# Story on the Ericksen-Leslie system of liquid crystal with and without the penalty function

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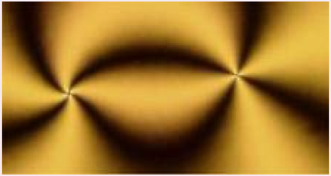
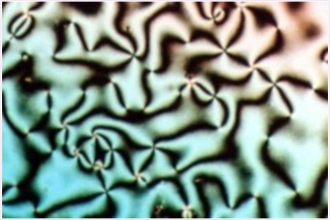
# outline


1. Ericksen-Leslie system with penalty function
2. modelling
3. Numerical Method
   - $C^0$ finite element method
   - Simple case: "1+2" model
   - Numerical results and discussion
4. Ericksen-Leslie system without penalty function
   - Energy stable scheme
   - Numerical results and discussion
5. Conclusions

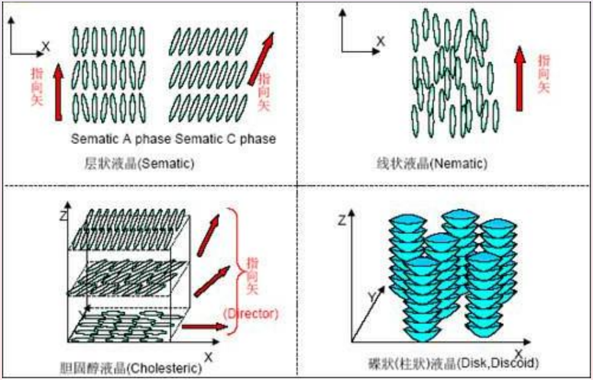
# Liquid crystal: vortex





# Liquid crystal: a very important type of complex fluids

Main types of liquid crystal:



# Transport of directors

- Define :

  $\mathbf{X}$ Lagrangian coordinate
  $\mathbf{x}$ Eulerian coordinate
  F $\frac{\partial \mathbf{x}}{\partial \mathbf{X}}$
  $\mathbf{u}$ velocity of the liquid crystal flow

- Transport of $F$ (Chain Rule):

$$F_t + \mathbf{u} \cdot \nabla F = \nabla \mathbf{u} \cdot F$$

- Transport of $F^{-T}$:

$$F_t^{-T} + \mathbf{u} \cdot \nabla F^{-T} = -(\nabla \mathbf{u})^T \cdot F^{-T}$$

# Transport of directors

- For rodlike shape:

$$\mathbf{d}(\mathbf{x}, t) = F \cdot \mathbf{d}_0(\mathbf{X})$$

$$\mathbf{d}_t + \mathbf{u} \cdot \nabla \mathbf{d} = \frac{\mathrm{d}}{\mathrm{dt}} F \cdot \mathbf{d}_0(X) = (\nabla \mathbf{u}) F \cdot \mathbf{d}_0(X) = (\nabla \mathbf{u}) \mathbf{d}$$

- For disklike shape:

$$\mathbf{d}(\mathbf{x}, t) = F^{-T} \mathbf{d}_0(\mathbf{X})$$

$$\mathbf{d}_t + \mathbf{u} \cdot \nabla \mathbf{d} = \frac{\mathrm{d}}{\mathrm{dt}} F^{-T} \cdot \mathbf{d}_0(\mathbf{X}) = -(\nabla \mathbf{u})^T F^{-T} \cdot \mathbf{d}_0(\mathbf{X}) = -(\nabla \mathbf{u})^T \mathbf{d}$$

# Transport of directors

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# Transport of directors

For $E$ generated by $-(\beta\nabla\mathbf{u} + (1+\beta)(\nabla\mathbf{u})^T)$ where $-1 \leq \beta \leq 0$

$$\frac{\mathrm{d}}{\mathrm{dt}}E = -(\beta\nabla\mathbf{u} + (1+\beta)(\nabla\mathbf{u})^T)E$$

and $\mathbf{d}$ transported by

$$\mathbf{d}(\mathbf{x}, t) = E \cdot \mathbf{d}_0(\mathbf{X})$$

we have

$$\mathbf{d}_t + \mathbf{u}\cdot\nabla\mathbf{d} = \frac{\mathrm{d}}{\mathrm{dt}}E \cdot \mathbf{d}_0(\mathbf{X}) = -(\beta\nabla\mathbf{u} + (1+\beta)(\nabla\mathbf{u})^T)\mathbf{d}$$

*G. B. Jeffery, The Motion of Ellipsoidal Particles Immersed in a Viscous Fluid, Proceeding of Royal Society of London, 1922.*

## Transport of directors

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# Coupled system

$$
\begin{aligned}
&\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} + \nabla p - \nu \Delta \mathbf{u} - \lambda \nabla \cdot \Big( (\nabla \mathbf{d})^T (\nabla \mathbf{d}) \\
&\qquad\qquad + \beta(\Delta \mathbf{d} - \mathbf{f}(\mathbf{d}))\mathbf{d}^T + (\beta + 1)\mathbf{d}(\Delta \mathbf{d} - \mathbf{f}(\mathbf{d}))^T \Big) = 0 \\
&\nabla \cdot \mathbf{u} = 0 \\
&\frac{\partial \mathbf{d}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{d} + (\beta \nabla \mathbf{u} + (1+\beta)(\nabla \mathbf{u})^T)\mathbf{d} - \gamma(\Delta \mathbf{d} - \mathbf{f}(\mathbf{d})) = 0
\end{aligned}
$$

With initial and boundary conditions:

$$
\mathbf{u}|_{t=0} = \mathbf{u}_0, \quad \mathbf{d}|_{t=0} = \mathbf{d}_0, \quad \mathbf{u}|_{\partial\Omega} = \mathbf{u}_0|_{\partial\Omega} = \mathbf{g}_{\mathbf{u}}, \quad \mathbf{d}|_{\partial\Omega} = \mathbf{d}_0|_{\partial\Omega} = \mathbf{g}_{\mathbf{d}}.
$$

where $\quad \mathbf{f}(\mathbf{d}) = (1/\epsilon^2)(|\mathbf{d}|^2 - 1)\mathbf{d}$

# Energy law

Independent to the parameter $\beta$, we have energy law

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

where

$$E = \frac{1}{2}\|\mathbf{u}\|^2_{L^2(\Omega)} + \frac{\lambda}{2}\|\nabla \mathbf{d}\|^2_{L^2(\Omega)} + \lambda\int_\Omega F(\mathbf{d})\mathrm{dx}$$

and $F = \frac{1}{4\epsilon^2}(|\mathbf{d}|^2 - 1)^2$

# About the energy law

- These energy laws are particularly important when the singularities are involved in our study of hydrodynamical motions of these liquid crystal materials. The physical singularities we are seeking/tracking are those energetically admissible ones.
- For this reason, one of the crucial problems in solving the system is that how to preserving the energy law.

# Reformulated energy law

$$\frac{\mathrm{d}}{\mathrm{dt}}E = -\left(\nu\|\nabla\mathbf{u}\|^2_{L^2(\Omega)} + \frac{\lambda}{\gamma}\|\mathbf{d}_t + (\mathbf{u}\cdot\nabla)\mathbf{d}\|^2_{L^2(\Omega)}\right)$$

where

$$E = \frac{1}{2}\|\mathbf{u}\|^2_{L^2(\Omega)} + \frac{\lambda}{2}\|\nabla\mathbf{d}\|^2_{L^2(\Omega)} + \lambda\int_\Omega F(\mathbf{d})\mathrm{dx}$$

make $C^0$ finite element method feasible.

