

This is the final peer-reviewed accepted manuscript of:

Nochetto, R.H., Ruggeri, M., Yang, S., GAMMA-CONVERGENT PROJECTION-FREE FINITE ELEMENT METHODS FOR NEMATIC LIQUID CRYSTALS: THE ERICKSEN MODEL (2022) SIAM Journal on Numerical Analysis, 60 (2), pp. 856-887

The final published version is available online at:
<https://dx.doi.org/10.1137/21M1407495>

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1 **GAMMA-CONVERGENT PROJECTION-FREE FINITE ELEMENT**
2 **METHODS FOR NEMATIC LIQUID CRYSTALS:**
3 **THE ERICKSEN MODEL***

4 RICARDO H. NOCHETTO[†], MICHELE RUGGERI[‡], AND SHUO YANG[§]

5 **Abstract.** The Ericksen model for nematic liquid crystals couples a director field with a scalar
6 degree of orientation variable, and allows the formation of various defects with finite energy. We
7 propose a simple but novel finite element approximation of the problem that can be implemented
8 easily within standard finite element packages. Our scheme is projection-free and thus circumvents
9 the use of weakly acute meshes, which are quite restrictive in 3D but are required by recent algorithms
10 for convergence. We prove stability and Γ -convergence properties of the new method in the presence
11 of defects. We also design an effective nested gradient flow algorithm for computing minimizers that
12 controls the violation of the unit-length constraint of the director. We present several simulations in
13 2D and 3D that document the performance of the proposed scheme and its ability to capture quite
14 intriguing defects.

15 **Key words.** liquid crystals, finite element method, Γ -convergence, gradient flow, defect, energy
16 minimization

17 **AMS subject classifications.** 65N30, 35J70, 65Z05

18 **1. Introduction.**

19 **1.1. Liquid crystals with variable degree of orientation.** Liquid crystals
20 (LCs) are a mesophase between crystalline solid and isotropic liquid. They are a
21 host of numerous potential applications in engineering and science, in particular in
22 materials science [1, 5, 10]. Nematic LCs are made of rod-like molecules with no
23 positional order that tend to point in a preferred direction. LC materials are thus
24 anisotropic.

25 We consider the one-constant Ericksen model for nematic LCs with variable de-
26 gree of orientation [17], which lies between the Oseen–Frank director model and the
27 Landau–de Gennes Q -tensor model [16, 29]. The state of the LC is described in terms
28 of a vector field \mathbf{n} and a scalar function s , which satisfy the constraints $|\mathbf{n}| = 1$ and
29 $-1/(d-1) < s < 1$ for the space dimension $d = 2, 3$. The director \mathbf{n} indicates the
30 preferred orientations of the LC molecules, while s represents the degree of alignment
31 that the molecules have with respect to \mathbf{n} , both in the sense of local probabilistic av-
32 erage. A schematic illustration of their meaning is given in Figure 1. The equilibrium

*Submitted to the editors DATE.

Funding: This project started while RHN and MR were in residence at the Institute for Computational and Experimental Research in Mathematics (ICERM) during the workshop *Numerical Methods and New Perspectives for Extended Liquid Crystalline Systems* in 2019 (grant DMS-1439786). MR acknowledges partial support of the Austrian Science Fund (FWF) through the special research program *Taming complexity in partial differential systems* (grant F65) and of the Erwin Schrödinger International Institute for Mathematics and Physics (ESI), given during the workshop *New Trends in the Variational Modeling and Simulation of Liquid Crystals*. RHN and SY acknowledge partial support of the National Science Foundation (grant DMS-1908267).

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33 state is given by an admissible pair (s, \mathbf{n}) that minimizes the Ericksen energy

34 (1.1)
$$E[s, \mathbf{n}] = \frac{1}{2} \int_{\Omega} (\kappa |\nabla s|^2 + s^2 |\nabla \mathbf{n}|^2) + \int_{\Omega} \psi(s),$$

35 where $\kappa > 0$ is constant; the constraint on s is enforced by the double well potential
36 ψ . We refer to [4, 21] for early analysis of the Ericksen model.

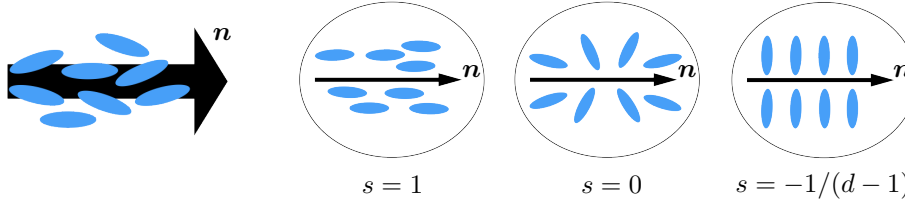


FIG. 1. Schematic illustration of $\mathbf{n}(x)$ and $s(x)$, in microscopic scale near a fixed $x \in \Omega \subset \mathbb{R}^d$. Note that $s = 1$ represents the state of perfect alignment in which all molecules in the local ensemble are parallel to \mathbf{n} . Likewise, $s = -1/(d-1)$ represents the state of perpendicular alignment. The case $s = 0$ corresponds to a defect in the LC material, an isotropic distribution of molecules in the local ensemble that do not lie along any preferred direction.

37 If s can be approximated by a nonvanishing constant, then the energy (1.1) re-
38 duces to the Oseen–Frank energy $E[\mathbf{n}] \propto \int_{\Omega} |\nabla \mathbf{n}|^2$, whose minimizers are harmonic
39 maps and have been extensively studied, e.g., in [27, 14]. However, the simpler Oseen–
40 Frank model has severe limitations in capturing defects: It only admits point defects
41 with finite energy for $d = 3$. In contrast, the Ericksen model (1.1) allows for
42 $\mathbf{n} \notin H^1(\Omega)$ and compensates blow-up of $\nabla \mathbf{n}$ by letting s vanish, which is the mech-
43 anism for the formation of a variety of line and plane defects; see, e.g., [21] for a
44 proof of the fact that the singular set of a minimizer of (1.1) can have positive Haus-
45 dorff dimension. This physical process leads to a *degenerate* Euler–Lagrange equation
46 for \mathbf{n} that poses serious difficulties to formulate mathematically sound algorithms to
47 approximate (1.1) and study their convergence.

48 **1.2. Numerical analysis of the Ericksen model.** Several numerical methods
49 for the Oseen–Frank model have been proposed [22, 3, 7, 9]. Finite element methods
50 (FEMs) for the Ericksen model are designed in [6, 23, 24, 30, 15]; see also the recent
51 review [12]. In contrast to [6], a fundamental structure of (1.1) is exploited in [23, 24]
52 to design and analyze FEMs that handle the inherent degeneracy of (1.1) without
53 regularization and enforce the constraint $|\mathbf{n}| = 1$ robustly. Stability and convergence
54 properties via Γ -convergence are proved in [23, 24], pioneering results in this setting.
55 They hinge on a clever discrete energy that mimics the structure of (1.1) discretely
56 but, unfortunately, is cumbersome to implement in standard software packages and
57 requires weakly acute meshes. The latter ensures that the projection of discrete
58 director fields onto the unit sphere is energy decreasing, and thus compatible with the
59 quasi-gradient flow, but is quite restrictive and difficult to implement for $d = 3$ and
60 domains with nontrivial topology.

61 **1.3. Contributions.** In this work, we propose a projection-free FEM that avoids
62 dealing with weakly acute meshes. Without the projection step, the unit-length con-
63 straint $|\mathbf{n}| = 1$ is no longer satisfied exactly but instead is relaxed at each step of our
64 iterative solver, a nested gradient flow. The latter guarantees control of the violation

65 of $|\mathbf{n}| = 1$ and asymptotic enforcement of it. We summarize the chief novelties and
 66 advantages of our approach as follows.

67 • *Shape-regular meshes.* Partitions of Ω are assumed to be only shape-regular,
 68 which allows for the use of software with general mesh generators such as Netgen [26].
 69 Avoiding weakly acute meshes is important in 3D to deal with interesting but nontrivial
 70 geometries as documented in section 5. An earlier work achieving this goal is [30],
 71 which presents a mass-lumped FEM with a consistent stabilization term involving
 72 $s^2 \nabla \mathbf{n}^\top \mathbf{n}$ for the generalized Ericksen energy.

73 • *Standard algorithm.* Our novel discretization of (1.1) is straightforward, requires
 74 no stabilization, and is easy to implement in standard software packages such as
 75 NGSolve [26]. In contrast to [23, 24], our FEM does no longer exploit the structure
 76 of (1.1), but its analysis does.

77 • *Γ -convergence.* The analysis of our FEM hinges heavily on the underlying
 78 structure of (1.1), which is fully discussed in section 2 and relies on the notion of
 79 L^2 -gradient on \mathbf{n} [18, Theorem 6.2]; see Proposition 2.1 below. Such a notion was
 80 already used in [11] in the context of the uniaxial Q-tensor LC model. We prove
 81 stability and Γ -convergence. Our results are similar to those in [23, 24, 30], but the
 82 use of the discrete structure is new.

83 • *Linear solver.* We propose a nested gradient flow that, despite the nonlinear nature
 84 of the problem, is *fully linear* to compute minimizers. The inner loop to advance
 85 the director \mathbf{n} for fixed degree of orientation s is allowed to subiterate. This turns
 86 out to induce an acceleration mechanism for the computation and motion of defects.
 87 For a recent acceleration technique based on a domain decomposition approach, we
 88 refer to [15]. Our nested gradient flow iterations fall within the Γ -convergence frame-
 89 work provided a CFL-type condition is imposed on the discretization parameters (see
 90 Proposition 4.3). However, well-posedness and stability of the algorithm are guaran-
 91 teed without any such CFL restriction.

92 • *Numerical experiments.* We present several simulations in section 5. Some aim
 93 to compare the new algorithm with the existing literature in terms of performance
 94 and ability to capture defects. Other experiments explore 3D intriguing configurations
 95 such as the propeller defect and challenging variations of the Saturn ring defect.

96 • *Boundary conditions.* Since we do not impose the unit-length constraint $|\mathbf{n}| = 1$,
 97 the treatment of boundary data could be simplified and their properties weakened.
 98 This potentially affects the regularization procedure for the lim-sup property and the
 99 possible presence of defects at the boundary of Ω . We do not explore these issues in
 100 this paper but rather in future extension to the Q-tensor model.

101 **1.4. Outline.** The remainder of this work is organized as follows. In the next
 102 subsection, we collect some general notation used throughout the paper. In section 2,
 103 we describe the Ericksen model for LCs with variable degree of orientation and discuss
 104 its key structure. In section 3, we introduce our discretization of the model and
 105 state our Γ -convergence result. In section 4, we present our iterative scheme for the
 106 computation of discrete local minimizers. In section 5, we show numerical experiments
 107 illustrating effectiveness and efficiency of our method, as well as its flexibility to deal
 108 with complex defects in 3D. We postpone the proofs of most results to section 6.

109 **1.5. General notation.** We denote by $\mathbb{N} = \{1, 2, \dots\}$ the set of natural num-
 110 bers and set $\mathbb{N}_0 := \mathbb{N} \cup \{0\}$. For $d = 2, 3$, we denote the unit sphere in \mathbb{R}^d by
 111 $\mathbb{S}^{d-1} = \{x \in \mathbb{R}^d : |x| = 1\}$. We denote by $B_r(x)$ the ball of radius $r > 0$ centered at
 112 $x \in \mathbb{R}^d$. For (spaces of) vector- or matrix-valued functions, we use bold letters, e.g.,
 113 for a generic domain $\Omega \subset \mathbb{R}^d$, we denote both $L^2(\Omega; \mathbb{R}^d)$ and $L^2(\Omega; \mathbb{R}^{d \times d})$ by $\mathbf{L}^2(\Omega)$.

114 We denote by $\langle \cdot, \cdot \rangle$ both the scalar product of $\mathbf{L}^2(\Omega)$ and the duality pairing between
 115 $\mathbf{H}^1(\Omega)$ and its dual, with the ambiguity being resolved by the arguments. We use
 116 the notation \lesssim to denote *smaller than or equal to up to a multiplicative constant*, i.e.,
 117 we write $A \lesssim B$ if there exists a constant $c > 0$, which is clear from the context and
 118 always independent of the discretization parameters, such that $A \leq cB$.

119 **2. Problem formulation.** Let $\Omega \subset \mathbb{R}^d$ ($d = 2, 3$) be a bounded Lipschitz do-
 120 main. In the Ericksen model, the state of the LC is described in terms of a unit-length
 121 vector field $\mathbf{n} : \Omega \rightarrow \mathbb{S}^{d-1}$ and a scalar function $s : \Omega \rightarrow (-1/(d-1), 1)$. Equilibrium
 122 configurations are minimizers of the energy $E[s, \mathbf{n}] = E_1[s, \mathbf{n}] + E_2[s]$ in (1.1), where

$$123 \quad (2.1) \quad E_1[s, \mathbf{n}] := \frac{1}{2} \int_{\Omega} (\kappa |\nabla s|^2 + s^2 |\nabla \mathbf{n}|^2), \quad E_2[s] := \int_{\Omega} \psi(s).$$

124 The double well potential $\psi : (-1/(d-1), 1) \rightarrow \mathbb{R}_{\geq 0}$ satisfies the following proper-
 125 ties [17]:

- 126 • $\psi \in C^2(-1/(d-1), 1)$,
- 127 • $\lim_{s \rightarrow 1^-} \psi(s) = +\infty = \lim_{s \rightarrow -1/(d-1)^+} \psi(s)$,
- 128 • $\psi(0) > \psi(s^*) = \min_{s \in (-1/(d-1), 1)} \psi(s) = 0$ for some $s^* \in (0, 1)$,
- 129 • $\psi'(0) = 0$.

130 In (2.1), $E_1[s, \mathbf{n}]$ is the one-constant approximation of the elastic energy proposed
 131 in [17], while $E_2[s]$ is a potential energy which confines the variable s within the
 132 physically admissible interval $(-1/(d-1), 1)$. The presence of the weight s^2 in the
 133 second term of $E_1[s, \mathbf{n}]$ allows for blow-up of $\nabla \mathbf{n}$, namely $\mathbf{n} \notin \mathbf{H}^1(\Omega)$, in the *singular*
 134 *set* Σ , where defects may occur:

$$135 \quad (2.2) \quad \Sigma := \{x \in \Omega : s(x) = 0\}.$$

136 To complete the setting, we define the set of admissible functions where we seek
 137 minimizers of (2.1). Note that, allowing for a director $\mathbf{n} \notin \mathbf{H}^1(\Omega)$, one encounters at
 138 least two difficulties: On the one hand, it is not clear how to interpret the gradient of
 139 \mathbf{n} appearing in $E_1[s, \mathbf{n}]$. On the other hand, the trace of \mathbf{n} on the boundary of Ω is
 140 not well-defined, so that one cannot impose Dirichlet conditions on \mathbf{n} in the standard
 141 way. To cope with these problems, following [4, 21], we introduce the auxiliary variable
 142 $\mathbf{u} = s\mathbf{n}$. Then, the product rule formally yields that

$$143 \quad (2.3) \quad \nabla \mathbf{u} = \mathbf{n} \otimes \nabla s + s \nabla \mathbf{n}.$$

144 Since $|\mathbf{n}| = 1$, the identities $\nabla \mathbf{n}^\top \mathbf{n} = \mathbf{0}$ and $|\mathbf{n} \otimes \nabla s| = |\nabla s|$ are valid. It follows that
 145 the above decomposition of $\nabla \mathbf{u}$ is orthogonal, i.e.,

$$146 \quad (2.4) \quad |\nabla \mathbf{u}|^2 = |\mathbf{n} \otimes \nabla s|^2 + s^2 |\nabla \mathbf{n}|^2 = |\nabla s|^2 + s^2 |\nabla \mathbf{n}|^2.$$

147 In particular, $E_1[s, \mathbf{n}]$ can be rewritten in terms of s and $\mathbf{u} = s\mathbf{n}$ as

$$148 \quad (2.5) \quad E_1[s, \mathbf{n}] = \tilde{E}_1[s, \mathbf{u}] = \frac{1}{2} \int_{\Omega} ((\kappa - 1) |\nabla s|^2 + |\nabla \mathbf{u}|^2).$$

149 In the latter, the degree of orientation and the auxiliary field are decoupled. In
 150 particular, this reveals that, for (s, \mathbf{n}) such that $E_1[s, \mathbf{n}] < \infty$, $\mathbf{u} = s\mathbf{n} \in \mathbf{H}^1(\Omega)$ even
 151 though $\mathbf{n} \notin \mathbf{H}^1(\Omega)$.

