Director Fields on Manifolds, a Diffuse Domain Approach

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Abstract

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1 Introduction

2 Director Field

Throughout this paper we consider a director field to be a smooth(beside isolated points) vectorfield $\mathbf{p}$ with unit length on a singely connected subset of $\mathcal{R}^3$. For the special case of surfaces S we also require $\mathbf{p} \in TS$ or $\mathbf{p} \cdot \mathbf{n} = 0$($\mathbf{n}$ surface normal).

The established modelling of director field dynamics $\mathbf{p}(\mathbf{x}, t)$ bases on definition of a free energy(E)/energy density(e) with dynamics driven by a gradient flow $\frac{\partial \mathbf{p}}{\partial t} = -\frac{\delta e}{\delta \mathbf{p}}$.

A well known defintion of such a energy is the elastic Frank Oseen energy(cite 3), penalizing three basic deformations(splay, twist and bend) in the director

$$E = \int_\Omega \underbrace{\frac{K_1}{2}(\nabla \cdot \mathbf{p})^2}_{\text{splay}} + \underbrace{\frac{K_2}{2}(\mathbf{p} \cdot [\nabla \times \mathbf{p}])^2}_{\text{twist}} + \underbrace{\frac{K_3}{2}\|\mathbf{p} \times [\nabla \times \mathbf{p}]\|^2}_{\text{bend}} \, \mathbf{d}\Omega$$

Applying the widely used One Constant Approximation(cite 3) $K_1 = K_2 = K_3 = K_o$ and incorporating $\|\mathbf{p}\| = 1$ allows us to simplify this energy functional to

$$E = \int_\Omega \frac{K_0}{2}\|\nabla \mathbf{p}\|_F^2 \, \mathbf{d}\Omega \tag{1}$$

$$\|\nabla \mathbf{p}\|_F^2 = \sum_{ij} (\nabla_i \mathbf{p}_j)^2 \tag{2}$$

For time beeing we consider only passive dynamics(without external forces, continously driving the system) relaxating from an intial state to the equilibrium. Please note that in this type of dynamics the resting points/equilibrium manifold of the system are also defined by a solution of a constraint minimization problem

$$\text{find } \mathbf{p} \quad \text{such that :} \tag{3}$$

$$\min E(\mathbf{p}) \text{ and} \tag{4}$$

$$\|\mathbf{p}\| = 1 \tag{5}$$

$$\text{furthermore for surface } \mathbf{p} \cdot \mathbf{n} = 0 \tag{6}$$

The solution to (3) is smooth beside a zero-meassured set of isolated points[2] called defects $\{\tilde{\mathbf{x}}_i\}_i$. At this points at least one of the state constraints on $\mathbf{p}$ is void. The amount of defects dictated by choosen boundary conditions and topological properties of the domain/surface. Further this defects can be endowed with a characteristic number, called Index $\mathbf{Ind}(\tilde{\mathbf{x}})$ (cite). For director fields exists three basic types called vortex, source/sink and saddle. In special case of closed surfaces Poincare Hopf theorem(cite) states that any director field must satisfy $\sum_i \mathbf{Ind}(\tilde{\mathbf{x}}_i) = \chi(S)$, where $\chi(S)$ is the Euler characteristic of the surface(an overview of Euler characteristics see appendix).

Figure 1: types of defects: vortex, source/sink and saddle point

2.1 Diffuse Domain Modelling

What is Diffuse Domain: The proposed approach bases on the diffuse interface approach for domain description. Central idea in our approach is to embed the relevant domain Ω in a favorable shaped domain $\tilde{\Omega}$ and to approximate the boundary between Ω and $\tilde{\Omega} \setminus \Omega$ by a diffuse interface. Using a suitable smooth phase field function we can asymptotically express the charcteristic function χ_Ω by

$$\begin{aligned} \phi(\mathbf{x}) &= \frac{1}{2}\left(\tanh\left(\frac{d(\mathbf{x},\Omega)}{2\epsilon_\phi}\right)\right) \\ \chi_\Omega(\mathbf{x}) &= \lim_{\epsilon_\phi \to 0} \phi(\mathbf{x}) \end{aligned}$$

Motivation: Main advantage of this kind of numerical approach is that surfaces can be defined easyly(by a suitable distance field) and we do not have to discriminate between surface or domain. This comes in handy for surface/-domain evolutions involving strong deformations or topological changes.

