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ROBUST FINITE DIFFERENCE SCHEMES FOR A NONLINEAR VARIATIONAL WAVE EQUATION MODELING LIQUID CRYSTALS.

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ABSTRACT. We consider a nonlinear variational wave equation that models the dynamics of nematic liquid crystals. Finite difference schemes, that either conserve or dissipate a discrete version of the energy, associated with these equations, are designed. Numerical experiments, in both one and two-space dimensions, illustrating the stability and efficiency of the schemes are presented. An interesting feature of these schemes is their ability to approximate both the conservative as well as the dissipative weak solution of the underlying system.

1. INTRODUCTION

1.1. **The model.** The dynamics of nematic liquid crystals is an important object of study in both physics and engineering. Many popular models of nematic liquid crystals consider a medium consisting of thin rods that are allowed to rotate about their center of mass but are not allowed to translate. Under the assumption that the medium is not flowing and deformations only occur when the mean orientation of long molecules is changed, one can describe the the orientation of the molecules at each location $\mathbf{x} \in \mathbb{R}^3$ and time $t \in \mathbb{R}$ using a field of unit vectors

$$\mathbf{n} = \mathbf{n}(\mathbf{x}, t) \in \mathcal{S}^2.$$

This field \mathbf{n} is termed as the *director field*.

Given a director field \mathbf{n} , the well-known Oseen-Frank potential energy density \mathbf{W} , associated with this field, is given by

$$(1.1) \quad \mathbf{W}(\mathbf{n}, \nabla \mathbf{n}) = \alpha |\mathbf{n} \times (\nabla \times \mathbf{n})|^2 + \beta (\nabla \cdot \mathbf{n})^2 + \gamma (\mathbf{n} \cdot (\nabla \times \mathbf{n}))^2.$$

The positive constants α, β and γ are elastic constants of the liquid crystal. Note that each term on the right hand side of (1.1) arises from different types of distortions. For instance, the term $\alpha |\mathbf{n} \times (\nabla \times \mathbf{n})|^2$ corresponds to the bending of the medium, the term $\beta (\nabla \cdot \mathbf{n})^2$ corresponds to a type of deformation called splay, and the term $\gamma (\mathbf{n} \cdot (\nabla \times \mathbf{n}))^2$ corresponds to the twisting of the medium.

For the special case of $\alpha = \beta = \gamma$, the potential energy density (1.1) reduces to

$$\mathbf{W}(\mathbf{n}, \nabla \mathbf{n}) = \alpha |\nabla \mathbf{n}|^2,$$

which corresponds to the potential energy density used in harmonic maps into the sphere \mathcal{S}^2 . The constrained elliptic system of equations for \mathbf{n} , derived from the potential (1.1) using a variational principle, and the parabolic flow associated with it, are widely studied, see [1, 4, 6] and references therein.

However in the regime where inertial effects are dominant (over the viscosity), it is more natural to model the propagation of orientation waves in the director field by employing the principle of least action [12] i.e.,

$$(1.2) \quad \frac{\delta}{\delta u} \iint (\mathbf{n}_t^2 - \mathbf{W}(\mathbf{n}, \nabla \mathbf{n})) \, dx \, dt = 0, \quad \mathbf{n} \cdot \mathbf{n} = 1.$$

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Again in the special case of $\alpha = \beta = \gamma$, this variational principle (1.2) yields the equation for harmonic wave maps from $(1+3)$ -dimensional Minkowski space into the two sphere, see [3, 13, 14] and references therein.

1.1.1. *One-dimensional planar waves.* Planar deformations are of great interest in the study of nematic liquid crystals. In particular, if we assume that the deformation depends on a single space variable x , the director field \mathbf{n} has a special form:

$$\mathbf{n} = \cos u(x, t)\mathbf{e}_x + \sin u(x, t)\mathbf{e}_y.$$

Here, the unknown $u \in \mathbb{R}$ measures the angle of the director field to the x -direction, and \mathbf{e}_x and \mathbf{e}_y are the coordinate vectors in the x and y directions, respectively. In this case, the variational principle (1.2) reduces to

$$(1.3) \quad \begin{cases} u_{tt} - c(u)(c(u)u_x)_x = 0, & (x, t) \in \Pi_T, \\ u(x, 0) = u_0(x), & x \in \mathbb{R}, \\ u_t(x, 0) = u_1(x), & x \in \mathbb{R}. \end{cases}$$

where $\Pi_T = \mathbb{R} \times [0, T]$ with fixed $T > 0$, and the wave speed $c(u)$ given by

$$(1.4) \quad c^2(u) = \alpha \cos^2 u + \beta \sin^2 u,$$

for some positive constants α, β . The form (1.3) is the standard form of the nonlinear variational wave equation considered in the literature.

If we consider the following *energy*:

$$(1.5) \quad \mathcal{E}(t) = \int_{\mathbb{R}} (u_t^2 + c^2(u)u_x^2) dx,$$

a simple calculation shows that smooth solutions of the variational wave equation (1.3) *conserve* this energy i.e, they satisfy

$$(1.6) \quad \frac{d\mathcal{E}(t)}{dt} \equiv 0.$$

1.1.2. *Two-dimensional planar waves.* Similarly, if the deformation depends on two space variables x, y , the director field has the form:

$$\mathbf{n} = \cos u(x, y, t)\mathbf{e}_x + \sin u(x, y, t)\mathbf{e}_y,$$

with u being the angle to the $x - y$ plane. The corresponding wave equation is given by,

$$(1.7) \quad \begin{cases} u_{tt} - c(u)(c(u)u_x)_x - b(u)(b(u)u_y)_y - a'(u)u_x u_y - 2a(u)u_{xy} = 0, & (x, y, t) \in \mathbb{Q}_T, \\ u(x, y, 0) = u_0(x, y), & (x, y) \in \mathbb{R}^2, \\ u_t(x, y, 0) = u_1(x, y), & (x, y) \in \mathbb{R}^2. \end{cases}$$

where $\mathbb{Q}_T = \mathbb{R}^2 \times [0, T]$ with $T > 0$ fixed, $u : \mathbb{Q}_T \rightarrow \mathbb{R}$ is the unknown function and a, b, c are given by

$$\begin{aligned} c^2(u) &= \alpha \cos^2 u + \beta \sin^2 u, \\ b^2(u) &= \alpha \sin^2 u + \beta \cos^2 u, \\ a(u) &= \frac{\alpha - \beta}{2} \sin(2u). \end{aligned}$$

for some constants α and β . Furthermore, smooth solutions of (1.7) also *conserve* the following energy:

$$(1.8) \quad \begin{aligned} \mathcal{E}(t) &= \iint_{\mathbb{R}^2} (u_t^2 + c^2(u)u_x^2 + b^2(u)u_y^2 + 2a(u)u_x u_y) dx dy \\ &= \iint_{\mathbb{R}^2} (u_t^2 + \alpha(\cos(u)u_x + \sin(u)u_y)^2 + \beta(\sin(u)u_x - \cos(u)u_y)^2) dx dy, \end{aligned}$$

i.e, smooth solutions satisfy (1.6) with respect to the above energy.

1.2. Mathematical issues. It is well known that the solution of the initial value problem, even for the one-dimensional planar wave equation (1.3) develops singularities in finite time, even if the initial data are smooth [7]. Hence, solutions of (1.3) are defined in the sense of distributions, i.e.,

Definition 1.1. Set $\Pi_T = \mathbb{R} \times (0, T)$. A function

$$u(t, x) \in L^\infty([0, T]; W^{1,p}(\mathbb{R})) \cap C(\Pi_T), u_t \in L^\infty([0, T]; L^p(\mathbb{R})),$$

for all $p \in [1, 3 + q]$, where $q > 0$ is some positive constant is a weak solution of the initial value problem (1.3) if it satisfies:

- For all test functions $\varphi \in \mathcal{D}(\mathbb{R} \times [0, T])$

$$(1.9) \quad \iint_{\Pi_T} (u_t \varphi_t - c^2(u) u_x \varphi_x - c(u) c'(u) (u_x)^2 \varphi) dx dt = 0.$$

- $u(\cdot, t) \rightarrow u_0$ in $C([0, T]; L^2(\mathbb{R}))$ as $t \rightarrow 0^+$.
- $u_t(\cdot, t) \rightarrow v_0$ as a distribution in Π_T when $t \rightarrow 0^+$.

It is highly non-trivial to extend the solution after the appearance of singularities. In particular, the choice of this extension is non-unique. Two distinct types of solutions, the so-called *conservative* and *dissipative* solutions are known. To illustrate this difference, one considers initial data for which the solution vanishes identically at some specific (finite) time. At this point, at least two possibilities exist: to continue with the trivial zero solution, termed as the dissipative solution. As an alternative, one can show that there exists a nontrivial solution that appears as a natural continuation of the solution prior to the critical time. This solution is denoted the conservative solution as it preserves the total energy of the system. This dichotomy makes the question of well-posedness of the initial value problem (1.3) very difficult. Additional admissibility conditions are needed to select a physically relevant solution. The specification of such admissibility criteria is still open.

Although the problem of global existence and uniqueness of solutions to the Cauchy problem of the nonlinear variational wave equation (1.3) is still open, several recent papers have explored related questions or particular cases of (1.3). It has been demonstrated in [9] that (1.3) is rich in structural phenomena associated with weak solutions. In fact rewriting the highest derivatives of (1.3) in conservative form

$$u_{tt} - (c^2(u) u_x)_x = -c(u) c'(u) u_x^2,$$

we see that the strong precompactness in L^2 of the derivatives $\{u_x\}$ of a sequence of approximate solutions is essential in establishing the existence of a global weak solution. However, the equation shows the phenomenon of persistence of oscillations [5] and annihilation in which a sequence of exact solutions with bounded energy can oscillate forever so that the sequence $\{u_x\}$ is not precompact in L^2 , but the weak limit of the sequence is still a weak solution.

There has been a number of papers concerning the existence of weak solutions of the Cauchy problem (1.3), starting with the papers by Zhang and Zheng [15, 16, 17, 18, 19, 20], Bressan and Zheng [2] and Holden et al [10]. In [19], the authors show existence of a global weak solution, using method of Young measures, for initial data $u_0 \in H^1(\mathbb{R})$ and $u_1 \in L^2(\mathbb{R})$. The function c is assumed to be smooth, bounded, positive with derivative that is non-negative and strictly positive on the initial data u_0 .

A different approach to the study of (1.3) was taken by Bressan and Zheng [2]. Here, they rewrote the equation in new variables such that the singularities disappeared. They show that for u_0 absolutely continuous with $(u_0)_x, u_1 \in L^2(\mathbb{R})$, the Cauchy problem (1.3) allows a global weak solution with the following properties: the solution u is locally Lipschitz continuous and the map $t \rightarrow u(t, \cdot)$ is continuously differentiable with values in $L^p_{loc}(\mathbb{R})$ for $1 \leq p < 2$.

In [10], Holden and Raynaud prove the existence of a global semigroup for conservative solutions of (1.3), allowing for concentration of energy density on sets of zero measure. Furthermore they also allow for initial data u_0, u_1 that contain measures. The proof involves constructing the solution by introducing new variables related to the characteristics, leading to a characterization

of singularities in the energy density. They also prove that energy can only focus on a set of times of zero measure or at points where $c'(u)$ vanishes.

In contrast to the one-dimensional case, hardly any rigorous wellposedness or even qualitative results are available for the two-dimensional version of the variational wave equation (1.7).

1.3. Numerical schemes. Given the nonlinear nature of the variational wave equations (1.3) and (1.7), explicit solution formulas are hard to obtain. Consequently, robust numerical schemes for approximating the variational wave equation, are very important in the study of nematic liquid crystals. However, there is a paucity of efficient numerical schemes for these equations. Within the existing literature, we can refer to [8], where the authors present some numerical examples to illustrate their theory. In recent years, a semi-discrete finite difference scheme for approximating one-dimensional equation (1.3) was considered in [11]. The authors were even able to prove convergence of the numerical approximation, generated by their scheme, to the *dissipative* solutions of (1.3). However, the underlying assumptions on the wave speed c (positivity of the derivative of c) precludes consideration of realistic wave speeds given by (1.4). Another recent paper dealing with numerical approximation of (1.3) is [10]. Here, the authors use their analytical construction to define a numerical method that can approximate the *conservative* solution. However, the method is computationally very expensive as there is no time marching.

1.4. Aims and scope of the current paper. The above discussion clearly highlights the lack of robust and efficient numerical schemes to simulate the nonlinear variational wave equation (1.3). In particular, one needs a scheme that is both efficient, simple to implement and is able to approximate the solutions of (1.3) accurately. Furthermore, one can expect both *conservative* as well as *dissipative* solutions of the variational wave equation (1.3), after singularity formation. Hence, it is essential to design schemes that approximate these different types of solutions.

