widetilde{U})$ and $\partial F(U, \cdot)/\partial(V, \widetilde{V})$ of F are defined by

$$\frac{\partial \varphi(V, \cdot)}{\partial(U, \widetilde{U})} := \begin{cases} \frac{F(U,V)-F(\widetilde{U},V)}{U-\widetilde{U}}, & U \neq \widetilde{U}, \\ \partial_u F(U, V), & U = \widetilde{U}, \end{cases} \qquad \frac{\partial \varphi(\cdot, U)}{\partial(V, \widetilde{V})} := \begin{cases} \frac{F(U,V)-F(U,\widetilde{V})}{V-\widetilde{V}}, & V \neq \widetilde{V}, \\ \partial_v F(U, V), & V = \widetilde{V}. \end{cases}$$

For more precise information about the difference quotient we refer to [11].

3 Structure-Preserving Schemes

We give several schemes which are derived by applying the idea given in [2] and [10] easily. We first introduce difference formulas for product and composite function. Obviously, it holds that

$$\begin{aligned} \delta_n^+ (f^{(n)} \cdot g^{(n)}) &= \delta_n^+ f^{(n)} \cdot g^{(n)} + f^{(n+1)} \cdot \delta_n^+ g^{(n)} && (3.1) \\ &= \delta_n^+ f^{(n)} \cdot g^{(n+1)} + f^{(n)} \cdot \delta_n^+ g^{(n)} && (3.2) \\ &= \delta_n^+ f^{(n)} \cdot \left(\frac{g^{(n+1)} + g^{(n)}}{2} \right) + \left(\frac{f^{(n+1)} + f^{(n)}}{2} \right) \cdot \delta_n^+ g^{(n)}, && (3.3) \end{aligned}$$

etc. From a similar observation, we also see that

$$\delta_n^+ \varphi(f^{(n)}, g^{(n)}) = \delta_n^+ f^{(n)} \cdot \frac{\partial \varphi(\cdot, g^{(n)})}{\partial (f^{(n+1)}, f^{(n)})} + \delta_n^+ g^{(n)} \cdot \frac{\partial \varphi(f^{(n+1)}, \cdot)}{\partial (g^{(n+1)}, g^{(n)})} \tag{3.4}$$

$$= \delta_n^+ f^{(n)} \cdot \frac{\partial \varphi(\cdot, g^{(n+1)})}{\partial (f^{(n+1)}, f^{(n)})} + \delta_n^+ g^{(n)} \cdot \frac{\partial \varphi(f^{(n)}, \cdot)}{\partial (g^{(n+1)}, g^{(n)})} \tag{3.5}$$

$$= \delta_n^+ f^{(n)} \cdot \left(\frac{\partial \varphi(\cdot, g^{(n)})}{\partial (f^{(n+1)}, f^{(n)})} + \frac{\partial \varphi(\cdot, g^{(n+1)})}{\partial (f^{(n+1)}, f^{(n)})} \right) + \delta_n^+ g^{(n)} \cdot \left(\frac{\partial \varphi(f^{(n)}, \cdot)}{\partial (g^{(n+1)}, g^{(n)})} + \frac{\partial \varphi(f^{(n+1)}, \cdot)}{\partial (g^{(n+1)}, g^{(n)})} \right). \tag{3.6}$$

Let us give examples. We can derive various structure-preserving finite difference schemes for (1.3)–(1.5) by the combination of choice of (3.1)–(3.3) and (3.4)–(3.6). The first example is the following:

$$\delta_n^+ W_k^{(n)} = \delta_k^{\langle 1 \rangle} \left(\frac{V_k^{(n+1)} + V_k^{(n)}}{2} \right), \tag{3.7}$$

$$\delta_n^+ V_k^{(n)} = \delta_k^{\langle 1 \rangle} \left(\frac{\partial \varphi(\cdot, \Theta_k^{(n)} + \tau_0)}{\partial (W_k^{(n+1)}, W_k^{(n)})} \right), \tag{3.8}$$

$$-(\Theta_k^{(n)} + \tau_0) \delta_n^+ \left(\frac{\partial \varphi(W_k^{(n)}, \cdot)}{\partial (\Theta_k^{(n)} + \tau_0, \Theta_k^{(n-1)} + \tau_0)} \right) = \delta_k^{\langle 2 \rangle} \Theta_k^{(n)}, \quad k = 1, 2, \ldots, K, \tag{3.9}$$

with the periodic boundary condition:

$$W_{K+k}^{(n)} = W_k^{(n)}, \quad V_{K+k}^{(n)} = V_k^{(n)}, \quad \Theta_{K+k}^{(n)} = \Theta_k^{(n)}. \tag{3.10}$$

