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Numerical simulation of liquid crystals

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Abstract. We consider the numerical simulation of nematic liquid crystal flows, modeled by a simplified version of [2] the Ericksen-Leslie model, imposing a nonconvex constraint on the director field. Computational experiments are used to compare the two approaches.

Keywords: Nematic liquid crystals, Ericksen-Lislie model, harmonic map heat flow, finite element method, discrete scheme.

AMS classification: 65M12, 65M60, 35K55, 35Q35.

§1. Introduction

In this paper, we consider a simplified version of the Ericksen- Leslie model, see for example Lin and Liu [2]. This model is a modified Navier- Stokes system that takes into account the liquid crystallinity, coupled with the Ginzburg-Landau equations.

$$\mathbf{v}_t - \nu\,\Delta\mathbf{v} + (\mathbf{v}.\nabla)\mathbf{v} + \nabla p + \lambda\,\nabla\cdot(\nabla\mathbf{d}\odot\nabla\mathbf{d}) = 0 \qquad \text{in } \Omega_T := (0,T)\times\Omega, \tag{1}$$

$$\mathbf{d}_t + (\mathbf{v}.\nabla)\mathbf{d} - \gamma\Delta\mathbf{d} = \gamma|\Delta\mathbf{d}|^2\mathbf{d} \qquad \text{in } \Omega_T, \tag{2}$$

$$\nabla\cdot\mathbf{v} = 0 \qquad \text{in } \Omega_T, \tag{3}$$

and the nonconvex constraint

$$|\mathbf{d}(t,x)| = 1, \tag{4}$$

and with the initial and boundary conditions

$$\mathbf{v}(0,\mathbf{x}) = \mathbf{v}_0(\mathbf{x}), \qquad \mathbf{d}(0,\mathbf{x}) = \mathbf{d}_0(\mathbf{x}), \quad \forall\mathbf{x}\in\Omega. \tag{5}$$

$$\mathbf{v}(t,\mathbf{x}) = 0, \qquad \partial_{\mathbf{n}}\mathbf{d}(t,\mathbf{x}) = 0, \qquad \forall(t,\mathbf{x})\in\partial\Omega_T. \tag{6}$$

The unknowns are the time-dependent divergence-free velocity field $\mathbf{v}(t,\mathbf{x})$, the pressure $p(t,\mathbf{x})$ of the fluid and the director field $\mathbf{d}(t,\mathbf{x})$ representing the orientation of the liquid crystal molecules. The fluid is confined in an open bounded domain Ω of $\mathbb{R}^3$ with a lipschitz boundary $\partial\Omega$. In the above, the vector $\mathbf{n}$ denotes the outward pointing unit normal and the matrix product is defined as

$$(\nabla\mathbf{d}\odot\nabla\mathbf{d})_{ij} = \sum_{k=1}^{2}\frac{\partial\mathbf{d}_k}{\partial\mathbf{x}_i}\frac{\partial\mathbf{d}_k}{\partial\mathbf{x}_j}.$$

The constraint (4) causes difficulties from both analytical and numerical points of view. A widely used approach is to approximate this constraint by a penalty function such as the

Ginzburg-Landau approximation $\mathbf{f}_\epsilon(\mathbf{d}) = \epsilon^{-2}(|\mathbf{d}|^2 - 1)\mathbf{d}$, for $0 < \epsilon \ll 1$. This penalisation function exhibits a potential structure, i.e., there exists a potential function $\mathbf{F}_\epsilon(\mathbf{d}) = \frac{\epsilon^{-2}}{4}(|\mathbf{d}|^2 - 1)^2$ such that $\mathbf{f}_\epsilon(\mathbf{d}) = \nabla_{\mathbf{d}}(\mathbf{F}_\epsilon(\mathbf{d}))$.
Accordingly, the penalised model reads as

$$\mathbf{v}_t - \nu\,\Delta\mathbf{v} + (\mathbf{v}.\nabla)\mathbf{v} + \nabla p + \lambda\,\nabla\cdot\,(\nabla\mathbf{d}\odot\nabla\mathbf{d}) = 0 \qquad \text{in } \Omega_T := (0,T)\times\Omega, \tag{7}$$