To this end, we will construct robust finite difference schemes for approximating the variational wave equation in both one and two space dimensions. The key design principle will be energy conservation (dissipation). As pointed out before, smooth solutions of (1.3) and (1.7) are energy conservative. After singularity formation, either this energy is conserved or dissipated. We will design numerical schemes that imitate this energy principle. In other words, our schemes will either conserve a discrete form of the energy (1.5) or dissipate it. Hence, we construct both energy conservative schemes as well as energy dissipative schemes for the variational wave equation, in both one and two space dimensions. Extensive numerical experiments are presented to illustrate that the energy conservative (dissipative) schemes converge to the conservative (dissipative) solution of the variational wave equation as the mesh is refined. To the best of our knowledge, these are the first finite difference schemes that can approximate the conservative solutions of the one-dimensional variational wave equation. Furthermore, we present the first set of numerical schemes to approximate the two-dimensional version of these equations. Our energy conservative (dissipative) schemes are based on either rewriting the wave equation as a first-order system of equations or using a Hamiltonian formulation of our system.

The rest of the paper is organized as follows: In section 2, we present energy conservative and energy dissipative schemes for the one-dimensional equation (1.3). Numerical experiments illustrating these schemes are presented in section 3. The two-dimensional schemes are presented in section 4.

2. NUMERICAL SCHEMES FOR THE ONE-DIMENSIONAL VARIATIONAL WAVE EQUATION (1.3)

2.1. The grid and notation. We begin by introducing some notation needed to define the finite difference schemes. Throughout this paper, we reserve Δx and Δt to denote two small positive numbers that represent the spatial and temporal discretization parameters, respectively, of the numerical schemes. For $j \in \mathbb{N}_0 = \mathbb{N} \cup \{0\}$, we set $x_j = j\Delta x$, and for $n = 0, 1, \dots, N$, where $N\Delta t = T$ for some fixed time horizon $T > 0$, we set $t_n = n\Delta t$. For any function $g = g(x)$ admitting point values we write $g_j = g(x_j)$, and similarly for any function $h = h(x, t)$ admitting point values we write $h_j^n = h(x_j, t_n)$. We also introduce the spatial and temporal grid cells

$$I_j = [x_{j-\frac{1}{2}}, x_{j+\frac{1}{2}}), \quad I_j^n = I_j \times [t_n, t_{n+1}).$$

Furthermore we introduce the jump, and respectively, the average of any grid function ρ across the interface $x_{j+\frac{1}{2}}$

$$\begin{aligned}\bar{\rho}_{j+\frac{1}{2}} &:= \frac{\rho_j + \rho_{j+1}}{2}, \\ \llbracket \rho \rrbracket_{j+\frac{1}{2}} &:= \rho_{j+1} - \rho_j.\end{aligned}$$

The following identities are readily verified:

$$(2.1) \quad \begin{aligned}\llbracket uv \rrbracket_{j+\frac{1}{2}} &= \bar{u}_{j+\frac{1}{2}} \llbracket v \rrbracket_{j+\frac{1}{2}} + \llbracket u \rrbracket_{j+\frac{1}{2}} \bar{v}_{j+\frac{1}{2}}, \\ v_j &= \bar{v}_{j\pm\frac{1}{2}} \mp \frac{1}{2} \llbracket v \rrbracket_{j\pm\frac{1}{2}}.\end{aligned}$$

2.2. A first-order system for (1.3). It is easy to check that the variational wave equation (1.3) can be rewritten as a first-order system by introducing the independent variables:

$$\begin{aligned}v &:= u_t \\ w &:= c(u)u_x.\end{aligned}$$

Then, for smooth solutions, equation (1.3) is equivalent to the following system for (v, w, u) ,

$$(2.2) \quad \begin{cases} v_t - (c(u)w)_x = -c_x(u)w \\ w_t - (c(u)v)_x = 0, \\ u_t = v. \end{cases}$$

Furthermore, the energy associated with the above equation is

$$(2.3) \quad \mathcal{E}(t) = \int_{\mathbb{R}} (v^2 + w^2) dx.$$

Again, we can check that smooth solutions of (2.2) preserve this energy. Weak solutions can be either energy conservative or energy dissipative.

2.3. Energy Preserving Scheme Based On System (2.2). Our objective is to design a (semi-discrete) finite difference scheme such that the numerical approximations conserve a discrete version of the energy (2.3). To this end, we suggest the following finite difference scheme:

$$(2.4) \quad \begin{aligned}(v_j)_t - \frac{1}{\Delta x} \left(\bar{c}_{j+\frac{1}{2}} \bar{w}_{j+\frac{1}{2}} - \bar{c}_{j-\frac{1}{2}} \bar{w}_{j-\frac{1}{2}} \right) &= -\frac{1}{2\Delta x} \left(\llbracket c \rrbracket_{j+\frac{1}{2}} \bar{w}_{j+\frac{1}{2}} + \llbracket c \rrbracket_{j-\frac{1}{2}} \bar{w}_{j-\frac{1}{2}} \right), \\ (w_j)_t - \frac{1}{\Delta x} \left(\bar{c} \bar{v}_{j+\frac{1}{2}} - \bar{c} \bar{v}_{j-\frac{1}{2}} \right) &= 0, \\ (u_j)_t &= v_j.\end{aligned}$$

The energy conservative property of this semi-discrete scheme is presented in the following theorem:

Theorem 2.1. *Let $v_j(t)$ and $w_j(t)$ be approximate solutions generated by the scheme (2.4). Then*

$$\partial_t \left(\frac{\Delta x}{2} \sum_j (v_j^2(t) + w_j^2(t)) \right) = 0.$$

Proof. We start by multiplying the first equation of (2.4) by v_j and second equation by w_j respectively. Using relations (2.1), we have

$$\begin{aligned}& \frac{1}{2} \frac{d}{dt} (v_j^2 + w_j^2) \\ &= \frac{1}{\Delta x} \bar{v}_{j+\frac{1}{2}} \bar{c}_{j+\frac{1}{2}} \bar{w}_{j+\frac{1}{2}} - \frac{1}{2\Delta x} \llbracket v \rrbracket_{j+\frac{1}{2}} \bar{c}_{j+\frac{1}{2}} \bar{w}_{j+\frac{1}{2}} \\ &\quad - \frac{1}{\Delta x} \bar{v}_{j-\frac{1}{2}} \bar{c}_{j-\frac{1}{2}} \bar{w}_{j-\frac{1}{2}} - \frac{1}{2\Delta x} \llbracket v \rrbracket_{j-\frac{1}{2}} \bar{c}_{j-\frac{1}{2}} \bar{w}_{j-\frac{1}{2}} \\ &\quad - \frac{1}{2\Delta x} \bar{v}_{j+\frac{1}{2}} \llbracket c \rrbracket_{j+\frac{1}{2}} \bar{w}_{j+\frac{1}{2}} + \frac{1}{4\Delta x} \llbracket v \rrbracket_{j+\frac{1}{2}} \llbracket c \rrbracket_{j+\frac{1}{2}} \bar{w}_{j+\frac{1}{2}}\end{aligned}$$

$$\begin{aligned}
& -\frac{1}{2\Delta x}\bar{v}_{j-\frac{1}{2}}\llbracket c \rrbracket_{j-\frac{1}{2}}\bar{w}_{j-\frac{1}{2}} - \frac{1}{4\Delta x}\llbracket v \rrbracket_{j-\frac{1}{2}}\llbracket c \rrbracket_{j-\frac{1}{2}}\bar{w}_{j-\frac{1}{2}} \\
& + \frac{1}{\Delta x}\bar{w}_{j+\frac{1}{2}}\bar{c}v_{j+\frac{1}{2}} - \frac{1}{2\Delta x}\llbracket w \rrbracket_{j+\frac{1}{2}}\bar{c}v_{j+\frac{1}{2}} - \frac{1}{\Delta x}\bar{w}_{j-\frac{1}{2}}\bar{c}v_{j-\frac{1}{2}} - \frac{1}{2\Delta x}\llbracket w \rrbracket_{j-\frac{1}{2}}\bar{c}v_{j-\frac{1}{2}},
\end{aligned}$$

which implies

$$(2.5) \quad \frac{1}{2} \frac{d}{dt} (v_j^2 + w_j^2) = \frac{1}{\Delta x} (H_{j+\frac{1}{2}} - H_{j-\frac{1}{2}}) - \frac{1}{2\Delta x} (\llbracket cvw \rrbracket_{j+\frac{1}{2}} + \llbracket cvw \rrbracket_{j-\frac{1}{2}}),$$

where

$$H_{j+\frac{1}{2}} = \bar{v}_{j+\frac{1}{2}}\bar{c}_{j+\frac{1}{2}}\bar{w}_{j+\frac{1}{2}} + \frac{1}{4}\llbracket v \rrbracket_{j+\frac{1}{2}}\llbracket c \rrbracket_{j+\frac{1}{2}}\bar{w}_{j+\frac{1}{2}} + \bar{w}_{j+\frac{1}{2}}\bar{c}v_{j+\frac{1}{2}}.$$

Next, multiplying (2.5) by Δx and summing over j gives

$$\begin{aligned}
\frac{d}{dt} \left(\frac{\Delta x}{2} \sum_j (v_j^2 + w_j^2) \right) &= \sum_j (H_{j+\frac{1}{2}} - H_{j-\frac{1}{2}}) - \frac{1}{2} \sum_j (\llbracket cvw \rrbracket_{j+\frac{1}{2}} + \llbracket cvw \rrbracket_{j-\frac{1}{2}}) \\
&= 0.
\end{aligned}$$

This proves the theorem. \square

2.4. Energy dissipating Scheme Based On System (2.2). We expect the above designed energy conservative scheme (2.4) to approximate a conservative solution of the underlying system (1.3). In order to be able to approximate a dissipative solution of (1.3), we propose the following modification of the energy conservative scheme (2.4):

$$\begin{aligned}
(v_j)_t - \frac{1}{\Delta x} (\bar{c}_{j+\frac{1}{2}}\bar{w}_{j+\frac{1}{2}} - \bar{c}_{j-\frac{1}{2}}\bar{w}_{j-\frac{1}{2}}) \\
(2.6) \quad &= -\frac{1}{2\Delta x} (\llbracket c \rrbracket_{j+\frac{1}{2}}\bar{w}_{j+\frac{1}{2}} + \llbracket c \rrbracket_{j-\frac{1}{2}}\bar{w}_{j-\frac{1}{2}}) + \frac{1}{2\Delta x} (s_{j+\frac{1}{2}}\llbracket v \rrbracket_{j+\frac{1}{2}} - s_{j-\frac{1}{2}}\llbracket v \rrbracket_{j-\frac{1}{2}}) \\
(w_j)_t - \frac{1}{\Delta x} (\bar{c}v_{j+\frac{1}{2}} - \bar{c}v_{j-\frac{1}{2}}) &= \frac{1}{2\Delta x} (s_{j+\frac{1}{2}}\llbracket w \rrbracket_{j+\frac{1}{2}} - s_{j-\frac{1}{2}}\llbracket w \rrbracket_{j-\frac{1}{2}}), \\
(u_j)_t &= v_j,
\end{aligned}$$

where we have chosen $s_{j\pm\frac{1}{2}} = \max\{c_j, c_{j\pm 1}\}$ i.e., the maximum local wave speed.

