

Active nematic fluid films

P. Rangamani[†]

Department of Mechanical and Aerospace Engineering, University of California San Diego, La Jolla, CA 92093-0411, USA

(Received 3 February 2023; accepted 13 February 2023)

Coupling surface deformations with active stresses in two-dimensional nematic liquid crystal films leads to a rich area of investigation, particularly in biological fluid mechanics across multiple scales from tissue mechanics to cell membrane mechanics. In Al-Izzi & Morris (*J. Fluid Mech.*, vol. 957, 2023, A4), the authors derive the complete set of governing equations for such systems. Their results provide an extended theoretical framework with which active nematic fluid films with in-plane flow and out-of-plane deformation can be analysed. To illustrate the potential applications of this framework, a few specific biologically inspired examples are discussed.

Key words: membranes

1. Introduction

Interfacial fluid phenomena are of interest in a wide range of applications including biological materials such as membranes formed by lipid bilayers and two-dimensional liquid crystal films. The development of a theoretical framework that describes the governing equations for these interfaces has been of long-standing interest to both the fluids and biophysics community. The dynamics of a fluid interface for a Newtonian fluid is concisely given in Scriven (1960). Inspired by these works and by the observations that lipid bilayers behave as fluid membranes (Singer & Nicolson 1972), the governing equations for deformable membranes with bending elasticity and viscous flow were derived a few years ago (Arroyo & DeSimone 2009; Rangamani *et al.* 2013). These studies have led to multiple insights into how the viscosity of the fluid film can interact with the bending elasticity, foremost of which is the description of the Scriven–Love number and its implications (Al-Izzi, Sens & Turner 2020; Sahu *et al.* 2020). This dimensionless number captures the competition between the viscous and bending forces in the membrane. Building on these prior works, we now focus on the two-dimensional active nematic fluids and their governing equations as described in Al-Izzi & Morris (2023).

