CONVERGENT STRUCTURE-PRESERVING FINITE ELEMENT METHODS FOR NEMATIC LIQUID CRYSTALS

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ABSTRACT

Liquid crystals (LCs) are materials which exhibit properties intermediate between isotropic liquids and crystalline solids. The Ericksen model describes nematic LCs in terms of a unit-length vector field (director) and a scalar function (degree of orientation). Equilibrium states of the LC are given by admissible pairs that minimize an energy functional, which consists of the sum of Oseen-Frank-like energies and a double well potential. The resulting Euler-Lagrange equations are degenerate for the director, which poses serious difficulties to formulate mathematically sound algorithms for their approximation. We propose a simple but novel finite element approximation of the problem that can be implemented easily within standard finite element packages. The scheme does not employ a projection to impose the unit-length constraint on the director and thus circumvents the use of weakly acute meshes, which are quite restrictive in 3D but are required by recent algorithms for convergence. We show stability and Gamma-convergence properties of the new method in the presence of defects. We also discuss an effective nested gradient flow algorithm for computing minimisers that controls the violation of the unit-length constraint. We present several simulations in 2D and 3D that document the performance of the proposed scheme and its ability to capture quite intriguing defects. This is joint work [1] with Ricardo H. Nochetto (University of Maryland) and Shuo Yang (Tsinghua University).

References

[1] R. H. Nochetto, M. Ruggeri, S. Yang. *Gamma-convergent projection-free finite element methods for nematic liquid crystals: The Ericksen model.* SIAM J. Numer. Anal. 60, 2 (2022), 856-887.

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