On the application of finite differences, method of lines and pseudo-spectral methods to smectic-C liquid crystals

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Abstract

Purpose – The purpose of this paper is to derive a dynamic equation for modelling the behaviour of smectic-C liquid crystals under the effect of an electric field.
Design/methodology/approach – The model equation is solved using a finite difference approximation, method of lines and pseudo-spectral methods. The solutions are compared for accuracy and efficiency. Comparison is made of the efficiency of finite differences, method of lines and pseudo-spectral methods.
Findings – The Fourier pseudo-spectral method is shown to be the most efficient approach.
Originality/value – This work is original; a computational comparison of numerical schemes applied to liquid crystals has not been found in the literature.

Keywords Finite differences, Methods, Crystals, States of matter, Fluids
Paper type Research paper

1. Introduction

Liquid crystals are considered to be condensed matter that exhibit both properties of crystalline solids and simple liquids (de Gennes, 1974). The molecules arrange themselves in a crystal-like manner, but flow like a liquid. As a consequence of this property, liquid crystals generally possess orientational order, while losing some or all of their positional order. Orientational order is defined to be a measure of the tendency of the molecules to align along a unit vector, known as the director, whereas positional order is the extent to which the position of an average molecule or group of molecules shows translational symmetry. The amount of order in a liquid crystal is quite small relative to that of a crystal, but can be manipulated with mechanical, magnetic or electric forces. Liquid crystals are anisotropic fluids that consist of rod or disc-like organic molecules which tend to align themselves along a common axis in space known as the director, **n** (Stewart, 2004). There are many different types of liquid crystal states, depending upon the amount of order in the material. The two main liquid crystal states are nematic and smectic liquid crystals. Smectic liquid crystals also consist of different types, namely, smectic-A, B, C, D, E, F, G, H and I (Gray and Goodby, 1985). The difference between these liquid crystals, is again the amount of order that they each possess.

For over 20 years now, research into liquid crystals has contributed greatly to optical displays and screens. Since they exhibit unique optical properties, i.e. they scatter light strongly, they are known to be of use in various applications in diverse

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fields, such as engineering, physics, chemistry, biology, medical research and pharmacy.

In this paper, we consider a nonlinear diffusion equation that models the effect of an applied electric filed across a sample of smectic-C (SmC) liquid crystals. This nonlinear partial differential equation is solved numerically using a finite difference approximation, method of lines and pseudo-spectral methods which include sinc and Fourier methods. We compare the accuracy and efficiency of the four algorithms. Our goal is to find an algorithm; that starts with an initial configuration $u = u_0(x)$, that tends to the steady state in the most efficient way. Efficiency is measured in terms of the time taken for each method to reach the steady state at some fixed final time.

We first consider a finite difference approximation to the nonlinear partial differential equation (Smith, 1985). We consider a central difference approximation to the spatial derivatives and a first-order forward difference approximation to the time derivative. We find that the finite difference approximation has poor convergence at the boundaries due to high-frequency oscillations. These high-frequency oscillations at the boundaries may occur because of a mismatch of the initial and boundary conditions at the boundaries. This is not the case in this paper. To overcome these high-frequency oscillations, the forward approximation in time should be replaced with an implicit high order approximation. The interested reader is referred to the papers by Khaliq *et al.* (2007, 2009) and Yousuf (2008) in which high-order schemes are discussed.

We overcome the high-frequency oscillations at the boundary by using the method of lines and pseudo-spectral methods (Fornberg, 1996; Trefethen, 2000; Boyd, 2001). In the case of pseudo-spectral methods, we use sinc (Stenger, 1981; Lund and Bowers, 1992; Bellomo *et al.*, 2001) and Fourier methods (Nielsen and Janssen, 2001; Holmas *et al.*, 2008). We specifically use the sinc and Fourier methods because the model equation contains trigonometric functions. The forward difference approximation in time means that the finite difference approach leads to a numerical approximation in terms of matrix multiplication. The method of lines and pseudo-spectral approximations produces a nonlinear system of ordinary differential equations which we solve using the stiff nonlinear ordinary differential equation solver ode15s in MATLAB. Sinc and Fourier methods approximate the spatial derivative in the model equation by dense differentiation matrices. The package DMSuite (A MATLAB Differentiation Matrix Suite (Weideman and Reddy, 2000)) is used to generate these matrices. We show that the Fourier pseudo-spectral method is the most efficient solution method.

This paper is divided up as follows. In section 2, the nonlinear model is derived and non-dimensionalized. In section 3, the numerical solutions of the model equation are obtained using a finite difference method, method of lines, sinc method and Fourier method. The results of these methods are then compared. Concluding remarks are made in section 4.

2. Smectic-C liquid crystals

Smectic liquid crystals possess translational order, which is a condition in which the molecules have some arrangement in space. Molecules in this phase are arranged in well-defined, equally spaced layers, they move only within these layers while the layers themselves slide over one another like soap. Within the layers, the molecules tend to align in the same direction described by the director **n**. This director **n** makes an angle θ with the layer normal **a**. θ is referred to as the smectic tilt angle and is usually temperature dependent. However, it may vary due to competition between boundary

conditions, elastic effects or smectic layer compressional effects (Stewart, 2007). It was shown by Stewart *et al.* (1994) that θ increases as temperature decreases.

SmC liquid crystals consist of elongated rod-like molecules which can be easily polarized due to their dipole substituents. This phase is formed when the directors of the liquid crystals tilts away from the layer normal at an angle θ. From X-ray diffraction, it is shown that molecules are randomly arranged within structured layers. It is assumed that the tilt directions of the molecules align in the same direction as shown in Figure 1.

Since the molecules in this phase rotate rapidly about their long molecular axes and because of possible polarization field effects, SmC liquid crystals are said to be biaxial (i.e. 2D unstructured layers with a tilted molecular arrangement). Within the layers, molecules are said to rotate about the z-axis in a cone-shaped as illustrated in Figure 2.