*Ping Lin, Chun Liu, Hui Zhang, J. Comp. Phys., 227 (2007), 1411-1427*

# Weak formulation and continuous energy law

From the director equation we can express:

$$\Delta \mathbf{d} = \frac{1}{\gamma}\left(\mathbf{d}_t + (\mathbf{u}\cdot\nabla)\mathbf{d} + (D_\beta(\mathbf{u}))\mathbf{d} + \gamma \mathbf{f}(\mathbf{d})\right)$$

where $D_\beta(\mathbf{u}) = \beta\nabla\mathbf{u} + (\beta+1)(\nabla\mathbf{u})^T$, we then have

$$\begin{aligned}
\nabla\cdot\Big((\nabla\mathbf{d})^T\nabla\mathbf{d}\Big) &= \frac{1}{\gamma}(\nabla\mathbf{d})^T\left(\mathbf{d}_t + (\mathbf{u}\cdot\nabla)\mathbf{d} + D_\beta(\mathbf{u})\mathbf{d}\right) + \nabla\left(|\nabla\mathbf{d}|^2/2 + F(\mathbf{d})\right)\\
\nabla\cdot\Big((\Delta\mathbf{d} - \mathbf{f}(\mathbf{d})\mathbf{d}^T)\Big) &= \frac{1}{\gamma}\nabla\cdot\Big((\mathbf{d}_t + (\mathbf{u}\cdot\nabla)\mathbf{d} + D_\beta(\mathbf{u})\mathbf{d})\mathbf{d}^T\Big)\\
\nabla\cdot\Big(\mathbf{d}(\Delta\mathbf{d} - \mathbf{f}(\mathbf{d}))^T\Big) &= \frac{1}{\gamma}\nabla\cdot\Big(\mathbf{d}(\mathbf{d}_t + (\mathbf{u}\cdot\nabla)\mathbf{d} + D_\beta(\mathbf{u})\mathbf{d})^T\Big)
\end{aligned}$$

# Weak formulation

Find $\mathbf{u} \in \mathbf{W}^{1,2+\sigma}_{\mathbf{g_u}}(\Omega)$, $p \in \mathbf{L}^2_0(\Omega)$, $\mathbf{d} \in \mathbf{W}^{1,2+\sigma}_{\mathbf{g_d}}(\Omega)$ such that

$$
\begin{aligned}
&\int_\Omega \Big( \mathbf{u}_t \cdot \mathbf{v} + (\mathbf{u}\cdot\nabla)\mathbf{u}\cdot\mathbf{v} - p(\nabla\cdot\mathbf{v}) + \nu\nabla\mathbf{u} : \nabla\mathbf{v} + \frac{\lambda}{\gamma}\left(\mathbf{d}_t + (\mathbf{u}\cdot\nabla)\mathbf{d} + D_\beta(\mathbf{u})\mathbf{d}\right)\cdot(\mathbf{v}\cdot\nabla)\mathbf{d} \\
&\qquad\qquad + \frac{\lambda}{\gamma}\left(\mathbf{d}_t + (\mathbf{u}\cdot\nabla)\mathbf{d} + D_\beta(\mathbf{u})\mathbf{d}\right)\cdot D_\beta(\mathbf{v})\mathbf{d}\Big)\,\mathrm{dx} = 0, \qquad \forall \mathbf{v} \in \mathbf{W}^{1,2+\sigma}_0(\Omega) \\
&\int_\Omega (\nabla\cdot\mathbf{u})q\,\mathrm{dx} = 0, \qquad \forall q \in L^2(\Omega) \\
&\int_\Omega \left(\mathbf{d}_t\cdot\mathbf{e} + (\mathbf{u}\cdot\nabla)\mathbf{d}\cdot\mathbf{e} + D_\beta(\nabla\mathbf{u})\mathbf{d}\cdot\mathbf{e} + \gamma(\nabla\mathbf{d} : \nabla\mathbf{e} + \mathbf{f}(\mathbf{d})\cdot\mathbf{e})\right)\mathrm{dx} = 0, \qquad \forall \mathbf{e} \in \mathbf{W}^{1,2+\sigma}_0
\end{aligned}
$$

where ":" represents an inner product of two matrices.

Energy law can be easily obtained by taking $\mathbf{v} = \mathbf{u}$ and $\mathbf{e} = (\lambda/\gamma)\mathbf{d}_t$.

# A modified midpoint scheme

$$\int_\Omega \Big( \mathbf{u}_{\bar t}^{n+1}\cdot\mathbf{v} + (\mathbf{u}_h^{n+\frac12}\cdot\nabla)\mathbf{u}_h^{n+\frac12}\cdot\mathbf{v} + \frac12(\nabla\cdot\mathbf{u}_h^{n+\frac12})\mathbf{u}_h^{n+\frac12}\cdot\mathbf{v} - p_h^{n+\frac12}(\nabla\cdot\mathbf{v}) + \nu\nabla\mathbf{u}_h^{n+\frac12} : \nabla\mathbf{v}$$
$$+\frac{\lambda}{\gamma}\Big(\mathbf{d}_{\bar t}^{n+1} + (\mathbf{u}_h^{n+\frac12}\cdot\nabla)\mathbf{d}_h^{n+\frac12} + D_\beta(\mathbf{u}_h^{n+\frac12})\mathbf{d}_h^{n+\frac12}\Big)\cdot(\mathbf{v}\cdot\nabla)\mathbf{d}_h^{n+\frac12}$$
$$+\frac{\lambda}{\gamma}\Big(\mathbf{d}_{\bar t}^{n+1} + (\mathbf{u}_h^{n+\frac12}\cdot\nabla)\mathbf{d}_h^{n+\frac12} + D_\beta(\mathbf{u}_h^{n+\frac12})\mathbf{d}_h^{n+\frac12}\Big)\cdot D_\beta(\mathbf{v})\mathbf{d}_h^{n+\frac12}\Big)\,\mathrm{dx} = 0, \quad (4$$

$$\int_\Omega (\nabla\cdot\mathbf{u}_h^{n+\frac12})q\,\mathrm{dx} = 0, \quad (5$$

$$\int_\Omega \Big(\mathbf{d}_{\bar t}^{n+1}\cdot\mathbf{e} + (\mathbf{u}_h^{n+\frac12}\cdot\nabla)\mathbf{d}_h^{n+\frac12}\cdot\mathbf{e} + D_\beta(\mathbf{u}_h^{n+\frac12})\mathbf{d}_h^{n+\frac12}\cdot\mathbf{e}$$
$$+\gamma\nabla\mathbf{d}_h^{n+\frac12} : \nabla\mathbf{e} + \frac{\gamma}{\epsilon^2}\mathbf{g}_h(\mathbf{d}_n^n, \mathbf{d}_h^{n+1})\cdot\mathbf{e}\Big)\,\mathrm{dx} = 0, \quad (6$$

for all $(\mathbf{v}, q, \mathbf{e}) \in \mathcal{W}_0^h$, where $\mathbf{u}_{\bar t}^{n+1} = \frac{\mathbf{u}_h^{n+1}-\mathbf{u}_h^n}{\Delta t}$, $\mathbf{d}_{\bar t}^{n+1} = \frac{\mathbf{d}_h^{n+1}-\mathbf{d}_h^n}{\Delta t}$, $\mathbf{u}_h^{n+\frac12} = \frac12(\mathbf{u}_h^{n+1}+\mathbf{u}_h^n)$, $\mathbf{d}_h^{n+\frac12} = \frac12(\mathbf{d}_h^{n+1}+\mathbf{d}_h^n)$, $p_h^{n+\frac12} = \frac12(p_h^{n+1}+p_h^n)$, and

$$\mathbf{g}_h(\mathbf{d}_n^n, \mathbf{d}_h^{n+1}) = \frac{(|\mathbf{d}_h^{n+1}|^2-1)+(|\mathbf{d}_h^n|^2-1)}{2}\,\frac{\mathbf{d}_h^{n+1}+\mathbf{d}_h^n}{2}$$

# Discrete energy law

Take $\mathbf{v} = \mathbf{u}_h^{n+\frac{1}{2}}$ and $\mathbf{e} = \mathbf{d}_{\bar{t}}^{n+1}$, we can then obtain a discrete energy law:

$$\left(\frac{1}{2}\|\mathbf{u}_h^{n+1}\|_{\mathbf{L}^2}^2 + \frac{\lambda}{2}\|\nabla \mathbf{d}_h^{n+1}\|_{\mathbf{L}^2}^2 + \lambda \int_\Omega F(\mathbf{d}_h^{n+1})\right)_{\bar{t}} =$$

$$-\left(\nu\|\nabla \mathbf{u}_h^{n+\frac{1}{2}}\|_{\mathbf{L}^2}^2 + \frac{\lambda}{\gamma}\|\mathbf{d}_{\bar{t}}^{n+1} + (\mathbf{u}_h^{n+\frac{1}{2}} \cdot \nabla)\mathbf{d}_h^{n+\frac{1}{2}} + D_\beta(\mathbf{u}_h^{n+\frac{1}{2}})\mathbf{d}_h^{n+\frac{1}{2}}\|_{\mathbf{L}^2}^2\right)$$

# Example

We consider the hydrodynamic liquid crystal model , where the initial director field $\mathbf{d}(\mathbf{x}) = \tilde{\mathbf{d}}(\mathbf{x})/\sqrt{|\tilde{\mathbf{d}}(\mathbf{x})|^2 + \epsilon^2}$, and

$$\tilde{\mathbf{d}}(\mathbf{x}) = (x_1^2 + x_2^2 - \alpha^2, 2\alpha x_2).$$

We simply choose $\alpha = 0.5$. This director field has singularities at $\mathbf{x} = (\pm\alpha, 0)$ with unit degrees of opposite signs.