Modell Equations Beside this implicite treatment of the domain we follow the explicit domain approach and enforce the constraints on $\mathbf{p}$ by using penality terms. Namely we add following terms to the energy functional

$$\begin{gathered} \phi\frac{K_n}{4}\left(\|\mathbf{p}\|^2 - 1\right)^2 \\ \phi\frac{K_t}{2}\|\mathbf{p}\cdot\mathbf{n}\|^2 \ , \ \mathbf{n} = \frac{\nabla\phi}{|\nabla\phi|} \end{gathered}$$

Both penality Terms have been restricted to the relevant domain, which allows us to negelect $\mathbf{p} = 0 \ \forall \mathbf{x} \notin \Omega$ and prescribe homogeneous Neumann boundary conditions on the containing domain $\Omega \subset \tilde{\Omega}$ ($\tilde{\Omega}$ ussually a box shaped domain).

$$E = \int_\Omega \phi\frac{K_0}{2}\|\nabla\mathbf{p}\|_F^2 + \phi\frac{K_n}{4}\left(\|\mathbf{p}\|^2 - 1\right)^2 + \phi\frac{K_t}{2}\|\mathbf{p}\cdot\mathbf{n}\|^2 \, \mathbf{d}\Omega \tag{7}$$

This form of the energy functional can also be motivated by applying the diffuse domain formulation(introduced in cite 3) to the governing/evolution equations

$$\begin{aligned} \frac{\partial\mathbf{p}}{\partial t} = h = -\frac{\delta e}{\delta\mathbf{p}} &\qquad S(t) \\ \frac{\partial\phi\mathbf{p}}{\partial t} = \phi h = -\frac{\delta\phi e}{\delta\mathbf{p}} &\qquad \Omega \\ \int_\Omega \phi e \, \mathbf{d}\Omega = \int_{S(t)} e \, \mathbf{d}S(t) & \end{aligned}$$

Considering the cases of stationary and time dependent phasefields we obtain

evolution equation

$$\frac{\partial \phi \mathbf{p}}{\partial t} = \phi \frac{\partial \mathbf{p}}{\partial t} \qquad \phi = \phi(\mathbf{x})$$
$$\frac{\partial \phi \mathbf{p}}{\partial t} = \phi \frac{\partial \mathbf{p}}{\partial t} + \mathbf{p} \frac{\partial \phi}{\partial t} \qquad \phi = \phi(\mathbf{x}, t)$$

With this extended/diffuse free energy functional the evolution equations(for stationary phasefields) reads as

$$\tilde{\phi} \frac{\partial \mathbf{p}}{\partial t} - \tilde{\phi} K_o \triangle \mathbf{p} \tag{8}$$
$$+\phi K_t \left(\frac{\nabla \phi}{|\nabla \phi|} \otimes \frac{\nabla \phi}{|\nabla \phi|}^T \right) \cdot \mathbf{p} + \phi K_n \left(\|\mathbf{p}\|^2 - 1 \right) \mathbf{p} = \quad 0 \quad \tilde{\Omega} \tag{9}$$
$$\frac{\partial \mathbf{p}}{\partial \mathbf{n}} = \quad 0 \quad \tilde{\Gamma} \tag{10}$$

For numerical solution procedures the phase has been regularized for time derivative and laplace term ($\tilde{\phi} = \max(\phi, 10e-4)$) and a linearization of $\left(\|\mathbf{p}\|^2 - 1 \right) \mathbf{p}$ has been applied, for details see Appendix.

Demarcated numerical approximations between explicit domain and spherical harmonics modelling(detailes descripiton of these methods see appendix A).

- spherical harmonics: $\mathbf{p} \in TS$, so single penality term for $\|\mathbf{p}\| = 1$
- explicit domain: $\mathbf{p} \in \mathcal{R}^3$, penality terms for $\|\mathbf{p}\| = 1$ and tangential direction $\mathbf{p} \cdot \mathbf{n} = 0$
- diffuse domain: dynamics as in explicit domain(two penality terms) but domain is asymptotically described by phasefield

To solve the approaches of explicit and diffuse domain we use finite Elements on hierarchic adaptive meshes provided by `AMDiS` .

2.2 Modell Validation - Minimal Energy Configurations on Unit Sphere

We compare the modell with analytical known directorfield with minimal defect configuration of source sink type on the unit sphere. For the unit sphere a energy minimal director field satisfying (3) with source/sink defect configuration(along z axis) can be described by

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

To investigate convergence of out modell torwards this state we consider two asymptotics. First asymptotic we let $\epsilon_\phi \to 0$ to approach the explicit surface/sharp interface limit and second we ramp up $K_t = K_n$ to approach the

constraints $\|\mathbf{p}\| = 1$ and $\mathbf{p} \cdot \mathbf{n} = 0$. Throughout the calculations we keep a fixed $K_o = 1$
We perform several simulations starting at noise director field until engery relaxes. From this simulations we select the minimal energy director field configurations exhibiting the source/sink defect configuration. Due to the rotational invariance of the analytical configurations we rotate the evaluated configuration to match the defect axis(source-sink) with z-Axis and compute the L^2 difference between analytical and evaluated configuration.