We show that the above scheme dissipates energy in the following theorem:

Theorem 2.2. *Let $v_j(t)$ and $w_j(t)$ be approximate solutions generated by the scheme (2.6). Then one can prove that*

$$\partial_t \left(\frac{\Delta x}{2} \sum_j (v_j^2(t) + w_j^2(t)) \right) \leq 0.$$

Proof. First note that $s_{j\pm\frac{1}{2}}$ are positive for all j , since $c_j > 0$ for all j . Emulating the calculations of previous theorem, i.e., first multiplying the first equation of (2.6) by $\Delta x v_j$ and second equation by $\Delta x w_j$ respectively, and summing over all j we have

$$\begin{aligned}
\frac{d}{dt} \left(\frac{\Delta x}{2} \sum_j (v_j^2 + w_j^2) \right) \\
&= \sum_j (H_{j+\frac{1}{2}} - H_{j-\frac{1}{2}}) - \frac{1}{2} \sum_j (\llbracket cvw \rrbracket_{j+\frac{1}{2}} + \llbracket cvw \rrbracket_{j-\frac{1}{2}}) \\
&+ \frac{1}{2} \sum_j s_{j+\frac{1}{2}}\bar{v}_{j+\frac{1}{2}}\llbracket v \rrbracket_{j+\frac{1}{2}} - \frac{1}{4} \sum_j s_{j+\frac{1}{2}}\llbracket v \rrbracket_{j+\frac{1}{2}}^2 - \frac{1}{2} \sum_j s_{j-\frac{1}{2}}\bar{v}_{j-\frac{1}{2}}\llbracket v \rrbracket_{j-\frac{1}{2}} \\
&- \frac{1}{4} \sum_j s_{j-\frac{1}{2}}\llbracket v \rrbracket_{j-\frac{1}{2}}^2 + \frac{1}{2} \sum_j s_{j+\frac{1}{2}}\bar{w}_{j+\frac{1}{2}}\llbracket w \rrbracket_{j+\frac{1}{2}} - \frac{1}{4} \sum_j s_{j+\frac{1}{2}}\llbracket w \rrbracket_{j+\frac{1}{2}}^2
\end{aligned}$$

$$-\frac{1}{2} \sum_j s_{j-\frac{1}{2}} \bar{w}_{j-\frac{1}{2}} \llbracket w \rrbracket_{j-\frac{1}{2}} - \frac{1}{4} \sum_j s_{j-\frac{1}{2}} \llbracket w \rrbracket_{j-\frac{1}{2}}^2$$

Next, define

$$\begin{aligned} K_{j+\frac{1}{2}} &= H_{j+\frac{1}{2}} + \frac{1}{2} s_{j+\frac{1}{2}} \bar{v}_{j+\frac{1}{2}} \llbracket v \rrbracket_{j+\frac{1}{2}} + \frac{1}{2} s_{j+\frac{1}{2}} \bar{w}_{j+\frac{1}{2}} \llbracket w \rrbracket_{j+\frac{1}{2}} \\ M_{j+\frac{1}{2}} &= \frac{1}{4} s_{j+\frac{1}{2}} \left(\llbracket v \rrbracket_{j+\frac{1}{2}}^2 + \llbracket w \rrbracket_{j+\frac{1}{2}}^2 \right). \end{aligned}$$

Then we have

$$\begin{aligned} \frac{d}{dt} \left(\frac{\Delta x}{2} \sum_j (v_j^2 + w_j^2) \right) &= \sum_j \left(K_{j+\frac{1}{2}} - K_{j-\frac{1}{2}} \right) - \frac{1}{2} \sum_j \left(\llbracket cvw \rrbracket_{j+\frac{1}{2}} + \llbracket cvw \rrbracket_{j-\frac{1}{2}} \right) \\ &\quad - \sum_j \left(M_{j+\frac{1}{2}} + M_{j-\frac{1}{2}} \right) \leq 0. \end{aligned}$$

This proves the theorem. \square

Hence, the scheme (2.6) is energy stable (dissipating) and we expect it to converge to a dissipative solution of (1.3) as the mesh is refined. We remark that energy dissipation results by adding *numerical viscosity* (scaled by the maximum wave speed) to the energy conservative scheme (2.4).

2.5. A first-order system for (1.3) based on Riemann invariants. We can also rewrite the one-dimensional variational wave equation (1.3) as a first-order system of equations by introducing the Riemann invariants:

$$\begin{aligned} R &:= u_t + c(u)u_x \\ S &:= u_t - c(u)u_x. \end{aligned}$$

Again, for smooth solutions, equation (1.3) is equivalent to the following system in non-conservative form for (R, S, u) ,

$$(2.7) \quad \begin{cases} R_t - c(u)R_x = \frac{c'(u)}{4c(u)} (R^2 - S^2), \\ S_t + c(u)S_x = -\frac{c'(u)}{4c(u)} (R^2 - S^2), \\ u_t = \frac{R+S}{2}. \end{cases}$$

Observe that one can also rewrite the equation (1.3) in conservative form for (R, S, u) ,

$$(2.8) \quad \begin{cases} R_t - (c(u)R)_x = -\frac{c_x(u)}{2} (R - S), \\ S_t + (c(u)S)_x = -\frac{c_x(u)}{2} (R - S), \\ u_t = \frac{R+S}{2}. \end{cases}$$

The corresponding energy associated with the system (2.7) is

$$(2.9) \quad \mathcal{E}(t) = \frac{1}{2} \int_{\mathbb{R}} (R^2 + S^2) dx.$$

A simple calculation shows that smooth solutions of (2.7) satisfy the energy identity:

$$(2.10) \quad (R^2 + S^2)_t - (c(u)(R^2 - S^2))_x = 0.$$

Hence, the fact that the total energy (2.9) is conserved follows from integrating the above identity in space and assuming that the functions R, S decay at infinity.

2.6. Energy Preserving Scheme Based On System (2.8). We also propose the following energy conservative scheme based on the Riemann invariant system (2.8): to (2.8)

$$\begin{aligned}
(2.11) \quad & (R_j)_t - \frac{1}{\Delta x} \left(\bar{c}_{j+\frac{1}{2}} \bar{R}_{j+\frac{1}{2}} - \bar{c}_{j-\frac{1}{2}} \bar{R}_{j-\frac{1}{2}} \right) \\
& = -\frac{R_j}{4\Delta x} \left(\llbracket c \rrbracket_{j+\frac{1}{2}} + \llbracket c \rrbracket_{j-\frac{1}{2}} \right) + \frac{S_j}{4\Delta x} \left(\llbracket c \rrbracket_{j+\frac{1}{2}} + \llbracket c \rrbracket_{j-\frac{1}{2}} \right) \\
& (S_j)_t + \frac{1}{\Delta x} \left(\bar{c}_{j+\frac{1}{2}} \bar{S}_{j+\frac{1}{2}} - \bar{c}_{j-\frac{1}{2}} \bar{S}_{j-\frac{1}{2}} \right) \\
& = -\frac{R_j}{4\Delta x} \left(\llbracket c \rrbracket_{j+\frac{1}{2}} + \llbracket c \rrbracket_{j-\frac{1}{2}} \right) + \frac{S_j}{4\Delta x} \left(\llbracket c \rrbracket_{j+\frac{1}{2}} + \llbracket c \rrbracket_{j-\frac{1}{2}} \right), \\
& (u_j)_t = \frac{R_j + S_j}{2}.
\end{aligned}$$

We have the following theorem for the scheme:

Theorem 2.3. *Let $R_j(t)$ and $S_j(t)$ be approximate solutions generated by the scheme (2.11). Then*

$$\partial_t \left(\frac{\Delta x}{2} \sum_j (R_j^2(t) + S_j^2(t)) \right) = 0.$$

Proof. Proof of this theorem is very similar to Theorem 2.1. We multiply R_j to the first equation of (2.11), S_j to the second equation of (2.11) and add resulting equations. This yields,

$$\begin{aligned}
& \frac{1}{2} \frac{d}{dt} (R_j^2 + S_j^2) \\
& = \frac{1}{\Delta x} \bar{R}_{j+\frac{1}{2}} \bar{c}_{j+\frac{1}{2}} \bar{R}_{j+\frac{1}{2}} - \frac{1}{2\Delta x} \llbracket R \rrbracket_{j+\frac{1}{2}} \bar{c}_{j+\frac{1}{2}} \bar{R}_{j+\frac{1}{2}} \\
& \quad - \frac{1}{\Delta x} \bar{R}_{j-\frac{1}{2}} \bar{c}_{j-\frac{1}{2}} \bar{R}_{j-\frac{1}{2}} - \frac{1}{2\Delta x} \llbracket R \rrbracket_{j-\frac{1}{2}} \bar{c}_{j-\frac{1}{2}} \bar{R}_{j-\frac{1}{2}} \\
& \quad - \frac{R_j^2}{4\Delta x} \left(\llbracket c \rrbracket_{j+\frac{1}{2}} + \llbracket c \rrbracket_{j-\frac{1}{2}} \right) + \frac{R_j S_j}{4\Delta x} \left(\llbracket c \rrbracket_{j+\frac{1}{2}} + \llbracket c \rrbracket_{j-\frac{1}{2}} \right) \\
& \quad - \frac{1}{\Delta x} \bar{S}_{j+\frac{1}{2}} \bar{c}_{j+\frac{1}{2}} \bar{S}_{j+\frac{1}{2}} + \frac{1}{2\Delta x} \llbracket S \rrbracket_{j+\frac{1}{2}} \bar{c}_{j+\frac{1}{2}} \bar{S}_{j+\frac{1}{2}} \\
& \quad + \frac{1}{\Delta x} \bar{S}_{j-\frac{1}{2}} \bar{c}_{j-\frac{1}{2}} \bar{S}_{j-\frac{1}{2}} - \frac{1}{2\Delta x} \llbracket S \rrbracket_{j-\frac{1}{2}} \bar{c}_{j-\frac{1}{2}} \bar{S}_{j-\frac{1}{2}} \\
& \quad + \frac{S_j^2}{4\Delta x} \left(\llbracket c \rrbracket_{j+\frac{1}{2}} + \llbracket c \rrbracket_{j-\frac{1}{2}} \right) - \frac{R_j S_j}{4\Delta x} \left(\llbracket c \rrbracket_{j+\frac{1}{2}} + \llbracket c \rrbracket_{j-\frac{1}{2}} \right)
\end{aligned}$$

Next, multiplying by Δx and summing over all j gives

$$\begin{aligned}
\frac{d}{dt} \left(\frac{\Delta x}{2} \sum_j (R_j^2 + S_j^2) \right) & = \sum_j \left(F_{j+\frac{1}{2}} - F_{j-\frac{1}{2}} \right) - \frac{1}{2} \sum_j \left(\llbracket c \frac{R^2}{2} \rrbracket_{j+\frac{1}{2}} + \llbracket c \frac{R^2}{2} \rrbracket_{j-\frac{1}{2}} \right) \\
& \quad + \frac{1}{2} \sum_j \left(\llbracket c \frac{S^2}{2} \rrbracket_{j+\frac{1}{2}} + \llbracket c \frac{S^2}{2} \rrbracket_{j-\frac{1}{2}} \right) = 0,
\end{aligned}$$

where

$$F_{j+\frac{1}{2}} = \bar{R}_{j+\frac{1}{2}} \bar{c}_{j+\frac{1}{2}} \bar{R}_{j+\frac{1}{2}} - \bar{R}_{j+\frac{1}{2}} \bar{c}_{j+\frac{1}{2}} \bar{R}_{j+\frac{1}{2}}.$$

This proves the theorem. \square

2.7. Energy Dissipating Scheme Based On System (2.8). In-order to approximate dissipative solutions, we add some numerical viscosity to the energy conservative scheme (2.11) to obtain,

$$\begin{aligned}
(R_j)_t &- \frac{1}{\Delta x} \left(\bar{c}_{j+\frac{1}{2}} \bar{R}_{j+\frac{1}{2}} - \bar{c}_{j-\frac{1}{2}} \bar{R}_{j-\frac{1}{2}} \right) \\
&= -\frac{R_j}{4\Delta x} \left(\llbracket c \rrbracket_{j+\frac{1}{2}} + \llbracket c \rrbracket_{j-\frac{1}{2}} \right) \\
&\quad + \frac{S_j}{4\Delta x} \left(\llbracket c \rrbracket_{j+\frac{1}{2}} + \llbracket c \rrbracket_{j-\frac{1}{2}} \right) + \frac{1}{2\Delta x} \left(s_{j+\frac{1}{2}} \llbracket R \rrbracket_{j+\frac{1}{2}} - s_{j-\frac{1}{2}} \llbracket R \rrbracket_{j-\frac{1}{2}} \right), \\
(S_j)_t &+ \frac{1}{\Delta x} \left(\bar{c}_{j+\frac{1}{2}} \bar{S}_{j+\frac{1}{2}} - \bar{c}_{j-\frac{1}{2}} \bar{S}_{j-\frac{1}{2}} \right) \\
&= -\frac{R_j}{4\Delta x} \left(\llbracket c \rrbracket_{j+\frac{1}{2}} + \llbracket c \rrbracket_{j-\frac{1}{2}} \right) \\
&\quad + \frac{S_j}{4\Delta x} \left(\llbracket c \rrbracket_{j+\frac{1}{2}} + \llbracket c \rrbracket_{j-\frac{1}{2}} \right) + \frac{1}{2\Delta x} \left(s_{j+\frac{1}{2}} \llbracket S \rrbracket_{j+\frac{1}{2}} - s_{j-\frac{1}{2}} \llbracket S \rrbracket_{j-\frac{1}{2}} \right), \\
(u_j)_t &= \frac{R_j + S_j}{2}.
\end{aligned} \tag{2.12}$$

where we have chosen $s_{j\pm\frac{1}{2}} = \max\{c_j, c_{j\pm 1}\}$, i.e., the maximum local wave speed.

