XVIII INTERNATIONAL CONFERENCE ON HYPERBOLIC PROBLEMS
THEORY, NUMERICS, APPLICATIONS
Málaga, June 20-24, 2022

Convergence analysis of a fully discrete energy-stable numerical scheme for the Q-tensor flow of liquid crystals

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Liquid crystals constitute a state of matter that is intermediate between solids and liquids. On one hand, they have properties that are typical for fluids, in particular they have the ability to flow, on the other hand, they exhibit properties of solids, as an example, their molecules are oriented in a crystal-like manner. A common characteristic of materials exhibiting a liquid crystal phase is that they consist of elongated molecules of identical size. They may be pictured as 'rods' or 'ribbons' and are subject to molecular interactions that make them align alike.

Liquid crystals play an important role in nature. One generally distinguishes three types of liquid crystals, nematics, cholesterics and smectics. We focus here on the numerical discretization of a liquid crystal model for nematic liquid crystals, the so-called Q-tensor model by Landau and de Gennes. The main orientation of the liquid crystal molecules is represented by the Q-tensor, a symmetric, trace-free matrix that is assumed to minimize the Landau-de Gennes free energy.

$$E_{LG}(Q) = \int_\Omega \mathcal{F}_B(Q) + \mathcal{F}_E(Q),$$

in equilibrium situations. Here $\Omega \in \mathbb{R}^n$, $n = 2, 3$, is the spatial domain occupied by the liquid crystal molecules, $\mathcal{F}_B$ is a bulk potential and $\mathcal{F}_E$ is the elastic energy given by

$$\mathcal{F}_B(Q) = \frac{a}{2}\operatorname{tr}(Q^2) - \frac{b}{3}\operatorname{tr}(Q^3) + \frac{c}{4}(\operatorname{tr}(Q^2))^2, \quad \mathcal{F}_E(Q) = \frac{L_1}{2}|\nabla Q|^2 + \frac{L_2}{2}|\operatorname{div} Q|^2 + \frac{L_3}{2}\sum_{i=1}^{3}\partial_i Q_{jk}\partial_j Q_{ik},$$

where a, b, c, L_1, L_2, L_3 are constants with $c, L_1, L_2, L_3 > 0$.

Non-equilibrium situations can be described by the gradient flow,

$$\begin{aligned}\frac{\partial Q_{ij}}{\partial t} = M\Bigg(&L_1\Delta Q_{ij} + \frac{L_2+L_3}{2}\left(\sum_{k=1}^{3}(\partial_{ik}Q_{jk} + \partial_{jk}Q_{ik}) - \frac{2}{3}\sum_{k,\ell=1}^{3}\partial_{k\ell}Q_{k\ell}\delta_{ij}\right)\\ &- \left(aQ_{ij} - b\left((Q^2)_{ij} - \frac{1}{n}\operatorname{tr}(Q^2)\delta_{ij}\right) + c\operatorname{tr}(Q^2)Q_{ij}\right)\Bigg),\end{aligned} \tag{1}$$

where $M > 0$ is a constant, and one approach to obtaining equilibrium states is to follow this gradient flow. Adding the dynamics of mean flow of the liquid crystal fluid to this, one obtains the Beris-Edwards system.

Our goal is to show that a fully discrete version of the numerical method for the Q-tensor flow constructed by Zhao et al. [1] is convergent. This method takes as a basis the reformulation of the Q-tensor flow using the auxiliary variable r:

$$r(Q) = \sqrt{2\left(\frac{a}{2}\operatorname{tr}(Q^2) - \frac{b}{3}\operatorname{tr}(Q^3) + \frac{c}{4}\operatorname{tr}^2(Q^2) + A_0\right)}, \tag{2}$$

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where A_0 is a constant ensuring that r is positive. Defining

$$S(Q) = aQ - b\left[Q^2 - \frac{1}{n}\text{tr}(Q^2)I\right] + c\text{tr}(Q^2)Q, \tag{3}$$

it follows that

$$\frac{\delta r(Q)}{\delta Q} = \frac{S(Q)}{r(Q)} := P(Q). \tag{4}$$

for symmetric, trace free tensors Q. Then one can formally write the gradient flow (1) as a system for (Q, r):

$$Q_t = M\left(L_1\Delta Q + \frac{L_2+L_3}{2}\alpha(Q) - rP(Q)\right) := MH, \tag{5a}$$

$$r_t = P(Q) : Q_t, \tag{5b}$$

where

$$\alpha(Q)_{ij} = \sum_{k=1}^{3}(\partial_{ik}Q_{jk} + \partial_{jk}Q_{ik}) - \frac{2}{3}\sum_{k,\ell=1}^{3}\partial_{k\ell}Q_{k\ell}\delta_{ij}.$$

