Numerical modeling of Defect Dynamics in Nematic Liquid Crystals

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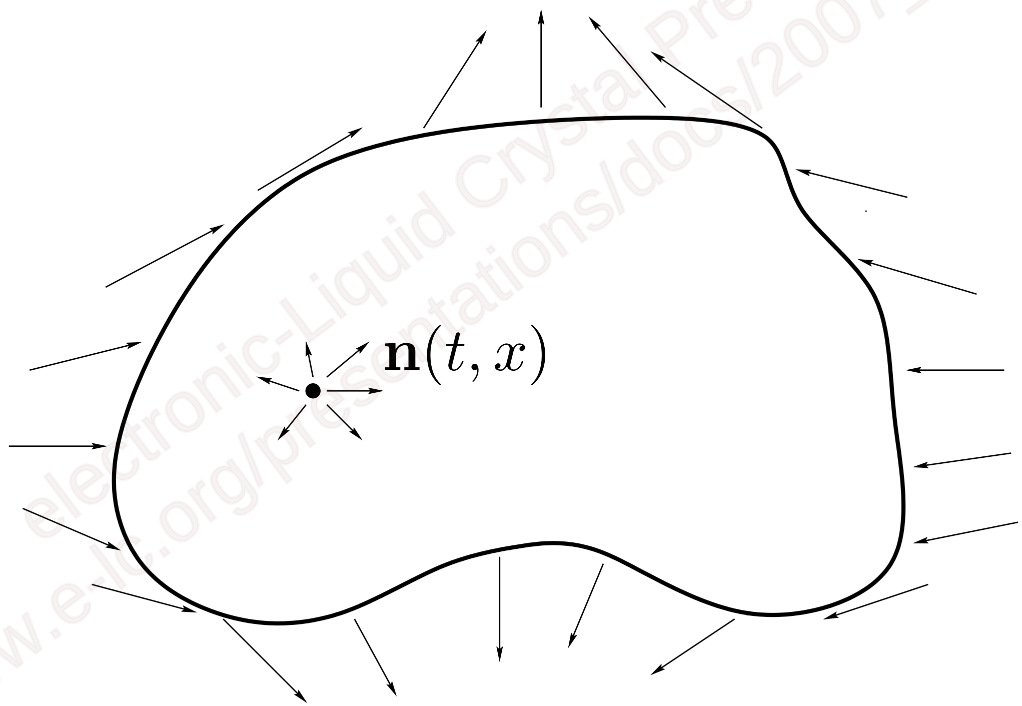
Open Problem

Harmonic Mapping Problem: Mimimize

$$I(\mathbf{n}) = \int_\Omega (1/2)|\nabla \mathbf{n}|^2, \quad \mathbf{n} \in \{\mathbf{n} \in U \mid |\mathbf{n}| = 1\}$$



Open Problem

- Numerical Approximation:

$$\mathbf{n}_h \in \mathcal{P}_k(K)^d \text{ and } |\mathbf{n}_h| = 1 \quad \Rightarrow \quad \mathbf{n}_h \text{ constant}$$

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- Lagrangian: Find a stationary value of

$$L(\mathbf{n},\theta) = \int_\Omega (1/2)|\nabla \mathbf{n}|^2 - \theta(|\mathbf{n}|^2 - 1), \qquad (\mathbf{n},\theta) \in U \times \Theta$$

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- Discrete Problem: $(\mathbf{n}_h, \theta_h)$ is a stationary value of

$$L(\mathbf{n}_h, \theta_h) = \int_\Omega (1/2)|\nabla \mathbf{n}_h|^2 - \theta_h(|\mathbf{n}_h|^2 - 1), \qquad (\mathbf{n}_h, \theta_h) \in U_h \times \Theta_h$$

where $U_h \times \Theta_h \subset U \times \Theta$ are finite element subspaces.

Open Problem

Open Problem: Let

$$\mathcal{Z}_h = \left\{ \mathbf{n}_h \in U_h \;\middle|\; \int_\Omega \theta_h (|\mathbf{n}_h|^2 - 1) = 0,\ \theta_h \in \Theta_h \right\}.$$

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Characterize the finite element spaces $U_h \times \Theta_h \subset U \times \Theta$ such that

- (Stability) If $\mathbf{n} \in U$, $|\mathbf{n}| = 1$, then

$$\inf_{\mathbf{z}_h \in \mathcal{Z}_h} \|\mathbf{n} - \mathbf{z}_h\|_U \leq C \inf_{\mathbf{n}_h \in U_h} \|\mathbf{n} - \mathbf{n}_h\|_U$$

- (Consistency) $(\mathbf{n}_h, \theta_h) \to (\mathbf{n}, \theta)$ where $(\mathbf{n}, \theta)$ is a stationary value of L on $U \times \Theta$.

