RELAXATION METHODS FOR LIQUID CRYSTAL PROBLEMS

By

SAN-YIH LIN

AND

MITCHELL LUSKIN

IMA Preprint Series # 332

June 1987

INSTITUTE FOR MATHEMATICS AND ITS APPLICATIONS

UNIVERSITY OF MINNESOTA

514 Vincent Hall

206 Church Street S.E.

Minneapolis, Minnesota 55455

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RELAXATION METHODS FOR LIQUID CRYSTAL PROBLEMS

SAN-YIH LIN[†] AND MITCHELL LUSKIN[‡]

Abstract. A point relaxation method for the liquid crystal problem is proposed and analyzed. The liquid crystal problem is a minimization problem with a *nonconvex* local constraint. We prove that the energy of successive iterates is non-increasing for the point relaxation method with relaxation parameter ω satisfying $0 < \omega < 2$ for a class of material constants. We also show that the difference between successive iterates converges to zero, and that limit points of the iteration sequence are minima with respect to perturbations which are supported at a point and which satisfy the constraint. Numerical results are given which demonstrate the improved rate of convergence for overrelaxation.

Key words. relaxation method, liquid crystals

AMS(MOS) subject classifications. 65K10

1. Introduction.

The liquid crystal problem [2,6,7,8,10] is to minimize the bulk energy of the liquid crystal

$$(1.1) \quad \mathcal{W}(n) = \int_{\Omega} W(\nabla n, n) dx$$

where $\Omega \subseteq \mathbb{R}^3$ is the region occupied by the material, $n : \Omega \rightarrow \mathbb{R}^3$ is the optic axis, and $W(\nabla n, n)$ is the Oseen-Frank free energy density. Since n is the optic axis, the *nonconvex* local (pointwise) constraint

$$(1.2) \quad |n(x)| = 1, \quad x \in \Omega,$$

holds where $|\cdot|$ is the Euclidean norm. The problem is also constrained by boundary conditions

$$(1.3) \quad n(x) = n_0(x), \quad x \in \partial\Omega,$$

where $\partial\Omega$ is the boundary of Ω .

It has recently been shown that minimum energy solutions to the liquid crystal problem exist [9]. These minimum energy solutions in general have point discontinuities at point

[†]School of Mathematics, University of Minnesota, Minneapolis, Minnesota 55455. The work of this author was supported by the National Science Foundation, Grant DMS 835-1080, and by a grant from the Minnesota Supercomputer Institute.

[‡]School of Mathematics, University of Minnesota, Minneapolis, Minnesota 55455. The work of this author was supported by the National Science Foundation, Grant DMS 835-1080, and by a grant from the Minnesota Supercomputer Institute. Part of this work was done while the author was supported as a visitor at the Institute for Mathematics and its Applications, University of Minnesota.

defects [1,8,15]. Computational results obtained by the relaxation method analyzed here gave the first demonstration that point defects of degree greater than one are unstable [3]. In this paper we give a proof that the energy of successive iterates is non-increasing. We also show that the difference between successive iterates converges to zero, and that limit points of the iteration sequence are minima with respect to perturbations which are supported at a point and which satisfy the constraint. This is the first analysis of the relaxation method for a problem with a *nonconvex* local (pointwise) constraint that we know of. Analyses of the relaxation method for unconstrained problems and for problems with convex local constraints can be found in [4,5,12,16,17]. We note that although symmetric eigenvalue problems can be formulated as optimization problems with global nonconvex constraints, relaxation methods for eigenvalue problems utilize the Rayleigh quotient formulation of the problem as an unconstrained nonconvex optimization problem [11, 14].

In section 4, we give the results of numerical experiments which demonstrate that over relaxation greatly improves the rate of convergence for the liquid crystal problem. In fact, the relationship between the rate of convergence and the relaxation parameter is similar to that found for unconstrained problems.

