An Angular Momentum Method for the Wave Map to the Sphere

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The Problem

We want to develop a numerical method to simulate wave maps to the sphere. By *wave maps* we mean vector functions $d = (d_1, d_2, d_3)$ satisfying the constrained wave equation

$$d_{tt} - \Delta d = \gamma d, \quad |d| = 1, \quad \text{in } (0,\infty) \times \Omega, \tag{1}$$

$\Omega = [0,1]^n$ or $\Omega = \mathbb{T}^n$, $n = 2,3$ with periodic or Neumann boundary conditions.

- γ is a Langrange multiplier enforcing $|d| = 1$.
- Dotting (1) with d, we find $\gamma = |\nabla d|^2 - |d_t|^2$, so (1) is higly nonlinear.
- Singularities may develop in the solutions, cf. Figure 3.
- Ensuring that numerical approximations conserve the constraint and a discrete version of the energy is crucial to obtain a stable method.

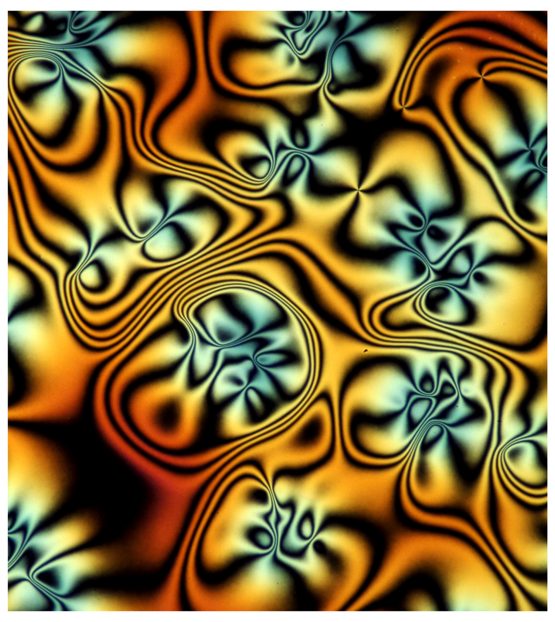

Figure 1: Defects (singularities in d) in a nematic liquid crystal

Application: Liquid Crystals

Nematic liquid crystals are materials that exhibit intermediate states between the liquid and the solid phase. They consist of elongated molecules that tend to align along the same axis, [3].

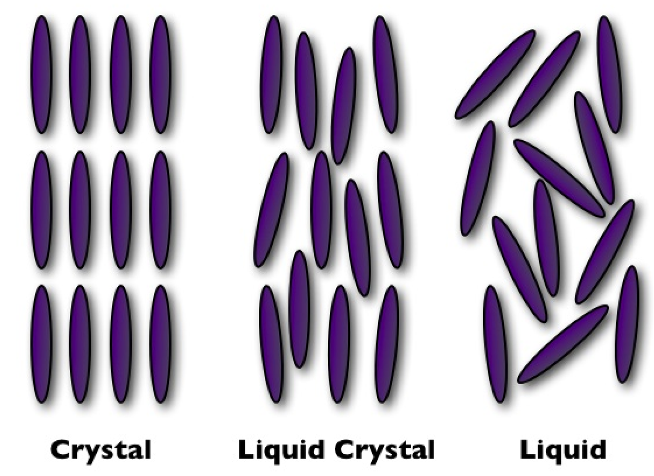

Figure 2: Schematic view of the molecules of a liquid crystal

- The *director field* $d(x)$ describes this main orientation of the molecules.
- Its dynamics can be described by the Euler-Lagrange equations corresponding to the *Oseen-Frank elastic energy*,

$$W_{OF} = \frac{1}{2}K_1(\nabla \cdot d)^2 + \frac{1}{2}K_2(d \cdot (\nabla \times d))^2 + \frac{1}{2}K_3(d \times (\nabla \times d))^2,$$

  where K_1, K_2, and K_3 are material constants, including inertia effects.
- (1) corresponds to the special case when $K_1 = K_2 = K_3 = 1$, the *one-constant approximation*.