152 We say that a triple $(s, \mathbf{n}, \mathbf{u})$ satisfies the *structural condition* if

$$153 \quad (2.6) \quad -\frac{1}{d-1} < s < 1, \quad |\mathbf{n}| = 1, \quad \text{and} \quad \mathbf{u} = s\mathbf{n} \quad \text{a.e. in } \Omega.$$

154 In view of the above discussion, we are led to consider the following admissible class:

$$155 \quad (2.7) \quad \mathcal{A} := \{(s, \mathbf{n}, \mathbf{u}) \in H^1(\Omega) \times \mathbf{L}^\infty(\Omega) \times \mathbf{H}^1(\Omega) : (s, \mathbf{n}, \mathbf{u}) \text{ satisfies (2.6)}\}.$$

156 For triples $(s, \mathbf{n}, \mathbf{u}) \in \mathcal{A}$, it is possible to characterize the gradient of \mathbf{n} occurring in
 157 $E_1[s, \mathbf{n}]$ using a weaker notion of differentiability. To this end, we recall the following
 158 definition [18, Theorem 6.2]: We say that \mathbf{n} is L^2 -differentiable at $x \in \Omega$, and we
 159 denote its L^2 -gradient at x by $\nabla \mathbf{n}(x)$, if

$$160 \quad \int_{B_r(x)} |\mathbf{n}(y) - \mathbf{n}(x) - \nabla \mathbf{n}(x)(y - x)|^2 dy = o(r^2) \quad \text{as } r \rightarrow 0.$$

161 It is well known that the notion of L^2 -differentiability is weaker than the existence of
 162 an L^2 -integrable weak gradient, in the sense that every H^1 -function is L^2 -differentiable
 163 almost everywhere and its L^2 -gradient coincides with the weak gradient; see, e.g., [18,
 164 Theorem 6.2].

165 In the following proposition, we establish that if $(s, \mathbf{n}, \mathbf{u}) \in \mathcal{A}$, then \mathbf{n} is L^2 -
 166 differentiable and the decomposition (2.4) holds almost everywhere outside of the
 167 singular set Σ in (2.2). Its proof will be presented in subsection 6.1.

168 PROPOSITION 2.1 (orthogonal decomposition). *Let $(s, \mathbf{n}, \mathbf{u}) \in \mathcal{A}$. Then, \mathbf{n} is*
 169 *L^2 -differentiable a.e. in $\Omega \setminus \Sigma$. In particular, its L^2 -gradient is given by*

$$170 \quad (2.8) \quad \nabla \mathbf{n} = s^{-1}(\nabla \mathbf{u} - \mathbf{n} \otimes \nabla s) \quad \text{a.e. in } \Omega \setminus \Sigma.$$

171 Moreover, the following identity holds

$$172 \quad (2.9) \quad |\nabla \mathbf{u}|^2 = |\nabla s|^2 + s^2 |\nabla \mathbf{n}|^2 \quad \text{a.e. in } \Omega \setminus \Sigma.$$

173 This allows us to give a precise meaning to $E_1[s, \mathbf{n}]$ in (2.1). Depending on the
 174 context, we interpret $\nabla \mathbf{n}$ in the sense of L^2 -gradient in $\Omega \setminus \Sigma$ and $\int_{\Sigma} s^2 |\nabla \mathbf{n}|^2 = 0$,
 175 or we alternatively replace Ω by $\Omega \setminus \Sigma$ as domain of integration or even use the
 176 representation $\tilde{E}_1[s, \mathbf{u}]$ of (2.5).

177 Turning to boundary conditions, let $\Gamma_D \subseteq \partial\Omega$ be a relatively open subset of the
 178 boundary such that $|\Gamma_D| > 0$, where we aim to impose Dirichlet boundary conditions.
 179 These, in the context of LCs, are usually referred to as *strong anchoring* conditions.
 180 To this end, given a triple $(g, \mathbf{q}, \mathbf{r}) \in W^{1,\infty}(\mathbb{R}^d) \times \mathbf{L}^\infty(\mathbb{R}^d) \times \mathbf{W}^{1,\infty}(\mathbb{R}^d)$ satisfying the
 181 structural condition (2.6), we consider the following restricted admissible class that
 182 incorporates boundary conditions:

$$183 \quad (2.10) \quad \mathcal{A}(g, \mathbf{r}) := \{(s, \mathbf{n}, \mathbf{u}) \in \mathcal{A} : s|_{\Gamma_D} = g|_{\Gamma_D} \text{ and } \mathbf{u}|_{\Gamma_D} = \mathbf{r}|_{\Gamma_D}\}.$$

184 Overall, we are interested in the following constrained minimization problem: Find
 185 $(s^*, \mathbf{n}^*, \mathbf{u}^*) \in \mathcal{A}(g, \mathbf{r})$ such that

$$186 \quad (2.11) \quad (s^*, \mathbf{n}^*, \mathbf{u}^*) = \underset{(s, \mathbf{n}, \mathbf{u}) \in \mathcal{A}(g, \mathbf{r})}{\operatorname{arg\,min}} E[s, \mathbf{n}].$$

187 To conclude this section, let $\delta_0 > 0$ be sufficiently small. Some of our results
 188 below will require the following technical assumptions on the Dirichlet data, namely

$$189 \quad (2.12) \quad -\frac{1}{d-1} + \delta_0 \leq g(x) \leq 1 - \delta_0 \quad \text{for all } x \in \mathbb{R}^d,$$

$$190 \quad (2.13) \quad g \geq \delta_0 \quad \text{on } \Gamma_D,$$

192 and on the double well potential, namely

$$193 \quad (2.14) \quad \begin{aligned} \psi(s) &\geq \psi(1 - \delta_0) && \text{for all } s \geq 1 - \delta_0, \\ \psi(s) &\geq \psi\left(-\frac{1}{d-1} + \delta_0\right) && \text{for all } s \leq -\frac{1}{d-1} + \delta_0, \end{aligned}$$

194 and ψ is monotone in $(-1/(d-1), -1/(d-1) + \delta_0)$ and in $(1 - \delta_0, 1)$. Note that (2.13)
195 implies that $\mathbf{q} = g^{-1}\mathbf{r}$ is $\mathbf{W}^{1,\infty}$ on Γ_D so that imposing the Dirichlet condition
196 $\mathbf{n}|_{\Gamma_D} = \mathbf{q}|_{\Gamma_D}$ on the physical variable \mathbf{n} is equivalent to imposing $\mathbf{u}|_{\Gamma_D} = \mathbf{r}|_{\Gamma_D}$ on
197 the auxiliary variable \mathbf{u} . Finally, the property (2.14) is consistent with the fact that
198 $\psi(s) \rightarrow +\infty$ as $s \rightarrow -1/(d-1)$ and $s \rightarrow 1$.

199 **3. Γ -convergent finite element discretization.** We assume Ω to be a poly-
200 topal domain and consider a shape-regular family $\{\mathcal{T}_h\}$ of simplicial meshes of Ω (in the
201 sense of, e.g., [8, Definitions 3.3–3.4]) parametrized by the mesh size $h = \max_{K \in \mathcal{T}_h} h_K$,
202 where $h_K = \text{diam}(K)$. We stress that we do not require any mesh to be weakly acute
203 (we refer to [8, Remark 3.12] for a discussion of this assumption for $d = 2, 3$). We
204 denote by \mathcal{N}_h the set of vertices of \mathcal{T}_h . For any $K \in \mathcal{T}_h$, we denote by $\mathcal{P}^1(K)$ the
205 space of first-order polynomials on K . We consider the space of \mathcal{T}_h -piecewise affine
206 and globally continuous functions

$$207 \quad V_h := \{v_h \in C^0(\bar{\Omega}) : v_h|_K \in \mathcal{P}^1(K) \text{ for all } K \in \mathcal{T}_h\}.$$

208 Let $\mathbf{V}_h := (V_h)^d$ be the corresponding space of vector-valued polynomials. We denote
209 by I_h both the nodal interpolant $I_h : C^0(\bar{\Omega}) \rightarrow V_h$ and its vector-valued counterpart
210 $I_h : \mathbf{C}^0(\bar{\Omega}) \rightarrow \mathbf{V}_h$.

211 For $s_h \in V_h$ and $\mathbf{n}_h \in \mathbf{V}_h$, let the discrete energy be $E^h[s_h, \mathbf{n}_h] = E_1^h[s_h, \mathbf{n}_h] +$
212 $E_2^h[s_h]$ with

$$213 \quad (3.1) \quad E_1^h[s_h, \mathbf{n}_h] := \frac{1}{2} \int_{\Omega} (\kappa |\mathbf{n}_h \otimes \nabla s_h|^2 + s_h^2 |\nabla \mathbf{n}_h|^2), \quad E_2^h[s_h] := \int_{\Omega} \psi(s_h).$$

214 Note that E^h is consistent, in the sense that $E^h[s, \mathbf{n}] = E[s, \mathbf{n}]$ if $(s, \mathbf{n}, \mathbf{u}) \in \mathcal{A}(g, \mathbf{r})$.

215 We say that a triple $(s_h, \mathbf{n}_h, \mathbf{u}_h) \in V_h \times \mathbf{V}_h \times \mathbf{V}_h$ satisfies the *discrete structural*
216 *condition* if

$$217 \quad (3.2) \quad -\frac{1}{d-1} < s_h(z) < 1, \quad |\mathbf{n}_h(z)| \geq 1, \quad \text{and} \quad \mathbf{u}_h(z) = s_h(z)\mathbf{n}_h(z) \quad \text{for all } z \in \mathcal{N}_h.$$

218 In (3.2), the requirements prescribed by the continuous structural condition (2.6) are
219 imposed only at the vertices of the mesh, which is practical. Moreover, the unit-length
220 constraint for the director is relaxed, since \mathbf{n}_h may attain also values outside of the
221 unit sphere.

222 Let $\varepsilon > 0$, $g_h = I_h[g]$, and $\mathbf{r}_h = I_h[\mathbf{r}]$. We consider the following discrete
223 minimization problem: Find $(s_h^*, \mathbf{n}_h^*, \mathbf{u}_h^*) \in \mathcal{A}_{h,\varepsilon}(g_h, \mathbf{r}_h)$ such that

$$224 \quad (3.3) \quad (s_h^*, \mathbf{n}_h^*, \mathbf{u}_h^*) = \underset{(s_h, \mathbf{n}_h, \mathbf{u}_h) \in \mathcal{A}_{h,\varepsilon}(g_h, \mathbf{r}_h)}{\arg \min} E_h[s_h, \mathbf{n}_h],$$

225 where the discrete restricted admissible class is defined as

$$226 \quad (3.4) \quad \mathcal{A}_{h,\varepsilon}(g_h, \mathbf{r}_h) := \{(s_h, \mathbf{n}_h, \mathbf{u}_h) \in V_h \times \mathbf{V}_h \times \mathbf{V}_h : \\ 227 \quad (s_h, \mathbf{n}_h, \mathbf{u}_h) \text{ satisfies (3.2), } \|I_h[|\mathbf{n}_h|^2] - 1\|_{L^1(\Omega)} \leq \varepsilon, \\ 228 \quad s_h(z) = g_h(z), \text{ and } u_h(z) = r_h(z) \text{ for all } z \in \mathcal{N}_h \cap \Gamma_D\}.$$

231 In the following theorem, we show that the discrete energy (3.1) converges towards
 232 the continuous one (2.1) in the sense of Γ -convergence.

233 **THEOREM 3.1** (Γ -convergence). *Suppose that $\varepsilon \rightarrow 0$ as $h \rightarrow 0$. Then, the*
 234 *following two properties are satisfied:*

235 (i) *Lim-sup inequality (consistency): Let $\Gamma_D = \partial\Omega$. Let the assumptions (2.12)–(2.14)*
 236 *hold. If $(s, \mathbf{n}, \mathbf{u}) \in \mathcal{A}(g, \mathbf{r})$, then there exists a sequence $\{(s_h, \mathbf{n}_h, \mathbf{u}_h)\} \subset \mathcal{A}_{h,\varepsilon}(g_h, \mathbf{r}_h)$*
 237 *such that $\|\mathbf{n}_h\|_{\mathbf{L}^\infty(\Omega)} = 1$, $s_h \rightarrow s$ in $H^1(\Omega)$, $\mathbf{n}_h \rightarrow \mathbf{n}$ in $\mathbf{L}^2(\Omega \setminus \Sigma)$, $\mathbf{u}_h \rightarrow \mathbf{u}$ in*
 238 *$\mathbf{H}^1(\Omega)$, as $h \rightarrow 0$, and*

$$239 \quad (3.5) \quad E[s, \mathbf{n}] \geq \limsup_{h \rightarrow 0} E^h[s_h, \mathbf{n}_h].$$

240 (ii) *Lim-inf inequality (stability): Let $\{(s_h, \mathbf{n}_h, \mathbf{u}_h)\} \subset \mathcal{A}_{h,\varepsilon}(g_h, \mathbf{r}_h)$ be a sequence such*
 241 *that $E^h[s_h, \mathbf{n}_h] \leq C$ and $\|\mathbf{n}_h\|_{\mathbf{L}^\infty(\Omega)} \leq C$, where $C \geq 1$ is a constant independent*
 242 *of h . Then, there exist $(s, \mathbf{n}, \mathbf{u}) \in \mathcal{A}(g, \mathbf{r})$ and a subsequence of $\{(s_h, \mathbf{n}_h, \mathbf{u}_h)\}$ (not*
 243 *relabelled) such that $s_h \rightarrow s$ in $H^1(\Omega)$, $\mathbf{n}_h \rightarrow \mathbf{n}$ in $\mathbf{L}^2(\Omega \setminus \Sigma)$, $\mathbf{u}_h \rightarrow \mathbf{u}$ in $\mathbf{H}^1(\Omega)$ as*
 244 *$h \rightarrow 0$, and*

$$245 \quad (3.6) \quad E[s, \mathbf{n}] \leq \liminf_{h \rightarrow 0} E^h[s_h, \mathbf{n}_h].$$

246 The proof of [Theorem 3.1](#) is deferred to [subsections 6.2](#) and [6.3](#). The assump-
 247 tion $\Gamma_D = \partial\Omega$ in part (i) is needed to apply a regularization result from [\[23\]](#) (see
 248 [Lemma 6.2](#) below). The properties established in [Theorem 3.1](#) are slight variations
 249 of the properties required by the standard definition of Γ -convergence; see, e.g., [\[13,](#)
 250 [Definition 1.5\]](#). However, they still allow to prove the convergence of discrete global
 251 minimizers.

252 **COROLLARY 3.2** (convergence of discrete global minimizers). *Let $\Gamma_D = \partial\Omega$ and*
 253 *suppose that the assumptions (2.12)–(2.14) hold. Let $\{(s_h, \mathbf{n}_h, \mathbf{u}_h)\} \subset \mathcal{A}_{h,\varepsilon}(g_h, \mathbf{r}_h)$ be*
 254 *a sequence of global minimizers of the discrete energy (3.1) such that $\|\mathbf{n}_h\|_{\mathbf{L}^\infty(\Omega)} \leq C$,*
 255 *where $C \geq 1$ is a constant independent of h . Then, every cluster point $(s, \mathbf{n}, \mathbf{u})$ belongs*
 256 *to $\mathcal{A}(g, \mathbf{r})$ and is a global minimizer of the continuous energy (2.1).*

257 **4. Computation of discrete local minimizers.** In this section, we propose
 258 an effective algorithm to compute discrete local minimizers of (3.1). The method is
 259 based on a discretization of the (nonphysical) energy-decreasing dynamics driven by
 260 the system of gradient flows

$$261 \quad \partial_t \mathbf{n} + \delta_{\mathbf{n}} E^h[s, \mathbf{n}] = 0,$$

$$262 \quad \partial_t s + \delta_s E^h[s, \mathbf{n}] = 0,$$

264 where $\delta_{\mathbf{n}} E^h[s, \mathbf{n}]$ and $\delta_s E^h[s, \mathbf{n}]$ denote the Gâteaux derivatives of the energy with
 265 respect to the order parameters, i.e.,

$$266 \quad \langle \delta_{\mathbf{n}} E^h[s, \mathbf{n}], \phi \rangle = \langle \delta_{\mathbf{n}} E_1^h[s, \mathbf{n}], \phi \rangle = \kappa \langle \mathbf{n} \otimes \nabla s, \phi \otimes \nabla s \rangle + \langle s \nabla \mathbf{n}, s \nabla \phi \rangle,$$

$$267 \quad \langle \delta_s E^h[s, \mathbf{n}], w \rangle = \langle \delta_s E_1^h[s, \mathbf{n}], w \rangle + \langle \delta_s E_2^h[s, \mathbf{n}], w \rangle$$

$$268 \quad = \kappa \langle \mathbf{n} \otimes \nabla s, \mathbf{n} \otimes \nabla w \rangle + \langle s \nabla \mathbf{n}, w \nabla \mathbf{n} \rangle + \langle \psi'(s), w \rangle.$$

270 Let us introduce the ingredients of the scheme. First, let

$$271 \quad V_{h,D} := \{v_h \in V_h : v_h(z) = 0 \text{ for all } z \in \mathcal{N}_h \cap \Gamma_D\} \quad \text{and} \quad \mathbf{V}_{h,D} := (V_{h,D})^d$$

272 be the spaces of discrete functions satisfying homogeneous Dirichlet conditions on Γ_D .
 273 Given $\mathbf{n}_h \in \mathbf{V}_h$, we consider the subspace of $\mathbf{V}_{h,D}$ consisting of all discrete functions
 274 with nodal values orthogonal to those of \mathbf{n}_h at all vertices:

$$275 \quad \mathcal{K}_h[\mathbf{n}_h] := \{\phi_h \in \mathbf{V}_{h,D} : \mathbf{n}_h(z) \cdot \phi_h(z) = 0 \text{ for all } z \in \mathcal{N}_h\}.$$

276 The space $\mathcal{K}_h[\mathbf{n}_h]$ can be interpreted as a discretization of the space of tangential vari-
 277 ations $\mathcal{K}[\mathbf{n}] := \{\phi \in \mathbf{H}^1(\Omega) : \mathbf{n} \cdot \phi = 0 \text{ a.e. in } \Omega\}$, which naturally occurs in the vari-
 278 ational formulation of problems with a unit-length constraint; see, e.g., [8, Lemma 7.1]
 279 for the harmonic map equation.

