Nematics

Mathematical & Physical Aspects

Nematics
Mathematical and Physical Aspects

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Foreword

This volume (*)

NEMATICS
Mathematical and Physical aspects

constitutes the proceedings of a workshop which was held at l'Université de Paris Sud (Orsay) in May 1990. This meeting was an Advanced Research Workshop sponsored by NATO. We gratefully acknowledge the help and support of the NATO Science Committee.

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INTRODUCTION

DEFECTS, SINGULARITIES AND PATTERNS IN NEMATIC LIQUID CRYSTALS : Mathematical and Physical Aspects

A. Mathematical aspects.

There are three principal models used to represent the mechanical properties of nematic liquid crystals. In increasing order of realism and complexity, these are:

(a) the harmonic mappings from a tri-dimensional domain into the sphere,

(b) the Oseen-Frank model,

(c) the Ericksen model.

Among these models, only the Ericksen model allows the possibility of line singularities, which are in fact physically observed.

During this workshop, recent progress was described concerning the following three questions.

1. Minima of relaxed energies associated with the two first models.

H. Brezis, R. Hardt, M. Giaquinta, and J. Soucek presented some new existence and regularity results on the minima of the relaxed energy of the Dirichlet functional for harmonic maps and of the Oseen-Frank functional for nematics. Moreover, explicit formula were given for the relaxed energies for both of these models. This relaxed energy was used to construct a large number of critical points of the non-relaxed energy, which could turn out to be metastable states of the nematic liquid crystal. Surprisingly, energy infima calculated over different natural classes of mappings (regular maps, equivariant maps, Sobolev spaces) result in different energy levels, giving rise to so-called gap phenomena. This leads to natural questions of density presented by F. Bethuel. For example, smooth maps on the unit ball B^3 in three dimensions into the unit sphere S^2 are not dense in the Sobolev space $H^1(B^3,S^2)$. However, maps which have a finite number of point singularities are dense in $H^1(B^3,S^2)$.

2. Minima of the Ericksen functional.

This recent model for nematics which was proposed by Ericksen allows both line and point singularities. F.-H. Lin presented regularity results and estimates of the size of the singular set by using the fact that this singular set is also the zero set of a certain harmonic map from a domain in R3 into a three dimensional cone in R4. E. Virga studied the precise behavior of some solutions with line singularities. A related functional for ferromagnetic material has been studied by D. Kinderlehrer.

3. Solutions of evolution equations associated with the problem of harmonic maps.

New results about heat flow equations for harmonic maps were presented by Y. Chen, J. Grotowski, R. Gulliver, N. Kikuchi, R. Musina, J. Rubinstein, and M. Struwe. (See also the paper of K.-C. Chang and W.-Y. Ding, who were unable to attend the workshop.) These results include partial regularity, blow-up in finite time, evolution of defects, of fibers and non-uniqueness for the heat flow, as well as similar results for the wave equation.

B. Physical aspects.

The following three topics represent the work of many different researchers.

1. Nematic liquid crystal polymers.

After a review of the topology and the properties of basic defects in usual nematic phases, M. Kléman presented an experimental and theoretical description of the characteristics of the defects observed in some new nematic liquid crystal polymers. Recent important results include that these polymers have a strongly anisotropic elastic behavior and that defects have static and dynamical characteristics different from those of classical nematics, in particular, singular lines of degree 1/2 are observed, but no point singularities. Experiments show the presence of a locally biaxial order. In cholesterics, such as D. N. A., distortion and frustration tendencies have been noticed.

2. Defects in flows of nematic fluids.

An original experiment was presented by P. Cladis on the patterns and defects occurring in a Taylor-Couette flow for a properly oriented nematic. The situation is more complex than in the case of usual isotropic fluids, where similar experimentals have exhibited anisotropic effects. Here, a classically anisotropic phenomenon is studied with an anisotropic fluid, which causes rich and complex phenomena. Most of the questions are not yet solved concerning the nonlinearities and the conditions for the appearance of defects, which are here disclination lines in the nematic ordering.