A unit vector **n** is defined, as mentioned above, to represent the projection of the molecules. Although at a given temperature the tilt angle, θ, is constant, the direction is not specified and is chosen at will. This direction may be described by a orthogonal unit projection **c** onto the plane of the layers, and is known as the c-director of the structure. It is perpendicular to layer normal **a** and parallel to the the director **n** (Stewart and Momoniat, 2004), as indicated in Figure 2. ϕ is known as the orientation angle of **c** from the x-axis. This angle describes the orientation of the director, **n**. i.e. the position of the liquid crystal rotating around the z-axis, projected onto the x-y plane.

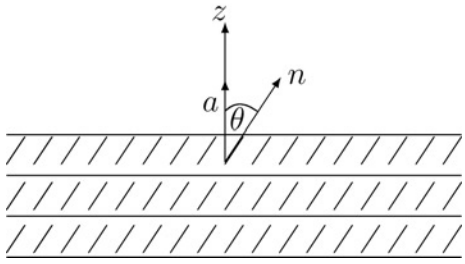
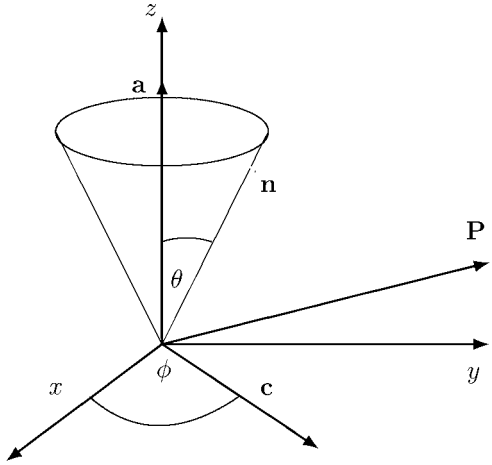


Figure 1.
SmC liquid crystals, arranged in well defined layers and molecules are tilted at an angle θ to the director, **a**



Notes: The unit vector **c** describes the direction of the molecules, which is parallel to the projection of **n** and perpendicular to **a**

Figure 2.
The director **n** makes an angle θ with the layer normal **a**

When the molecules in this phase are chiral, (i.e. they differ from their mirror image) they lie next to each other in a skewed orientation. Chiral refers to the unique ability to selectively reflect one component of circularly polarized light (Stewart and Momoniat, 2004; PLC, n.d.). This state is referred to as the smectic-C* (SmC*) phase. Experiments have shown that SmC* liquid crystals are ferroelectric, which means they are substances which obtain spontaneous electric polarization, **P** (PLC, n.d.). The polarization exists parallel to the smectic layers and perpendicular to the molecules, and the magnitude is determined by molecular considerations although its existence depends only on symmetry (Stewart *et al.*, 1994). Just as in the SmC phase, the director in the SmC* phase makes an angle θ with respect to the layer normal. The difference being, θ rotates from layer to layer producing a helical structure (Figure 3). That is, the director in this phase is neither parallel nor perpendicular to the layers, but rotates from one layer to the next and always lies on the surface of the fictitious cone.

Now consider an external electric field **E** as shown in Figure 4, being applied across a sample of SmC. This is given by the equation:

$$\mathbf{E} = E_0\left(1 + \frac{\epsilon}{2}\cos(\omega\epsilon t)\right)(\cos\alpha, 0, \sin\alpha), \tag{1}$$

where $0 < \alpha \ll 1$, and E_0 is the magnitude of the electric field. **E** is not constant, it varies according to time and has an oscillating amplitude of $\frac{\epsilon}{2}$. However, in this article ϵ will be set equal to zero.

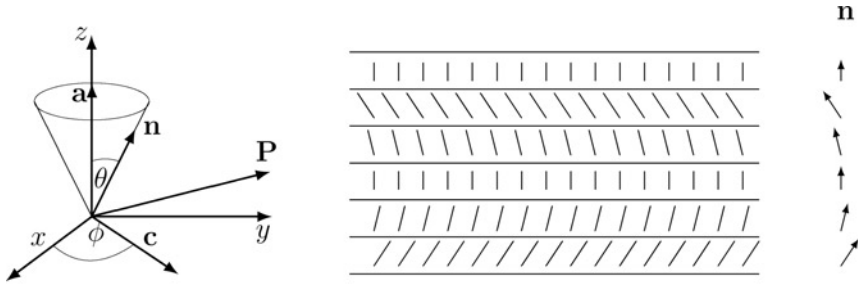


Figure 3.
SmC* liquid crystals with spontaneous polarization **P**

Notes: The director **n** rotates around the fictitious cone

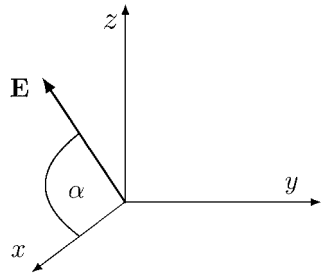


Figure 4.
The field is tilted at a constant angle $\alpha \geq 0$

From Figure 3 the following are given:

$$\mathbf{n} = \mathbf{a}\cos\theta + \mathbf{c}\sin\theta, \tag{2}$$

$$\mathbf{a} = (0, 0, 1), \tag{3}$$

$$\mathbf{c} = (\cos\phi(z,t), \sin\phi(z,t), 0), \tag{4}$$

$$\mathbf{b} = (-\sin\phi(z,t), \cos\phi(z,t), 0), \tag{5}$$

where $\mathbf{b} = \mathbf{a} \times \mathbf{c}$ and the orientation angle ϕ is dependent upon x and t only. The spontaneous polarization, which is a characteristic of SmC liquid crystals, is in the same direction of the vector $\mathbf{b}$ and is denoted by:

$$\mathbf{P} = P_0\mathbf{b}, \tag{6}$$

where $P_0 > 0$ is the magnitude of the polarization.