280 For the treatment of the double well potential, we follow a convex splitting ap-
 281 proach (see, e.g., [31]): We assume the splitting $\psi = \psi_c - \psi_e$, where ψ_c and ψ_e are
 282 both convex and ψ_c is quadratic.

283 The *time* discretization of the gradient flow for the director and the degree of
 284 orientation are based on the constant time-step sizes $\tau_n > 0$ and $\tau_s > 0$, respectively.
 285 Moreover, we consider the difference quotient $d_t s_h^{i+1} := (s_h^{i+1} - s_h^i)/\tau_s$.

286 In the following algorithm, we state the proposed numerical scheme for the com-
 287 putation of discrete local minimizers of (3.1). We assume that (2.13) is satisfied so
 288 that imposing Dirichlet boundary conditions directly for the director is allowed. Let
 289 $\text{tol} > 0$ denote a tolerance.

Algorithm 4.1 alternating direction discrete gradient flow

Input: $s_h^0 \in V_h$, $\mathbf{n}_h^0 \in \mathbf{V}_h$ such that $|\mathbf{n}_h^0(z)| = 1$ for all $z \in \mathcal{N}_h$, $\mathbf{n}_h^0(z) = \mathbf{r}_h(z)/g_h(z)$
 and $s_h^0(z) = g_h(z)$ for all $z \in \mathcal{N}_h \cap \Gamma_D$.

Outer loop: For all $i \in \mathbb{N}_0$, iterate (i)–(ii):

(i) Inner loop: Given (\mathbf{n}_h^i, s_h^i) , let $\mathbf{n}_h^{i,0} = \mathbf{n}_h^i$. For all $\ell \in \mathbb{N}_0$, iterate (i-a)–(i-b):

(i-a) Compute $\mathbf{t}_h^{i,\ell} \in \mathcal{K}_h[\mathbf{n}_h^{i,\ell}]$ such that

$$(4.1) \quad \begin{aligned} \langle \mathbf{t}_h^{i,\ell}, \phi_h \rangle_* + \tau_n \kappa \langle \mathbf{t}_h^{i,\ell} \otimes \nabla s_h^i, \phi_h \otimes \nabla s_h^i \rangle + \tau_n \langle s_h^i \nabla \mathbf{t}_h^{i,\ell}, s_h^i \nabla \phi_h \rangle \\ = -\kappa \langle \mathbf{n}_h^{i,\ell} \otimes \nabla s_h^i, \phi_h \otimes \nabla s_h^i \rangle - \langle s_h^i \nabla \mathbf{n}_h^{i,\ell}, s_h^i \nabla \phi_h \rangle \end{aligned}$$

for all $\phi_h \in \mathcal{K}_h[\mathbf{n}_h^{i,\ell}]$;

(i-b) Update $\mathbf{n}_h^{i,\ell+1} := \mathbf{n}_h^{i,\ell} + \tau_n \mathbf{t}_h^{i,\ell}$;

until

$$(4.2) \quad |E_1^h[s_h^i, \mathbf{n}_h^{i,\ell+1}] - E_1^h[s_h^i, \mathbf{n}_h^{i,\ell}]| < \text{tol}.$$

If $\ell_i \in \mathbb{N}_0$ denotes the smallest integer for which the stopping criterion (4.2)
 is satisfied, define $\mathbf{n}_h^{i+1} := \mathbf{n}_h^{i,\ell_i+1}$.

(ii) Compute $s_h^{i+1} \in V_h$ such that $s_h^{i+1}(z) = g_h(z)$ for all $z \in \mathcal{N}_h \cap \Gamma_D$ and

$$(4.3) \quad \begin{aligned} \langle d_t s_h^{i+1}, w_h \rangle + \kappa \langle \mathbf{n}_h^{i+1} \otimes \nabla s_h^{i+1}, \mathbf{n}_h^{i+1} \otimes \nabla w_h \rangle \\ + \langle s_h^{i+1} \nabla \mathbf{n}_h^{i+1}, w_h \nabla \mathbf{n}_h^{i+1} \rangle + \langle \psi'_c(s_h^{i+1}), w_h \rangle = \langle \psi'_e(s_h^i), w_h \rangle \end{aligned}$$

for all $w_h \in V_{h,D}$.

Output: Sequence of approximations $\{(s_h^i, \mathbf{n}_h^i)\}_{i \in \mathbb{N}_0}$.

290 In Algorithm 4.1, $\langle \cdot, \cdot \rangle_*$ denotes the scalar product of the metric used in the
 291 discrete gradient flow (4.1) for the director. In this work, we consider the following

292 two choices for $\langle \cdot, \cdot \rangle_*$, dictated by numerical convenience:

$$293 \quad (4.4) \quad \langle \phi, \psi \rangle_* = \langle \phi, \psi \rangle \quad (L^2\text{-metric}),$$

$$294 \quad (4.5) \quad \langle \phi, \psi \rangle_* = \langle h^\alpha \nabla \phi, \nabla \psi \rangle \quad \text{with } 0 < \alpha \leq 2 \quad (\text{weighted } H^1\text{-metric}).$$

296 In (4.5), the H^1 -metric is weakened by a positive power of the mesh size h . Note that
 297 the choice $\alpha = 0$ corresponds to a full H^1 -gradient flow, which is not appropriate since
 298 the director does not belong to $\mathbf{H}^1(\Omega)$ in general (e.g., in the presence of defects).
 299 On the other hand, if $\alpha = 2$, a standard scaling argument shows that the resulting
 300 metric is equivalent to the L^2 -metric in (4.4).

301 In the convex splitting of ψ , we adopt a semi-implicit approach: The convex
 302 and quadratic part ψ_c is treated implicitly, while the concave one ψ_e is treated ex-
 303 plicitly. This leads to a linear and positive definite contribution to the left-hand side
 304 of (4.3). Moreover, the resulting discretization is unconditionally stable (see, e.g., [23,
 305 Lemma 4.1]). Altogether, both (4.1) and (4.3) are linear symmetric positive definite
 306 systems in the unknowns $\mathbf{t}_h^{i,\ell}$ and s_h^{i+1} . The orthogonality constraint in (4.1) can be
 307 imposed at the linear algebraic level by introducing a Lagrange multiplier associated
 308 with it (see, e.g., the discussion in [8, Section 7.2.5]) or via a null-space method as
 309 done, e.g., in [25, 23, 20]. In this work, we implement it using a Lagrange multiplier.

310 Although in most of our numerical experiments we will set $\tau_{\mathbf{n}} = \tau_s$, we observed
 311 that in some situations the flexibility of choosing different time-step sizes in (4.1)
 312 and (4.3) is decisive in order to move defects in numerical simulations (see, e.g., the
 313 experiment in subsection 5.3 below).

314 In the following proposition, we prove well-posedness and an energy-decreasing
 315 property of Algorithm 4.1.

316 PROPOSITION 4.1 (properties of Algorithm 4.1). *Algorithm 4.1 is well-posed and*
 317 *energy decreasing. Specifically, for all $i \in \mathbb{N}_0$, the following assertions hold:*

- 318 (i) *For all $\ell \in \mathbb{N}_0$, (4.1) admits a unique solution $\mathbf{t}_h^{i,\ell} \in \mathcal{K}_h[\mathbf{n}_h^{i,\ell}]$;*
- 319 (ii) *The inner loop terminates in a finite number of iterations, i.e., there exists $\ell \in \mathbb{N}_0$*
 320 *such that the stopping criterion (4.2) is met;*
- 321 (iii) *(4.3) admits a unique solution $s_h^{i+1} \in V_h$ such that $s_h^{i+1}(z) = g_h(z)$ for all $z \in$*
 322 *$\mathcal{N}_h \cap \Gamma_D$.*
- 323 (iv) *There holds*

$$324 \quad (4.6) \quad E^h[s_h^{i+1}, \mathbf{n}_h^{i+1}] - E^h[s_h^i, \mathbf{n}_h^i] \leq - \left(\tau_s \|d_t s_h^{i+1}\|_{L^2(\Omega)}^2 + \tau_{\mathbf{n}} \sum_{\ell=0}^{\ell_i} \|\mathbf{t}_h^{i,\ell}\|_*^2 \right) \\ - \left(\tau_s^2 E_1^h[d_t s_h^{i+1}, \mathbf{n}_h^{i+1}] + \tau_{\mathbf{n}}^2 \sum_{\ell=0}^{\ell_i} E_1^h[s_h^i, \mathbf{t}_h^{i,\ell}] \right).$$

325 *In particular, there holds $E^h[s_h^{i+1}, \mathbf{n}_h^{i+1}] \leq E^h[s_h^i, \mathbf{n}_h^i]$ and equality holds if and only*
 326 *if $(s_h^{i+1}, \mathbf{n}_h^{i+1}) = (s_h^i, \mathbf{n}_h^i)$ (equilibrium state).*

327 Remark 4.2 (energy decrease). The right-hand side of (4.6) characterizes the en-
 328 ergy decrease guaranteed by each step of Algorithm 4.1 and comprises two contribu-
 329 tions: The term

$$330 \quad - \left(\tau_s \|d_t s_h^{i+1}\|_{L^2(\Omega)}^2 + \tau_{\mathbf{n}} \sum_{\ell=0}^{\ell_i} \|\mathbf{t}_h^{i,\ell}\|_*^2 \right)$$

331 is the energy decrease due to the gradient-flow nature of [Algorithm 4.1](#). The term

$$332 \quad - \left(\tau_s^2 E_1^h [d_t s_h^{i+1}, \mathbf{n}_h^{i+1}] + \tau_n^2 \sum_{\ell=0}^{\ell_i} E_1^h [s_h^i, \mathbf{t}_h^{i,\ell}] \right)$$

333 is the numerical dissipation due to the backward Euler methods used for the time
334 discretization.

335 In practical implementations of [Algorithm 4.1](#), the outer loop is terminated when

$$336 \quad (4.7) \quad |E^h [s_h^{i+1}, \mathbf{n}_h^{i+1}] - E^h [s_h^i, \mathbf{n}_h^i]| < \text{tol.}$$

337 Since the algorithm fulfills a monotone energy-decreasing property, the stopping cri-
338 terion is met in a finite number of iterations.

339 The approximations \mathbf{n}_h^{i+1} of the director generated by [Algorithm 4.1](#) do not sat-
340 isfy the unit-length constraint at the vertices of the mesh, as in [23, 24]. However,
341 the following proposition, proved in [subsection 6.4](#), shows that violation of this con-
342 straint can be controlled by the time-step size τ_n , independently of the number of
343 iterations. Moreover, the uniform boundedness in $L^\infty(\Omega)$ of the sequence required
344 by the Γ -convergence result (cf. [Theorem 3.1\(ii\)](#)) can be guaranteed if the discretiza-
345 tion parameters satisfy a suitable CFL-type condition. However, we stress that such
346 condition is not necessary for the well-posedness and the stability of the algorithm.

347 **PROPOSITION 4.3** (properties of discrete director field). *Let $j \geq 1$. The following*
348 *holds.*

349 (i) *Suppose that the norm induced by the metric $\langle \cdot, \cdot \rangle_*$ used in (4.1) is an upper bound*
350 *for the L^2 -norm, i.e., there exists $C_* > 0$ such that*

$$351 \quad (4.8) \quad \|\phi_h\|_{L^2(\Omega)} \leq C_* \|\phi_h\|_* \quad \text{for all } \phi_h \in \mathbf{V}_{h,D}.$$

352 *Then, the approximations generated by [Algorithm 4.1](#) satisfy*

$$353 \quad (4.9) \quad \|I_h [|\mathbf{n}_h^j|^2 - 1]\|_{L^1(\Omega)} \leq C_1 \tau_n E^h [s_h^0, \mathbf{n}_h^0],$$

354 *where $C_1 > 0$ depends only on C_* and the shape-regularity of $\{\mathcal{T}_h\}$.*

355 (ii) *Suppose τ_n fulfills the following CFL-type condition*

$$356 \quad (4.10) \quad \begin{aligned} \tau_n h_{\min}^{-d} &\leq C^* && \text{if } \langle \cdot, \cdot \rangle_* \text{ is chosen as (4.4),} \\ \tau_n h_{\min}^{2-d-\alpha} |\log h_{\min}|^2 &\leq C^* && \text{if } \langle \cdot, \cdot \rangle_* \text{ is chosen as (4.5),} \end{aligned}$$

357 *where $h_{\min} := \min_{K \in \mathcal{T}_h} h_K$ and $C^* > 0$ is arbitrary. Then, the approximations*
358 *generated by [Algorithm 4.1](#) satisfy*

$$359 \quad (4.11) \quad \|\mathbf{n}_h^j\|_{L^\infty(\Omega)} \leq 1 + C_2 E^h [s_h^0, \mathbf{n}_h^0],$$

360 *where $C_2 > 0$ is proportional to $C^* > 0$ in (4.10) with proportionality constant de-*
361 *pending on the shape-regularity of $\{\mathcal{T}_h\}$.*

362 To conclude this section, we discuss the design of [Algorithm 4.1](#) with special em-
363 phasis on its nested structure and distinct roles of τ_n and τ_s . Obviously, τ_n controls
364 the violation of the unit-length constraint according to (4.9), but the roles of subit-
365 erations in (4.1) and τ_s in (4.3) is more subtle and deserves further elaboration. The
366 presence of defects is associated with values $s_h^i(x_j)$ close to zero at nodes x_j , which

367 in turn act as weights in the equation (4.1) for the tangential updates $\mathbf{t}_h^{i,\ell}$ of the
 368 director field $\mathbf{n}_h^{i,\ell}$. The fast decrease to zero of $s_h^i(x_j)$, relative to the growth of $\nabla \mathbf{n}_h^i$
 369 in its vicinity, impedes further changes of $\mathbf{n}_h^i(x_j)$ because they are not energetically
 370 favorable: The defect is thus pinned at the same location x_j for many iterations.
 371 Experiments with Algorithm 4.1 reveal defect pinning if $\tau_n = \tau_s$ and one step of (4.1)
 372 per step of (4.3) is utilized. The subiterations within the inner loop (4.1) allow $\mathbf{n}_h^{i,\ell}$
 373 to adjust to the current value of s_h^i . This mimics an approximate optimization step
 374 but with unit length and max norm control dictated by Proposition 4.3. In contrast,
 375 full optimization has been proposed in [23, 24, 30] instead of (4.1), followed by nodal
 376 projection onto the unit sphere, whereas one step of a weighted gradient flow (4.1) has
 377 been advocated in [11] for the Q -tensor model. On the other hand, since τ_s penalizes
 378 changes of s_h^i , smaller values of τ_s relative to τ_n delay changes of s_h^i in favor of changes
 379 of \mathbf{n}_h^i . This does not fix the stiff character of (4.1), studied in [15], but does remove
 380 defect pinning. Several numerical experiments in section 5 document this finding.

381 **5. Numerical experiments.** In this section, we present a series of numerical
 382 experiments that explore the accuracy of Algorithm 4.1 and its ability to approximate
 383 rather complex defects of nematic LCs in 2D and 3D. In both cases, these results
 384 complement the theory of sections 3 and 4 and extend it.

385 We have implemented Algorithm 4.1 within the high performance multiphysics
 386 finite element software Netgen/NGSolve [26]. To solve the constrained variational
 387 problem (4.1), we adopt a saddle point approach. The ensuing linear systems are
 388 solved using the built-in conjugate gradient solver of Netgen/NGSolve, while the
 389 visualization relies on ParaView [2].

390 All pictures below obey the following rules. The vector field depicts the director
 391 \mathbf{n} , whereas the color scale refers to the degree of orientation s . Blue regions indicate
 392 areas with values of s close to zero, which signify the occurrence of defects, while
 393 the red ones indicate regions with largest values of s ($s \approx 0.75$ in our simulations),
 394 where the director encodes the local orientation of the LC molecules. We generate
 395 unstructured, generally non-weakly acute, meshes within Netgen with desirable mesh
 396 size h_0 but the effective maximum size h of tetrahedra in 3D may only satisfy $h \approx h_0$.
 397 For the sake of reproducibility, we will specify h_0 when dealing with unstructured 3D
 398 meshes.