2. The Relaxation Method for the Liquid Crystal Problem.

To formulate the problem more precisely we introduce the space of admissible functions

$$(2.1) \quad \mathcal{A}(n_0) = \{u \in H^1(\Omega; \mathbb{R}^3) : |u(x)| = 1 \text{ for } x \in \Omega \text{ and } u = n_0 \text{ on } \partial\Omega\}$$

where n_0 is defined on the boundary, $\partial\Omega$, and $|n_0| = 1$. The Oseen-Frank free energy density is given by

$$(2.2) \quad \begin{aligned} W(\nabla u, u) = & \frac{\kappa_1}{2}(\operatorname{div} u)^2 + \frac{\kappa_2}{2}(u \cdot \operatorname{curl} u)^2 + \frac{\kappa_3}{2}|u \times \operatorname{curl} u|^2 \\ & + \frac{\nu}{2}(\operatorname{tr}(\nabla u)^2 - (\operatorname{div} u)^2) \end{aligned}$$

where the material constants satisfy $k_i > 0$ for $i = 1, 2, 3$. The liquid crystal problem is then to find $n \in \mathcal{A}(n_0)$ such that

$$(2.3) \quad \int_{\Omega} W(\nabla n, n) dx = \inf_{u \in \mathcal{A}(n_0)} \int_{\Omega} W(\nabla u, u) dx.$$

Our analysis applies to the special case $\kappa_1 = \kappa_2 = \kappa_3 = \kappa$. In this case,

$$(2.4) \quad W(\nabla u, u) = \frac{\kappa}{2}|\nabla u|^2.$$

However, our computational results show that the relaxation method converges for the general case of $\kappa_i > 0$ for $i = 1, 2, 3$ [13]. In what follows, we shall assume that $\kappa_1 = \kappa_2 = \kappa_3 = \kappa = 1$.

For simplicity of exposition, we shall assume that $\Omega = (0, 1) \times (0, 1) \times (0, 1)$ and we shall define the regular lattice for $h = 1/(M + 1)$ and M a positive integer by

$$(2.5) \quad x_{ijk} = (ih, jh, kh), \quad 0 \leq i, j, k \leq M + 1.$$

The values of functions U defined on the lattice are denoted by U_{ijk} . Clearly, we want to compute N such that

$$N_{ijk} \approx n(x_{ijk})$$

where $n(x)$ is the solution to problem defined by (2.3). Next, we introduce the space of admissible lattice functions by

$$(2.6) \quad \begin{aligned} \tilde{\mathcal{A}}(n_0) = \{U : & |U_{ijk}| = 1 \text{ for } 0 \leq i, j, k \leq M + 1 \\ & \text{and } U_{ijk} = n_0(x_{ijk}) \text{ for } x_{ijk} \in \partial\Omega\} \end{aligned}$$

and we define the discrete bulk energy by

$$(2.7) \quad \begin{aligned} \tilde{\mathcal{W}}(U) = & \sum_{i=0}^M \sum_{j=0}^M \sum_{k=0}^M \left(\left| \frac{U_{i+1,jk} - U_{ijk}}{h} \right|^2 \right. \\ & \left. + \left| \frac{U_{i,j+1,k} - U_{ijk}}{h} \right|^2 + \left| \frac{U_{ij,k+1} - U_{ijk}}{h} \right|^2 \right) h^3. \end{aligned}$$

The approximation problem is to determine $N \in \tilde{\mathcal{A}}(n_0)$ so that

$$(2.8) \quad \tilde{\mathcal{W}}(N) = \inf_{U \in \tilde{\mathcal{A}}(n_0)} \tilde{\mathcal{W}}(U)$$

The above approximation problem can be directly generalized in the usual way to regions Ω which are the union of non-intersecting rectangular parallelepipeds and to non-uniform grids. Further, general regions Ω can be first approximated by such a union of non-intersecting rectangular parallelepipeds.

The relaxation algorithm for $\omega = 1$ is to cycle through the lattice points. At a given lattice point x_{ijk} we update the approximation N_{ijk} by computing the value of the minimum for the energy functional $\tilde{\mathcal{W}}$ with respect to variations of U_{ijk} satisfying the constraint $|U_{ijk}| = 1$ and such that $U_{\alpha\beta\gamma}$ is held fixed for $x_{\alpha\beta\gamma} \neq x_{ijk}$ at $U_{\alpha\beta\gamma} = N_{\alpha\beta\gamma}$. In the unconstrained case, this gives the classical Gauss-Seidel algorithm for harmonic functions.

We now describe the relaxation algorithm for relaxation parameter ω . For simplicity of exposition we shall assume that the lattice points are ordered lexicographically. Our analysis is valid without modification for arbitrary orderings and for general regions Ω . Let N^0 be the initial guess for the minimum N . We denote by N^ℓ the approximation given by the ℓ^{th} iteration.

