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APPROXIMATION OF LIQUID CRYSTAL FLOWS

CHUN LIU[*] AND NOEL J. WALKINGTON[†]

Abstract. The numerical solution of the flow of a liquid crystal governed by a particular instance of the Ericksen–Leslie equations is considered. Convergence of finite element approximations is established under appropriate regularity hypotheses, and numerical experiments exhibiting the interaction of singularities and the coupling of the director and momentum equations are presented.

Key words. Liquid Crystals, Finite Element Approximation, Convergence.

1. Introduction. In this paper, we study the numerical simulation of the following system:

$$u_t + (u \cdot \nabla)u - \nu\, div D(u) + \nabla p - \lambda\, div(\nabla d \otimes \nabla d) = 0$$

$$\nabla \cdot u = 0, \tag{1.1}$$

$$d_t + (u \cdot \nabla)d - \gamma(\Delta d - f(d)) = 0$$

with initial and boundary conditions

$$u|_{t=0} = u_0, \qquad d|_{t=0} = d_0, \qquad u|_{\partial\Omega} = 0, \qquad d|_{\partial\Omega} = d_0$$

where $u,\, d : \Omega \times \Re^+ \longrightarrow \Re^2$ and $\Omega \subset \Re^2$. In the above, $D(u) = (1/2)(\nabla u + (\nabla u)^T)$ is the stretching tensor,

$$(\nabla d \otimes \nabla d)_{ij} = \sum_{k=1}^{2} \frac{\partial d_k}{\partial x_i}\frac{\partial d_k}{\partial x_j}$$

and $f(d) = (1/\epsilon^2)(|d|^2 - 1)d$ is a penalty function used to approximate the constraint $|d| = 1$ and is the gradient of the scalar valued function $F(d) = (1/4\epsilon^2)(|d|^2 - 1)^2$.

The above system was motivated by Ericksen-Leslie equations describing the flow of nematic liquid crystals. A nematic flow behaves like a regular liquid with molecules of similar size; however, it displays anisotropic properties due to the molecule alignment, which is usually described by the local director field n.

In many experiments and theoretical works, slow motion of the liquid crystal is assumed and the behavior of the director field n is studied in the absence of the velocity fields. Under this assumption, there are many interesting results on the distribution and motion of defects [8, 9, 12, 17, 19]. The main idea is to minimize the Oseen-Frank energy associated with the director field:

$$E(n) = K_1|div\, n|^2 + K_2(n \cdot curl\, n)^2 + K_3(n \times curl\, n)^2.$$

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Note that when the constants are equal, this energy becomes the Dirichlet energy $K|\nabla n|^2$ plus a constant term which can be determined by the "strong anchoring condition" (Dirichlet boundary conditions) of n on the boundary. From the mathematical point of view, this is closely related to the theory of the calculus of variations and especially work on harmonic maps [5, 12].

In many situations the flow velocity does disturb the alignment of the molecule. More importantly the converse is also true; that is, a change in the alignment will induce velocity. This implies that, if the initial fluid velocity is zero, the evolution of the director field will induce a velocity, and this velocity will in turn affect the evolution of the director field. In this process, we can not assume that the velocity field will remain small.

The Ericksen-Leslie system was derived from the macroscopic point of view and involves many coupling terms between the two vector fields [6, 7, 16, 15]. In [19], Lin introduced the simplified system (1.1) consisting of a Navier-Stokes type of equation coupled with a gradient flow equation similar to that of of harmonic maps. This system retains some important properties of the original Ericksen-Leslie equations and at the same time is amenable to rigorous analysis.

The first equation in system (1.1) is the equation for the conservation of linear momentum. It contains the usual Navier-Stokes equation describing the flow of an isotropic fluid and the term $\lambda\, div(\nabla d \otimes \nabla d)$ which is anisotropic. The second equation represents the property of incompressibility of the liquid, and the third equation is associated with conservation of the angular momentum. The term $f(d)$ is simply the Ginzburg-Landau approximation of the constraint $|n| = 1$ for small ϵ.

This system exhibits many interesting properties. For instance, the director field satisfies the maximum principle; that is, its magnitude will not achieve a maximum at any interior point of the space-time domain. Substituting a stationary solution $(u, d) = (0, d_0)$ into the system, shows that d_0 not only has to satisfy the equation $\Delta d - f(d) = 0$, but also an extra constraint $(\nabla d)^T \Delta d = \nabla \phi$, where ϕ is a scalar function. This implies certain regularity of d_0. Moreover, system (1.1) admits the following energy law:

$$\frac{dE}{dt} = -\left(\nu\|D(u)\|^2_{L^2(\Omega)} + \lambda\gamma\|\Delta d - f(d)\|^2_{L^2(\Omega)}\right)$$

where

$$E = (1/2)\|u\|^2_{L^2(\Omega)} + (\lambda/2)\|d\|^2_{H^1_0(\Omega)} + \lambda \int_\Omega F(d)$$

Using energy estimates, Lin and Liu [21] were able to prove local existence of classical solutions and global existence of the weak solutions to the system (1.1) with

$$u \in L^2[0, T,\ H^1(\Omega)] \cap L^\infty[0, T,\ L^2(\Omega)], \qquad d \in L^2[0, T,\ H^2(\Omega)] \cap L^\infty[0, T,\ H^1(\Omega)].$$

For any fixed ϵ, they also proved that the one dimensional space-time Hausdorff measure of the singular set of "suitable" weak solutions is zero. Some of their results extended to the general Ericksen-Leslie equations [22].

Recently much work has appeared on the related Ginzburg-Landau equation

$$u_t - \Delta u = (1/\epsilon^2)(1 - |u|^2)u,$$

where $u : \Omega \times \Re^+ \to \Re^2$ with boundary condition

$$u|_{\partial\Omega} = g, \qquad deg(g; \partial\Omega) = d.$$

This is the gradient flow of the Ginzburg-Landau functional:

$$E^\epsilon_\Omega(u) = \int_\Omega (1/2)|\nabla u|^2 + (1/4\epsilon^2)(|u|^2 - 1)^2$$

Bethuel, Brezis and Helein [1] show that as $\epsilon \to 0$ the singular set of the solution contains only isolated singular points $\{a_i\}$ with degree one; moreover,

$$\inf\{E^\epsilon_\Omega(u) \mid u|_{\partial\Omega} = g\} = \pi d \log(1/\epsilon) + \gamma d + \min\{W_g(a_i)\} + o(1)$$

where W_g is the "renormalized" energy, and $\gamma \geq 0$ is a universal constant.

Lin [18, 20], Jerrard and Soner [13] and others study the dynamic motion of the defects. They proved that the motion of the singularities of the solution follows the gradient flow associated with the renormalized energy:

$$\frac{da_i}{dt} = -\frac{\delta W_g}{\delta a_i}$$

In our numerical examples, we illustrate several interesting properties of the motion of the defects of (1.1). For instance, when two defects of opposite degree move towards each other their relative velocity increases, indicating the Ginzburg–Landau like effect of the second equation. However, the examples clearly show the significant effect of the velocity on the motion of defects.

In this paper, we use prove that the numerical approximations using a finite element approximation of the spatial domain and implicit Euler time stepping will converge to the solution of (1.1). Examples of approximations computed using this scheme are given in Section 4 which illustrate the interesting behavior exhibited when defects in the director field are present. In the next section we recall the energy estimates discovered by Lin and Liu [21] and variants that are applicable to the numerical schemes analyzed in Section 3.

