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MINIMIZATION OF THE LANDAU - DE GENNES FREE ENERGY FOR LIQUID CRYSTALS IN A RECTANGULAR GEOMETRY

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Abstract

We will describe a finite difference code for computing equilibrium configurations, of the order-parameter tensor field for nematic liquid crystals, in rectangular regions, by minimization of the Landau - de Gennes Free Energy functional. The implementation of the free energy functional described here includes electric and magnetic fields, quadratic gradient terms, and scalar bulk terms through sixth order. The inclusion of the electric field term in the free energy equation allows modelling of the dielectric tensor (which is proportional to the Q-tensor) as a function of the radiation field. Boundary conditions include the effects of strong surface anchoring. The target architectures for our implementation are SIMD machines, with interconnection networks which can be configured as 2 or 3 dimensional grids, such as the Wavetracer DTC. We also discuss the relative efficiency of a number of iterative methods for the solution of the linear systems arising from this discretization on such architectures and illustrate some results for a disclination problem on a rectangular region.

I. Introduction : The Problem

We consider a finite difference approximation of the equilibrium configuration of liquid crystals in a slab,

$$\Omega = \{(x, y, z) : 0 \leq x \leq a, 0 \leq y \leq b, 0 \leq z \leq c\}.$$

Following Gartland [3], we will use the Landau-de Gennes formulation, and seek a tensor order parameter field Q that minimizes the free energy of the system. In this case, the free energy can be expressed as

$$F(Q) = F_{\text{vol}}(Q) + F_{\text{surf}}(Q) = \int_{\Omega} f_{\text{vol}}(Q) + \int_{\partial\Omega} f_{\text{surf}}(Q)\,,$$

where Q(x) is a 3×3 symmetric, traceless tensor and where Ω and $\partial\Omega$ represent the interior and surface of the slab respectively. In this implementation we limit ourselves to strong anchoring on the surface of Ω. This corresponds to Dirichlet boundary conditions on $q_i, i = 1, \ldots, 5$, and in such cases

$$F_{\text{surf}}(Q) = \int_{\partial\Omega} f_{\text{surf}}(Q) = 0.$$

The term $F_{\text{vol}}(Q)$ represents an approximation of the interior free energy. To describe $F_{\text{vol}}(Q)$, we will use the convention that summation over repeated indices is implied and

that indices separated by commas represent partial derivatives. With these conventions $F_{\text{vol}}(Q)$ has the following form, (see, for instance [7]):

$$\begin{aligned} f_{\text{vol}}(Q) \;:=\; & \frac{1}{2}L_1 Q_{\alpha\beta,\gamma}Q_{\alpha\beta,\gamma} + \frac{1}{2}L_2 Q_{\alpha\beta,\beta}Q_{\alpha\gamma,\gamma} + \frac{1}{2}L_3 Q_{\alpha\beta,\gamma}Q_{\alpha\gamma,\beta} + \frac{1}{2}A\,\text{trace}(Q^2) \\ & -\frac{1}{3}B\,\text{trace}(Q^3) + \frac{1}{4}C\,\text{trace}(Q^2)^2 + \frac{1}{5}D\,\text{trace}(Q^2)\text{trace}(Q^3) \qquad (1) \\ & +\frac{1}{6}M\,\text{trace}(Q^2)^3 + \frac{1}{6}M'\,\text{trace}(Q^3)^2 - \Delta\chi_{\text{max}}H_\alpha Q_{\alpha\beta}H_\beta - \Delta\epsilon_{\text{max}}E_\alpha Q_{\alpha\beta}E_\beta\,. \end{aligned}$$

where L_1, L_2, and L_3 are elastic constants, A, B, C, D, M, and M' are bulk constants, and H, $\Delta\chi_{\text{max}}$, E, and $\Delta\epsilon_{\text{max}}$ are the field terms and constants associated with the magnetic and electrical fields respectively.

For $P \in \Omega$, the tensor $Q(P)$ will be represented in the form,

$$Q(P) = (Q_{\alpha\beta})_{\alpha,\beta=1}^{3} = q_1(P)\phi_1 + q_2(P)\phi_2 + q_3(P)\phi_3 + q_4(P)\phi_4 + q_5(P)\phi_5 \qquad (2)$$

where $\{q_\ell(P)\}_{\ell=1}^5$ are real-valued functions on Ω and the ϕ_i are a basis for the prescribed tensor field [2, 3].

