CECAM SCHOOL
Liquid Crystal Modelling and Simulation: A Comprehensive Introduction
Ettore Majorana Centre – Erice (TP) July 14–18, 2017

AIM AND SCOPE

Liquid crystals (LCs) are anisotropic fluids endowed with orientational order but with a positional order either reduced with respect to crystals, like in smectics, or absent altogether, as in nematics. There exists a variety of thermotropic LC phases ranging from uniaxial and biaxial nematics to a zoo of smectics [1], to LC polymers and elastomers [2]. They are formed by molecules of increasing complexity, from the low molar mass ones – like the cyano-biphenyls used for LC displays, with a few tens of atoms per molecule [3] – to those of polymeric size, with orders-of-magnitude increase in the number of constituent atoms. Given the complexity of these systems, it is not surprising that completely different families of models have rather independently developed over time, dealing either with molecular aspects and design [4–6] or, at the opposite extreme, tackling a macroscopic description in terms of vector fields [7–10].

Nowadays, technological interest in LCs is strongly reviving, due to new emerging applications, rather remote from the now almost mature LC display technology, ranging from organic electronics to optics and nanostructured materials [11–15]. Simultaneously and independently, our present-day capability to perform predictive molecular dynamics (MD) simulations on large enough LC samples paves the way to a hitherto unpractised association of bottom-up approaches with hydrodynamic modelling and device design. This context, and the long time elapsed after the last CECAM event (Lausanne 2008) devoted to LCs, motivated us to organise a school addressing concurrently computational models of LCs developed and practised by different communities. We aim at bringing together leading experts of the different modelling approaches and students with different backgrounds, in an effort to train a new generation of young researchers that, being familiar with manifold methodologies, can succeed in creating a new unified approach.

Since LCs are an archetype of soft matter, ideas and techniques developed for modelling and simulating them form a benchmark and a toolbox of general utility for dealing with other forms of soft matter. This school, where foundational issues will be introduced with care, may hence appeal also to students who are not specifically interested in working on LCs.

SUMMARY OF CONTENTS

The contents of the school are organised into five main topics, shortly presented in the 'Description' section under the 'Details' tag. Each topic is illustrated here in greater detail, and accompanied by suitable references, listed in the 'Key references' section under the 'Details' tag).

Topic 1: Bottom-up models of LCs: atomistic, molecular, lattice models

In principle, one of the most important challenges in the molecular design of LCs is to relate a specific molecular structure to collective physical observables. This task may seem a desperate one, in view of the variety of chemical species forming typical mesogenic molecules, the number of ways they can be connected, their internal flexibility, and the ensuing difficulties in defining a realistic set of interactions. Fortunately, several important observable properties are less abstruse and more easily accessed than others. In fact, simple spin lattice models [16, 17] can be extremely useful, particularly for nematics, where only orientational order matters.

In off-lattice molecular models, comparatively more refined, each molecule is represented by a rigid body whose shape – e.g., ellipsoidal or sphero-cylindrical – mimics that of the real molecule. Elongated or disc-like or chiral particles can be endowed just with hard-core repulsive properties [18, 19] or, more realistically, with attractive-repulsive interactions. The Gay-Berne (GB) model [20, 21], where a molecule is represented as an anisotropic Lennard-Jones particle, is the current prototype model of this kind. Models in this class [22–29] have been extensively applied to study order, pair correlations and dynamics, and even to simulate LC displays. Chains of ellipsoidal GB beads have also been employed for modelling polymers or LC elastomers.

In the most refined bottom-up approach, each molecule is represented in full chemical detail as a connected set of atoms. Models of this kind, being much more computationally demanding, have developed more recently. Typically, a quantum chemistry study is performed first, to characterise geometry, charge distribution and torsional potentials. Then, particles are treated classically and their evolution is time-integrated with Newtonian MD techniques. An essential – though often neglected – component of this approach is the construction of a set of force fields (FF). Current simulations show that well tuned FFs can yield nematic-isotropic transition temperatures within a few degrees from experiment [3, 30, 31] and predict observables that are often within the experimental error bar from the measured ones. Theoretical assumptions implicitly used in simpler models can now be put to test against results from atomistic simulations [32]. On the application side, these simulations are proving essential to study ordering and anchoring of LCs at interfaces with substrates and in applications to organic electronics [33–36].