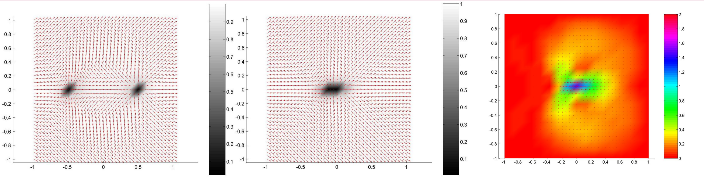

Figure 5.1: Initial director field and director and flow fields at the annihilation time $t = 0.26$ with $\beta = -0.2$.

# Annihilation time with different parameters

| $\beta$ | 0.0 | -0.2 | -0.5 | -0.8 | -1.0 |
|---|---|---|---|---|---|
| Annihilation time | 0.267 | 0.262 | 0.251 | 0.238 | 0.231 |

Table: $\beta$ vs time

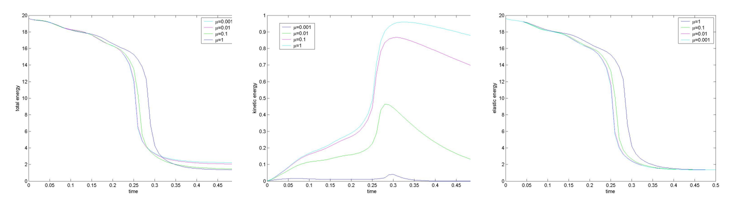


Figure 5.5: Energy vs time

# Simple case: "1+2" model

Assuming that $\Omega = [-1,1] \times [-1,1]$, $\mathbf{u} = (0, v(z,x), 0)^T, p = p(z,x), \mathbf{d} = (0, d_2(z,x), d_3(z,x))^T, (z,x) \in \Omega$, the full model can be simplified as follows for this shear flow case

$$v_t = \mu \triangle v + \lambda \tau_z, \tag{7}$$

$$\tau = \beta d_3(\triangle d_2 - f_2) + (\beta + 1) d_2(\triangle d_3 - f_3), \tag{8}$$

$$d_{2t} + \beta d_3 v_z = \gamma(\triangle d_2 - f_2), \tag{9}$$

$$d_{3t} + (1+\beta) d_2 v_z = \gamma(\triangle d_3 - f_3), \tag{10}$$

where $f_i = (4/\varepsilon^2)(d_2^2 + d_3^2 - 1)d_i, i = 2,3$ with the initial data $v^0 = \xi z, d_2^0, d_3^0$ and the boundary conditions:

$$\left.\frac{\partial v}{\partial z}\right|_{z=\pm 1} = \xi, \quad \left.\frac{\partial v}{\partial x}\right|_{x=\pm 1} = 0, \tag{11}$$

$$\frac{\partial d_i}{\partial \mathbf{n}} = -\frac{2}{\delta}(d_i - d_i^0), \ i = 2,3 \quad on \quad \partial\Omega. \tag{12}$$

# Finite difference method

For the space discretization we adopt the semi-implicit scheme and use the forward difference scheme for the time discretization,

$$\frac{d_{2\,j,i}^{\,n+1} - d_{2\,j,i}^{\,n}}{dt} + \beta d_{3\,ji}^{\,n} \frac{\delta_{0z} v_{j,i}^{n}}{2h} = \gamma \left( \frac{\delta_z^2 d_{2\,j,i}^{\,n+1} + \delta_x^2 d_{2\,j,i}^{\,n+1}}{h^2} - f_{3\,j,i}^{\,n} \right),$$

$$\frac{d_{3\,j,i}^{\,n+1} - d_{3\,j,i}^{\,n}}{dt} + (1+\beta) d_{2\,j,i}^{\,n} \frac{\delta_{0z} v_{j,i}^{n}}{2h} = \gamma \left( \frac{\delta_z^2 d_{3\,j,i}^{\,n+1} + \delta_x^2 d_{3\,j,i}^{\,n+1}}{h^2} - f_{3\,j,i}^{\,n} \right)$$

$$\tau_{j,i}^{n} = \beta d_{3\,j,i}^{\,n} \frac{1}{\gamma} \left( \frac{d_{2\,j,i}^{\,n+1} - d_{2\,j,i}^{\,n}}{dt} + \beta d_{3\,j,i}^{\,n} \frac{\delta_{0z} v_{j,i}^{n}}{2h} \right)$$

$$+(\beta+1) d_{2\,j,i}^{\,n} \frac{1}{\gamma} \left( \frac{d_{3\,j,i}^{\,n+1} - d_{3\,j,i}^{\,n}}{dt} + (1+\beta) d_{2\,j,i}^{\,n} \frac{\delta_{0z} v_{j,i}^{n}}{2h} \right),$$

$$\frac{v_{j,i}^{n+1} - v_{j,i}^{n}}{dt} = \mu \left( \frac{\delta_z^2 v_{j,i}^{n+1} + \delta_x^2 v_{j,i}^{n+1}}{h^2} \right) + \lambda \frac{\delta_{0z} \tau_{ji}^{n}}{2h},$$

where $\delta_{0z} v^n_{j,i} = v^n_{j,i+1} - v^n_{j,i-1}$, $\delta^2_z d_{j,i} = d_{j,i+1} + d_{j,i-1} - 2d_{j,i}$, $\delta^2_x d_{j,i} = d_{j+1,i} + d_{j-1,i} - 2d_{j,i}$.
${f_k}^n_{j,i} = (4/\varepsilon^2)[({d_2}^n_{j,i})^2 + ({d_3}^n_{j,i})^2 - 1]{d_k}^n_{j,i}, k = 2, 3,\ h = 2/M$. The discretization of the boundary conditions are as follows

$$\frac{{d_k}^{n+1}_{j,M} - {d_k}^{n+1}_{j,M-1}}{h} = -\frac{2}{\delta}({d_k}^{n+1}_{j,M} - {d_k}^{0}_{j,M}), \tag{13}$$

$$\frac{{d_k}^{n+1}_{j,1} - {d_k}^{n+1}_{j,0}}{h} = \frac{2}{\delta}({d_k}^{n+1}_{j,0} - {d_k}^{0}_{j,0}), \tag{14}$$

$$\frac{{d_k}^{n+1}_{M,i} - {d_k}^{n+1}_{M-1,i}}{h} = -\frac{2}{\delta}({d_k}^{n+1}_{M,i} - {d_k}^{0}_{M,i}), \tag{15}$$

$$\frac{{d_k}^{n+1}_{1,i} - {d_k}^{n+1}_{0,i}}{h} = \frac{2}{\delta}({d_k}^{n+1}_{0,i} - {d_k}^{0}_{0,i}), \tag{16}$$

$$\frac{v^{n+1}_{j,M} - v^{n+1}_{j,M-1}}{h} = \xi, \quad \frac{v^{n+1}_{j,1} - v^{n+1}_{j,0}}{h} = \xi, \tag{17}$$

$$v^{n+1}_{M,i} = v^{n+1}_{M-1,i}, \quad v^{n+1}_{0,i} = v^{n+1}_{1,i}. \tag{18}$$

# Impact of parameters

We set the mesh grid $M \times M = 40 \times 40$ and the time step $dt = 1 \times 10^{-4}$. We mainly focus on the impact of $\beta$ and $\xi$ and the other parameters are set to be:$\gamma = 1, \mu = 1, \lambda = 1, \varepsilon = 0.1, \delta = 5 \times 10^{-5}$.

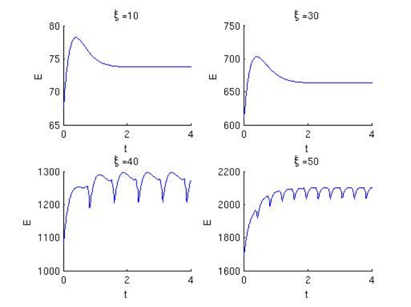


Figure: $\beta = -0.5$, energy function with different $\xi$

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# Impact of parameters

Here we investigate what impact on system with different $\beta$. We fix the shear rate $\xi = 30$ and the other parameters are same as previous page.

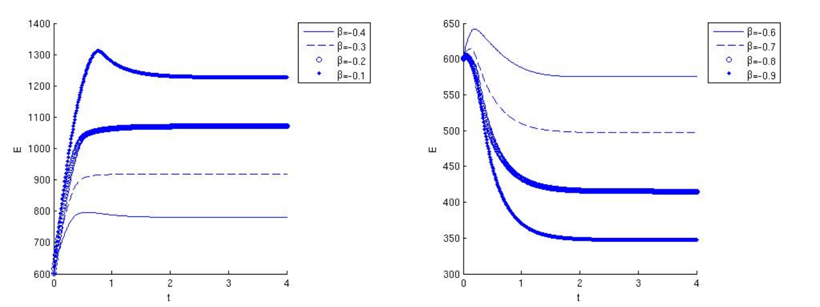


Figure: $\xi = 30$, energy function with different $\beta$.