II. The Implementation

To discretize our problem we begin by dividing the slab Ω into $I \times J \times K$ regions

$$v(i,j,k) = \{(x,y,z) : i\Delta x \le x \le (i+1)\Delta x, j\Delta y \le y \le (j+1)\Delta y, k\Delta z \le z \le (k+1)\Delta z\}$$

for $0 \le i \le I-1$, $0 \le j \le J-1$, and $0 \le k \le K-1$, where $\Delta x = a/I$, $\Delta y = b/J$, $\Delta z = c/K$.

Using the points $P = (x_i, y_j, z_k)$, where $x_i = i\Delta x$, $y_j = j\Delta y$, $z_k = k\Delta z$, which are located in the lower left-hand corner of the $v(i,j,k)$, we represent the discrete interior free energy integral by

$$\int_\Omega f_{\text{vol}}(Q) \approx \sum_{i,j,k} f_{\text{vol}}(Q(x_i,y_j,z_k)) \times volume(v(i,j,k)). \qquad (3)$$

Note that (1) involves derivatives of the functions $\{q_\ell(P)\}_{\ell=1}^5$ with respect to the x, y, and z coordinates. For interior points P, these derivatives can be approximated using central difference approximations.

Thus, we have the following approximation of the **Landau-de Gennes free energy** which is second order accurate:

$$F(Q) \approx \sum_{i,j,k} f_{\text{vol}}(Q(x_i,y_j,z_k)) \times volume(v(i,j,k)) = \sum_{i,j,k} h(x_i,y_j,z_k). \qquad (4)$$

With the discretization (4), we have reduced the problem to one of minimizing $\sum_{i,j,k} h(x_i,y_j,z_k)$ over all choices of $\{q_\ell(x_i,y_j,z_k)\}_{\ell=1}^5$. This unconstrained discrete minimization problem can be attacked in the standard way. That is, seek a solution of the non-linear system of equations

$$g(\hat{\ell},\hat{i},\hat{j},\hat{k}) := \frac{\partial \sum_{i,j,k} h(x_i,y_j,z_k)}{\partial q_{\hat{\ell}}(x_{\hat{i}},y_{\hat{j}},z_{\hat{k}})} = 0, \qquad (5)$$

for $1 \leq \hat{i} \leq I-1$, $1 \leq \hat{j} \leq J-1$, $1 \leq \hat{k} \leq K-1$, and $\hat{\ell} = 1 \ldots 5$. A standard approach, to solving non-linear systems such as these, is to use Newton's method.

In the next section, we will describe the type of computer architecture we use for our implementation, and sketch the details of that implementation.

III. The Architecture

Our target architecture is a Single Instruction Multiple Data stream (SIMD) computer, so called, since each of the processors execute the same instruction in lock-step on the data stored in its associated local memory. The platform chosen for this implementation was the Wavetracer Data Transport Computer (DTC), situated in the Department of Mathematics and Computer Science at Kent State. The minimal configuration, the DTC-4, has 4096 processors. These can be configured either as a $16 \times 16 \times 16$ cube, for three dimensional applications, or as a 64×64 square, for two dimensional applications. The assumption here is that most applications, correspond to physical problems in 2 or 3 dimensions, and thus a 2 and 3 dimensional interconnection network is the most efficient for their solution.

The traditional mode of solution of problems on a SIMD machine involves assigning one processor of the array per node in the problem space. To provide the ability to consider problems with more nodes than are available in the array, the DTC provides the ability to partition the memory of each processor to provide a larger number of *virtual processors*.

For the minimization problem we are considering, each discretization point, P, of the slab is associated with a virtual processor. Each set of 5 unknowns $\{q_\ell(P)\}_{\ell=1,5}$, at the point P, is stored in a single virtual processor's memory. For each $\{q_\ell(P)\}_{\ell=1,5}$ there is also a corresponding row of the Jacobian matrix. The nonzero constants of that row are also stored in the virtual processor memory. The set of processors with which a given processor, P, must communicate in order to update its row of the Jacobian is called the stencil of P. The finite difference approximation described here yields a relatively small and compact stencil. In the problem discussed below, the stencil will consist of processors which are at most two steps away from the given processor.

