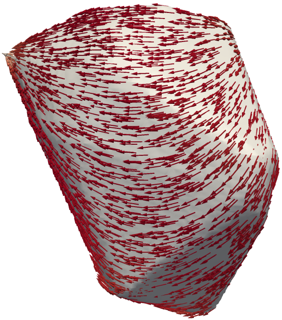
Orientation Fields on Evolving Surfaces
A Diffuse Domain Approach

27.04.2015

1. Problem Setup
2. Diffuse Domain Modelling for stationary Surfaces
   - Model
   - Validation
3. Diffuse Domain Modelling for evolving Surfaces
   - Shell Coalescence
   - Cahn Hilliard Surface Evolution
   - Onsager Relations
   - Coupled Dynamics

Problem



Problem:

- Find Vectorfield $\mathbf{p}$ on $S = \partial B \subset \mathcal{R}^3$ such that:

$$\text{minimize distortion energy } E(\mathbf{p})$$
$$\mathbf{p} \cdot \mathbf{n} = 0 \text{ and } \|\mathbf{p}\| = 1 \text{ on } S$$

- B bounded, connected Set

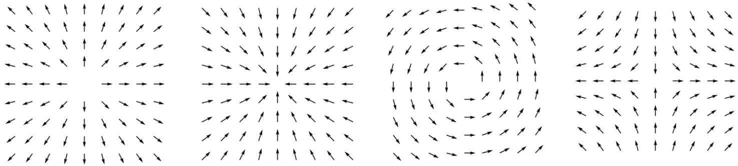
Geometric Frustration: [1]

- physical preferred local order cannot propagate throughout the system
- order is locally broken $\rightarrow$ defects
- curvature plays crucial role in position of defects

Defects in Orientation Fields

Poincare Hopf Theorem

Let M be a compact orientable differentiable Manifold. Let v be a Vector Field on M with isolated Zeroes.
Then the Sum of the Indices is over all the isolated Zeroes of v equals the Euler Characteristic of M.



- different Types of Zeroes/Defects with different Indices Source(+1), Sink(+1), Vortex(+1) and Saddlepoint(-1)
- Euler Characteristic: Sphere/Ellipsoid = 2, Torus = 0

Existing Approaches

Frank Oseen Energy

$$E = \int_S \frac{K_o}{2} \|\nabla \mathbf{p}\|_F^2 + \text{Penality Terms}\, \mathbf{d}S$$

Spherical Harmonics

$\mathbf{p} \in TS$

$$\frac{K_n}{4}\left(\|\mathbf{p}\|^2 - 1\right)^2$$

Explicit Domain

$\mathbf{p} \in \mathcal{R}^3$

$$\frac{K_t}{2}(\mathbf{p}\cdot\mathbf{n})^2 + \frac{K_n}{4}\left(\|\mathbf{p}\|^2 - 1\right)^2$$

Constitutive Equation

$$\frac{\partial \mathbf{p}}{\partial t} = -\frac{\delta e}{\delta \mathbf{p}}$$

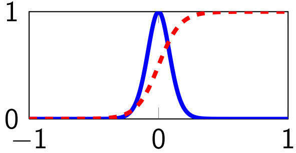
molecular Field $h = -\frac{\delta e}{\delta \mathbf{p}_i}$ (generalized force)

Diffuse Domain Model

diffuse approximation of B and S

$$\chi_B = \lim_{\epsilon_\phi \to 0} c$$

$$\chi_S = \lim_{\epsilon_\phi \to 0} B(c)$$



$\Omega \setminus B \leftarrow S \rightarrow B$

Free Energy and Constitutive Equation

$$E = \int_\Omega B(c) \frac{K_o}{2} \|\nabla \mathbf{p}\|_F^2 \, \mathbf{d}\Omega + \int_\Omega B(c) \left(\frac{K_t}{2} (\mathbf{p} \cdot \mathbf{n})^2 + \frac{K_n}{4} \left(\|\mathbf{p}\|^2 - 1\right)^2 \right) \mathbf{d}\Omega$$