We then propose the following numerical method to solve system (5)

$$\begin{cases} D_t^+ Q_{ijk}^n = M\left(L_1\Delta_h Q_{ijk}^{n+\frac{1}{2}} - r_{ijk}^{n+\frac{1}{2}}\overline{P}_{ijk}^{n+\frac{1}{2}} + \frac{L_2+L_3}{2}\alpha_{ijk}^{n+\frac{1}{2}}\right) := MH_{ijk}^{n+\frac{1}{2}} \\ r_{ijk}^{n+1} - r_{ijk}^n = \overline{P}_{ijk}^{n+\frac{1}{2}} : (Q_{ijk}^{n+1} - Q_{ijk}^n) \end{cases} \tag{6}$$

Here, Q_{ijk}^n is an approximation for Q and r_{ijk}^n is an approximation of r at spatial point (x_i, y_j, z_k) and time step n.

In this work, we have shown that weak solutions of (5) are in fact weak solutions of (1) and so achieve convergence to the original system (1). To the best of our knowledge, this is the first convergence proof for a numerical scheme discretizing (1). The proof is based on the derivation of discrete energy stability of the fully discrete scheme, then using this to derive the existence of a precompact sequence that allows us to pass to the limit in the approximations. We proceed to showing Lipschitz continuity of the function P and use a Lax-Wendroff type argument to show that the limit of the approximating sequence is a weak solution of (5). The last step is to show that weak solutions of (5) are in fact weak solutions of (1). We achieve this through showing that a weak form of the chain rule holds in this case. We conclude with numerical experiments in 2D. Our scheme and analysis is for the 3D case but adaptions to 2D can be made easily. For example, dynamics of defects is presented in

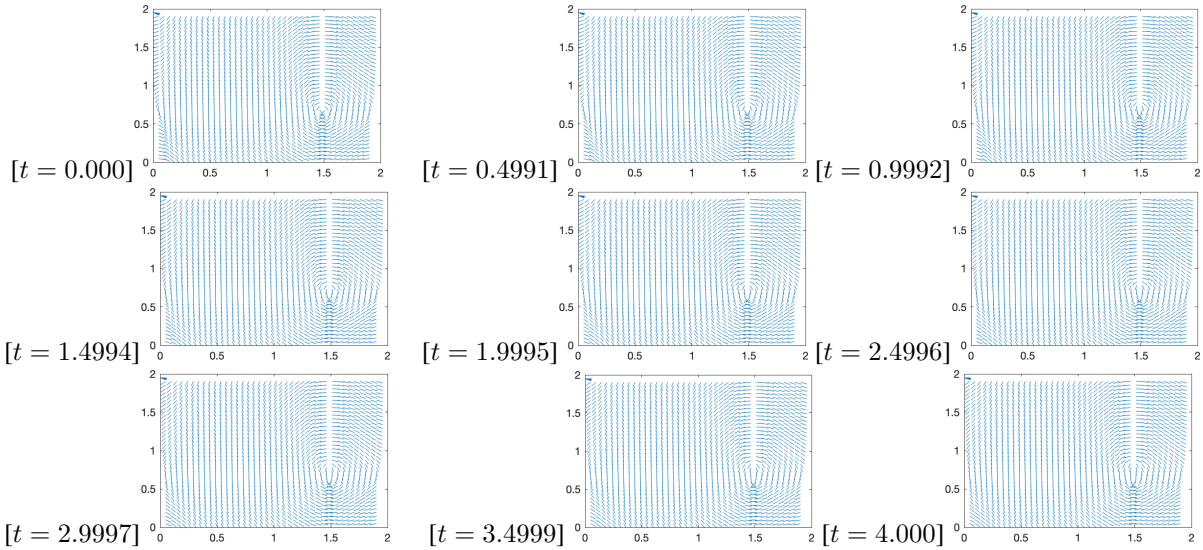

Figure 1: Simulation for defects of liquid crystals

Acknowledgements

This research is sponsored by NSF-DMS 1912854

References

[1] J. Zhao, X. Yang, Y. Gong, and Q. Wang. A novel linear second order unconditionally energy stable scheme for a hydrodynamic Q-tensor model of liquid crystals. *Comput. Methods Appl. Mech. Engrg.*, 318:803–825, 2017.