399 We stress that, unlike FEMs proposed in previous works [24, 23], the energy-
 400 decreasing property of Algorithm 4.1 (cf. Proposition 4.1) does not rely on meshes
 401 being weakly acute. Except for simple 3D geometries, such meshes are hard, to
 402 impossible, to construct. This is the case of the cylinder domain in subsection 5.3
 403 and the Saturn ring configurations in subsection 5.5, for which mesh flexibility is of
 404 fundamental importance to capture topologically complicated defects.

405 Throughout this section, we consider the double well potential $\psi(s) = c_{\text{dw}}(\psi_c(s) -$
 406 $\psi_e(s))$ with

$$407 \quad (5.1) \quad \psi_c(s) := 63s^2, \quad \psi_e(s) := -16s^4 + \frac{64}{3}s^3 + 57s^2 - 0.5625,$$

408 where $c_{\text{dw}} \geq 0$. Note that, for $c_{\text{dw}} > 0$, ψ has a local minimum at $s = 0$ and a
 409 global minimum at $s = \hat{s} := 0.750025$ such that $\psi(\hat{s}) = 0$. Moreover, in view of
 410 Proposition 4.3, we measure the violation of the unit-length constraint in terms of the
 411 quantity

$$412 \quad (5.2) \quad \text{err}_{\mathbf{n}} := \|I_h[|\mathbf{n}_h^N|^2 - 1]\|_{L^1(\Omega)},$$

413 where \mathbf{n}_h^N denotes the final approximation of the director generated by [Algorithm 4.1](#).
 414 Furthermore, unless otherwise specified, we choose the L^2 -metric (4.4) in (4.1), and
 415 we set the tolerance $\text{tol} = 10^{-6}$ in both (4.2) and (4.7).

416 **5.1. Point defect in 2D.** In striking contrast with the Oseen–Frank model, the
 417 Ericksen model allows point defects to have finite energy in 2D: The blow-up of $|\nabla \mathbf{n}|$
 418 near a defect is compensated by infinitesimal values of s for the energy $E[s, \mathbf{n}]$ in (1.1)
 419 to stay bounded. We examine this basic mechanism with simulations of a point defect
 420 in 2D and study the influence of the discretization parameters on the performance of
 421 [Algorithm 4.1](#).

422 We consider the unit square $\Omega = (0, 1)^2$, and set $\kappa = 2$ in (1.1) as well as $c_{\text{dw}} =$
 423 $0.1(0.3)^{-2}$ in (5.1). We impose Dirichlet boundary conditions for s and \mathbf{n} on $\partial\Omega$,
 424 namely

$$425 \quad (5.3) \quad g = \hat{s} \quad \text{and} \quad \mathbf{q} = \mathbf{r}/g = \frac{(x - 0.5, y - 0.5)}{|(x - 0.5, y - 0.5)|} \quad \text{on } \partial\Omega.$$

426 To initialize [Algorithm 4.1](#), we consider a constant degree of orientation $s_h^0 = \hat{s}$ in Ω
 427 and a director \mathbf{n}_h^0 exhibiting an off-center point defect located at $(0.24, 0.24)$. Due
 428 to the imposed boundary conditions and for symmetry reasons, we expect that an
 429 energy-decreasing dynamics moves the defect to the center of the square; see [Figure 2](#).

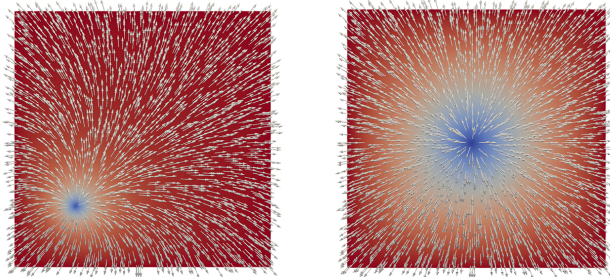


FIG. 2. Point defect experiment of [subsection 5.1](#): Plot of the approximation (s_h^1, \mathbf{n}_h^1) after the first iteration (left) and of the final approximation (s_h^N, \mathbf{n}_h^N) (right). The gradient flow algorithm moves the defect to the center of the domain.

430 In our first experiment, we consider a uniform mesh \mathcal{T}_h of the unit square con-
 431 sisting of 2048 right triangles. The resulting mesh size is $h = \sqrt{2}2^{-5}$. Moreover, we
 432 set $\tau_{\mathbf{n}} = \tau_s = 0.1$ and compare the results obtained for different choices of the metric
 433 $\langle \cdot, \cdot \rangle_*$ in (4.1); cf. (4.4)–(4.5). [Table 1](#) displays the outputs for each run. On the one
 434 hand, we observe that using the L^2 -metric leads to the fastest dynamics in terms of
 435 both number of iterations and CPU time. On the other hand, the violation of the
 436 unit-length constraint is smaller for the weighted H^1 -metrics. For smaller values of α
 437 in the weighted H^1 -metric, [Algorithm 4.1](#) terminates with a configuration exhibiting
 438 defect pinning at an off-center location. The expected equilibrium state, depicted in
 439 [Figure 2](#) (right), can be restored when reducing the time-step size τ_s .

440 In our second experiment, we investigate the effect of mesh refinement and changes
 441 of the time-step size on the results. To this end, we first repeat the simulation using
 442 three uniform meshes with $h = \sqrt{2}2^{-5-\ell}$ ($\ell = 0, 1, 2$); we set $\tau_{\mathbf{n}} = 0.12^{-2\ell}$, in
 443 agreement with the CFL condition in (4.10) for the L^2 -metric and $d = 2$. We collect
 444 the results of computations in [Table 2](#) (top), and observe that both $\min(s_h^N)$ and $\text{err}_{\mathbf{n}}$

metric	N	$E^h[s_h^N, \mathbf{n}_h^N]$	$\min(s_h^N)$	$\text{err}_{\mathbf{n}}$	CPU time
L^2	60	2.984	0.0757	0.0404	64.83
weighted H^1 , $\alpha = 2.0$	67	2.944	0.0750	0.0370	98.65
weighted H^1 , $\alpha = 1.9$	65	2.938	0.0754	0.0362	111.69
weighted H^1 , $\alpha = 1.8$	67	2.932	0.0755	0.0353	130.17
weighted H^1 , $\alpha = 1.7$	80	2.926	0.0760	0.0342	154.92

TABLE 1

Point defect experiment of [subsection 5.1](#): Final outputs of [Algorithm 4.1](#) for different choices of metric $\langle \cdot, \cdot \rangle_*$, namely total number of iterations N , value of the energy $E^h[s_h^N, \mathbf{n}_h^N]$ for the equilibrium state, smallest value of the final s_h^N , error in the unit-length constraint in [\(5.2\)](#), and the CPU time.

445 decrease about linearly with h , whereas the energy $E^h[s_h^N, \mathbf{n}_h^N]$ slightly decreases. The
 446 linear decay of $\text{err}_{\mathbf{n}}$ with respect to $\tau_{\mathbf{n}}$ established in [\(4.9\)](#) is not observed. This can
 447 be explained by the increase of $E^h[s_h^0, \mathbf{n}_h^0]$ upon refinement, attributable to the fact
 448 that \mathbf{n}_h^0 has a point defect while s_h^0 is constant and does not compensate the blow-up
 449 of $\nabla \mathbf{n}_0$.

450 In our third experiment, we aim to empirically confirm the first-order convergence
 451 of the error $\text{err}_{\mathbf{n}}$ in [\(5.2\)](#) with respect to $\tau_{\mathbf{n}}$ established in [Proposition 4.3](#); see [\(4.9\)](#).
 452 To this end, we consider a fixed mesh with $h = \sqrt{2}2^{-5}$, we set $\tau_{\mathbf{n}} = (0.1)2^{-5-\ell}$
 453 ($\ell = 0, 1, 2$) as well as $\text{tol} = 10^{-5}\tau_{\mathbf{n}}$ in both [\(4.2\)](#) and [\(4.7\)](#). The computational
 454 results, collected in [Table 2](#) (bottom), confirm the expected linear decay of the error.

h	N	$E^h[s_h^N, \mathbf{n}_h^N]$	$\min(s_h^N)$	$\text{err}_{\mathbf{n}}$	CPU time
$\sqrt{2}2^{-5}$	60	2.984	0.0757	0.0404	64.83
$\sqrt{2}2^{-6}$	61	2.940	0.0422	0.0232	592.23
$\sqrt{2}2^{-7}$	133	2.939	0.0289	0.0100	7919.25

$\tau_{\mathbf{n}}$	$\text{err}_{\mathbf{n}}$
$(0.1)2^{-5}$	0.00610
$(0.1)2^{-6}$	0.00346
$(0.1)2^{-7}$	0.001927

TABLE 2

Point defect experiment of [subsection 5.1](#): Final outputs of [Algorithm 4.1](#) for different uniform meshes with mesh size h and time steps $\tau_{\mathbf{n}} = Ch^2$ (top) and different time step sizes $\tau_{\mathbf{n}}$ with fixed mesh size $h = \sqrt{2}2^{-5}$ (bottom).

455 **5.2. Plane defect in 3D.** We simulate a plane defect in the unit cube $\Omega =$
 456 $(0, 1)^3$ located at $\{z = 0.5\}$, according to [\[29, Section 6.4\]](#). We set $\kappa = 0.2$ in [\(1.1\)](#)
 457 and $c_{\text{dw}} = 0$ in [\(5.1\)](#). We impose Dirichlet boundary conditions on the top and bottom
 458 faces Γ_D of the cube

$$\begin{aligned}
 459 \quad g &= \hat{s}, \quad \mathbf{q} = \mathbf{r}/g = (1, 0, 0) \text{ on } \partial\Omega \cap \{z = 0\}, \\
 460 \quad g &= \hat{s}, \quad \mathbf{q} = \mathbf{r}/g = (0, 1, 0) \text{ on } \partial\Omega \cap \{z = 1\}.
 \end{aligned}$$

462 The exact solution is $\mathbf{n}(z) = (1, 0, 0)$ for $z < 0.5$ and $\mathbf{n}(z) = (0, 1, 0)$ for $z > 0.5$, while
 463 $s(z) = 0$ on $z = 0.5$ and linear on $(0, 0.5) \cup (0.5, 1)$ [\[29, Section 6.4\]](#). Our numerical
 464 results are consistent with those in [\[23, Section 5.3\]](#). To initialize [Algorithm 4.1](#), we

465 set $s_h^0 = \hat{s}$ and \mathbf{n}_h^0 to be a regularized point defect away from the center of the cube.
 466 **Figure 3** displays the three components of \mathbf{n}_h^k and s_h^k evaluated along the vertical line
 467 $(0.5, 0.5, z)$ for iterations $k = 1, 31, 79$ computed on a uniform mesh with $h = \sqrt{3}0.05$
 468 and $\tau_{\mathbf{n}} = \tau_s = 0.01$.

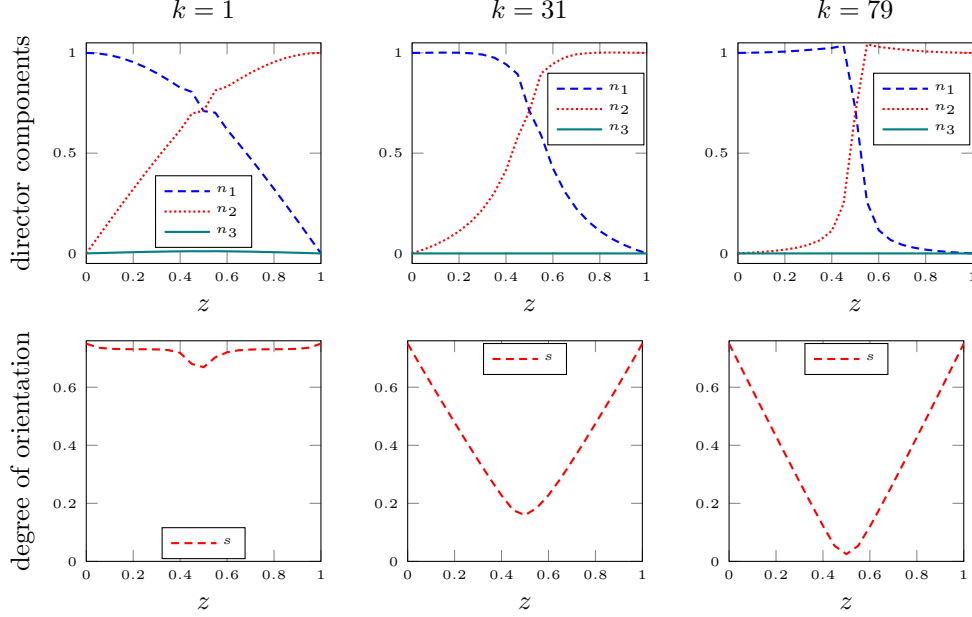


FIG. 3. Plane defect of [subsection 5.2](#): Plots of the three components of \mathbf{n}_h^k (first row) and plots of s_h^k (second row) for iterations $k = 1, 31, 79$. In the final configuration ($k = N = 79$), the energy is $E^h[s_h^N, \mathbf{n}_h^N] = 0.247$, $\min(s_h^N) = 0.0101$, and $\text{err}_{\mathbf{n}} = 0.0556$. Moreover, there is a transition layer between about $z = 0.4$ and $z = 0.6$, and s_h is almost linear in $(0, 0.4)$ and $(0.6, 1)$.

469 **5.3. Effect of κ on equilibria.** The value of the constant $\kappa > 0$ in (1.1) plays
 470 a crucial role in the formation of defects. For large values of κ , the dominant term
 471 in $E_1[s, \mathbf{n}]$ is $\int_{\Omega} \kappa |\nabla s|^2$ that prevents variations of s . Typically s tends to be close
 472 to a (usually positive) constant and the model behaves much like the simpler Oseen–
 473 Frank model, where defects are less likely to occur (and no defects with finite energy
 474 beyond point defects are allowed in 3D). On the other hand, for small values of κ ,
 475 the energy is dominated by $\int_{\Omega} s^2 |\nabla \mathbf{n}|^2$, which allows s to become zero to compensate
 476 large gradients of \mathbf{n} , and defects are then more likely to occur. In this section, we
 477 investigate this dichotomy numerically.

478 We consider a cylindrical domain Ω in 3D with lateral boundary Γ_D

$$479 \quad \Omega = \{(x, y, z) \in \mathbb{R}^3 : (x - 0.5)^2 + (y - 0.5)^2 < 0.5^2, 0 < z < 1\},$$

$$480 \quad \Gamma_D = \{(x, y, z) \in \mathbb{R}^3 : (x - 0.5)^2 + (y - 0.5)^2 = 0.5^2, 0 < z < 1\},$$

482 and impose the Dirichlet conditions on Γ_D

$$483 \quad (5.4) \quad g = \hat{s} \quad \text{and} \quad \mathbf{q} = \mathbf{r}/g = \frac{(x - 0.5, y - 0.5, 0)}{|(x - 0.5, y - 0.5, 0)|},$$

484 The top and bottom faces of Ω are treated as free boundaries and the double well
 485 potential ψ is neglected, i.e., $c_{\text{dw}} = 0$ in (5.1). The analysis in [29, Section 6.5]

486 predicts that minimizers of the energy exhibit a line defect along the central axis of the
 487 cylinder if κ is sufficiently small, whereas they are smooth (no defects) if κ is
 488 sufficiently large.

489 **Figure 4** displays the final configurations obtained for $\kappa = 0.2$ and $\kappa = 2$. To
 490 discretize Ω , we consider an unstructured mesh generated by Netgen with $h_0 = 0.05$.
 491 For both values of κ , we set \hat{s} as initial condition for the degree of orientation. For
 492 $\kappa = 0.2$, we set $\tau_n = 0.1$ and $\tau_s = 10^{-3}$ and take as initial condition for the director
 493 field an off-center point defect located at the slice $z = 0.5$. For $\kappa = 2$, we set
 494 $\tau_n = \tau_s = 0.01$ and initialize \mathbf{n}_h^0 as an off-center point defect located at the slice
 495 $z = 0.25$. These computational results are consistent with those in [23] and confirm
 496 the predicted effect of κ [29, Section 6.5].