The lexicographical ordering is defined by

$$(\alpha, \beta, \gamma) < (i, j, k)$$

if $\alpha < i$ or $\alpha = i, \beta < j$ or $\alpha = i, \beta = j, \gamma < k$.

To define the algorithm it is convenient to define the following subset of the space of admissible lattice functions

$$(2.9) \quad \begin{aligned} \tilde{\mathcal{A}}_{ijk}^\ell &= \{U \in \tilde{\mathcal{A}}(n_0) : \\ U_{\alpha\beta\gamma} &= N_{\alpha\beta\gamma}^\ell \text{ if } (\alpha, \beta, \gamma) < (i, j, k) \\ U_{\alpha\beta\gamma} &= N_{\alpha\beta\gamma}^{\ell-1} \text{ if } (\alpha, \beta, \gamma) > (i, j, k) \} \end{aligned}$$

The algorithm is then defined by updating N at the lattice point x_{ijk} during the ℓ^{th} iteration cycle by

(1) computing $V \in \tilde{\mathcal{A}}_{ijk}^\ell$ so that

$$(2.10) \quad \tilde{\mathcal{W}}(V) = \inf_{U \in \tilde{\mathcal{A}}_{ijk}^\ell} \tilde{\mathcal{W}}(U),$$

(2) updating N by

$$(2.11) \quad \tilde{N}_{ijk}^\ell = \omega V_{ijk} + (1 - \omega) \tilde{N}_{ijk}^{\ell-1}$$

and

$$(2.12) \quad N_{ijk}^\ell = \frac{\tilde{N}_{ijk}^\ell}{|\tilde{N}_{ijk}^\ell|}.$$

Now it is easy to check that for $U \in \tilde{\mathcal{A}}_{ijk}^\ell$ since $|U_{ijk}| = 1$, we have

$$(2.13) \quad \begin{aligned} \tilde{\mathcal{W}}(U) &= 6h|U_{ijk}|^2 - 2h\langle B_{ijk}^\ell, U_{ijk} \rangle + c \\ &= 6h - 2h\langle B_{ijk}^\ell, U_{ijk} \rangle + c \end{aligned}$$

where

$$(2.14) \quad \begin{aligned} B_{ijk}^\ell &= N_{i-1,jk}^\ell + N_{i,j-1,k}^\ell + N_{ij,k-1}^\ell \\ &\quad + N_{ij,k+1}^{\ell-1} + N_{i,j+1,k}^{\ell-1} + N_{ij,k+1}^{\ell-1} \end{aligned}$$

and c is constant which depends on $N_{\alpha\beta\gamma}^\ell$ for $(\alpha, \beta, \gamma) < (i, j, k)$ and $N_{\alpha\beta\gamma}^{\ell-1}$ for $(\alpha, \beta, \gamma) > (i, j, k)$. Thus, if $B_{ijk}^\ell \neq 0$, then

$$(2.15) \quad V_{ijk} = \frac{B_{ijk}^\ell}{|B_{ijk}^\ell|}.$$

Our computational experiments have demonstrated that we can expect that $B_{ijk}^\ell \neq 0$ for all i, j, k, ℓ (The initial guess N^o could be chosen so that $B_{111}^1 = 0$, but this problem can be easily resolved by arbitrarily assigning N_{111}^1 so that $|N_{111}^1| = 1$). In fact, we expect that there exists a positive constant ρ such that

$$(2.16) \quad |B_{ijk}^\ell| \geq \rho$$

for all i, j, k, ℓ . This is just a statement of the computational fact that singularities for the discrete problem are not found at lattice points. Numerical experiments which demonstrate this fact will be given in section 4. Hence, the algorithm can be written in the simple and compact form

$$(2.17) \quad \tilde{N}_{ijk}^\ell = \omega \frac{B_{ijk}^\ell}{|B_{ijk}^\ell|} + (1 - \omega) N_{ijk}^{\ell-1},$$

$$(2.18) \quad N_{ijk}^\ell = \frac{\tilde{N}_{ijk}^\ell}{|\tilde{N}_{ijk}^\ell|}.$$

We note that

$$\tilde{N}_{ijk}^\ell = 0$$

only if $\omega = \frac{1}{2}$ and

$$\frac{B_{ijk}^\ell}{|B_{ijk}^\ell|} = -N_{ijk}^{\ell-1}.$$

We have always found in our computational experiments that

$$(2.19) \quad \tilde{N}_{ijk}^\ell \neq 0.$$

In any case, we give the results of numerical experiments in section 4 which show that the best rates of convergence are obtained for $1 \leq \omega < 2$. Thus, we do not have very much interest in the case $\omega = \frac{1}{2}$.

