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Solution of the Landau-de-Gennes Equations of Liquid Crystal Physics on a SIMD Computer *

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Abstract

We will describe a scalable parallel finite difference algorithm for computing the equilibrium configurations, of the order-parameter tensor field for nematic liquid crystals, in rectangular and ellipsoidal regions, by minimization of the Landau - de Gennes free energy functional. In this formulation, we solve for a symmetric traceless 3×3 tensor at each point. Our implementation of the free energy functional includes surface, gradient and scalar bulk terms, together with the effects of electric or magnetic fields. Boundary conditions can include both strong and weak surface anchoring. The target architectures for our implementation are primarily SIMD machines, with 2 or 3 dimensional rectangular grid networks, such as the Wavetracer DTC or the MasPar MP-1 as opposed to hypercube networks such as the Thinking Machines Corporation CM-2.

1 Introduction: The Problem

We will describe a finite difference approximation of the equilibrium configuration of liquid crystals in an ellipsoidal region,

$$\Omega = \{(ar \sin(\phi) \cos(\theta), br \sin(\phi) \sin(\theta), cr \cos(\phi)) : 0 \leq r \leq 1, 0 \leq \theta < 2\pi, 0 \leq \phi < \pi\},$$

where a , b and c are the three semi-axes of the ellipsoid. See [2] for the details of the finite difference approximation for rectangular regions. As in Gartland [3], we use the Landau-de Gennes formulation which expresses the free energy in terms of a tensor order parameter field Q , and the free energy is then given by

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

where $Q(x)$ is a 3×3 symmetric, traceless tensor and where Ω and $\partial\Omega$ represent the interior and surface of the ellipsoid respectively.

The representation of $f_{\text{vol}}(Q)$ uses the convention that summation over repeated indices is implied and that indices separated by commas represent partial derivatives. It is given

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by (see, for instance [5])

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

where L_1 , L_2 , and L_3 are elastic constants; A , B , C , D , E , and E' 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. The surface free density f_{surf} has the form

$$(2) \quad f_{\text{surf}}(Q) := \frac{1}{2}V \text{trace}((Q - Q_0)^2)$$

where Q_0 is a tensor associated with the type of anchoring of the surface elements and V is prescribed constant.

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

$$\begin{aligned} Q(P) &= (Q_{\alpha\beta})_{\alpha,\beta=1}^3 \\ &= q_1(P)E_1 + q_2(P)E_2 + q_3(P)E_3 + q_4(P)E_4 + q_5(P)E_5 \\ &= q_1(P) \begin{pmatrix} \frac{\sqrt{3}-3}{6} & 0 & 0 \\ 0 & \frac{\sqrt{3}+3}{6} & 0 \\ 0 & 0 & -\frac{\sqrt{3}}{3} \end{pmatrix} + q_2(P) \begin{pmatrix} \frac{\sqrt{3}+3}{6} & 0 & 0 \\ 0 & \frac{\sqrt{3}-3}{6} & 0 \\ 0 & 0 & -\frac{\sqrt{3}}{3} \end{pmatrix} \\ &\quad + q_3(P) \begin{pmatrix} 0 & \frac{\sqrt{2}}{2} & 0 \\ \frac{\sqrt{2}}{2} & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} + q_4(P) \begin{pmatrix} 0 & 0 & \frac{\sqrt{2}}{2} \\ 0 & 0 & 0 \\ \frac{\sqrt{2}}{2} & 0 & 0 \end{pmatrix} \\ &\quad + q_5(P) \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{2}}{2} \\ 0 & \frac{\sqrt{2}}{2} & 0 \end{pmatrix}, \end{aligned}$$

similar to that in Gartland [4], where $\{q_\ell(P)\}_{\ell=1}^5$ are real-valued functions on Ω .