The total electric energy density that occurs when the electric field is applied across a liquid crystal is given by de Gennes (1974) and Stewart and Momoniat (2004):

$$\omega_{elec} = -\mathbf{P}\cdot\mathbf{E} - \frac{1}{2}\epsilon_0\epsilon_a(\mathbf{n}\cdot\mathbf{E})^2, \tag{7}$$

where ϵ_0 is the permittivity of free space given as $\epsilon_0 = 8.854 \times 10^{-12}\,\mathrm{F.m}^{-1}$ and ϵ_a is the dielectric anisotropy.

The bulk energy density is given by:

$$\omega_{bulk} = \frac{1}{2}B_3\left(\frac{\partial\phi}{\partial x}\right)^2, \tag{8}$$

where B_3 is the positive elastic constant related to the rotation of the $\mathbf{c}$ director observed from layer to layer.

Using the above equations, along with the four constraints of SmC continuum theory (Leslie *et al.*, 1991):

$$\mathbf{a}\cdot\mathbf{a} = 1, \quad \mathbf{c}\cdot\mathbf{c} = 1, \quad \mathbf{a}\cdot\mathbf{c} = 0, \quad \nabla\times\mathbf{a} = 0,$$

the dynamic equation is given as (Stewart and Momoniat, 2004):

$$\begin{aligned} 2\lambda_5\frac{\partial\phi}{\partial t} = {} & B_3\frac{\partial^2\phi}{\partial z^2} - P_0E_0\cos\alpha\cos\phi - \epsilon_0\epsilon_aE_0^2\cos\phi\sin^2\theta\cos^2\alpha\sin\phi \\ & - \epsilon_0\epsilon_aE_0^2\cos\theta\sin\alpha\sin\theta\cos\alpha\sin\phi. \end{aligned} \tag{9}$$

For simplicity, we non-dimensionalize the above dynamic equation so the results can be compared to those results already obtained by other authors.

In Stewart and Momoniat (2004), it was shown that when the following scaled variables were introduced:

$$T = \frac{1}{4}t(2\lambda_5)^{-1}\epsilon_0|\epsilon_a|E_0^2\cos^2\alpha\sin\theta, \tag{10}$$

$$X = \frac{1}{2} x B^{-\frac{1}{2}} (\epsilon_0 |\epsilon_a| E_0^2 \cos^2 \alpha \sin \theta)^{\frac{1}{2}}, \tag{11}$$

where it is assumed that $\epsilon_a < 0$, the dynamic equation can be non-dimensionalized to:

$$\phi_T = \phi_{XX} + 2a \cos \phi + 4b \sin \phi + 2\phi(2\phi). \tag{12}$$

The subscripts denote partial differentiation with respect to the indicated variables and a and b are introduced as dimensionless parameters given by:

$$a = 2P_0 (\epsilon_0 \epsilon_a E_0 \cos \alpha \sin^2 \theta)^{-1}, \tag{13}$$

$$b = \tan \alpha \cot \theta. \tag{14}$$

A further transformation:

$$u(X, T) = 2\phi(X, T) - \pi, \tag{15}$$

results in the non-dimensional equation in a standard form (Stewart, 1998):

$$u_T = u_{XX} - 4a \sin\left(\frac{u}{2}\right) - 4 \sin u + 8b \cos\left(\frac{u}{2}\right). \tag{16}$$

Stewart and Momoniat (2004) obtain an implicit approximate solution to Equation (16).

Of physical importance is the steady state solution of Equation (16) given by $u(x, t) = F(x)$. The steady state solution can be found by solving:

$$\frac{d^2F}{dx^2} = 4a \sin\left(\frac{u}{2}\right) 4 \sin u - 8b \cos\left(\frac{u}{2}\right). \tag{17}$$

Stewart and Momoniat (2004) have shown that appropriate boundary conditions for solving Equation (16) are given by the clamped boundary conditions:

$$u(-\infty, t) = u(\infty, t) = 0. \tag{18}$$

We use bvp4c in MATLAB to obtain a numerical solution to the nonlinear second-order ordinary differential Equation (17). The steady state solution is important in terms of assessing the validity of the numerical results we obtain later. We impose the clamped boundary conditions as:

$$F(\pm 5) = 0. \tag{19}$$

We plot the variation in the steady profile in Figure 5. Changing the constant a has no influence on the steady profile. Changing the constant b increases or decreases the height of the steady profile.

The steady solution is physically important in the theory of liquid crystals. We motivate this importance by considering the effect of a magnetic field on iron filings. When a magnetic field is applied the iron fillings move and align in the same direction without any further movement until the magnetic field is removed. SmC liquid crystals have polarizable constituents and are easily polarized when an electric current is

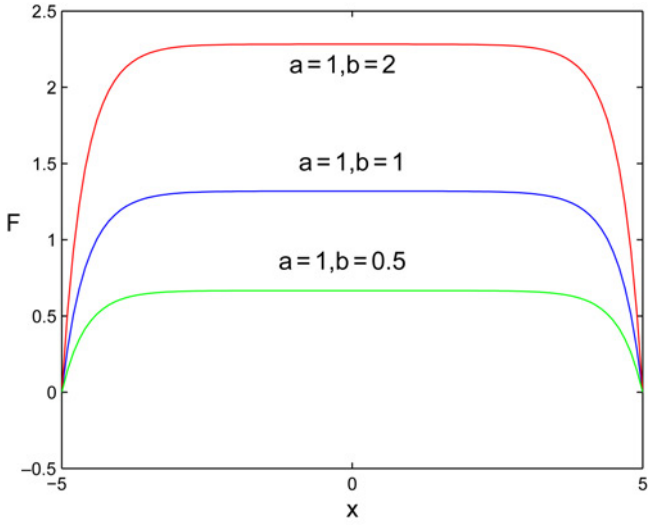


Figure 5.
Plot showing the variation in the steady profile obtained from a numerical solution of (17) solved subject to (19) using bvp4c in MATLAB

applied. This polarized state of the liquid crystal is represented by the steady solution to the model Equation (16).