# Defects

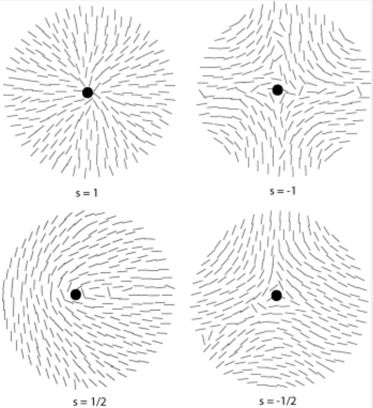


Figure: Defects with different strength.

# Defects

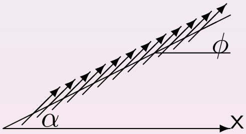


Figure: $\phi = s\alpha + c$

where $\alpha$ is made by director orientation along the polar line(x-axis) and $\phi$ is made by director end along the polar line(x-axis) and $c$ is a constant. The director is on the polar line if $s = 1$ and $c = 0$ and on a circle if $s = 1$ and $c = \frac{\pi}{2}$.

# Defects

Now we define the complex function $g_{s_j}(X - X_j^0)$ as follows

$$g_{s_j}(X - X_j^0) = \|X - X_j^0\|[\cos(\phi_j) + i\sin(\phi_j)] = ||X - X_j^0||e^{i\phi_j},$$
$$\phi_j = s_j\alpha_j + c,$$

Multiply all this complex function :

$$g_0(X) = \begin{cases} \prod_{j=1}^{N} \frac{g_{s_j}(X - X_j^0)}{||X - X_j^0||}, & X \in \Omega \setminus \{X_j^0, j = 1, \cdots, N\}, \\ 0, & X \in \{X_j^0, j = 1, \cdots, N\}. \end{cases} \quad (19)$$

Thus we can get the initial value $d_2^0(X)$ and $d_3^0(X)$ from the complex function $g_0(X)$ as follows

$$d_2^0(X) = Im(g_0(X)), \quad d_3^0(X) = Re(g_0(X)). \quad (20)$$

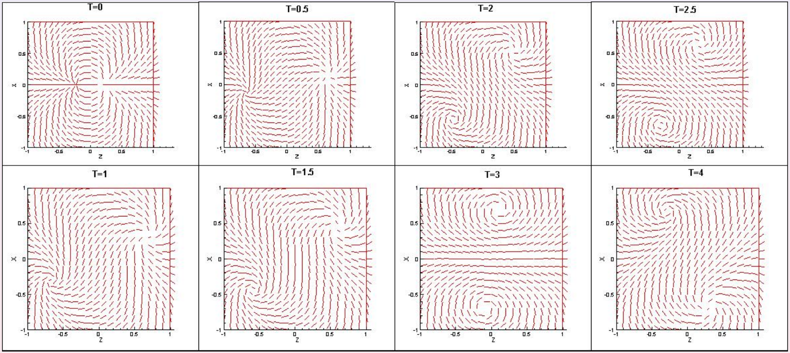


Figure: case1-(a)
$N = 2, X_1^0 = (-0.2, 0), X_2^0 = (0.2, 0), s_1 = s_2 = 1, \xi = 3.$

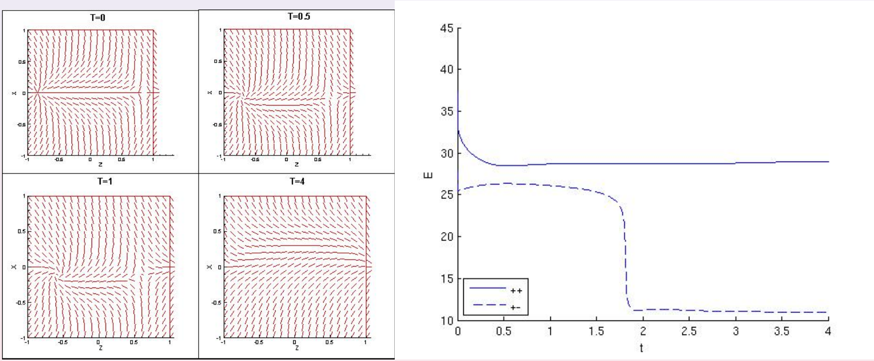


Figure: left:case1-
(b) $N = 2, X_1^0 = (-0.85, 0), X_2^0 = (0.85, 0), s_1 = 1, s_2 = -1,\ \xi = 3.$
right: energy function

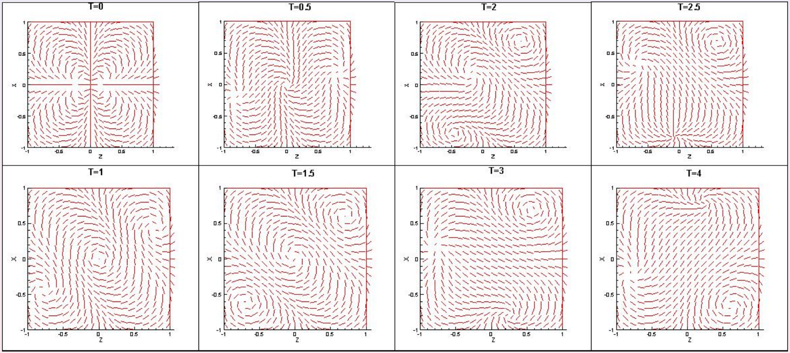


Figure: case2-(a)$N = 3, X_1^0 = (-0.2, 0), X_2^0 = (0, 0), X_3^0 = (0.2, 0), s_1 = s_2 = s_3 = 1, \xi = 3.$

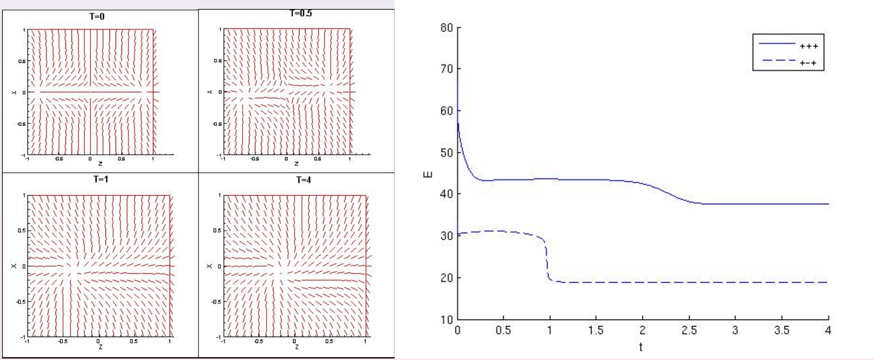


Figure: left:case2-(b)$N = 3, X_1^0 = (-0.85, 0), X_2^0 = (0, 0), X_3^0 = (0.85, 0), s_1 = s_3 = 1, s_2 = -1, \xi = 3.$ right:energy function

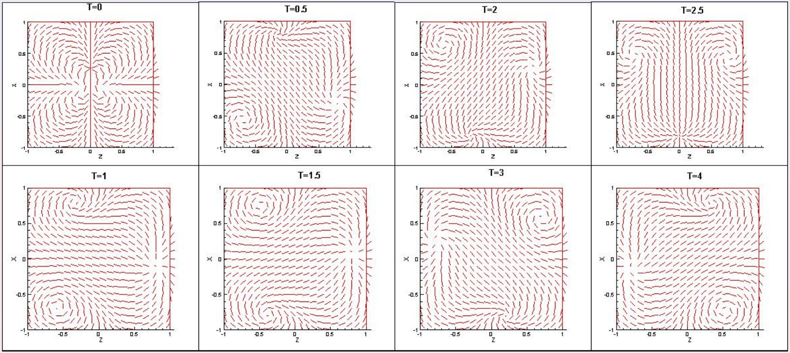


Figure: case2-(c):$N = 3, X_1^0 = (-0.1 \times \sqrt{3}, -0.1), X_2^0 = (0, 0.2), X_3^0 = (0.1 \times \sqrt{3}, -0.1), s_1 = s_2 = s_3 = 1, \xi = 3.$

