Chair:
Prof. Paolo Biscari

DOCTORAL PROGRAM IN MATHEMATICAL MODELS AND METHODS IN ENGINEERING

Equations are everywhere! Between the atmosphere and the wing of a spaceship, in the blood flowing in an artery, on the demarcation line between ice and water at the poles, in the motion of the tides, in the charge density of a semiconductor, in the compression algorithms of a signal sending images from outer space. Such equations represent real problems. The Mathematical Engineer can see and understand the nature of these equations, and can develop models in order to understand their relevant qualities and solve real problems.
This PhD program aims at training young researchers by providing them with a strong mathematical background and with ability to apply their knowledge to the solution of real-world problems that arise in various areas of science, technology, industry, finance, management, whenever advanced methods are required in analysis, design, planning, decision and control activities. PhD students carry out their research both in the development of new mathematical methods and in the implementation and improvement of advanced techniques in connection with specific contexts and applications.
The Faculty of the PhD program is responsible for the organization of the training and research activities of the PhD students. Decisions of the Faculty comply with the requirements and standards of the Doctoral School of the Politecnico di Milano. A Chairman is elected within the Faculty, for representative and coordination activities.
Admission of students to the PhD program is decided after examination of the candidates. Students applying to our program must provide their CV, along with reference and motivation letters.
After admission, each student is assigned a tutor. The tutor is a member of the Faculty who assists the student in the early stages of his career, especially in the choice of the courses and in identifying a thesis advisor.
The overall activity of the PhD students can be quantified in 180 credits. The PhD program has a duration of three years.
Activity can be classified into:

- introductory courses (no minimum number of credits required);
- main courses (at least 40 credits);
- specialized research training, including seminars, tutoring activity, participation to workshops/conferences, and scientific publications (at least 20 credits);
- development of a doctoral thesis (at least 90 credits).

At the end of each academic year, the PhD students report to the Faculty about their activity. The students report about attendance of courses and exams (and the corresponding grades), participation in various scientific activities (seminars, conferences, summer schools etc.), planning and intermediate results on their research project and preparation of the PhD thesis, and any other relevant activity. At the annual meeting the students also receive a grade by the Faculty. A negative grade may entail repetition of the current year of doctoral study (with suspension of the grant, if any) or exclusion from the PhD program, depending on the Faculty's decision. Mobility of PhD students to other institutions is strongly encouraged and financial support is provided to this purpose.

Among others, let us mention some typical types of professional skills and possible occupations of the graduated Doctors: analytic and numerical treatment of differential models for physical and industrial problems, quantitative methods in finance and risk management, operations research and optimisation, statistical modelling and data analysis.

Placement of graduated Doctors is expected in the following positions: research and development divisions of businesses, businesses involved in innovative design activities, financial institutions such as banks or insurance companies, public or private research centres, public and/or governmental agencies for social, economical, scientific study, planning or evaluation, Universities.

Since the PhD program in Mathematical Models and Methods in Engineering (formerly, Mathematical Engineering) has been active since the year 2001, we expect that a larger number of institutions and businesses will soon become more and more aware of the professional skills and expertise of graduated doctors.

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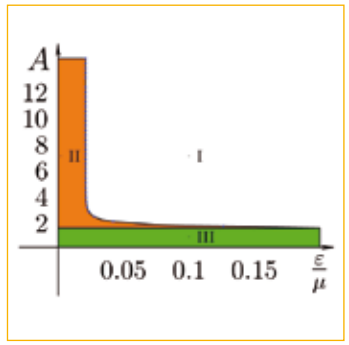
STRAIN-INDUCED DEFECT IN NEMATIC ELASTOMERS