3. Analysis of the Relaxation Method.

We can define the admissible lattice function $N^{ijk\ell} \in \tilde{\mathcal{A}}(n_0)$ by

$$(3.1) \quad N_{\alpha\beta\gamma}^{ijk\ell} = \begin{cases} N_{\alpha\beta\gamma}^\ell & \text{if } (\alpha, \beta, \gamma) \leq (i, j, k), \\ N_{\alpha\beta\gamma}^{\ell-1} & \text{if } (\alpha, \beta, \gamma) > (i, j, k). \end{cases}$$

We shall now show that the relaxation algorithm is monotonically nonincreasing for $0 < \omega < 2$ at each step of the algorithm. In what follows we shall always assume that (2.16) and (2.19) hold.

THEOREM 1. For $0 < \omega < 2$ we have that

$$(3.2) \quad \tilde{\mathcal{W}}(N^{ijk\ell}) \leq \tilde{\mathcal{W}}(N^{\alpha\beta\gamma\ell})$$

if $(i, j, k) > (\alpha, \beta, \gamma)$ and

$$(3.3) \quad \tilde{\mathcal{W}}(N^{ijk\ell}) \leq \tilde{\mathcal{W}}(N^{\alpha\beta\gamma\lambda})$$

if $\ell > \lambda$.

Proof of Theorem 1. We note that

$$\begin{aligned} N^{1,1,0,\ell} &= N^{\ell-1}, \\ N^{i,j,0,\ell} &= N^{i,j-1,M\ell}, \\ N^{M,M,M,\ell} &= N^\ell. \end{aligned}$$

Thus, it is sufficient to demonstrate that

$$(3.4) \quad \tilde{\mathcal{W}}(N^{ijk\ell}) \leq \tilde{\mathcal{W}}(N^{ij,k-1,\ell})$$

for $1 \leq k \leq M$. Now by (2.13),

$$(3.5) \quad \tilde{\mathcal{W}}(N^{ijk\ell}) = -2h\langle B_{ijk}^\ell, N_{ijk}^\ell \rangle + c_1$$

and

$$(3.6) \quad \tilde{\mathcal{W}}(N^{ij,k-1,\ell}) = -2h\langle B_{ijk}^\ell, N_{ijk}^{\ell-1} \rangle + c_1$$

where c_1 is a constant which depends on $N_{\alpha\beta\gamma}^\ell$ for $(\alpha, \beta, \gamma) < (i, j, k)$ and $N_{\alpha\beta\gamma}^{\ell-1}$ for $(\alpha, \beta, \gamma) > (i, j, k)$. Hence, (3.4) follows from

$$-\langle B_{ijk}^\ell, N_{ijk}^\ell \rangle \leq -\langle B_{ijk}^\ell, N_{ijk}^{\ell-1} \rangle$$

or

$$(3.7) \quad -\langle \frac{B_{ijk}^\ell}{|B_{ijk}^\ell|}, N_{ijk}^\ell \rangle \leq -\langle \frac{B_{ijk}^\ell}{|B_{ijk}^\ell|}, N_{ijk}^{\ell-1} \rangle.$$

Since N_{ijk}^ℓ is given by (2.17) and (2.18), (3.7) follows from the following lemma

LEMMA 1. Suppose that $u, v \in \mathbf{R}^3$ are unit vectors, $|u| = |v| = 1$, that $0 < \omega < 2$, and that

$$\omega u + (1 - \omega)v \neq 0.$$

Then

$$(3.8) \quad -\langle u, \frac{\omega u + (1 - \omega)v}{|\omega u + (1 - \omega)v|} \rangle \leq -\langle u, v \rangle.$$

Proof of Lemma 1. First, we note that the assumption $\omega u + (1 - \omega)v \neq 0$ only excludes the case $\omega = \frac{1}{2}$ and $u = -v$.