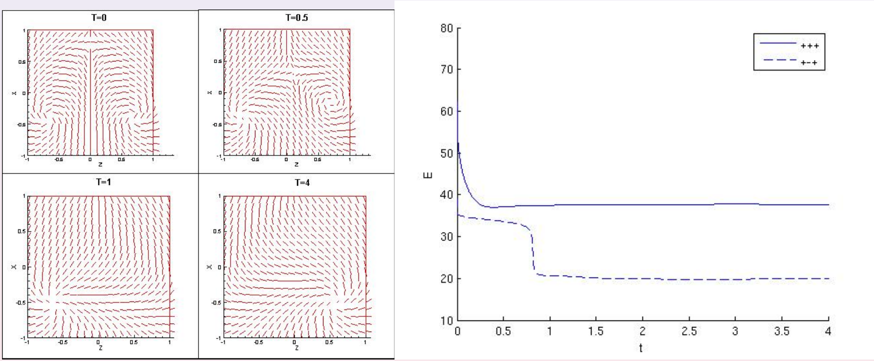


Figure: left:case2-(d), $N = 3, X_1^0 = (-0.4 \times \sqrt{3}, -0.4), X_2^0 = (0, 0.8), X_3^0 = (0.4 \times \sqrt{3}, -0.4), s_1 = s_3 = 1, s_2 = -1, \xi = 3.$
right:energy function

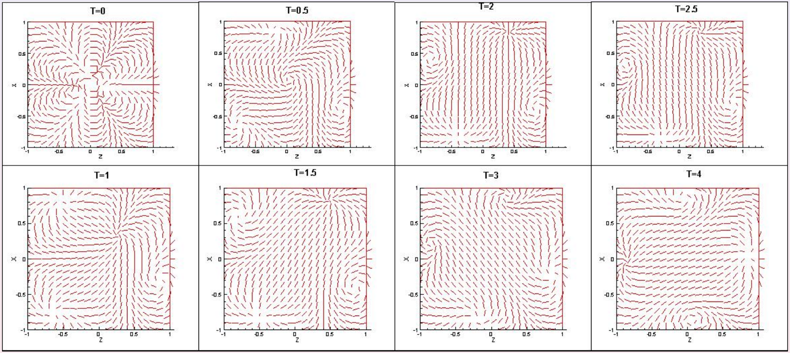


Figure: case3-(a): $N = 4, X_1^0 = (-0.1 \times \sqrt{3}, -0.1), X_2^0 = (0, 0.2), X_3^0 = (0.1 \times \sqrt{3}, -0.1), X_0^0 = (0, 0), s_0 = s_1 = s_2 = s_3 = 1, \xi = 3.$

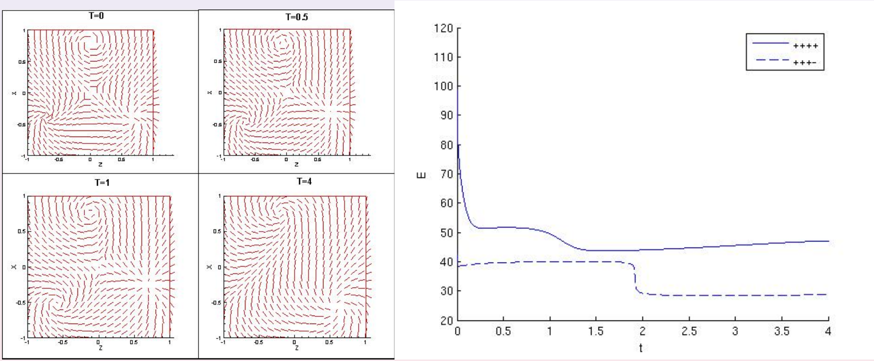


Figure: left:case3-(b),
$N = 4, X_1^0 = (-0.4 \times \sqrt{3}, -0.4), X_2^0 = (0, 0.8), X_3^0 = (0.4 \times \sqrt{3}, -0.4), X_0^0 = (0, 0), s_1 = s_2 = s_3 = 1, s_0 = -1, \xi = 3.$
right:energy function

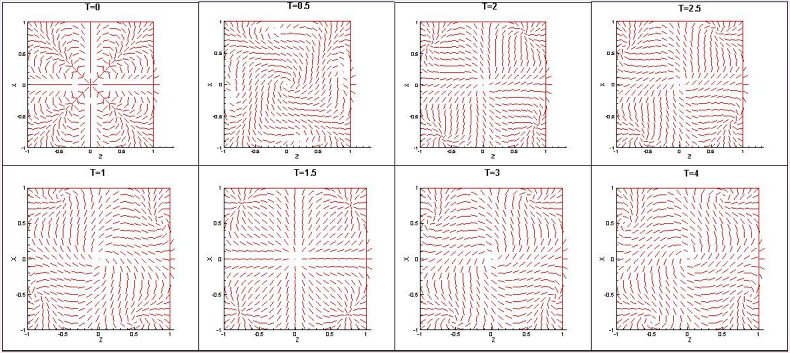


Figure: case4-(a): $N = 5, X_1^0 = (-0.2, 0), X_2^0 = (0, 0.2), X_3^0 = (0.2, 0), X_4^0 = (0, -0.2), X_0^0 = (0, 0), s_0 = s_1 = s_2 = s_3 = s_4 = 1, \xi = 3.$

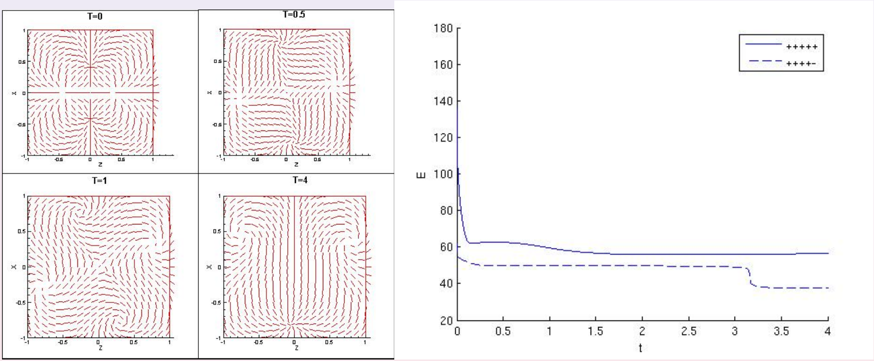


Figure: left:case4-(b),
$N = 5, X_1^0 = (-0.4, 0), X_2^0 = (0, 0.4), X_3^0 = (0.4, 0), X_4^0 = (0, -0.4), X_0^0 = (0, 0), s_1 = s_2 = s_3 = s_4 = 1, s_0 = -1, \xi = 3.$
right:energy function

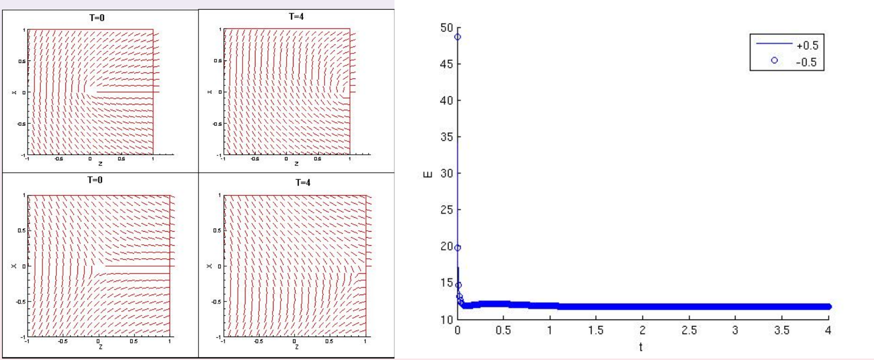


Figure: left(up: $s = +\frac{1}{2}$; down: $s = -\frac{1}{2}$) right: energy function

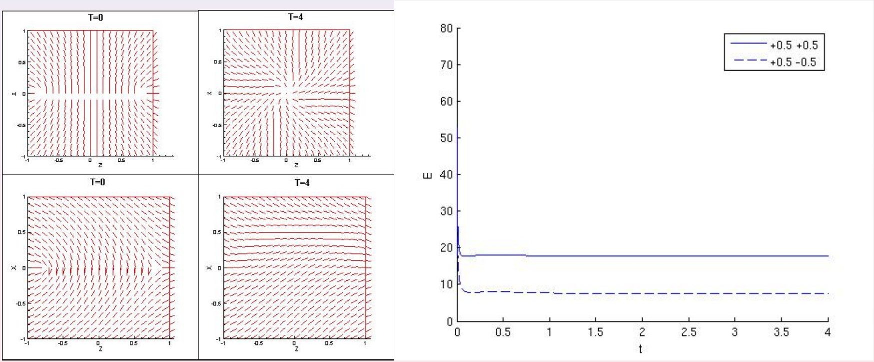


Figure: left(up: $s_1 = s_2 = +\frac{1}{2}$; down: $s_1 = +\frac{1}{2}, s_2 = -\frac{1}{2}$) right:energy function