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Variation: For the evolution equation consider

$$L(\mathbf{n}, \theta) = \int_0^T \int_\Omega (1/2)|\nabla \mathbf{n}|^2 + \theta \mathbf{n}.\mathbf{n}_t$$

Open Problem

Alternative: Let $\epsilon > 0$, $U_h \subset U$ and minimize

$$I_\epsilon(\mathbf{n}_h) = \int_\Omega (1/2)|\nabla \mathbf{n}_h|^2 + (1/\epsilon)^2(|\mathbf{n}_h|^2 - 1)^2 \quad \mathbf{n}_h \in U_h$$

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Problem:

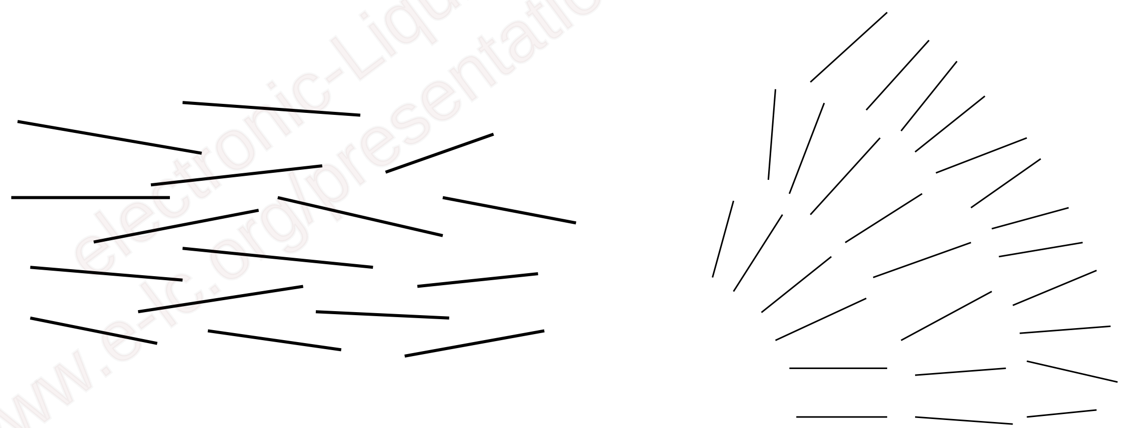
- The "best" ϵ probably depends upon the *specific problem* and h.
- For linear problems penalty methods perform terribly when compared with finite element approximations satisfying the Babuska-Brezzi conditions.

Nematic Liquid Crystal Flows

Problem: Software for solving the Ericksen Lesslie equations is not widely available.

- Experiments (interpretation, parameter identification, etc.)
- Defect Dynamics (Gartland, Sonner, Virga, & Cermelli, Fried)
- Device Design (simulation)

Nematics: Rod-like molecules with orientation $\mathbf{n}(t, x)$



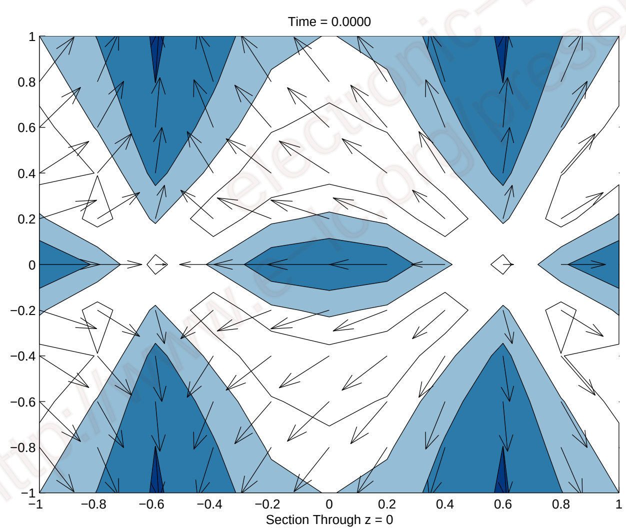
Nematic Semetic

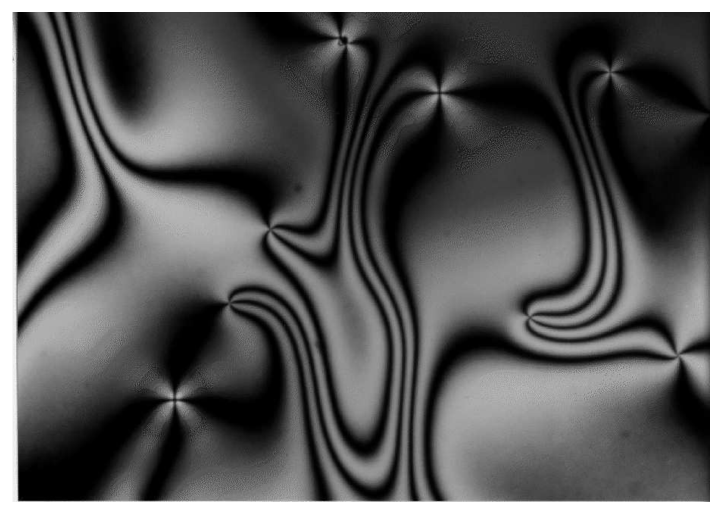
Nematic Liquid Crystal Flows

Goal: *Routine* simulation of (nematic) liquid crystal flows

Software must be

- Accurate: e.g. second order or better
- Reliable: provably correct.
- User Friendly: flexible, easy to use, 2d/3d.
- Efficient: modest run times for modest flows.
- Powerful: exploit parallelism for complex problems