$$\mathbf{d}_t + (\mathbf{v}.\nabla)\mathbf{d} - \gamma(\Delta\mathbf{d} - \mathbf{f}_\epsilon(\mathbf{d})) = 0 \qquad \text{in } \Omega_T, \tag{8}$$

$$\nabla\cdot\mathbf{v} = 0 \qquad \text{in } \Omega_T, \tag{9}$$

subject to the initial and the boundary conditions (5) and (6).

Two fully discrete finite element methods for the system (1)-(3) and (7)-(9) have been recently studied by R. Becker, X. Feng, and A. Prohl [1], where the convergence of finite element approximations is established but the schemes do not satisfy the constraint (4). In this note, we are interested in a modification satisfying this contraint.

The paper is organized as follows. In the next section, we recall the energy estimates proven by Lin and Liu [2]. In section 3, we develop our modified scheme and in section 4, we prove that this scheme satisfies the constraint (4). Computational examples are given to prove the efficiency of the method.

§2. Energy estimates

It was observed in [2] that by using the differential identity $\nabla\cdot(\nabla\mathbf{z}\odot\nabla\mathbf{z}) = (\nabla\mathbf{z})^T\Delta\mathbf{z} + \frac{1}{2}\nabla(|\nabla\mathbf{z}|^2)$, the equation (7) can be rewritten as follows:

$$\mathbf{v}_t - \nu\,\Delta\mathbf{v} + (\mathbf{v}.\nabla)\mathbf{v} + \nabla p + \frac{\lambda}{2}\,\nabla(|\nabla\mathbf{d}|^2) + \lambda(\nabla\mathbf{d})^T\Delta\mathbf{d} = 0. \tag{10}$$

Notice that the term $\frac{\lambda}{2}\,\nabla(|\nabla\mathbf{d}|^2)$ can be absorbed into the definition of the pressure. Hence the system (7)–(9) satisfies the following basic energy law:

$$\frac{dE}{dt} = -\Big(\nu\|\nabla\mathbf{v}\|^2_{L^2(\Omega)} + \lambda\gamma\|\Delta\mathbf{d} - \mathbf{f}_\epsilon(\mathbf{d})\|^2_{L^2(\Omega)}\Big), \tag{11}$$

where

$$E = \frac{1}{2}\|\mathbf{v}\|^2_{L^2(\Omega)} + \frac{\lambda}{2}\|\nabla\mathbf{d}\|^2_{L^2(\Omega)} + \lambda\int_\Omega \mathbf{F}_\epsilon(\mathbf{d}).$$

This estimate was used by Lin and Liu [2] to establish existence, uniqueness and regularity of solutions to the coupled liquid crystal problem. The energy law (11) is obtained by multiplying the equation (10) by $\mathbf{v}$ and the director equation (8) by $-(\Delta\mathbf{d} - \mathbf{f}_\epsilon(\mathbf{d})$ and adding the two. The crucial observation is that the main term from the momentum equation $\nabla\mathbf{d}^T(\Delta\mathbf{d})\cdot\mathbf{v}$, cancels with the convective term $(\mathbf{v}\cdot\nabla)\mathbf{d}\cdot(-\Delta\mathbf{d}) = -\nabla\mathbf{d}^T(\Delta\mathbf{d})\mathbf{v}$ in the director equation. We have also, by using the facts $\operatorname{div}\mathbf{v} = 0$ and $\mathbf{v} = 0$ on $\partial\Omega$, that

$$\int_\Omega (\mathbf{v}\cdot\nabla)\mathbf{v}\cdot\mathbf{v}\,\mathrm{d}\mathbf{x} = \int_\Omega \mathbf{v}\cdot\nabla p\,\mathrm{d}\mathbf{x} = \int_\Omega (\mathbf{v}\cdot\nabla)\mathbf{d}\cdot\mathbf{f}_\epsilon(\mathbf{d})\,\mathrm{d}\mathbf{x} = \int_\Omega \mathbf{v}\cdot\nabla\Big(\frac{|\mathbf{d}|^2}{2}\Big)\,\mathrm{d}\mathbf{x} = 0.$$