Let the discrete energy $E_d = E_d(\boldsymbol{W}^{(n)}, \boldsymbol{V}^{(n)}, \boldsymbol{\Theta}^{(n-1)}, \boldsymbol{\Theta}^{(n)})$, the discrete momentum $M_d = M_d(\boldsymbol{W}^{(n)})$ and the discrete entropy $S_d = S_d(\boldsymbol{W}^{(n)}, \boldsymbol{\Theta}^{(n-1)}, \boldsymbol{\Theta}^{(n)})$ be defined by

$$E_d := \sum_{k=0}^{K}{}'' \left\{ \frac{1}{2} |V_k^{(n)}|^2 + \varphi(W_k^{(n)}, \Theta_k^{(n)} + \tau_0) - (\Theta_k^{(n)} + \tau_0) \frac{\partial \varphi(W_k^{(n)}, \cdot)}{\partial (\Theta_k^{(n)} + \tau_0, \Theta_k^{(n-1)} + \tau_0)} \right\} \Delta x,$$

$$M_d := \sum_{k=0}^{K}{}'' W_k^{(n)} \Delta x, \qquad S_d := -\sum_{k=0}^{K}{}'' \frac{\partial \varphi(W_k^{(n)}, \cdot)}{\partial (\Theta_k^{(n)} + \tau_0, \Theta_k^{(n-1)} + \tau_0)} \Delta x.$$

Then the following conservation laws

$$\delta_n^+ E_d(\boldsymbol{W}^{(n)}, \boldsymbol{V}^{(n)}, \boldsymbol{\Theta}^{(n-1)}, \boldsymbol{\Theta}^{(n)}) = 0, \qquad \delta_n^+ M_d(\boldsymbol{W}^{(n)}) = 0$$

hold and under the assumptions of positivity of temperature the increasing law

$$\delta_n^+ S_d(\boldsymbol{W}^{(n)}, \boldsymbol{\Theta}^{(n-1)}, \boldsymbol{\Theta}^{(n)}) \geq 0$$

holds. Indeed, it is easily seen from (3.7) and (2.4) that

$$\delta_n^+ M_d(\boldsymbol{W}^{(n)}) = \sum_{k=0}^{K}{}'' \delta_n^+ W_k^{(n)} \Delta x = \sum_{k=0}^{K}{}'' \delta_k^{\langle 1 \rangle} \left(\frac{V_k^{(n+1)} + V_k^{(n)}}{2} \right) \Delta x = 0.$$

Next, observing

$$\begin{aligned}
&\delta_n^+ \left\{ \varphi(W_k^{(n)}, \Theta_k^{(n)} + \tau_0) - (\Theta_k^{(n)} + \tau_0) \frac{\partial \varphi(W_k^{(n)}, \cdot)}{\partial(\Theta_k^{(n)} + \tau_0, \Theta_k^{(n-1)} + \tau_0)} \right\} \\
&= \delta_n^+ W_k^{(n)} \frac{\partial \varphi(\cdot, \Theta_k^{(n)} + \tau_0)}{\partial(W_k^{(n+1)}, W_k^{(n)})} + \delta_n^+ \Theta_k^{(n)} \frac{\partial \varphi(W_k^{(n+1)}, \cdot)}{\partial(\Theta_k^{(n+1)} + \tau_0, \Theta_k^{(n)} + \tau_0)} \\
&\quad - \delta_n^+ \Theta_k^{(n)} \frac{\partial \varphi(W_k^{(n+1)}, \cdot)}{\partial(\Theta_k^{(n+1)} + \tau_0, \Theta_k^{(n)} + \tau_0)} - (\Theta_k^{(n)} + \tau_0) \delta_n^+ \left(\frac{\partial \varphi(W_k^{(n)}, \cdot)}{\partial(\Theta_k^{(n)} + \tau_0, \Theta_k^{(n-1)} + \tau_0)} \right) \\
&= \delta_n^+ W_k^{(n)} \frac{\partial \varphi(\cdot, \Theta_k^{(n)} + \tau_0)}{\partial(W_k^{(n+1)}, W_k^{(n)})} - (\Theta_k^{(n)} + \tau_0) \delta_n^+ \left(\frac{\partial \varphi(W_k^{(n)}, \cdot)}{\partial(\Theta_k^{(n)} + \tau_0, \Theta_k^{(n-1)} + \tau_0)} \right),
\end{aligned}$$

