The Mathematics of Liquid Crystals: Final Report

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Liquid crystals are materials that flow like liquids but retain orientational and in some cases positional order due to the arrangement of their constituent molecules. They were discovered in the late 19th century, but it was only in the 1960s that their immense technological potential for electronic displays began to be realized, leading to their present widespread use in computers, televisions, watches and other applications. At about the same time mathematicians became interested in theoretical models for liquid crystals that had been developed by Oseen, Frank and others, and a fertile period ensued in which the models were refined and attacked using powerful tools of nonlinear analysis.

Fig. 1: Ubiquitous liquid crystalline order: smectic basmati rice with defects. [1]

The Mathematics of Liquid Crystals Programme aimed to take advantage of a second wave of interest by mathematicians in the area, stimulated in part by the newer tensor order-parameter theory of de Gennes, in part by recently discovered liquid crystalline materials such as liquid crystal elastomers and active nematics, and in part by the developing potential of nonlinear and topological analysis to address the challenges of describing liquid crystal defects and other phenomena. At the same time many of the mathematical issues arising in the study of liquid crystals, such as the rigorous passage from atomic and molecular to continuum models and the mathematical description of defects, are of core interest in the description of solids, fluids and other types of soft matter, with a clear potential for cross-fertilization. The proposal for the MLC Programme was prepared with the help of a large number of world experts in different aspects of the subject (chemistry, physics, simulation, nonlinear analysis), most of whom spent extended periods at the Institute.

The many topics addressed in the workshops, seminars, informal lecture courses, discussion groups and individual interactions included the following:

- Density functional theory for single and multi-component liquid crystal systems, its use to predict quantities such as elastic constants and surface behaviour, and its relation to continuum theories.
- Generic equivariant bifurcation theory and its role in phase transitions.
- Phenomenological and molecular theories based on order parameters, their microscopic derivation, dependence on particle shapes, symmetries, bifurcations and eigenvalue constraints.
- Atomistic and molecular dynamics simulations of liquid crystal systems.
- Analysis of the Landau – de Gennes Q-tensor theory, its relation to director models, and the contrasting descriptions of defects in these different models.
- Topology and defect structures in liquid crystal colloid mixtures.
- Smectic and chiral structures: focal conic domains and torons.
- Dynamics of liquid crystal flows, well-posedness in director and Q-tensor models, bifurcation analysis of shear flows.

- Liquid crystalline solids, their microstructures, mechanical consequences of their LC defects, and use in elastomeric motors.
- Models of active liquid crystals in biology (in which the constituent particles are self-propelled) and their flows (see Fig. 2).

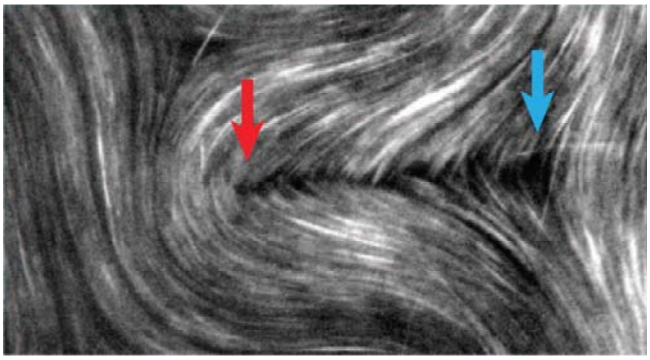

Fig. 2: Biologically related active microtubule liquid crystal domains extend, buckle and internally self-fracture. [2]

Numerous research projects were initiated, establishing new connections and international collaborations between mathematicians, physicists, chemists, materials scientists and biologists, from starting research students to established researchers.

Programme activities included four very successful one week workshops on different aspects of liquid crystals, one of which was a satellite meeting at the University of Oxford. An additional one day Turing Gateway meeting brought together mathematicians and representatives of industry producing liquid crystal materials and devices. The British Liquid Crystal Society also held their annual meeting in Cambridge to benefit from the INI Programme, with several participants giving invited lectures. In the area of soft matter there was a significant synergy with the parallel INI Programme on *Mathematical Modelling and Analysis of Complex Fluids and Active Media in Evolving Domains*, with a number of mutual talks and a joint workshop session, which enabled a fruitful interaction between the two communities. The Rothschild Visiting Professor for the programme was Tom Lubensky (University of Pennsylvania), and the Microsoft Research Visiting Fellow Epifanio Virga (Università degli Studi di Pavia).

A special effort was made to involve young researchers. A two-day meeting for young researchers was held in which every participant gave a short presentation and had individual mentoring sessions with senior researchers attending the Programme, some of whom gave talks on open problems in the field. The last two weeks of the Programme were also organized in conjunction with the I-CAMP 2013 Summer School, in which about 80 young researchers attended an intensive programme of lectures and other activities in Cambridge.

The Programme experimented with and exploited the internet and social media in various ways. For example a Remote Poster Session using Google+Hangout was held between participants and graduate students and faculty at the Liquid Crystal Institute at Kent State University. The intent was to bring together participants at the INI Programme with geographically separated students and faculty for real-time face-to-face discussions in small groups using social media, and to assess the ease of setting up and the overall effectiveness of such interactions. This proved very successful, and the graduate students at Kent State who prepared the online posters and related short videos were particularly pleased with the ability to interact with world experts in the field at the INI, who viewed the posters from their offices.

Another innovation was the delivery of two outstanding remote seminars by interactive video-link. The first, by Professor Yuka Tabe (Waseda University, Tokyo), concerned orientational motion and flow due to vapour transport through membranes of chiral liquid crystals. The second, by Professor Nicholas

Abbott from (Chemical and Biological Engineering, University of Wisconsin-Madison), described the remarkable discovery of endotoxin-induced ordering transitions in liquid crystalline droplets, which provides a novel way of detecting this bacterial infection-signalling chemical, previously only possible by using the blood of horseshoe crabs: given the potential industrial impact of this simple detection scheme, a special invitation to attend the remote seminar was extended to affiliates of the Turing Gateway Initiative.

Finally, an interview with Professor Jerry Ericksen was conducted by video-conference from the University of Oregon (see http://sms.cam.ac.uk/media/1486552), in which he describes his perspectives on liquid crystals, including the issues he and Frank Leslie faced in their famous work on the continuum theory, together with other aspects of his distinguished career in mechanics.

Together with the frequent viewing of streamed lectures, either in real time or later, these activities are examples of how colleagues, unable to attend in person, were able both to contribute greatly to the scope of the Programme and to benefit from it. The archive of videos of lectures from the Programme will form an important source of material for researchers in the area which will extend the influence of the Programme into the future. However it is hoped to achieve this in a more proactive way by setting up a web-based resource for open problems in the mathematics of liquid crystals, based initially on those identified during the Programme.

[1] V. Narayan, N. Menon and S. Ramaswamy, "Nonequilibrium steady states in a vibrated-rod monolayer: tetratic, nematic and smectic correlations." J. Stat. Mech. (2006) P01005

[2] T. Sanchez, D.T.N. Chen, S. J. DeCamp, M. Heymann and Z. Dogic, "Spontaneous motion in hierarchically assembled active matter", Nature **491**, 431 (2012)