The three lectures devoted to this topic will cover the following themes, summarised in the titles labelled T1 in the School Schedule on pp. 6–7:

An introduction to bottom-up modelling and simulation: the Metropolis Monte Carlo and MD methods. Lattice and molecular models of LCs. Phase transitions and how to locate them. Order parameters and correlation functions. Predictive atomistic modelling of LCs: force fields; applications to realistic LC systems in the bulk and at interfaces; comparison with experiments; ways of testing common modelling assumptions, such as molecular rigidity and uniaxiality.

Topic 2: Approximate statistical mechanics methods

We find it especially useful to expose young researchers in computational science and engineering also to ideas and techniques from approximate statistical mechanics that, while not directly applicable to simulation, do help setting the computational scene and may provide enlightening insights and expedient shortcuts.

Non-equilibrium mean-field theories [37–41] have highlighted the molecular mechanisms underlying the phenomenologically successful linear-viscosity theory of nematic LCs by Ericksen and Leslie [42, 43] and provided some understanding of the intricate issues associated with rotational diffusion in nematic and discotic LCs. More recently, molecular field theories have succeeded in explained the rich phase portrait behaviour observed in bent-core and biaxial nematics [44, 45].

The three lectures devoted to this topic will cover the following themes, summarised in the titles labelled T2 in the Schedule on pp. 6–7:

Molecular field theories of nematics and smectics. Extended mean field theories. Landau-de Gennes theory. Ginzburg criterion and fluctuations. Dynamical phenomena. Bulk, surface and defect phenomena.

Topic 3: Hydrodynamical models

Hydrodynamical models of LCs are an established part of continuum physics [8], presently progressing in new, uncharted directions [9, 10]. Their introduction and first developments in the sixties [42, 43] – extremely controversial at the time – is definitely to be considered one of the most innovative and fertile contributions of modern continuum mechanics to condensed matter physics [7].

Recently introduced relaxational theories formalise the idea of coupling a solid-like elastic response with a dissipative, viscous-like evolution of the relaxed state. They hold promise to provide a unified formalism covering the complex macroscopic behaviour of soft matter, typically intermediate between the behaviours conventionally considered solid or fluid-like. Applied to nematic LCs, these theories proved able to explain their peculiar frequency-dependent viscoelastic response [46], while at the same time lowering the number of independent macroscopic phenomenological viscosity coefficients [47].

A clever use of some versatile finite element (FE) code is mandatory to perform parametric studies of essentially nonlinear continuum models [48], as is necessary to extract meaningful physical information out or them, or to use them as an aid to device design.

The three lectures devoted to this topic will cover the following themes, summarised in the titles labelled T3 in the School Schedule on pp. 6–7:

Vector and tensor nematic order parameters. Nematic LCs and nematic elastomers. Free energy functionals and relaxational dissipation. Finite element implementation: conceptual underpinnings and tools of the trade.

Topic 4: Complex topological defects in constrained LCs

Topological defects are one of the most intriguing features of nematic LCs [49]. They may originate from boundary conditions, phase boundaries and/or solid-particle inclusions, and exhibit a complex evolution, including transformations, annihilations and pattern formation, strongly influenced – if not dictated – by topological constraints [50, 51]. The panorama is further enriched by chiral LCs [52]: dispersing colloidal particles in a chiral medium generates complex meso-structures such as knots and vortices [53, 54]. As a consequence, the study of topological defects in chiral LCs is presently a very active field of investigation.