We have the following theorem illustrating the energy dissipation associated with (2.12)

Theorem 2.4. *Let $R_j(t)$ and $S_j(t)$ be approximate solutions generated by the scheme (2.12). Then,*

$$\partial_t \left(\frac{\Delta x}{2} \sum_j (R_j^2(t) + S_j^2(t)) \right) \leq 0.$$

Proof. Emulating the calculations of previous theorem, i.e., multiplying the first equation of (2.12) by R_j and second equation by S_j respectively, we have

$$\begin{aligned}
\frac{d}{dt} \left(\frac{\Delta x}{2} \sum_j (R_j^2 + S_j^2) \right) &= \sum_j \left(F_{j+\frac{1}{2}} - F_{j-\frac{1}{2}} \right) \\
&- \frac{1}{2} \sum_j \left(\llbracket c \frac{R^2}{2} \rrbracket_{j+\frac{1}{2}} + \llbracket c \frac{R^2}{2} \rrbracket_{j-\frac{1}{2}} \right) + \frac{1}{2} \sum_j \left(\llbracket c \frac{S^2}{2} \rrbracket_{j+\frac{1}{2}} + \llbracket c \frac{S^2}{2} \rrbracket_{j-\frac{1}{2}} \right) \\
&+ \frac{1}{2} \sum_j s_{j+\frac{1}{2}} \bar{R}_{j+\frac{1}{2}} \llbracket R \rrbracket_{j+\frac{1}{2}} - \frac{1}{4} \sum_j s_{j+\frac{1}{2}} \llbracket R \rrbracket_{j+\frac{1}{2}}^2 - \frac{1}{2} \sum_j s_{j-\frac{1}{2}} \bar{R}_{j-\frac{1}{2}} \llbracket R \rrbracket_{j-\frac{1}{2}} \\
&- \frac{1}{4} \sum_j s_{j-\frac{1}{2}} \llbracket R \rrbracket_{j-\frac{1}{2}}^2 + \frac{1}{2} \sum_j s_{j+\frac{1}{2}} \bar{S}_{j+\frac{1}{2}} \llbracket S \rrbracket_{j+\frac{1}{2}} - \frac{1}{4} \sum_j s_{j+\frac{1}{2}} \llbracket S \rrbracket_{j+\frac{1}{2}}^2 \\
&- \frac{1}{2} \sum_j s_{j-\frac{1}{2}} \bar{S}_{j-\frac{1}{2}} \llbracket S \rrbracket_{j-\frac{1}{2}} - \frac{1}{4} \sum_j s_{j-\frac{1}{2}} \llbracket S \rrbracket_{j-\frac{1}{2}}^2
\end{aligned}$$

Next, define

$$\begin{aligned}
G_{j+\frac{1}{2}} &= F_{j+\frac{1}{2}} + \frac{1}{2} s_{j+\frac{1}{2}} \bar{R}_{j+\frac{1}{2}} \llbracket R \rrbracket_{j+\frac{1}{2}} + \frac{1}{2} s_{j+\frac{1}{2}} \bar{S}_{j+\frac{1}{2}} \llbracket S \rrbracket_{j+\frac{1}{2}} \\
N_{j+\frac{1}{2}} &= \frac{1}{4} s_{j+\frac{1}{2}} \left(\llbracket R \rrbracket_{j+\frac{1}{2}}^2 + \llbracket S \rrbracket_{j+\frac{1}{2}}^2 \right).
\end{aligned}$$

Then we have

$$\frac{d}{dt} \left(\frac{\Delta x}{2} \sum_j (R_j^2 + S_j^2) \right) = \sum_j \left(G_{j+\frac{1}{2}} - G_{j-\frac{1}{2}} \right) - \sum_j \left(N_{j+\frac{1}{2}} + N_{j-\frac{1}{2}} \right)$$

$$-\frac{1}{2} \sum_j \left(\left[\left[c \frac{R^2}{2} \right] \right]_{j+\frac{1}{2}} + \left[\left[c \frac{R^2}{2} \right] \right]_{j-\frac{1}{2}} \right) + \frac{1}{2} \sum_j \left(\left[\left[c \frac{S^2}{2} \right] \right]_{j+\frac{1}{2}} + \left[\left[c \frac{S^2}{2} \right] \right]_{j-\frac{1}{2}} \right) \leq 0.$$

This proves the theorem. □

2.8. Energy Preserving Scheme Based On a Variational Formulation. All the above schemes were designed by rewriting the variational wave equation (1.3) as first-order systems and approximating these systems. However, one also design an energy conservative scheme by approximating the nonlinear wave equation (1.3) directly. To this end. we write the nonlinear wave equation (1.3) in the general form:

$$(2.13) \quad u_{tt} = -\frac{\delta H}{\delta u},$$

with $H = H(u, u_x) := \frac{1}{2}c^2(u)u_x^2$ being a part of the "Hamiltonian", and $\frac{\delta H}{\delta u}$ being the variational derivative of function $H(u, u_x)$ with respect to u .

In general, it is easy to show that for (2.13)

$$(2.14) \quad \frac{d}{dt} \int_{\mathbb{R}} \left(\frac{1}{2}u_t^2 + H(u, u_x) \right) dx = 0.$$

In fact, this is a direct consequence of the fact that

$$(2.15) \quad \frac{\delta H}{\delta u} = \frac{\partial H}{\partial u} - \frac{d}{dx} \left(\frac{\partial H}{\partial u_x} \right).$$

We also note that for equation (1.3),

$$\frac{\delta H}{\delta u} = c(u)c'(u)u_x^2 - (c^2(u)u_x)_x = -c^2(u)u_{xx} - c(u)c'(u)u_x^2 = -c(u)(c(u)u_x)_x.$$

Based on above observations, we propose the following scheme for (1.3)

$$(2.16) \quad (u_j)_{tt} + c(u_j)c'(u_j)(D^0 u_j)^2 - D^0 (c^2(u_j)D^0 u_j) = 0.$$

This scheme happens to be energy preserving as shown in the following theorem:

Theorem 2.5. *Let $u_j(t)$ be approximate solution generated by the scheme (2.16). Then we have*

$$\partial_t \left(\frac{\Delta x}{2} \sum_j ((u_j)_t^2 + c^2(u_j) (D^0 u_j)^2) \right) = 0.$$

Proof. We start by calculating

$$\begin{aligned} & \partial_t \left(\frac{\Delta x}{2} \sum_j ((u_j)_t^2 + c^2(u_j) (D^0 u_j)^2) \right) \\ &= \Delta x \sum_j \left((u_j)_t (u_j)_{tt} + c(u_j)c'(u_j) (D^0 u_j)^2 (u_j)_t + c^2(u_j)D^0 u_j D^0 (u_j)_t \right) \\ &= \Delta x \sum_j \left((u_j)_t (u_j)_{tt} + c(u_j)c'(u_j) (D^0 u_j)^2 (u_j)_t - D^0 (c^2(u_j)D^0 u_j) (u_j)_t \right) \\ &= 0. \end{aligned}$$

□

3. NUMERICAL EXPERIMENTS

In this section, we will test the numerical schemes developed in the previous section on several examples. The semi-discrete schemes (2.4), (2.6), (2.11) and (2.12) are integrated in time using a third order SSP-Runge Kutta method. The timestep Δt is chosen such that it satisfies the CFL-condition

$$(3.1) \quad \Delta t = \theta \frac{\Delta x}{\sup_u c(u)}$$

for some $0 \leq \theta \leq 0.5$. We denote by N the number of gridpoints in the spatial dimension.

3.1. Gaussian pulse. As a first test problem we consider (1.3) augmented with the initial data

$$(3.2) \quad \begin{aligned} u_0(x) &= \frac{\pi}{4} + \exp(-x^2), \\ u_1(x) &= -c(u_0(x)) (u_0)_x(x), \end{aligned}$$

on the domain $D = [-15, 15]$ with periodic boundary conditions and the function $c(u)$ given by

$$(3.3) \quad c(u) = \sqrt{\alpha \cos^2(u) + \beta \sin^2(u)},$$

where α, β are positive constants. For this experiment, we choose $\alpha = 0.5$ and $\beta = 4.5$. This Cauchy problem has already been numerically investigated in [8] and [11]. We compute approximations by the schemes at times, $T = 1, 10$. In Figure 3.1 the approximations computed by

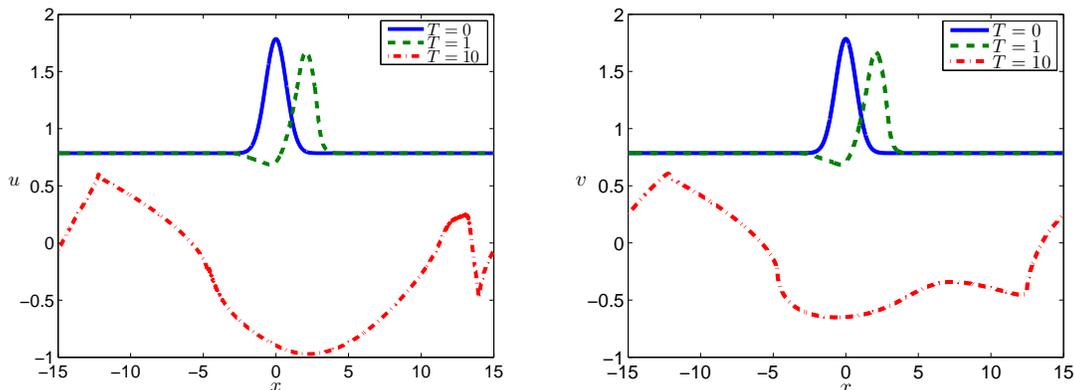


FIGURE 3.1. Approximations of u in (1.3), (3.2), (3.3) computed by scheme (2.4) and scheme (2.6) on a grid with $N_x = 15 \cdot 2^{12}$ points at time $T = 1, 10$ and with CFL-number $\theta = 0.05$. Left: Approximation by energy conservative scheme (2.4), Right: Approximation by energy dissipative scheme (2.6).

scheme (2.4) and (2.6) with CFL-number $\theta = 0.05$ at times $T = 1, 10$ are shown. We observe that at time $T = 1$ the approximated solution appears smooth whereas at time $T = 10$, we observe kinks in the solution indicating that singularities have appeared by this time.

As schemes (2.4) and (2.6), are based on the first-order system (2.2), we plot the quantities v and w in Figures 3.2 and 3.3, and observe high frequency oscillations in the approximations computed by the energy-conservative scheme (2.4). This is not unexpected as there is no numerical viscosity in this approximations and the high frequency oscillations are a manifestation of this effect. Furthermore, at time $T = 1$, the two approximations computed by (2.4) and (2.6) look alike, whereas we observe visible differences at time $T = 10$.

Similarly, the approximations computed with schemes (2.11) and (2.16) are qualitatively very close to those computed by the energy conservative scheme (2.4), whereas the approximations computed with (2.12) resembled those computed with (2.6). Furthermore, as predicted by our analysis and shown in Figure 3.4, the conservative schemes almost preserve the discrete L^2 -energy

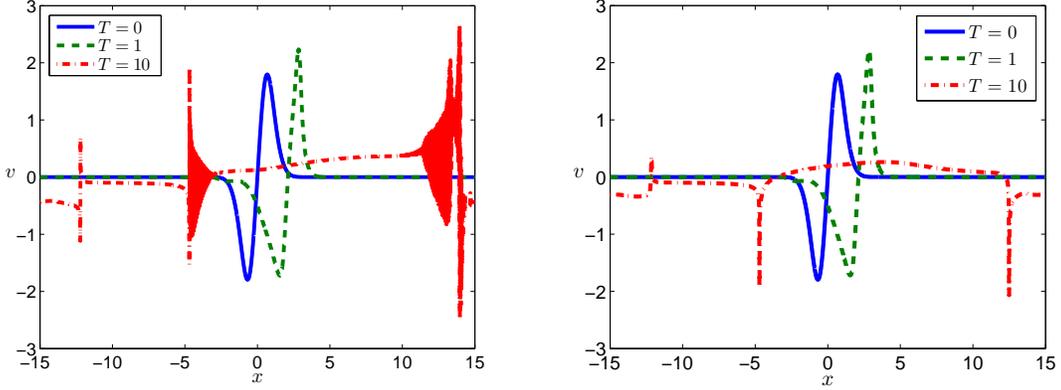


FIGURE 3.2. Approximations of the quantity v in (2.2), (3.2), (3.3) computed by scheme (2.4) and scheme (2.6) on a grid with $N_x = 15 \cdot 2^{12}$ points at time $T = 1, 10$ and with CFL-number $\theta = 0.05$. Left: Approximation by scheme (2.4), Right: Approximation by scheme (2.6).

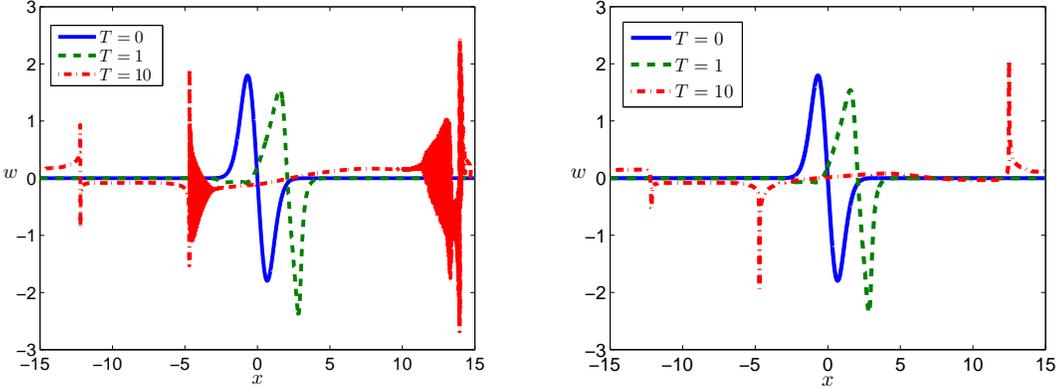


FIGURE 3.3. Approximations of the quantity w in (2.2), (3.2), (3.3) computed by scheme (2.4) and scheme (2.6) on a grid with $N_x = 15 \cdot 2^{12}$ points at time $T = 1, 10$ and with CFL-number $\theta = 0.05$. Left: Approximation by scheme (2.4), Right: Approximation by scheme (2.6).

over time whereas the approximations computed by the dissipative schemes lose energy by a significant amount. Note the difference in scales (in the Y-axis) between the adjacent plots in figure 3.4.