[†] Email address for correspondence: prangamani@ucsd.edu

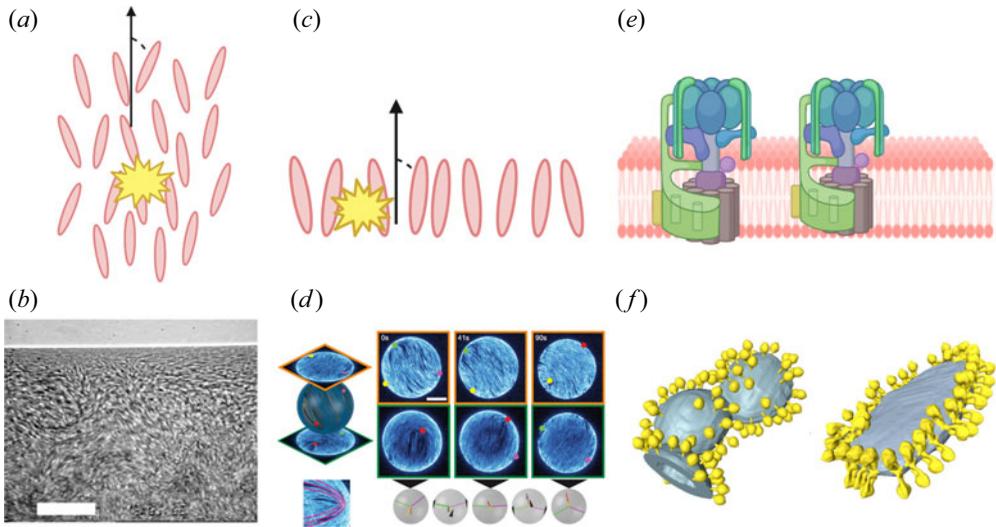


Figure 1. (a) Three-dimensional nematic liquid crystals have long-range orientational order but no positional order. The director is the black arrow and represents the average orientation of the liquid crystals. Presence of activity (represented by yellow) leads to hydrodynamic flows as shown in a bacterial suspension in (b), scale bar 35 μm . Image adapted with permission from Dombrowski *et al.* (2004). (c) Two-dimensional liquid crystals with activity also have a director field associated with them and presence of activity on such surfaces can lead to flow patterns as observed in panel (d). These experiments were conducted using active nematic liquid crystals on lipid bilayers; image adapted with permission from Keber *et al.* (2014). (e) Lipid bilayers with embedded motor proteins such as adenosine triphosphate (ATP) synthases shown as a schematic. (f) The interaction of the ATP synthases alters the surface curvature of the lipid membrane. The left image shows monomeric ATP synthases and the right image shows dimeric ATP synthases. Image adapted with permission from Davies *et al.* (2012). Figure created with BioRender.com.

2. Overview

Nematic liquid crystals are rod-shaped molecules that do not have a translational order but instead have a long-range orientational order, which is represented by a director field (figure 1a). A specific biological example of such systems in three dimensions is bacterial suspensions, shown in figure 1(b), (Dombrowski *et al.* 2004). The coupling of nematic liquid crystals and thin film deformation has been studied by different groups with varying degrees of complexity (Nitschke, Reuther & Voigt 2020). Coupling deformation with a director field is a challenging mathematical problem, particularly for two-dimensional films. The effect of surface geometry on the order parameter was explored in detail in Napoli & Vergori (2012). Steigmann (2013) worked out a detailed theory for lipid membranes with tilt and distension based on three-dimensional liquid crystal theory, and explored how the deformation and the director field exhibit coupled behaviours in special cases (Rangamani & Steigmann 2014; Rangamani *et al.* 2014) (figure 1c). These prior studies did not consider the interactions of the director field with the surface flows or the role played by the activity of the inclusions on the surface.

Al-Izzi & Morris (2023) derive the governing equations for active nematic fluids on deformable curved surface for nematic liquid crystals in the one-constant limit of the Frank free energy and derive the general form of the tangential and normal force balance equations. The activity of these liquid crystals, which characterizes their ability to convert stored energy or energy from the environment into motion, is described using an active stress tensor. They obtain the full dynamical equations that describe the polarization

dynamics, the constant director and incompressibility constraints and the tangential and normal balances. Analysis of these equations reveals both the dimensionless Scriven–Love number described above for isotropic coupling and a new ‘liquid crystalline Scriven–Love’ number that captures the anisotropic coupling terms. The dimensionless active stress, which results from comparing the tangential stresses with bending stress, is an analogue of the Föppl–von-Kármán number. These dimensionless numbers complete the analysis and allow for a comparison between isotropic fluid films and anisotropic fluids films for in-plane and out-of-plane stresses. Further, the authors apply their equations to some example cases. On tubes with active nematics, they find that contractile active stresses lead to the case of an ‘active pearling’ instability while extensile active stresses lead to ‘ruffles’.

There are many potential applications for the model developed in Al-Izzi & Morris (2023). Consider the field of membrane biophysics as a specific example. Cellular membranes contain many proteins that diffuse in the plane of the membrane. The dynamics of defects associated with active nematic liquid crystals on lipid vesicles was experimentally determined in Keber *et al.* (2014) (figure 1d). Deformation of the membrane in response to any curvature-inducing proteins is often modelled as a spontaneous curvature, a ‘catch-all’ input parameter that essentially forces the curvature of the surface. Coupling of the diffusion of such curvature-inducing proteins with membrane flow was discussed in Mahapatra, Saintillan & Rangamani (2020, 2021). However, many of these proteins are active, undergoing conformational changes or phosphorylation state changes due to biochemical reactions or interactions with the environment. Active proteins in cellular membranes can act as hydrodynamic dipoles, and analysis of hydrodynamic collective effects of active proteins in lipid bilayers showed that this activity can contribute to the diffusion enhancement and drift in the plane of the membrane (Mikhailov & Kapral 2015). The activity of these proteins could then influence the nematic order parameter and the deformation of the membrane without the need for specific-curvature-inducing domains on the bilayer. Al-Izzi & Morris (2023) discuss active pearling of a cylindrical tube. Such active pearling could be relevant to the function of membrane-embedded motor proteins in cellular systems. Prominent examples of such a system are the ATP synthases on mitochondrial membranes, which produce ATP in cells (figure 1e) (Nirody, Budin & Rangamani 2020). Applications of models such as those developed in Al-Izzi & Morris (2023) can shed light into how the activity of ATP synthases and local lipid environment may be coupled. Davies *et al.* (2012) showed that the curvature of the mitochondrial membranes depends on the interactions between ATP synthases (figure 1f). The long-range effects of active inclusions in deformable surfaces and the effect of non-uniform distribution of inclusion in local and long-range transport will be important to understand in general conditions and with applications to specific examples. Thus, this study paves the path forward for us to gain fundamental insight into some extremely complex, small length scale (nm– μm), active nematic thin fluid films.