Ericksen's Equations

Linear Momentum Equation:

$$\rho\dot{\mathbf{v}} - div(T) = \rho\mathbf{f}, \qquad div(\mathbf{v}) = 0,$$

Angular Momentum Equation: (short rod like molecules)

$$\rho\bar{r}^2\ddot{\mathbf{n}} + \mathbf{g} - div(C) = \rho\mathbf{m}, \qquad |\mathbf{n}| = 1.$$

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$$\rho\bar{r}^2\ddot{\mathbf{n}} + \mathbf{g} - div(C) = \rho\mathbf{m}, \qquad |\mathbf{n}| = 1.$$

- $T = -pI + T_{elastic} + T_{viscous}$ is the Cauchy stress tensor.
- $C = C_{elastic}$ is the couple tensor.
- $\mathbf{g} = \theta\mathbf{n} + \mathbf{g}_{elastic} + \mathbf{g}_{viscous}$ (cancels moments parallel to $\mathbf{n}$).

Notation: $\dot{\mathbf{n}} = \mathbf{n}_t + (\mathbf{v}.\nabla)\mathbf{n}, \qquad div(T)_i = T_{ij,j}$

Stresses and Couples

Elastic Energy: $\mathcal{W}(\mathbf{n}, \nabla\mathbf{n})$ frame indifferent

$$T_{elastic} = (\nabla\mathbf{n})^T \left[\frac{\partial\mathcal{W}}{\partial\nabla\mathbf{n}}\right] \qquad C = \left[\frac{\partial\mathcal{W}}{\partial\nabla\mathbf{n}}\right] \qquad \mathbf{g}_{elastic} = \left(\frac{\partial\mathcal{W}}{\partial\mathbf{n}}\right)$$

Oseen-Frank Energy:

$$\mathcal{W}_{OF}(\mathbf{n}, \nabla\mathbf{n}) = (k_1/2)\, div(\mathbf{n})^2 + (k_2/2)\, (\mathbf{n}.curl(\mathbf{n}) + q)^2$$
$$+(k_3/2)\, |\mathbf{n} \times curl(\mathbf{n})|^2 + (1/2)(k_2 + k_4)\, \left(tr((\nabla\mathbf{n})^2) - div(\mathbf{n})^2\right)$$

Viscous Stress: (Leslie)

$$\begin{aligned} T_{viscous} &= \alpha_1(\mathbf{n}^T D(\mathbf{v})\mathbf{n})\mathbf{n} \otimes \mathbf{n} + \alpha_2\mathbf{N} \otimes \mathbf{n} + \alpha_3\mathbf{n} \otimes \mathbf{N} \\ &\quad +\mu D(\mathbf{v}) + \alpha_5 D(\mathbf{v})\mathbf{n} \otimes \mathbf{n} + \alpha_6\mathbf{n} \otimes D(\mathbf{v})\mathbf{n} \end{aligned}$$

$$\mathbf{g}_{viscous} = (\alpha_3 - \alpha_2)\mathbf{N} + (\alpha_6 - \alpha_5)D(\mathbf{v})\mathbf{n}$$

Standard FEM

Linear Momentum:

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Angular Momentum:

$$\mathbf{g} - div(C) = \rho\mathbf{m},$$

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Natural Weak Statement:

$$\int_\Omega \rho \dot{\mathbf{v}}.\mathbf{w} + T : (\nabla \mathbf{w}) = \int_\Omega \rho \mathbf{f}.\mathbf{w},$$

$$\int_\Omega \mathbf{g}.\mathbf{e} + C : (\nabla \mathbf{e}) = \int_\Omega \rho \mathbf{m}.\mathbf{e},$$

Numerics: (i) Select a time stepping scheme
(ii) Discretize spatial variation using standard (Lagrange) FEM
(iii) Approximate the constraints . . .

Model System (Lin-Liu)

Linear Momentum:

$$\rho\dot{\mathbf{v}} - div\left(-pI + \mu D(\mathbf{v}) + k(\nabla\mathbf{n})^T(\nabla\mathbf{n})\right) = \rho\mathbf{f}, \quad div(\mathbf{v}) = 0$$

Angular Momentum:

$$\gamma\dot{\mathbf{n}} - div\,(k\nabla\mathbf{n}) + \theta\mathbf{n} = \rho\mathbf{m}, \qquad |\mathbf{n}| = 1$$

Notation:

- $\dot{\mathbf{n}} = \mathbf{n}_t + (\mathbf{v}.\nabla)\mathbf{n}$ (convective derivative)
- $(\nabla\mathbf{n})_{\alpha\beta} = \partial\mathbf{n}_\alpha/\partial x_\beta$ (gradient of a vector)
- $D(\mathbf{v}) = (1/2)\left((\nabla\mathbf{v}) + (\nabla\mathbf{v})^T\right)$ (stretching tensor)
- $div(\mathbf{v}) = v_{\beta,\beta} = \sum_\beta \partial\mathbf{v}_\beta/\partial x_\beta$ (classical divergence)
- $div(T)_\alpha = T_{\alpha\beta,\beta}$ (divergence of a tensor)

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$$\int_\Omega \rho\dot{\mathbf{v}}.\mathbf{w} - p\,div(\mathbf{w}) + \mu D(\mathbf{v}) : D(\mathbf{w}) + k(\nabla\mathbf{n})^T(\nabla\mathbf{n}) : (\nabla\mathbf{w}) = \int_\Omega \rho\mathbf{f}.\mathbf{w}$$

$$\int_\Omega \gamma\dot{\mathbf{n}}.\mathbf{e} + k(\nabla\mathbf{n}) : (\nabla\mathbf{e}) + \theta\mathbf{n}.\mathbf{e} = \int_\Omega \rho\mathbf{m}.\mathbf{e}$$

Problem: Putting $\mathbf{w} = \mathbf{v}$ and $\mathbf{e} = \mathbf{n}_t$ (or $\dot{\mathbf{n}}$) gives a mess!