If w, v are unit vectors, then

$$(3.9) \quad \langle w, w - v \rangle = \langle v, v - w \rangle$$

(Let R be the orthogonal matrix

$$R = I - 2 \frac{v - w}{|v - w|} \otimes \frac{v - w}{|v - w|}.$$

Then $Rv = w$ and $Rw = v$. Thus

$$\langle w, w - v \rangle = \langle Rw, R(w - v) \rangle = \langle v, v - w \rangle.$$

Hence,

$$(3.10) \quad |w - v|^2 = \langle w - v, w - v \rangle = \langle w, w - v \rangle - \langle v, w - v \rangle = 2\langle w, w - v \rangle.$$

We apply (3.10) with

$$w = \frac{\omega u + (1 - \omega)v}{|\omega u + (1 - \omega)v|}$$

to obtain

$$(3.11) \quad \begin{aligned} \left| \frac{\omega u + (1 - \omega)v}{|\omega u + (1 - \omega)v|} - v \right|^2 &= 2 \left\langle \frac{\omega u + (1 - \omega)v}{|\omega u + (1 - \omega)v|}, \frac{\omega u + (1 - \omega)v}{|\omega u + (1 - \omega)v|} - v \right\rangle \\ &= \frac{2\omega}{|\omega u + (1 - \omega)v|} \left\langle u, \frac{\omega u + (1 - \omega)v}{|\omega u + (1 - \omega)v|} - v \right\rangle \\ &\quad + \frac{2(1 - \omega)}{|\omega u + (1 - \omega)v|} \left\langle v, \frac{\omega u + (1 - \omega)v}{|\omega u + (1 - \omega)v|} - v \right\rangle \\ &= \frac{2\omega}{|\omega u + (1 - \omega)v|} \left\langle u, \frac{\omega u + (1 - \omega)v}{|\omega u + (1 - \omega)v|} - v \right\rangle \\ &\quad - \frac{(1 - \omega)}{|\omega u + (1 - \omega)v|} \left| \frac{\omega u + (1 - \omega)v}{|\omega u + (1 - \omega)v|} - v \right|^2. \end{aligned}$$

Thus, it follows that

$$\begin{aligned}
(3.12) \quad & \left[1 + \frac{(1-\omega)}{|\omega u + (1-\omega)v|}\right] \left| \frac{\omega u + (1-\omega)v}{|\omega u + (1-\omega)v|} - v \right|^2 \\
&= \frac{2\omega}{|\omega u + (1-\omega)v|} \langle u, \frac{\omega u + (1-\omega)v}{|\omega u + (1-\omega)v|} - v \rangle.
\end{aligned}$$

Since

$$\frac{2\omega}{|\omega u + (1-\omega)v|} > 0,$$

to prove Lemma 1 it is sufficient to demonstrate that

$$(3.13) \quad 1 + \frac{(1-\omega)}{|\omega u + (1-\omega)v|} = \frac{|\omega u + (1-\omega)v| + (1-\omega)}{|\omega u + (1-\omega)v|} \geq 0$$

Now (3.13) is clearly valid for $0 < \omega \leq 1$. For $1 \leq \omega < 2$, we note that by the triangle inequality

$$|\omega u| \leq |\omega u + (1-\omega)v| + |(\omega-1)v|$$

or

$$\omega \leq |\omega u + (1-\omega)v| + \omega - 1.$$

Thus,

$$(3.14) \quad 1 \leq |\omega u + (1-\omega)v|.$$

Hence,

$$(3.15) \quad |\omega u + (1-\omega)v| + (1-\omega) \geq 2 - \omega > 0.$$

This completes the proof of Lemma 1. $\square$

Since $\tilde{W}(N^\ell)$ is a non-negative, non-increasing sequence, there exists $E \geq 0$ such that

$$(3.16) \quad \lim_{\ell \rightarrow \infty} \tilde{W}(N^\ell) = E$$

We shall prove that the difference between successive iterates converges to zero. First, we need the following lemma.