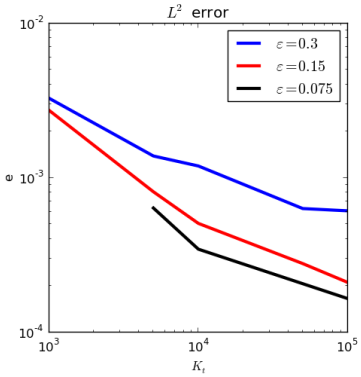

Figure 2: L^2 error vs $K_t = K_n \to \infty$ and $\epsilon_\phi \to 0$

2.3 Modell Validation - Defect Trajectories on Unit Sphere

As second approach to validate our modell we compare defect trajectories on the unit sphere. By choosing a suitable initial value we define a predictable/well defined final equilibrium state. For comparision we use two established numerical schemes, namely the epxlicit domain formulation and the formulation in spherical harmonics.
As initial Value we define a non minimum energy director field with four defects summing up to the correct topological charge of 2. Namely two sinks(each +1), one source +1 and a saddle point −1 arranged on the great circle of the xy plane. To prescribe the final state we position the saddle point a bit closer($\tilde{\lambda}$) to one sink.
This initial value is obtained by evaluating a preliminary director field $\mathbf{e}$ which is projected into tangential space and normalized afterwards.

$$\begin{array}{rcl} |x_2| \geq \cos\frac{\pi}{4} & : & \mathbf{e} = [-x_1, 0, -x_3]^T \\ x_1 \geq \cos\frac{\pi}{4} & : & \mathbf{e} = [0, x_2, x_3]^T \\ x_1 \leq -\cos\frac{\pi}{4} & : & \mathbf{e} = \left[0, \sin\left(\pi\left(x_2 - \tilde{\lambda}\right)\right), -\sin\left(\pi x_3\right)\right]^T \\ \text{otherwise} & : & \mathbf{e} = \left[|x_2/\cos\frac{\pi}{4}| - 1, x_2/\cos\frac{\pi}{4}, 0\right]^T \end{array}$$

This initial configuration will converge to a minimum energy configuration consiting of a source and sink configuration(still located in XY plane). In the transient saddle point and the closer sink will annihilate each other.

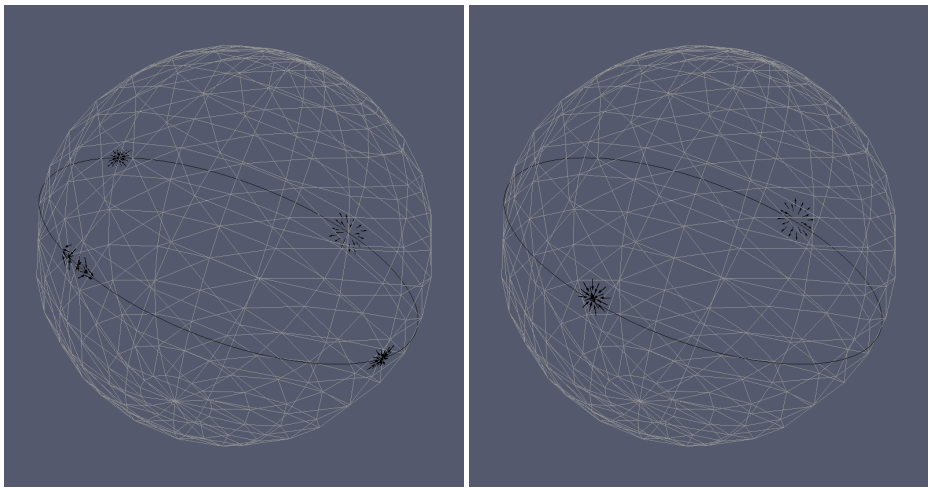

Figure 3: intial and final defects on sphere

In the modell we use penality coefficients as $K_o = 1$ and $K_t = K_n = 1000$, and for the initial value $\tilde{\lambda} = 0.01$
To compare the results of the three modells we plot the trajectories of the four defects in the XY plane via the azimuthal angle φ_i over time