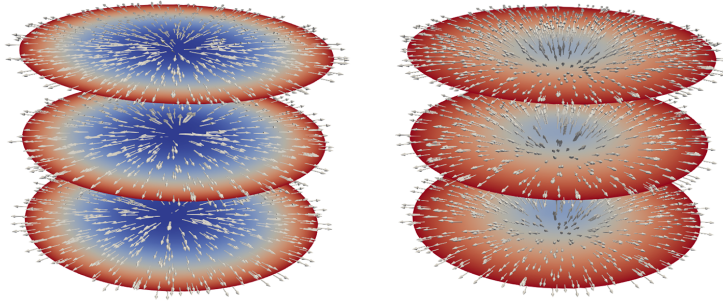


FIG. 4. *Effect of κ in subsection 5.3: Equilibria for $\kappa = 0.2$ (left) and $\kappa = 2$ (right). Both pictures show s_h^N and \mathbf{n}_h^N on the slices $z = 0.2, 0.5, 0.8$. If $\kappa = 0.2$, the final configuration exhibits a line defect along the central axis of the cylinder; the final energy is $E^h[s_h^N, \mathbf{n}_h^N] = 0.806$, $\min(s_h^N) = -7.33 \times 10^{-4}$, $\text{err}_n = 0.0778$, and $N = 226$. If $\kappa = 2$, the z -component of the director is not zero. This behavior is usually referred to as fluting effect or escape to the third dimension [29, Section 6.5.1]. Moreover, the degree of orientation is bounded well away from zero; the final energy is $E^h[s_h^N, \mathbf{n}_h^N] = 2.635$, $\min(s_h^N) = 0.224$, $\text{err}_n = 0.044$, and $N = 17$.*

497 **5.4. Propeller defect.** In this section, we investigate a new defect discovered
 498 in [23, Section 5.4]. We consider a setup similar to the one discussed in subsection 5.3,
 499 except that the domain is the unit cube $\Omega = (0, 1)^3$, and we again set $c_{dw} = 0$ in (5.1).
 500 The top and bottom faces of the cube are treated as free boundary, while the same
 501 strong anchoring conditions as in (5.4) are imposed on the vertical faces Γ_D of the
 502 cube (lateral boundary). The initial conditions are $s_h^0 = \hat{s}$ for the degree of orientation
 503 and an off-center point defect located on the slice $z = 0.5$ for the director. The domain
 504 is discretized using an unstructured mesh generated by Netgen with $h_0 = 0.025$, and
 505 we set $\tau_n = 0.02$. We consider the values $\kappa = 2$ and $\kappa = 0.1$. For $\kappa = 2$ and $\tau_s = 0.2$,
 506 the computational results agree with those of subsection 5.3: The equilibrium state
 507 is smooth and is characterized by a nonzero z -component (fluting effect).

508 For $\kappa = 0.1$, the final configuration reported in [23, Section 5.4, Figure 5] con-
 509 sists of two plane defects intersecting at the vertical symmetry axis of the cube, the
 510 so-called propeller defect. Whether this was a numerical artifact due to the inherent
 511 symmetries of the structured uniform weakly acute meshes used in [23] for simulation
 512 was an intriguing open question that we now answer. Owing to the flexibility of our
 513 approach regarding meshes, we repeated the experiment using an unstructured non-
 514 symmetric mesh with $\tau_s = 10^{-4}$. Our computational results confirm the emergence
 515 of the propeller defect in Figure 5, which in turn displays the director field \mathbf{n}_h^k at
 516 iterations $k = 0, 1, 2766$ with colors indicating the size of s_h^k .

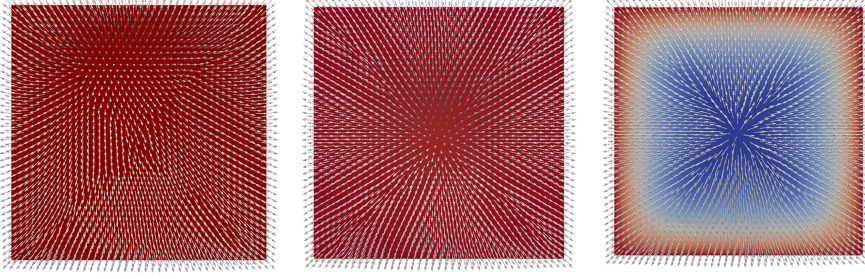


FIG. 5. Propeller defect of [subsection 5.4](#): Evolution of the order parameters on the top face of the cube ($z = 1$). Plots of the initial state (s_h^0, \mathbf{n}_h^0) (left), of the intermediate approximation (s_h^1, \mathbf{n}_h^1) obtained after the first iteration (middle), and of the equilibrium state (s_h^N, \mathbf{n}_h^N) after 2766 iterations (right). In the initial state, due to the off-center point defect at $z = 0.5$, there is a corresponding region on the slice for $z = 1$ where \mathbf{n} is aligned with z -direction. After the first iteration, in which \mathbf{n} is minimized for fixed $s = \hat{s}$, by symmetry the defect has moved to the center on $z = 0.5$. Correspondingly, on the top surface of the cube, the region where \mathbf{n} is aligned with the z -axis was moved to the center. The final state is a propeller defect consisting of a planar X-like configuration extruded in the z -direction. The final energy is $E^h[s_h^N, \mathbf{n}_h^N] = 0.592$, $\min(s_h^N) = -1.575 \times 10^{-4}$, $\text{err}_{\mathbf{n}} = 0.0265$, and $N = 2766$.

517 **5.5. Colloidal effects in nematic LCs.** Colloidal particles suspended in a
 518 nematic LC can induce interesting topological defects and distortions [19, 28]. One
 519 prominent example is the so-called *Saturn ring defect*, a director configuration char-
 520 acterized by a circular ring singularity surrounding a spherical particle and located
 521 around its equator. Such defects are typically nonorientable and captured within the
 522 Landau–de Gennes Q -tensor model [11, 12], but the Ericksen model yields similar
 523 orientable defects under suitable boundary conditions [24]. We confirm the ability of
 524 [Algorithm 4.1](#) to produce similar configurations.

525 In this section, we exploit the flexibility of [Algorithm 4.1](#) regarding meshes,
 526 together with the built-in Constructive Solid Geometry (CSG) approach of Net-
 527 gen/NGSolve, to explore numerically the formation of Saturn-ring-like defects induced
 528 by nonspherical or multiple particles.

529 **5.5.1. One ellipsoidal particle.** Let $\Omega_c = (0, 1)^3$ be the unit cube and let
 530 $\Omega_s \subset \Omega_c$ be an ellipsoid centered at $(0.5, 0.5, 0.5)$ with axes parallel to the coordinate
 531 axes and semiaxis lengths equal to 0.3 (x -direction), 0.075 (y -direction), and 0.075
 532 (z -direction); Ω_s has an aspect ratio 1 : 4. The computational domain is then $\Omega :=$
 533 $\Omega_c \setminus \overline{\Omega_s}$. We set $\kappa = 1$ in (1.1) as well as $c_{\text{dw}} = 0.2$ in (5.1). On $\partial\Omega = \partial\Omega_c \cup \partial\Omega_s$, we
 534 impose strong anchoring conditions

$$535 \quad (5.5) \quad g = \hat{s} \text{ on } \partial\Omega, \quad \mathbf{q} = \mathbf{r}/g = \boldsymbol{\nu} \text{ on } \partial\Omega_s, \quad \text{and} \quad \mathbf{q} = \mathbf{r}/g = \mathbf{n}_{sr} \text{ on } \partial\Omega_c,$$

536 where $\boldsymbol{\nu} : \partial\Omega_s \rightarrow \mathbb{S}^2$ denotes the outward-pointing unit normal vector of Ω_s and
 537 $\mathbf{n}_{sr} : \partial\Omega_s \rightarrow \mathbb{S}^2$ smoothly interpolates between the constant values $(0, 0, -1)$ on the
 538 bottom face and $(0, 0, 1)$ on the top face of the cube (see [24, Figure 11]). These
 539 boundary conditions are essential in order to induce the defect. The initial conditions
 540 for [Algorithm 4.1](#) are given by

$$541 \quad (5.6) \quad s_h^0 = \hat{s} \text{ in } \Omega \quad \text{and} \quad \mathbf{n}_h^0(z) = \begin{cases} (0, 0, 1) & z \in \Omega \text{ and } z_3 \geq 0.5, \\ (0, 0, -1) & z \in \Omega \text{ and } z_3 < 0.5, \\ \mathbf{q}(z) & z \in \partial\Omega, \end{cases}$$

542 for $z = (z_1, z_2, z_3) \in \mathcal{N}_h$. **Figure 6** displays cuts of the final configuration obtained
 543 using **Algorithm 4.1** with an unstructured mesh with $h_0 = 0.05$ and time-step sizes
 544 $\tau_{\mathbf{n}} = \tau_s = 0.01$.

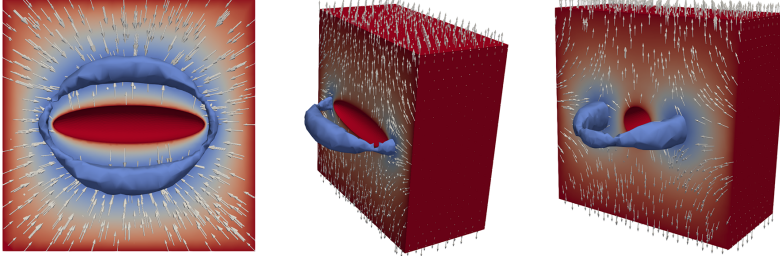


FIG. 6. *Saturn ring experiment of subsection 5.5.1. Three different perspectives of the Saturn ring defect around an ellipsoidal particle: slice $z = 0.5$ (left), a 3D view clipped at $y = 0.5$ (middle), and a 3D view clipped at $x = 0.5$ (right). The blue ring surrounding the particle, the iso-surface for $s = 0.15$, provides a good approximation of the defect. We stress that neither the distance between the defect and the particle nor the defect diameter are constant, which is a consequence of the anisotropic shape of the particle. The final energy is $E^h[s_h^N, \mathbf{n}_h^N] = 7.263$, $\min(s_h^N) = 0.0128$, $\text{err}_{\mathbf{n}} = 0.145$, and $N = 33$.*

545 **5.5.2. Multiple spherical particles.** We conclude this section with two novel
 546 and challenging simulations involving multiple spherical colloidal particles. In both
 547 cases, the domain has the form $\Omega := \Omega_c \setminus \overline{\Omega_s}$, where $\Omega_c \subset \mathbb{R}^3$ denotes a simply
 548 connected domain (representing the LC container), whereas $\Omega_s \subset \Omega_c$ denotes the
 549 region occupied by spherical colloidal particles. We set $\kappa = 1$ in (1.1) and $c_{\text{dw}} = 0.2$
 550 in (5.1). Moreover, boundary and initial conditions are suitable extensions to the
 551 multiple particle case of (5.5) and (5.6) considered in subsection 5.5.1.

552 **Figure 7** shows the equilibrium state corresponding to $\Omega_c = (0, 1)^3$ and a pair
 553 of disjoint spherical colloids Ω_s with radii 0.1 and centered at $(0.3, 0.5, 0.5)$ and
 554 $(0.7, 0.5, 0.5)$. **Algorithm 4.1** employs an unstructured mesh with $h_0 = 0.025$ and
 555 time-step sizes $\tau_{\mathbf{n}} = \tau_s = 0.0025$. A novel *fat figure “8”* defect forms.

556 **Figure 8** depicts the equilibrium state corresponding to $\Omega_c = (-0.1, 1.1)^3$ and
 557 a colloidal region consisting of six spheres. The latter have radii 0.1 and centers
 558 located at $(0.2, 0.5, 0.5)$, $(0.8, 0.5, 0.5)$, $(0.5, 0.2, 0.5)$, $(0.5, 0.8, 0.5)$, $(0.5, 0.5, 0.2)$, and
 559 $(0.5, 0.5, 0.8)$ distributed symmetrically with respect to the cube center. **Algorithm 4.1**
 560 utilizes an unstructured mesh with $h_0 = 0.05$ and time-step sizes $\tau_{\mathbf{n}} = \tau_s = 0.005$.

561 **6. Proofs.** In this section, we present the proofs of the results discussed in
 562 sections 2 to 4.

563 **6.1. L^2 -differentiability of admissible directors.** We now prove that any
 564 admissible director field, despite not being in $\mathbf{H}^1(\Omega)$, is L^2 -differentiable in $\Omega \setminus \Sigma$. We
 565 refer to [11] for a similar argument for a line field.

566 *Proof of Proposition 2.1.* Since $(s, \mathbf{n}, \mathbf{u}) \in \mathcal{A}$, we have that $s \in H^1(\Omega)$ and $\mathbf{u} =$
 567 $s\mathbf{n} \in \mathbf{H}^1(\Omega)$. Then, for almost all $x \in \Omega$ (specifically, for all Lebesgue points of
 568 $(s, \mathbf{u}, \nabla s, \nabla \mathbf{u})$), s and \mathbf{u} are L^2 -differentiable and their L^2 -gradients coincide with

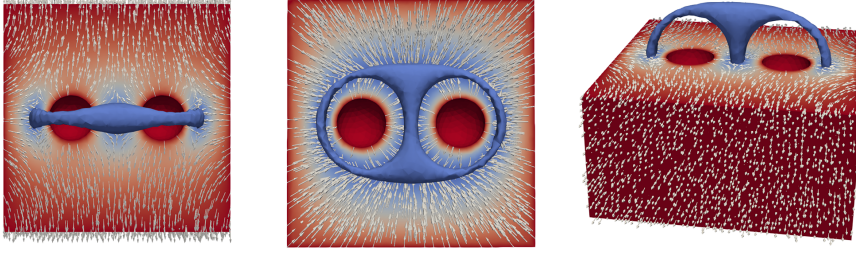


FIG. 7. *Two-particle experiment of subsection 5.5.2. Fat figure “8” defect around two spherical colloids viewed from different perspectives: slice $y = 0.5$ (left), slice $z = 0.5$ (middle), and a 3D view clipped at $y = 0.5$ (right). The blue ring surrounding the particle is the iso-surface for $s = 0.12$, which provides a good approximation of the defect. The final energy is $E^h[s_h^N, \mathbf{n}_h^N] = 7.656$, $\min(s_h^N) = 0.0146$, $\text{err}_{\mathbf{n}} = 0.0972$, and $N = 57$.*

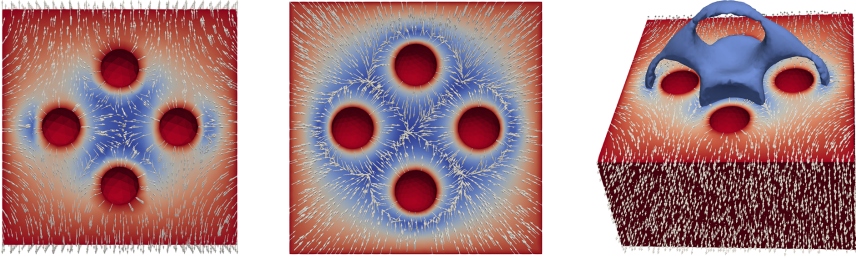


FIG. 8. *Six-particle experiment of subsection 5.5.2. Defect around six spherical colloids viewed from different perspectives: slice $y = 0.5$ (left), slice $z = 0.5$ (middle), and a 3D view clipped at $y = 0.5$ (right); the slice $x = 0.5$ is similar to $y = 0.5$. The blue ring surrounding the particles is the iso-surface for $s = 0.22$, which provides a good approximation of the defect. Therefore the defect appears to be a combination of a large Saturn ring defect around particles with center in the plane $z = 0.5$ and a planar X-like configuration with axis $x = 0.5, y = 0.5, -0.1 < z < 1$. The final energy is $E^h[s_h^N, \mathbf{n}_h^N] = 12.562$, $\min(s_h^N) = -0.0079$, $\text{err}_{\mathbf{n}} = 0.163$, and $N = 61$.*

569 their respective weak gradients for a.e. $x \in \Omega$, i.e., as $r \rightarrow 0$, it holds that

$$570 \quad \int_{B_r(x)} |s(y) - s(x) - \nabla s(x) \cdot (y - x)|^2 dy = o(r^2),$$

$$571 \quad \int_{B_r(x)} |\mathbf{u}(y) - \mathbf{u}(x) - \nabla \mathbf{u}(x)(y - x)|^2 dy = o(r^2);$$

572

573 see [18, Theorem 6.2]. For almost all $x \in \Omega \setminus \Sigma$ (specifically, for all Lebesgue points
574 of $(s, \mathbf{n}, \mathbf{u}, \nabla s, \nabla \mathbf{u})$ in $x \in \Omega \setminus \Sigma$), in view of the identity (2.3), we define the quantity

$$575 \quad (6.1) \quad \nabla \mathbf{n}(x) := \frac{\nabla \mathbf{u}(x) - \mathbf{n}(x) \otimes \nabla s(x)}{s(x)}.$$

576 Let $r > 0$. It holds that

$$\begin{aligned}
 & \int_{B_r(x)} |\mathbf{n}(y) - \mathbf{n}(x) - \nabla \mathbf{n}(x)(y-x)|^2 dy \\
 & \lesssim \frac{1}{s(x)^2} \int_{B_r(x)} |\mathbf{u}(y) - \mathbf{u}(x) - \nabla \mathbf{u}(x)(y-x)|^2 dy \\
 & \quad + \frac{1}{s(x)^2} \int_{B_r(x)} |s(y) - s(x) - \nabla s(x) \cdot (y-x)|^2 |\mathbf{n}(y)|^2 dy \\
 & \quad + \frac{|\nabla s(x)|^2}{s(x)^2} \int_{B_r(x)} |\mathbf{n}(y) - \mathbf{n}(x)|^2 |y-x|^2 dy = o(r^2)
 \end{aligned}$$