$$\frac{\partial B(c)\, \mathbf{p}}{\partial t} = B(c)\, h$$

Evolution Equations

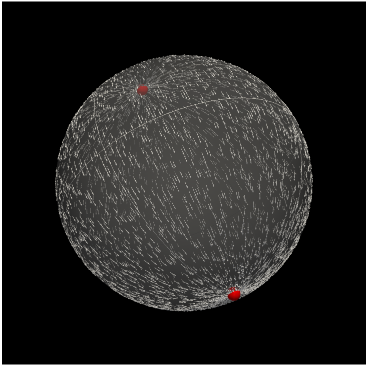
Diffuse Domain Evolution Equations

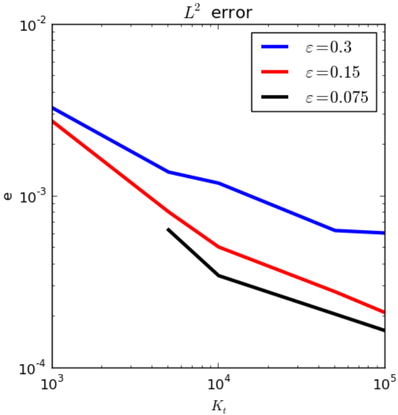
$$\begin{aligned} \tilde{B}(c)\frac{\partial \mathbf{p}}{\partial t} - K_o \nabla \cdot \tilde{B}(c) \nabla \mathbf{p} & \\ + B(c) K_t \left(\mathbf{n} \otimes \mathbf{n}^T\right) \cdot \mathbf{p} + B(c) K_n \left(\|\mathbf{p}\|^2 - 1\right) \mathbf{p} &= 0 \quad \Omega \\ \frac{\partial \mathbf{p}}{\partial \mathbf{n}} &= 0 \quad \Gamma \end{aligned}$$

- normal extended intial values on S, $\mathbf{n} \approx \frac{\nabla c}{|\nabla c|}$
- $B(c) = \tilde{C} c^2 (1-c)^2$

$\Rightarrow$ `AMDiS` **can be applied straight forward**

Analytical Solution on Unit Sphere





$$\mathbf{p}(\mathbf{x}) = \frac{1}{\sqrt{1 - \mathbf{x}_3^2}} \begin{bmatrix} \mathbf{x}_1 \mathbf{x}_3 \\ \mathbf{x}_2 \mathbf{x}_3 \\ \mathbf{x}_3^2 - 1 \end{bmatrix}$$

Defect Trajectories on Unit Sphere

start at non minimal energy configuration with deterministic defect behaviour

$\Rightarrow$ compare diffuse domain model to results of other methods

$\Rightarrow$ Spherical-Harmonics and Explicit Domain approach

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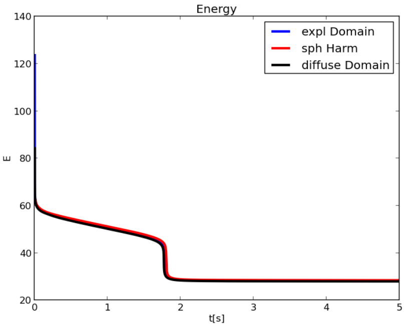

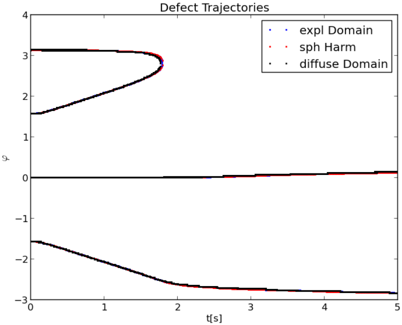

Outline

1. informative example: shell coalescence 3D and director fields
    - decoupled dynamics $\rightarrow$ sequence of minimal energy states, on prescribed surfaces
    - get a idea about possible interactions
2. basic surface relaxation coupled with director field dynamics
    - use basic free energy driven surface evolution $\rightarrow$ Cahn Hilliard
    - use Onsager Relations to develop possible coupling mechanisms
    - investigate influence of coupling on relaxation trajectorie
3. continous forced system

Equilibrium Configurations on evolving Surface

Surface evolution is presicribed by external results [2]

- **intial state:** "touching spheres", 4 defects with toplogical charge 4
- **intermediate state:** saddle points occur, 6 defects with topological charge 2
- **critical event:** pair of source/sink gets annihilated by merging with saddle points, 2 defects with topological charge 2
- **late phase:** remaining defect pair relocates to final position, topological charge 2

Model - Surface Evolution

Surface Evolution defined by Cahn Hilliard Interface Evolution

Free Energy

$$E = \int_\Omega K_c \left(\frac{1}{\epsilon} B(c) + \frac{\epsilon}{2}|\nabla c|^2\right) \, \mathbf{d}\Omega$$

Constitutive Equation given by Diffusive Transport and Chemical Potential μ (generalized force $\triangle\mu$)