3. Numerical solutions

In this section, the non-dimensional Equation (16) is solved numerically using a finite difference approximation, methods of lines, sinc method and Fourier method. As indicated earlier, the finite difference approach leads to a numerical approximation in terms of matrix multiplication. The method of lines and pseudo-spectral approximations lead to a nonlinear system of ordinary differential equations. This nonlinear system is solved using ode15s in MATLAB.

For the sinc and Fourier methods, the spatial derivative in Equation (16) is approximated by a dense differentiation matrix, unlike the finite difference approach in which the spatial derivative is approximated by a tridiagonal matrix. The nonlinear functions are approximated by either a sinc or Fourier approximation depending on which method is being used. We use the package DMSuite (A MATLAB Differentiation Matrix Suite (Weideman and Reddy, 2000)) to obtain the differentiation matrices for the sinc and Fourier methods.

The model Equation (16) is solved subject to the boundary conditions (18). We assume an initial Gaussian configuration given by:

$$u(x,0) = e^{-x^2}. \tag{20}$$

3.1 A finite difference approximation

A finite difference approximation is one of the simplest methods used in numerical analysis to approximate a solution to a differential equation (see e.g. Smith, 1985). We approximate the time derivative by the forward difference:

$$u_T \approx \frac{u_{i,j+1} - u_{i,j}}{\Delta T} \tag{21}$$

and the spatial derivative by the central difference approximation:

$$u_{XX} \approx \frac{u_{i+1,j} - 2u_{i,j} + u_{i-1,j}}{(\Delta X)^2} \tag{22}$$

We divide the spatial domain $[-a, a]$ into n equidistant subintervals. We have $u_{i,j} = u(X_i, T_j)$, $X_i = -a + i\Delta x$, $i = 10, 1, 2, \ldots, n$ and $\Delta x = 2a/n$. The boundary conditions (18) are approximated by $u(-a, t) = u(a, t) = 0$. In this paper, we choose $a = 4$.

Substituting the difference approximations (21) and (22) into (16) we obtain:

$$\frac{u_{i,j+1} - u_{i,j}}{\Delta T} = \left(\frac{u_{i+1,j} - 2u_{i,j} + u_{i-1,j}}{(\Delta X)^2}\right) - 4a\sin\left(\frac{u_{i,j}}{2}\right) - 4\sin u_{i,j} + 8b\cos\left(\frac{u_{i,j}}{2}\right).$$

Therefore,

$$\begin{aligned} u_{i,j+1} = u_{i,j} + \frac{\Delta T}{(\Delta X)^2}(u_{i+1,j} - 2u_{i,j} + u_{i-1,j}) - 4a\Delta T\sin\left(\frac{u_{i,j}}{2}\right) - 4\Delta T\sin u_{i,j} \\ + 8b\Delta T\cos\left(\frac{u_{i,j}}{2}\right) - 4a\Delta T\sin\left(\frac{u_{i,j}}{2}\right) - 4\Delta T\sin u_{i,j} - 8b\Delta T\cos\left(\frac{u_{i,j}}{2}\right). \end{aligned} \tag{23}$$

Now let:

$$\kappa = \frac{\Delta T}{2\lambda_5(\Delta X)^2}, \quad \overline{A} = 4a\Delta T, \quad \overline{B} = 4\Delta T, \quad \overline{C} = 8b\Delta T.$$

The boundary conditions $u(-a, t) = u(a, t) = 0$ are given by:

$$u_{0,j} = 0, \quad u_{n,j} = 0.$$

From this the following system is obtained:

$$\begin{bmatrix} u_{0,j+1} \\ u_{1,j+1} \\ u_{2,j+1} \\ \vdots \\ \vdots \\ u_{n-1,j+1} \\ u_{n,j+1} \end{bmatrix} = \begin{bmatrix} 0 & 0 & 0 & \ldots & \ldots & \ldots & 0 \\ \kappa & (1-2\kappa) & \kappa & 0 & \ldots & \vdots & 0 \\ 0 & \kappa & (1-2\kappa) & \kappa & \ldots & \vdots & 0 \\ \vdots & \vdots & \vdots & \ldots & \vdots & \vdots & \vdots \\ \vdots & \vdots & \vdots & \ldots & \vdots & \vdots & \vdots \\ 0 & 0 & \vdots & \ldots & \kappa & (1-2\kappa) & \kappa \\ 0 & 0 & \ldots & \ldots & \ldots & 0 & 0 \end{bmatrix}$$

$$\times \begin{bmatrix} u_{0,j} \\ u_{1,j} \\ u_{2,j} \\ \vdots \\ \vdots \\ u_{n-1,j} \\ u_{n,j} \end{bmatrix} - \overline{A} \begin{bmatrix} \sin\left(\frac{u_{0,j}}{2}\right) \\ \sin\left(\frac{u_{1,j}}{2}\right) \\ \sin\left(\frac{u_{2,j}}{2}\right) \\ \vdots \\ \vdots \\ \sin\left(\frac{u_{n-1,j}}{2}\right) \\ \sin\left(\frac{u_{n,j}}{2}\right) \end{bmatrix} - \overline{B} \begin{bmatrix} \sin u_{0,j} \\ \sin u_{1,j} \\ \sin u_{2,j} \\ \vdots \\ \vdots \\ \sin u_{n-1,j} \\ \sin u_{n,j} \end{bmatrix} + \overline{C} \begin{bmatrix} \cos\left(\frac{u_{0,j}}{2}\right) \\ \cos\left(\frac{u_{1,j}}{2}\right) \\ \cos\left(\frac{u_{2,j}}{2}\right) \\ \vdots \\ \vdots \\ \cos\left(\frac{u_{n-1,j}}{2}\right) \\ \cos\left(\frac{u_{n,j}}{2}\right) \end{bmatrix} - P.$$

The vector P given by:

$$P = \begin{bmatrix} \overline{C}\cos\left(\frac{u_{0,j}}{2}\right) \\ 0 \\ 0 \\ \vdots \\ \vdots \\ 0 \\ \overline{C}\cos\left(\frac{u_{n,j}}{2}\right) \end{bmatrix},$$

is included to accommodate for the boundary conditions. This is the only necessary term since $\sin 0 = 0$. We perform the matrix multiplications in MATLAB.