LEMMA 2. Suppose that $u, v \in \mathbb{R}^3$ are unit vectors, $|u| = |v| = 1$, that $0 < \omega < 2$, and that

$$\omega u + (1-\omega)v \neq 0.$$

Then

$$(3.17) \quad \left| \frac{\omega u + (1 - \omega)v}{|\omega u + (1 - \omega)v|} - v \right|^2 \leq \max(2, \frac{2\omega}{2 - \omega}) \langle u, \frac{\omega u + (1 - \omega)v}{|\omega u + (1 - \omega)v|} - v \rangle.$$

Proof of Lemma 2. It follows from (3.12) that

$$(3.18) \quad \left| \frac{\omega u + (1 - \omega)v}{|\omega u + (1 - \omega)v|} - v \right|^2 = \frac{2\omega}{|\omega u + (1 - \omega)v| + (1 - \omega)} \langle u, \frac{\omega u + (1 - \omega)v}{|\omega u + (1 - \omega)v|} - v \rangle$$

For $0 < \omega \leq \frac{1}{2}$, we note by the triangle inequality that

$$(3.19) \quad |(1 - \omega)v| \leq |\omega u + (1 - \omega)v| + |\omega u|$$

or

$$(3.20) \quad 1 - 2\omega \leq |\omega u + (1 - \omega)v|.$$

Thus,

$$(3.21) \quad \frac{2\omega}{|\omega u + (1 - \omega)v| + (1 - \omega)} \leq \frac{2\omega}{(1 - 2\omega) + (1 - \omega)} = \frac{2\omega}{2 - 3\omega} \leq 2.$$

For $\frac{1}{2} \leq \omega \leq 1$, by the triangle inequality we have that

$$|\omega u| \leq |\omega u + (1 - \omega)v| + |(1 - \omega)v|$$

or

$$2\omega - 1 \leq |\omega u + (1 - \omega)v|.$$

Thus,

$$(3.22) \quad \frac{2\omega}{|\omega u + (1 - \omega)v| + (1 - \omega)} \leq \frac{2\omega}{(2\omega - 1) + (1 - \omega)} = \frac{2\omega}{\omega} = 2$$

Finally, for $1 \leq \omega < 2$ we have by (3.14) that

$$(3.23) \quad \frac{2\omega}{|\omega u + (1 - \omega)v| + (1 - \omega)} \leq \frac{2\omega}{1 + (1 - \omega)} = \frac{2\omega}{2 - \omega}.$$

This completes the proof of Lemma 2. $\square$

We can now prove that the difference between successive iterates converges to zero.

THEOREM 2. Let $0 < \omega < 2$. Then

$$(3.24) \quad \lim_{\ell \rightarrow \infty} |N_{ijk}^\ell - N_{ijk}^{\ell-1}| = 0 \text{ for } i, j, k = 1, \dots, M.$$

Proof of Theorem 2. It follows from Lemma 2 with $u = \frac{B_{ijk}^\ell}{|B_{ijk}^\ell|}$ and $v = N_{ijk}^{\ell-1}$ that

$$(3.25) \quad \begin{aligned} |N_{ijk}^\ell - N_{ijk}^{\ell-1}|^2 &\leq \max(2, \frac{2\omega}{2-\omega}) \langle \frac{B_{ijk}^\ell}{|B_{ijk}^\ell|}, N_{ijk}^\ell - N_{ijk}^{\ell-1} \rangle \\ &= \frac{\max(2, \frac{2\omega}{2-\omega})}{2h\rho} [\tilde{W}(N^{ij,k-1,\ell}) - \tilde{W}(N^{ijk\ell})] \\ &\leq \frac{\max(2, \frac{2\omega}{2-\omega})}{2h\rho} [\tilde{W}(N^{ij,k-1,\ell}) - E]. \end{aligned}$$

By Theorem 1,

$$\lim_{\ell \rightarrow \infty} \tilde{W}(N^{ij,k-1,\ell}) = E$$

This completes the proof of Theorem 2. $\square$

Finally, we shall prove that limit points of the iteration sequence are minima with respect to perturbations which are supported at a point and which satisfy the constraint.

THEOREM 3. Let $\hat{N} \in \tilde{\mathcal{A}}(n_0)$ be a limit point of the iteration sequence

$$\{N^{\alpha\beta\gamma\lambda} : \alpha, \beta, \gamma = 1, \dots, M; \lambda = 1, 2, \dots\} \subset \tilde{\mathcal{A}}(n_0)$$

for $0 < \omega < 2$. Let $P \in \tilde{\mathcal{A}}(n_0)$ have the property that for some (i, j, k) we have $P_{\alpha\beta\gamma} = \hat{N}_{\alpha\beta\gamma}$ for $(\alpha, \beta, \gamma) \neq (i, j, k)$. Then