3. Outlook

Deformable nematic shells appear in a wide range of biological systems ranging across length scales from tissues to subcellular components such as cellular membranes. Many of these components also carry activity and deform their shape in response to activity. Recent experiments described in Guillaumat *et al.* (2022) and simulations described in Zhang & Yeomans (2023) highlight the role of active forces in determining tissue architecture. The development of governing equations that describe the interaction of the activity with the nematic order parameter, such as the work done in Al-Izzi & Morris (2023),

is a step forward in our ability to investigate multiple physics, particularly in complex biological systems. These predictions set the stage for the investigation of both long-range interactions in these fluid films and short length scale molecular dynamic simulations to identify how the interactions between order parameter and activity can perturb the system. There now arises an exciting possibility of even making comparisons with experimental measurements; see Watkins *et al.* (2011) for beautiful grazing incidence X-ray diffraction measurements of textures induced on a lipid bilayer surface by cholera toxin molecules. For further in-depth investigation and generation of quantitative results, computational tools, including numerical schemes to solve the governing equations and molecular dynamic simulations to obtain small length scale parameters, will be needed (see Huang *et al.* 2013; Sauer 2018).

Acknowledgements. The author would like to thank Dr A. Chandrasekaran, S. Llewellyn Smith and D. Saintillan, and Y. Chen for their feedback and many discussions on this topic.

Declaration of interests. The author reports no conflict of interest.

Author ORCIDs.

© P. Rangamani <https://orcid.org/0000-0001-5953-4347>.