From Figure 6, it can be seen that a finite difference approximation results in high oscillations at the boundaries. This technique is unable to produce a smooth solution for

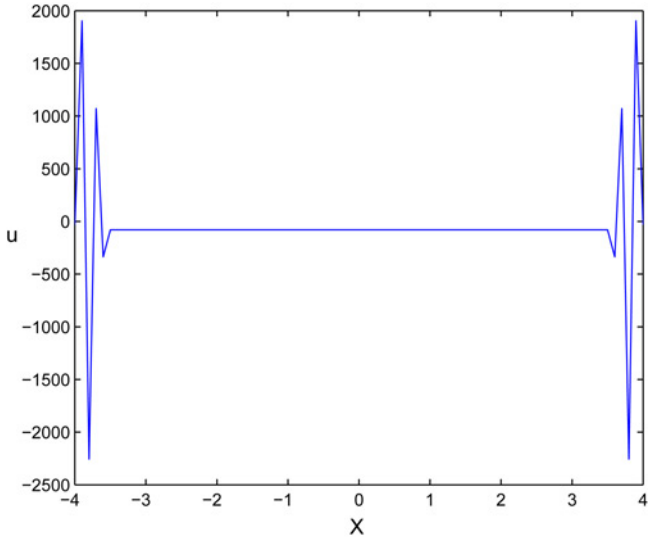


Figure 6.
Numerical solution of the dynamic model (16) obtained using the finite difference approach for $n = 250$ and $\Delta T = 0.01$ showing high-frequency oscillations at the boundary

our model and therefore we look at method of lines and pseudo-spectral methods for results.

3.2 Method of lines

In the method of lines, the spatial derivative in Equation (16) is approximated by the central difference approximation.

$$u_{XX} = \frac{u_{i+1}(T) - 2u_i(T) + u_{i-1}(T)}{h^2}. \tag{24}$$

The time derivative is evaluated as a time derivative at $X = X_i$. The model Equation (16) becomes:

$$\begin{aligned} u_i'(T) = \frac{1}{h^2}(u_{i+1}(T) - 2u_i(T) + u_{i-1}(T)) - 4a\sin\left(\frac{u_i(T)}{2}\right) \\ - 4\sin u_i(T) + 8b\cos\left(\frac{u_i(T)}{2}\right). \end{aligned} \tag{25}$$

The boundary conditions $u(-a,t) = u(a,t) = 0$ are approximated by:

$$u_0(T) = 0, \quad u_n(T) = 0. \tag{26}$$

We obtain the system:

$$\begin{bmatrix} u_0'(T) \\ u_1'(T) \\ u_2'(T) \\ \vdots \\ \vdots \\ u_{n-1}'(T) \\ u_n'(T) \end{bmatrix} = \frac{1}{h^2}\begin{bmatrix} 0 & 0 & 0 & \dots & \dots & \dots & 0 \\ 1 & -2 & 1 & \dots & \dots & \dots & 0 \\ 0 & 1 & -2 & 1 & \dots & \dots & 0 \\ \vdots & & \ddots & \ddots & & & \vdots \\ \vdots & & & \ddots & \ddots & \ddots & \vdots \\ 0 & \dots & \dots & \dots & \dots & 1 & -2 \\ 0 & \dots & \dots & \dots & \dots & 0 & 0 \end{bmatrix}\begin{bmatrix} u_0(T) \\ u_1(T) \\ u_2(T) \\ \vdots \\ \vdots \\ u_{n-1}(T) \\ u_n(T) \end{bmatrix} - 4a\begin{bmatrix} \sin\frac{u_0(T)}{2} \\ \sin\frac{u_1(T)}{2} \\ \sin\frac{u_2(T)}{2} \\ \vdots \\ \vdots \\ \sin\frac{u_{n-1}(T)}{2} \\ \sin\frac{u_n(T)}{2} \end{bmatrix}$$

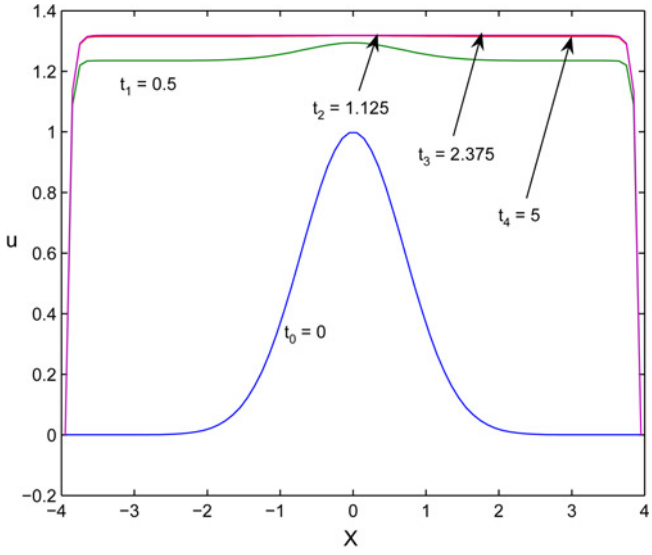
$$- 4\begin{bmatrix} \sin u_0(T) \\ \sin u_1(T) \\ \sin u_2(T) \\ \vdots \\ \vdots \\ \sin u_{n-1}(T) \\ \sin u_n(T) \end{bmatrix} + 8b\begin{bmatrix} \cos\frac{u_0(T)}{2} \\ \cos\frac{u_1(T)}{2} \\ \cos\frac{u_2(T)}{2} \\ \vdots \\ \vdots \\ \cos\frac{u_{n-1}(T)}{2} \\ \cos\frac{u_n(T)}{2} \end{bmatrix} - \begin{bmatrix} 8b\cos\frac{u_0(T)}{2} \\ 0 \\ 0 \\ \vdots \\ \vdots \\ 0 \\ 8b\cos\frac{u_n(T)}{2} \end{bmatrix}.$$

The nonlinear system of ordinary differential equations is solved using ode15s in MATLAB. In Figure 7, we plot the solutions obtained from solving Equation (27). We note in Figure 7 that the curve for the steady state is not smooth. The solution is negative at the boundaries. While the method of lines has significantly reduced the oscillations at the boundaries. We still have not achieved a smooth result.