The Method

We introduce the *angular momentum* $w = d_t \times d$, so that the wave map equation (1) can be reformulated as

$$\begin{aligned} d_t &= d \times w, \\ w_t &= \Delta d \times d. \end{aligned} \tag{2}$$

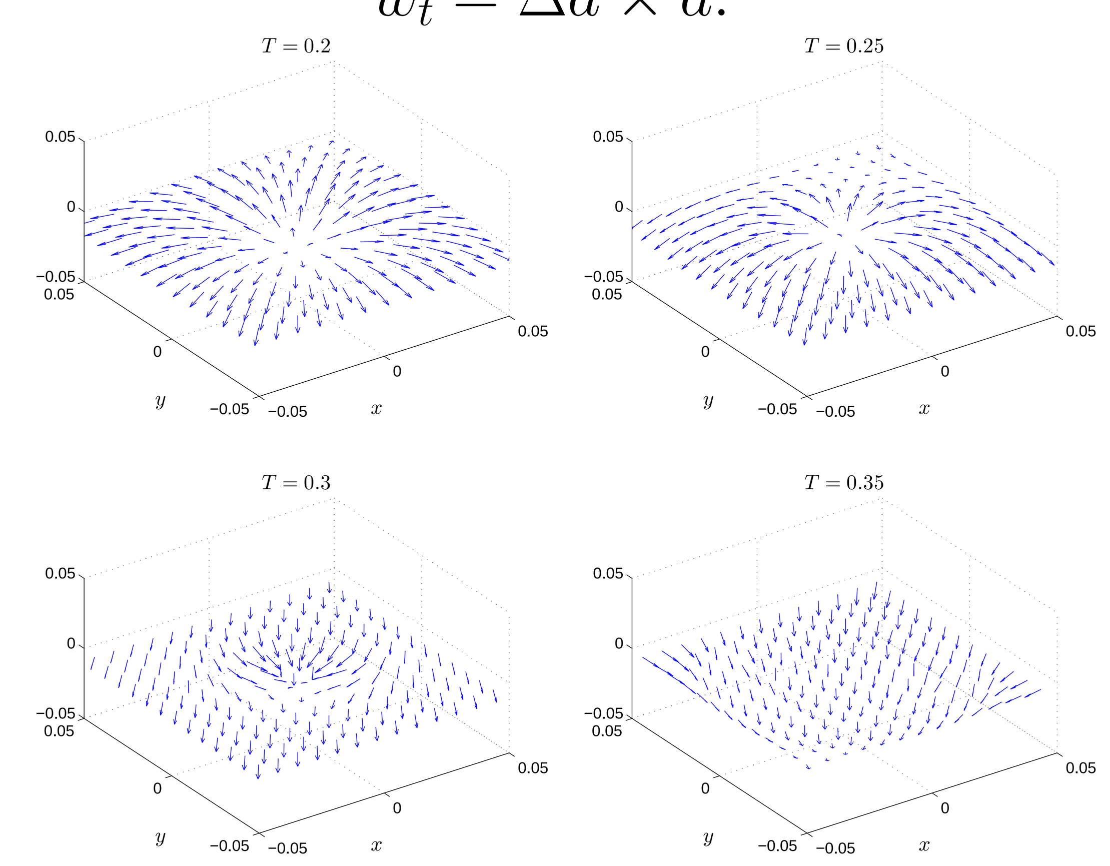

Figure 3: The approximation of (2) by the difference method (4) for an initial data developing a singularity at $x = 0$, $N = 2^7$; [2].

- Preservation of the constraint $|d| = 1$ is inherit in the equation, no need for Lagrange multiplier.
- The energy $\mathcal{E}$ is formally preserved,

$$\mathcal{E}(t) := \int_\Omega \left(|w|^2 + |\nabla d|^2\right)(t)dx = \mathcal{E}(0). \tag{3}$$

- It can easily be cast into a finite difference method:

$$\begin{aligned} \frac{d_{\underline{i}}^{m+1} - d_{\underline{i}}^m}{\Delta t} &= d_{\underline{i}}^{m+1/2} \times w_{\underline{i}}^{m+1/2}, \\ \frac{w_{\underline{i}}^{m+1} - w_{\underline{i}}^m}{\Delta t} &= \Delta_{\underline{i}}\, d_{\underline{i}}^{m+1/2} \times d_{\underline{i}}^{m+1/2}, \end{aligned} \tag{4}$$

  where $f^{m+1/2} := \frac{f^m + f^{m+1}}{2}$ is the average of two time steps, $f_{\underline{i}}^m \approx f(m\Delta t, x_{\underline{i}})$, $x_{\underline{i}} := x_{i,j,k} = (ih, jh, kh)$, for time step and grid sizes $\Delta t, h > 0$, and $\Delta_{\underline{i}}$ is a standard discretization of the Laplace operator.