Model System (Lin-Liu)

Linear Momentum: $div\big((\nabla \mathbf{n})^T(\nabla \mathbf{n})\big) = (1/2)\nabla(|\nabla \mathbf{n}|^2) + (\nabla \mathbf{n})^T \Delta \mathbf{n}$

$$\rho \dot{\mathbf{v}} - div\big(-\tilde{p}I + \mu D(\mathbf{v})\big) + k(\nabla \mathbf{n})^T \Delta \mathbf{n} = \rho \mathbf{f}$$

Angular Momentum: $div(\nabla \mathbf{n}) = \Delta \mathbf{n}$

$$\gamma \dot{\mathbf{n}} - k\Delta \mathbf{n} + \theta \mathbf{n} = \rho \mathbf{m}$$

Alternative Weak Statement

$$\int_\Omega \rho \dot{\mathbf{v}}.\mathbf{w} - \tilde{p}\, div(\mathbf{w}) + \mu D(\mathbf{v}) : D(\mathbf{w}) + k\Delta \mathbf{n}.(\mathbf{w}.\nabla)\mathbf{n} = \int_\Omega \rho \mathbf{f}.\mathbf{w}$$

$$\int_\Omega \gamma \dot{\mathbf{n}}.\mathbf{e} - k\Delta \mathbf{n}.\mathbf{e} + \theta \mathbf{n}.\mathbf{e} = \int_\Omega \rho \mathbf{m}.\mathbf{e}$$

Model System (Lin-Liu)

Put $\mathbf{w} = \mathbf{v}$ and $\mathbf{e} = \dot{\mathbf{n}}$

$$\frac{d}{dt}\int_\Omega (\rho/2)|\mathbf{v}|^2 + \int_\Omega \mu|D(\mathbf{v})|^2 + k\Delta\mathbf{n}.(\mathbf{v}.\nabla)\mathbf{n} = \int_\Omega \rho\mathbf{f}.\mathbf{v}$$

$$\int_\Omega \gamma|\dot{\mathbf{n}}|^2 - k\Delta\mathbf{n}.\left(\mathbf{n}_t + (\mathbf{v}.\nabla)\mathbf{n}\right) + \theta\mathbf{n}.\dot{\mathbf{n}} = \int_\Omega \rho\mathbf{m}.\dot{\mathbf{n}}$$

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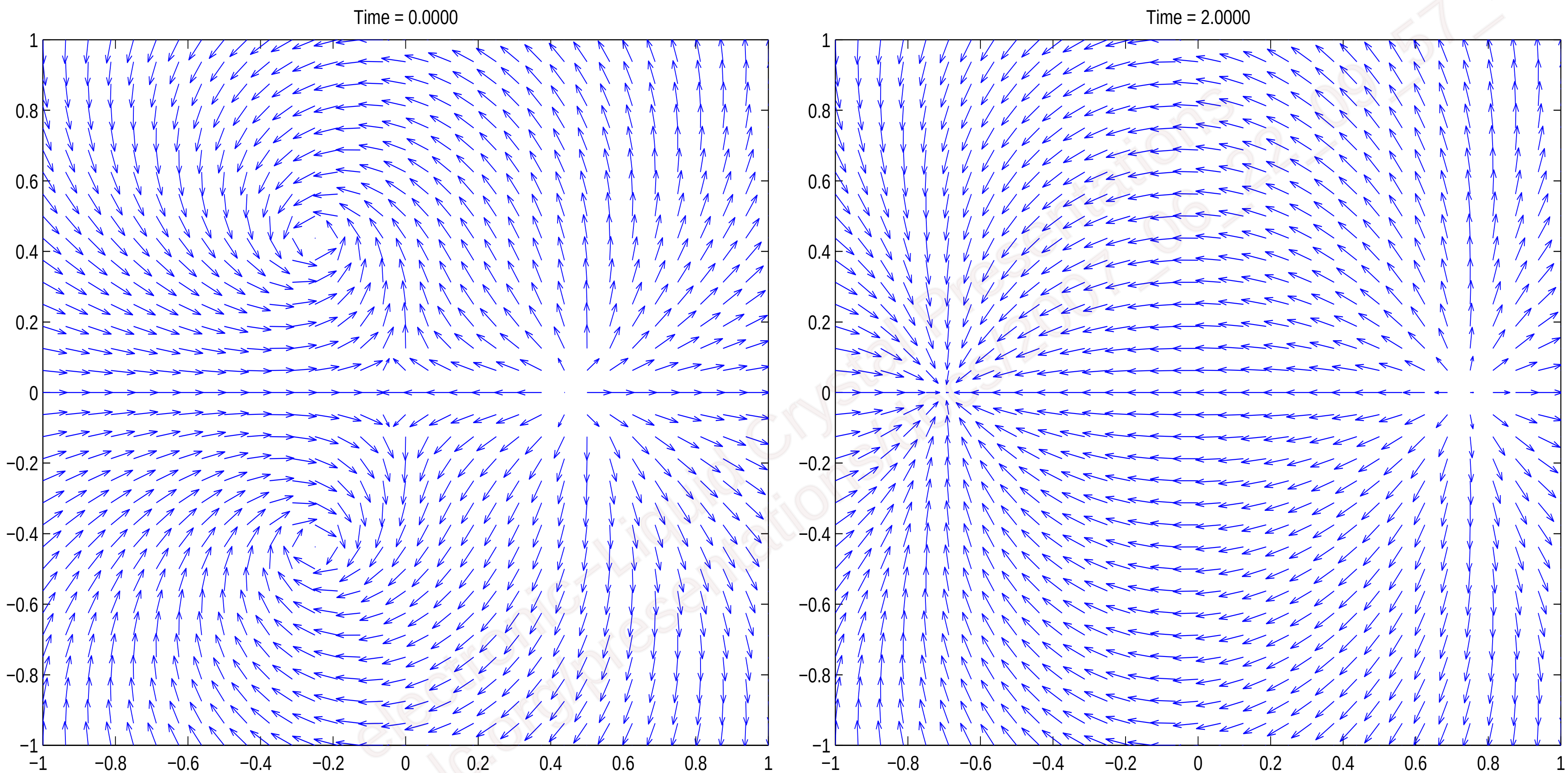
Energy Estimate:

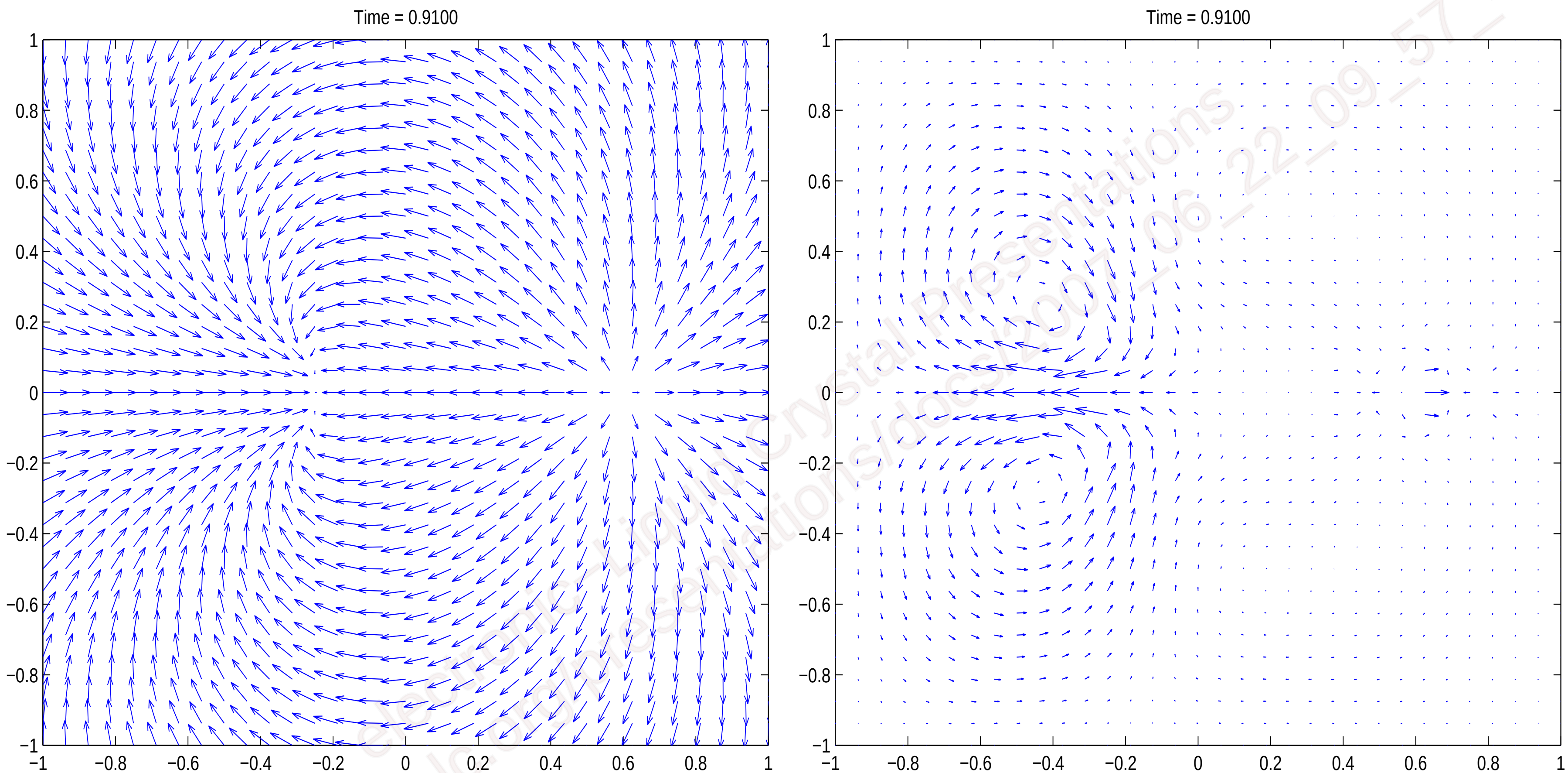
$$\frac{d}{dt}\int_\Omega \left\{(\rho/2)|\mathbf{v}|^2 + (k/2)|\nabla\mathbf{n}|^2\right\} + \int_\Omega \left\{\mu|D(\mathbf{v})|^2 + \gamma|\dot{\mathbf{n}}|^{\mathbf{2}}\right\} = \int_\Omega \rho\left(\mathbf{f}.\mathbf{v} + \mathbf{m}.\dot{\mathbf{n}}\right)$$