Paolo Finotelli

Nematic elastomers offer a quite interesting and promising example of complex material in which the optical properties of nematic liquid crystals interact with the mechanical degrees of freedom of macroscopic elastic systems such as common rubber.
Nematic elastomers may be used in several applications, but above all, they are one of the best material-candidates to constitute artificial muscles. This reveals the importance of studying any energy aspect regarding nematic elastomers both from the mathematical and the physical/chemical approach.
This work is concerned with nematic elastomers. We are interested in understanding their possible transitions among two stationary configurations. One exhibits a defect of strength +1 while the other is the so called Cladis-Kl´eman solution, from the name of the two scientists who for the first time described the "escape in the third dimension" or "3-dimensional escape" in nematic liquid crystals. These two different configurations involve different characteristic lengths. We computed how their free energy varies with the strain ratio, defined as the ratio between the radius of the deformed sample of elastomer and the radius of the elastomer in a reference state. Our research work has been focused in the study of disclinations in nematic elastomers, and more precisely in the analysis of how they can be induced and/or avoided by suitably treating the system in the cross-linking phase or by the application of macroscopic deformations.
We considered a right cylindrical sample, cross-linked with the nematic degrees of freedom, i.e. the average direction along which the molecules point, identified by a unit vector called the director of the phase, and is usually given the symbol **n**. We forced the director to lie along the principal and along the radial axis of the cylinder. The main objective of the Thesis is to ascertain whether the minimized free-energy will be characterized by a disclinations on the cylinder axis, called defect configuration, or will exhibit a 3-dimensional escape in this case we talk about Cladis-Kl´eman configuration. More specifically we identified two Cladis-Kl´eman configurations: the radial-Cladis-Kl´eman configuration and the uniform-Cladis- Kl´eman configuration.
The Thesis is organized as follows. *Chapter 1* gives a brief introduction to nematic elastomers. *Chapter 2* is devoted to give a bird's-eye view on liquid crystals, one of fundamental components of nematic elastomers.
However nematic elastomers do not simply exhibit a simply superposition of liquid crystals and polymers' properties. On the contrary they show completely new effects that we cannot find elsewhere in Nature.
The other components of nematic elastomers are polymers. Polymers are completely different from liquid crystals but are peculiar materials too. *Chapter 3* is dedicated to explain their nature and properties. In particular we focused on nematic liquid crystals elastomers which show very peculiar behaviors. For example, thermal phase transformations give rise to significative spontaneous shape changes. Under some particular conditions they deform completely softly, in the sense that they deform without any application of stress, as true liquids do. The principal responsible of these unique behaviors is the cross-linking among chains to constitute a rubbery network. It is also interesting to note that the most important properties of cross-linked elastomers are established without any information about how chains elongate or flatten spontaneously. In case of more molecular details are needed, a qualitative study on nematic elastomers can be done by adopting a simple model keep into account the characteristic orientational order.
We have already emphasized the importance of the director **n**. A lot of studies and papers on nematic elastomers do not take into account that, during the crosslinking, it is possible to force the director to lie along a particular direction. This has several interesting consequences.
In *Chapter 4* we showed the existence of transitions when $\mathbf{n}_0$, the director at the time of cross-linking, is directed along the principal axis of the cylindrical sample of nematic elastomer.
In *Chapter 5* we analyzed the case of director at cross-linking lying along the radial direction, i.e. $\mathbf{n}_0 = \mathbf{e}_r$. Where $\mathbf{e}_r$ is the unit vector of the radial direction in cylindrical coordinates. Once again we showed the existence of transitions even if their features are completely different in regards to the ones found in *Chapter 4*.
Finally in *Chapter 6* we have summarized and discussed the results we found in this work.
In addiction we thought it was useful to write two appendices, *Appendix A* and *Appendix B*, where it has been demonstrated the existence of minimizers in nematic elastomers.
Basically the most remarkable result appears to be the identification of a critical value of the strain ratio such that the escaped configuration is always preferred on one side of the critical value, while a defect configuration may or may not occur on the other side, depending on the relative value of the nematic and elastomeric coherence lengths. Such critical value was determined both when $\mathbf{n}_0 = \mathbf{e}_z$ and $\mathbf{n}_0 = \mathbf{e}_r$.
We emphasize that generally in literature the shape tensor at cross-linking, is considered to be isotropic. This assumption simplifies the calculations a lot. Differently from this general way to operate we assumed to work with an uniaxial, positive definite and symmetric shape tensor of the following general form $\mathbf{L} = \alpha\mathbf{I} + \beta\mathbf{n} \otimes \mathbf{n}$ where **n** is the director while α and β are two scalar parameters obeying particular conditions.
Several nematic elastomers studies adopt the further simplification det**L** = 1.
We chose to generalized as much as possible our results, so we dropped this additional constraint. We calculated the optimized values of detL. This is another peculiar- 2 ity of this Thesis.
Our principal mathematical tool of analysis was to introduce a series of approximations inspired by the Boundary Layer Theory, that allowed us, among the other things, to obtain analytical estimates of both the configurations' details and their free energy.
To end up we think it is useful to show, just to give an example, one result we got.
Let consider the director lying originally along the z-axis, and $A_{crit} > 1$ more precisely A_{crit} = 1:4678:



1. A_{crit}= 1:4678. I=Def; II=R-CK; III=U-CK

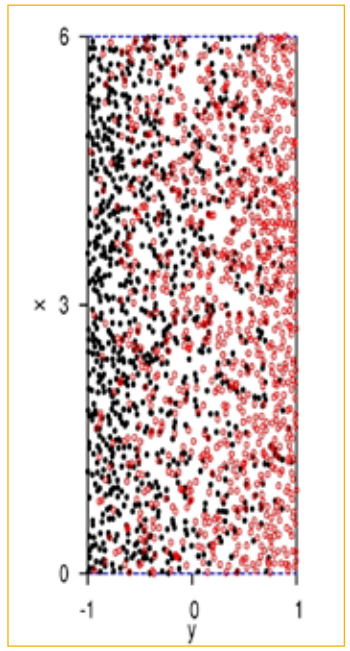
The plot shows that when A < A_{crit} the uniform Cladis-Kl´eman second case configuration is the preferred configuration, while for A > A_{crit} then the preferred configuration is either the defect or the radial Cladis-Kl´eman configuration depending on the value of A_{crit} and ε/μ. Where ε and μ are the characteristic lengths of the Landau-de Gennes and elastomeric potential.

SUPERFLUID FLOWS IN WALL-BOUNDED GEOMETRIES

Luca Galantucci

This dissertation illustrates the theoretical and numerical study performed on two--dimensional Helium II thermal channel counterflows. The principal motivation of the investigation described in this dissertation is the recent development of innovative flow visualization techniques in superfluid helium based on micron-size tracers and laser-induced fluorescence of metastable helium molecules whose measurements potentially represent the experimental counterpart of the numerical results obtained in this work. After an initial introductory part describing the peculiar properties of the quantum liquid phase Helium II and the characteristics of the different flow regimes observable in a counterflow channel, we illustrate the analytical deduction of the laminar steady solutions of the Hall-Vinen- Bekharevich-Khalatnikov (HVBK) equations applying to our cartesian geometry the approach employed in the past to investigate Helium II counterflows in cylindrical capillaries. Subsequently, we outline the characteristics of the two--dimensional Lagrangian algorithm elaborated ex--novo during this research project, focusing in particular the attention on the numerical re-nucleation models elaborated in order to account for the superfluid vorticity production/ destruction mechanisms which are intrinsically three-dimensional processes. The numerical re-nucleation models developed are indicated with (a), (b) and (c) and correspond respectively to random vortex re-insertion in the channel, vortex re-insertion on the channel axis and vortex re-insertion near the channel walls. The employment of these models also prevents from the generation of infinitesimal length- scales which would trigger numerical instabilities.