577

578 as $r \rightarrow 0$. This shows that $\nabla \mathbf{n}(x)$ is the L^2 -gradient of \mathbf{n} at x . Moreover, (2.9) follows
 579 from a direct computation. In fact, in view of (6.1), there holds that

$$\begin{aligned}
 s(x)^2 |\nabla \mathbf{n}(x)|^2 &= |\nabla \mathbf{u}(x) - \mathbf{n}(x) \otimes \nabla s(x)|^2 \\
 &= |\nabla \mathbf{u}(x)|^2 + |\mathbf{n}(x) \otimes \nabla s(x)|^2 - 2 \nabla \mathbf{u}(x) : [\mathbf{n}(x) \otimes \nabla s(x)] \\
 &= |\nabla \mathbf{u}(x)|^2 - |\nabla s(x)|^2,
 \end{aligned}$$

580

581 where the last equality follows from the identities

$$|\mathbf{n}(x) \otimes \nabla s(x)|^2 = \sum_{i,j=1}^d n_i(x)^2 (\partial_j s(x))^2 = \sum_{j=1}^d (\partial_j s(x))^2 = |\nabla s(x)|^2$$

582

583 and for a.e $x \in \Omega \setminus \Sigma$

$$\begin{aligned}
 \nabla \mathbf{u}(x) : [\mathbf{n}(x) \otimes \nabla s(x)] &= \sum_{i,j=1}^d \partial_j u_i(x) n_i(x) \partial_j s(x) = \frac{1}{s(x)} \sum_{i,j=1}^d \partial_j u_i(x) u_i(x) \partial_j s(x) \\
 &= \frac{1}{2s(x)} \sum_{i,j=1}^d \partial_j |u_i(x)|^2 \partial_j s(x) = \frac{1}{2s(x)} \sum_{j=1}^d \partial_j |\mathbf{u}(x)|^2 \partial_j s(x) \\
 &= \frac{1}{2s(x)} \sum_{j=1}^d \partial_j (s(x)^2) \partial_j s(x) = \sum_{j=1}^d (\partial_j s(x))^2 = |\nabla s(x)|^2.
 \end{aligned}$$

584

585 This concludes the proof. \square

586 **6.2. Lim-sup inequality (consistency).** We start with two results from [23]
 587 that we state without proofs. The first one shows that the degree of orientation s
 588 can be truncated near the end points of the domain of definition $(-1/(d-1), 1)$ of ψ
 589 without increasing the energy $E[s, \mathbf{n}]$. We refer to [23, Lemma 3.1] for a proof.

590 **LEMMA 6.1** (truncation of s). *Let the assumptions (2.12) and (2.14) hold. Let*
 591 *$(s, \mathbf{n}, \mathbf{u}) \in \mathcal{A}(g, \mathbf{r})$. For all $0 < \rho \leq \delta_0$, define*

$$s_\rho(x) := \min \left\{ 1 - \rho, \max \left\{ -\frac{1}{d-1} + \rho, s(x) \right\} \right\} \quad \text{and} \quad \mathbf{u}_\rho(x) := s_\rho(x) \mathbf{n}(x)$$

592

593 for a.e. $x \in \Omega$. Then, $(s_\rho, \mathbf{n}, \mathbf{u}_\rho) \in \mathcal{A}(g, \mathbf{r})$ and $E_1[s_\rho, \mathbf{n}] \leq E_1[s, \mathbf{n}]$, $E_2[s_\rho] \leq E_2[s]$.

594 A simple consequence of [Lemma 6.1](#), based on the convergence of the charac-
 595 teristic function $\chi_{\{s_\rho=s\}} \rightarrow \chi_\Omega$ as $\rho \rightarrow 0$, is that $\|(s, \mathbf{u}) - (s_\rho, \mathbf{u}_\rho)\|_{H^1(\Omega)^{1+d}} \rightarrow 0$ as
 596 $\rho \rightarrow 0$. The second result is about regularization of admissible functions but pre-
 597 serving the structural condition [\(2.6\)](#) and boundary values. This is a rather tricky
 598 two-scale process fully discussed in [\[23, Proposition 3.2\]](#).

599 **LEMMA 6.2** (regularization of functions in $\mathcal{A}(g, \mathbf{r})$). *Let the assumptions [\(2.12\)](#)*
 600 *and [\(2.13\)](#) hold, and suppose that $\Gamma_D = \partial\Omega$. Let $(s, \mathbf{n}, \mathbf{u}) \in \mathcal{A}(g, \mathbf{r})$ and $\rho \leq \delta_0$ such*
 601 *that $-1/(d-1) + \rho \leq s(x) \leq 1 - \rho$ for a.e. $x \in \Omega$. Then, for all $\sigma > 0$, there*
 602 *exists a triple $(s_\sigma, \mathbf{n}_\sigma, \mathbf{u}_\sigma) \in \mathcal{A}(g, \mathbf{r})$ such that $s_\sigma \in W^{1,\infty}(\Omega)$ and $\mathbf{u}_\sigma \in \mathbf{W}^{1,\infty}(\Omega)$.*
 603 *Moreover, there holds $\|(s, \mathbf{u}) - (s_\sigma, \mathbf{u}_\sigma)\|_{H^1(\Omega)^{1+d}} \leq \sigma$, $\|\mathbf{n} - \mathbf{n}_\sigma\|_{\mathbf{L}^2(\Omega \setminus \Sigma)} \leq \sigma$, and*
 604 *$-1/(d-1) + \rho \leq s_\sigma(x) \leq 1 - \rho$ for all $x \in \Omega$.*

605 We recall the following classical local inverse estimates (see, e.g., [\[8, Lemma 3.5\]](#)),
 606 which will be used in several points of the upcoming analysis: For all $v_h \in V_h$,
 607 $1 \leq p, r \leq \infty$, and $K \in \mathcal{T}_h$, there holds

$$608 \quad \|\nabla v_h\|_{\mathbf{L}^p(K)} \leq Ch_K^{-1} \|v_h\|_{L^p(K)} \quad \text{and} \quad \|v_h\|_{L^p(K)} \leq Ch_K^{d(r-p)/(pr)} \|v_h\|_{L^r(K)},$$

609 where $C > 0$ is a constant depending only on the shape-regularity of $\{\mathcal{T}_h\}$.

610 It is well known that the Lagrange interpolation operator $I_h : C(\bar{\Omega}) \rightarrow V_h$ is not
 611 stable in $H^1(\Omega)$ unless $d = 1$. We exploit stability in $L^\infty(\Omega)$ to derive stability in
 612 $W^{1,p}(\Omega)$ for $p > d$.

613 **LEMMA 6.3** ($W^{1,p}$ -stability of Lagrange interpolant). *Let $v \in W^{1,p}(\Omega)$ for $d <$*
 614 *$p \leq \infty$. Then*

$$615 \quad (6.2) \quad \|\nabla I_h[v]\|_{\mathbf{L}^p(K)} \leq C \|\nabla v\|_{\mathbf{L}^p(K)} \quad \text{for all } K \in \mathcal{T}_h,$$

616 where $C > 0$ depends only on the shape-regularity of $\{\mathcal{T}_h\}$.

617 *Proof.* Let $K \in \mathcal{T}_h$ be an arbitrary element and let $\bar{v}_K = f_K v$. An inverse
 618 estimate gives

$$619 \quad \|\nabla I_h[v]\|_{\mathbf{L}^p(K)}^p \leq |K| \|\nabla I_h[v - \bar{v}_K]\|_{\mathbf{L}^\infty(K)}^p \lesssim h_K^{d-p} \|v - \bar{v}_K\|_{L^\infty(K)}^p.$$

620 The Bramble–Hilbert estimate yields $\|v - \bar{v}_K\|_{L^\infty(K)} \lesssim h_K^{1-d/p} \|\nabla v\|_{\mathbf{L}^p(K)}$ and ends
 621 the proof. \square

622 Applying a standard density argument in $W^{1,p}(\Omega)$, for $d < p < \infty$, we deduce

$$623 \quad (6.3) \quad \lim_{h \rightarrow 0} \|v - I_h[v]\|_{W^{1,p}(\Omega)} = 0 \quad \text{for all } v \in W^{1,p}(\Omega).$$

624 We have collected all the ingredients to show the existence of a recovery sequence
 625 (lim-sup inequality).

626 *Proof of [Theorem 3.1](#)(i).* For the sake of clarity, we decompose the proof into
 627 seven steps.

628 *Step 1: Regularization.*

629 Let $(s, \mathbf{n}, \mathbf{u}) \in \mathcal{A}(g, \mathbf{r})$. For all $k \in \mathbb{N}$ such that $1/k \leq \delta_0$, let $0 < \sigma_k \leq 1/k$ be
 630 sufficiently small. Applying successively [Lemma 6.1](#) (with $\rho = 1/k$) and [Lemma 6.2](#)
 631 (with $\sigma = \sigma_k$), we obtain $(s_k, \mathbf{n}_k, \mathbf{u}_k) \in \mathcal{A}(g, \mathbf{r})$ satisfying $(s_k, \mathbf{u}_k) \in [W^{1,\infty}(\Omega)]^{1+d}$
 632 and $-1/(d-1) + 1/k \leq s_k \leq 1 - 1/k$ in Ω for all k . Moreover, we have that

$$633 \quad \|(s, \mathbf{u}) - (s_k, \mathbf{u}_k)\|_{H^1(\Omega)^{1+d}} \leq \sigma_k \quad \text{and} \quad \|\mathbf{n} - \mathbf{n}_k\|_{\mathbf{L}^2(\Omega \setminus \Sigma)} \leq \sigma_k.$$

634 Since $(s, \mathbf{n}, \mathbf{u}) \in \mathcal{A}(g, \mathbf{r})$, [Proposition 2.1](#) guarantees that \mathbf{n} is L^2 -differentiable a.e. in
 635 $\Omega \setminus \Sigma$, with its L^2 -gradient given by (2.8) and that the identity (2.9) holds. The same
 636 result is valid for \mathbf{n}_k a.e. in $\Omega \setminus \Sigma_k$, where $\Sigma_k := \{x \in \Omega : s_k(x) = 0\}$.

637 We have convergence of the energy: $E[s_k, \mathbf{n}_k] \rightarrow E[s, \mathbf{n}]$ as $k \rightarrow \infty$. To see this,
 638 we first observe that, thanks to (2.5), we have that
 639

$$640 \quad E_1[s_k, \mathbf{n}_k] = \tilde{E}_1[s_k, \mathbf{u}_k] = \frac{1}{2} \int_{\Omega} (\kappa - 1) |\nabla s_k|^2 + |\nabla \mathbf{u}_k|^2$$

$$641 \quad \rightarrow \frac{1}{2} \int_{\Omega} (\kappa - 1) |\nabla s|^2 + |\nabla \mathbf{u}|^2 = \tilde{E}_1[s, \mathbf{u}] = E_1[s, \mathbf{n}] \quad \text{as } k \rightarrow \infty.$$

643 Moreover, the monotonicity of ψ in $(-1/(d-1), -1/(d-1) + \delta_0)$ and in $(1 - \delta_0, 1)$
 644 translates into $\psi(s_k) \geq 0$ increasing and converging pointwise to $\psi(s)$, whence the
 645 monotone convergence theorem gives

$$646 \quad E_2[s_k] = \int_{\Omega} \psi(s_k) \rightarrow \int_{\Omega} \psi(s) = E_2[s] \quad \text{as } k \rightarrow \infty.$$

647 Let $\epsilon > 0$ be arbitrary. The above convergences guarantee the existence of $k \in \mathbb{N}$
 648 such that $\sigma_k < \epsilon$, $|E[s_k, \mathbf{n}_k] - E[s, \mathbf{n}]| < \epsilon$ and $|(\Sigma_k \setminus \Sigma) \cup (\Sigma \setminus \Sigma_k)| < \epsilon$. Let such a
 649 $k \in \mathbb{N}$ be fixed for the rest of the proof.

650 *Step 2: Discretization.*

651 Let $s_{k,h} := I_h[s_k]$ and $\mathbf{u}_{k,h} := I_h[\mathbf{u}_k]$. Let $\mathbf{n}_{k,h} \in \mathbf{V}_h$ be defined as

$$652 \quad \mathbf{n}_{k,h}(z) := \begin{cases} \mathbf{u}_{k,h}(z)/s_{k,h}(z) = \mathbf{u}_k(z)/s_k(z) & \text{if } z \in \mathcal{N}_h \cap (\Omega \setminus \Sigma_k), \\ \text{an arbitrary unit vector} & \text{if } z \in \mathcal{N}_h \cap \Sigma_k. \end{cases}$$

653 Note that, by construction, $(s_{k,h}, \mathbf{n}_{k,h}, \mathbf{u}_{k,h})$ satisfies the discrete structural condi-
 654 tion (3.2) and $\|\mathbf{n}_{k,h}\|_{L^\infty(\Omega)} = 1$. Moreover, since $0 = \|I_h[|\mathbf{n}_{k,h}|^2] - 1\|_{L^1(\Omega)} \leq \epsilon$ as
 655 well as $s_{k,h}(z) = g_h(z)$ and $\mathbf{u}_{k,h}(z) = \mathbf{r}_h(z)$ for all $z \in \mathcal{N}_h \cap \Gamma_D$, we deduce that
 656 $(s_{k,h}, \mathbf{n}_{k,h}, \mathbf{u}_{k,h}) \in \mathcal{A}_{h,\epsilon}(g_h, \mathbf{r}_h)$.

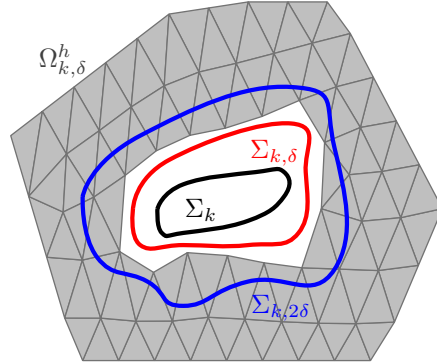


FIG. 9. A schematic illustration of the mutual relations of the sets defined in Steps 1–2 of the proof of [Theorem 3.1\(i\)](#) (*lim-sup inequality*). Note that the set $\Sigma_k \subset \Omega$ is closed, as it is the preimage of a closed set with respect to the continuous function s_k , but it might be more topologically complicated than in the picture.

657 Given $\delta > 0$, we consider the sets

$$658 \quad \Sigma_{k,\delta} := \{x \in \Omega : |s_k(x)| \leq \delta\} \quad \text{and} \quad \Omega_{k,\delta}^h := \bigcup \{K \in \mathcal{T}_h : K \cap \Sigma_{k,\delta} = \emptyset\}.$$

659 Note that, by construction, there holds $\Omega_{k,\delta}^h \subset \Omega \setminus \Sigma_{k,\delta}$; see [Figure 9](#).

660 Let $K \in \mathcal{T}_h$ such that $K \cap \Sigma_{k,\delta} \neq \emptyset$. In particular, there exists $x_0 \in K \cap \Sigma_{k,\delta}$.
661 For $x_1 \in K$ arbitrary, the Lipschitz continuity of s_k yields

$$662 \quad |s_k(x_1)| \leq |s_k(x_0)| + |s_k(x_1) - s_k(x_0)| \leq \delta + \|\nabla s_k\|_{\mathbf{L}^\infty(\Omega)} h.$$

663 Hence, $\Omega \setminus \Omega_{k,\delta}^h \subset \Sigma_{k,2\delta}$ provided h and δ are such that $h\|\nabla s_k\|_{\mathbf{L}^\infty(\Omega)} \leq \delta$; see [Figure 9](#).

664 Now, for any $x \in \Omega_{k,\delta}^h$, we infer that

$$665 \quad |s_k(x) - s_{k,h}(x)| \leq \|s_k - s_{k,h}\|_{L^\infty(\Omega_{k,\delta}^h)} = \|s_k - I_h[s_k]\|_{L^\infty(\Omega_{k,\delta}^h)} \lesssim h\|\nabla s_k\|_{\mathbf{L}^\infty(\Omega_{k,\delta}^h)},$$

666 whence

$$667 \quad |s_{k,h}(x)| \geq |s_k(x)| - |s_k(x) - s_{k,h}(x)| > \delta - Ch\|\nabla s_k\|_{\mathbf{L}^\infty(\Omega_{k,\delta}^h)} > \delta/2$$

668 provided h and δ are such that $Ch\|\nabla s_k\|_{\mathbf{L}^\infty(\Omega)} < \delta/2$. Hence, for this range of
669 parameters, we can define $\tilde{\mathbf{n}}_k := \mathbf{u}_{k,h}/s_{k,h}$ in $\Omega_{k,\delta}^h$. Note that, by definition, the
670 relation $\mathbf{n}_{k,h} = I_h[\tilde{\mathbf{n}}_k]$ in $\Omega_{k,\delta}^h$ holds.