$$(3.26) \quad \tilde{W}(\hat{N}) \leq \tilde{W}(P)$$

Proof. Suppose there did exist $P \in \tilde{\mathcal{A}}(n_0)$ such that for some (i, j, k) we have $P_{\alpha\beta\gamma} = \hat{N}_{\alpha\beta\gamma}$ for $(\alpha, \beta, \gamma) \neq (i, j, k)$ and

$$(3.27) \quad \tilde{W}(P) < \tilde{W}(\hat{N})$$

It then follows by (2.13) that

$$(3.28) \quad \hat{N}_{ijk} \neq \frac{B_{ijk}}{|B_{ijk}|}$$

where

$$\begin{aligned} B_{ijk} &= \hat{N}_{i-1,jk} + \hat{N}_{i,j-1,k} + \hat{N}_{i,j,k-1} \\ &\quad + \hat{N}_{i+1,jk} + \hat{N}_{i,j+1,k} + \hat{N}_{i,j,k+1}. \end{aligned}$$

Define $S \in \tilde{\mathcal{A}}(n_0)$ by

$$S_{\alpha\beta\gamma} = \hat{N}_{\alpha\beta\gamma} \quad \text{for } (\alpha, \beta, \gamma) \neq (i, j, k)$$

and

$$(3.29) \quad S_{ijk} = \frac{\omega \frac{B_{ijk}}{|B_{ijk}|} + (1 - \omega) \hat{N}_{ijk}}{|\omega \frac{B_{ijk}}{|B_{ijk}|} + (1 - \omega) \hat{N}_{ijk}|}.$$

Since $S_{ijk} \neq \hat{N}_{ijk}$, we obtain from (2.13) and (3.17) that

$$(3.30) \quad \tilde{\mathcal{W}}(S) < \tilde{\mathcal{W}}(\hat{N}).$$

Now since $\hat{N}$ is a limit point of the iteration sequence

$$\{N^{\alpha\beta\gamma\lambda} : \alpha, \beta, \gamma = 1, \dots, M; \lambda = 1, 2, \dots\}$$

and since by Theorem 2

$$\lim_{\ell \rightarrow \infty} |N_{\alpha\beta\gamma}^{\ell} - N_{\alpha\beta\gamma}^{\ell-1}| = 0 \text{ for } \alpha, \beta, \gamma = 1, \dots, M,$$

it follows that $\hat{N}$ is a limit point of the iteration sequence

$$\{N^{ij,k-1,\ell} : \ell = 1, 2, \dots\}.$$

It then follows that S is a limit point of the iteration sequence

$$\{N^{ijk\ell} : \ell = 1, 2, \dots\}.$$

Thus, by the continuity of $\tilde{\mathcal{W}}$ there exists a positive integer L such that

$$(3.31) \quad |\tilde{\mathcal{W}}(N^{ijkL}) - \tilde{\mathcal{W}}(S)| < \tilde{\mathcal{W}}(\hat{N}) - \tilde{\mathcal{W}}(S).$$

Now $\tilde{\mathcal{W}}(\hat{N}) = E$. Thus, from (3.31) we conclude that

$$\tilde{\mathcal{W}}(N^{ijkL}) < E.$$

However, Theorem 1 implies the contradiction that $\tilde{\mathcal{W}}(N^{ijkL}) \geq E$. Thus, there must not exist a $P \in \tilde{\mathcal{A}}(n)$ such that for some (i, j, k) we have $P_{\alpha\beta\gamma} = \hat{N}_{\alpha\beta\gamma}$ for $(\alpha, \beta, \gamma) \neq (i, j, k)$ and $\tilde{\mathcal{W}}(P) < \tilde{\mathcal{W}}(\hat{N})$. This completes the proof of Theorem 3. $\square$

4. Numerical Results.

In this section, we shall present some numerical results to show that over-relaxation greatly improves the rate of convergence for the liquid crystal problem. We shall show that the relationship between the rate of convergence and the relaxation parameter is similar to that found for classical unconstrained problems. More detailed convergence studies are given in [13].