§3. Fully discrete finite element methods for the Ericksen-Leslie model

We assume that $\mathcal{T}_h$ is a quasi-uniform triangulation of a bounded polygonal domain $\Omega \subset \mathbb{R}^2$ into triangles of diameter $h > 0$, i.e., $\overline{\Omega} = \bigcup_{K \in \mathcal{T}_h} \overline{K}$. Let $\mathcal{N}_h$ denote the set of all nodes of $\mathcal{T}_h$. We introduce the space

$$\mathbf{Y}_h = \left\{ \mathbf{a}_h \in C(\overline{\Omega}, \mathbb{R}^2) : \mathbf{a}_h|_K \in P_1(K, \mathbb{R}^2) \right\},$$

and $\mathcal{I}_h : C(\overline{\Omega}, \mathbb{R}^2) \longrightarrow \mathbf{Y}_h$: the nodal interpolation operator such that $\mathcal{I}_h \Phi = \sum_{\mathbf{z} \in \mathcal{N}_h} \Phi(\mathbf{z}) \varphi_{\mathbf{z}}$, where $\{\varphi_{\mathbf{z}} : \mathbf{z} \in \mathcal{N}_h\} \subset \mathbf{Y}_h$. Choose

$$\mathbf{X}_h = \left\{ \mathbf{v}_h \in C^0(\overline{\Omega}, \mathbb{R}^2) \cap H_0^1(\Omega, \mathbb{R}^2); \mathbf{v}_h/K \in P_2(K, \mathbb{R}^2) \right\},$$
$$M_h = \left\{ q_h \in \mathbf{L}_0^2(\Omega);\ q_h/K \in P_0(K) \right\},$$

and

$$\mathbf{V}_h = \{ \mathbf{v}_h \in \mathbf{X}_h :\ (\operatorname{div} \mathbf{v}_h, q_h) = 0\ \forall q_h \in M_h \}.$$

In the following, we use the L^2-orthogonal projections $Q_{\mathbf{Y}_h} : \mathbf{L}^2(\Omega, \mathbb{R}^2) \longrightarrow \mathbf{Y}_h$, $Q_{\mathbf{V}_h} : \mathbf{L}^2(\Omega, \mathbb{R}^3) \longrightarrow \mathbf{V}_h$ and the H^1-orthogonal projection $R_h : H^1(\Omega, \mathbb{R}^2) \longrightarrow \mathbf{Y}_h$.

In [1], the authors study a first fully discrete finite element approximation for the regularized problem (7)-(9), which uses the couple $(\mathbf{X}_h, M_h)$ of finite dimensional spaces for the velocity and for a new pressure $\widetilde{p} = \hat{p} + \lambda \mathbf{F}_\epsilon(\mathbf{d})$, where $\hat{p} = p + \frac{\lambda}{2} |\nabla \mathbf{d}|^2$.

Algorithm 1.

(1) Set $\mathbf{v}_h^0 := Q_{\mathbf{V}_h} \mathbf{v}_0{}^\epsilon$ and $\mathbf{d}_h^0 := R_{\mathbf{Y}_h} \mathbf{d}_0^\epsilon$.

