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HIGH-ORDER ENERGY STABLE NUMERICAL SCHEMES FOR A NONLINEAR VARIATIONAL WAVE EQUATION MODELING NEMATIC LIQUID CRYSTALS IN TWO DIMENSIONS

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Abstract. We consider a nonlinear variational wave equation that models the dynamics of the director field in nematic liquid crystals with high molecular rotational inertia. Being derived from an energy principle, energy stability is an intrinsic property of solutions to this model. For the two-dimensional case, we design numerical schemes based on the discontinuous Galerkin framework that either conserve or dissipate a discrete version of the energy. Extensive numerical experiments are performed verifying the scheme's energy stability, order of convergence and computational efficiency. The numerical solutions are compared to those of a simpler first-order Hamiltonian scheme. We provide numerical evidence that solutions of the 2D variational wave equation loose regularity in finite time. After that occurs, dissipative and conservative schemes appear to converge to different solutions.

Key words. Nonlinear variational wave equation, energy preserving scheme, energy stable scheme, discontinuous Galerkin method, higher order scheme.

1. Introduction

1.1. The Equation. Liquid crystals (LCs) are mesophases, i.e., intermediate states of matter between the liquid and the crystal phase. They possess some of the properties of liquids (e.g. formation, fluidity) as well as some crystalline properties (e.g. electrical, magnetic, etc.) normally associated with solids. The nematic phase is the simplest of the liquid crystal mesophases, and is close to the liquid phase. It is characterized by long-range orientational order, i.e., the long axes of the molecules tend to align along a preferred direction, which can be considered invariant under rotation by an angle of π. The state of a nematic liquid crystals is usually given by two linearly independent vector fields; one describing the fluid flow and the other describing the dynamics of the preferred axis, which is defined by a vector $\mathbf{n}$ giving its local orientation. Under the assumption of constant degree of orientation, the magnitude of the *director field* $\mathbf{n}$ is usually taken to be unity. In the present work we focus exclusively on the dynamics of the director field (independently of any coupling with the fluid flow), a map

$$\mathbf{n} : \mathbb{R}^3 \times [0, \infty) \to \mathbb{S}^2$$

from the Euclidean space to the unit ball.

We consider the elastic dynamics of the liquid crystal director field in the inertia-dominated case (zero viscosity). Associated with the director field $\mathbf{n}$, the classical Oseen-Frank elastic energy density $\mathcal{W}$ is given by

$$\mathcal{W}(\mathbf{n}, \nabla\mathbf{n}) = \alpha \left|\mathbf{n} \times (\nabla \times \mathbf{n})\right|^2 + \beta \left(\nabla \cdot \mathbf{n}\right)^2 + \gamma \left(\mathbf{n} \cdot (\nabla \times \mathbf{n})\right)^2 . \quad (1)$$

The constants α, β and γ are elastic material constants of the liquid crystal, and are associated with the three basic types of deformations of the medium; bend, splay and twist; respectively. Each of these constants must be positive in order

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to guarantee the existence of the minimum configuration of the energy $\mathcal{W}$ in the undistorted nematic configuration.

The one constant approximation ($\alpha = \beta = \gamma$) often provides a valuable tool to reach a qualitative insight into distortions of nematic configurations. Observe that, in this case the potential energy density (1) reduces to the Dirichlet energy

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

This corresponds to the potential energy density used in harmonic maps into the sphere $\mathbb{S}^2$. The stability of the general Oseen–Frank potential energy equation, derived from the potential (1) using a variational principle, is studied by Ericksen and Kinderlehrer [8]. For the parabolic flow associated to (1), see [3, 7] and references therein.

In the regime in which inertial effects dominate viscosity, the dynamics of the director $\mathbf{n}$ is governed by the least action principle

$$\mathbb{J}(\mathbf{n}) = \iint \left(\mathbf{n}_t^2 - \mathcal{W}(\mathbf{n}, \nabla\mathbf{n})\right)\, dx\, dt, \qquad \mathbf{n}\cdot\mathbf{n} = 1. \tag{2}$$

Standard calculations reveal that the *Euler-Lagrange* equation associated to $\mathbb{J}$ is given by

$$\mathbf{n}_{tt} = \operatorname{div}\left(\mathcal{W}_{\nabla\mathbf{n}}(\mathbf{n}, \nabla\mathbf{n})\right) - \mathcal{W}_{\mathbf{n}}(\mathbf{n}, \nabla\mathbf{n}), \tag{3}$$

and is termed the variational wave equation. Introducing the *energy* and *energy density*

$$\mathcal{E}(t) = \int \left(\mathbf{n}_t^2 + \mathcal{W}(\mathbf{n}, \nabla\mathbf{n})\right)\, dx, \qquad \mathbf{E}(t, x) = \mathbf{n}_t^2 + \mathcal{W}(\mathbf{n}, \nabla\mathbf{n}),$$

it is easy to check the identities

$$\mathcal{E}' = 0, \qquad \mathbf{E}_t = \operatorname{div}\left(\mathcal{W}_{\nabla\mathbf{n}}(\mathbf{n}, \nabla\mathbf{n})\mathbf{n}_t\right),$$

in light of (3). Given the formidable difficulties in the mathematical analysis of (3), it is customary to investigate the particular case of a planar director field configuration.

The physical implications of considering the inertia-dominated regime warrants a comment. Indeed, in many experimental situations the inertial forces acting on the director are orders of magnitude smaller than the dissipative. For this reason, the inertial term is often neglected in modelling [9, 25, 26]. It was however noted early by Leslie [21] that inertial forces might be significant in cases where the director field is subjected to large accelerations. In general, inertia will be more significant in the small time-scale dynamics of the director. For this reason, their inclusion can be warranted in, e.g., liquid crystal acoustics [19], mechanical vibrations [27] and in cases with and external oscillating magnetic field [28].

1.1.1. One-dimensional planar waves. Planar deformations are central in the mathematical study of models for nematic liquid crystals. A simple such model can be derived by assuming that the deformation depends on a single space variable x and that the director field $\mathbf{n}$ in confined to the x-y plane. In this case we can write the director as

$$\mathbf{n} = (\cos u(x, t),\, \sin u(x, t),\, 0).$$