In a more general context, J. Lajzerowicz presented a study of the chiral interaction between two line singularities in a three dimensional space. This system shows a transition localization-delocalization, chiral interaction favoring localization. An exact computation of the twist angle and of its fluctuations was described.

3. Experimental and theoretical studies of turbulence phenomena in nematics which are subjected to various excitations.

After a presentation of the instabilities which occur at the interface between two fluid motions, P. Huerre focussed on the important question of vortex pairing. He showed that the pairing process occurs mainly by causing defects (edge dislocations) of the periodic flow structure which develops at the interface.

L. M. Pismen presented a complete study of the motion of defects in nematics, by using a dissipative Ginzburg-Landau equation. He computed (using matched asymptotic expansions with the numerical solution in the core region) the velocity of a vortex solution of the (real or complex) Ginzburg-Landau equation which is subjected to a weak external field. Also, the speed of the interacting vortices was estimated as a function of their distance using the quasi-stationary approximation of the phase field.

A nematic layer subjected to some constraint may develop a convection organized in rolls. E. Guazzeli has analysed the defects inside a structure of rolls in the framework of mixed-type elasticity, as in lamellar systems or smetic layers. In the case of an electrical constraint, A. Joets has shown experimentally the topology, the role and the instabilities of defects in the transition to chaos. The defects appear as "germs" of the most unstable structure. In the sama system, R. Ribotta has shown the existence of nonlinear waves. These waves being ordered structures of space-time, they also show the same type of defects (point defects and line defects). Numerical simulations of a Ginzburg-Landau model reproduce certain experimental findings. P. Coullet showed how this type of model is related to the broken symmetries of the system at the convection point and also gives rise to new examples of defects. In the more particular case of electro-hydrodynamic instabilities, W. Pesch showed that the Ginzburg-Landau model should include an extra term which physically represents large scale flows, and W. Zimmermann showed how noise can change some bifurcations. Also, the Ginzburg-Landau equation was used by J. Lega to simulate the occurrence of defects in nonlinear waves in phase interaction , and by D. Walgraef to study the effect of spatial forcing.

C. Numerical aspects.

Numerical studies using an original algorithm of the stability of defects of the mathematical solutions to harmonic maps were presented by F. Alouges. They confirm theoretical results and lead to interesting questions concerning energy gap phenomena. Nonlinear projection methods have been shown by Y. Saad.

Acknowledgments

We would like to thank all the Speakers, Contributors and Participants who have made of this worshop a very interesting meeting. We would like also to thank A. Joets, R. Ribotta and F. Weissler for their help in the organisation and Mrs D. Le Meur and S.Souriou for their technical assistance.

Paris le 29 Octobre 1990

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Contents (*)

(*) The names of the authors who have given a talk during the meeting are written in italics

AN ENERGY-DECREASING ALGORITHM FOR HARMONIC MAP

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ABSTRACT. We study a new algorithm to compute harmonic maps from a domain of R^3 into S^2. The novelty of this algorithm is that the renormalisation step speeds up the convergence. We also apply it to the evolution problem.

I. Introduction

The study of a liquid crystal in a domain $\Omega \subset \mathbb{R}^3$, is, by the Oseen-Frank model, very related with the study of harmonic mappings from Ω into S^2 (see [7]). Therefore, some authors have studied this problem from a numerical point of view. The problem is a minimization problem under quadratic constraints ($|u(x)|^2 = 1$ a.e.) :

$$\text{find } u \in H^1_g(\Omega, S^2) = \{u \in H^1(\Omega, \mathbb{R}^3);\ |u(x)|^2 = 1 \text{ a.e.}, u\,|_{\partial\Omega} = g\}$$

which minimizes the quantity

$$E(u) = \int_\Omega |\nabla u|^2 dx \text{ for a given boundary data } g.$$

Several methods have been studied (see [3,4,8]) which are based on the following principle:
1)· Start with an initial guess u_0
2)· for $n = 0...$ until convergence
2.1) find a v such that $E(v) \leq E(u^n)$ which eventually does not satisfy the constraint,
2.2) renormalize v, that is set $u^{n+1} = \frac{v}{|v|}$.
Different methods can be used during 2.1) (gradient methods, multistep methods, splitting methods), but the energy is not often controlled during 2.2), and so, this second step can increase the energy and therefore make 2.1) useless.
The purpose of this paper is to present an algorithm which use the step 2.2) to speed up the convergence : we construct it to be sure that the energy decreases during 2.2).

