

# RECENT DEVELOPMENTS IN THE ANALYSIS AND MODELLING OF LIQUID CRYSTALS

15 – 16 March 2010

Mathematical Institute, University of Oxford  
24-29 St Giles', Oxford, OX1 3LB

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# RECENT DEVELOPMENTS IN THE ANALYSIS AND MODELLING OF LIQUID CRYSTALS

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*Mathematical Institute, University of Oxford*

24-29 St Giles', Oxford OX1 3LB

MONDAY		TUESDAY	
10:00	Registration & Coffee	9:00	Fang-Hua Lin
10:30	Peter Palfy-Muhoray	10:00	Coffee
11:30	Eduard Feireisl	10:30	Mikhail Osipov
12:30	Lunch	11:30	Apala Majumdar
14:00	David R. J. Chillingworth	12:30	Lunch
15:00	Luc Nguyen	14:00	Jonathan Robbins
16:00	Tea	15:00	Valeriy Slastikov
16:30	Antonio DeSimone	16:00	Tea
17:30	Drinks Reception	16:30	Pedro Pereira
19:15	Dinner at Brasenose	17:30	Claudio Zannoni

# RECENT DEVELOPMENTS IN THE ANALYSIS AND MODELLING OF LIQUID CRYSTALS

## Programme

### Monday 15 March

10:00 *Registration at Mathematical Institute and Morning Coffee*

10:30 **One order parameter tensor mean field theory for biaxial LCs**  
Peter Palffy-Muhoray (Kent State)

11:30 **On a non-isothermal model for nematic liquid crystals**  
Eduard Feireisl (Prague)

12:30 *Lunch*

14:00 **Biaxiality, Phase Transitions and Symmetry**  
David R.J.Chillingworth (Southampton)

15:00 **Refined approximation for Landau-de Gennes energy minimizers**  
Luc Nguyen (Oxford)

16:00 *Tea*

16:30 **Mechanics of nematic elastomers: modeling, analysis, and numerical simulation**  
Antonio DeSimone (SISSA)

17:30 *Drinks Reception at the Mathematical Institute*

19:15 *Dinner at Brasenose College*

# RECENT DEVELOPMENTS IN THE ANALYSIS AND MODELLING OF LIQUID CRYSTALS

## Programme

### Tuesday 16 March

9:00 **Flows of liquid crystals and incompressible viscoelastic fluids**  
Fang-Hua Lin (Courant Institute)

10:00 ***Morning Coffee***

10:30 **Molecular models for biaxial nematic liquid crystals**  
Mikhail Osipov (Strathclyde)

11:30 **Nematic Liquid Crystals - from Maier-Saupe to continuum theories**  
Apala Majumdar (Oxford)

12:30 ***Lunch***

14:00 **Onsager model for biaxial liquid crystals / Nonabelian homotopy invariants and the Dirichlet energy of tangent director fields**  
Jonathan Robbins (Bristol)

15:00 **Spatial Onsager Model for nematics**  
Valeriy Slastikov (Bristol)

16:00 ***Tea***

16:30 **Some Moving Boundary Problems in the Continuum Theory of Nematic Liquid Crystals**  
Pedro Pereira (Lisbon)

17:30 **From Generic to Atomistic Models. How relevant are the details?**  
Claudio Zannoni (Bologna)

18:30 ***Conference Close***

**RECENT DEVELOPMENTS IN THE ANALYSIS  
AND MODELLING OF LIQUID CRYSTALS**

**Titles & Abstracts**

**The Mathematical Institute**

**University of Oxford**

**15 - 16 March 2010**

## **Peter Palfy-Muhoray (Kent State)**

### **One order parameter tensor mean field theory for biaxial LCs**

I will present a simple one tensor mean field model of biaxial nematic liquid crystals. The salient feature of this approach is that material parameters appear explicitly in the order parameter tensor. The free energy is constructed from a mean field potential based on anisotropic dispersion interactions. The order parameter tensor and its elements are identified, and self-consistent equations for these are obtained by minimizing the free energy. The self-consistent equations are solved numerically. The results are illustrated in a 3D ternary phase diagram. The phase behavior can be simply related to molecular parameters. The results may be useful for designing molecules that show a thermotropic biaxial phase.

*Joint work with Xiaoyu Zheng (Kent State University)*

## **Eduard Feireisl (Prague)**

### **On a non-isothermal model for nematic liquid crystals**

We propose a new model describing the evolution of a liquid crystal substance in the nematic phase under the influence of temperature changes. The existence is shown in the framework of distributional solutions, without any essential restriction on the size of the data and the length of the time interval.