Specific textures to be discussed theoretically and simulated practically at the school will include nematic liquid crystals in porous networks [55], colloidal nematics and cholesterics [52], defect mediated structures, topological colloidal crystals [54] and nematic braids with knots and links [40]. Also the most recent findings in this area will be presented, including hopfions and torons in thin cholesteric layers [56], blue phases, colloidal and confined blue phases, and skyrmion structures [57].

The three lectures devoted to this topic will cover the following themes, summarised in the titles labelled T4 in the School Schedule on pp. 6–7:

Topological defects in nematics and cholesterics: from hedgehogs to disclinations. Confinement, surface anchoring, stable nematic fields with defects. Effects of chirality, example of nematic and cholesteric droplets, visualisation of structures and simulation of polarised light microscopy (POM) pictures. Nematic LCs in pores, LC shells, colloidal nematics and cholesterics, defect-mediated structures, topological colloidal crystals, nematic braids with knots and link. Hopfions and torons in thin cholesteric layers, blue phases, colloidal and confined blue phases, skyrmion structures.

Topic 5: Modelling LC devices

Liquid crystals represent a fascinating and challenging field, in which complex modelling and simulation can be promptly utilised to design new devices with a strong potential for industrial applications. A perfect example is provided by nematic LC elastomer motors, where macroscopic rotation and steady torque is produced by heat, light or solvent vapor without the transfer of angular momentum [58, 59]. Cholesteric liquid crystals are self-assembled photonic band-gap materials, which can give rise to distributed feedback lasing without

any external laser cavity [13]. Nematic liquid crystals can exhibit very fast (nanosecond) switching under the influence of electric fields without any director reorientation [60].

All these peculiar nematic effects, with high potential spin-offs for technology, can be understood in terms of simple model descriptions, which, however, require numerical methods for their solution. Different methods (energy minimisation, transfer matrix methods and Fokker-Planck evolution on a sphere) will be introduced and used, while the hands-on training will be mostly devoted to the implementation of numerical solutions.

The four lectures devoted to this topic will cover the following themes, summarised in the titles labelled T5 in the School Schedule on pp. 6–7:

Nematic LC elastomer motors. Cholesteric LCs as self-assembled photonic band-gap materials. Nanosecond switching of nematic LCs. Photonic devices, organic field-effect transistor (OFET), photovoltaics.

GENERAL ORGANISATION

The school will be run at the Ettore Majorana Centre in Erice, from July 14th to July 18th, 2017. Participants are expected to arrive on Thursday, July 13th, and leave on Wednesday, July 19th. The opportunity of running the school in this environment gives a big boost to its activities. The Centre boasts a first-class infrastructure for courses and meetings. Its location in the small historical hilltown of Erice – an attractive and peaceful place with affordable lodging and food options – offers a perfect venue for a fully residential school. All participants, lecturers and instructors included, will certainly benefit from that.

Each of the five main topics of the school is organised as a mini-course, comprising three or four lectures and one extended hands-on session. Overall, as many as 10 hours are allotted to practical work, subdivided into five sessions lasting 2 hours and a half each (see *Hands-on Sessions* for more information). The total time allotted to ex-cathedra tuition is 20 hours, distributed into 16 lectures. A detailed timetable is given in the School Schedule on pp. 6–7.

In order to foster mutual acquaintance and for a deeper involvement into the school, the participants will be given the opportunity to present their own work during a dedicated poster session on Day 1 (Friday, July 14th). Active interaction with lecturers and instructors will be invited during lectures and practicals, and informal discussion encouraged during the (rather generous) coffee and lunch breaks. A brief journey with an informal dinner is planned for the evening of Day 3 (Sunday, July 16th). The whole afternoon of Day 5 (Tuesday, July 18th) is dedicated to a freewheeling discussion, organised into two question-and-answer sessions, where the roles of asking and answering questions will not be rigidly distributed.