II. Three remarks – Construction of the algorithm :

The method we used is based on the following three remarks :

R1
If $v \in H^1(\Omega, \mathbb{R}^3)$ verifies $|v(x)| \geq 1$ a.e., we have the following inequality

$$II-1 \qquad \left|\nabla\left(\frac{v(x)}{|v(x)|}\right)\right|^2 \leq |\nabla v(x)|^2 \text{ a.e.}$$

Hence, the energy of such a v decreases by renormalizing it.

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Thanks to this remark, we now do have a way of decreasing the energy by renormalization. It remains to find a vectorfield v in $H^1(\Omega, \mathbb{R}^3)$ of norm greater than 1 a.e.

R2

$$\left[\begin{array}{l}\text{Giving } u^n \in H^1_g(\Omega, S^2) \text{ a good way to find } v \text{ in } H^1_g(\Omega, \mathbb{R}^3) \\ \text{with } |v(x)| \geq 1 \text{ a.e. is to search } v \text{ under the form} \\ v(x) = u^n(x) - w(x) \text{ where } w \in H^1_0(\Omega, \mathbb{R}^3);\ w(x) \cdot u^n(x) = 0 \text{ a.e.} \\ \text{Consequently, we will have} \\ |v(x)|^2 = |u^n(x) - w(x)|^2 = 1 + |w(x)|^2 \geq 1 \text{ a.e.}\end{array}\right.$$

This very simple remark is also very important because we now have transformed a quadratic constraint ($|u^n(x)|^2 = 1$) into a linear one ($u^n(x) \cdot w(x) = 0$).

R3

$$\left[\begin{array}{l}\text{We have to compute } w \text{ such that } w(x) \cdot u^n(x) = 0 \text{ a.e.} \\ \text{let us choose the best one, that is, the solution of the} \\ \text{following minimization problem :} \\ (P_{u^n}) \qquad \underset{w \in H^1_0(\Omega, \mathbb{R}^3),\ w \cdot u = 0 \text{ a.e.}}{\text{Min}} \int_\Omega |\nabla(u^n - w)|^2\, dx.\end{array}\right.$$

Let $K_u = \{w \in H^1_0(\Omega, \mathbb{R}^3)$ such that $w(x) \cdot u^n(x) = 0$ a.e.$\}$; K_u is a closed convex (K_u is a linear space) subset of $H^1(\Omega, \mathbb{R}^3)$, hence, the solution of (P_{u^n}) is just the projection of u^n on K_{u^n} with respect to the H^1_0 scalar product. It follows from this, that the solution w^n of (P_{u^n}) is unique. Moreover, since K_u is a linear space, we have the following equality:

$$II - 2 \qquad \int_\Omega |\nabla(u^n - w^n|^2\, dx + \int_\Omega |\nabla w^n|^2\, dx = \int_\Omega |\nabla u^n|^2\, dx.$$

We are now able to construct the algorithm :

1)· Start with an initial guess $u_0 \in H^1_g(\Omega, S^2)$;

2)· For $n = 0...$, until the convergence :

2.1)· Solve (P_{u^n}) and call w^n the solution ;

2.2)· Set $u^{n+1} = \dfrac{u^n - w^n}{|u^n - w^n|}$.

The formula $II - 2$ gives

$$\int_\Omega |\nabla(u^n - w^n|^2\, dx \leq \int_\Omega |\nabla u^n|^2\, dx,$$

therefore the step 2.1) decreases the energy.

The formula $II - 1$ gives

$$\int_\Omega |\nabla u^{n+1}|^2\, dx = \int_\Omega \left|\nabla \frac{u^n - w^n}{|u^n - w^n|}\right|^2 dx \leq \int_\Omega |\nabla(u^n - w^n)|^2\, dx,$$

So the step 2.2) also decreases the energy.

