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A fast Huygens sweeping method for capturing paraxial multi-color optical self-focusing in nematic liquid crystals

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ABSTRACT

We propose a numerically efficient algorithm for simulating the multi-color optical self-focusing phenomena in nematic liquid crystals. The propagation of the nematicon is modeled by a parabolic wave equation coupled with a nonlinear elliptic partial differential equation governing the angle between the crystal and the direction of propagation. Numerically, the paraxial parabolic wave equation is solved by a fast Huygens sweeping method, while the nonlinear elliptic PDE is handled by the alternating direction explicit (ADE) method. The overall algorithm is shown to be numerically efficient for computing high frequency beam propagations.

1. Introduction

We propose an efficient numerical method to simulate light beams (the so-called nematicons) propagating inside a nematic liquid crystal (NLC). When the incident beam has a large enough intensity and frequency, the corresponding energy will reorientate the NLC cells. This change in the material property will then divert the motion of the incident beam, and sometimes it might even create self-focusing of the beam leading to a further concentration of energy. The self-focused spot, known as the focal spot, has its intensity and position affected by the settings. In many situations, this also leads to an off-axis meandering (undulation) which is then followed by a break-up (filamentation) of the beam. Because of these interesting unique optical and electrical properties, such a material has a wide range of applications from various types of display panel to telecommunication devices. We refer interested readers to [3,7] for a more complete introduction to the properties of NLC and the research field. Some experimental results can be found in [5,2].

Mathematically, we follow the discussion in [27] and model the orientation of the nematic field by an elliptic partial differential equation (PDE) while the optical field is governed by a paraxial parabolic wave equation with a nonlinear interaction with the underlying nematic field. Some analysis of this coupled nonlinear system can be found in, for example, [39,14]. This coupled nonlinear system can also be extended and applied to various related phenomenon including arbitrary degree of nonlinearity [10] and multi-color nematicons [36,37,35].

Numerically, it is challenging to solve the hyperbolic PDE in the high frequency regime. Since the high wavenumber in the parabolic wave equation introduces extremely rapid transverse oscillations across beams, typical direct methods such as finite-difference or finite-element methods require a very fine mesh to resolve the oscillations in the solution.

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Because of the usual Courant–Fredrichs–Lewy condition for a hyperbolic-type PDE, the overall computational cost could be very high. An alternative to resolve these highly oscillatory wave function is to use asymptotic methods. In a series of studies [30,31,19,20], we have considered the geometrical optics approximation for acoustic wave equations and their corresponding inverse problems. In geophysical applications, Gaussian beam superpositions have been proposed for seismic wave modeling [9] and for seismic wave migration [13]. Based on [32,38], we have developed a purely Eulerian approach to compute the Gaussian beam solution in [23]. In the context of quantum mechanics where one has to solve the Schrödinger equation, some variants of Gaussian beams including the frozen Gaussian beams and Gaussian wave packets have been used to construct approximate solutions to the Schrödinger equation in the semi-classical regime [16,11,12]. However, these formulations were all based on the Lagrangian framework. In [21,22] we proposed an Eulerian formulation of Gaussian beams for the Schrödinger equation by generalizing [23,25]. We have recently proposed a novel method in [24], called the fast Huygens sweeping method, for solving the Schrödinger equation in the semi-classical regime [33,8] by incorporating the short-time Wentzel–Kramers–Brillouin–Jeffreys (WKBJ) propagator into Huygens' principle. Even though the WKBJ solution is valid only for a short time period due to the occurrence of caustics, the Huygens' principle allows us to construct the global-in-time semi-classical solution. To further improve the computational efficiency, we have developed in [24] analytic approximation formulas for the short-time WKBJ propagator by using the Taylor expansion in time.

There are two main contributions in this paper. We notice that the original Huygens sweeping method as proposed in [24] has a lower bound in the step size for time. This will hinder a detailed visualization of the beam self-focusing and interaction. In the first part of the paper, we will propose a simple strategy to relax the lower bound on the time marching step using a forward–backward step marching approach. In the second part of the work, we will replace the simple iterative solver for the nematic field as discussed in [27] by the alternative direction explicit (ADE) method [18]. The method has been shown to be unconditionally stable for elliptic type problems and, therefore, it is computationally extremely efficient for our application. In the example section, we are going to demonstrate that the computational complexity of our proposed approach is of order of approximately $O(N^d)$ where N is the number of grid points used in each of the physical direction and d is the overall dimension of the problem. Because of this improvement in the computational efficiency, we are now able to carry out detailed studies of the behavior of multiple frequency wave propagations in nonlinear media like NLC even in high dimensions.

The rest of the paper is organized as follows. In Section 2, we will briefly summarize the background of the project and some necessary components of the proposed algorithm. With these new developments in the numerical algorithm for different equations, we propose in Section 3 an efficient implementation for modeling the propagation of beams with multiple colors in nematic liquid crystals.

2. Background

In this section, we will summarize the mathematical formulation for modeling the nematic liquid crystals. Then we will introduce briefly two numerical methods including the fast Huygens sweeping method and the alternating direction explicit (ADE) method in the following subsections which will be the building blocks of the overall algorithm.

2.1. A paraxial model for multi-color optical self-focusing

As suggested by [27], the paraxial model represents a particular form and inherits features from the actual time-independent electromagnetic wave and nematic liquid crystal model. We consider the time-harmonic vectorial Maxwell's equations and the static Frank free-energy nematic equation [39]:

$$\nabla \times \nabla \times \mathbf{E} - k^2[\mathbf{E} + \alpha(\mathbf{n}\cdot\mathbf{E})\mathbf{n}] = 0\,,$$
$$\mathbf{n} \times [(\Delta\mathbf{n}) + (\mathbf{n}\cdot\mathbf{E}^*)\mathbf{E} + (\mathbf{n}\cdot\mathbf{E})\mathbf{E}^*] = 0\,,$$

with simplification made by imposing the *paraxial substitution* [28]:

$$\mathbf{E} = \begin{pmatrix} U \\ 0 \\ H \end{pmatrix} e^{ikz} \text{ and } \mathbf{n} = \begin{pmatrix} \sin\theta \\ 0 \\ \cos\theta \end{pmatrix}.$$

Assuming that the wavenumber $k \gg 1$ is large with a slowly varying envelope approximation in a medium with small anisotropy α, we can conclude that the longitudinal electric field H becomes negligible compared to the transverse component U. Let θ be the nematic field representing the angles between the NLC rod-like cells and the direction of propagation (z in our case) [6]. We have

$$2ik\frac{\partial}{\partial z}U + (\Delta_\perp + k^2\alpha\sin^2\theta)U = 0, \tag{1}$$
$$\left(\frac{\partial}{\partial z^2} + \Delta_\perp\right)\theta + |U|^2\sin 2\theta = 0\,, \tag{2}$$

with the initial conditions $U(x, z = 0) = U_0(x)$ and $\theta(x, z = 0) = 0$. We impose the following Dirichlet boundary conditions: $U(x_{\min}, z) = U(x_{\max}, z) = 0$ and $\theta(x_{\min}, z) = \theta(x_{\max}, z) = 0$. For the nonlinear elliptic equation, we further set $\theta_z(x, z_{\max}) = 0$.