# Ericksen-Leslie system without penalty function

F.H. Lin (1989) proposed a simplified E-L system

$$\mathbf{d}_t + (\mathbf{u} \cdot \nabla)\mathbf{d} = \triangle \mathbf{d} + |\nabla \mathbf{d}|^2 \mathbf{d}, \tag{21}$$

$$|\mathbf{d}| = 1, \tag{22}$$

$$\mathbf{u}_t + \mathbf{u} \cdot \nabla \mathbf{u} + \nabla P = \triangle \mathbf{u} - \nabla \cdot ((\nabla \mathbf{d})^T \nabla \mathbf{d}), \tag{23}$$

$$\nabla \cdot \mathbf{u} = 0. \tag{24}$$

With the boundary conditions and initial conditions

$$\mathbf{u} = 0, \quad \frac{\partial \mathbf{d}}{\partial \mathbf{n}} = \mathbf{0}, \quad \text{on} \quad \partial\Omega \times (0, T), \tag{25}$$

$$\mathbf{d}(\mathbf{x}, 0) = \mathbf{d}_0(\mathbf{x}), \quad \mathbf{u}(\mathbf{x}, 0) = \mathbf{u}_0(\mathbf{x}), \quad \text{in} \quad \Omega, \tag{26}$$

the system satisfies the energy relation

$$\frac{d}{dt}(\frac{1}{2}\|\mathbf{u}\|^2 + \frac{1}{2}\|\nabla \mathbf{d}\|^2) + \|\nabla \mathbf{u}\|^2 + \|\triangle \mathbf{d} + |\nabla \mathbf{d}|^2 \mathbf{d}\|^2 = 0, \tag{27}$$

The constraint $|\mathbf{d}| = 1$ is difficulty to at the discrete level. Thus many works for this system are based on the discretization of the penalized problem.

However, we find that the sphere constraint $|\mathbf{d}| = 1$ is satisfied automatically due to the equation (21).

### Theorem

*Assume* $(\mathbf{u}, \mathbf{d})$ *is the smooth solution of the following equation:*

$$\mathbf{d}_t + (\mathbf{u} \cdot \nabla)\mathbf{d} = \triangle \mathbf{d} + |\nabla \mathbf{d}|^2 \mathbf{d}, \tag{28}$$

*in* $\Omega \times (0, T)$ *with* $\mathbf{d}(\mathbf{x}, 0) = \mathbf{d}_0(\mathbf{x})$. *If the initial condition satisfies* $|\mathbf{d}_0| = 1$, *then* $|\mathbf{d}| = 1$ *constantly.*

Hence, we can rewrite the system (21)-(24) by denoting $\mathbf{d}(\mathbf{x}, t) = \mathbf{d}(x, y, t) = (\cos\theta(x, y, t),\ \sin\theta(x, y, t))^T$, where $\mathbf{x} = (x, y) \in \Omega \subset \mathbb{R}^2$.

The whole system (21)-(24), denoting $\tilde{P} = P + \frac{1}{2}|\nabla\theta|^2$, reads as:

$$\theta_t + (\mathbf{u}\cdot\nabla)\theta - \triangle\theta = 0, \tag{29}$$

$$\mathbf{u}_t + \mathbf{u}\cdot\nabla\mathbf{u} + \nabla\tilde{P} - \triangle\mathbf{u} + \triangle\theta\nabla\theta = 0, \tag{30}$$

$$\nabla\cdot\mathbf{u} = 0, \tag{31}$$

with the boundary conditions and initial conditions

$$\mathbf{u} = 0, \quad \nabla\theta\cdot\mathbf{n} = 0, \quad \text{on} \quad \partial\Omega\times(0, T), \tag{32}$$

$$\theta(\mathbf{x}, 0) = \theta_0(\mathbf{x}), \quad \mathbf{u}(\mathbf{x}, 0) = \mathbf{u}_0(\mathbf{x}), \quad \text{in} \quad \Omega, \tag{33}$$

Then the system (29)-(31) satisfies the following energy law:

$$\frac{d}{dt}E + \|\triangle\theta\|^2 + \|\nabla\mathbf{u}\|^2 = 0, \tag{34}$$

where $E = \frac{1}{2}\|\mathbf{u}\|^2 + \frac{1}{2}\|\nabla\theta\|^2$.

# Energy stable scheme

Given the initial conditions $\theta^0$, $\mathbf{u}^0$ and $P^0$, having computed for $\theta^n$, $\mathbf{u}^n$, $P^n$ and $\tilde{P}^n = P^n + \frac{1}{2}|\nabla\theta^n|^2$ for $n > 0$, we compute $\theta^{n+1}$, $\mathbf{u}^{n+1}$, $P^{n+1}$ by

**Step 1.**

$$\frac{\theta^{n+1} - \theta^n}{\delta t} + (\mathbf{u}_*^n \cdot \nabla)\theta^n = \triangle\theta^{n+1}, \tag{35}$$

with

$$\mathbf{u}_*^n = \mathbf{u}^n - \delta t[\frac{\theta^{n+1} - \theta^n}{\delta t} + (\mathbf{u}_*^n \cdot \nabla)\theta^n]\nabla\theta^n. \tag{36}$$

# Energy stable scheme

**Step 2.**

$$\frac{\tilde{\mathbf{u}}^{n+1} - \mathbf{u}_*^n}{\delta t} + (\mathbf{u}^n \cdot \nabla)\tilde{\mathbf{u}}^{n+1} - \triangle \tilde{\mathbf{u}}^{n+1} + \nabla \tilde{P}^n = 0, \tag{37}$$

$$\tilde{\mathbf{u}}^{n+1}|_{\partial\Omega} = 0. \tag{38}$$

**Step 3.**

$$\frac{\mathbf{u}^{n+1} - \tilde{\mathbf{u}}^{n+1}}{\delta t} + \nabla(\tilde{P}^{n+1} - \tilde{P}^n) = 0, \tag{39}$$

$$\nabla \cdot \mathbf{u}^{n+1} = 0, \tag{40}$$

$$\mathbf{u}^{n+1} \cdot \mathbf{n}|_{\partial\Omega} = 0. \tag{41}$$

And

$$P^{n+1} = \tilde{P}^{n+1} - \frac{1}{2}|\nabla\theta^{n+1}|^2. \tag{42}$$

# Energy stable scheme

**Theorem**

*The scheme* (35)-(41) *is stable, with the following discrete energy dissipation law:*

$$E^{n+1} + \frac{\delta t^2}{2}\|\nabla \tilde{P}^{n+1}\|^2 + \delta t\|\frac{\theta^{n+1}-\theta^n}{\delta t} + (\mathbf{u}_* \cdot \nabla)\theta^n\|^2 + \delta t\|\nabla \tilde{\mathbf{u}}^{n+1}\|^2 \le E^n + \frac{\delta t^2}{2}\|\nabla \tilde{P}^n\|^2, \tag{43}$$

*where* $E^n = \frac{1}{2}\|\mathbf{u}^n\|^2 + \frac{1}{2}\|\nabla\theta^n\|^2$.

# Ericksen-Leslie system without penalty function

**Example 1** Initial conditions:

$$\mathbf{u}_0 \equiv \mathbf{0}, \quad \theta_0(\mathbf{x}) = \theta_0(x, y) = 2\pi(\cos(x) - \sin(y)). \tag{44}$$

We choose mesh size $h = 1/50$, time step size $\delta t = 0.001$.

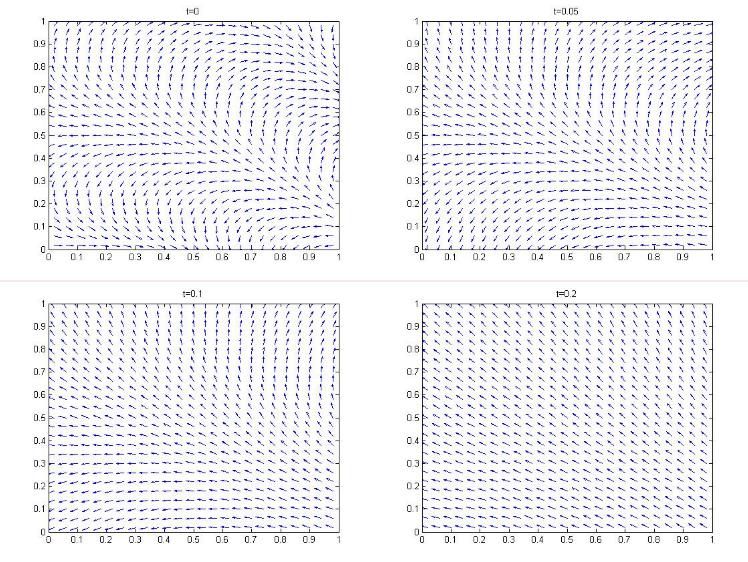


Figure: Numerical results of **d**.