To investigate the possibility of different limit solutions approximated by the conservative and dissipative schemes, we compute reference approximations by schemes (2.4) and (2.6) at times $T = 1, 10$, with CFL-number $\theta = 0.05$ on a grid with cell size $\Delta x = 2^{-11}$ (i.e. the number of grid points is $N_x = 15 \cdot 2^{12}$) and test the convergence of the schemes towards these reference solutions. We measure the distance to the reference solutions in the following discrete relative L^2 -distance,

$$(3.4) \quad d^2(\mathbf{a}^N, \mathbf{b}^N) := 200 \times \frac{(\sum_j (a_j^N - b_j^N)^2)^{1/2}}{(\sum_j (a_j^N)^2)^{1/2} + (\sum_j (b_j^N)^2)^{1/2}}$$

for vectors $\mathbf{a}^N = (\dots, a_{j-1}^N, a_j^N, a_{j+1}^N, \dots)$, $\mathbf{b}^N = (\dots, b_{j-1}^N, b_j^N, b_{j+1}^N, \dots)$. The distances to the conservative and dissipative reference solution respectively, are shown in Tables 3.1, 3.2, 3.3 and 3.4. From Tables 3.1 and 3.2, we see that at time $T = 1$, all approximations to the variable u

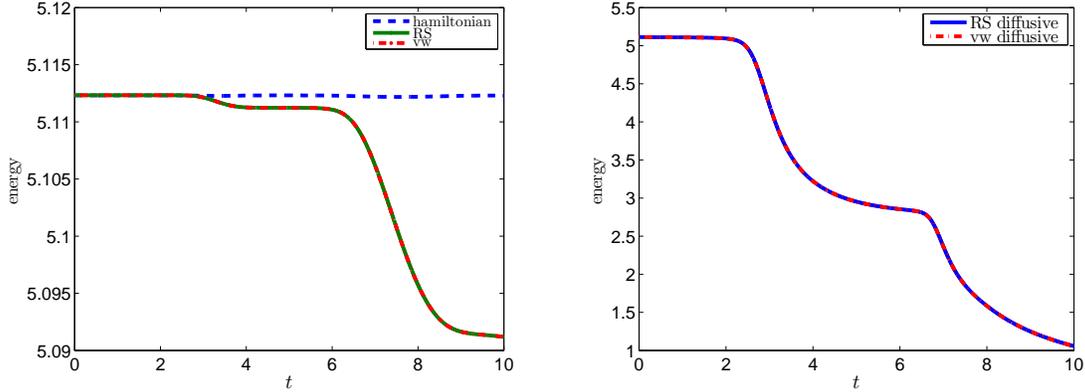


FIGURE 3.4. Evolution of discrete energies over time, Left: Energies for the conservative schemes (2.4), (2.11), (2.16), Right: Energies for the diffusive schemes (2.6), (2.12).

Δx	(2.4)	(2.6)	(2.11)	(2.12)	(2.16)
2^{-2}	3.2367	8.4373	3.2710	8.5292	2.8605
2^{-3}	1.1274	4.9475	1.1314	4.9974	1.0724
2^{-4}	0.4723	2.7432	0.4727	2.7693	0.4644
2^{-5}	0.2217	1.4592	0.2217	1.4726	0.2206
2^{-6}	0.1088	0.7557	0.1088	0.7625	0.1087
2^{-7}	0.0541	0.3852	0.0541	0.3886	0.0541
2^{-8}	0.0269	0.1946	0.0269	0.1963	0.0269
2^{-9}	0.0131	0.0978	0.0131	0.0986	0.0131

TABLE 3.1. $d^2(\mathbf{u}_{\Delta x}^N, \mathbf{u}_{\text{ref}}^N)$ for different mesh resolutions, $T = 1$, CFL-number $\theta = 0.05$, $\mathbf{u}_{\Delta x}^N$ approximation computed by the various schemes at different mesh resolutions, $\mathbf{u}_{\text{ref}}^N$ the reference solution computed by scheme (2.4).

Δx	(2.4)	(2.6)	(2.11)	(2.12)	(2.16)
2^{-2}	3.2353	8.4145	3.2700	8.5065	2.8565
2^{-3}	1.1280	4.9240	1.1322	4.9740	1.0713
2^{-4}	0.4735	2.7194	0.4741	2.7455	0.4647
2^{-5}	0.2234	1.4352	0.2235	1.4486	0.2219
2^{-6}	0.1117	0.7316	0.1118	0.7384	0.1114
2^{-7}	0.0594	0.3611	0.0594	0.3645	0.0593
2^{-8}	0.0363	0.1705	0.0363	0.1722	0.0362
2^{-9}	0.0276	0.0737	0.0276	0.0746	0.0276

TABLE 3.2. $d^2(\mathbf{u}_{\Delta x}^N, \mathbf{u}_{\text{ref}}^N)$ for different mesh resolutions, $T = 1$, CFL-number $\theta = 0.05$, $\mathbf{u}_{\Delta x}^N$ approximation computed by the various schemes at different mesh resolutions, $\mathbf{u}_{\text{ref}}^N$ the dissipative reference solution computed by scheme (2.6).

seem to converge to both reference solutions, so the two reference solutions are very close to each other.

However, at time $T = 10$, the approximations of the conservative schemes still seem to be converging to the reference solution computed by (2.4) whereas no convergence can be observed for the energy dissipative schemes (2.6) and (2.12) (Table 3.3). Similarly, the dissipative schemes seem to be converging to the dissipative reference solution whereas the distance of the conservative

Δx	(2.4)	(2.6)	(2.11)	(2.12)	(2.16)
2^{-2}	49.9592	95.6001	52.2856	96.0428	66.2850
2^{-3}	75.9922	75.1585	76.9143	75.2326	78.6955
2^{-4}	71.5391	75.4320	71.9087	75.4286	72.5368
2^{-5}	52.2962	75.9529	52.4645	75.9412	52.7209
2^{-6}	36.9257	74.3883	36.9673	74.3799	36.9809
2^{-7}	25.7497	72.4280	25.7554	72.4241	25.6531
2^{-8}	16.4966	71.5233	16.4962	71.5220	16.2811
2^{-9}	9.4041	71.8735	9.4031	71.8734	9.0068

TABLE 3.3. $d^2(\mathbf{u}_{\Delta x}^N, \mathbf{u}_{\text{ref}}^N)$ for different mesh resolutions, $T = 10$, CFL-number $\theta = 0.05$, $\mathbf{u}_{\Delta x}^N$ approximation computed by the various schemes at different mesh resolutions, $\mathbf{u}_{\text{ref}}^N$ the reference solution computed by the energy-conservative scheme (2.4).

Δx	(2.4)	(2.6)	(2.11)	(2.12)	(2.16)
2^{-2}	60.0811	81.5763	59.6149	81.9256	62.0062
2^{-3}	71.5451	50.5324	72.0433	50.5400	72.7812
2^{-4}	67.0084	41.7781	67.1806	41.8145	67.4443
2^{-5}	59.7701	34.6851	59.7986	34.7138	59.8481
2^{-6}	62.0292	27.4402	62.0238	27.4533	62.0309
2^{-7}	64.0325	20.2404	64.0339	20.2445	64.0901
2^{-8}	67.1313	13.6321	67.1327	13.6326	67.2587
2^{-9}	70.3864	7.9905	70.3874	7.9899	70.6403

TABLE 3.4. $d^2(\mathbf{u}_{\Delta x}^N, \mathbf{u}_{\text{ref}}^N)$ for different mesh resolutions, $T = 10$, CFL-number $\theta = 0.05$, $\mathbf{u}_{\Delta x}^N$ approximation computed by the various schemes at different mesh resolutions, $\mathbf{u}_{\text{ref}}^N$ the reference solution computed by the dissipative scheme (2.6).

approximations computed by (2.4), (2.11) and (2.16) to the dissipative reference solution remains (approximately) constant despite mesh refinement (Table 3.4). We conclude that the energy-conservative schemes converge to a different limit solution than the energy-dissipative schemes in this example. Furthermore, as the conservative schemes preserve energy, the limit of these schemes is the conservative solution. Similarly, the dissipative schemes converge to a solution that has lower energy than the initial data. Hence, this solution appears to be a dissipative solution of (1.3). This dichotomy of solutions is also illustrated in Figure 3.5 where the difference of conservative and dissipative solutions (realized as limits of the energy conservative and energy dissipative schemes, respectively) is apparent at time $T = 10$ (after singularity formation).

3.2. Traveling wave with infinite local energy. As a second example we consider a traveling wave solution of (1.3), that is a solution of the form

$$(3.5) \quad u(t, x) = \psi(x - st),$$

where $s \in \mathbb{R}$ is the wave speed. Glassey, Hunter and Zheng have shown in [9], that the function ψ is given as the solution of the ODE

$$(3.6) \quad \psi' \sqrt{|s^2 - c^2(\psi)|} = k,$$

where k is an integration constant. If $|s| \notin [c_0, c_1]$, where

$$c_0 = \min_{v \in \mathbb{R}} c(v), \quad c_1 = \max_{v \in \mathbb{R}} c(v),$$

the solution to the ODE (3.6) is smooth and unbounded on \mathbb{R} . If $|s| \in [c_0, c_1]$ on the other hand, then exists $u_0 \in [0, \pi/2]$ such that $|s| = c(u_0)$ and ψ' has a singularity. One can then construct a bounded traveling wave solution as

$$\psi(\xi) = u_0, \quad \text{for } \xi \leq \xi_0,$$

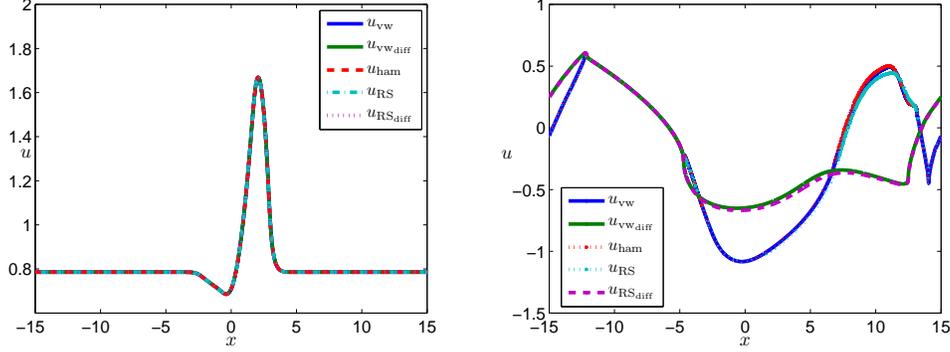


FIGURE 3.5. Approximations of (1.3), (3.2), (3.3) computed by schemes (2.4), (2.6), (2.11), (2.12) and (2.16) on a grid with $15 \cdot 2^{10}$ points and CFL-number $\theta = 0.2$. Left: At time $T = 1$, Right: At time $T = 10$.

$$(3.7) \quad \int_{u_0}^{\psi(\xi)} \sqrt{|c^2(u_0) - c^2(v)|} dv = k_1(\xi - \xi_0), \quad \text{for } \xi_0 \leq \xi \leq \psi^{-1}(\pi - u_0),$$

$$\psi(\xi) = \pi - u_0, \quad \text{for } \xi \geq \psi^{-1}(\pi - u_0),$$

for any $u_0 \in [0, \pi/2]$, any $\xi_0 \in \mathbb{R}$ and $k_1 > 0$. We choose (for this example) $s = \sqrt{\alpha}$, since for this case, we obtain an explicit expression for ψ , namely, for $\alpha = 0.5$ and $\beta = 1.5$, the function

$$(3.8) \quad \psi(\xi) = \begin{cases} 0 & \xi \leq 0, \\ \cos^{-1}(-2\xi + 1), & 0 < \xi < 1, \\ \pi, & \xi \geq 1, \end{cases}$$

with

$$(3.9) \quad \psi'(\xi) = \begin{cases} 0 & \xi \leq 0, \\ \frac{1}{\sqrt{\xi - \xi^2}}, & 0 < \xi < 1, \\ 0, & \xi \geq 1, \end{cases}$$

is a traveling wave solution. This function has infinite local energy as demonstrated in [9]. We compute approximations to the solution at time $T = 0.5$ and $T = 1$, when it has the form

$$(3.10) \quad u(T, x) = \begin{cases} 0 & x \leq \sqrt{\alpha}T, \\ \cos^{-1}(-2(x - \sqrt{\alpha}T) + 1), & \sqrt{\alpha}T < x < 1 + \sqrt{\alpha}T, \\ \pi, & x \geq 1 + \sqrt{\alpha}T. \end{cases}$$

In Figure 3.6, we plot the approximations of (3.10) computed by the different schemes on a mesh with $\Delta x = 2^{-13}$ gridpoints and CFL-number $\theta = 0.4$ at time $T = 0.5$ and $T = 1$. We observe that in the lower part between $y = 0$ and $y = 0.4$, the approximations appear to differ from the exact solution, and the discrepancy increases with time T . However, as we can see from Tables 3.5 and 3.6 it appears all that all the schemes but the hamiltonian scheme converge, at however, a very slow rate. This slow rate of convergence is not unexpected given the presence of strong singularities (with infinite local energy).