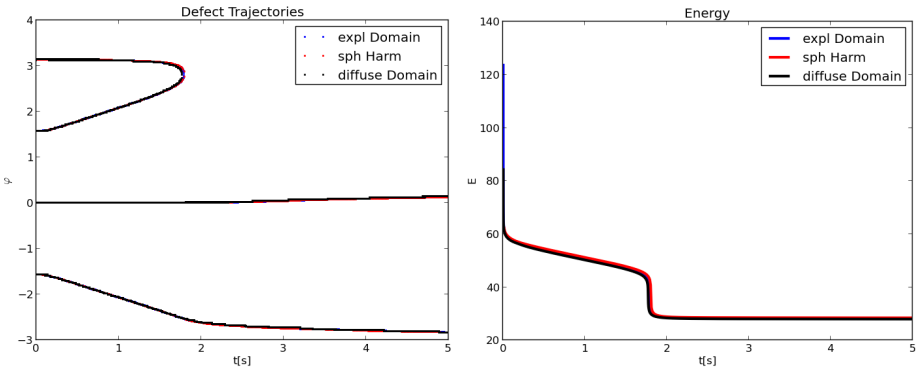

Figure 4: Defect Trajectories in XYplane, Energies

- dynamics of defects match: critical event of annihilation of saddle and source defect is reproduced, final configurations match
- energy transients match
- diffuse domain parameters???

3 Application - Surface Evolution and Defect Position

3.1 Sphere to Ellipsoid and Defect Repositioning

3.2 Shell Coalescence

From [3] we know series of axissymetric surfaces describing the process of coalescence of two shells(by a single coalescence factor). We use this to investigate the defect position on each surface. This matches a evolution with decoupled dynamics of surface evolution(slow) and orientation field relaxation(fast).

3.3 Coupling Cahn Hilliard and Orientation Fields

3.3.1 Decoupled Shell Coalesence and Director Fields

We use the well known Cahn-Hilliard equations to describe a surface evolution towards a minimal surface/interface while preserving the initial volume. As model problem we will investigate the coalesence of two seperated spherical shells. We assume director field evolution as fast compared to the surface evolution, leading to a decoupling of those evolutions and a scenario closely related to the one discused in section 3.2
Finally we compare the coalesence driven by decoupled Cahn-Hilliard surface evolution with a coalesence driven by coupled Cahn-Hilliard and Director Field evolution(modell see below).
Additional Test, limit case with surface evolution and director field both fast.
The surface/interface evolution of Cahn Hilliard is defined by energy minimization while conserving the quanitity $\int_\Omega c \, \mathbf{d}\Omega$. c can be interpreted e.g. as the (diffuse) domains two inmiscible fluids in Ω where $c = 1$ denotes the one fluid while $c = 0$ indicates the other fluid.

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

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

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

Please note that an intuitive approach by choosing $\frac{\partial c}{\partial t} = -\frac{\delta e_C}{\delta c}$ would not preserve $\int_\Omega c \, \mathbf{d}\Omega$. Therefore we choose a Onsager Coefficient of $D\triangle\left(.\right)$ to obtain Fick's law of diffusive transport(which is mass conserving) as evolution equation.
We introduced the Parameter K_c which can be interpreted as a relaxation parameter defining the speed of interface evolution. Namely for $K_c \ll 1$ we have slow/dampend evolution.

3.3.2 Coupling Cahn Hilliard Surface Evolution and Director Field

Instead of using a prescribed phase field ϕ to define a surface we use the result of the diffuse interface evolution equation of Cahn-Hilliard. We use the diffuse

interface between the two fluids given by $B(c) = 36/\gamma\,(1-c)^2\,c^2$ as phase field for the director field evolution. A suitable energy functional combining those evolution reads as

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

Applying the Onsager scheme and identifing fluxes of system with $\frac{\partial c}{\partial t}$ and $\frac{\partial B(c)\mathbf{p}}{\partial t}$ we obtain conjugated forces μ and $h = -\frac{\delta e_{\mathbf{p}}}{\delta \mathbf{p}}$(molecular field). Since the interface $B(c)$ is time dependent we arrive at following director field flux term

$$\frac{\partial B(c)\,\mathbf{p}}{\partial t} = B(c)\,\frac{\partial \mathbf{p}}{\partial t} + \frac{36}{\gamma}\left(4c^3 - 2c\right)\mathbf{p}\ \underbrace{\frac{\partial c}{\partial t}}_{\approx O(K_C)}$$

Assuming dynamics close to equilibrium we can apply linear response coupling between flux and forces and yield following couplings

$$\begin{aligned}\frac{\partial c}{\partial t} &= D\triangle\mu && +\Lambda\mathbf{p}\cdot h\\ \frac{\mathrm{D}\mathbf{p}}{\mathrm{D}t} &= \Lambda\mathbf{p}\mu && +h\end{aligned}$$