3.3 Sinc method

To implement the sinc method, we use the boundary conditions (26). The spatial derivative in Equation (16) is approximated by a sinc differential matrix given in Weideman and Reddy (2000). We obtain the system:

$$\begin{bmatrix} u_1'T \\ u_2'(T) \\ \vdots \\ \vdots \\ \vdots \\ u_{n-1}'(T) \\ u_n'(T) \end{bmatrix} = \kappa \begin{bmatrix} 0 & 0 & 0 & \dots & \dots & \dots & 0 \\ 2 & -\frac{\pi^2}{3} & 2 & \dots & \dots & \dots & \\ -\frac{1}{2} & 2 & -\frac{\pi^2}{3} & \dots & \dots & \dots & -\frac{1}{2} \\ \vdots & & \ddots & \ddots & & & \vdots \\ \vdots & & & \ddots & \ddots & \ddots & \vdots \\ \frac{2(-1)^{(n-1)}}{(n-2)^2} & \dots & & \dots & \dots & -\frac{\pi^2}{3} & 2 \\ 0 & \dots & \dots & \dots & 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} u_1(T) \\ u_2(T) \\ \vdots \\ \vdots \\ \vdots \\ u_{n-1}(T) \\ u_n(T) \end{bmatrix}$$



Notes: The solutions tends to the steady state in a stable manner

Figure 7.
Numerical solution of the model Equation (16) obtained using the method of lines for $n = 250$ and $\Delta T = 0.01$

$$-\overline{A}\begin{bmatrix} \sin\left(\frac{u_1(T)}{2}\right) \\ \sin\left(\frac{u_2(T)}{2}\right) \\ \vdots \\ \sin\left(\frac{u_{n-1}(T)}{2}\right) \\ \sin\left(\frac{u_n(T)}{2}\right) \end{bmatrix} - \overline{B}\begin{bmatrix} \sin u_1(T) \\ \sin u_2(T) \\ \vdots \\ \sin u_{n-1}(T) \\ \sin u_n(T) \end{bmatrix} + \overline{C}\begin{bmatrix} \cos\left(\frac{u_1(T)}{2}\right) \\ \cos\left(\frac{u_2(T)}{2}\right) \\ \vdots \\ \cos\left(\frac{u_{n-1}(T)}{2}\right) \\ \cos\left(\frac{u_n(T)}{2}\right) \end{bmatrix} - \begin{bmatrix} 8b\cos\left(\frac{u_1(T)}{2}\right) \\ 0 \\ \vdots \\ 0 \\ 8b\cos\left(\frac{u_n(T)}{2}\right) \end{bmatrix},$$

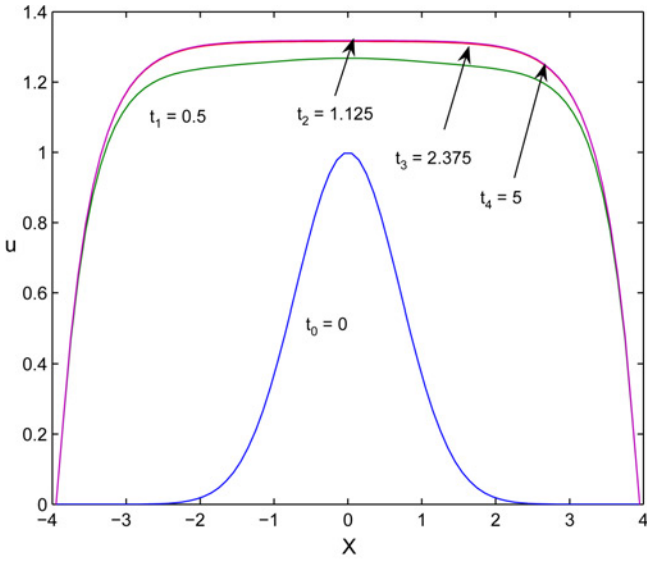
where:

$$\kappa = \frac{1}{h^2}, \quad \overline{A} = 4a, \quad \overline{B} = 4, \quad \overline{C} = 8b. \tag{27}$$

The nonlinear system of ordinary differential Equation (27) is solved using ode15s in MATLAB. We plot the results in Figure 8. We note from Figure 8 that the steady state solution is reached without oscillations at the boundaries. These results compare well to those obtained by Ried *et al.* (2000) in which electrically driven hybrid instabilities in SmC liquid crystal films are described.