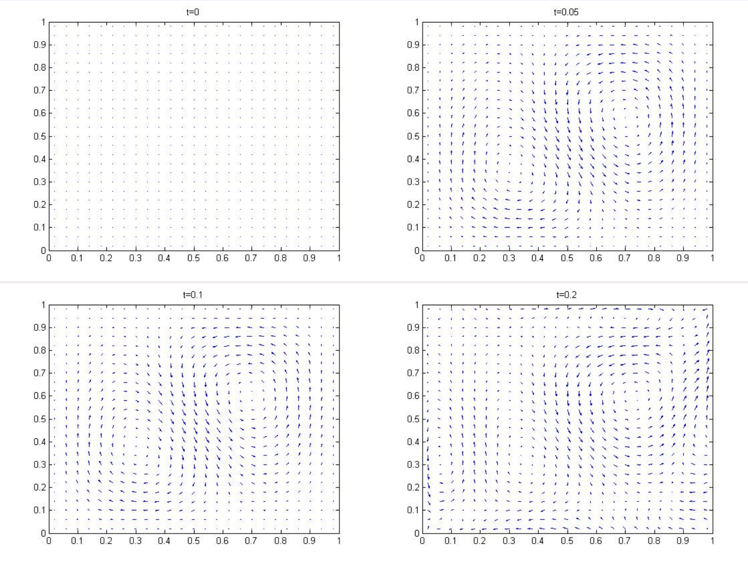


Figure: Numerical results of $\mathbf{u}$.

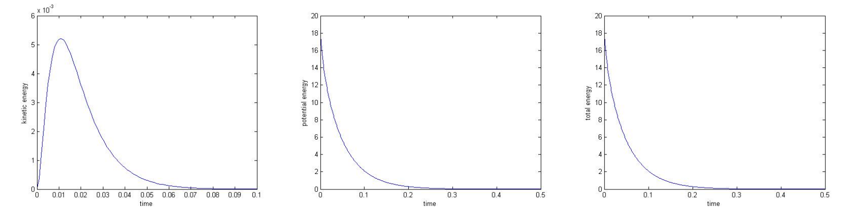


Figure: Evolution in time of the energies. Kinetic energy(left), potential energy(middle) and total energy(right).

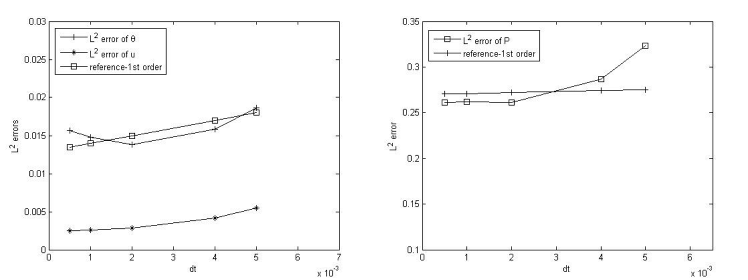


Figure: $L^2$ errors of velocity and function $\theta$(left) and pressure(right).

# Example 2

Initial conditions:

$$\mathbf{u}_0 \equiv \mathbf{0}, \ \mathbf{d}_0 = \frac{\tilde{\mathbf{d}}}{|\tilde{\mathbf{d}}|},$$
$$\text{where } \tilde{\mathbf{d}} = ((x-0.5)^2 + (y-0.5)^2 - 0.09, y - 0.5)^T,$$

so we choose the initial $\theta_0(x, y) \in [0, 2\pi]$ satisfying $(\cos\theta_0, \sin\theta_0)^T = \mathbf{d}_0$. This director field has singularities at $(0.2, 0.5)$ and $(0.8, 0.5)$ with unit degrees of opposite signs. We choose mesh size $h = 1/55$, the time step size $\delta t = 0.001$

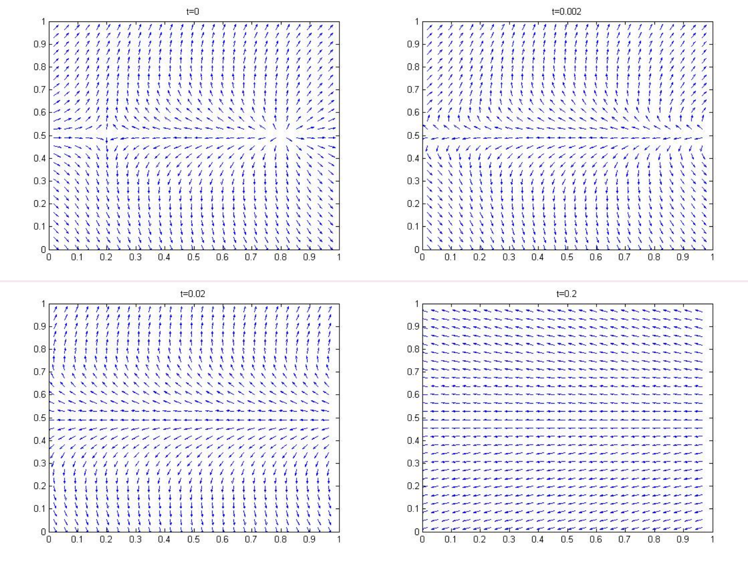


Figure: Numerical results of **d**.

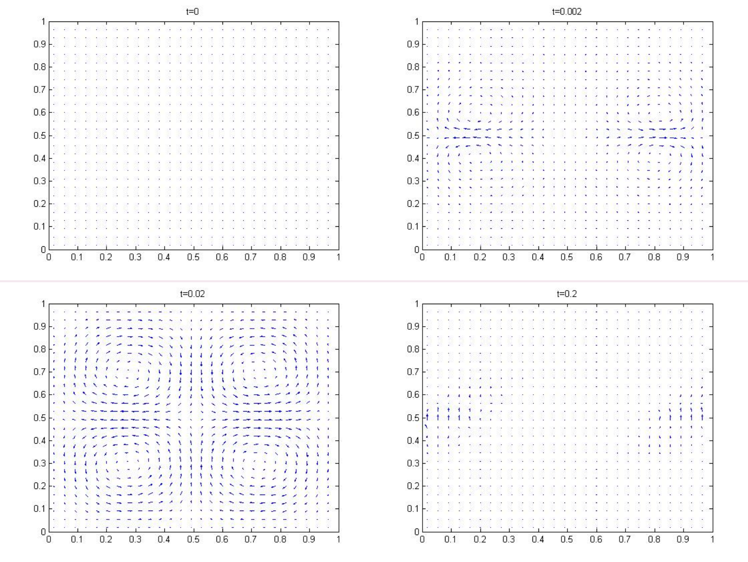


Figure: Numerical results of $\mathbf{u}$.

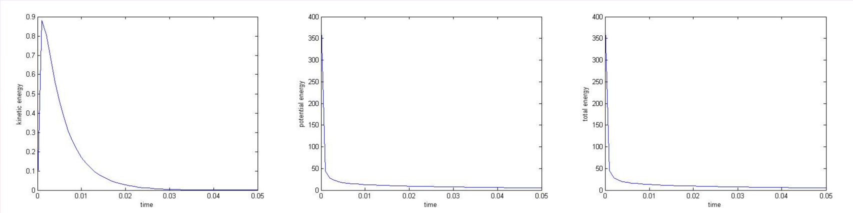


Figure: Evolution in time of the energies. Kinetic energy(left), potential energy(middle) and total energy(right).

# Example 3

We choose the singularities to be $(0.35, 0.5)$ and $(0.65, 0.5)$. The mesh size $h = 1/55$, and the time step size $\delta t = 0.001$.
$\mathbf{u}_0$ is set as in **Example 2**.