3.3. Multiplicity of dissipative solutions. The above numerical experiments clearly illustrate that one set of schemes converge to a conservative solution whereas another to a dissipative solution of the variational wave equation (1.3). Is there uniqueness within these two classes of solutions? A priori, it seems that in contrast to conservative solutions, one might be able to construct multiple dissipative solutions by varying the amount and rate of energy dissipation. We study this

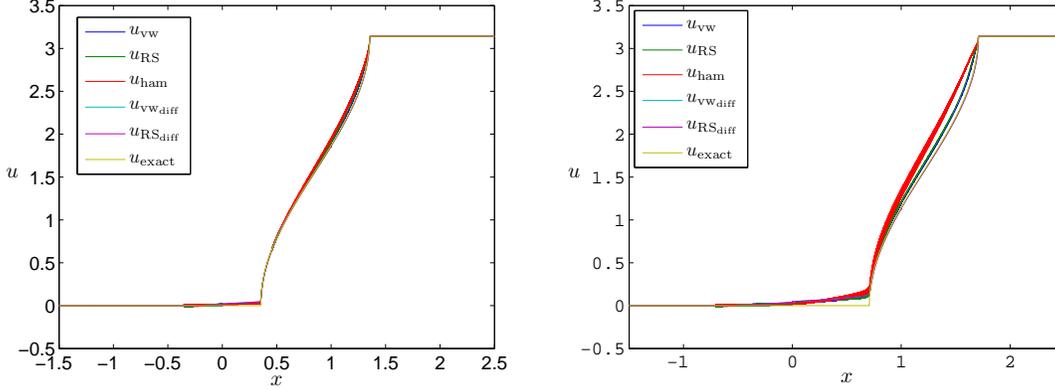


FIGURE 3.6. Approximations of (3.10) computed by schemes (2.4), (2.6), (2.11), (2.12) and (2.16) on a grid with cell size $\Delta x = 2^{-13}$ points and CFL-number $\theta = 0.4$. Left: At time $T = 0.5$, Right: At time $T = 1$.

scheme	(2.4)	(2.11)	(2.16)	(2.6)	(2.12)
$\Delta x = 2^{-5}$	6.2205	6.2292	4.4418	5.0283	5.1028
$\Delta x = 2^{-6}$	4.6404	4.6546	3.3480	3.8852	3.9214
$\Delta x = 2^{-7}$	3.4806	3.4937	2.5925	2.9698	2.9897
$\Delta x = 2^{-8}$	2.7565	2.7672	2.2064	2.3253	2.3367
$\Delta x = 2^{-9}$	2.3243	2.3365	2.0482	1.8115	1.8181
$\Delta x = 2^{-10}$	2.1222	2.1437	2.0499	1.4261	1.4300
$\Delta x = 2^{-11}$	2.0401	2.0828	2.1209	1.1282	1.1306
$\Delta x = 2^{-12}$	1.9870	2.0666	2.2118	0.8970	0.8984
$\Delta x = 2^{-13}$	1.8997	2.0318	2.2988	0.7167	0.7175

TABLE 3.5. $d^2(\mathbf{u}_{\Delta x}, \mathbf{u}_{\text{exact}})$ between the exact solution (3.10) and the approximations for different mesh resolutions, $T = 0.5$, $\theta = 0.2$.

scheme	(2.4)	(2.11)	(2.16)	(2.6)	(2.12)
$\Delta x = 2^{-5}$	11.7380	11.6747	10.2197	11.7075	11.4846
$\Delta x = 2^{-6}$	9.2074	9.1694	8.1966	9.5308	9.4172
$\Delta x = 2^{-7}$	7.4764	7.4783	6.9984	7.7588	7.6963
$\Delta x = 2^{-8}$	6.2859	6.3612	6.4006	6.2545	6.2171
$\Delta x = 2^{-9}$	5.4966	5.7117	6.3075	5.0454	5.0213
$\Delta x = 2^{-10}$	4.8401	5.2414	6.4866	4.0728	4.0568
$\Delta x = 2^{-11}$	4.1818	4.7290	6.7554	3.2958	3.2850
$\Delta x = 2^{-12}$	3.5273	4.1234	7.0079	2.6766	2.6695
$\Delta x = 2^{-13}$	2.9187	3.4861	7.1997	2.1830	2.1783

TABLE 3.6. $d^2(\mathbf{u}_{\Delta x}, \mathbf{u}_{\text{exact}})$ between the exact solution (3.10) and the approximations for different mesh resolutions, $T = 1$, $\theta = 0.4$.

possibility by modifying the dissipative scheme (2.6) to

$$\begin{aligned}
 (v_j)_t & - \frac{1}{\Delta x} \left(\bar{c}_{j+\frac{1}{2}} \bar{w}_{j+\frac{1}{2}} - \bar{c}_{j-\frac{1}{2}} \bar{w}_{j-\frac{1}{2}} \right) \\
 & = - \frac{1}{2\Delta x} \left(\llbracket c \rrbracket_{j+\frac{1}{2}} \bar{w}_{j+\frac{1}{2}} + \llbracket c \rrbracket_{j-\frac{1}{2}} \bar{w}_{j-\frac{1}{2}} \right) + \frac{\kappa}{2\Delta x} \left(s_{j+\frac{1}{2}} \llbracket v \rrbracket_{j+\frac{1}{2}} - s_{j-\frac{1}{2}} \llbracket v \rrbracket_{j-\frac{1}{2}} \right) \\
 (w_j)_t & - \frac{1}{\Delta x} \left(\bar{c} v_{j+\frac{1}{2}} - \bar{c} v_{j-\frac{1}{2}} \right) = \frac{\kappa}{2\Delta x} \left(s_{j+\frac{1}{2}} \llbracket w \rrbracket_{j+\frac{1}{2}} - s_{j-\frac{1}{2}} \llbracket w \rrbracket_{j-\frac{1}{2}} \right) \\
 (u_j)_t & = v_j,
 \end{aligned}
 \tag{3.11}$$

by adding κ to scale the numerical viscosity in (2.6)¹. We investigate the above question by setting κ to different values, resulting in different amounts of energy-loss and possibly, convergence to different dissipative solutions. We test the convergence of resulting numerical approximations by (3.11) of (1.3), (3.2), (3.3) for $\kappa = 0.01, 0.05, 0.1, 1, 2, 5, 10, 20$ towards the reference solutions from Section 3.1, computed by both schemes (2.4) and (2.6). The distances d^2 as defined in (3.4) are displayed in Tables 3.7 (dissipative reference solution) for time $T = 10$ (after singularity formation) and CFL-number $\theta = 0.05$.

$\Delta x \setminus \kappa$	0.01	0.05	0.1	1	2	5	10	20
2^{-2}	54.93	47.42	43.86	81.58	142.49	162.03	166.35	169.59
2^{-3}	71.27	63.95	47.50	50.53	85.11	151.50	162.14	166.37
2^{-4}	66.01	48.50	31.36	41.78	50.76	108.55	151.64	162.18
2^{-5}	58.34	28.33	17.25	34.69	41.71	56.59	108.74	151.68
2^{-6}	51.59	11.03	8.19	27.44	34.54	44.12	56.61	108.79
2^{-7}	37.25	3.40	2.84	20.24	27.31	36.80	44.11	56.61
2^{-8}	24.40	3.62	0.7	13.63	20.15	29.60	36.8	44.11
2^{-9}	18.93	4.88	3.01	7.99	13.59	22.39	29.6	36.8

TABLE 3.7. $d^2(\mathbf{u}_{\Delta x}, \mathbf{u}_{\text{ref}})$ between the dissipative reference solution computed by (2.6) and the approximations by (3.11) for different mesh resolutions and diffusion coefficient κ , $T = 10$, $\theta = 0.05$.

The results, presented Table 3.7, clearly show that all the approximations (computed with different values of the diffusion coefficient κ), clearly converge to the same dissipative reference solution. Furthermore, we have listed the discrete energy ratio

$$(3.12) \quad E_{\text{rel}} = \frac{\sum_j \{(v_j^M)^2 + (w_j^M)^2\}}{\sum_j \{(v_j^0)^2 + (w_j^0)^2\}},$$

where v_j^0, w_j^0 are the approximations at the initial time and v_j^M, w_j^M are the approximations at the final time T . From Table 3.8, we observe that these ratios seem to converge to ≈ 0.2 for all the tested κ , showing that there is a universal rate of energy dissipation, associated with the dissipative solutions (at least in this example).

$\Delta x \setminus \kappa$	0.01	0.05	0.1	1	2	5	10	20
2^{-2}	0.8438	0.5002	0.3326	0.0740	0.0257	0.0052	0.0014	0.0003
2^{-3}	0.8021	0.4899	0.3124	0.1291	0.0702	0.0171	0.0051	0.0014
2^{-4}	0.7086	0.3760	0.2505	0.1630	0.1269	0.0515	0.0170	0.0051
2^{-5}	0.6174	0.2939	0.214	0.1779	0.1615	0.1095	0.0514	0.0170
2^{-6}	0.5304	0.2368	0.2034	0.1842	0.1769	0.1526	0.1094	0.0514
2^{-7}	0.4216	0.2122	0.2037	0.1891	0.1837	0.1730	0.1525	0.1094
2^{-8}	0.3331	0.2081	0.2051	0.1943	0.1889	0.1817	0.1729	0.1525
2^{-9}	0.2801	0.2076	0.2060	0.1987	0.1942	0.1871	0.1817	0.1729

TABLE 3.8. E_{rel} as in (3.12) for different mesh resolutions and diffusion coefficient κ , $T = 10$, $\theta = 0.05$.

3.4. Time stepping schemes. Energy conservation for the schemes (2.4) and (2.11) has only been proved in the semi-discrete setting. Some time integration routine needs to be used in order to obtain a fully discrete scheme. The choice of the time integration scheme might lead to some energy dissipation or production. We explore this issue by integrating the energy conservative scheme (2.4) in time using different Runge-Kutta methods, namely the 2nd-order strong stability preserving (SSPRK2) method, the 3rd-order SSPRK3 and the standard RK4 procedure. Furthermore, a

¹In a similar way, we generalize scheme (2.12).

standard Leap-Frog (LF) time-stepping procedure has also been used for the sake of comparison. It can be readily shown that the fully discrete scheme, combining leap-frog time stepping with the energy conservative scheme (2.4) conserves the discrete energy:

$$\Delta x \sum_j \{v_j^n v_j^{n+1} + w_j^n w_j^{n+1}\},$$

for all time levels n .

To illustrate the energy balance of the above time stepping procedures, we have computed the energy ratio (3.12) for the variational wave equation (1.3), (3.2), (3.3), $\alpha = 0.5$, $\beta = 4.5$; with different time-stepping methods, for all the above mentioned time-stepping schemes at CFL-numbers $\theta = 0.1, 0.2, 0.4$. The results of the mesh refinement study are displayed in Table 3.9.

Δx	θ	SSPRK2	SSPRK3	RK4	lf
2^{-2}	0.4	1.1006	0.9761	0.9996	1.0018
2^{-3}	0.4	1.1602	0.9660	0.9994	1.0017
2^{-4}	0.4	1.5334	0.9285	0.9984	1.0016
2^{-5}	0.4	2.3257	0.8699	0.9968	1.0011
2^{-6}	0.4	4.8354	0.8022	0.9939	1.0008
2^{-7}	0.4	7.4642	0.7197	0.9886	1.0008
2^{-8}	0.4	6.0891	0.6684	0.9794	1.0008
2^{-2}	0.2	1.0111	0.9969	1.0000	1.0004
2^{-3}	0.2	1.0153	0.9954	1.0000	1.0004
2^{-4}	0.2	1.0361	0.9895	0.9999	1.0004
2^{-5}	0.2	1.0740	0.9790	0.9999	1.0003
2^{-6}	0.2	1.1509	0.9619	0.9998	1.0002
2^{-7}	0.2	1.3280	0.9302	0.9996	1.0002
2^{-8}	0.2	1.8364	0.8822	0.9993	1.0002
2^{-2}	0.1	1.0014	0.9996	1.0000	1.0001
2^{-3}	0.1	1.0018	0.9994	1.0000	1.0001
2^{-4}	0.1	1.0042	0.9987	1.0000	1.0001
2^{-5}	0.1	1.0084	0.9973	1.0000	1.0001
2^{-6}	0.1	1.0158	0.9949	1.0000	1.0000
2^{-7}	0.1	1.0307	0.9904	1.0000	1.0001
2^{-8}	0.1	1.0584	0.9825	1.0000	1.0001

TABLE 3.9. E_{rel} as in (3.12) for scheme (2.4), problem (1.3), (3.2), (3.3), for different mesh resolutions, time stepping methods and CFL-numbers $\theta = 0.1, 0.2, 0.4$, $T = 10$.