where we have used (3.4) and (3.2), we obtain from (3.7)–(3.9) that

$$\begin{aligned}
\delta_n^+ E_d &= \sum_{k=0}^{K}{}'' \Bigg\{ \delta_n^+ V_k^{(n)} \frac{V_k^{(n+1)} + V_k^{(n)}}{2} + \delta_n^+ W_k^{(n)} \frac{\partial \varphi(\Theta_k^{(n)} + \tau_0, \cdot)}{\partial(W_k^{(n+1)}, W_k^{(n)})} \\
&\qquad - (\Theta_k^{(n)} + \tau_0) \delta_n^+ \left(\frac{\partial \varphi(\cdot, W_k^{(n)})}{\partial(\Theta_k^{(n)} + \tau_0, \Theta_k^{(n-1)} + \tau_0)} \right) \Bigg\} \Delta x \\
&= \sum_{k=0}^{K}{}'' \Bigg(\delta_k^{\langle 1 \rangle} \left(\frac{\partial \varphi(\cdot, \Theta_k^{(n)} + \tau_0)}{\partial(W_k^{(n+1)}, W_k^{(n)})} \right) \cdot \frac{V_k^{(n+1)} + V_k^{(n)}}{2} \\
&\qquad + \delta_k^{\langle 1 \rangle} \left(\frac{V_k^{(n+1)} + V_k^{(n)}}{2} \right) \cdot \frac{\partial \varphi(\cdot, \Theta_k^{(n)} + \tau_0)}{\partial(W_k^{(n+1)}, W_k^{(n)})} - \delta_k^{\langle 2 \rangle} \Theta_k^{(n)} \Bigg) \Delta x \\
&= 0,
\end{aligned}$$

with the help of (2.1) and (2.5). We also see that

$$\begin{aligned}
\delta_n^+ S_d &= - \sum_{k=0}^{K}{}'' \delta_n^+ \left(\frac{\partial \varphi(W_k^{(n)}, \cdot)}{\partial(\Theta_k^{(n)} + \tau_0, \Theta_k^{(n-1)} + \tau_0)} \right) \Delta x \\
&= \sum_{k=0}^{K}{}'' \frac{\delta_k^{\langle 2 \rangle} (\Theta_k^{(n)} + \tau_0)}{\Theta_k^{(n)} + \tau_0} \Delta x \\
&= \sum_{k=0}^{K}{}'' \left(\frac{|\delta_k^+ \Theta_k^{(n)}|^2}{(\Theta_k^{(n)} + \tau_0)(\Theta_{k+1}^{(n)} + \tau_0)} + \frac{|\delta_k^- \Theta_k^{(n)}|^2}{(\Theta_k^{(n)} + \tau_0)(\Theta_{k-1}^{(n)} + \tau_0)} \right) \Delta x,
\end{aligned}$$

from (2.3) and $\delta_k^{\pm}(1/f_k) = \delta_k^{\pm} f_k/(f_k f_{k\pm 1})$. We thus complete the proof.

Next, we shall consider the different choices of (3.1)–(3.3) and (3.4)–(3.6). If we use (3.5) and (3.1), we see that

$$\begin{aligned}
&\delta_n^+ \left\{ \varphi(W_k^{(n)}, \Theta_k^{(n)} + \tau_0) - (\Theta_k^{(n)} + \tau_0) \frac{\partial \varphi(W_k^{(n)}, \cdot)}{\partial(\Theta_k^{(n)} + \tau_0, \Theta_k^{(n-1)} + \tau_0)} \right\} \\
&= \delta_n^+ W_k^{(n)} \frac{\partial \varphi(\cdot, \Theta_k^{(n+1)} + \tau_0)}{\partial(W_k^{(n+1)}, W_k^{(n)})} + \delta_n^+ \Theta_k^{(n)} \frac{\partial \varphi(W_k^{(n)}, \cdot)}{\partial(\Theta_k^{(n+1)} + \tau_0, \Theta_k^{(n)} + \tau_0)} \\
&\qquad - \delta_n^+ \Theta_k^{(n)} \frac{\partial \varphi(W_k^{(n)}, \cdot)}{\partial(\Theta_k^{(n)} + \tau_0, \Theta_k^{(n-1)} + \tau_0)} - (\Theta_k^{(n+1)} + \tau_0) \delta_n^+ \left(\frac{\partial \varphi(W_k^{(n)}, \cdot)}{\partial(\Theta_k^{(n)} + \tau_0, \Theta_k^{(n-1)} + \tau_0)} \right) \\
&= \delta_n^+ W_k^{(n)} \frac{\partial \varphi(\cdot, \Theta_k^{(n+1)} + \tau_0)}{\partial(W_k^{(n+1)}, W_k^{(n)})} - (\Theta_k^{(n+1)} + \tau_0) \delta_n^+ \left(\frac{\partial \varphi(W_k^{(n)}, \cdot)}{\partial(\Theta_k^{(n)} + \tau_0, \Theta_k^{(n-1)} + \tau_0)} \right),
\end{aligned}$$