(2) For $m = 1, ..., M$, let $\mathbf{f}_h^m := \left| \mathbf{d}_h^m \right|^2 \mathbf{d}_h^m - \mathbf{d}_h^{m-1}$. *Find* $(\mathbf{v}_h^m, \mathbf{d}_h^m, \tilde{p}_h^m, \mathbf{w}_h^m) \in \mathbf{X}_h \times \mathbf{Y}_h \times M_h \times \mathbf{Y}_h$ *such that, for all* $(\mathbf{u}_h, \mathbf{a}_h, q_h, \mathbf{b}_h) \in \mathbf{X}_h \times \mathbf{Y}_h \times M_h \times \mathbf{Y}_h$,

$$\begin{aligned}
&(d_t\, \mathbf{v}_h^m, \mathbf{u}_h) + \nu (\nabla \mathbf{v}_h^m, \nabla \mathbf{u}_h) + \left((\mathbf{v}_h^{m-1}.\nabla)\, \mathbf{v}_h^m, \mathbf{u}_h \right) + \frac{1}{2} \left((\operatorname{div} \mathbf{v}_h^{m-1})\, \mathbf{v}_h^m, \mathbf{u}_h \right) \\
&\qquad\qquad + (\tilde{p}_h^m, \operatorname{div} \mathbf{u}_h) - \lambda \left((\nabla \mathbf{d}_h^{m-1})^T\, \mathbf{w}_h^m, \mathbf{u}_h \right) = \langle \mathbf{g}(t_m, .), \mathbf{u}_h \rangle, \\
&(d_t\, \mathbf{d}_h^m, \mathbf{a}_h) + \left((\mathbf{v}_h^m.\nabla)\, \mathbf{d}_h^{m-1}, \mathbf{a}_h \right) + \gamma (\mathbf{w}_h^m, \mathbf{a}_h) = 0, \\
&(\operatorname{div} \mathbf{v}_h^m, q_h) = 0, \\
&(\nabla \mathbf{d}_h^m, \nabla \mathbf{b}_h) + (\mathbf{f}_\epsilon^m, \mathbf{b}_h)_h - (\mathbf{w}_h^m, \mathbf{b}_h) = 0.
\end{aligned}$$

Moreover, they have proved that the solution of Algorithm 1 verifies a discrete energy law, see [1] for more details. Next they study the following discrete scheme for the system (1)-(3), where an implicit treatment of the coupling terms is used in contrast to the semi-implicit discretization in Algorithm1. The discrete Laplacian $\Delta_h : W^{1,2}(\Omega) \rightarrow \mathbf{Y}_h$ and a temporal discretisation using the implicit midpoint rule are used.

Algorithm 2.

(1) Let $\mathbf{v}_h^0 := Q_{\mathbf{V}_h} \mathbf{v}^0$ and $\mathbf{d}_h^0 := \mathcal{I}_h\, \mathbf{d}^0$.

(2) Let $m = 1, ..., M$. *Find* $(\mathbf{v}_h^m, \mathbf{d}_h^m, \hat{p}_h^m) \in \mathbf{X}_h \times \mathbf{Y}_h \times M_h$ *such that, for all* $(\mathbf{u}_h, \mathbf{a}_h, q_h) \in \mathbf{X}_h \times \mathbf{Y}_h \times M_h$, *there holds*

$$\begin{aligned}(d_t\, \mathbf{v}_h^m, \mathbf{u}_h) + \nu(\nabla \mathbf{v}_h^m, \nabla \mathbf{u}_h) + \Big((\mathbf{v}_h^{m-1}.\nabla)\, \mathbf{v}_h^m, \mathbf{u}_h\Big) + \frac{1}{2}\,\Big((\operatorname{div} \mathbf{v}_h^{m-1})\, \mathbf{v}_h^m, \mathbf{u}_h\Big)& \\ - (\hat{p}_h^m, \operatorname{div} \mathbf{u}_h) - \lambda\Big((\nabla \mathbf{d}_h^{m-1})^T\, \Delta_h \mathbf{d}^{m-\frac{1}{2}}, \mathbf{u}_h\Big) &= \langle \mathbf{g}(t_m, .), \mathbf{u}_h\rangle, \\ (\operatorname{div} \mathbf{v}_h^m, q_h) &= 0, \\ (d_t\, \mathbf{d}_h^m, \mathbf{a}_h) + \Big((\mathbf{v}_h^m.\nabla)\, \mathbf{d}_h^{m-1}, \mathbf{a}_h\Big) + \gamma\Big(\mathbf{d}_h^{m-\frac{1}{2}} \times (\mathbf{d}_h^{m-\frac{1}{2}} \times \Delta_h \mathbf{d}_h^{m-\frac{1}{2}}),\ \mathbf{a}_h\Big) &= 0,\end{aligned}$$

where $\mathbf{d}_h^{m-\frac{1}{2}} = \frac{1}{2}(\mathbf{d}_h^{m-1} + \mathbf{d}_h^m)$.