3.4 Fourier method

The Fourier method reduces to a similar system as for the sinc method. The Fourier differentiation matrix for the spatial derivative in Equation (16) is given in Weideman and Reddy (2000). We obtain the system for N even:



Notes: The solutions tends to the steady state in a stable manner

Figure 8.
Numerical solution of the model Equation (16) obtained using the sinc method for $n = 250$ and $\Delta T = 0.01$

$$\begin{bmatrix} u_1'T \\ u_2'(T) \\ \vdots \\ \vdots \\ \vdots \\ u_{n-1}'(T) \\ u_n'(T) \end{bmatrix} =$$

$$\begin{bmatrix} 0 & 0 & 0 & \cdots & \cdots & \cdots & 0 \\ \frac{1}{2}\csc^2\left(\frac{h}{2}\right) & -\frac{\pi^2}{3h^2}-\frac{1}{6} & \frac{1}{2}\csc^2\left(\frac{h}{2}\right) & \cdots & \cdots & \cdots & \\ -\frac{1}{2}\csc^2(h) & \frac{1}{2}\csc^2\left(\frac{h}{2}\right) & -\frac{\pi^2}{3h^2}-\frac{1}{6} & \frac{1}{2}\csc^2\left(\frac{h}{2}\right) & \cdots & \cdots & \cdots \\ \vdots & & \ddots & \ddots & & & \vdots \\ \vdots & & & \ddots & \ddots & \ddots & \vdots \\ \cdots & \cdots & \cdots & \cdots & \cdots & -\frac{\pi^2}{3h^2}-\frac{1}{6} & \frac{1}{2}\csc^2\left(-\frac{h}{2}\right) \\ 0 & \cdots & \cdots & \cdots & 0 & 0 & 0 \end{bmatrix}$$

$$\times \begin{bmatrix} u_1(T) \\ u_2(T) \\ \vdots \\ \vdots \\ \vdots \\ u_{n-1}(T) \\ u_n(T) \end{bmatrix} - \overline{A} \begin{bmatrix} \sin\left(\frac{u_1(T)}{2}\right) \\ \sin\left(\frac{u_2(T)}{2}\right) \\ \vdots \\ \vdots \\ \vdots \\ \sin\left(\frac{u_{n-1}(T)}{2}\right) \\ \sin\left(\frac{u_n(T)}{2}\right) \end{bmatrix} - \overline{B} \begin{bmatrix} \sin u_1(T) \\ \sin u_2(T) \\ \vdots \\ \vdots \\ \vdots \\ \sin u_{n-1}(T) \\ \sin u_n(T) \end{bmatrix} + \overline{C} \begin{bmatrix} \cos\left(\frac{u_1(T)}{2}\right) \\ \cos\left(\frac{u_2(T)}{2}\right) \\ \vdots \\ \vdots \\ \vdots \\ \cos\left(\frac{u_{n-1}(T)}{2}\right) \\ \cos\left(\frac{u_n(T)}{2}\right) \end{bmatrix}$$

$$- \begin{bmatrix} 8b\cos\left(\frac{u_1(T)}{2}\right) \\ 0 \\ \vdots \\ \vdots \\ \vdots \\ 0 \\ 8b\cos\left(\frac{u_n(T)}{2}\right) \end{bmatrix}, \tag{28}$$

and

$$\begin{bmatrix} u_1'T \\ u_2'(T) \\ \vdots \\ \vdots \\ \vdots \\ u_{n-1}'(T) \\ u_n'(T) \end{bmatrix} = \kappa \begin{bmatrix} 0 & 0 & 0 \ \dots \ \dots & \dots & 0 \\ \frac{1}{2}\csc^2\left(\frac{h}{2}\right)\cot\left(\frac{h}{2}\right) & -\frac{\pi^2}{3h^2}-\frac{1}{12} & \dots \ \dots \ \dots & \dots & \\ \vdots & \frac{1}{2}\csc^2\left(\frac{h}{2}\right)\cot\left(\frac{h}{2}\right) & \dots \ \dots \ \dots & \dots & \dots \\ \vdots & & \ddots \ \ddots & & \vdots \\ \vdots & & & \ddots \ \ddots & \vdots \\ \dots & \dots & \dots \ \dots \ \dots & -\frac{\pi^2}{3h^2}-\frac{1}{12} & \frac{1}{2}\csc^2\left(-\frac{h}{2}\right)\cot\left(-\frac{h}{2}\right) \\ 0 & \dots & \dots \ \dots & 0 & 0 \end{bmatrix}$$

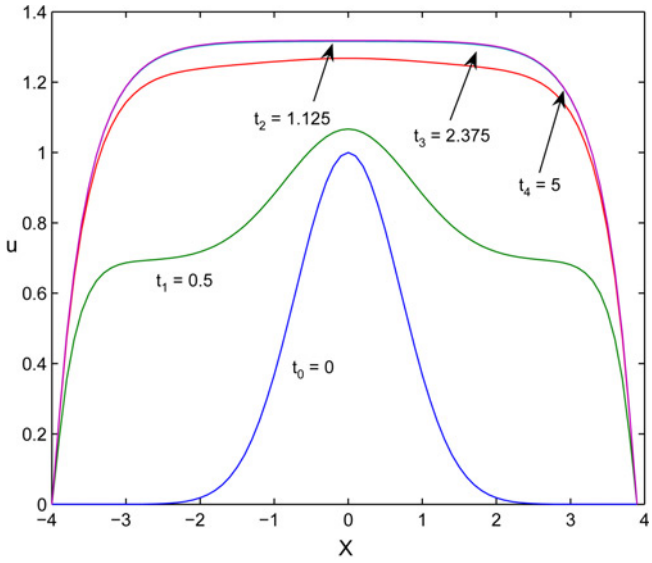
$$\times \begin{bmatrix} u_1(T) \\ u_2(T) \\ \vdots \\ \vdots \\ \vdots \\ u_{n-1}(T) \\ u_n(T) \end{bmatrix} - \overline{A} \begin{bmatrix} \sin\left(\frac{u_1(T)}{2}\right) \\ \sin\left(\frac{u_2(T)}{2}\right) \\ \vdots \\ \vdots \\ \vdots \\ \sin\left(\frac{u_{n-1}(T)}{2}\right) \\ \sin\left(\frac{u_n(T)}{2}\right) \end{bmatrix} - \overline{B} \begin{bmatrix} \sin u_1(T) \\ \sin u_2(T) \\ \vdots \\ \vdots \\ \vdots \\ \sin u_{n-1}(T) \\ \sin u_n(T) \end{bmatrix} \tag{29}$$

$$+ \overline{C} \begin{bmatrix} \cos\left(\frac{u_1(T)}{2}\right) \\ \cos\left(\frac{u_2(T)}{2}\right) \\ \vdots \\ \vdots \\ \vdots \\ \cos\left(\frac{u_{n-1}(T)}{2}\right) \\ \cos\left(\frac{u_n(T)}{2}\right) \end{bmatrix} - \begin{bmatrix} 8b\cos\left(\frac{u_1(T)}{2}\right) \\ 0 \\ \vdots \\ \vdots \\ \vdots \\ 0 \\ 8b\cos\left(\frac{u_n(T)}{2}\right) \end{bmatrix},$$

for N odd. We once again use ode15s in MATLAB to solve the resulting system. The results are plotted in Figure 9. As in the case of the sinc method, the steady state solution is smooth with out oscillations at the boundary.