2 The Implementation

We discretize the problem by dividing the ellipsoid Ω into $I \times J \times K$ regions

$$v(i, j, k) = \{(ar \sin(\phi) \cos(\theta), br \sin(\phi) \sin(\theta), cr \cos(\phi))\},$$

for $1 \leq i \leq I$, $0 \leq j \leq J$, and $0 \leq k \leq K$, where for given

i, j, k , $r_i - \frac{\Delta r}{2} \leq r \leq r_i + \frac{\Delta r}{2}$, $\phi_j - \frac{\Delta \phi}{2} \leq \phi \leq \phi_j + \frac{\Delta \phi}{2}$, $\theta_k - \frac{\Delta \theta}{2} \leq \theta \leq \theta_k + \frac{\Delta \theta}{2}$, where $r_i = i\Delta r$, $\phi_j = j\Delta \phi$, $\theta_k = k\Delta \theta$ and where $\Delta r = \frac{1}{I+1/2}$, $\Delta \phi = \frac{\pi}{J}$, and $\Delta \theta = \frac{2\pi}{K+1}$, and one region centered at the origin

$$\begin{aligned} v(0, 0, 0) = & \{(ar \sin(\phi) \cos(\theta), br \sin(\phi) \sin(\theta), cr \cos(\phi)) : 0 \leq r \leq \frac{1}{2}\Delta r, 0 \leq \theta < 2\pi, \\ & 0 \leq \phi \leq \pi\}. \end{aligned}$$

The discrete interior free energy integral is then given by

$$(3) \quad \int_{\Omega} f_{\text{vol}}(Q) \approx \sum_{i,j,k} f_{\text{vol}}(Q(r_i, \phi_j, \theta_k)) \times \text{volume}(v(i, j, k)).$$

The x , y , and z derivatives in (1) are approximated using the chain rule and central difference approximations of the derivatives of $\{q_\ell(P)\}_{\ell=1}^5$ with respect to r , θ and ϕ . Exceptions occur when $r = 0$, $\phi = 0$, and $\phi = \pi$. In those cases the x , y , and z derivatives can be approximate using direct divided difference approximations of $\partial/\partial x$, $\partial/\partial y$, and $\partial/\partial z$, provided we require that $\pi/2$ be an integer multiple of both $\Delta\theta$ and $\Delta\phi$. With this formulation, we can approximate $f_{\text{vol}}(Q(P))$ accurately using the values of $\{q_\ell(P)\}_{\ell=1}^5$ at P and at 6 points immediately adjacent to P .

By our choice of Δr , the points on the surface of the ellipsoid are $(r_{I+1}, \phi_j, \theta_k) = ((I + \frac{1}{2})\Delta r, j\Delta\phi, k\Delta\theta)$, for $0 < j < J$, $0 \leq k < K$. Upon setting $a(j, k) = \{(r_{I+1}, \phi, \theta) : \phi_j - \frac{\Delta\phi}{2} \leq \phi \leq \phi_j + \frac{\Delta\phi}{2}, \theta_k - \frac{\Delta\theta}{2} \leq \theta \leq \theta_k + \frac{\Delta\theta}{2}\}$, $0 \leq j \leq J$, $0 \leq k \leq K$, we can approximate the surface energy by

$$(4) \quad \int_{\partial\Omega} f_{\text{surf}}(Q) \approx \sum_{j,k} f_{\text{surf}}(Q(r_{I+1}, \phi_j, \theta_k)) \times \text{area}(a(j, k)),$$

where $f_{\text{surf}}(Q(r_{I+1}, \phi_j, \theta_k))$ can be evaluated using only the data at the point $(r_{I+1}, \phi_j, \theta_k)$.

Using (3) and (4), we have the following approximation of the Landau-de Gennes free energy which is second order accurate.

$$(5) \quad \begin{aligned} F(Q) &\approx \sum_{i,j,k} f_{\text{vol}}(Q(r_i, \phi_j, \theta_k)) \times \text{volume}(v(i, j, k)) \\ &+ \sum_{j,k} f_{\text{surf}}(Q(r_{I+1}, \phi_j, \theta_k)) \times \text{area}(a(j, k)) \\ &= \sum_{i,j,k} h(r_i, \phi_j, \theta_k), \end{aligned}$$

where $h(r_i, \phi_j, \theta_k)$ can be evaluated using the values of $\{q_\ell\}_{\ell=1}^5$ at (r_i, ϕ_j, θ_k) and six adjacent points.