Simulation of Singularities



Evolution of three degree $+1$ singularities surrounding a degree -1 singularity.

Simulation of Singularities



Director field and backflow near the annihilation time.

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Numerical Issues:

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- To date, only the implicit Euler time stepping scheme has been considered.
- Extension to the full Ericksen Leslie system?

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Linear Momentum:

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Angular Momentum:

$$\gamma\dot{\mathbf{n}} - k\Delta\mathbf{n} + \theta\mathbf{n} = \rho\mathbf{m}$$

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Eliminate $k\Delta\mathbf{n}$ from the momentum equation

Linear Momentum:

$$\rho\dot{\mathbf{v}} - div\big(-\tilde{p}I + \mu D(\mathbf{v})\big) + (\nabla\mathbf{n})^T(\gamma\dot{\mathbf{n}} - \rho\mathbf{m}) = \rho\mathbf{f}$$

Angular Momentum:

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Model System (Lin-Liu)

Weak Statement:

$$\int_\Omega \Big\{\rho\dot{\mathbf{v}}.\mathbf{w} - \tilde{p}\, div(\mathbf{w}) + \mu D(\mathbf{v}) : D(\mathbf{w})$$

$$+\left(\gamma\dot{\mathbf{n}} - \rho\mathbf{m}\right).(\mathbf{w}.\nabla)\mathbf{n}\Big\} = \int_\Omega \rho\mathbf{f}.\mathbf{w}$$

$$\int_\Omega \gamma\dot{\mathbf{n}}.\mathbf{e} + k(\nabla\mathbf{n}) : (\nabla\mathbf{e}) + \theta\mathbf{n}.\mathbf{e} = \int_\Omega \rho\mathbf{m}.\mathbf{e}$$

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$$\int_\Omega \gamma\dot{\mathbf{n}}.\mathbf{e} + k(\nabla\mathbf{n}) : (\nabla\mathbf{e}) + \theta\mathbf{n}.\mathbf{e} = \int_\Omega \rho\mathbf{m}.\mathbf{e}$$

Energy Estimate: Put $\mathbf{w} = \mathbf{v}$ and $\mathbf{e} = \mathbf{n}_t$

$$\frac{d}{dt}\int_\Omega \{(\rho/2)|\mathbf{v}|^2 + (k/2)|\nabla\mathbf{n}|^2\}$$

$$+ \int_\Omega \{\mu|D(\mathbf{v})|^2 + \gamma|\dot{\mathbf{n}}|^{\mathbf{2}}\} = \int_\Omega \rho\,(\mathbf{f}.\mathbf{v} + \mathbf{m}.\dot{\mathbf{n}})$$

Model System (Lin-Liu)

Numerical Schemes

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    Lowest order DG scheme is implicit Euler

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  - If stability follows upon setting $\mathbf{e} = \mathbf{d}_t$ then use CG

    Lowest order CG scheme is the trapezoid rule
- Solutions of the numerical scheme are bounded independently of ϵ

Model System (Lin-Liu)

DG Scheme: $\mathbf{v}, \mathbf{w} \in \mathcal{P}_\ell(t^{n-1}, t^n, V_h)$

$$\int_{t^{n-1}}^{t^n} \int_\Omega \Big\{ \rho \dot{\mathbf{v}}.\mathbf{w} \quad - \quad \tilde{p}\, div(\mathbf{w}) + \mu D(\mathbf{v}) : D(\mathbf{w}) + (\gamma \dot{\mathbf{n}} - \rho \mathbf{m}).(\mathbf{w}.\nabla)\mathbf{n} \Big\}$$

$$+ \quad \int_\Omega (\mathbf{v}_+^{n-1} - \mathbf{v}_-^{n-1}).\mathbf{w}_+^{n-1} = \int_{t^{n-1}}^{t^n} \int_\Omega \rho \mathbf{f}.\mathbf{w}$$

Pressure: $p, q \in \mathcal{P}_\ell(t^{n-1}, t^n, P_h)$

$$\int_{t^{n-1}}^{t^n} \int_\Omega div(\mathbf{v}) q = 0$$

CG Scheme: $\mathbf{d} \in \mathcal{P}_\ell(t^{n-1}, t^n, D_h)$ but $\mathbf{e} \in \mathcal{P}_{\ell-1}(t^{n-1}, t^n, D_h)$

$$\int_{t^{n-1}}^{t^n} \int_\Omega \gamma \dot{\mathbf{n}}.\mathbf{e} + k(\nabla \mathbf{n}) : (\nabla \mathbf{e}) + DF(\mathbf{d}).\mathbf{e} = \int_{t^{n-1}}^{t^n} \int_\Omega \rho \mathbf{m}.\mathbf{e}$$