REFERENCES

- AL-IZZI, S.C. & MORRIS, R.G. 2023 Morphodynamics of active nematic fluid surfaces. *J. Fluid Mech.* **957**, A4
- AL-IZZI, S.C., SENS, P. & TURNER, M.S. 2020 Shear-driven instabilities of membrane tubes and dynamin-induced scission. *Phys. Rev. Lett.* **125** (1), 018101.
- ARROYO, M. & DESIMONE, A. 2009 Relaxation dynamics of fluid membranes. *Phys. Rev. E* **79** (3 Pt 1), 031915.
- DAVIES, K.M., ANSELMINI, C., WITTIG, I., FARALDO-GOMEZ, J.D. & KUHLBRANDT, W. 2012 Structure of the yeast F1Fo-ATP synthase dimer and its role in shaping the mitochondrial cristae. *Proc. Natl Acad. Sci.* **109** (34), 13602–13607.
- DOMBROWSKI, C., CISNEROS, L., CHATKAEW, S., GOLDSTEIN, R.E. & KESSLER, J.O. 2004 Self-concentration and large-scale coherence in bacterial dynamics. *Phys. Rev. Lett.* **93** (9), 098103.
- GUILLAMAT, P., BLANCH-MERCADER, C., PERNOLLET, G., KRUSE, K. & ROUX, A. 2022 Integer topological defects organize stresses driving tissue morphogenesis. *Nat. Mater.* **21**, 588–597.
- HUANG, M.-J., KAPRAL, R., MIKHAILOV, A.S. & CHEN, H.-Y. 2013 Coarse-grain simulations of active molecular machines in lipid bilayers. *J. Chem. Phys.* **138** (19), 195101.
- KEBER, F.C., LOISEAU, E., SANCHEZ, T., DECAMP, S.J., GIOMI, L., BOWICK, M.J., MARCHETTI, M.C., DOGIC, Z. & BAUSCH, A.R. 2014 Topology and dynamics of active nematic vesicles. *Science* **345** (6201), 1135–1139.
- MAHAPATRA, A., SAINTILLAN, D. & RANGAMANI, P. 2020 Transport phenomena in fluid films with curvature elasticity. *J. Fluid Mech.* **905**, A8.
- MAHAPATRA, A., SAINTILLAN, D. & RANGAMANI, P. 2021 Curvature-driven feedback on aggregation–diffusion of proteins in lipid bilayers. *Soft Matt.* **17** (36), 8373–8386.
- MIKHAILOV, A.S. & KAPRAL, R. 2015 Hydrodynamic collective effects of active protein machines in solution and lipid bilayers. *Proc. Natl Acad. Sci. USA* **112** (28), E3639–E3644.
- NAPOLI, G. & VERGORI, L. 2012 Extrinsic curvature effects on nematic shells. *Phys. Rev. Lett.* **108** (20), 207803.
- NIRODY, J.A., BUDIN, I. & RANGAMANI, P. 2020 ATP synthase: evolution, energetics, and membrane interactions. *J. Gen. Physiol.* **152** (11), e201912475.
- NITSCHKE, I., REUTHER, S. & VOIGT, A. 2020 Liquid crystals on deformable surfaces. *Proc. Math. Phys. Engng Sci.* **476** (2241), 20200313.
- RANGAMANI, P., AGRAWAL, A., MANDADAPU, K.K., OSTER, G. & STEIGMANN, D.J. 2013 Interaction between surface shape and intra-surface viscous flow on lipid membranes. *Biomech. Model. Mechanobiol.* **12** (4), 833–845.
- RANGAMANI, P., BENJAMINI, A., AGRAWAL, A., SMIT, B., STEIGMANN, D.J. & OSTER, G. 2014 Small scale membrane mechanics. *Biomech. Model. Mechanobiol.* **13** (4), 697–711.

Active nematic fluid films

- RANGAMANI, P. & STEIGMANN, D.J. 2014 Variable tilt on lipid membranes. *Proc. Math. Phys. Engng Sci.* **470** (2172), 20140463.
- SAHU, A., GLISMAN, A., TCHOUFAG, J. & MANDADAPU, K.K. 2020 Geometry and dynamics of lipid membranes: the Scriven–Love number. *Phys. Rev. E* **101** (5), 052401.
- SAUER, R.A. 2018 On the computational modeling of lipid bilayers using thin-shell theory. In *The Role of Mechanics in the Study of Lipid Bilayers* (ed. D.J. Steigmann), pp. 221–286. Springer.
- SCRIVEN, L.E. 1960 Dynamics of a fluid interface equation of motion for newtonian surface fluids. *Chem. Engng Sci.* **12** (2), 98–108.
- SINGER, S.J. & NICOLSON, G.L. 1972 The fluid mosaic model of the structure of cell membranes. *Science* **175** (4023), 720–731.
- STEIGMANN, D.J. 2013 A model for lipid membranes with tilt and distension based on three-dimensional liquid crystal theory. *Int'l J. Non-Linear Mech.* **56**, 61–70.
- WATKINS, E.B., MILLER, C.E., MAJEWSKI, J. & KUHL, T.L. 2011 Membrane texture induced by specific protein binding and receptor clustering: active roles for lipids in cellular function. *Proc. Natl Acad. Sci. USA* **108** (17), 6975–6980.
- ZHANG, G. & YEOMANS, J.M. 2023 Active forces in confluent cell monolayers. *Phys. Rev. Lett.* **130** (3), 038202.