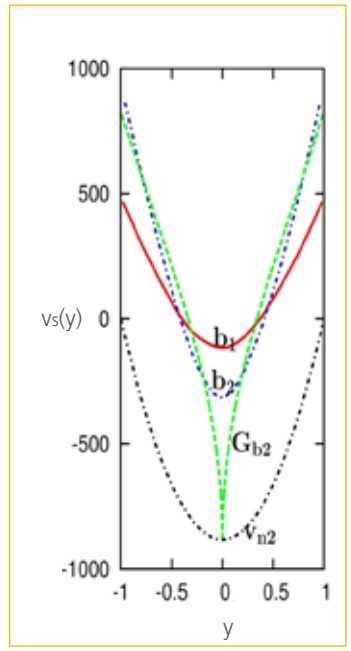
The impact of these re-nucleation models on the steady-state vortex configurations, the mesoscopic vortex-density profiles across the channel and the coarse--grained superfluid velocity profiles is then investigated via the results obtained with the numerical simulations performed. The steady state vortex configurations show that the vortices spatially organize themselves in patterns determined by the polarized motion of the vortices and the re-nucleation models adopted. The self- consistent density profiles for case (a) observed for different values of the vortex number employed in the simulations suggests that the random re-nucleation model is the most appropriate model to describe the nucleation phenomena in two-dimensional idealized counterflow systems. This thesis



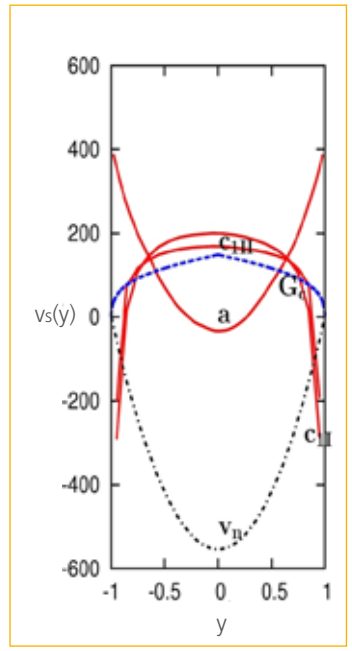
1. Steady state vortex configuration for case (a). Positive and negative vortices are respectively denoted by empty red and filled black circles.

is supported by the coarse-grained superfluid velocity profile computed for case (a): it perfectly matches the functional form of the normal fluid velocity profile, as observed in past numerical studies.

The consistency between the numerical profiles computed and the analytical solutions previously determined is also carefully analyzed. The resulting



2. Coarse-grained superfluid velocity vs for case (b). The subscripts 1 and 2 indicate respectively a number of vortices equal to N_1=1876 and N_2=4800. Gb_2 is the analytical solution for N_2= 4800, v_n is the normal fluid velocity profile.



3.Coarse-grained superfluid velocity vs for cases (a) and (c). The subscripts I and II indicate two different wall-nucleation distances for case (c) . G_c is the analytical solution for case (c) and N_1=1876, v_n is the normal fluid velocity profile.

agreement is very good exception made near the singularities of the analytical solutions where the analytical framework elaborated predicts an unphysical infinite superfluid vorticity corresponding to an infinite number of vortices. Finally, the last issue addressed in this dissertation concerns the comparison between Helium II counterflows and other quantum fluid systems in terms of the statistical distribution (PDFs) of the superfluid velocity components. We examined the power-law scaling of the PDF tails concluding that the characteristic scaling in channel regions where the flow is not influenced by the large-scale anisotropies of the flow is -4. In all the regions, however, the PDFs clearly show a non-Gaussian behaviour confirming that this characteristic is effectively peculiar to quantum turbulent flows being as well observable in Onsager gases and in Bose Einstein Condensates (BECs). This intermittent character of the superfluid velocity fields investigated in this idealized two-dimensional system also confirms the conjecture according to which the power-law-tails do not necessarily arise from the high-magnitude superfluid velocity fields generated by vortex reconnections.

STUDY OF PARAMETER DEPENDENCE FOR HYPERBOLIC SYSTEMS

Monica Gamba

Most mathematical models need to be complemented with data and parameters that specify the physical characteristics of the simulated systems among the class of systems spanned by the model.
These data may concern the system geometry, the boundary and initial conditions, the external forces. The parameters may be physical or model constants prescribing the constitutive laws of the system.
In many situations, the data and parameters cannot be exactly specified, because of some limitations in experimental data available (for instance in the measurement or identification of model constant), in the knowledge of the system (for instance in early design stage where the forcing and boundary conditions may not be precisely defined yet), or because of inherent variability of the system (for instance due to dimensional tolerances in production and assembly process, variability in operating conditions, etc..).
Therefore it is essential that any algorithm is robust with respect to variations of the parameters and data. Furthermore, it may be very useful to know the functional dependence of the results with respect of the parameters and data in order to better understand and exploit the model. The knowledge of the functional dependence of the results with respect of the parameters and data is the best instrument that allows, for example, to:

- Tune the model: usually simulations must be validated against measurements performed on the real systems. If, from the physical measurements, we know the responses of the system, by simply inverting the functional dependence, we can identify the exact value of one or more parameters for the simulated system.
- Characterize the robustness and controllability of the system: evaluating the bounds of the functional dependence, we can have information on the variation of the system response that is relevant in the design and optimization process.
- Perform risk analysis: by assigning a probability law to the parameters and or data, it is straightforward and computationally cheap to determine, using the functional dependence, the probabilities of the system exceeding certain critical values or operation thresholds.
- These probabilities can be used to conduct reliability or risk assessment analyses.
- Manage variability: in cases where there are many parameters or data that we know with finite precision, a key question concerns their relative impacts on the response of the system. This is required in order to identify the most crucial parameters and establish effective strategies for managing, observing and eventually reducing the range of variability of these parameters.

There is a vast literature on intrusive methods for uncertainty quantification. Those methods are focused on the computation of the probability distribution of the output of the computation, given a probability distribution of the parameters in input.
The general idea of those methods stems from the polynomial chaos introduced by Wiener . The other basic fact about these methods is that the equations under study are projected on a suitable basis for the probability space, and such projection is then integrated.
We present a new approach to the problem of studying systems depending on parameters and data, and specifically of computing the functional dependence of the response of the system with respect to the parameters.
Unlike the methods for uncertainty quantification and propagation, this technique is not focused on the computation of the probability distribution of the response of the system, but on the determination of the functional dependence of the output with respect to the parameters.
To this purpose, we call a parameter $x \in R_n$ "uncertain" when it ranges in some multi-interval, say $x \in X_0 = [x_1^a, x_1^b] \times \ldots \times [x_N^a, x_N^b]$, but we do not assign to it any probability distribution. The method is intrusive and it relies on automatic differentiation algorithms. Therefore it does not require changes on the numerical algorithms used to solve the system, nor significant changes in the equations describing the model; rather, by making extensive use of object oriented programming, it only requires a minor adaptation of the algorithms used to compute the system response with fixed values of the parameters.
The basic idea comes from the Taylor Models (TM) developed by Berz and Makino to study dynamical systems whose initial data are intervals. Moreover, the method extensively uses techniques that are commonly adopted in the setting of computer assisted proof.
Then, we seek the functional dependence expressed as a truncated series expansion in a finite dimensional subspace of the more appropriate Banach space for the specific problem under study.
We focus the attention on computing the functional dependence of the result of the numerical integration of a non linear hyperbolic systems with respect to one or more parameters. Since hyperbolic systems can generate discontinuities such as shock and contact waves, they could be a very good benchmark test for this technique. We choose as an example of a non linear hyperbolic system a well known system of conservation laws of the gas dynamics, the one dimensional Euler equations, that model the fluid dynamic of a compressible gas in a pipe. We seek the functional dependence of the physical variables that describes the fluid dynamics with respect to a parameter that describes the type of gas that we have inside the pipe.
First we seek the functional dependence expressed as a truncated Taylor polynomial expansion and we introduce a measure of the error that we have reconstructing the fluid dynamic field by evaluating the functional dependence at fixed value of the parameter.
The results obtained show that is impossible to reach a descriptions of the discontinuities as accurate as we want through a functional dependence due to the presence of singularities close to the real axis on the physical variables maps.
Knowing a priori the shape of the region of analyticity, it is possible to deform it in the domain of the Taylor expansion by a change of variable with an holomorphic map.
Then, we change the representation of the functional dependence by expressing it as a truncated Chebyshev expansion. Since the Chebyshev expansion of a function analytic in a thin region around the real axis converges, we can obtain a description of the discontinuities as accurate as we want.
The drawback is that we lose the direct information on the derivatives that we have with the Taylor expansion.