A discrete energy law is also proved for the solutions of this scheme. The main contribution in this note is to change the term $\Big((\mathbf{v}_h^m.\nabla)\, \mathbf{d}_h^{m-1}, \mathbf{a}_h\Big)$ in Algorithm 2 by $\frac{1}{2}\Big((\mathbf{v}_h^m.\nabla)\, \mathbf{d}_h^{m-\frac{1}{2}}, \mathbf{a}_h\Big) - \frac{1}{2}(\mathbf{d}^{m-\frac{1}{2}}, \mathbf{v}_h^m.\nabla \mathbf{a}_h)$.

Then, the new Algorithm reads as follows:

Algorithm 3.

(1) Let $\mathbf{v}_h^0 := Q_{\mathbf{V}_h} \mathbf{v}^0$ and $\mathbf{d}_h^0 := \mathcal{I}_h\, \mathbf{d}^0$.

(2) Let $m = 1, ..., M$. *Find* $(\mathbf{v}_h^m, \mathbf{d}_h^m, \hat{p}_h^m) \in \mathbf{X}_h \times \mathbf{Y}_h \times M_h$ *such that, for all* $(\mathbf{u}_h, \mathbf{a}_h, q_h) \in \mathbf{X}_h \times \mathbf{Y}_h \times M_h$, *there holds*

$$\begin{aligned}(d_t\, \mathbf{v}_h^m, \mathbf{u}_h) + \nu(\nabla \mathbf{v}_h^m, \nabla \mathbf{u}_h) + \Big((\mathbf{v}_h^{m-1}.\nabla)\, \mathbf{v}_h^m, \mathbf{u}_h\Big) + \frac{1}{2}\,\Big((\operatorname{div} \mathbf{v}_h^{m-1})\, \mathbf{v}_h^m, \mathbf{u}_h\Big)& \\ - (\hat{p}_h^m, \operatorname{div} \mathbf{u}_h) - \lambda\Big((\nabla \mathbf{d}_h^{m-1})^T\, \Delta_h \mathbf{d}^{m-\frac{1}{2}}, \mathbf{u}_h\Big) &= \langle \mathbf{g}(t_m, .), \mathbf{u}_h\rangle, \\ (\operatorname{div} \mathbf{v}_h^m, q_h) &= 0, \\ (d_t\, \mathbf{d}_h^m, \mathbf{a}_h) + \frac{1}{2}\Big((\mathbf{v}_h^m.\nabla)\, \mathbf{d}_h^{m-\frac{1}{2}}, \mathbf{a}_h\Big) - \frac{1}{2}(\mathbf{d}^{m-\frac{1}{2}}, \mathbf{v}_h^m.\nabla \mathbf{a}_h)& \\ + \gamma\Big(\mathbf{d}_h^{m-\frac{1}{2}} \times (\mathbf{d}_h^{m-\frac{1}{2}} \times \Delta_h \mathbf{d}_h^{m-\frac{1}{2}}),\ \mathbf{a}_h\Big) &= 0,\end{aligned}$$

and with a judicious choice of the test function $\mathbf{a}_h = \mathbf{d}_h^{m-\frac{1}{2}}$, and by supposing that $\mathbf{d}_h^0 \in \mathbf{Y}_h$ satisfies $|\mathbf{d}_h^0| = 1$, the director field $\mathbf{d}$ satisfies the constraint (4).

§4. Numerical examples

In this section, we present and we compare numerical results using the algorithms 2 and 3. We use Newton's method for the solution of the nonlinear system at each time step. For this purpose, three Newton iterations are sufficient in our computations.