2. Estimates and Weak Forms of the Liquid Crystal Equations.

2.1. Energy Estimates. A key discovery of Lin and Liu [21] was the existence of energy estimates (Liaponov functions) for the coupled liquid crystal equations. One essential step was to write the Navier Stokes equations (1.1) in non–divergence form:

$$u_t + (u \cdot \nabla)u - \nu\, div D(u) + \nabla p + \lambda\left[(1/2)\nabla(\nabla d \cdot \nabla d) + (\nabla d)^T \Delta d\right] = 0$$

Notice that the term $(\lambda/2)(\nabla d \cdot \nabla d)$ can be absorbed into the definition of the pressure.

Proceeding formally we can multiply this equation by u (and recall that we're assuming Dirichlet boundary data) to get

$$\frac{1}{2}\frac{d}{dt}||u||^2_{L^2(\Omega)} + \nu||D(u)||^2_{L^2(\Omega)} + \int_\Omega (u \cdot \nabla)u \cdot u + \lambda \int_\Omega \Delta d^T (\nabla d) u = 0.$$

Similarly we may take the inner product of the director equation with $-(\Delta d - f(d))$ to obtain

$$\frac{d}{dt}\left((1/2)||d||^2_{H^1_0(\Omega)} + \int_\Omega F(d)\right)$$
$$- \int_\Omega \left(\Delta d^T(\nabla d)u - (u \cdot \nabla)d \cdot f(d)\right) + \gamma||\Delta d - f(d)||^2_{L^2(\Omega)} = 0.$$

The identities

$$\int_\Omega (u\cdot\nabla)u\cdot u = (1/2)\int_\Omega u\cdot\nabla|u|^2 = 0$$

and

$$\int_\Omega (u\cdot\nabla)d\cdot f(d) = \int_\Omega u\cdot\nabla F(d) = 0$$

give the fundamental estimate

$$\frac{d}{dt}\left((1/2)||u||^2_{L^2(\Omega)} + (\lambda/2)||d||^2_{H^1_0(\Omega)} + \int_\Omega \lambda F(d)\right)$$
$$+\nu||D(u)||^2_{L^2(\Omega)} + \lambda\gamma||\Delta d - f(d)||^2_{L^2(\Omega)} = 0.$$

Defining the energy $E(t) = E(u(t), d(t))$ by

$$E = (1/2)||u||^2_{L^2(\Omega)} + (\lambda/2)||d||^2_{H^1_0(\Omega)} + \lambda\int_\Omega F(d)$$

then E non–increasing as a function of time. Note that this provides a uniform bound on the penalty term $F(d)$. This estimate on the solution was used by Lin and Liu [21] to establish existence, uniqueness, and regularity of solutions to the coupled liquid crystal problem.

To obtain the fundamental energy estimate it was necessary to multiply the director equation by the function $-(\Delta d - f(d))$. When Galerkin methods are used to approximate the solution of the pde's, such functions will not be in the Galerkin sub–spaces due to the nonlinearity of f, and, in general, the energy estimate fails to hold. We can still obtain estimates by multiplying the director equation by $-\Delta d$, and these do carry over to Galerkin approximations; however, these estimates now depend upon the penalty parameter ϵ. This procedure gives

$$(1/2)\frac{d}{dt}\left(||u||^2_{L^2(\Omega)} + \lambda||d||^2_{H^1_0(\Omega)}\right) + \nu||D(u)||^2_{L^2(\Omega)} + \lambda\gamma||\Delta d||^2_{L^2(\Omega)} = \lambda\gamma\int_\Omega f(d)\cdot\Delta d.$$

Recalling the penalty term is of the form $f(d) = DF(d)$ the term on the right simplifies to,

$$\int_\Omega f(d)\cdot\Delta d = \int_\Omega -tr\left[(\nabla d)^T D^2F(d)(\nabla d)\right] + \int_{\partial\Omega} f(d_0)^T(\nabla d)n$$

where tr is the trace of a matrix. Since the penalty term is used to enforce the constraint $|d| = 1$, typically $f(d_0) = 0$ and F is convex on the set $|d| \geq 1$. The term on the right can then be bounded by

$$\int_\Omega f(d)\cdot\Delta d \leq \left(\max_{|d|\leq 1}|D^2F(d)|\right)||\nabla d||^2_{L^2(\Omega)}.$$

For example, when $F(d) = (1/4\epsilon^2)(|d|^2-1)^2$ one has

$$\epsilon^2\int_\Omega f(d)\cdot\Delta d = -(1/2)||\nabla|d|^2||^2_{L^2(\Omega)} - \int_\Omega(|d|^2-1)|\nabla d|^2 \leq ||\nabla d||^2_{L^2(\Omega)}.$$

In this situation Gronwall's inequality gives bounds on the solution of the form

$$\begin{aligned} &\|u(t)\|^2_{L^2(\Omega)} + \lambda\|d(t)\|^2_{H^1_0(\Omega)} \\ &\qquad + \int_0^t \nu\|D(u(s))\|^2_{L^2(\Omega)} + \lambda\gamma\|\Delta d(s)\|^2_{L^2(\Omega)}\, ds \le C\exp(t/\epsilon^2), \end{aligned} \tag{2.1}$$

where the constant C depends upon the initial data and is independent of ϵ.

Notice that the maximum principle could have been used in place of the convexity argument. Multiplying the director equation by d and rearranging the derivatives shows that $|d|$ satisfies

$$\frac{d}{dt}|d|^2 + (u \cdot \nabla)|d|^2 - \gamma\Delta|d|^2 = -2\gamma(|\nabla d|^2 + f(d) \cdot d)$$

At a maximum it is clear that the left hand side is non-negative. If $f(d) \cdot d > 0$ for $|d| > 1$ then it is clear that any maximum of $|d|^2$ must satisfy $|d| \le 1$. Thus if the initial data satisfies $|d| \le 1$ then this inequality continue to hold at later times.

2.2. Bounds on Pressure. The estimates above bound the velocity and director fields but not the pressure. The sharpest bounds on the pressure are obtained by taking the divergence of the momentum equation to get

$$-\Delta p = (\nabla \otimes \nabla) \cdot (u \otimes u + (\nabla d)^T(\nabla d))$$

where

$$(\nabla \otimes \nabla) \cdot A = \sum_{i,j} \partial^2 A_{ij}/\partial x_i \partial x_j .$$

If Ω was the whole of space Calderon Zigmund theory [3, 10] would immediately give estimates on the pressure. On a bounded domain the following holds [22, 24].

THEOREM 2.1. *Let $\Omega \subset \Re^3$ be smooth and*

$$u \in L^2[0, T,\ H^1(\Omega)] \cap L^\infty[0, T,\ L^2(\Omega)] \qquad d \in L^2[0, T,\ H^2(\Omega)] \cap L^\infty[0, T,\ H^1(\Omega)]$$

and p satisfy the above equation, then $p \in L^{5/3}[0, T; L^{5/3}(\Omega)]$ and $\nabla p \in L^{5/3}[0, T; L^{15/14}(\Omega)]$.
Other regularity results for the Navier Stokes equations may be found in [23, 25, 26].

When constructing Galerkin approximations, stability of the pressure is obtained using the following lemma due to Ladyzenskya [11].