Ericksen Leslie Equations

$$\rho\dot{\mathbf{v}} - div\,(-pI + T_v + T_e) = \rho\mathbf{f}, \qquad \mathbf{g}_v + \mathbf{g}_e - div(C) + \theta\mathbf{n} = \rho\mathbf{m}$$

Elastic Terms:

$$T_e = (\nabla\mathbf{n})^T \left[\frac{\partial\mathcal{W}}{\partial\nabla\mathbf{n}}\right] \qquad C = \left[\frac{\partial\mathcal{W}}{\partial\nabla\mathbf{n}}\right] \quad \mathbf{g}_e = \left(\frac{\partial\mathcal{W}}{\partial\mathbf{n}}\right)$$

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Crucial Identity:

$$div\left((\nabla\mathbf{n})^T\left[\frac{\partial\mathcal{W}}{\partial\nabla\mathbf{n}}\right]\right) = \nabla\mathcal{W}(\mathbf{n},\nabla\mathbf{n}) + (\nabla\mathbf{n})^T\left(div\left[\frac{\partial\mathcal{W}}{\partial\nabla\mathbf{n}}\right] - \left(\frac{\partial\mathcal{W}}{\partial\mathbf{n}}\right)\right),$$

or

$$\begin{aligned} div(T_e) &= \nabla\mathcal{W}(\mathbf{n},\nabla\mathbf{n}) + (\nabla\mathbf{n})^T\left(div(C) - \mathbf{g}_e\right) \\ &= \nabla\mathcal{W}(\mathbf{n},\nabla\mathbf{n}) + (\nabla\mathbf{n})^T\left(\mathbf{g}_v - \rho\mathbf{m} + \theta\mathbf{n}\right) \end{aligned}$$

Ericksen Leslie Equations

Linear Momentum:

$$\rho \dot{\mathbf{v}} - div\left(-\tilde{p}I + T_v\right) + (\nabla \mathbf{n})^T \left(\mathbf{g}_v - \rho \mathbf{m}\right) = \rho \mathbf{f}$$

Angular Momentum:

$$\mathbf{g}_v + \left(\frac{\partial \mathcal{W}}{\partial \mathbf{n}}\right) - div\left(\left[\frac{\partial \mathcal{W}}{\partial \nabla \mathbf{n}}\right]\right) + \theta \mathbf{n} = \rho \mathbf{m}$$

Weak Statement

$$\int_\Omega \left\{ \rho \dot{\mathbf{v}}.\mathbf{w} - \tilde{p}\, div(\mathbf{w}) + T_v : (\nabla \mathbf{w}) + \left(\mathbf{g}_v - \rho \mathbf{m}\right).(\mathbf{w}.\nabla)\mathbf{n} \right\} = \int_\Omega \rho \mathbf{f}.\mathbf{w}$$

$$\int_\Omega \left\{ \mathbf{g}_v.\mathbf{e} + \left(\frac{\partial \mathcal{W}}{\partial \mathbf{n}}\right).\mathbf{e} + \left[\frac{\partial \mathcal{W}}{\partial \nabla \mathbf{n}}\right] : (\nabla \mathbf{e}) + \theta \mathbf{n}.\mathbf{e} \right\} = \int_\Omega \rho \mathbf{m}.\mathbf{e}$$

Ericksen Leslie Equations

Energy Estimate: Put $\mathbf{w} = \mathbf{v}$ and $\mathbf{e} = \mathbf{n}_t$

$$\frac{d}{dt}\int_\Omega \left((\rho/2)|\mathbf{v}|^2 + \mathcal{W}(\mathbf{n}, \nabla\mathbf{n})\right)$$

$$+ \int_\Omega (T_v : (\nabla\mathbf{v}) + \mathbf{g}_v.\dot{\mathbf{n}}) = \int_\Omega \rho\,(\mathbf{f}.\mathbf{v} + \mathbf{m}.\dot{\mathbf{n}})$$

Viscous Terms:

$$T_v : (\nabla\mathbf{v}) + \mathbf{g}_v.\dot{\mathbf{n}}$$

$$\geq \quad \mu|D(\mathbf{v})|^2 + \alpha_1|\mathbf{n}^T D(\mathbf{v})\mathbf{n}|^2 + \gamma\left(|\mathbf{N}|^2 + |D(\mathbf{v})\mathbf{n}|^2\right)$$