We observe that for ‘higher’ CFL-numbers, such as 0.4, the leap frog scheme performs best whereas the 2nd and 3rd order SSPRK methods can produce/dissipative energy of significant amplitude. However, for lower CFL numbers, the standard RK4 also performs adequately in terms of energy balance, vis a vis the leap frog time stepping scheme.

4. NUMERICAL SCHEMES IN TWO-SPACE DIMENSIONS

As in the one-dimensional case, we will design energy conservative and energy dissipative finite difference discretizations of the two-dimensional version of the nonlinear variational wave equation (1.7) by rewriting it as a first-order system. To this end, we introduce three new independent variables:

$$\begin{aligned} p &:= u_t, \\ v &:= \cos(u)u_x + \sin(u)u_y, \\ w &:= \sin(u)u_x - \cos(u)u_y, \end{aligned}$$

Then, for smooth solutions, equation (1.7) is equivalent to the following system for (p, v, w, u) ,

$$(4.1) \quad \begin{cases} p_t - \alpha(\phi(u)v)_x - \alpha(\psi(u)v)_y - \beta(\psi(u)w)_x + \beta(\phi(u)w)_y - \alpha v w + \beta v w = 0, \\ v_t - (\phi(u)p)_x + p\phi_x - (\psi(u)p)_y + p\psi_y + p w = 0, \\ w_t - (\psi(u)p)_x + p\psi_x + (\phi(u)p)_y - p\phi_y - p v = 0, \\ u_t = v \end{cases}$$

where $\phi(u) := \cos(u)$, and $\psi(u) := \sin(u)$.

4.1. The grid. We introduce some notation needed to define the finite difference schemes in two dimensions. we reserve $\Delta x, \Delta y$ and Δt to denote three small positive numbers that represent the spatial and temporal discretization parameters, respectively, of the numerical schemes. Given $\Delta x, \Delta y, \Delta t > 0$, let D^\pm denote the discrete forward and backward differences, respectively, in the spatial direction, i.e.,

$$\begin{aligned} D_x^\pm g(x, y) &= \pm \frac{1}{\Delta x} (g(x \pm \Delta x, y) - g(x, y)), & D_y^\pm g(x, y) &= \pm \frac{1}{\Delta y} (g(x, y \pm \Delta y) - g(x, y)), \\ D_x^0 g(x, y) &= \frac{1}{2} (D_x^+ g(x) + D_x^- g(x)), & D_y^0 g(x, y) &= \frac{1}{2} (D_y^+ g(x) + D_y^- g(x)). \end{aligned}$$

for any function $g : \mathbb{R} \times \mathbb{R} \rightarrow \mathbb{R}$ admitting pointvalues. Similarly, we let D_t^\pm denote the forward and backward differences, respectively, in the time direction, i.e.,

$$D_t^\pm h(x, y, t) = \pm \frac{1}{\Delta t} (h(x, y, t \pm \Delta t) - h(x, y, t))$$

for any function $h : \mathbb{Q}_T \rightarrow R$ admitting pointvalues. For $i, j \in \mathbb{N}_0 = \mathbb{N} \cup \{0\}$, we set $x_i = i\Delta x$, $y_j = j\Delta y$ and for $n = 0, 1, \dots, N$, where $N\Delta t = T$ for some fixed time horizon $T > 0$, we set $t_n = n\Delta t$. For any function $g = g(x, y)$ admitting pointvalues we write $g_{i,j} = g(x_i, y_j)$, and similarly for any function $h = h(x, y, t)$ admitting pointvalues we write $h_{i,j}^n = h(x_i, y_j, t_n)$. We also introduce the *Cartesian* spatial and temporal grid cells

$$I_{i,j} = [x_{i-\frac{1}{2}}, x_{i+\frac{1}{2}}) \times [y_{j-\frac{1}{2}}, y_{j+\frac{1}{2}}), \quad I_{i,j}^n = I_{i,j} \times [t_n, t_{n+1}).$$

Furthermore we introduce the jump, and respectively, the average of a quantity w across the interfaces $x_{i+\frac{1}{2}}$ and $y_{j+\frac{1}{2}}$

$$\begin{aligned} \bar{w}_{i,j+\frac{1}{2}} &:= \frac{w_{i,j} + w_{i,j+1}}{2}, \\ \bar{w}_{i+\frac{1}{2},j} &:= \frac{w_{i,j} + w_{i+1,j}}{2}, \\ \llbracket w \rrbracket_{i,j+\frac{1}{2}} &:= w_{i,j+1} - w_{i,j}, \\ \llbracket w \rrbracket_{i+\frac{1}{2},j} &:= w_{i+1,j} - w_{i,j}. \end{aligned}$$

The following identities are readily verified:

$$(4.2) \quad \begin{aligned} \llbracket uv \rrbracket_{i,j+\frac{1}{2}} &= \bar{u}_{i,j+\frac{1}{2}} \llbracket v \rrbracket_{i,j+\frac{1}{2}} + \llbracket u \rrbracket_{i,j+\frac{1}{2}} \bar{v}_{i,j+\frac{1}{2}}, \\ \llbracket uv \rrbracket_{i+\frac{1}{2},j} &= \bar{u}_{i+\frac{1}{2},j} \llbracket v \rrbracket_{i+\frac{1}{2},j} + \llbracket u \rrbracket_{i+\frac{1}{2},j} \bar{v}_{i+\frac{1}{2},j}, \\ v_{i,j} &= \bar{v}_{i,j\pm\frac{1}{2}} \mp \frac{1}{2} \llbracket v \rrbracket_{i,j\pm\frac{1}{2}}, \\ v_{i,j} &= \bar{v}_{i\pm\frac{1}{2},j} \mp \frac{1}{2} \llbracket v \rrbracket_{i\pm\frac{1}{2},j}. \end{aligned}$$

4.2. Energy conservative scheme. Based on the first-order system (4.1), We propose the following finite difference scheme to approximate the two-dimensional version of the nonlinear variational wave equation (1.7):

(4.3)

$$\begin{aligned}
& (p_{i,j})_t - \frac{\alpha}{\Delta x} \left(\bar{\phi} v_{i+\frac{1}{2},j} - \bar{\phi} v_{i-\frac{1}{2},j} \right) - \frac{\alpha}{\Delta y} \left(\bar{\psi} v_{i,j+\frac{1}{2}} - \bar{\psi} v_{i,j-\frac{1}{2}} \right) - \frac{\beta}{\Delta x} \left(\bar{\psi} w_{i+\frac{1}{2},j} - \bar{\psi} w_{i-\frac{1}{2},j} \right) \\
& \quad + \frac{\beta}{\Delta y} \left(\bar{\phi} w_{i,j+\frac{1}{2}} - \bar{\phi} w_{i,j-\frac{1}{2}} \right) - \alpha v_{i,j} w_{i,j} + \beta v_{i,j} w_{i,j} = 0, \\
& (v_{i,j})_t - \frac{1}{\Delta x} \left(\bar{\phi}_{i+\frac{1}{2},j} \bar{p}_{i+\frac{1}{2},j} - \bar{\phi}_{i-\frac{1}{2},j} \bar{p}_{i-\frac{1}{2},j} \right) + \frac{1}{2\Delta x} \bar{p}_{i+\frac{1}{2},j} \llbracket \phi \rrbracket_{i+\frac{1}{2},j} + \frac{1}{2\Delta x} \bar{p}_{i-\frac{1}{2},j} \llbracket \phi \rrbracket_{i-\frac{1}{2},j} \\
& \quad - \frac{1}{\Delta y} \left(\bar{\psi}_{i,j+\frac{1}{2}} \bar{p}_{i,j+\frac{1}{2}} - \bar{\psi}_{i,j-\frac{1}{2}} \bar{p}_{i,j-\frac{1}{2}} \right) + \frac{1}{2\Delta y} \bar{p}_{i,j+\frac{1}{2}} \llbracket \psi \rrbracket_{i,j+\frac{1}{2}} + \frac{1}{2\Delta y} \bar{p}_{i,j-\frac{1}{2}} \llbracket \psi \rrbracket_{i,j-\frac{1}{2}} \\
& \quad \quad + p_{i,j} w_{i,j} = 0, \\
& (w_{i,j})_t - \frac{1}{\Delta x} \left(\bar{\psi}_{i+\frac{1}{2},j} \bar{p}_{i+\frac{1}{2},j} - \bar{\psi}_{i-\frac{1}{2},j} \bar{p}_{i-\frac{1}{2},j} \right) + \frac{1}{2\Delta x} \bar{p}_{i+\frac{1}{2},j} \llbracket \psi \rrbracket_{i+\frac{1}{2},j} + \frac{1}{2\Delta x} \bar{p}_{i-\frac{1}{2},j} \llbracket \psi \rrbracket_{i-\frac{1}{2},j} \\
& \quad + \frac{1}{\Delta y} \left(\bar{\phi}_{i,j+\frac{1}{2}} \bar{p}_{i,j+\frac{1}{2}} - \bar{\phi}_{i,j-\frac{1}{2}} \bar{p}_{i,j-\frac{1}{2}} \right) - \frac{1}{2\Delta y} \bar{p}_{i,j+\frac{1}{2}} \llbracket \phi \rrbracket_{i,j+\frac{1}{2}} - \frac{1}{2\Delta y} \bar{p}_{i,j-\frac{1}{2}} \llbracket \phi \rrbracket_{i,j-\frac{1}{2}} \\
& \quad \quad - p_{i,j} v_{i,j} = 0, \\
& (u_{i,j})_t = v_{i,j}.
\end{aligned}$$

The above scheme preserves a discrete version of the energy as reported in the following theorem:

Theorem 4.1. *Let $p_{ij}(t)$, $v_{i,j}(t)$ and $w_{i,j}(t)$ be approximate solutions generated by the scheme (4.3). Then*

$$\partial_t \left(\frac{\Delta x \Delta y}{2} \sum_i \sum_j (p_{i,j}^2(t) + \alpha v_{i,j}^2(t) + \beta w_{i,j}^2(t)) \right) = 0.$$

Proof. The proof of this theorem is identical to Theorem 2.1. In fact multiplying the first equation of (4.3) by $p_{i,j}$, second equation by $v_{i,j}$ and third equation by $w_{i,j}$ respectively, adding those resulting equations and using relations (4.2) we obtain the desired result. \square

4.3. Energy dissipative scheme. As in the one-dimensional case, we can add some *numerical viscosity* to the energy conservative scheme (4.3) to obtain the following energy dissipative scheme for approximating the variational wave equation (1.7):