IV. Infinite Slab Case

In this paper we shall confine our consideration to the case of an infinite slab. Assuming the slab is infinite in the z-direction and imposing boundary conditions, which do not vary with z, effectively reduces the problem to a two dimensional problem on a rectangle:

$$\Omega := \{(x, y) : 0 \leq x \leq a,\ 0 \leq y \leq b\}.$$

The Euler-Lagrange equations, corresponding to (1), form a system of non-linear elliptic partial differential equations. Discretizing this system of equations produces the discrete Euler-Lagrange equations. Using standard central-difference approximations for the partial derivatives produces a 9-point stencil (in our implementation) at each nodal point in the domain. Since nearest-neighbor communications are efficient on the Wavetracer's mesh array of processors, the communication costs are minimal.

In order to solve the resulting non-linear system of equations we use an Inexact Newton's method. Let $G : R^n \to R^n$ be a function representing the discrete Euler-Lagrange

equations. The function G depends on the $5n$ unknowns

$$G(\mathbf{x}) = G\left(q_1^1, \ldots, q_5^1, q_1^2, \ldots, q_5^2, \ldots, q_1^n, \ldots q_5^n\right),$$

where $n = (I-1) \times (J-1)$ is the number of interior nodal points. The method requires solving a large sparse linear system $G'(\mathbf{x}_k)\mathbf{s}_k = -G(\mathbf{x}_k)$, where $G'(\mathbf{x})$ is the Jacobian of the system, and then updating the unknowns. Inexact Newton methods use some form of iterative procedure to solve the linear system approximately. Several iterative techniques such as SOR and multi-grid were tested on this inner problem with varying success. Note that the matrix $G'(\mathbf{x}_k)$ is singular at bifurcation and turning points and can be indefinite near these points. This can cause convergence problems when solving the inner linear system.

V. Iterative Solvers

Several classical iterative schemes were used to solve the inner sparse linear system for $q_1, \ldots, q_5$ at each nodal point. Each method had certain advantages and disadvantages when used as a solver on the Wavetracer. Both point and block versions of the following schemes were tried for the numerical simulations:

1. Multi-colored SOR (sor and blocksor)
2. Multi-level Multi-colored SOR (ml-sor and ml-blsor)
3. Multi-grid (mg and blockmg)
4. Multi-level multi-grid (ml-mg and ml-blmg)

The blocking scheme used involves blocking the $q_1, \ldots, q_5$ at each nodal point and using a block-iterative technique such as block-SOR.

A multi-coloring scheme was used for the SOR iterations [6] in order to introduce parallelism into the method. Only 4 colors were needed in the case considered here, since there is only a 9-point stencil at each node. The parameter ω was chosen to be the *optimal* ω for the simple Laplacian model, since the matrix in our linear system has a similar structure to the Laplacian matrix. Numerical experimentation showed that this was a good choice for this problem.

Multi-grid methods [5] are a class of fast linear solvers which are widely used. These methods performed well in our numerical simulations. When multi-grid was combined with a multi-level scheme [1, 4], it performed exceptionally well. Multi-level V-cycle multi-grid gave the best overall performance in our numerical simulations.

Preconditioned conjugate gradient schemes were tried on a simpler model problem [2] and were found to perform less efficiently than the methods considered above.

VI. Numerical Results

To illustrate the comparative speeds of the different solvers a test problem with the following known solution was used:

$$q_1 = x,\ q_2 = x^2,\ q_3 = y,\ q_4 = y^2,\ q_5 = xy.$$

Dirichlet (strong anchoring) conditions at the boundary were used. The simulations were performed in single precision on a Wavetracer DTC-4 with a 64×64 grid of processors.

In addition to the residuals, the errors can also be computed after each outer iteration, since the true solution is known. Initial guesses were chosen so that the initial maximum error at all points, except the boundary points, was 1.0. The iterations were continued until the maximum residual for the system was reduced by a factor of 10^6. Table 1 gives the results of these numerical simulations.

	real	user	syst	max q-resid	max q-error	outer iters
sor	148.7	7.6	12.9	9.1(-2)	2.4(-5)	34
blocksor	106.3	6.4	6.5	7.9(-2)	1.3(-5)	17
ml-sor	100.5	6.2	9.7	6.1(-2)	2.0(-5)	25(3,1,2,5,14)
ml-blsor	105.0	7.4	7.6	8.2(-2)	1.1(-5)	18(3,1,2,4,8)
mg	42.2	2.2	1.9	3.4(-2)	4.7(-5)	4
blockmg	60.9	4.1	1.6	3.0(-2)	4.2(-5)	4
ml-mg	36.3	2.8	2.8	4.6(-2)	3.9(-6)	8(4,1,1,1,1)
ml-blmg	50.5	3.8	2.7	4.6(-2)	3.9(-6)	8(4,1,1,1,1)

Table 1: Timings for Sample Problem on the Wavetracer DTC for $I = J = 64$.

