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Computational Mathematics Seminar Series

A Numerical Scheme for the Generalized Ericksen Model of Liquid Crystals With Applications to Virus DNA Packing

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Digital Media Center 1034
October 30, 2018 - 03:30 pm

Abstract:

We consider the generalized Ericksen model of liquid crystals, which is an energy with 8 independent ``elastic'' constants that depends on two order parameters n (director) and s (variable degree of orientation). In addition, we present a new finite element discretization for this energy, that can handle the degenerate elliptic part without regularization, is stable and it Gamma-converges to the continuous energy. Moreover, it does not require the mesh to be weakly acute (which was an important assumption in our previous work). A minimization scheme for computing discrete minimizers will also be discussed.

Furthermore, we include other effects such as weak anchoring (normal and tangential), as well as fully coupled electro-statics with flexo-electric and order-electric effects. We also present several simulations (in 2-D and 3-D) illustrating the effects of the different elastic constants and electric field parameters.

At the end of the talk, we discuss a problem about the packing of DNA inside viral capsids. We show how the generalized Ericksen model can be used to simulate the packing of DNA inside viral capsids, and to estimate packing pressures inside the capsid. This part is joint with Carme Calderer (UMN), Dmitry Golovaty (U. Akron).

Speaker's Bio:

Shawn Walker received his Ph.D. from the University of Maryland, College Park. He held a postdoctoral position at the Courant Institute (New York University), and joined the LSU faculty in 2010 in the computational mathematics group. He is now an associate professor in the mathematics department at LSU. He researches numerical methods to solve complex physical problems that arise in fluids and material science. He has won two NSF grants for work on developing numerical methods for partial differential equation (PDE) models of multi-physics and geometric evolution problems using finite element methods, as well as mesh generation, and PDE-constrained (shape) optimization. He also won an NSF CAREER award on "Numerical Methods For Liquid Crystals And Their Optimal Design" to develop advanced computational methods to better understand liquid crystal physics and enable material science applications of liquid crystals.

This lecture has refreshments @ 03:00 pm