LEMMA 2.2. *If $\Omega \subset \Re^n$ is a bounded Lipschitz domain and $p \in L^2(\Omega)$ then there exists $c > 0$ such that*

$$\sup_{\|v\|_{H^1_0(\Omega)}=1} \int_\Omega p(\nabla \cdot v) \ge c\|p\|_{L^2(\Omega)/\Re}$$

Rearranging the momentum equation shows that if $v \in H^1_0(\Omega)$ then

$$(-p, \nabla \cdot v) = (u_t + (u \cdot \nabla)u, v) + \nu(D(u), D(v)) + \lambda((\nabla d)^T(\nabla d), (\nabla v))$$

thus if $u \in L^2[0, T,\ H^1(\Omega)] \cap H^1[0, T,\ H^{-1}(\Omega)]$ and $d \in L^2[0, T,\ H^2(\Omega)]$ then the lemma shows $p \in L^2[0, T,\ L^2(\Omega)/\Re]$. The construction of discrete subspaces satisfying Ladyzinskia's lemma is well studied [2, 11]. and we will consider such subspaces below.

2.3. Weak Problem. The energy estimates derived in this section indicate that the following weak form of the coupled liquid crystal problem will be well posed. Find $u \in H^1[0,T,\ H^{-1}(\Omega)] \cap L^2[0,T,\ H^1_0(\Omega)]$, $p \in L^2[0,T,\ L^2(\Omega)/\Re]$ and $d \in H^1[0,T,\ H^1_0(\Omega)] \cap L^2[0,T,\ H^2(\Omega) \cap H^1_0(\Omega)]$ such that

$$\int_\Omega (u_t \cdot v + (1/2)\left[(u \cdot \nabla)u \cdot v - (u \cdot \nabla)v \cdot u)\right] - \nu D(u) \cdot D(v) \\ - p(\nabla \cdot v) + \Delta d^T (\nabla d) v) = 0$$

$$\int_\Omega (\nabla \cdot u) q = 0 \tag{2.2}$$

$$\int_\Omega (\nabla d_t \cdot \nabla e - \Delta e^T (\nabla d) u + \gamma(\Delta d - f(d)) \cdot \Delta e) = 0$$

for all $(v, q, e) \in L^2[0,T,\ H^1_0(\Omega)] \times L^2[0,T,\ L^2(\Omega)/\Re] \times L^2[0,T,\ H^2(\Omega) \cap H^1_0(\Omega)]$. Notice that when extending the definition of $(u \cdot \nabla)u$ to functions that may not satisfy $\nabla \cdot u = 0$ we chose to preserve the skew symmetry, $((u \cdot \nabla)u, u) = 0$.

Solutions of this weak problem are approximated using implicit finite differences for time derivative and the finite element method for approximating the spatial terms. Let

$$\mathcal{H} = H^1_0(\Omega) \times L^2(\Omega)/\Re \times (H^2(\Omega) \cap H^1_0(\Omega))$$

and let $\mathcal{H}_h = \mathcal{U}_h \times \mathcal{P}_h \times \mathcal{W}_h \subset \mathcal{H}$ be a finite dimensional subspace of $\mathcal{H}$ given by a finite element discretization of Ω. If $\tau > 0$ represents a time step and $(u^n, p^n, d^n) \in \mathcal{H}_h$ is an approximation of $u(t^n) = u(n\tau)$ etc. then the approximation at time $t^{n+1} = (n+1)\tau$ is is computed as the solution of $(u_h, p_h, d_h) \in \mathcal{H}_h$,

$$\int_\Omega ((1/\tau)(u_h - u^n) \cdot v + (1/2)\left[(u_h \cdot \nabla)u_h \cdot v - (u_h \cdot \nabla)v \cdot u_h)\right] - \nu D(u_h) \cdot D(v) \\ - p_h(\nabla \cdot v) + \Delta d_h^T (\nabla d_h) v) = 0$$

$$\int_\Omega (\nabla \cdot u_h) q = 0 \tag{2.3}$$

$$\int_\Omega \left(\frac{1}{\tau} \nabla (d_h - d^n) \cdot \nabla e - \Delta e^T (\nabla d_h) u_h + \gamma(\Delta d_h - f(d_h)) \cdot \Delta e \right) = 0$$

for all $(v, q, e) \in \mathcal{H}_h$.

3. Error Estimate of the Discrete Scheme. In this section we show that solutions of the approximate weak problem (2.3) converge to those of the continuous problem (2.2). We chose to concentrate on the convergence of the finite element approximations and, in particular, do not reproduce discrte versions of the existance results in [21] for (2.3).

3.1. Notation. Since much of the analysis is independent of the specifics of the problem at hand we introduce notation that facilitates some abstraction.

NOTATION 3.1. *If* $\mathbf{u} = (u, d)$, *and* $\mathbf{v} = (v, e)$ *define* $A\mathbf{u}$ *to be the linear monotone part of the spatial operator occurring in the weak form of coupled liquid crystal problem.*

$$A(\mathbf{u}, \mathbf{v}) = \int_\Omega \nu D(u) \cdot D(v) + \lambda\gamma \Delta d \cdot \Delta e \tag{3.1}$$

The remaining portion of the spatial operator is written as a linear term $B(.,.)$ *and a nonlinear part* $G\mathbf{u}$ *with*

$$B(p, \mathbf{v}) = \int_\Omega p(\nabla \cdot v) \tag{3.2}$$

$$(G\mathbf{u}, \mathbf{v}) = \int_\Omega (1/2)\left[(u \cdot \nabla)u \cdot v + (u \cdot \nabla)v \cdot u\right] + \lambda \Delta d^T (\nabla d) \cdot v - \lambda (u \cdot \nabla) d \cdot \Delta e + \lambda\gamma f(d) \cdot \Delta e \tag{3.3}$$

Since $B(p, \mathbf{v}) = B(p, (v, d))$ *is independent of* d *we will occasionally write* $B(p, v)$ *for this term.*

The inner product $(.,.)$ *on* $H = L^2(\Omega) \times H^1_0(\Omega)$ *is defined by*

$$(\mathbf{u}, \mathbf{v}) = \int_\Omega uv + \lambda \nabla d \cdot \nabla e \tag{3.4}$$

and we denote the associated norm by $|.|$.

Notice that A *is strictly monotone and*

$$A(\mathbf{u} - \mathbf{v}, \mathbf{u} - \mathbf{v}) = \|\mathbf{u} - \mathbf{v}\|^2 \equiv \nu \|D(u - v)\|^2_{L^2(\Omega)} + \lambda\gamma \|\Delta(d - e)\|^2_{L^2(\Omega)} \tag{3.5}$$

The norm $\|.\|$ *is equivalent to the usual norm on* $V = H^1_0(\Omega) \times (H^2(\Omega) \cap H^1_0(\Omega))$, *and we will denote the dual norm on* V' *by* $\|.\|_*$. *We identify* V *as a subset of* V' *by pivoting through* H, $V \hookrightarrow H \hookrightarrow V'$, *and in this situation* $\|(u, d)\|^2_* = \|u\|^2_{H^{-1}(\Omega)} + \|d\|^2_{L^2(\Omega)}$

Using this notation we may write the weak problem for the liquid crystal problem as

$$(\mathbf{u}_t, \mathbf{v}) + A(\mathbf{u}, \mathbf{v}) + B(p, \mathbf{v}) = (G\mathbf{u}, \mathbf{v}), \qquad B(q, \mathbf{u}) = 0,$$

for all $\mathbf{v} \in V$ and $q \in L^2(\Omega)/\Re$. The approximate scheme becomes

$$(\mathbf{u}^{n+1} - \mathbf{u}^n, \mathbf{v}) + \tau A(\mathbf{u}^{n+1}, \mathbf{v}) + \tau B(p^{n+1}, \mathbf{v}) = \tau(G\mathbf{u}^{n+1}, \mathbf{v})$$

for all $\mathbf{v} \in \mathcal{U}_h \times \mathcal{W}_h$ and $B(q, \mathbf{u}^{n+1}) = 0$ for all $q \in \mathcal{P}_h$.