With the discretization (5), we have reduced the problem to one of minimizing

$$(6) \quad \min \sum_{i,j,k} h(r_i, \phi_j, \theta_k)$$

over all choices of $\{q_\ell(r_i, \phi_j, \theta_k)\}_{\ell=1}^5$. To solve this unconstrained discrete minimization problem, we use Newton's method to find solutions of

$$(7) \quad g(\hat{\ell}, \hat{i}, \hat{j}, \hat{k}) := \frac{\partial \sum_{i,j,k} h(r_i, \phi_j, \theta_k)}{\partial q_\ell(r_{\hat{i}}, \phi_{\hat{j}}, \theta_{\hat{k}})} = 0,$$

for $0 \leq \hat{i} \leq I+1$, $0 \leq \hat{j} \leq J$, $0 \leq \hat{k} \leq K$, and $\hat{\ell} = 1 \dots 5$.

Each iteration of Newton's method involves solving a linear system, whose matrix is the Jacobian of (7), and then using that solution to update the iterate and the Jacobian, after which the process is repeated. Issues relating to the efficient generation of the Jacobian of (7) and to efficient methods for solving the linear system in the Newton's procedure are the primary concerns of this project.

The machine used for the implementation of this project was the Wavetracer Data Transport Computer (DTC-4), located in the Department of Mathematics and Computer Science at Kent State. The processors of the DTC-4 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 Wavetracer DTC-4 provides the ability to partition the memory of each processor to provide a larger number of *virtual processors*.

At each point of the ellipsoid the tensor order parameter Q is defined in terms of the 5 unknowns $\{q_\ell(P)\}_{\ell=1,5}$, and each set of 5 unknowns $\{q_\ell(P)\}_{\ell=1,5}$ is stored in a single virtual

processor. For each $q_\ell(P)$ there is also a corresponding row of the Jacobian matrix. The nonzero constants of that row are also stored in the memory of the processor associated with the discretization point P . Each non-zero constant, in a row of the Jacobian associated with P , also corresponds to another virtual processor with which the values of $\{q_\ell(P)\}_{\ell=1,5}$ at P must be communicated when the Jacobian matrix is updated.

In our implementation, the stencil of an interior processor P , i.e. the set of processors with which P , must communicate in order to update its row of the Jacobian, consists of all processors that are exactly 2 processors away from P . Exceptional stencils occur for processors located on the boundary of the array. To efficiently handle these exceptional situations, we group processors into equivalency classes: two processors are equivalent if their stencils have the same representation. We process these equivalency classes starting from the most general class (interior points) through to the least general classes (usually processors on the corners of the array). All operations performed on a given equivalency class are also performed on all less general classes. Nonexistent connections occurring in a less general class are avoided via zero coefficients. We achieve substantial parallelism from the fact that when we process a given equivalency class we only need process those connections which do not occur in a more general equivalency class.

The procedure described above produces a program which stores the geometry of the problem in the SIMD code itself, and as such, that program is both difficult to produce and to maintain. However, the alternative, i.e. storing the stencil as pointers in a processor's local memory, requires substantial sequential processing unless the machine permits (and the Wavertracer does not permit it) parallel, indirect, network addressing.

To circumvent the programming difficulties associated with storing the geometry of the problem in the program code, we have developed a symbolic algebra program which takes as input a list of points and their stencils and produces the layered SIMD code described above. The symbolic algebra program is quite easily maintainable and extensible. Using it, we will be able to produce SIMD code for other geometries such as cylinders which are of interest to liquid crystal researchers.

In the ellipsoidal case, our investigation into the choice of the linear solvers to be used in the Newton step is only in its preliminary stages. However, results from [2] and [6] suggest that multilevel methods (see, for instance [1]) may be the best choice, at least in those cases where the Jacobian of (7) is positive definite.

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