We have constructed, for a given $u_0 \in H^1_g(\Omega, S^2)$, a sequence $(u_n)_{n\in\mathbb{N}}$ such that

$$\begin{cases} \forall n \geq 0 \quad u_n \in H^1_g(\Omega, S^2) \\ \forall n \geq 0 \quad E\left(u^{n+1}\right) \leq E\left(u^n\right) \end{cases}$$

We deduce from these properties the

THEOREM. *Up to a subsequence still called* $(u_n)_{n\in\mathbb{N}}$ *we have* $u_n \rightharpoonup u_\infty$ *in* H^1 *where* $u_\infty \in H^1_g(\Omega, S^2)$ *is harmonic. Moreover, the sequence* $(w_n)_{n\in\mathbb{N}}$ *strongly converges to 0 in* $H^1(\Omega, \mathbb{R}^3)$.

The second assertion comes from II.2 which gives

$$\sum_{k=1}^{n} \int_\Omega \left|\nabla w^k\right|^2 \leq E(u^0) - E(u^n) \quad \forall n \in \mathbb{N}.$$

III. Numerical implementation

We implement this algorithm using finite differences. More precisely, we set $\Omega = C^3$ the unit cube of $\mathbb{R}^3$ and we split C^3 into M^3 small identical cubes. A vector field U defined on Ω is approximated by $(M+1)^3$ unit-vector values $u(i,j,k)$ at the vertices of the small cubes $u(i,j,k) \sim U(ih, jh, kh)$ for $1 \leq i,j,k \leq M$, where h is the space step : $h = \dfrac{1}{M+1}$. Then the energy is discretized classically by setting

$$\tilde{E}(u) = \left(\sum_{i,j,k=0}^{M-1} \left| \frac{u(i+1,j,k) - u(i,j,k)}{h} \right|^2 + \left| \frac{u(i,j+1,k) - u(i,j,k)}{h} \right|^2 + \right.$$
$$\left. + \left| \frac{u(i,j,k+1) - u(i,j,k)}{h} \right| \right) h^3$$

The remaining difficulty is the resolution of the problem (P_u). We use here an augmented-Lagrangian technique : let

$$L(w,\omega) = \frac{1}{2}\tilde{E}(u-w) + \frac{r}{2} \sum_{i,j,k=0}^{M-1} [u(i,j,k) \cdot w(i,j,k)] h^3$$
$$+ \sum_{i,j,k=0}^{M-1} [u(i,j,k) \cdot w(i,j,k)] \omega(i,j,k)$$

where ω is real-valued, u and w are vector-valued.

The standard theorems about quadratic lagrangian show that L has a unique saddle point which we have calculated with an algorithm of optimal descent applied to the dual functionnal : $\omega \longrightarrow -\operatorname{Min}_w L(w,\omega)$ (see [6] for example). Concerning this method, the results are the following :

- very few iterations are necessary to solve the problem (P) when the optimal r is chosen (Figure 1 shows the rate of convergence of the constraint to 0, for different values of r, in logarithmic scale).
- The energy of $u - w$ does not change after the second iteration. The other iterations just give w with more accuracy.
- The energy gained by solving (P) (step 2.1)) is of the same order than those gained by renormalizing the solution (step 2.2)). The Figure 2 compares these two energies in logarithmic scale.

IV. Another way to solve (P)

The Euler equations of the problem (P) are :

$$IV - 1 \qquad \begin{cases} \Delta(u^n - w) = \lambda u^n; \\ w \in H_0^1; \\ w \cdot u^n = 0 \ a.e. \end{cases}$$