The arguments used to derive the bounds (2.1) for the continuous solution carry over directly to the Euler scheme giving

$$|\mathbf{u}^n|^2 + \sum_{m=1}^{n} \tau \|\mathbf{u}^m\|^2 \leq C|\mathbf{u}^0|^2 \exp(n\tau/\epsilon^2) \tag{3.6}$$

where ϵ is small parameter appearing in the penalty term f.

3.2. Discrete Spaces. It is well known that when approximating the Navier Stokes equations it is necessary that the discrete velocity and pressure spaces, $\mathcal{U}_h$ and $\mathcal{P}_h$, satisfy the discrete Babuska–Brezzi condition, [2].

$$\sup_{||u_h||_{\mathcal{U}_h}=1} B(p_h, u_h) \geq c||p_h||_{\mathcal{P}_h}$$

for all $p_h \in \mathcal{P}_h$ where $c > 0$ is independent of h. This condition guarantees that the discrete divergence free space $\tilde{\mathcal{U}}_h = \{u_h \in \mathcal{U}_h \mid B(q_h, u_h) = 0 \,\forall\, q_h \in \mathcal{P}_h\}$ well approximates its continuous counterpart $\tilde{\mathcal{U}} = \{u \in \mathcal{U} \mid B(q, u) = 0 \,\forall\, q \in \mathcal{P}\}$ as indicated in the following lemma.

LEMMA 3.2. *Let the discrete Babuska–Brezzi condition hold, then there is a constant $C > 0$ (independent of h) such that if $u \in \tilde{\mathcal{U}}$ then*

$$\inf_{u_h \in \tilde{\mathcal{U}}_h} ||u - u_h||_{\mathcal{U}} \leq C \inf_{u_h \in \mathcal{U}} ||u - u_h||_{\mathcal{U}}.$$

A proof of this lemma may be found in [2, 11].

When analyzing the discrete schemes the best projections of elements in $\mathcal{U} \times \mathcal{W}$ onto $\tilde{\mathcal{U}}_h \times \mathcal{W}_h$ with respect to both of the norms $|.|$ and $||.||$ will arise.

DEFINITION 3.3. *If $\tilde{\mathcal{U}}_h = \mathcal{U}_h \cap \{u \mid B(q, u) = 0 \,\forall\, q \in \mathcal{P}_h\}$ and $u \in H^1_0(\Omega)$, $d \in H^2(\Omega)$ the projections $\tilde{u}$, $\hat{u} \in \tilde{\mathcal{U}}_h$ and $\tilde{d}$, $\hat{d} \in \mathcal{W}_h$ are defined by*

$$(\tilde{u}, v) = (u, v) \qquad (\nabla\tilde{d}, \nabla e) = (\nabla d, \nabla e)$$

and

$$(D(\hat{u}), D(v)) = (D(u), D(v)) \qquad (\Delta\hat{d}, \Delta e) = (\Delta d, \Delta e)$$

for all $v \in \tilde{\mathcal{U}}_h$ and $e \in \mathcal{W}_h$.

Notice that $\tilde{\mathbf{u}} = (\tilde{u}, \tilde{d})$ is the best projection of $\mathbf{u} = (u, d)$ onto the subspace $\tilde{\mathcal{U}}_h \times \mathcal{W}_h$ in the norm $|.|$ and $\hat{\mathbf{u}} = (\hat{u}, \hat{d})$ is the best projection with norm $||.||$. We will need to estimate the difference $||\tilde{\mathbf{u}} - \hat{\mathbf{u}}||$. The following lemma is prototypical for the spaces used for finite element approximations.

LEMMA 3.4. *Let $\tilde{\mathcal{U}}_h \subset \mathcal{U}_h$, $\tilde{\mathcal{U}} \subset \mathcal{U}$, $\mathcal{U}_h \subseteq \mathcal{U}$, and $\mathcal{W}_h \subset \mathcal{W}$. Suppose that $|.|$ and $||.||$ are two Hilbert norms on $\mathcal{U} \times \mathcal{W}$. Let $\mathbf{u} \in \tilde{\mathcal{U}} \times \mathcal{W}$ and let $\tilde{\mathbf{u}}$ be the projection onto $\tilde{\mathcal{U}}_h \times \mathcal{W}_h$ under norm $|.|$ and $\hat{\mathbf{u}}$ be the projection with norm $||.||$ and suppose additionally*

- *The discrete spaces satisfy an inverse inequality of the form $||\mathbf{u}_h|| \leq (C/h)|\mathbf{u}_h|$ for $\mathbf{u}_h \in \mathcal{U}_h \times \mathcal{W}_h$*
- *The elliptic projection $\hat{\mathbf{u}}$ satisfies an inequality of the form*

$$(1/h)|\mathbf{u} - \hat{\mathbf{u}}| + ||\mathbf{u} - \hat{\mathbf{u}}|| \leq C \inf_{\mathbf{v}_h \in \mathcal{U}_h \times \mathcal{W}_h} ||\mathbf{u} - \mathbf{v}_h||$$

whenever $u \in \tilde{\mathcal{U}}$.

then

$$||\tilde{\mathbf{u}} - \hat{\mathbf{u}}|| \leq C \inf_{\mathbf{v}_h \in \mathcal{U} \times \mathcal{W}} ||\mathbf{u} - \mathbf{v}_h||$$

Proof. Using the inverse estimate we obtain

$$||\hat{\mathbf{u}} - \hat{\mathbf{u}}|| \leq (C/h)|\hat{\mathbf{u}} - \hat{\mathbf{u}}| \leq (C/h)(|\hat{\mathbf{u}} - \mathbf{u}| + |\mathbf{u} - \hat{\mathbf{u}}|) \leq (2C/h)|\mathbf{u} - \hat{\mathbf{u}}_h|$$

An application of the second hypothesis establishes the lemma. □

The inverse inequality holds for all the usual finite element spaces; and the second estimate will hold if the pair of spaces $(\mathcal{U}_h, \mathcal{P}_h)$ satisfy the Babuska–Brezzi condition and the domain is smooth enough for the Aubin–Nitsche technique to be used [4].

3.3. Error Estimate. Following [11] it is convenient to introduce the (temporal) consistency error $\varepsilon^{n+1} \in V'$

$$\begin{aligned}(\mathbf{u}(t^{n+1}) - \mathbf{u}(t^n), \mathbf{v}) + \tau A(\mathbf{u}(t^{n+1}), \mathbf{v}) - \tau B(p(t^{n+1}), \mathbf{v}) \\ = \tau(G\mathbf{u}(t^{n+1}), \mathbf{v}) + \tau(\varepsilon^{n+1}, \mathbf{v})\end{aligned} \tag{3.7}$$

Subtracting this equation from the one satisfied by the approximation gives

$$\begin{aligned}(\mathbf{u}(t^{n+1}) - \mathbf{u}^{n+1}, \mathbf{v}) + \tau A(\mathbf{u}(t^{n+1}) - \mathbf{u}^{n+1}, \mathbf{v}) - \tau B(p(t^{n+1}) - p^{n+1}, \mathbf{v}) \\ = (\mathbf{u}(t^n) - \mathbf{u}^n, \mathbf{v}) + \tau(G\mathbf{u}(t^{n+1}) - G\mathbf{u}^{n+1}, \mathbf{v}) + \tau(\varepsilon^{n+1}, \mathbf{v})\end{aligned}$$

for all $\mathbf{v} \in \mathcal{U}_h \times \mathcal{W}_h$.