$$\begin{aligned}
(4.4) \quad & (p_{i,j})_t - \frac{\alpha}{\Delta x} \left(\bar{\phi} v_{i+\frac{1}{2},j} - \bar{\phi} v_{i-\frac{1}{2},j} \right) - \frac{\alpha}{\Delta y} \left(\bar{\psi} v_{i,j+\frac{1}{2}} - \bar{\psi} v_{i,j-\frac{1}{2}} \right) - \frac{\beta}{\Delta x} \left(\bar{\psi} w_{i+\frac{1}{2},j} - \bar{\psi} w_{i-\frac{1}{2},j} \right) \\
& + \frac{\beta}{\Delta y} \left(\bar{\phi} w_{i,j+\frac{1}{2}} - \bar{\phi} w_{i,j-\frac{1}{2}} \right) - \alpha v_{i,j} w_{i,j} + \beta v_{i,j} w_{i,j} \\
& = \frac{1}{2\Delta y} \left(s_{i,j+\frac{1}{2}} \llbracket p \rrbracket_{i,j+\frac{1}{2}} - s_{i,j-\frac{1}{2}} \llbracket p \rrbracket_{i,j-\frac{1}{2}} \right) + \frac{1}{2\Delta x} \left(s_{i+\frac{1}{2},j} \llbracket p \rrbracket_{i+\frac{1}{2},j} - s_{i-\frac{1}{2},j} \llbracket p \rrbracket_{i-\frac{1}{2},j} \right), \\
& (v_{i,j})_t - \frac{1}{\Delta x} \left(\bar{\phi}_{i+\frac{1}{2},j} \bar{p}_{i+\frac{1}{2},j} - \bar{\phi}_{i-\frac{1}{2},j} \bar{p}_{i-\frac{1}{2},j} \right) + \frac{1}{2\Delta x} \bar{p}_{i+\frac{1}{2},j} \llbracket \phi \rrbracket_{i+\frac{1}{2},j} + \frac{1}{2\Delta x} \bar{p}_{i-\frac{1}{2},j} \llbracket \phi \rrbracket_{i-\frac{1}{2},j} \\
& - \frac{1}{\Delta y} \left(\bar{\psi}_{i,j+\frac{1}{2}} \bar{p}_{i,j+\frac{1}{2}} - \bar{\psi}_{i,j-\frac{1}{2}} \bar{p}_{i,j-\frac{1}{2}} \right) + \frac{1}{2\Delta y} \bar{p}_{i,j+\frac{1}{2}} \llbracket \psi \rrbracket_{i,j+\frac{1}{2}} + \frac{1}{2\Delta y} \bar{p}_{i,j-\frac{1}{2}} \llbracket \psi \rrbracket_{i,j-\frac{1}{2}} \\
& + p_{i,j} w_{i,j} = \frac{1}{2\Delta y} \left(\llbracket v \rrbracket_{i,j+\frac{1}{2}} - \llbracket v \rrbracket_{i,j-\frac{1}{2}} \right) + \frac{1}{2\Delta x} \left(\llbracket v \rrbracket_{i+\frac{1}{2},j} - \llbracket v \rrbracket_{i-\frac{1}{2},j} \right), \\
& (w_{i,j})_t - \frac{1}{\Delta x} \left(\bar{\psi}_{i+\frac{1}{2},j} \bar{p}_{i+\frac{1}{2},j} - \bar{\psi}_{i-\frac{1}{2},j} \bar{p}_{i-\frac{1}{2},j} \right) + \frac{1}{2\Delta x} \bar{p}_{i+\frac{1}{2},j} \llbracket \psi \rrbracket_{i+\frac{1}{2},j} + \frac{1}{2\Delta x} \bar{p}_{i-\frac{1}{2},j} \llbracket \psi \rrbracket_{i-\frac{1}{2},j} \\
& + \frac{1}{\Delta y} \left(\bar{\phi}_{i,j+\frac{1}{2}} \bar{p}_{i,j+\frac{1}{2}} - \bar{\phi}_{i,j-\frac{1}{2}} \bar{p}_{i,j-\frac{1}{2}} \right) - \frac{1}{2\Delta y} \bar{p}_{i,j+\frac{1}{2}} \llbracket \phi \rrbracket_{i,j+\frac{1}{2}} - \frac{1}{2\Delta y} \bar{p}_{i,j-\frac{1}{2}} \llbracket \phi \rrbracket_{i,j-\frac{1}{2}} \\
& - p_{i,j} v_{i,j} = \frac{\nu}{2\Delta y} \left(\llbracket w \rrbracket_{i,j+\frac{1}{2}} - \llbracket w \rrbracket_{i,j-\frac{1}{2}} \right) + \frac{\nu}{2\Delta x} \left(\llbracket w \rrbracket_{i+\frac{1}{2},j} - \llbracket w \rrbracket_{i-\frac{1}{2},j} \right), \\
& (u_{i,j})_t = v_{i,j}.
\end{aligned}$$

Following very similar arguments, as used in the proof of Theorem 2.2, we can prove the following theorem:

Theorem 4.2. *Let $p_{i,j}(t)$, $v_{i,j}(t)$ and $w_{i,j}(t)$ be approximate solutions generated by the scheme (4.4). Then*

$$\partial_t \left(\frac{\Delta x \Delta y}{2} \sum_i \sum_j (p_{i,j}^2(t) + \alpha v_{i,j}^2(t) + \beta w_{i,j}^2(t)) \right) \leq 0.$$

4.4. Numerical experiments. We illustrate the energy conservative scheme (4.3) and the energy dissipative scheme (4.4) by considering the first-order system (4.1) with the following initial data

$$(4.5a) \quad u_0(x, y) = 2 \cos(2\pi x) \sin(2\pi y),$$

$$(4.5b) \quad u_1(x, y) = \sin(2\pi(x - y)),$$

on the domain $D = [0, 1]^2$ with periodic boundary conditions and coefficients $\alpha = 0.5$, $\beta = 1.5$ in a , b and c at times $T = 2$ and $T = 4$. For the time integration we have chosen a 3rd order strong stability preserving Runge Kutta method for the energy-dissipative scheme and leap-frog time stepping for the energy-conservative scheme

Approximations computed by schemes (4.3), (4.4) respectively, on a mesh with 2048 points in each coordinate direction can be seen in Figures 4.1, 4.2, 4.3 and 4.4. From the above figures, we observe that both the conservative and dissipative schemes seem to resolve the solution in a stable manner. Although the two schemes seems to converge to the same limit at time $T = 2$, the limits, computed by the energy conservative and energy dissipative schemes differ at time $T = 4$. These results are also confirmed by a convergence study, performed in a manner analogous to the one-dimensional case. However, we omit the convergence tables for brevity in the exposition.

5. CONCLUSION

We have considered a nonlinear variational wave equation, that models (both one and two dimensional) planar waves in the dynamics of nematic liquid crystals. Our schemes are based on either the conservation or the dissipation of the energy associated with these equations. In the one-dimensional case, we rewrite the variational wave equation (1.3) in the form of two equivalent first-order systems. Energy conservative as well as energy dissipative schemes, approximating both

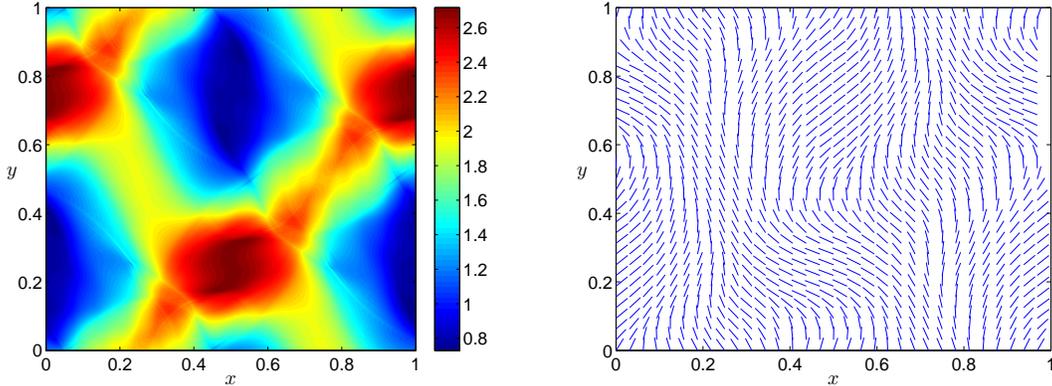


FIGURE 4.1. Approximations of the solution of (1.7) computed by scheme (4.3) on a grid with cell size $\Delta x = \Delta y = 2^{-11}$, CFL-number $\theta = 0.4$ at time $T = 2$. Left: the angle u , right: the corresponding director $\mathbf{n} = (\cos(u), \sin(u))$.

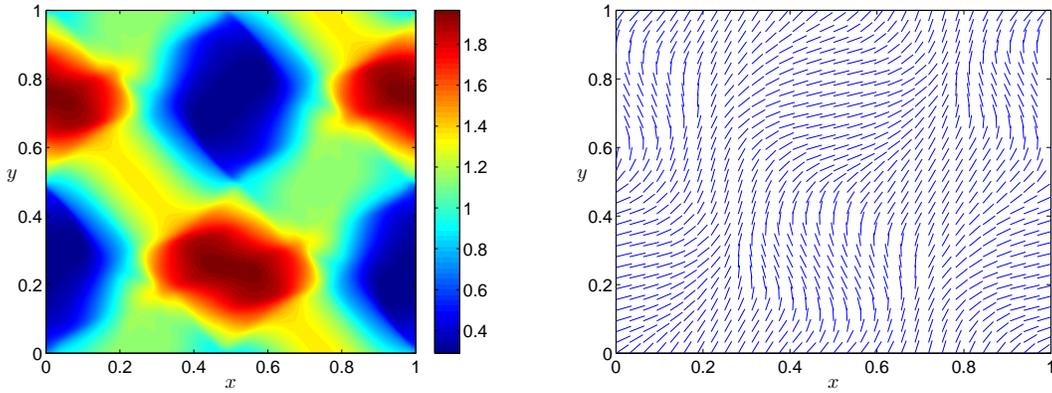


FIGURE 4.2. Approximations of the solution of (1.7) computed by scheme (4.4) on a grid with cell size $\Delta x = \Delta y = 2^{-11}$, CFL-number $\theta = 0.4$ at time $T = 2$. Left: the angle u , right: the corresponding director $\mathbf{n} = (\cos(u), \sin(u))$.

these formulations are derived. Furthermore, we also design an energy conservative scheme based on a Hamiltonian formulation of the variational wave equation (1.3). Numerical experiments, performed with these schemes, strongly suggest

- All the designed schemes resolved the solution (including possible singularities in the angle u) in a stable manner.
- The energy conservative schemes converge to a limit solution (as the mesh is refined), whose energy is preserved. This solution is a *conservative* solution of (1.3).
- The energy dissipative schemes also converge to a limit solution with energy being dissipated with time. This solution is a *dissipative* solution of the variational wave equation. Furthermore, this solutions appears to be unique. Varying the amount of numerical viscosity did not affect the limiting rate of entropy dissipation.

We also design both energy conservative as well as energy dissipative finite difference schemes for the two-dimensional version of the variational wave equation (1.7), based on the first-order system (4.1). Again, these schemes approximate the conservative, resp. dissipative, solutions efficiently.

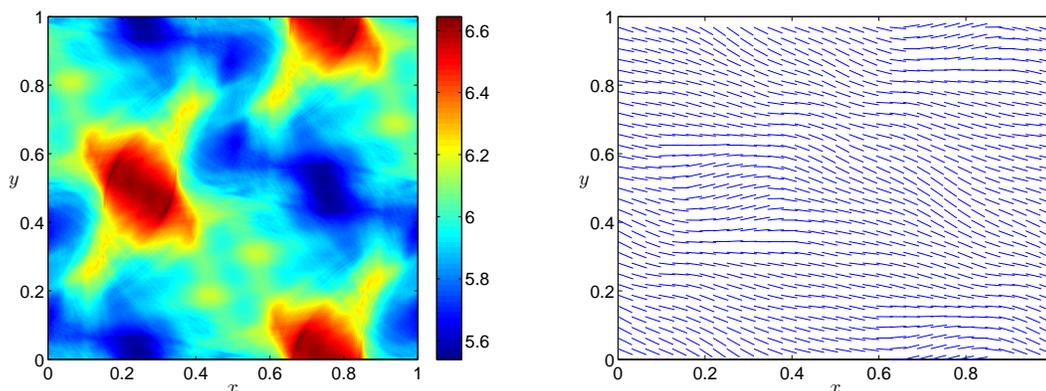


FIGURE 4.3. Approximations of the solution of (1.7) computed by scheme (4.3) on a grid with cell size $\Delta x = \Delta y = 2^{-11}$, CFL-number $\theta = 0.4$ at time $T = 4$. Left: the angle u , right: the corresponding director $\mathbf{n} = (\cos(u), \sin(u))$.

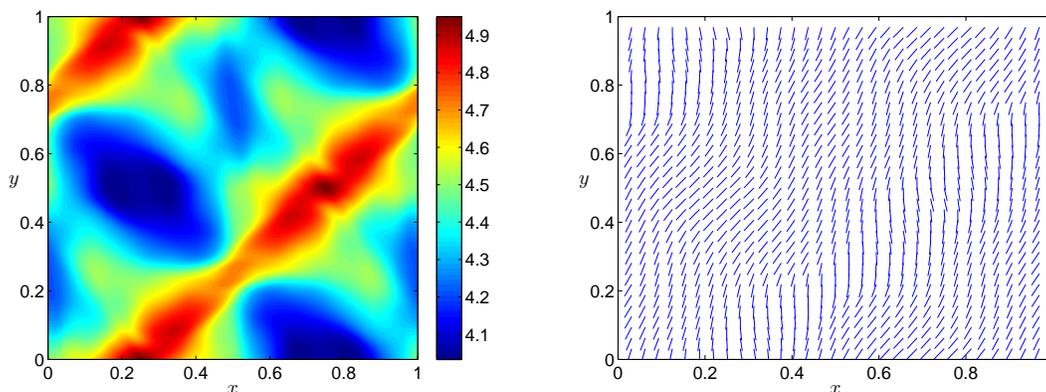


FIGURE 4.4. Approximations of the solution of (1.7) computed by scheme (4.4) on a grid with cell size $\Delta x = \Delta y = 2^{-11}$, CFL-number $\theta = 0.4$ at time $T = 4$. Left: the angle u , right: the corresponding director $\mathbf{n} = (\cos(u), \sin(u))$.

Thus, we have designed a stable, simple to implement, set of finite difference schemes that can approximate both the conservative as well as the dissipative solutions of the nonlinear variational wave equations. These schemes will be utilized in a forthcoming paper to study realistic modeling scenarios involving liquid crystals.

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