The Wavetracer DTC does not itself contain a micro-second timer. Consequently, all timings must be performed on the Sun 3/50 front end. The columns real, user and syst give the real (wall clock) time, the time spent in executing user code on the front end, and the time spent on systems tasks related to the program, including input/output. Maximum residuals and errors are computed over all grid points for $q_1, \ldots, q_5$. For the multi-level schemes the number of outer iterations performed at each level are given in parentheses in the last column of the table along with the total number of outer iterations needed for convergence.

The numerical results show that the multi-level multi-grid scheme gave the best overall performance. The above results are for the given test problem with known solution. Subsequent simulations performed on the more realistic liquid crystal problem, with Dirichlet boundary conditions, discussed below, produced results consistent with that of the above test problem.

Figure 1 gives the results for a liquid crystal problem with disclinations (nematic defects). The alignments of the tensor fields are simulated for two different anchoring conditions at the boundary. These are called disclinations of strengths one-half and one, respectively. We prescribe the director field on the boundary of Ω to be

$$n = \{cos(s\Theta), sin(s\Theta), 0\}$$

where Θ is the polar angle in the rectangular coordinate system. The director fields were calculated on a mesh with $I = J = 64$ but plotted on a coarser mesh to improve the resolution. The length of each director in the plot is proportional to the scalar order parameter (maximum eigenvalue of the Q-tensor) at that point. The figures show the equilibrium configurations of the director fields for $s = 0.5$ and $s = 1.0$, respectively. In both cases, as we approach the center of the field, the scalar order parameter at those points goes to zero and the field becomes isotropic. As we decrease the temperature, we expect this isotropic core to shrink eventually to a point defect.

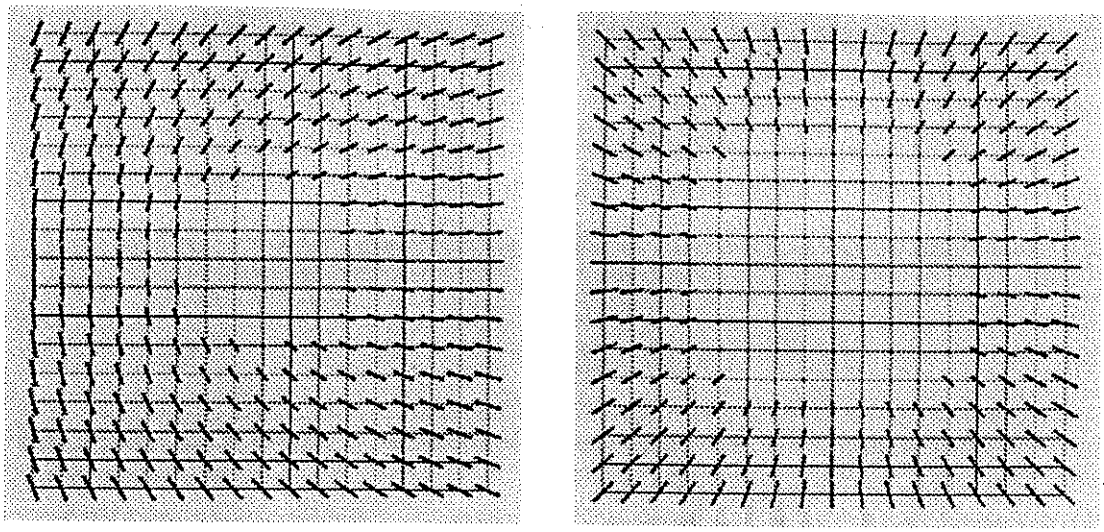

Figure 1: Director Field for liquid crystal problem with disclination

For these simulations the following values were used for the elastic and bulk constants: $L_1 = 1.0$, $L_2 = L_3 = 0.0$, $A = -3.0$, $B = C = D = M = M' = 1.0$. There were no magnetic or electric field terms present. The plots were generated using the apE graphics package licensed by Ohio State University.

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