Actually, these equations have a unique solution which is also w^n the solution of (P_{u^n}). We may calculate w^n using a relaxation method inspired by the Laplace problem. More precisely, we construct a sequence (w_ℓ) which will converge to w^n the solution of $IV - 1$ in the following way : choose $\omega \in]0, 2[$ for $1 \leq i, j, k \leq M - 1$; set

$$\begin{aligned} b_{i,j,k} = &\left(u^n_{i+1,j,k} + u^n_{i,j+1,k} + u^n_{i,j,k+1} + u^n_{i-1,j,k} + u^n_{i,j-1,k} + u^n_{i,j,k-1}\right) \\ &- \left(w_{\ell;i+1,j,k} + w_{\ell;i,j+1,k} + w_{\ell;i,j,k+1} + w_{\ell;i-1,j,k} + w_{\ell;i,j-1,k} + w_{\ell;i,j,k-1}\right) \end{aligned}$$

Then compute

$$\bar{w}_{i,j,k} = -\frac{1}{6}\left(b_{i,j,k} - \left(b_{i,j,k} \cdot u^n_{i,j,k}\right) u^n_{i,j,k}\right)$$

and

$$w_{\ell+1;i,j,k} = (1 - \omega)\bar{w}_{i,j,k} + \omega w_{\ell;i,j,k}$$

Since all the calculations are done in K_{u^n}, the constraint is always well satisfied. Moreover this method runs very much faster than the previous one. We will compare the results later.

V. Representing the solutions.

Inspired by R. Gulliver (see [5]), we have adapted a representation of the fibers of the solutions. A fiber of u is a set $u^{-1}(\{x, -x\})$ for a given value x in S^2. Hence we have chosen a few values x_i in S^2 and have drawn the associated fibers. Such a visualisation is very useful to see the singularities : in fact, since all singularities of the minimizers are of degree ± 1 (see [2]), we see the singularities in the pictures where all the fibers intersect. To give an example the usual harmonic map $u_0 : x \to \dfrac{x}{|x|}$ possesses fibers which are all straight lines intersecting at 0 (see Figure 4).

VI. Results

We first have tested an algorithm with an initial data which possesses a non-centered singularity, and which agrees with $\frac{x}{|x|}$ on the boundary (Figure 3). After some iterations we have obtained $\frac{x}{|x|}$ (Figure 4). Then we have tried initial data of the form

$$u_0 \equiv u_r(x) = \Pi^{-1} \circ r \circ \Pi\left(\frac{x}{|x|}\right)$$

where Π is the stereographic projection and r is holomorphic. Such data are harmonic (see [2]).

[Figures 5-5bis-6] $r(z) = z^2$; then u^{55} possesses two degree 1 singularities.

[Figures 7-8] $r(z) = z^3$; then u^{45} has three degree 1 singularities.

[Figures 9-10] $r(z) = 2z$; the singularity moves.

[Figures 11-12] u_0 is $z-$translating-invariant and covers almorst the sphere on the upper face. The minimizer has two singularities of degree $+1$ and -1.

All these results were confirmed by the relaxation method except in the case of $r(z) = z^3$ where the symmetry of the cube made a five-singularity-symmetric harmonic map appear [Figure 13].

VII. The evolution problem

The evolution problem associated to harmonic maps from Ω to S^2 reads :

$$VII-1 \qquad \begin{cases} \dfrac{\partial u}{\partial t} - \Delta u = u|\nabla u|^2; \\ u(0) = u_0 \ ; \ u\ |_{\partial\Omega} = g. \end{cases}$$

and it is possible to find weak solutions of this equation by successively minimizing

$$VII-2 \qquad \bar{E}(u) = E(u) + \int_\Omega \frac{|u - u(n\tau)|^2}{\tau} dx$$

over all $u \in H_g^1(\Omega, S^2)$ (see [1]).

In order to apply the preceding algorithm, we have to verify that $\bar{E}$ satisfies the energy-decrease of remark 1. But we obviously have :

if u, v are two vectors with $|u| = 1$ and $|v| \geq 1$, one has

$$|v - u|^2 = |v/|v| - u|^2 \text{ and so}$$

if $u \in H_g^1(\Omega, S^2)$ and $v \in H^1(\Omega, \mathbb{R}^3)$, $|v| \geq 1$ a.e.

$$|v(x) - u(x)|^2 \geq \left|\frac{v(x)}{|v(x)|} - u(x)\right|^2.$$