Writing $\mathbf{e}^{n+1} = (\tilde{u}(t^{n+1}) - u^{n+1}, \tilde{d}(t^{n+1}) - d^{n+1})$ and putting $\mathbf{v} = \mathbf{e}^{n+1}$ into the equation for the errors gives the basic estimate

$$\begin{aligned}(1/2)|\mathbf{e}^{n+1}|^2 + (\tau/2)||\mathbf{e}^{n+1}||^2 \leq (1/2)|\mathbf{e}^n|^2 + \tau B(p(t^{n+1}) - q_h, \mathbf{e}^{n+1}) + \\ \tau(G\mathbf{u}(t^{n+1}) - G\mathbf{u}^{n+1}, \mathbf{e}^{n+1}) + \tau(\varepsilon^{n+1}, \mathbf{e}^{n+1}) + (\tau/2)||\tilde{\mathbf{u}}^{n+1} - \hat{\mathbf{u}}^{n+1}||\end{aligned} \tag{3.8}$$

where $q_h \in \mathcal{P}_h$ is arbitrary.

The following lemma bounds each of the error terms on the right hand side of this equation.

LEMMA 3.5. *Let G be the operator defined in (3.3) and ε^{n+1} be the consistency error defined in (3.7), and assume that the penalty function F has been truncated to have quadratic growth outside the ball $|d| \leq 1$. If the solution $\mathbf{u} = (u, d)$ of the liquid crystal problem satisfies*

$$u \in C[0, T,\ H_0^1(\Omega)] \qquad u_t \in L^2[0, T,\ L^2(\Omega)]\ . \quad u_{tt} \in L^2[0, T,\ H^{-1}(\Omega)]$$

and

$$d \in C[0, T,\ H^2(\Omega)] \qquad d_t \in L^2[0, T,\ H^1(\Omega)] \qquad d_{tt} \in L^2[0, T,\ L^2(\Omega)]$$

then there is a constant $C > 0$, depending upon these norms and the bounds in (3.6) established for the approximate solution such that

$$||\varepsilon^{n+1}||_*^2 \leq \tau \int_{n\tau}^{(n+1)\tau} ||\mathbf{u}_{tt}||_*^2$$

and

$$(G\mathbf{u}(t^{n+1}) - G\mathbf{u}^{n+1}, \mathbf{e}^{n+1}) \leq C\ \left(||\mathbf{u}(t^{n+1}) - \tilde{\mathbf{u}}(t^{n+1})||^2 + |\mathbf{e}^{n+1}|^2\right) + (1/8)||\mathbf{e}^{n+1}||^2$$

The product norms $|.|$ and $||.||$ and dual norm $||.||_*$ are defined in Notation 3.1.

Proof. To bound the consistency error, note that the regularity hypotheses guarantee the each term in the weak form of the the coupled liquid crystal equations (2.2) is continuous. Evaluating (2.2) at $t = t^{n+1}$ and subtracting this from (3.7) gives

$$(\varepsilon^{n+1}, \mathbf{v}) = (1/\tau)(\mathbf{u}^{n+1} - \mathbf{u}^n, \mathbf{v}) - (\mathbf{u}_t(t^{n+1}), \mathbf{v}) = (1/\tau)\int_{n\tau}^{(n+1)\tau} (n\tau - t)(\mathbf{u}_{tt}, \mathbf{v})$$

It follows that

$$||\varepsilon^{n+1}||_*^2 \leq \left(\int_{n\tau}^{(n+1)\tau} ||\mathbf{u}_{tt}||_*\right)^2 \leq \tau \int_{n\tau}^{(n+1)\tau} ||\mathbf{u}_{tt}||_*^2$$

To avoid a plethora of superscripts, let us write the nonlinear term as $(G\mathbf{u} - G\mathbf{u}_h, \mathbf{e})$ where $\mathbf{e} = (e_u, e_d) = \tilde{\mathbf{u}} - \mathbf{u}_h$. We first break this term into two pieces

$$(G\mathbf{u} - G\mathbf{u}_h, \mathbf{e}) = (G\mathbf{u} - \tilde{\mathbf{u}}, \mathbf{e}) + (G\tilde{\mathbf{u}} - G\mathbf{u}_h, \mathbf{e}).$$

If the above terms are expanded out the expansion contains many trilinear terms and the nonlinear term involving the penalty function f.

The treatment of differences in trilinear forms is standard: one adds and subtracts various cross terms and groups them so that each piece is quadratic in the error. Judicious application of the Holder inequality and the Sobelov embedding theorem can be used to make the coefficient of $||\mathbf{e}||^2$ sufficiently small (e.g. less than 1/8). We illustrate this procedure for two typical terms.

$$\begin{aligned}
&\int_\Omega ((u \cdot \nabla)u - (\tilde{u} \cdot \nabla)\tilde{u}) \cdot e_u \\
&= \int_\Omega (((u - \tilde{u}) \cdot \nabla)u + (\tilde{u} \cdot \nabla)(u - \tilde{u})) \cdot e_u \\
&\leq (||u - \tilde{u}||_{L^4(\Omega)}||\nabla u||_{L^2(\Omega)} + ||\tilde{u}||_{L^4(\Omega)}||\nabla(u - \tilde{u})||_{L^2(\Omega)})||e_u||_{L^4(\Omega)} \\
&\leq C||u - \tilde{u}||_{H_0^1(\Omega)}||e_u||_{H_0^1(\Omega)} \\
&\leq C||D(u - \tilde{u})||_{L^2(\Omega)}^2 + \eta||e_u||_{H^1(\Omega)}^2
\end{aligned}$$

In the above we used Korn's inequality and the Sobelov embedding theorem, and note that the constant C depends upon various norms of u and $\tilde{u}$ which are bounded by hypothesis. The terms coupling the Navier Stokes and director equation are:

$$\begin{aligned}
&\int_\Omega \Big((e_u \cdot \nabla)\tilde{d} \cdot \Delta\tilde{d} - (e_u \cdot \nabla)d_h \cdot \Delta d_h - (\tilde{u} \cdot \nabla)\tilde{d} \cdot \Delta\tilde{d} + (u_h \cdot \nabla)d_h \cdot \Delta d_h\Big) \\
&= \int_\Omega (e_u \cdot \nabla)e_d \cdot \Delta\tilde{d} + (\tilde{u} \cdot \nabla)e_d \cdot \Delta e_d \\
&\leq ||\nabla e_d||_{L^4(\Omega)}(||e_u||_{L^4(\Omega)}||\Delta\tilde{d}||_{L^2(\Omega)} + ||\tilde{u}||_{L^4(\Omega)}||\Delta e_d||_{L^2(\Omega)})
\end{aligned}$$

The Sobelov embedding theorem (in dimension 3) bounds $||.||_{L^4(\Omega)}$ by $||\cdot||_{L^2(\Omega)}^{1/4}||\cdot||_{H^1(\Omega)}^{3/4}$ so application of the (scalar) Holder inequality use of regularity estimates to bound the term $||D^2 d||_{L^2(\Omega)}$ gives a suitable bound.

Since the penalty function F is assumed to have quadratic growth outside the ball $|d| \leq 1$, it's derivative f will be globally Lipschitz. In this situation we can compute

$$\int_\Omega (f(d) - f(\tilde{d})) \cdot \Delta e_d \leq |f|_{Lip}||d - \tilde{d}||_{L^2(\Omega)}||\Delta e_d||_{L^2(\Omega)}$$

and a similar inequality holds for $(f(\tilde{d}) - f(d_h)) \cdot \Delta e_d$. □

These estimates enable us to state the main theorem of this section concerning convergence of the discrete scheme.