671 To conclude this step, we observe that the L^2 -gradient $\nabla \mathbf{n}_k$ of \mathbf{n}_k exists a.e. in
672 $\Omega \setminus \Sigma_k$ and

$$673 \quad (6.4) \quad \int_{\Omega_{k,\delta}^h} |\nabla \mathbf{n}_k - \nabla \mathbf{n}_{k,h}|^2 \lesssim \int_{\Omega_{k,\delta}^h} |\nabla \mathbf{n}_k - \nabla \tilde{\mathbf{n}}_k|^2 + \int_{\Omega_{k,\delta}^h} |\nabla \tilde{\mathbf{n}}_k - \nabla \mathbf{n}_{k,h}|^2,$$

674 where $\nabla \tilde{\mathbf{n}}_k$ and $\nabla \mathbf{n}_{k,h}$ denote the weak gradients of $\tilde{\mathbf{n}}_k$ and $\mathbf{n}_{k,h}$, respectively, which
675 coincide elementwise with their classical gradients in $\Omega_{k,\delta}^h$. In the following two steps,
676 we will show that, for fixed $k \in \mathbb{N}$ (cf. Step 1), both two terms on the right-hand side
677 of (6.4) converge to 0 if $h, \delta \rightarrow 0$ in an appropriate way (note that we are completely
678 free to choose the speed of convergence of the parameters).

$$679 \quad \textit{Step 3: Proof of } \lim_{h,\delta \rightarrow 0} \int_{\Omega_{k,\delta}^h} |\tilde{\mathbf{n}}_k - \mathbf{n}_{k,h}|^2 + |\nabla \tilde{\mathbf{n}}_k - \nabla \mathbf{n}_{k,h}|^2 = 0.$$

680 Since $\mathbf{n}_{k,h} = I_h[\tilde{\mathbf{n}}_k]$ in $\Omega_{k,\delta}^h$, a classical local interpolation estimate yields that

$$681 \quad \int_{\Omega_{k,\delta}^h} |\nabla \tilde{\mathbf{n}}_k - \nabla \mathbf{n}_{k,h}|^2 = \sum_{\substack{K \in \mathcal{T}_h \\ K \cap \Sigma_{k,\delta} = \emptyset}} \int_K |\nabla(\tilde{\mathbf{n}}_k - I_h[\tilde{\mathbf{n}}_k])|^2 \lesssim \sum_{\substack{K \in \mathcal{T}_h \\ K \cap \Sigma_{k,\delta} = \emptyset}} h_K^2 \|D^2 \tilde{\mathbf{n}}_k\|_{\mathbf{L}^2(K)}^2.$$

682 Similarly, there holds

$$683 \quad \int_{\Omega_{k,\delta}^h} |\tilde{\mathbf{n}}_k - \mathbf{n}_{k,h}|^2 \lesssim \sum_{\substack{K \in \mathcal{T}_h \\ K \cap \Sigma_{k,\delta} = \emptyset}} h_K^4 \|D^2 \tilde{\mathbf{n}}_k\|_{\mathbf{L}^2(K)}^2.$$

684 Moreover, in view of $\tilde{\mathbf{n}}_k = \mathbf{u}_{k,h}/s_{k,h}$ in $\Omega_{k,\delta}^h$, explicit computations reveal that

$$685 \quad \partial_i \tilde{\mathbf{n}}_k = s_{k,h}^{-1} \partial_i \mathbf{u}_{k,h} - s_{k,h}^{-2} \partial_i s_{k,h} \mathbf{u}_{k,h} = s_{k,h}^{-1} (\partial_i \mathbf{u}_{k,h} - \partial_i s_{k,h} \tilde{\mathbf{n}}_k),$$

$$686 \quad \partial_j \partial_i \tilde{\mathbf{n}}_k = s_{k,h}^{-1} (s_{k,h}^{-1} \partial_j \partial_i s_{k,h} \mathbf{u}_{k,h} - \partial_j \partial_i s_{k,h} \tilde{\mathbf{n}}_k - \partial_j \partial_i s_{k,h} \tilde{\mathbf{n}}_k - s_{k,h}^{-1} \partial_j \partial_i s_{k,h} \mathbf{u}_{k,h}),$$

688 for all $1 \leq i, j \leq d$ (note that the second derivatives of the piecewise affine functions
689 $s_{k,h}$ and $\mathbf{u}_{k,h}$ vanish). Several applications of the generalized Hölder inequality, sta-
690 bility (6.2) in $W^{1,p}$ of the Lagrange interpolation operator I_h when $d < p \leq \infty$, in

691 conjunction with the lower bound $|s_{k,h}| > \delta/2$ in $\Omega_{k,\delta}^h$ and the uniform boundedness
 692 of $\mathbf{u}_{k,h}$ in $\mathbf{L}^\infty(\Omega)$, thus yield

$$\begin{aligned}
 & \|D^2 \tilde{\mathbf{n}}_k\|_{\mathbf{L}^2(K)} \lesssim \delta^{-3} \|\nabla s_{k,h}\|_{\mathbf{L}^8(K)}^2 \|\mathbf{u}_{k,h}\|_{\mathbf{L}^4(K)} \\
 & \quad + \delta^{-1} \|\nabla s_{k,h}\|_{\mathbf{L}^4(K)} \left(\delta^{-1} \|\nabla \mathbf{u}_{k,h}\|_{\mathbf{L}^4(K)} + \delta^{-2} \|\mathbf{u}_{k,h}\|_{\mathbf{L}^8(K)} \|\nabla s_{k,h}\|_{\mathbf{L}^8(K)} \right) \\
 693 & \quad + \delta^{-2} \|\nabla s_{k,h}\|_{\mathbf{L}^4(K)} \|\nabla \mathbf{u}_{k,h}\|_{\mathbf{L}^4(K)} \\
 & \lesssim |K|^{1/2} (\delta^{-3} \|\nabla s_k\|_{\mathbf{L}^\infty(K)}^2 + \delta^{-2} \|\nabla s_k\|_{\mathbf{L}^\infty(K)} \|\nabla \mathbf{u}_k\|_{\mathbf{L}^\infty(K)}).
 \end{aligned}$$

694 Altogether, we thus obtain the estimate

$$\begin{aligned}
 695 & \int_{\Omega_{k,\delta}^h} |\nabla \tilde{\mathbf{n}}_k - \nabla \mathbf{n}_{k,h}|^2 + \sum_{\substack{K \in \mathcal{T}_h \\ K \cap \Sigma_{k,\delta} = \emptyset}} h_K^{-2} \int_K |\tilde{\mathbf{n}}_k - \mathbf{n}_{k,h}|^2 \lesssim \sum_{\substack{K \in \mathcal{T}_h \\ K \cap \Sigma_{k,\delta} = \emptyset}} h_K^2 \|D^2 \tilde{\mathbf{n}}_k\|_{\mathbf{L}^2(K)}^2 \\
 696 & \lesssim h^2 (\delta^{-3} \|\nabla s_k\|_{\mathbf{L}^\infty(\Omega)}^2 + \delta^{-2} \|\nabla s_k\|_{\mathbf{L}^\infty(\Omega)} \|\nabla \mathbf{u}_k\|_{\mathbf{L}^\infty(\Omega)})^2, \\
 697 & \\
 698 &
 \end{aligned}$$

699 which yields the desired convergence, if $h\delta^{-3}$ goes to 0 as $h, \delta \rightarrow 0$.

$$700 \quad \textit{Step 4: Proof of } \lim_{h,\delta \rightarrow 0} \int_{\Omega_{k,\delta}^h} |\mathbf{n}_k - \tilde{\mathbf{n}}_k|^2 + |\nabla \mathbf{n}_k - \nabla \tilde{\mathbf{n}}_k|^2 = 0.$$

701 We first observe that

$$\begin{aligned}
 & \|\tilde{\mathbf{n}}_k - \mathbf{n}_k\|_{\mathbf{L}^p(\Omega_{k,\delta}^h)} = \|s_{k,h}^{-1} \mathbf{u}_{k,h} - s_k^{-1} \mathbf{u}_k\|_{\mathbf{L}^p(\Omega_{k,\delta}^h)} \\
 702 & \lesssim \delta^{-2} \|s_k - s_{k,h}\|_{\mathbf{L}^p(\Omega_{k,\delta}^h)} \|\mathbf{u}_{k,h}\|_{\mathbf{L}^\infty(\Omega_{k,\delta}^h)} + \delta^{-1} \|\mathbf{u}_{k,h} - \mathbf{u}_k\|_{\mathbf{L}^p(\Omega_{k,\delta}^h)} \\
 & \lesssim \delta^{-2} h \|\nabla s_k\|_{\mathbf{L}^\infty(\Omega)} + \delta^{-1} h \|\nabla \mathbf{u}_k\|_{\mathbf{L}^\infty(\Omega)},
 \end{aligned}$$

703 for all $1 \leq p < \infty$. This shows that $\|\tilde{\mathbf{n}}_k - \mathbf{n}_k\|_{\mathbf{L}^p(\Omega_{k,\delta}^h)} \rightarrow 0$ if $\delta^{-2}h \rightarrow 0$ as $h, \delta \rightarrow 0$.

704 To deal with the gradient part, we resort to available expressions of $\nabla \mathbf{n}_k$ and $\nabla \tilde{\mathbf{n}}_k$
 705 to write

$$\begin{aligned}
 706 & \int_{\Omega_{k,\delta}^h} |\nabla \mathbf{n}_k - \nabla \tilde{\mathbf{n}}_k|^2 = \int_{\Omega_{k,\delta}^h} |s_k^{-1} (\nabla \mathbf{u}_k - \mathbf{n}_k \otimes \nabla s_k) - s_{k,h}^{-1} (\nabla \mathbf{u}_{k,h} - \tilde{\mathbf{n}}_k \otimes \nabla s_{k,h})|^2 \\
 & \leq T_1 + T_2 + T_3,
 \end{aligned}$$

707 where

$$\begin{aligned}
 708 & T_1 := \int_{\Omega_{k,\delta}^h} |s_{k,h}^{-1} (\nabla \mathbf{u}_k - \nabla \mathbf{u}_{k,h})|^2, \quad T_2 := \int_{\Omega_{k,\delta}^h} |s_{k,h}^{-1} (\tilde{\mathbf{n}}_k \otimes \nabla s_{k,h} - \mathbf{n}_k \otimes \nabla s_k)|^2, \\
 709 & T_3 := \int_{\Omega_{k,\delta}^h} |(s_k^{-1} - s_{k,h}^{-1}) (\nabla \mathbf{u}_k - \mathbf{n}_k \otimes \nabla s_k)|^2. \\
 710 &
 \end{aligned}$$

711 Recalling again $|s_k|, |s_{k,h}| > \delta/2$ in $\Omega_{k,\delta}^h$, as well as (6.2)–(6.3), the asserted conver-
 712 gence follows from

$$\begin{aligned}
 713 & T_1 \lesssim \delta^{-2} \|\nabla (\mathbf{u}_k - I_h[\mathbf{u}_k])\|_{\mathbf{L}^2(\Omega)}^2, \\
 714 & T_2 \lesssim \delta^{-2} (\|\nabla s_{k,h}\|_{\mathbf{L}^4(\Omega_{k,\delta}^h)}^2 \|\tilde{\mathbf{n}}_k - \mathbf{n}_k\|_{\mathbf{L}^4(\Omega_{k,\delta}^h)}^2 + \|\mathbf{n}_k\|_{\mathbf{L}^4(\Omega_{k,\delta}^h)}^2 \|\nabla (s_k - I_h[s_k])\|_{\mathbf{L}^4(\Omega_{k,\delta}^h)}^2), \\
 715 & T_3 \lesssim \delta^{-4} \|s_k - I_h[s_k]\|_{\mathbf{L}^4(\Omega)}^2 \|\nabla \mathbf{u}_k - \mathbf{n}_k \otimes \nabla s_k\|_{\mathbf{L}^4(\Omega)}^2
 \end{aligned}$$

717 and the fact that the right-hand sides of these estimates converge to 0 for a suitably
718 faster convergence of h to 0 relative to that of δ .

719 *Step 5: Proof of* $\lim_{h,\delta \rightarrow 0} \int_{\Omega} s_{k,h}^2 |\nabla \mathbf{n}_{k,h}|^2 = \int_{\Omega \setminus \Sigma_k} s_k^2 |\nabla \mathbf{n}_k|^2$.

720 Let us assume that $h, \delta \rightarrow 0$ in such a way (h sufficiently faster than δ) that the
721 definitions and the convergence results established in Steps 2–4 are valid. Combining
722 Steps 3–4 gives

$$723 \quad (6.5) \quad \lim_{h,\delta \rightarrow 0} \int_{\Omega_{k,\delta}^h} |\nabla \mathbf{n}_k - \nabla \mathbf{n}_{k,h}|^2 = 0.$$

724 In order to exploit this property, we split the integral under consideration as

$$725 \quad (6.6) \quad \int_{\Omega} s_{k,h}^2 |\nabla \mathbf{n}_{k,h}|^2 = \int_{\Omega_{k,\delta}^h} s_{k,h}^2 |\nabla \mathbf{n}_{k,h}|^2 + \int_{\Omega \setminus \Omega_{k,\delta}^h} s_{k,h}^2 |\nabla \mathbf{n}_{k,h}|^2.$$

726 The fact that $s_{k,h} \rightarrow s_k$ strongly in $L^p(\Omega)$ as $h \rightarrow 0$ for $d < p < \infty$, according to
727 (6.3), together with $s_{k,h} \in L^\infty(\Omega)$ uniformly in h , $\nabla \mathbf{n}_k \in \mathbf{L}^\infty(\Omega \setminus \Sigma_{k,\delta})$ and (6.5),
728 yields

$$729 \quad \lim_{h,\delta \rightarrow 0} \left| \int_{\Omega_{k,\delta}^h} s_{k,h}^2 |\nabla \mathbf{n}_{k,h}|^2 - \int_{\Omega_{k,\delta}^h} s_k^2 |\nabla \mathbf{n}_k|^2 \right| = 0.$$

730 Since $\Omega \setminus \Sigma_{k,2\delta} \subset \Omega_{k,\delta}^h \subset \Omega \setminus \Sigma_{k,\delta}$ (recall Figure 9), we deduce

$$731 \quad \lim_{h,\delta \rightarrow 0} \int_{\Omega_{k,\delta}^h} s_{k,h}^2 |\nabla \mathbf{n}_{k,h}|^2 = \int_{\Omega \setminus \Sigma_k} s_k^2 |\nabla \mathbf{n}_k|^2.$$

732 Now, we consider the second term on the right-hand side of (6.6). Since $\Omega \setminus \Omega_{k,\delta}^h \subset$
733 $\Sigma_{k,2\delta}$ and $s_{k,h} \nabla \mathbf{n}_{k,h} = \nabla(s_{k,h} \mathbf{n}_{k,h}) - \mathbf{n}_{k,h} \otimes \nabla s_{k,h}$, using $\mathbf{u}_{k,h} = I_h[s_{k,h} \mathbf{n}_{k,h}]$, we see
734 that

$$\begin{aligned} & \int_{\Omega \setminus \Omega_{k,\delta}^h} s_{k,h}^2 |\nabla \mathbf{n}_{k,h}|^2 \\ 735 \quad & \lesssim \int_{\Sigma_{k,2\delta}} |\nabla(s_{k,h} \mathbf{n}_{k,h})|^2 + \int_{\Sigma_{k,2\delta}} |\mathbf{n}_{k,h} \otimes \nabla s_{k,h}|^2 \\ & \lesssim \int_{\Sigma_{k,2\delta}} |\nabla(s_{k,h} \mathbf{n}_{k,h}) - \nabla I_h[s_{k,h} \mathbf{n}_{k,h}]|^2 + \int_{\Sigma_{k,2\delta}} |\nabla \mathbf{u}_{k,h}|^2 + \int_{\Sigma_{k,2\delta}} |\nabla s_{k,h}|^2. \end{aligned}$$