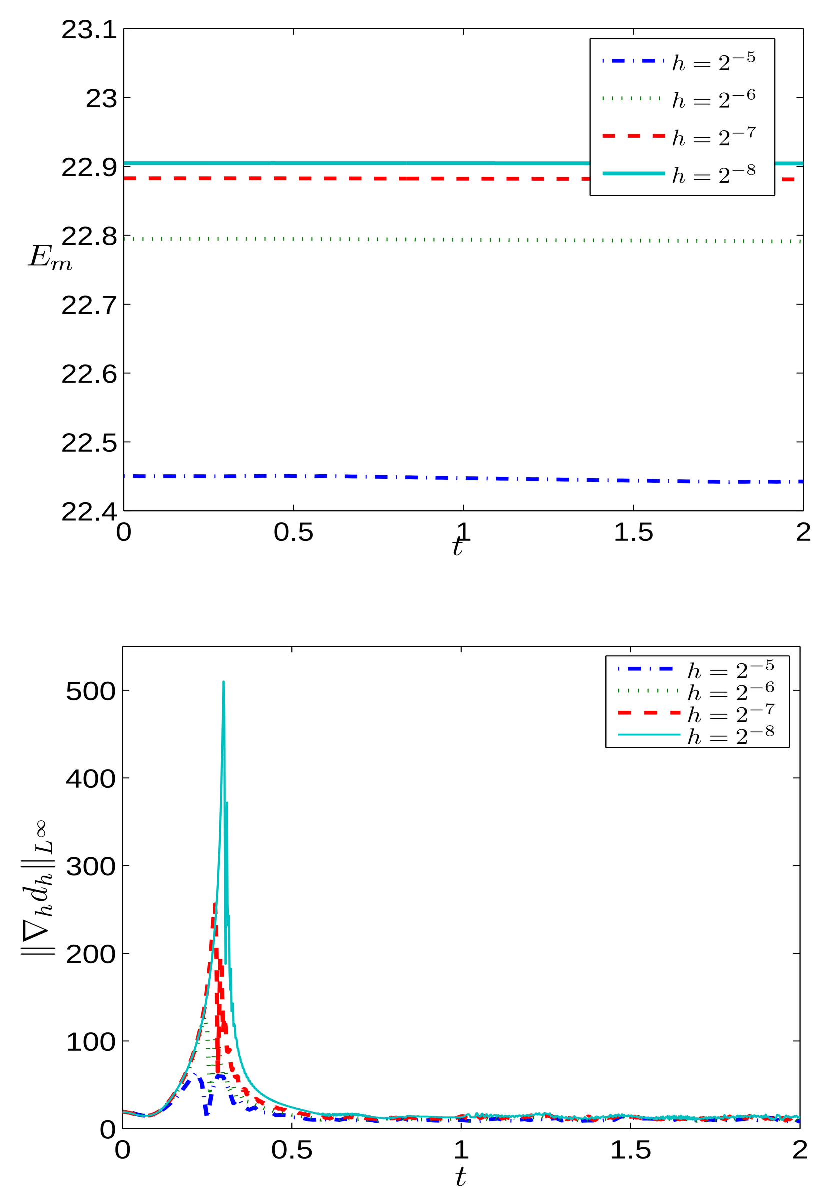

Figure 4: The evolution of the discrete energy $\mathcal{E}_m$ and the maximum of the gradient versus time for the same data as in Figure 3.

Future research directions

- Extension of the angular momentum method to general coefficients $K_1 \neq K_2 \neq K_3$,
- Inclusion of effects of electric and magnetic fields on liquid crystal dynamics and extend the work of [1],
- Incooperation of damping terms in the wave equation,
- Coupling of the director field with the convection by the flow of the fluid.

Conclusions

- The method conserves a discrete version of the energy, (3).
- The constraint $|d| = 1$ is satisfied at every gridpoint, that is, $|d_{\underline{i}}^m| = 1$ for all m and $\underline{i}$.
- Approximations can be shown to converge to a weak solution of (2).
- Fixpoint iteration can be used to solve the nonlinear system (4) in $\mathcal{O}(N^n \log N)$ operations up to a tolerance N^{-2}, N the number of degrees of freedom in one space dimension, linear stability condition for the time stepping: $\Delta t \leq CN^{-1}$, $C > 0$ a constant.
- The method is able to capture effects such as blow-up of solutions, cf. Figure 3.

Bibliography

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