The following example is taken from [1] to approximate smooth solutions of (1)–(3).

Example 1. We consider $\Omega = (-1, 1)^2$, and $\mathbf{v}_0 \equiv 0$, $\mathbf{d}_0 = (\sin(a), \cos(a))^\top$, where $a = 2.0\,\pi(\cos(x) - \sin(y))$. The parameters are taken as follows: $\lambda = \gamma = 1$, $\nu = 0.1$. The initial condition $\mathbf{d}_0$ and the final state are shown in Figure 1.

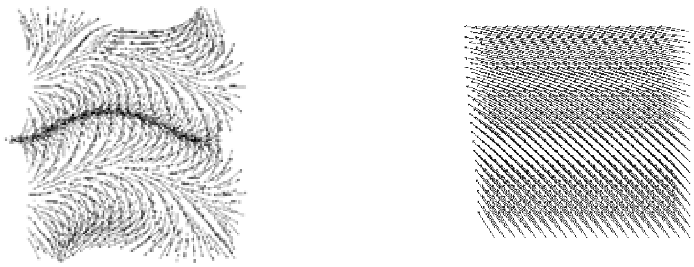

Figure 1: Algorithm 2: Initial (left) and final (right) director fields.

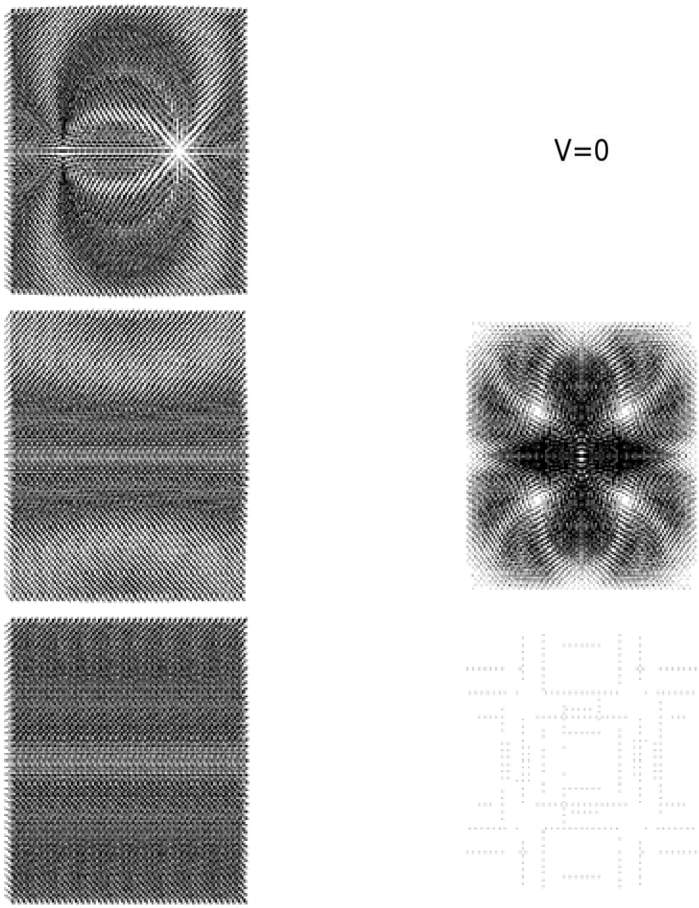

Figure 2: (Example 2) Using Algorithm 1. Snapshots at times $t = 0, 0.3, 0.9$ of $\{d_h^m\}$ (left) and $\{u_h^m\}$ (right).

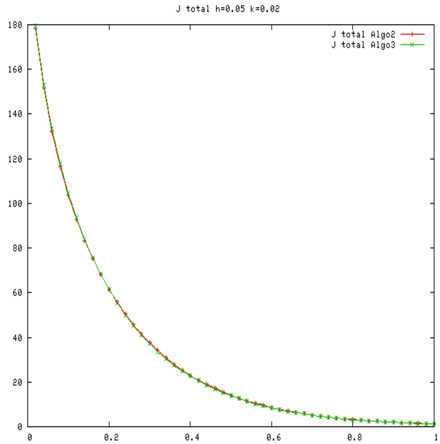

Figure 3: (Example 2) $\mathcal{J}_{total}$ with Algorithm 2 and Algorithm 3 for $k = 0.02$, $h = 0.05$ and $\eta = 0.1$.