Constitutive Equation

$$\mu = K_c \frac{\delta e_C}{\delta c}$$

$$\frac{\partial c}{\partial t} = \triangle\mu$$

Combined Free Energy

Free Energy - Directors on evolving Surface

$$E = \int_\Omega K_c \underbrace{\left(\frac{1}{\epsilon} B(c) + \frac{\epsilon}{2}|\nabla c|^2\right)}_{e_C} \mathbf{d}\Omega$$

$$+ \int_\Omega R(c) \underbrace{\frac{K_o}{2}\|\nabla \mathbf{p}\|_F^2}_{e_{P1}} \mathbf{d}\Omega$$

$$+ \int_\Omega R(c) \underbrace{\left(\frac{K_t}{2}(\mathbf{p}\cdot\mathbf{n})^2 + \frac{K_n}{4}\left(\|\mathbf{p}\|^2 - 1\right)^2\right)}_{e_{P2}} \mathbf{d}\Omega$$

conjugated flux-forces pairs: $\left(\frac{\partial c}{\partial t}, \triangle\mu\right)$ and $\left(\frac{\partial R(c)\mathbf{p}}{\partial t}, R(c)\, h\right)$, each with parities $(-1, 1)$

Onsager Relations

Constitutive Equations

$$\begin{aligned}\frac{\partial c}{\partial t} &= \triangle\mu + \Lambda\mathbf{p}\cdot R(c)\,h\\ \frac{\partial R(c)\,\mathbf{p}}{\partial t} &= \Lambda\mathbf{p}\triangle\mu + R(c)\,h\end{aligned}$$

Onsager Relations

Constitutive Equations

$$\begin{aligned}
\frac{\partial c}{\partial t} &= \triangle\mu + \Lambda\mathbf{p}\cdot R(c)\,h \\
\frac{\partial R(c)\,\mathbf{p}}{\partial t} &= \Lambda\mathbf{p}\triangle\mu + R(c)\,h
\end{aligned}$$

Rate of Dissipation

$$\Pi = -\left(\triangle\mu\frac{\partial c}{\partial t} + R(c)\,h\cdot\frac{\partial R(c)\mathbf{p}}{\partial t}\right)$$

$$\Pi = -\left((\triangle\mu)^2 + R(c)^2\,h^2 + \Lambda\left(1+R(c)\right)R(c)\,\mathbf{p}\cdot h\triangle\mu\right)$$

Onsager Relations

to preserve mass continuity of c and ensure $\Pi < 0$ we choose $\Lambda = 0$

Constitutive Equations

$$\begin{aligned}\frac{\partial c}{\partial t} &= \triangle\mu \\ \frac{\partial R(c)\,\mathbf{p}}{\partial t} &= R(c)\,h\end{aligned}$$

Coupling

$$\begin{aligned}\frac{\partial R(c)\,\mathbf{p}}{\partial t} &= R(c)\,\frac{\partial \mathbf{p}}{\partial t} + R'(c)\,\frac{\partial c}{\partial t}\mathbf{p} \\ \mu &= K_c\frac{\delta e_C}{\delta c} + (e_{p1}+e_{p2})\,\frac{\delta R(c)}{\delta c}\end{aligned}$$

Chemical Potential Coupling

Chemical Potential

for $R(c) = \left(\frac{1}{\epsilon} B(c) + \frac{\epsilon}{2} |\nabla c|^2\right) = e_C$:

$$\mu = \frac{\tilde{C}}{\epsilon} \left(c^3 - c\right) \left(K_c + e_{P1} + e_{P2}\right) - \epsilon \nabla \cdot \left(K_c + e_{P1} + e_{P2}\right) \nabla c$$

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non defect region:

$$e_{P1} + e_{P2} \approx 0$$

$$K_c$$

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non defect region:

$$e_{P1} + e_{P2} \approx 0$$

$$K_c$$

defect region:

$$\|\mathbf{p}\| \approx 0,\ \|\nabla\mathbf{p}\|_F \approx \frac{1}{r}$$

$$K_c + \frac{K_o}{2r} + \frac{K_n}{4}$$

Summary

Diffuse Domain Director Field Dynamics

- set up diffuse domain modelling for arbitrary stationary surfaces in 3D
- validated model's capacities to reproduce minimal energy states as well as defect dynamics

Basic Coupled Surface Director Field Evolution

- discussed several possible couplings between Cahn Hilliard and Director Dynamics
- highlighted possible influence of defects on surface relaxation

Outlook

- Quantive influence of defects in relaxation trajectorie of surface, at different values of K_c
- possible forcings on system:
  - external forces on surface
  - add chemical concentration to generate stress on $\mathbf{p}$
  - add chemical concentration to modify prefered curvature of surface
- apply Onsager relations to other surface evolutions
  - dendritic growth

Thanks for your attention!

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Modeling the coalescence of heterogenous amorphous particles.
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