where $\mathbf{N} = \dot{\mathbf{n}} - W(\mathbf{v})\mathbf{n}$

Ericksen Leslie Equations

Penalized Weak Statement $\mathbf{n} \sim \mathbf{d}$

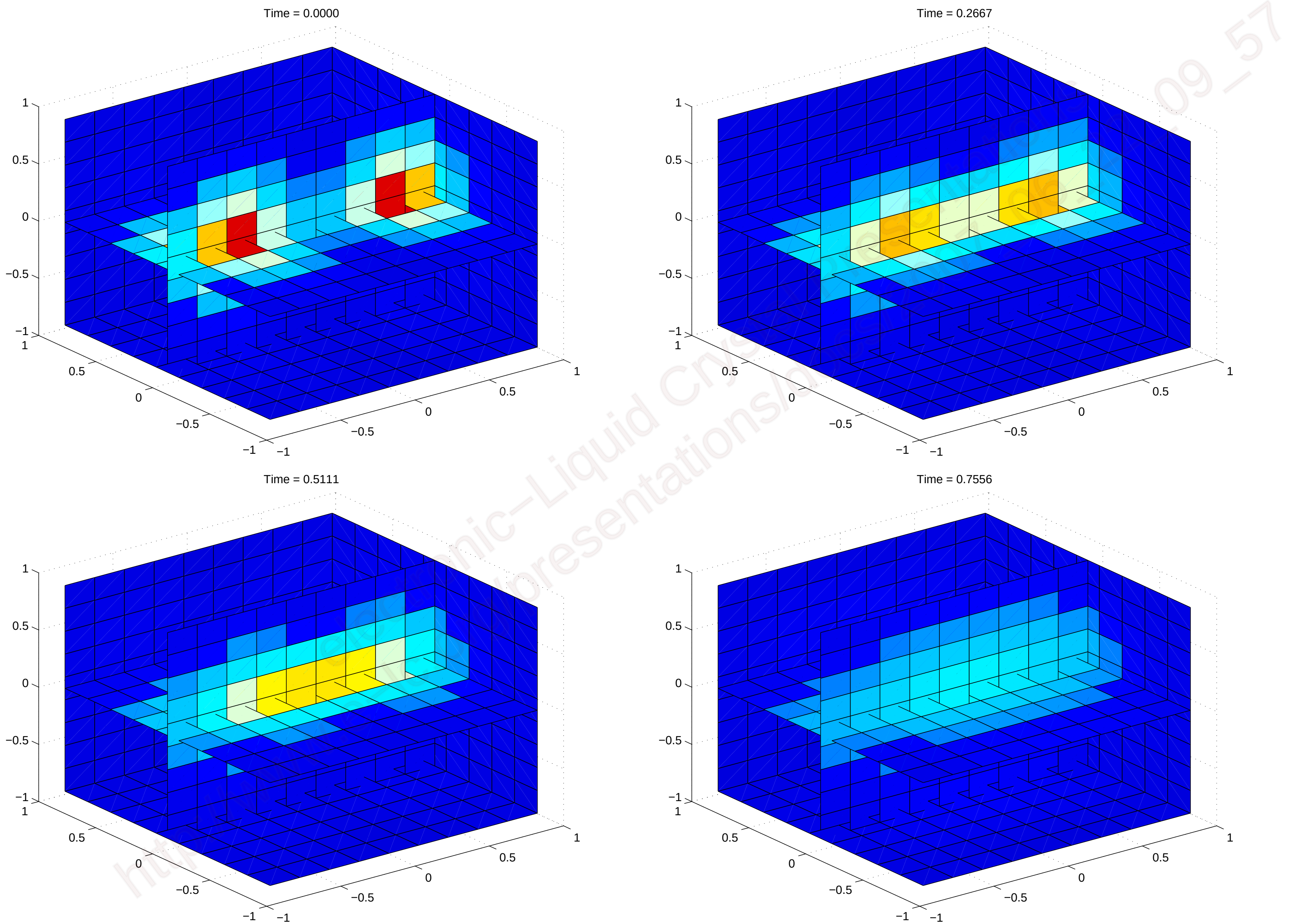
$$\int_\Omega \left\{ \rho \dot{\mathbf{v}}.\mathbf{w} - \tilde{p}\, div(\mathbf{w}) + T_v : (\nabla \mathbf{w}) + (g_v - \rho \mathbf{m}) .(\mathbf{w}.\nabla)\mathbf{d} \right\} = \int_\Omega \rho \mathbf{f}.\mathbf{w}$$

$$\int_\Omega \left\{ \mathbf{g}_v.\mathbf{e} + \left(\frac{\partial \mathcal{W}}{\partial \mathbf{d}} \right).\mathbf{e} + \left[\frac{\partial \mathcal{W}}{\partial \nabla \mathbf{d}} \right] : (\nabla \mathbf{e}) + DF(\mathbf{d}).\mathbf{e} \right\} = \int_\Omega \rho \mathbf{m}.\mathbf{e}$$

Penalized Energy Estimate: Put $\mathbf{w} = \mathbf{v}$ and $\mathbf{e} = \mathbf{d}_t$

$$\frac{d}{dt} \int_\Omega \left((\rho/2)|\mathbf{v}|^2 + \mathcal{W}(\mathbf{d}, \nabla \mathbf{d}) + F(\mathbf{d}) \right)$$
$$+ \int_\Omega \left\{ \mu |D(\mathbf{v})|^2 + \alpha_1 |\mathbf{d}^T D(\mathbf{v})\mathbf{d}|^2 + \gamma \left(|\mathbf{N}|^2 + |D(\mathbf{v})\mathbf{d}|^2 \right) \right\}$$
$$\leq \int_\Omega \rho \left(\mathbf{f}.\mathbf{v} + \mathbf{m}.\dot{\mathbf{d}} \right)$$

Annihilation of Singularities



Annihilation of Singularities