Therefore, by replacing the scheme (3.7)–(3.9) to

$$\begin{aligned}
&\delta_n^+ W_k^{(n)} = \delta_k^{\langle 1 \rangle} \left(\frac{V_k^{(n+1)} + V_k^{(n)}}{2} \right), \\
&\delta_n^+ V_k^{(n)} = \delta_k^{\langle 1 \rangle} \left(\frac{\partial \varphi(\cdot, \Theta_k^{(n+1)} + \tau_0)}{\partial(W_k^{(n+1)}, W_k^{(n)})} \right), \\
&- (\Theta_k^{(n+1)} + \tau_0) \delta_n^+ \left(\frac{\partial \varphi(W_k^{(n)}, \cdot)}{\partial(\Theta_k^{(n)} + \tau_0, \Theta_k^{(n-1)} + \tau_0)} \right) = \delta_k^{\langle 2 \rangle} \Theta_k^{(n+1)},
\end{aligned}$$

we can check energy and momentum conservation laws and the law of increasing entropy. In this way we can derive various structure-preserving numerical schemes.

4 Example of Numerical Simulation

In this section we give a guide for numerical experiments using a simple example in the case:

$$\varphi(w, \theta + \tau_0) = \frac{w^2}{2} - \frac{(\theta + \tau_0)^2}{2} + (\theta + \tau_0) w.$$

Obviously it satisfies (1.2). It follows from the definition of partial difference quotient that

$$\begin{aligned}
\frac{\partial \varphi(\cdot, \Theta_k^{(n)} + \tau_0)}{\partial(W_k^{(n+1)}, W_k^{(n)})} &= \frac{W_k^{(n+1)} + W_k^{(n)}}{2} + (\Theta_k^{(n)} + \tau_0), \\
\frac{\partial \varphi(W_k^{(n)}, \cdot)}{\partial(\Theta_k^{(n)} + \tau_0, \Theta_k^{(n-1)} + \tau_0)} &= -\frac{\Theta_k^{(n)} + \Theta_k^{(n-1)}}{2} - \tau_0 + W_k^{(n)}.
\end{aligned}$$

Then the numerical scheme (3.7)–(3.9) in this case is

$$\delta_n^+ W_k^{(n)} = \delta_k^{\langle 1 \rangle} \left(\frac{V_k^{(n+1)} + V_k^{(n)}}{2} \right), \tag{4.1}$$

$$\delta_n^+ V_k^{(n)} = \delta_k^{\langle 1 \rangle} \left(\frac{W_k^{(n+1)} + W_k^{(n)}}{2} + \Theta_k^{(n)} \right), \tag{4.2}$$

$$\delta_n^+ \left(\frac{\Theta_k^{(n)} + \Theta_k^{(n-1)}}{2} - W_k^{(n)} \right) = \frac{\delta_k^{\langle 2 \rangle} \Theta_k^{(n)}}{\Theta_k^{(n)} + \tau_0}, \tag{4.3}$$

and

$$E_d = \sum_{k=0}^{K}{}'' \left\{ \frac{1}{2}|V_k^{(n)}|^2 + \frac{1}{2}|W_k^{(n)}|^2 + \frac{(\Theta_k^{(n)} + \tau_0)(\Theta_k^{(n-1)} + \tau_0)}{2} \right\} \Delta x,$$

$$M_d := \sum_{k=0}^{K}{}'' W_k^{(n)} \Delta x, \qquad S_d := \sum_{k=0}^{K}{}'' \left\{ \frac{\Theta_k^{(n)} + \Theta_k^{(n-1)}}{2} + \tau_0 - W_k^{(n)} \right\} \Delta x.$$