4. Concluding remarks

In this paper, we have shown that a finite difference approximation to the model Equation (16) produces results with high oscillations at the boundaries. The method of lines approach reduces the oscillations at the boundaries. The steady solution is however not very smooth. The sinc and Fourier methods both obtain smooth steady solutions. A summary of the time taken for each of the programs to run is shown in



Notes: The solutions tends to the steady state in a stable manner

Figure 9.
Numerical solution of the model Equation (16) obtained using the Fourier method

	tfinal = 0.1	tfinal = 5
Sinc	0.9477	1.0107
Fourier	0.5393	0.6057
Method of lines	0.9177	0.9812

Table I.
Total times of methods

Table I. The Fourier method is the most efficient in terms of the time taken for the program to reach *tfinal*. This is because of the trigonometric terms which occur in the model Equation (16).

References

Bellomo, N., De Angelis, E., Graziano, L. and Romano, A. (2001), "Solution of nonlinear problems in applied sciences by generalized collocation methods and mathematica", *Computer & Mathematics with Applications*, Vol. 41, pp. 1343-63.

Boyd, J.P. (2001), *Chebyshev and Fourier Spectral Methods*, 2nd ed., Dover, New York, NY.

de Gennes, P.G. (1974), *The Physics of Liquid Crystals*, Clarendon, Oxford.

Fornberg, B. (1996), *A Practical Guide to Pseduospectral Methods*, Cambridge University Press, Cambridge.

Gray, G.W. and Goodby, J.W. (1985), "Smectic liquid crystals: textures and structures", *Acta Crystals*, Vol. B41, pp. 205-6.

Holmas, H., Clamond, D. and Langtangen, H.P. (2008), "A pseudospectral fourier method for a 1D incompressible two-fluid model", *International Journal of Numerical Methods in Fluids*, Vol. 58, pp. 639-58.

Khaliq, A.Q.M., Martin, J., Wade, B.A. and Yousuf, M. (2009), "Smoothing schemes for reaction-diffusion systems with nonsmooth data", *Journal of Computational and Applied Mathematics*, Vol. 223, pp. 374-86.

Khaliq, A.Q.M., Wade, B.A., Yousuf, M. and Vigo Augiar, J. (2007), "Higher order smoothing schemes for inhomogeneous parabolic problems with applications to nonsmooth payoff in option pricing", *Numerical Methods for Partial Differential Equations*, Vol. 23, pp. 1249-76.

Leslie, F.M., Stewart, I.W. and Nakagawa, M. (1991) "A continuum theory for smectic-C liquid crystals", *Molecular Crystals Liquid Crystals*, Vol. 198, pp. 443-54.

Lund, J. and Bowers, K.L. (1992), "Sinc methods for quadrature and differential equations", *Society for Industrial and Applied Mathematics*.

Nielsen, I.M.B. and Janssen, C.L. (2001), "A novel pseudospectral Fourier method for solving Poissons equation for a solute in a non-uniform dielectric", *Computer Physics Communication*, Vol. 136, pp. 29-36.

Ried, S., Pleiner, H. and Zimmermann, W. (2000), "Electrically driven hybrid instabilities in smectic C liquid crystal films", *Europhysics Letters*, Vol. 52, pp. 525-31.

Smith, G.D. (1985), *Numerical Solution of Partial Differential Equations: Finite Difference Methods*, Clarendon Press, Oxford.

Stenger, F. (1981), "Numerical methods based on Whitaker Cardinal or Sinc Functions", *SIAM Review*, Vol. 23, pp. 165-224.

Stewart, I.W. (1998), "Painlevè analysis for a semi-linear parabolic equation arising in smectic liquid crystals", *Journal of Applied Mathematics*, Vol. 61, pp. 47-60.

Stewart, I.W. (2004), *The Static and Dynamic Continuum Theory of Liquid Crystals*, Taylor and Francis, London and New York, NY.

Stewart, I.W. (2007), "The alignment of smectic-A liquid crystals with director tilt on the boundaries", *Journal of Physics A: Mathematical Theoretical*, Vol. 40, pp. 5297-318.

Stewart, I.W. and Momoniat, E. (2004), "Traveling waves in ferroelectric smectic-C liquid crystals", *Physical Reveiw E*, Vol. 69, p. 061714.

Stewart, I.W., Carlsson, T. and Leslie, F.M. (1994), "Chaotic instabilities in smectic-C liquid crystals", *Physical Review E*, Vol. 49, pp. 2130-40.

PLC (n.d.), "Introduction to liquid crystals", PLC, Case Western Reserve University, Cleveland, OH, available at: http://plc.cwru.edu/tutorial/enhanced/files/lc/Intro.html (accessed April 2007).

Trefethen, L.N. (2000), *Spectral Methods in MATLAB*, SIAM, Society for Industrial and Applied Mathematics, Philadelphia, PA.

Weideman, J.A.C. and Reddy, S.C. (2000), *A MATLAB Differentiation Matrix Suite*, ACM, New York, NY.

Yousuf, M. (2008), "On the class of high order time stepping schemes based on padè approximations for numerical solution of burgers' equation", *Applied Mathematics and Computation*, Vol. 205, pp. 442-53.

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