Please note that by the parities of fluxes$(-1,-1)$ and forces $(+1,+1)$ all couplings are dissipative. Considering the rate of dissipation in this evolution we obtain

need to be fixed

$$\Pi = -\left(D\left(\triangle\mu\right)^2 + h^2 + \underbrace{\Lambda\mathbf{p}\cdot h\triangle\mu}_{*}\right)$$

To ensure $\Pi < 0\ \forall t, \mathbf{x}$ we set $\Lambda = 0$. This choice of Λ also preserve the conservation of $\int_\Omega c\ \mathbf{d}\Omega$. Coupling of Surface evolution and director field is therefore limited to the chemical potential and the director field flux term(using c evolution equation).

$$\mu = \left(c^3 - c\right)\left(K_c + \frac{K_o}{2}\|\nabla\mathbf{p}\|_F^2 + \frac{K_n}{4}\left(\|\mathbf{p}\|^2 - 1\right)^2 + \frac{K_t}{2}\|\mathbf{p}\cdot\mathbf{n}\|^2\right) - K_c\gamma\triangle c$$
$$\frac{\partial B(c)\,\mathbf{p}}{\partial t} = B(c)\,\frac{\partial \mathbf{p}}{\partial t} + \left(\frac{36}{\gamma}\left(4c^3 - 2c\right)D\triangle\mu\right)\mathbf{p}$$

By this coupling the chemical potential is significantly reinforced at the defect. Considering the case(prevalent in our modelling) defects are expressed by $\|\mathbf{p}\| \approx 0$ we obtain a chemical Potential(in defect core region $\|\nabla\mathbf{p}\|_F^2 \approx 1$) as follows:

$$\mu = \left(c^3 - c\right)\left(K_c + \frac{K_o}{2} + \frac{K_n}{4}\right) - K_c\gamma\triangle c$$

With this formulation we expect the surface evolution to be drastically accelerated at defect locations(explicit modelling would involve $K_t = K_n \to \infty$!). In the limit case $K_c \ll K_o \ll K_n \approx K_t$ the surface evolution would be solely driven by the position of defects. The signifcant reinforcment of μ at defect locations will also lead to increased values of $D\triangle\mu$ which will have an impact on the director field fluxes, emphasising the structural difference of this modelling compared to the decoupled Evolution(described in 3.3.1)

A Orientation Fields on Unit Sphere by Spherical Harmonics and Explicit Domain Modelling

B Displacement Field for Interface Evolution

Coupling Navier Stokes and Cahn Hilliard we have the evolution equation(reactive coupling of μ and $\mathbf{v}$,see [1] for $D\triangle\mu = \nabla \cdot B(c)\nabla\mu$, D is usually set to almost zero to consider pure transport of the interface)

$$\frac{\partial c}{\partial t} = \underbrace{D\triangle\mu}_{1} - \underbrace{\mathbf{U}\cdot\nabla c}_{2}$$

For $D \neq 0$ the two terms can be interpreted as mean curvature flow(1) and normal transport(2) which together make up the interface Velocity $\mathbf{v}$

C Linearization of Diffuse Domain Evolution Equations

$$\begin{aligned} & \left(\|\mathbf{p}\|^2 - 1\right)\mathbf{p}_i \\ \approx\ & \|\tilde{\mathbf{p}}\|^2\tilde{\mathbf{p}}_i - \tilde{\mathbf{p}}_i + \left[\nabla\left(\|\tilde{\mathbf{p}}\|^2\tilde{\mathbf{p}}_i - \tilde{\mathbf{p}}_i\right)\right](\mathbf{p}_i - \tilde{\mathbf{p}}_i) \\ =\ & \sum_j \left[\tilde{\mathbf{p}}_j^2\mathbf{p}_i + 2\tilde{\mathbf{p}}_j\tilde{\mathbf{p}}_i\mathbf{p}_j\right] - \mathbf{p}_i - \sum_j \left[2\tilde{\mathbf{p}}_i\tilde{\mathbf{p}}_j^2\right] \end{aligned}$$

D Euler Characteristics for Surfaces

Table 1: topological charge for several surfaces

References

[1] S. Aland, John Lowengrub, and Axel Voigt. Two-phase flow in complex geometries: A diffuse domain approach. *CMES*, 57(1):77–108, 2010.

[2] Mark J. Bowick and Luca Giomi. Two-dimensional matter: order, curvature and defects. *Advances in Physics*, 58(5):449–563, 2009.

[3] Venkateshwarlu Yadha and Joseph J. Helble. Modeling the coalescence of heterogenous amorphous particles. *Journal of Aerosol Science*, 35(6):665 – 681, 2004.