ME – MTech (Res) Thesis Colloquium

Hybrid Finite-Difference Lattice Boltzmann Method for Tensorial Nematodynamics of Liquid Crystals

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ABSTRACT

Nematic liquid crystals are anisotropic soft materials whose rod-like molecules exhibit long-range orientational order, enabling them to flow like liquids while exhibiting anisotropy and elasticity. Despite their remarkable flow behaviour in microfluidic environments and their considerable potential for particle sorting and separation, the mechanisms governing the transport and manipulation of micron-sized particles in these complex fluids remain poorly understood. Developing numerical methods that accurately capture these phenomena is therefore essential for the design of nematic liquid crystal-based microfluidic devices. The nonlinear coupling between nematic orientational order and fluid flow, even in the creeping-flow regime, poses a significant challenge for the numerical modelling of nematic liquid crystals.

The present dissertation develops a hybrid finite-difference lattice Boltzmann solver coupled with the smoothed profile method to solve the tensorial nematodynamic equations in a two-dimensional domain and numerically investigate flow and particle transport in confined nematic liquid crystals. The proposed method is extensively validated against several benchmark problems involving nematic liquid crystals. The competing effects of flow-induced nematic alignment and elastic resistance to the director rotation are accurately reproduced in the simulations for shear flow of nematic liquid crystals. Rigid circular particles within shear flow of nematic liquid crystals exhibit cross-stream migration. The cross-stream migration of the particle reveals a strong dependence on the Ericksen number (*Er*). Here, *Er* denotes the ratio of viscous to elastic forces. The particle settles at the channel centreline for small *Er*. For larger *Er*, two off-centre equilibrium positions placed symmetrically about the channel centreline are observed, giving rise to a pitchfork-like bifurcation in the equilibrium transverse positions with respect to *Er*. The lift force computations on the particle at fixed transverse positions agree with the observed bifurcation behaviour in the equilibrium transverse positions. The topological configuration and the morphology of the Saturn ring defect show a close correlation with *Er*. An increase in *Er* demonstrates a change in the relative orientation of the Saturn ring defects, with the individual defects approaching each other closely on the particle periphery, losing their diametric symmetry. The particle-frame velocity contours confirm the strong coupling between momentum transport and orientational order evolution, with a distinct vertical symmetry observed at low *Er* that diminishes as *Er* increases and bifurcation occurs. Overall, the system dynamics are dictated by the anisotropic viscous and elastic forces/torques on the particle. The developed computational framework provides valuable insights into particle transport mechanisms in nematic liquid crystals and establishes a foundation for designing liquid crystal-based microfluidic systems.

ABOUT THE SPEAKER

Kalyan Kumar is currently pursuing an M.Tech. (Research) in the Department of Mechanical Engineering at the Indian Institute of Science (IISc), Bengaluru, under the supervision of Dr. Shubhadeep Mandal. His research focuses on the computational modelling of complex fluids, with particular emphasis on developing a smoothed-profile lattice Boltzmann framework for nematic liquid crystals.