Now we set $\boldsymbol{U}^{(n)} := [\boldsymbol{W}^{(n)}, \boldsymbol{V}^{(n)}, \boldsymbol{\Theta}^{(n)}]^T$ for K-dimensional vectors $\boldsymbol{W}^{(n)} = \{W_k^{(n)}\}_{k=1}^K$, $\boldsymbol{V}^{(n)} = \{V_k^{(n)}\}_{k=1}^K$ and $\boldsymbol{\Theta}^{(n)} = \{\Theta_k^{(n)}\}_{k=1}^K$, and define K-dimensional matrices

$$D_1 = \frac{1}{2\Delta x} \begin{bmatrix} 0 & 1 & 0 & & \cdots & -1 \\ -1 & 0 & 1 & 0 & \cdots & 0 \\ \vdots & \ddots & \ddots & \ddots & \ddots & \vdots \\ 0 & \cdots & -1 & 0 & 1 & 0 \\ 0 & \cdots & & -1 & 0 & 1 \\ 1 & \cdots & & & -1 & 0 \end{bmatrix}, \quad D_2 = \frac{1}{\Delta x^2} \begin{bmatrix} -2 & 1 & 0 & & \cdots & 1 \\ 1 & -2 & 1 & 0 & \cdots & 0 \\ \vdots & \ddots & \ddots & \ddots & \ddots & \vdots \\ 0 & \cdots & 1 & -2 & 1 & 0 \\ 0 & \cdots & & 1 & -2 & 1 \\ 1 & \cdots & & & 1 & -2 \end{bmatrix},$$

$$T^{(n)} = \begin{bmatrix} (\Theta_1^{(n)} + \tau_0)^{-1} & 0 & \cdots & 0 \\ 0 & (\Theta_2^{(n)} + \tau_0)^{-1} & & \\ \vdots & & \ddots & \vdots \\ 0 & \cdots & & (\Theta_K^{(n)} + \tau_0)^{-1} \end{bmatrix}.$$

Here D_1 and D_2 are matrix representations of $\delta_k^{\langle 1 \rangle}$ and $\delta_k^{\langle 2 \rangle}$ with the periodic boundary condition (3.10). By using these, we define the following $3K$-dimensional matrices

$$A_1 = \begin{bmatrix} \frac{1}{\Delta t}E & -\frac{1}{2}D_1 & O \\ -\frac{1}{2}D_1 & \frac{1}{\Delta t}E & O \\ -\frac{1}{\Delta t}E & O & \frac{1}{2\Delta t}E \end{bmatrix}, \quad A_2 = \begin{bmatrix} \frac{1}{\Delta t}E & \frac{1}{2}D_1 & O \\ \frac{1}{2}D_1 & \frac{1}{\Delta t}E & O \\ -\frac{1}{\Delta t}E & O & D_2 \end{bmatrix},$$

$$A_3 = \begin{bmatrix} O & O & O \\ O & O & O \\ O & O & \frac{1}{2\Delta t}E \end{bmatrix}, \quad \widetilde{T}^{(n)} = \begin{bmatrix} E & O & O \\ O & E & O \\ O & O & T^{(n)} \end{bmatrix},$$

where E and O are K-dimensional identity and zero matrices. Remark that the equation (4.3) is equivalent to

$$\frac{1}{2\Delta t}\Theta_k^{(n+1)} - \frac{1}{\Delta t}W_k^{(n+1)} = -\frac{1}{\Delta t}W_k^{(n)} + \frac{1}{2\Delta t}\Theta_k^{(n-1)} + \frac{\delta_k^{\langle 2\rangle}\Theta_k^{(n)}}{\Theta_k^{(n)} + \tau_0}.$$

Then the equations (4.1)–(4.3) with periodic boundary condition can be rewritten as

$$A_1\boldsymbol{U}^{(n+1)} = \widetilde{T}^{(n)}A_2\boldsymbol{U}^{(n)} + A_3\boldsymbol{U}^{(n-1)}.$$

We thus easily obtain $\boldsymbol{U}^{(n+1)} = A_1^{-1}(\widetilde{T}^{(n)}A_2\boldsymbol{U}^{(n)} + A_3\boldsymbol{U}^{(n-1)})$. Here we remark that in the first step, we need to prepare another calculation because (4.3) is two-step method. For example, by using

$$\delta_n^+\left(\Theta_k^{(0)} - W_k^{(0)}\right) = \frac{\delta_k^{\langle 2\rangle}\Theta_k^{(0)}}{\Theta_k^{(0)} + \tau_0}$$

instead of (4.3), we can perform the numerical simulation, and check numerical simulation works well satisfying the discrete version of (1.1). For the actual numerical simulation results we refer to the bachelor thesis by Yamada ([8]).

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