*Joint work with E. Rocca (Milano), G. Schimperna (Pavia)*

## **David R.J. Chillingworth (Southampton)**

### **Biaxiality, Phase Transitions and Symmetry**

Equilibrium states (phases) of liquid crystals are characteristically modelled as critical points of a free energy function defined on a suitable space of order parameters. To capture biaxial as well as uniaxial phases the order parameters in principle belong to the 25-dimensional space of linear transformations of  $V$ , where  $V$  is the 5-dimensional space of  $3 \times 3$  real traceless symmetric matrices. A common simplifying assumption reduces this dimension from 25 to four. Using invariant theory and singularity theory methods we give a full analysis of the bifurcation (i.e. phase transition) behaviour close to isotropy determined by any free energy function of the four order parameters having appropriate symmetry. The symmetry group itself exhibits interesting structure not always evident from the literature.

## **Pedro Pereira (Lisbon)**

### **Some Moving Boundary Problems in the Continuum Theory of Nematic Liquid Crystals**

Analytical solutions are considered for the equations of the continuum theory of nematic liquid crystals with small Ericksen number disturbed by the motion of thin plates. The resultant equations are a system of nonlinear partial differential equations to describe the spatial orientation of the director field in the one elastic constant approximation. Analytical bounding solutions based on maximum and minimum principles of differential equations are compared with Picard iterated solutions of a system of nonlinear integral equations. Moving boundary problems composed of ellipsoidal colloidal droplets which grow at the expense of a nematic phase are also discussed.

*Joint work with C. Atkinson*

## **Luc Nguyen (Oxford)**

### **Refined approximation for Landau-de Gennes energy minimizers.**

It is of interest to see how Oseen-Frank (OF) energy minimizers can be used to approximate Landau-de Gennes (LdG) energy minimizers, which depends on a small parameter  $L$ . The simplest approach is that LdG minimizers = OF minimizers + correction (\*), where the correction term is "small" for small  $L$ . Because of the failure of OF energy minimizer in predicting "line defects" it is possibly desirable to have a better understanding of the correction term. We show that the correction term is of size  $L$  so that (\*) becomes LdG minimizers = OF minimizer +  $F_{-1} L + o(L)$  in an appropriate sense. Furthermore, we will derive analytic relation between the OF minimizers and the first order term in the above asymptotic expansion.

## **Antonio DeSimone (SISSA)**

### **Mechanics of nematic elastomers: modeling, analysis, and numerical simulation.**

The deep understanding coming from the study of martensitic transformations in metals has often provided the tools for the accurate prediction of the mechanical response of other materials. Liquid crystal polymers and, in particular, nematic elastomers provide an example in this direction. Similarities in physical behavior e.g., soft elasticity, which is the analogue of superelasticity or stripe-domain instability, which is the analogue of mechanical twinning) have inspired the use of similar thermodynamic models and mathematical techniques based on the minimization of multi-well free-energies.

In this talk, we will review the recent progress on the modelling of martensitic-like microstructures in nematic elastomers, which has led to accurate coarse-grained models for the effective mechanical response. Highlights on current research will also be presented, with the aim of showing that nematic elastomers provide an extremely valuable model system to sharpen our understanding of material response governed by evolving microstructures.

## **Fang-Hua Lin (Courant Institute)**

### **Flows of liquid crystals and incompressible viscoelastic fluids**

The study of flows of liquid crystals plays an important role in understanding many other incompressible viscoelastic fluids. The equations describing these Non-Newtonian fluids are based on remarkably similar theories in physics and they have shared much of the mathematical properties as well. In this lecture I shall explain some recent works concerning some model equations, and to describe connections between them. I shall also try to present a couple fundamental unsolved mathematical questions regarding these equations.

## **Claudio Zannoni (Bologna)**

### **From Generic to Atomistic Models. How relevant are the details?**

Generic microscopic models both of lattice (e.g. Lebwohl-Lasher) and off-lattice (e.g. Gay-Berne) type have a long history and have greatly helped our understanding of the molecular origins of the macroscopic properties and of the phase organization of various types of liquid crystals (LC) and, as we shall see in the talk are still of great value. For instance lattice models simulations can be used to study defects in fairly complex systems such as thin nematic film coatings of colloidal particles of different shape [1,2] and molecular resolution models can be applied in the study of biaxial phases [3] and of model display devices [4]. More recently, fairly realistic atomistic models have been put forward [5] in an effort to

predict some of the important features of real mesogens like phase transition temperatures [6] and NMR observables for molecules in the bulk or at the nano-scale. In the talk we present recent relevant examples of applications of the various models and, following the indications coming from realistic models, we discuss which details of the generic models should be included in a next generation of simple or hybrid [7] models.

*Support from EU FP7-216025 Project BIND is gratefully acknowledged*

1. D. R. Nelson, *Nano Lett.*, 2, 1125 (2002).
2. G. Skacej and C. Zannoni, *Phys. Rev. Lett.*, 100, 197802 (2008); M. A. Bates, G. Skacej, C. Zannoni, *Soft Matter*, in press (2010), DOI: 10.1039/b917180k
3. R. Berardi, L. Muccioli and C. Zannoni, *J. Chem. Phys.* 128, 024905.1 (2008).
4. M. Ricci, M. Mazzeo, R. Berardi, P. Pasini and C. Zannoni, *Faraday Discuss.* 144, 171 (2010).
5. M. R. Wilson, *Internat. Rev. Phys. Chem.* 24, 421 (2005).
6. G. Tiberio, L. Muccioli, R. Berardi, C. Zannoni, *ChemPhysChem*, 10, 125 (2009).
7. O. Francescangeli, V. Stanic, S. I. Torgova, A. Strigazzi, N. Scaramuzza, C. Ferrero, I. P. Dolbnya, T. M. Weiss, R. Berardi, L. Muccioli, S. Orlandi and C. Zannoni, *Adv. Funct. Mater.* 19, 2592 (2009).