THEOREM 3.6. *Let $\{(u^n, p^n, d^n)\}_{n=0}^N$ be the solution of the discrete scheme (2.3), with subspaces*

$$\mathcal{H}_h = \mathcal{U}_h \times \mathcal{P}_h \times \mathcal{W}_h \subset H_0^1(\Omega) \times L^2(\Omega)/\Re \times (H^2(\Omega) \cap H_0^1(\Omega))$$

and assume that the penalty function F has been truncated to have quadratic growth outside the ball $|d| \leq 1$. Let $\tilde{\mathcal{U}}_h$ be the approximate divergence free subspace defined in 3.3. Suppose that the solution of the liquid crystal problem (2.2) satisfies

$$u \in C[0,T,\ H_0^1(\Omega)] \qquad u_t \in L^2[0,T,\ L^2(\Omega)] \qquad u_{tt} \in L^2[0,T,\ H^{-1}(\Omega)]$$

and

$$d \in C[0,T,\ H^2(\Omega)] \qquad d_t \in L^2[0,T,\ H^1(\Omega)] \qquad d_{tt} \in L^2[0,T,\ L^2(\Omega)]$$

and the $L^2(\Omega) \times H^1(\Omega)$ projection $(\tilde{u}, \tilde{d})$ of an element $(u,d) \in \mathcal{U} \times \mathcal{W}$ onto $\tilde{\mathcal{U}}_h \times \mathcal{W}_h$ satisfies (see Section 3.2)

$$\|u - \tilde{u}\|_{H_0^1(\Omega)} + \|d - \tilde{d}\|_{H^2(\Omega)} \leq \inf_{v_h \in \mathcal{U}_h} \|u - v_h\|_{H_0^1(\Omega)} + \inf_{e_h \in \mathcal{W}_h} \|d - e_h\|_{H^2(\Omega)}$$

then

$$\|u(t^n) - u^n\|_{L^2(\Omega)}^2 + \|d(t^n) - d^n\|_{H_0^1(\Omega)}^2 + \sum_{m=0}^{n} \tau \left(\|u(t^m) - u^m\|_{H_0^1(\Omega)}^2 + \|d(t^m) - d^m\|_{H^2(\Omega)}^2 \right)$$
$$\leq C\tau^2 + C\|u(0) - u^0\|_{L^2(\Omega)}^2 + \|d(0) - d^0\|_{H_0^1(\Omega)}^2 +$$
$$C \max_{0 \leq m \leq N} \left[\inf_{v_h \in \mathcal{U}_h} \|u(t^m) - v_h\|_{H^1(\Omega)}^2 + \inf_{q_h \in \mathcal{P}_h} \|p(t^m) - q_h\|_{L^2(\Omega)}^2 + \inf_{e_h \in \mathcal{W}_h} \|d(t^m) - e_h\|_{H^2(\Omega)}^2 \right]$$

for $0 \leq n \leq N$.

Proof. Substituting the estimates of Lemma 3.5 into equation (3.8) shows that

$$|\mathbf{e}^{n+1}|^2 + \tau\|\mathbf{e}^{n+1}\|^2 \leq (1 + C\tau)|\mathbf{e}^n|^2 + C\tau^2 \int_{n\tau}^{(n+1)\tau} \|\mathbf{u}_{tt}\|^2$$
$$C\tau\|p(t^{n+1}) - q^{n+1}\|_{L^2(\Omega)} + C\tau\|\mathbf{u}(t^{n+1}) - \tilde{\mathbf{u}}(t^{n+1})\|$$

where, as before, $\mathbf{e}^{n+1} = (\tilde{u}(t^{n+1}) - u^{n+1}, \tilde{d}(t^{n+1}) - d^{n+1})$, and $q^n \in \mathcal{P}_h$ is arbitrary. The discrete Gronwall inequality shows that

$$|\mathbf{e}^n|^2 + \sum_{m=0}^{n} \tau\|\mathbf{e}^m\|^2 \leq C\exp(Cn\tau) \left(|\mathbf{e}^0|^2 + \tau^2 \sum_{m=0}^{n} \tau \left[\|p(t^m) - q^m\|_{L^2(\Omega)} + \|\hat{\mathbf{u}}(t^m) - \tilde{\mathbf{u}}(t^m)\| \right] \right)$$

The proof now follows from an application of the triangle inequality and the approximation hypothesis assumed in the theorem. □

Remark: A similar estimate can be obtained for the pressure by using the discrete Babuska–Brezzi condtion and the ideas illustrated in Section 2.2.

4. Numerical Examples. The examples below were computed on the domain $\Omega = (0,1)^2$ with uniform square meshes. The velocity was approximated using piecewise biquadratic functions and the pressure using piecewise bilinear approximations. It is well known that these velocity–pressure spaces satisfy the Babuska–Brezzi condition stated in Section 3.2. The director field was approximated using bicubic Hermite polynomials. This choice of spaces will give a first order rate of convergence with respect to the mesh size h in the norm $||.||$ whenever the solution has the appropriate regularity.

All of the examples shown below were computed on a 16×16 mesh having a total of 4779 variables, and approximately 160 steps were used per unit of time. Newton's method was used to solve the nonlinear system of equations at each time step. Typically three to four Newton iterations were required per step to solve the system, and this method of solution took approximately 6 hours on a Sun Ultra Sparc to evolve the solution through one unit of time.

Our intention is to illustrate the interesting behavior exhibited by liquid crystal flows when singularities are present. Singularities are approximated in the initial data using functions of the form $d_0(x) = x/\sqrt{|x|^2 + \eta^2}$, and in this situation the analysis of the previous section is not strictly applicable, since singular solutions can not be well approximated by the finite element interpolants. However, the solution is smooth outside of a small set, and in this situation we expect the solution to be well approximated away from this exceptional set. Except when noted, the physical constants ν, λ and γ were all set to unity. The small parameter appearing in the penalty term, f, was set to $\epsilon = 0.05$ as was the small constant η used to regularize the singularities. If η is set to be much smaller the Hermite interpolant of the initial director field would develop oscillations on the 16×16 mesh.

4.1. Simple Annihilation of Singularities. To illustrate the annihilation of singularities a zero initial velocity field was specified and an initial director field $d_0 = \hat{d}/\sqrt{|\hat{d}|^2 + \eta^2}$ where

$$\hat{d}(x) = (x^2 + y^2 - \alpha^2, 2\alpha y),$$

and $\alpha = 1/2$. This director field has singularities at $(x,y) = (\pm\alpha, 0)$ with unit degrees of opposite signs. The evolution of this solution is shown in Figure 1 where the initial and final director fields are shown and also shown is the director and velocity fields close to the annihilation time $t = 0.25$.

4.2. Annihilation of Singularities in a Rotation Flow. This next example has the same initial director field as the previous example; however, this time the initial (and boundary) velocity field was chosen to be a rotating flow of the form $u = (-\omega y, \omega x)$ with $\omega = 20$ (approximately three revolutions per unit time). Figure 2 shows the director field at four different times; the initial field, the solution at $t = 0.1$ which clearly shows how the singularities are swirled around with the flow, and the solution just prior to annihilation at $t = 0.2$ and the steady state solution. In the absence of boundary conditions the director field would tend to a parallel state.

4.3. Degree Two Data with Four Singularities. As a final example we specified a zero initial velocity field and selected the initial director field to have three degree one singularities equally spaced about a circle of radius $1/4$ and a singularity having degree -1 at the center of the circle located at $(x, y) = (1/2, 1/2)$. The degree one singularities were chosen so that the solution was symmetric about the line $y = 1/2$ as shown in Figure 3.

