Active Nematodynamics on Curved Surfaces – The Influence of Geometric Forces on Motion Patterns of Topological Defects

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Abstract. We derive and numerically solve a surface active nematodynamics model. We validate the numerical approach on a sphere and analyse the influence of hydrodynamics on the oscillatory motion of topological defects. For ellipsoidal surfaces the influence of geometric forces on these motion patterns is addressed by taking into account the effects of intrinsic as well as extrinsic curvature contributions. The numerical experiments demonstrate the stronger coupling with geometric properties if extrinsic curvature contributions are present and provide a possibility to tune flow and defect motion by surface properties.

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1 Introduction

The driving force behind the huge interest in collective behaviour of active matter is the goal to understand the physics of natural materials. One well-studied class of active matter, which includes, for example, epithelia cells, elongated bacteria and filamentous particles inside living cells, can be described by the interaction of rod-shaped particles. This relates these systems to nematic liquid crystals with long-range orientational order between these particles. Adapting these theories and extending them by active components leads to the concept of ‘active nematics’, see [7] for a review. The active contribution
drives the system out of equilibrium and leads to spontaneous generation/annihilation of topological defects, destruction of long-ranged nematic order and the formation of active turbulence.

If such systems are confined on curved surfaces, topological constraints strongly influence the emerging spatiotemporal patterns. Using these topological constraints to guide collective cell behavior might be a key in morphogenesis [8] and active nematic films on surfaces have been proposed as a promising road to engineer synthetic materials that mimic living organisms [18]. As in passive systems the mathematical Poincaré-Hopf theorem forces topological defects to be present in the nematic film. On a sphere this leads to an equilibrium defect configuration with four +1/2 disclinations arranged as a tetrahedron [21]. The disclinations repel each other and this arrangement maximises their distance. In active systems unbalanced stresses drive this configuration out of equilibrium. But in contrast to planar active nematics with continuous creation and annihilation of defects the creation of additional defect pairs can be suppressed on curved surfaces, which is demonstrated in [18] for an active nematic film of microtubules and molecular motors, encapsulated within a spherical lipid vesicle. This provides an unique way to study the dynamics of the four defects in a controlled manner and led to the discovery of a tunable periodic state that oscillates between the tetrahedral and a planar defect configuration.

Various modeling approaches have been proposed to describe the periodic defect motion. They range from a coarse-grained model in which the +1/2 disclinations are effectively described by self-propelled particles with a velocity proportional to the activity [12]. On a sphere this approach leads to oscillations between the planar and tetrahedral configuration [18]. However, a quantitative comparison with the experimental results leads to differences, which become more evident for more general surfaces. For non-constant Gaussian curvature constraints local geometric properties influence the position of the defects and thus can be used to control defect dynamics. These effects are addressed with particle simulations [1, 2, 10]. We here consider a continuous description and also account for hydrodynamic effects. The considered model belongs to the class of ‘active nematodynamics’, it is a simplified Beris-Edwards model with active driving, see [17] for a review. We propose a thin-film limit of this modeling approach and numerically solve the corresponding surface model. Related models have been considered in [38, 45]. However, these models are based on a simplified surface Landau-de Gennes energy neglecting various curvature contributions [20]. For more detailed surface Landau-de Gennes models which also take extrinsic curvature contributions into account, see [15, 26, 29]. Another critical issue is the considered numerical approach for the Navier-Stokes-like equations. In [38, 45] it is based on a vorticity-stream function formulation and thus is restricted to surfaces which are topologically equivalent to a sphere [33]. More general numerical approaches have been proposed in [30, 41, 42]. We here combine such a general formulation with a numerical approach for a surface Landau-de Gennes model with intrinsic and extrinsic curvature contributions [29, 32] and demonstrate the relation between flow, topological defects and geometric properties of the surface for sur-