## **Apala Majumdar (Oxford)**

### **Nematic Liquid Crystals - from Maier-Saupe to continuum theories.**

We review the mean-field Maier-Saupe and continuum Landau-de Gennes theories for nematic liquid crystals. Using a maximum principle approach, we show that the Landau-de Gennes predictions are not consistent with the Maier-Saupe predictions in low-temperature regimes. We define a continuum energy functional that effectively interpolates between the Maier-Saupe energy and the Landau-de Gennes energy functional and can describe both spatially homogeneous and inhomogeneous systems. A key part of this definition is a thermotropic bulk potential which blows up whenever the Landau-de Gennes order parameter is inconsistent with the Maier-Saupe description. As a consequence, minimizers of this continuum energy functional are consistent with the Maier-Saupe predictions in all temperature regimes. We study the qualitative properties of these energy minimizers and also discuss phase transitions within this model.

*Joint work with John Ball.*

## **Jonathan Robbins (Bristol)**

### **Onsager model for biaxial liquid crystals / Nonabelian homotopy invariants and the Dirichlet energy of tangent director fields**

I'll discuss work on two problems related to liquid crystals.

The first concerns phase transitions in the Onsager model for biaxial liquid crystals. Building on the previous work of Fatkullin and Slastikov for the (uniaxial) Maier-Saupe interaction and using results from equivariant bifurcation theory, we obtain some rigorous results for the phase diagram for the (biaxial) London interaction.

*This is joint work with Valeriy Slastikov.*

The second problem is motivated by nematic liquid crystals in confined polyhedral geometries. We consider the Dirichlet energy of  $S^2$ -valued maps on a spherical polygon  $P$  which map the edges of  $P$  into the geodesics which contain them. In the case where  $P$  is an octant, we calculate the infimum Dirichlet energy as a function of homotopy type. For

nonconformal homotopy classes, this turns out to depend on an invariant of the (nonabelian) fundamental group of the  $n$ -times punctured sphere.

*This is joint work with Apala Majumdar and Maxim Zyskin.*

## **Valeriy Slastikov (Bristol)**

### **Spatial Onsager Model for nematics.**

We study a spatially extended Onsager-Maier-Saupe type of energy describing spatial variations of orientational ordering in nematic liquid crystals and show that it may be decomposed into Landau-deGennes-type and relative entropy-type contributions. Based on this decomposition we obtain the information about singularities of a liquid crystalline system.

*Joint work with Ibrahim Fatkullin*

## **Mikhail Osipov (Strathclyde)**

### **Molecular models for biaxial nematic liquid crystals**

A molecular-statistical theory of biaxial ordering and phase transitions in nematic liquid crystals is discussed in detail including the relation between tensor order parameters and molecular symmetry. In particular, the symmetry of the constituent molecules of the two recently discovered biaxial materials is considered. A molecular model of the biaxial and uniaxial nematic phases, composed of tetrapod-shaped molecules is developed using a simple model of a tetrapode composed of four mesogenic groups rigidly linked to the same centre. The coefficients of the effective interaction potential, used in the existing theory of biaxial nematics, are calculated numerically as functions of molecular model parameters by expansion of the total interaction potential for tetrapodes. Order parameters of the uniaxial and biaxial nematic phases are evaluated by direct minimization of the free energy at different temperatures, and the phase diagrams are obtained which enables one to study the dependence of the stability regions of all phases on the model parameters of a tetrapode molecule. A particular origin of the stability of the biaxial ordering in the nematic phase composed of tetrapode molecules, which has recently been discovered experimentally, is discussed in detail.

*Joint work with M.V.Gorkunov*

# Feedback Form

Thank you for attending Recent Developments in the Analysis and Modelling of Liquid Crystals Workshop.

We invite you to provide feedback on your experience and encourage you to use the space below for any comments or suggestions that you may have. We appreciate your feedback as it will assist us in our knowledge of how to make any necessary improvements for future conferences. We thank you in advance for your time.

Please circle the number that you think best suits each category.

	Excellent	Good	Average	Poor	Extremely Poor
Registration Process	5	4	3	2	1
Programme Information Pack	5	4	3	2	1
Presentations	5	4	3	2	1
Workshop Venue	5	4	3	2	1
Overall Experience of Workshop	5	4	3	2	1

Where did you find out about this workshop? \_\_\_\_\_

Please feel free to give any comments/suggestions that you may have:

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