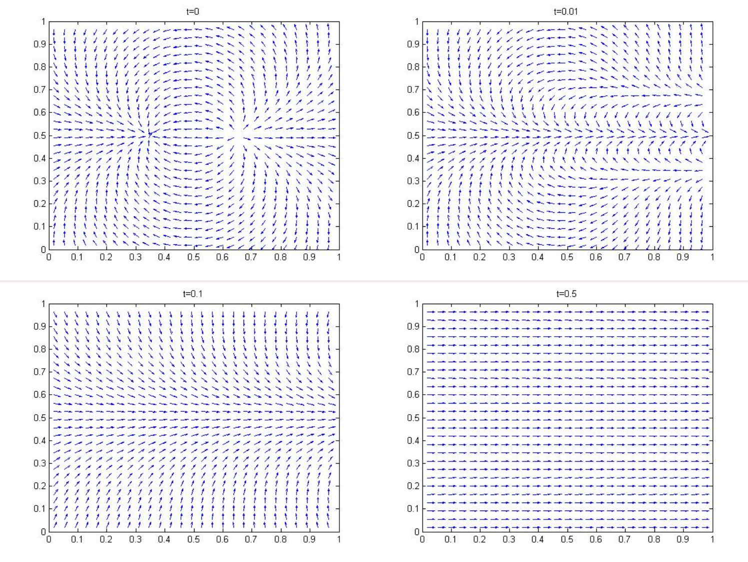


Figure: Numerical results of **d**.

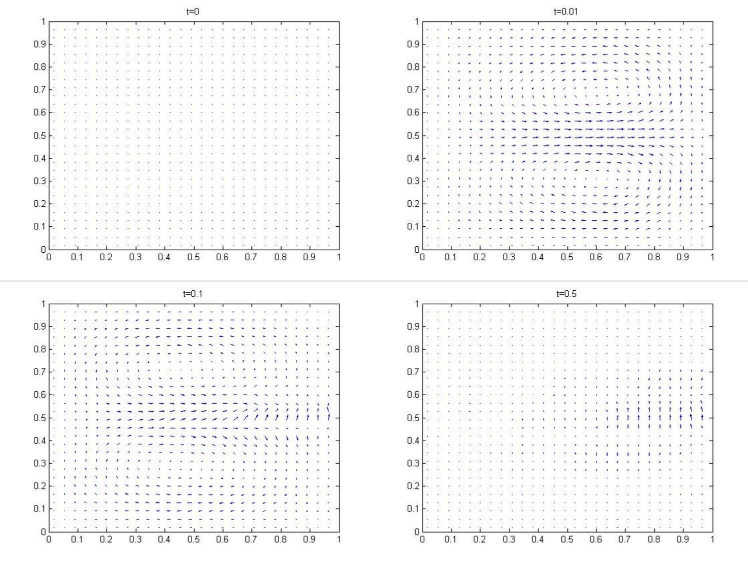


Figure: Numerical results of $\mathbf{u}$.

# Example 4

Initial velocity is set to be a rotating flow of the form:

$$\mathbf{u}_0 = 100(-y, x)^T,$$

$\mathbf{d}_0$ is set as in **Example 2**. And the mesh size $h = 1/55$, the time step size $\delta t = 0.0001$.

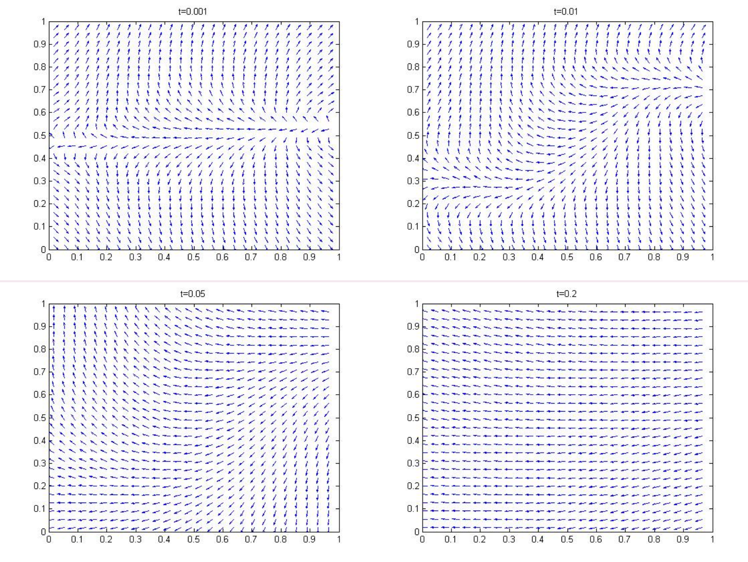


Figure: Numerical results of **d**.

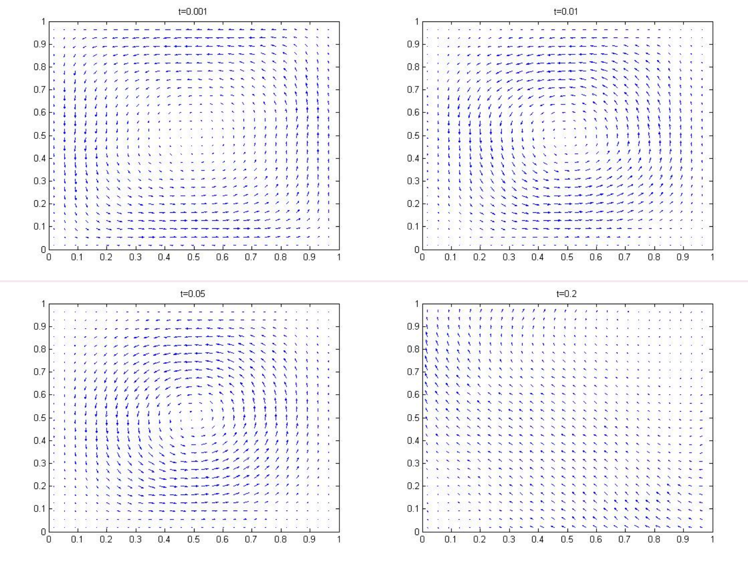


Figure: Numerical results of $\mathbf{u}$.

# References-1

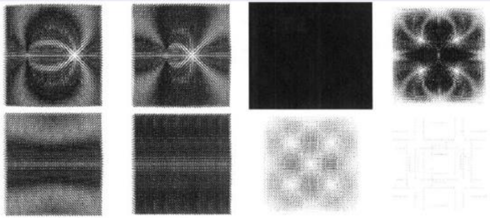

FIG. 5.4. *Example* 5.2, *using Algorithm* 3.1: *Snapshots at times* $t = 0, 0.3, 0.6, 0.9$ *of* $\{\mathbf{d}_h^m\}$ *(left) and* $\{\mathbf{u}_h^m\}$*(right). (The director and velocity fields are scaled by a factor of* 0.1 *and* 2.0, *respectively.)*

Figure: X.B Feng et al, SIAM J. Numer. Anal. 2008.

# References-2

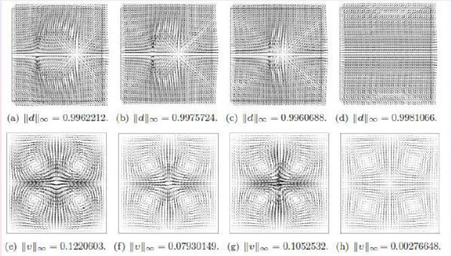


FIG. 1. *Evolution of the director field* (a)–(d) *and velocity field* (e)–(h) *for the annihilation of two singularities at times* $t = 0.1, 0.4, 0.6,$ *and* 1.

Figure: R. C. Cabrales, et al, SIAM J. Sci. Comput. 2015.

# References-3

**Theorem 1.1.** *Assuming the orientation field vector $d$ has a spherical expression*

$$d(x,t) = (\cos\theta(x,t), \sin\theta(x,t)\cos\psi(x,t), \sin\theta(x,t)\sin\psi(x,t))$$

*then the equations for $d$ can be reduced to the following system*

$$\begin{cases} \theta_t + u\cdot\nabla\theta = \Delta\theta - \sin\theta\cos\theta|\nabla\psi|^2 \\ \psi_t + u\cdot\nabla\psi = \Delta\psi + 2\cot\theta\nabla\theta\cdot\nabla\psi \end{cases}$$

*as long as*

$$\theta : \mathbb{R}^n \times \mathbb{R}_+ \to \mathbb{R} \setminus \bigcup_{k\in\mathbb{Z}} \{k\pi\}, \quad \psi : \mathbb{R}^n \times \mathbb{R}_+ \to \mathbb{R} \setminus \bigcup_{k\in\mathbb{Z}} \{k\pi\}.$$

Figure: X.D. Huang, Nonlinearity 2017.

# Numerical results and discussion

1. E-L system with penalty function can describe the annihilation of singularity.
2. E-L system including rotation term with penalty can describe the rotation beside annihilation of singularity.
3. For the "1+2" model with penalty function we show that the fact 同性排斥，异性相吸！
4. E-L model without penalty function is not physical model but include many mathematical analysis phenomena.

Thank you!