A PROJECTION-BASED TIME-SPLITTING FINITE ELEMENT METHOD FOR THE NUMERICAL APPROXIMATION OF NEMATIC LIQUID CRYSTALS FLOWS

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ABSTRACT. Liquid crystals, [3], are materials showing intermediate transitions between solid and liquid called mesophases. The mathematical theory describing liquid crystals attend the different degrees of the positional ordering of the molecules and their orientational ordering. This second ordering, alludes to the fact that the molecules tend to be locally aligned in a preferred direction. Such a direction is described by a unit vector $\boldsymbol{d}$ along the molecule if it is rod-shaped or perpendicular to the molecule if it is plate-shaped, by measuring the mean values of alignments. The simplest phase of liquid crystals is called nematic, which possesses an orientational ordering but not positional, thus, the molecules flow freely as in a disordered isotropic liquid phase while tend to be orientated along a direction.

Let $\Omega \subset \mathbb{R}^M, M = 2, 3$ a bounded domain and $T > 0$. We consider the following mathematical model for nematic liquid crystal to capture the coupling between the flow field and the dynamics of the director field:

$$
(1) \quad \begin{cases} \partial_t \boldsymbol{d} + \boldsymbol{u} \cdot \nabla \boldsymbol{d} + \beta(\nabla \boldsymbol{u})\boldsymbol{d} + (1+\beta)(\nabla \boldsymbol{u})^T \boldsymbol{d} + \gamma(\boldsymbol{f}_\varepsilon(\boldsymbol{d}) - \Delta \boldsymbol{d}) = \boldsymbol{0}, & \text{in } \Omega \times (0,T), \\ \partial_t \boldsymbol{u} + \boldsymbol{u} \cdot \nabla \boldsymbol{u} - \nu \Delta \boldsymbol{u} + \nabla p + \lambda \nabla \cdot ((\nabla \boldsymbol{d})^T \nabla \boldsymbol{d}) & \\ \qquad + \lambda \nabla \cdot (\beta(\boldsymbol{f}_\varepsilon(\boldsymbol{d}) - \Delta \boldsymbol{d})\boldsymbol{d}^T + (1+\beta)\boldsymbol{d}(\boldsymbol{f}_\varepsilon(\boldsymbol{d}) - \Delta \boldsymbol{d})^T) = \boldsymbol{0}, & \text{in } \Omega \times (0,T), \\ \nabla \cdot \boldsymbol{u} = 0, & \text{in } \Omega \times (0,T), \end{cases}
$$

where $\boldsymbol{u}$ is the velocity of the fluid, p is the pressure, and $\boldsymbol{d}$ is the orientation of the molecules. ν, λ, γ are positive constants representing the viscosity of the fluid, , the coupling coef- ficient representing the competition parameter between the kinetic energy and the elastic energy, and the parameter of elastic relaxation time. $\beta \in [-1, 0]$ is a constant associated with the aspect ratio of the ellipsoid particles, $\boldsymbol{f}_\varepsilon(\boldsymbol{d}) = \varepsilon^{-2}\left(|\boldsymbol{d}|^2 - 1\right)\boldsymbol{d}$, and $\varepsilon > 0$ are a function and a penalization parameter, respectively. The system (1) is supplemented by adequate initial and boundary conditions.

We develop a numerical algorithm to solve system (1), by following the ideas presented in [2]. The method is designed at two levels. First, at the differential level: we decouple the velocity, the pressure and the director. In this case, the director must be computed together with an auxiliary variable in order to deduce a priori energy estimates. Second, at the algebraic level: we can avoid computing such an extra variable because the auxiliary variable is approximated by a piecewise constant finite-element space and is coupled with the director by a linear system of equations. Therefore, the resulting numerical scheme can be written only in terms of the director variable. Additionally, the velocity-pressure is managed by a fractional step method of equal order for the velocity and the pressure (see [1]).

Finally, we perform some numerical simulations originally in presented in [4], to show the robustness and the efficiency of the proposed numerical scheme.

Keywords: Nematic liquid crystal; Finite elements; Projection method; Time-splitting method; stabilized methods.

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