The solution of this problem retains this symmetry; however, the two singularities above and below the axis of symmetry move towards the singularity at the center of the circle and it in turn moves along the x–axis towards them, and eventually they all meet and join to form a single singularity of degree one. This new singularity is then "repelled" by the remaining degree one singularity so they move apart along the x–axis to an equilibrium position determined by the boundary data. This evolution occurs even in the absence of a velocity field; that is, if we set $\lambda = 0$ so that the director and velocity fields decouple, and this is shown in Figure 3. However, when $\lambda = 1$ the resulting velocity field enhances the motion of the singularities and the time of annihilation decreases from $t = 1.35$ with $\lambda = 0$ to $t = 0.9$ when $\lambda = 1$. The director and velocity fields just before and slightly after annihilation for $\lambda = 1$ are shown in Figure 4. At this latter time the velocity field exhibits a pair of vortices enhancing the repulsion of the two remaining singularities with like sign.

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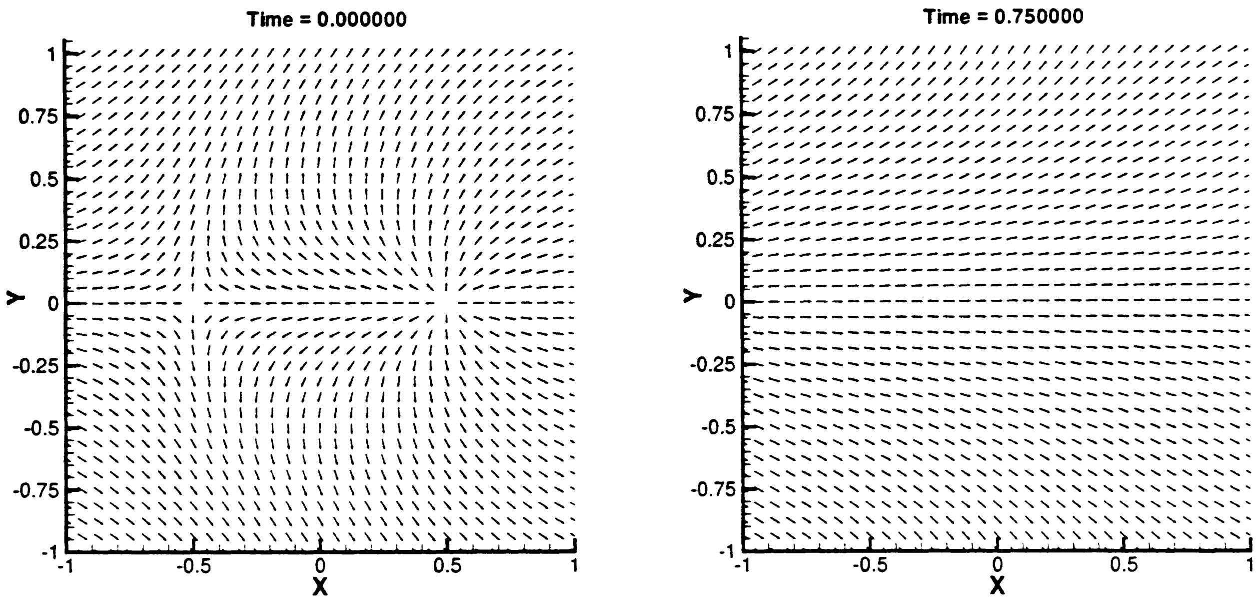
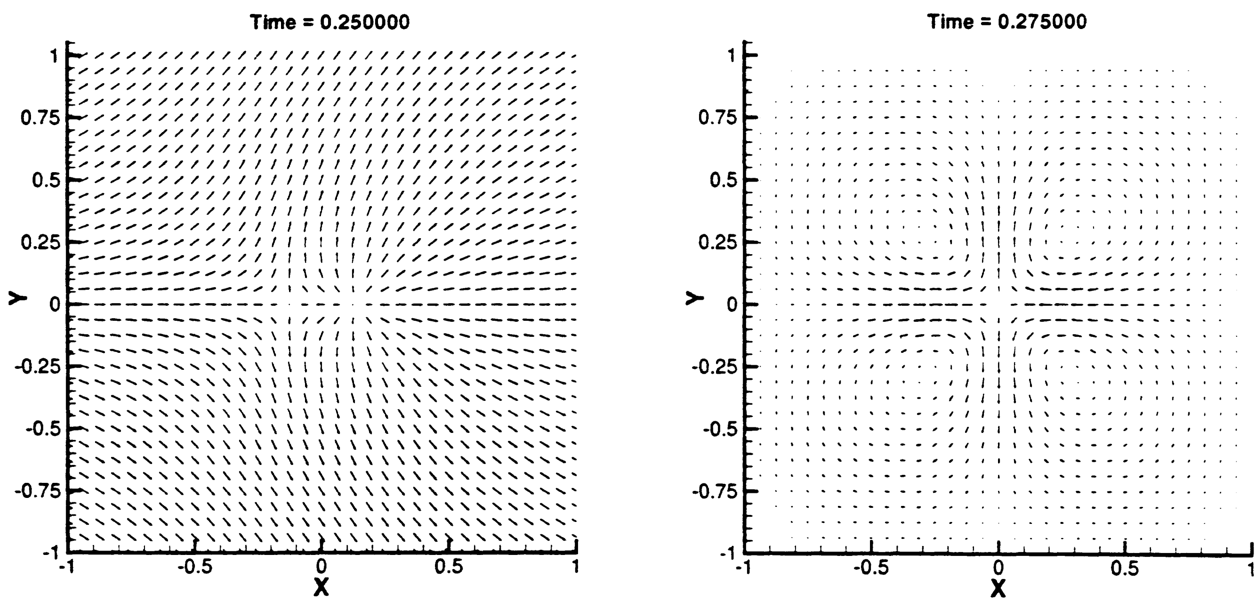