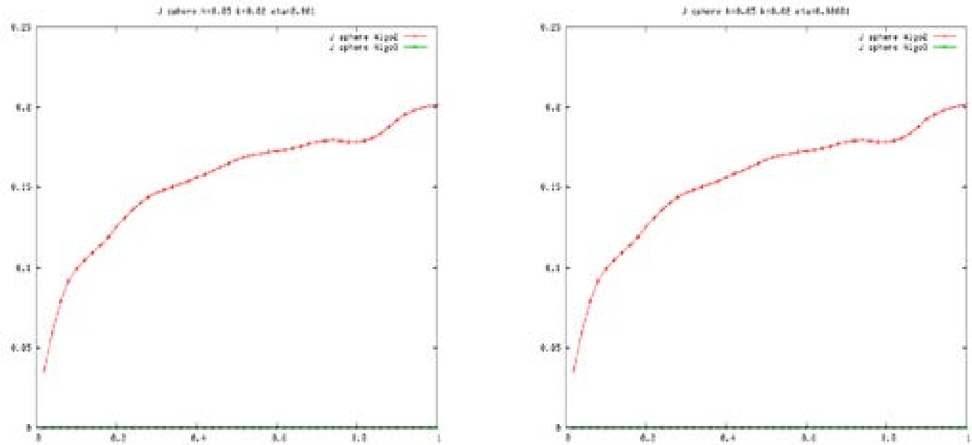

Figure 4: Comparison of Algorithm 2 and Algorithm 3 with Example 2 for $k = 0.02$, $h = 0.05$ and $\eta = 0.001$ (left), for $k = 0.02$, $h = 0.05$ and $\eta = 0.00001$ (right).

A uniform crisscross triangulation of Ω is used with uniform mesh size $h = 1/20, 1/40$ and $1/80$. Next, we present the results for Algorithm 1.

Example 2. We consider $\Omega = (-1,1)^2$, $\mathbf{v}_0 \equiv 0$ and $\mathbf{d}_0 = \hat{\mathbf{d}} \,/\, (|\hat{\mathbf{d}}|^2 + \eta^2)^{1/2}$, with $\hat{\mathbf{d}}(x,y) = (x^2 + y^2 - 0.25, y)^T$. The parameters are taken as follows: $\lambda = \gamma = 1$, $\nu = 0.1$, $\eta = 0.05$, $\epsilon = 0.05$, $k = 0.01$ and $h = 0.1$. The evolution of this solution is shown in Figure 2.

In order to compare the solutions of Algorithm 2 with those of Algorithm 3, we give some notations. Let $\mathcal{J}_{kin}(\mathbf{v}_h) = \frac{1}{2}\int_\Omega |\mathbf{v}_h|^2$ be the kinetic energy, $\mathcal{J}_{ela}(\mathbf{d}_h) = \frac{\lambda}{2}\int_\Omega |\nabla \mathbf{d}_h|^2$, the elastic energy and finally $\mathcal{J}_{total}(\mathbf{v}_h, \mathbf{d}_h) = \mathcal{J}_{kin}(\mathbf{v}_h) + \mathcal{J}_{ela}(\mathbf{d}_h)$, the total energy.

We then compare the total energy for the two algorithms on the same mesh with the same time step. As can be seen from Figure 3, we have exactly the same solutions with the two algorithms.

We define now, the sphere energy $\mathcal{J}_{sphere}(\mathbf{d}_h) = 1 - |\mathbf{d}_h|$. The results presented in Figure 4 show that the sphere energy for the Algorithm 3 is zero and the constraint (4) is satisfied in contrast to Algorithm 2.

References

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