We first present in Figure 1 the case for $M = 20$ and

$$n_0(x) = n_0(x_1, x_2, x_3) = (\cos(\frac{\pi x_3}{2}), \sin(\frac{\pi x_3}{2}), 0).$$

In this case, it is known that the minimization problem (2.8) has a solution [13] given by

$$(4.1) \quad N_{ijk} = (\cos(\frac{\pi kh}{2}), \sin(\frac{\pi kh}{2}), 0).$$

For our initial guess we take

$$(4.2) \quad N_{ijk}^0 = \frac{N_{ijk} + G_{ijk}}{|N_{ijk} + G_{ijk}|}$$

where the perturbation G_{ijk} is given by

$$(4.3) \quad G_{ijk} = .1 \sin(\pi ih) \sin(\pi jh) \sin(\pi kh)(1, 1, 1).$$

We define the error vector $\mathcal{E}^\ell$ by

$$(4.4) \quad \mathcal{E}^\ell = N - N^\ell$$

and we define the norm

$$\|\mathcal{E}\|^2 = \sum_{i=1}^M \sum_{j=1}^M \sum_{k=1}^M |\mathcal{E}_{ijk}|^2$$

Then to measure the average rate of convergence we define

$$(4.5) \quad R(\ell, \omega) = -\ell^{-1} \log \left[\frac{\|\mathcal{E}^\ell\|}{\|\mathcal{E}^0\|} \right].$$

For comparison, we give results in Figure 2 for the classical unconstrained Laplace problem with $M = 20$ and $n_0(x) = (\cos(\frac{\pi x_3}{2}), \sin(\frac{\pi x_3}{2}), 0)$. We define

$$\mathcal{H}(n_0) = \{U : U_{ijk} = n_0(x_{ijk}) \text{ for } x_{ijk} \in \partial\Omega\}.$$

Figure 1. Liquid crystal problem, $M = 20$, $n_0(x) = (\cos(\frac{\pi x_3}{2}), \sin(\frac{\pi x_3}{2}), 0)$.

The unconstrained or Laplace approximation problem is to determine $N \in \mathcal{H}(n_0)$ so that

$$(4.6) \quad \tilde{\mathcal{W}}(N) = \inf_{U \in \mathcal{H}(n_0)} \mathcal{W}(U).$$

In these results we use N^{100} as the exact solution, N , since we do not have an analytic expression for N .

Next, we give results for the problem with $M = 20$ and

$$(4.7) \quad n_0(x) = \frac{x - a}{|x - a|}$$

where $a = (\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$. For the liquid crystal problem (2.3) it is known [1] that the unique minima is given by

$$(4.8) \quad m(x) = \frac{x - a}{|x - a|}.$$

We note that $m(x)$ has a discontinuity at $x = a$. We give results in Figure 3 for the liquid crystal problem (2.8) and we give results in Figure 4 for the unconstrained problem. In both cases, we use N^{100} as the exact solution, N , and we use for our initial guess

$$N_{ijk}^0 = \frac{m(ih, jh, kh) + G_{ijk}}{|m(ih, jh, kh) + G_{ijk}|}$$

where $m(x)$ is given by (4.8) and G is given by (4.3).

Figure 2. Laplace problem, $M = 20$, $n_0(x) = (\cos(\frac{\pi x_a}{2}), \sin(\frac{\pi x_a}{2}), 0)$.

Finally, we shall give some computational results which show that singularities for the discrete problem are not found at lattice points. This implies that we should expect (2.19) to be valid. We consider again the case of the “point defect” defined by the boundary conditions (4.7). From (4.8) we see that the minimum for the continuous problem (2.3) has a discontinuity at $x = a$. If we solve the problem with $M = 20$, then $x = a$ is not a lattice point and we see from Figure 5 that in this case the discontinuity is at $x = a$.

However, if we solve this problem with $M = 19$, then $x = a$ is a lattice point and we see from Figure 6 that the discontinuity is not found at $x = a$. We note that the discontinuity will move to different points within a distance h of $x = a$ depending on the initial data.

Figure 3. Liquid crystal problem, $M = 20$, $n_0(x) = \frac{x}{|x|}$.

Figure 4. Laplace problem, $M = 20$, $n_0(x) = \frac{x}{|x|}$.

Figure 5. Liquid crystal problem, $M = 20$, $n_0(x) = \frac{x}{|x|}$. Orthogonal projection onto the plane $x_3 = \frac{1}{2}$ of the vectors in the plane $x_3 = \frac{1}{2}$.

Figure 6. Liquid crystal problem, $M = 19$, $n_0(x) = \frac{x}{|x|}$. Orthogonal projection onto the plane $x_3 = \frac{1}{2}$ of the vectors in the plane $x_3 = \frac{1}{2}$.

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