Initial (left) and Final (right) Director Fields



Director (left) and Velocity (right) Fields at Annihilation

Figure 1. Annihilation of Singularities

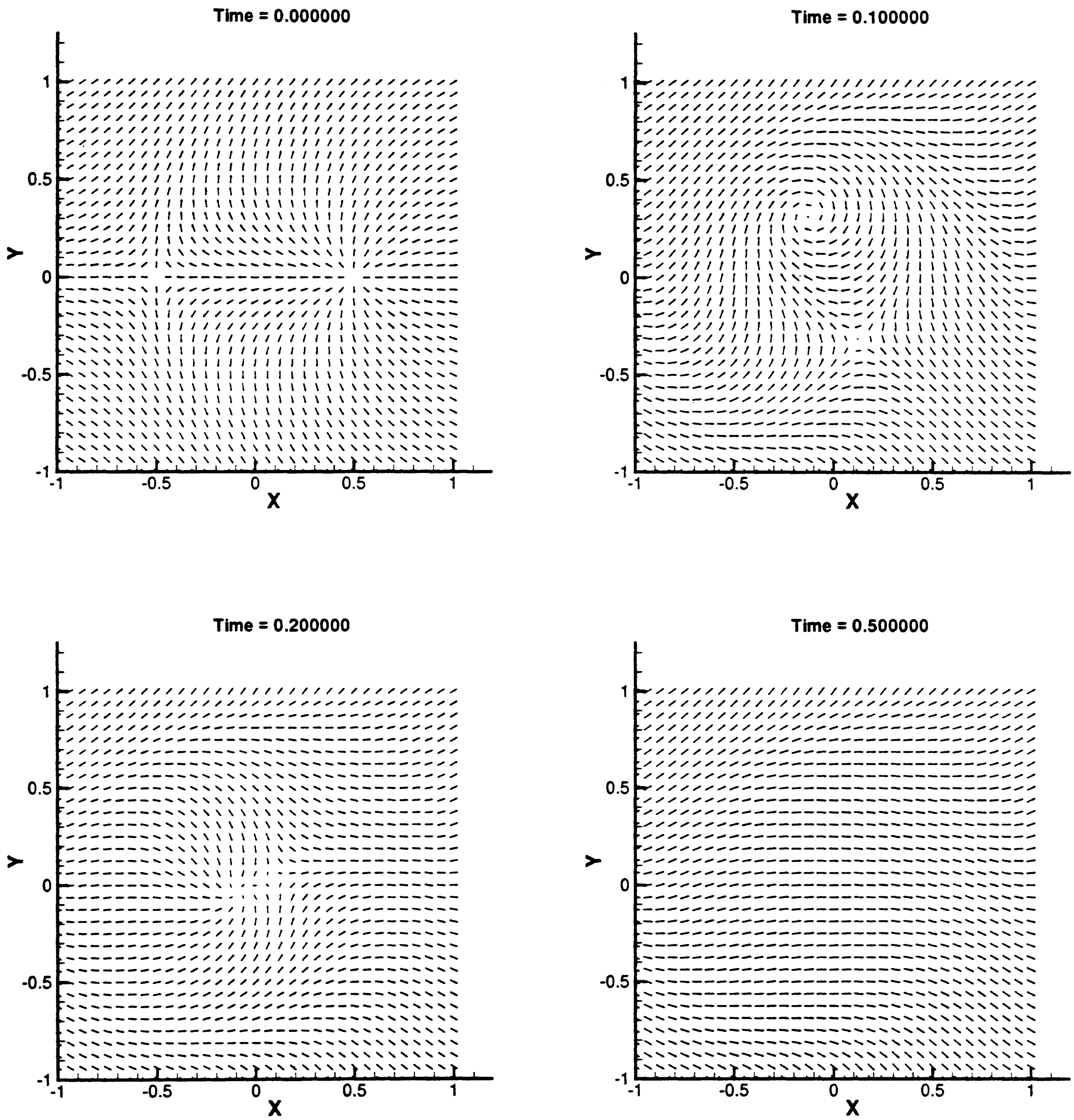


Figure 2. Annihilation of singularities in a rotating flow.

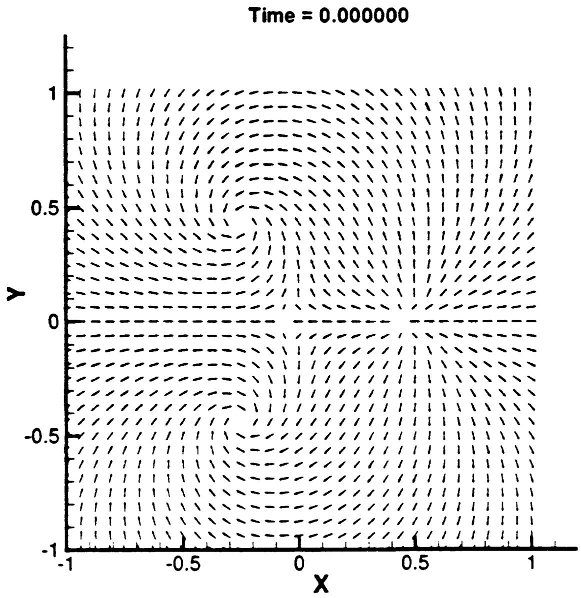


Figure 3. Four Defects with Total Degree Two
lambda = 0 (zero velocity)

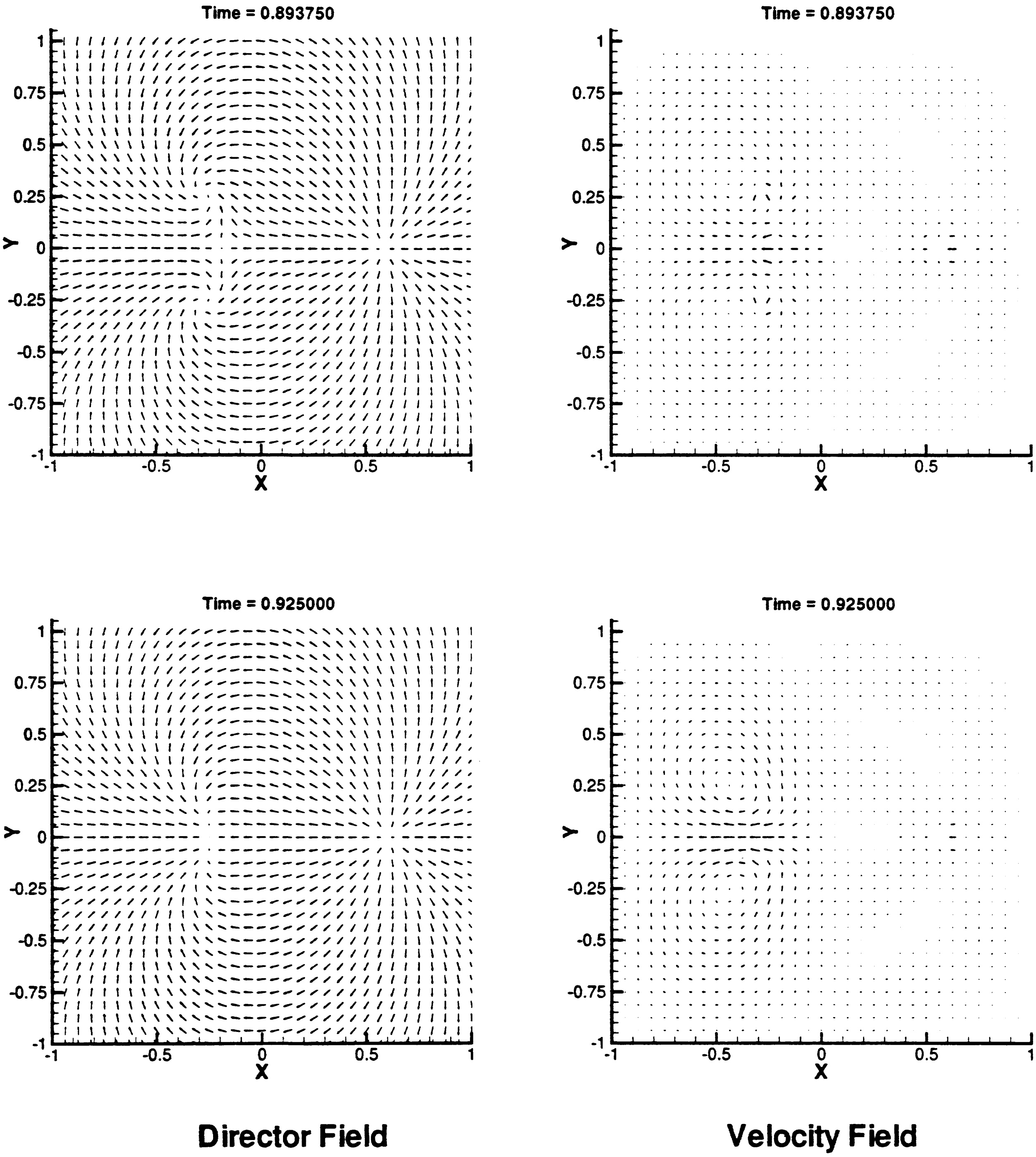


Figure 4. Four Defects with Total Degree Two Before and After Anhilation