HANDS-ON SESSIONS

All hands-on sessions will be so organised as to allow students to work on (computation-wise) simple, but realistic examples of the simulation/modelling techniques presented and discussed in the lectures. To grant a profitable one-to-one approach, the participants will be divided into small groups (3–4 students each) and advised to bring and use their own laptops. A complete modelling environment – available as a benefit also after the end of the school – will be provided as a virtual machine (based on the free open-source VirtualBox software (`wikipedia.org/wiki/VirtualBox`, `www.virtualbox.org`) with all the necessary software, procedures and documentation preinstalled. This virtual machine will be made available online to all enrolled participants well before the beginning of the school, to grant time to address and solve all unexpected compatibility issues that may arise. On top of that, we will rely on the computer facilities available at the Centre as an additional fallback solution.

The session on Monte Carlo and MD simulations of lattice and molecular models will be based on our home-made codes, as well as on the open-source LAMMPS simulator engine (`http://lammps.sandia.gov`). For visualisation, we will rely on the open-source viewers QMGA (`http://qmga.sourceforge.net`) and Ovito (`http://www.ovito.org`). The open-source computer algebra system Maxima (`http://maxima.sourceforge.net`) will be mostly used in the sessions on statistical-mechanics and device modelling. The finite element COMSOL Multiphysics software (`https://www.comsol.com`) will be adopted in the sessions on hydrodynamical models and device modelling.

SCHOOL SCHEDULE

Day 1 (Friday, July 14th)
08:30–09:00 Get-together and opening
09:00–10:15 T2: Introduction to LCs: order parameters (Biscari)
10:15–10:45 Coffee break
10:45–12:00 T4: Topological defects (Čopar)
12:00–13:00 T2: Molecular and mean field theories (Sluckin)
13:00–15:00 Lunch break
15:00–17:30 Practical work on T2, led by Turzi
17:30–18:00 *Coffee break*
18:00–19:30 Poster session

Day 2 (Saturday, July 15th)
09:00–10:15 T4: Constrained nematic and cholesteric LCs (Žumer)
10:15–11:15 T3: Nematic LCs and nematic elastomers (Biscari)
11:15–11:45 Coffee break
11:45–13:00 T2: Dynamical phenomena (Sluckin)
13:00–15:00 Lunch break
15:00–16:15 T4: Hopfions, torons, skyrmions; blue phases (Žumer)
16:15–16:45 Coffee break
16:45–19:15 Practical work on T4, led by Čopar

Day 3 (Sunday, July 16th)
09:00–10:15 T1: Bottom-up models of LCs (Zannoni)
10:15–11:15 T3: Free energy and relaxation (DiCarlo)
11:15–11:45 Coffee break
11:45–13:00 T5: Nematic LC elastomer motors (Palffy)
13:00–15:00 Lunch break
15:00–16:15 T1: Lattice and molecular models of LCs (Zannoni)
16:15–16:45 Coffee break
16:45–19:15 Practical work on T1, led by Berardi
20:00– Outing

Day 4 (Monday, July 17th)
09:00–10:15 T1: Predictive atomistic modelling of LCs (Zannoni)
10:15–11:15 T5: Photonic devices, OFET, photovoltaics (d'Alessandro)
11:15–11:45 Coffee break
11:45–13:00 T5: Cholesteric LCs (Palffy)
13:00–15:00 Lunch break
15:00–16:15 T3: Finite element implementation (DiCarlo & Teresi)
16:15–16:45 Coffee break
16:45–19:15 Practical work on T3, led by Teresi

Day 5 (Tuesday, July 18th)
09:00–10:15 T5: Nanosecond switching of NLCs (Palffy)
10:15–10:45 Coffee break
10:45–13:15 Practical work on T5, led by Zheng
13:15–15:15 Lunch break
15:15–16:45 Questions & Answers
16:45–17:15 Coffee break
17:15–18:45 Questions & Answers
18:45–19:00 Closure
19:00–19:15 Farewell toast

Topic Schedule at a Glance

	14am	14pm	15am	15pm	16am	16pm	17am	17pm	18am	18pm
T 1					L	LP	L			
T 2	LL	P	L							
T 3			L		L			LP		
T 4	L		L	LP						
T 5					L		LL		LP	

Legenda: L = Lecture, P = Practical work.