736 Combining an interpolation estimate with the fact that $s_{k,h}$ and $\mathbf{n}_{k,h}$ are piece-
737 wise affine, and exploiting an inverse estimate to bound $\|\nabla \mathbf{n}_{k,h}\|_{\mathbf{L}^\infty(K)}$ in terms
738 of $\|\mathbf{n}_{k,h}\|_{\mathbf{L}^\infty(K)} = 1$, yields

$$\begin{aligned} 739 \quad & \int_{\Sigma_{k,2\delta}} |\nabla(s_{k,h} \mathbf{n}_{k,h}) - \nabla I_h[s_{k,h} \mathbf{n}_{k,h}]|^2 \lesssim \sum_{\substack{K \in \mathcal{T}_h \\ K \cap \Sigma_{k,2\delta} \neq \emptyset}} h_K^2 \|D^2(s_{k,h} \mathbf{n}_{k,h})\|_{\mathbf{L}^2(K)}^2 \\ 740 \quad & \lesssim \sum_{\substack{K \in \mathcal{T}_h \\ K \cap \Sigma_{k,2\delta} \neq \emptyset}} h_K^2 \|\nabla s_{k,h}\|_{\mathbf{L}^2(K)}^2 \|\nabla \mathbf{n}_{k,h}\|_{\mathbf{L}^\infty(K)}^2 \lesssim \sum_{\substack{K \in \mathcal{T}_h \\ K \cap \Sigma_{k,2\delta} \neq \emptyset}} \|\nabla s_{k,h}\|_{\mathbf{L}^2(K)}^2. \\ 741 \end{aligned}$$

742 Using the $W^{1,p}$ -stability (6.2) of the nodal interpolant with $p > d$ for all elements
 743 $K \in \mathcal{T}_h$ with $K \cap \Sigma_{k,2\delta} \neq \emptyset$, we end up with the following as $h, \delta \rightarrow 0$

744

$$745 \int_{\Omega \setminus \Omega_{k,\delta}^h} s_{k,h}^2 |\nabla \mathbf{n}_{k,h}|^2 \lesssim \|\nabla \mathbf{u}_k\|_{\mathbf{L}^p(\Sigma_{k,3\delta})}^2 + \|\nabla s_k\|_{\mathbf{L}^p(\Sigma_{k,3\delta})}^2$$

$$746 \rightarrow \|\nabla \mathbf{u}_k\|_{\mathbf{L}^p(\Sigma_k)}^2 + \|\nabla s_k\|_{\mathbf{L}^p(\Sigma_k)}^2 = 0$$

748 (cf. [18, Theorem 4.4](iv)), because the Lipschitz continuity of s_k implies that all
 749 elements $K \in \mathcal{T}_h$ with $K \cap \Sigma_{k,2\delta} \neq \emptyset$ are contained in $\Sigma_{k,3\delta}$ provided $h\delta^{-1}$ is sufficiently
 750 small (cf. Step 2).

$$751 \textit{Step 6: Proof of } \lim_{h,\delta \rightarrow 0} \int_{\Omega} |\mathbf{n}_{k,h} \otimes \nabla s_{k,h}|^2 = \int_{\Omega} |\nabla s_k|^2.$$

752 We split the integral as

$$753 \int_{\Omega} |\mathbf{n}_{k,h} \otimes \nabla s_{k,h}|^2 = \int_{\Omega_{k,\delta}^h} |\mathbf{n}_{k,h} \otimes \nabla s_{k,h}|^2 + \int_{\Omega \setminus \Omega_{k,\delta}^h} |\mathbf{n}_{k,h} \otimes \nabla s_{k,h}|^2.$$

754 Exploiting the identity $\mathbf{n}_{k,h} \otimes \nabla s_{k,h} - \mathbf{n}_k \otimes \nabla s_k = (\mathbf{n}_{k,h} - \mathbf{n}_k) \otimes \nabla s_k + \mathbf{n}_{k,h} \otimes (\nabla s_{k,h} -$
 755 $\nabla s_k)$, and using the convergence results for $s_{k,h}$ and $\mathbf{n}_{k,h}$ in $\Omega_{k,\delta}^h$ from Steps 2–4, we
 756 readily see that

$$757 \lim_{h,\delta \rightarrow 0} \int_{\Omega_{k,\delta}^h} |\mathbf{n}_{k,h} \otimes \nabla s_{k,h}|^2 = \int_{\Omega \setminus \Sigma_k} |\mathbf{n}_k \otimes \nabla s_k|^2 = \int_{\Omega} |\nabla s_k|^2.$$

758 Moreover, employing $\Omega \setminus \Omega_{k,\delta} \subset \Sigma_{k,2\delta}$ together with (6.2) implies

$$759 \int_{\Omega \setminus \Omega_{k,\delta}^h} |\mathbf{n}_{k,h} \otimes \nabla s_{k,h}|^2 \lesssim \|\nabla s_{k,h}\|_{\mathbf{L}^2(\Sigma_{k,2\delta})}^2 \lesssim \|\nabla s_{k,h}\|_{\mathbf{L}^p(\Sigma_{k,2\delta})}^2 \lesssim \|\nabla s_k\|_{\mathbf{L}^p(\Sigma_{k,3\delta})}^2.$$

760 Finally, taking $h, \delta \rightarrow 0$ yields $\|\nabla s_k\|_{\mathbf{L}^p(\Sigma_{k,3\delta})} \rightarrow \|\nabla s_k\|_{\mathbf{L}^p(\Sigma_k)} = 0$, which leads to the
 761 desired limit.

762 *Step 7: End of the proof.*

763 Let $\epsilon > 0$ be the arbitrary value fixed in Step 1. The triangle inequality yields that

$$764 \|\mathbf{n}_{k,h} - \mathbf{n}_k\|_{\mathbf{L}^2(\Omega \setminus \Sigma)} \lesssim \|\mathbf{n}_{k,h} - \mathbf{n}_k\|_{\mathbf{L}^2(\Omega_{k,\delta}^h)} + \|\mathbf{n}_{k,h} - \mathbf{n}_k\|_{\mathbf{L}^2(\Sigma_{k,2\delta} \setminus \Sigma)}.$$

765 For the first term, the convergences in Steps 3–4 guarantee that $\|\mathbf{n}_{k,h} - \mathbf{n}_k\|_{\mathbf{L}^2(\Omega_{k,\delta}^h)} < \epsilon$
 766 if h, δ are chosen properly and sufficiently small. For the second term, we have

$$767 \|\mathbf{n}_{k,h} - \mathbf{n}_k\|_{\mathbf{L}^2(\Sigma_{k,2\delta} \setminus \Sigma)} \leq 2|\Sigma_{k,2\delta} \setminus \Sigma|^{1/2} \rightarrow 2|\Sigma_k \setminus \Sigma|^{1/2} \quad \text{as } \delta \rightarrow 0.$$

768 Since $|\Sigma_k \setminus \Sigma|^{1/2} < \epsilon^{1/2}$, we deduce that $\|\mathbf{n}_{k,h} - \mathbf{n}_k\|_{\mathbf{L}^2(\Omega \setminus \Sigma)} \lesssim \epsilon + \epsilon^{1/2}$ provided h, δ
 769 are sufficiently small.

770 Next, recall that $(s_{k,h}, \mathbf{u}_{k,h}) \rightarrow (s_k, \mathbf{u}_k)$ in $H^1(\Omega)^{1+d}$ as $h \rightarrow 0$ (thanks to (6.3))
 771 as well as $E_1^h[s_{k,h}, \mathbf{n}_{k,h}] \rightarrow E_1[s_k, \mathbf{n}_k]$ as $h, \delta \rightarrow 0$ (thanks to Steps 5–6). Furthermore,
 772 since $-1/(d-1) + 1/k \leq s_k \leq 1 - 1/k$ in Ω , assumption (2.14) guarantees that $0 \leq$
 773 $\psi(s_{k,h}) \leq \max\{\psi(-1/(d-1) + 1/k), \psi(1 - 1/k)\}$. Hence, the dominated convergence
 774 theorem implies that

$$775 \lim_{h \rightarrow 0} E_2^h[s_{k,h}] = \lim_{h \rightarrow 0} \int_{\Omega} \psi(I_h[s_k]) = \int_{\Omega} \lim_{h \rightarrow 0} \psi(I_h[s_k]) = \int_{\Omega} \psi(s_k) = E_2[s_k].$$

776 Altogether, we can therefore find sufficiently small $\delta > 0$ and $h > 0$ such that
 777 $\|s_{k,h} - s_k\|_{H^1(\Omega)} < \epsilon$, $\|\mathbf{u}_{k,h} - \mathbf{u}_k\|_{\mathbf{H}^1(\Omega)} < \epsilon$, $\|\mathbf{n}_{k,h} - \mathbf{n}_k\|_{\mathbf{L}^2(\Omega \setminus \Sigma)} \lesssim \epsilon + \epsilon^{1/2}$, and
 778 $|E^h[s_{k,h}, \mathbf{n}_{k,h}] - E[s_k, \mathbf{n}_k]| < \epsilon$. Combining these inequalities with those estab-
 779 lished in Step 1, we conclude that $\|s_{k,h} - s\|_{H^1(\Omega)} < 2\epsilon$, $\|\mathbf{u}_{k,h} - \mathbf{u}\|_{\mathbf{H}^1(\Omega)} < 2\epsilon$,
 780 $\|\mathbf{n}_{k,h} - \mathbf{n}\|_{\mathbf{L}^2(\Omega \setminus \Sigma)} \lesssim \epsilon + \epsilon^{1/2}$, and $|E^h[s_{k,h}, \mathbf{n}_{k,h}] - E[s, \mathbf{n}]| < 2\epsilon$. Since ϵ was arbitrary,
 781 this shows that the sequence $(s_h, \mathbf{n}_h, \mathbf{u}_h) := (s_{k,h}, \mathbf{n}_{k,h}, \mathbf{u}_{k,h}) \in \mathcal{A}_{h,\epsilon}(g_h, \mathbf{r}_h)$ satisfies
 782 the desired convergence towards $(s, \mathbf{n}, \mathbf{u}) \in \mathcal{A}(g, \mathbf{r})$ as well as $\lim_{h \rightarrow 0} E^h[s_h, \mathbf{n}_h] =$
 783 $E[s, \mathbf{n}]$. This implies the lim-sup inequality (3.5) and concludes the proof. \square

784 **6.3. Lim-inf inequality: Stability.** To show the lim-inf inequality, we first
 785 prove that admissible discrete pairs (s_h, \mathbf{n}_h) with uniformly bounded energy are uni-
 786 formly bounded in H^1 . In contrast to [23], we do not need to assume that \mathcal{T}_h is
 787 weakly acute.

788 LEMMA 6.4 (coercivity). *Let $\{(s_h, \mathbf{n}_h, \mathbf{u}_h)\} \subset V_h \times \mathbf{V}_h \times \mathbf{V}_h$ satisfy $\mathbf{u}_h =$
 789 $I_h[s_h, \mathbf{n}_h]$ and $|\mathbf{n}_h(z)| \geq 1$ for all $z \in \mathcal{N}_h$. Then, there exists a constant $C > 0$
 790 depending only on the shape-regularity of $\{\mathcal{T}_h\}$ and κ such that*

$$791 \quad C \max \left\{ \|\nabla \mathbf{u}_h\|_{\mathbf{L}^2(\Omega)}^2, \|\nabla(s_h, \mathbf{n}_h)\|_{\mathbf{L}^2(\Omega)}^2, \|\nabla s_h\|_{\mathbf{L}^2(\Omega)}^2 \right\} \leq E_1^h[s_h, \mathbf{n}_h].$$

792 *Proof.* Since $\|\mathbf{n}_h\|_{\mathbf{L}^\infty(K)} \geq 1$ for all $K \in \mathcal{T}_h$ and ∇s_h is piecewise constant, it
 793 holds that

$$\begin{aligned} \|\nabla s_h\|_{\mathbf{L}^2(\Omega)}^2 &\leq \sum_{K \in \mathcal{T}_h} \|\mathbf{n}_h\|_{\mathbf{L}^\infty(K)}^2 \|\nabla s_h\|_{\mathbf{L}^2(K)}^2 = \sum_{K \in \mathcal{T}_h} |K| \|\mathbf{n}_h\|_{\mathbf{L}^\infty(K)}^2 |\nabla s_h|_K|^2 \\ 794 \quad &\lesssim \sum_{K \in \mathcal{T}_h} |\nabla s_h|_K|^2 \|\mathbf{n}_h\|_{\mathbf{L}^2(K)}^2 = \|\mathbf{n}_h \otimes \nabla s_h\|_{\mathbf{L}^2(\Omega)}^2 \leq \frac{2}{\kappa} E_1^h[s_h, \mathbf{n}_h], \end{aligned}$$

795 where the hidden multiplicative constant depends only on the shape-regularity of
 796 $\{\mathcal{T}_h\}$. Let $\tilde{\mathbf{u}}_h = s_h \mathbf{n}_h$ and use the Hölder inequality in conjunction with (6.2) for
 797 $p > d$ and an inverse estimate to obtain

$$798 \quad \|\nabla I_h[\tilde{\mathbf{u}}_h]\|_{\mathbf{L}^2(K)} \lesssim |K|^{\frac{p-2}{2p}} \|\nabla I_h[\tilde{\mathbf{u}}_h]\|_{\mathbf{L}^p(K)} \lesssim |K|^{\frac{p-2}{2p}} \|\nabla \tilde{\mathbf{u}}_h\|_{\mathbf{L}^p(K)} \lesssim \|\nabla \tilde{\mathbf{u}}_h\|_{\mathbf{L}^2(K)}$$

799 for all $K \in \mathcal{T}_h$. Consequently, for $\mathbf{u}_h = I_h[\tilde{\mathbf{u}}_h]$ we deduce

$$800 \quad \|\nabla \mathbf{u}_h\|_{\mathbf{L}^2(\Omega)}^2 \lesssim \|\nabla \tilde{\mathbf{u}}_h\|_{\mathbf{L}^2(\Omega)}^2 \lesssim \|\mathbf{n}_h \otimes \nabla s_h\|_{\mathbf{L}^2(\Omega)}^2 + \|s_h \nabla \mathbf{n}_h\|_{\mathbf{L}^2(\Omega)}^2 \lesssim E_1^h[s_h, \mathbf{n}_h].$$

801 This completes the proof. \square

802 We are now ready to extract convergent subsequences and characterize their lim-
 803 its.

804 LEMMA 6.5 (characterization of limits). *Let $\{(s_h, \mathbf{n}_h, \mathbf{u}_h)\} \subset \mathcal{A}_{h,\epsilon}(g_h, \mathbf{r}_h)$ be a
 805 sequence such that $E_1^h[s_h, \mathbf{n}_h] \leq C$ and $\|\mathbf{n}_h\|_{\mathbf{L}^\infty(\Omega)} \leq C$, where $C > 0$ is a constant
 806 independent of h . Then, there exist a triple $(s, \mathbf{n}, \mathbf{u}) \in \mathcal{A}(g, \mathbf{r})$ and a subsequence (not
 807 relabeled) of $\{(s_h, \mathbf{n}_h, \mathbf{u}_h)\}$ satisfying the following properties:*

- 808 • As $h \rightarrow 0$, $(s_h, \mathbf{u}_h, s_h \mathbf{n}_h)$ converges towards $(s, \mathbf{u}, \mathbf{u})$ weakly in $H^1(\Omega) \times$
 809 $\mathbf{H}^1(\Omega) \times \mathbf{H}^1(\Omega)$, strongly in $L^2(\Omega) \times \mathbf{L}^2(\Omega) \times \mathbf{L}^2(\Omega)$, and pointwise a.e.
 810 in Ω ;
- 811 • \mathbf{n}_h converges towards \mathbf{n} strongly in $\mathbf{L}^2(\Omega \setminus \Sigma)$ and pointwise a.e. in $\Omega \setminus \Sigma$ as
 812 $h \rightarrow 0$ and $\epsilon \rightarrow 0$;

813 • \mathbf{n} is L^2 -differentiable a.e. in $\Omega \setminus \Sigma$ and the orthogonal decomposition $|\nabla \mathbf{u}|^2 =$
 814 $|\nabla s|^2 + s^2 |\nabla \mathbf{n}|^2$ is valid a.e. in $\Omega \setminus \Sigma$,
 815 where $\Sigma \subset \Omega$ is given by (2.2).

816 *Proof.* For the sake of clarity, we divide the proof into three steps.

817 *Step 1: Convergence of $\{s_h\}$, $\{\mathbf{u}_h\}$, and $\{s_h \mathbf{n}_h\}$.* Since the energy $E_1^h[s_h, \mathbf{n}_h]$
 818 is uniformly bounded, Lemma 6.4 (coercivity) gives uniform bounds in $H^1(\Omega) \times$
 819 $\mathbf{H}^1(\Omega) \times \mathbf{H}^1(\Omega)$ for the the sequence $\{(s_h, \mathbf{u}_h, s_h \mathbf{n}_h)\}$. With successive extractions
 820 of subsequences (not relabeled), one can show that there exists a limit $(s, \mathbf{u}, \tilde{\mathbf{u}}) \in$
 821 $H^1(\Omega) \times \mathbf{H}^1(\Omega) \times \mathbf{H}^1(\Omega)$ such that $(s_h, \mathbf{u}_h, s_h \mathbf{n}_h)$ converges to $(s, \mathbf{u}, \tilde{\mathbf{u}})$ weakly in
 822 $H^1(\Omega) \times \mathbf{H}^1(\Omega) \times \mathbf{H}^1(\Omega)$, strongly in $L^2(\Omega) \times \mathbf{L}^2(\Omega) \times \mathbf{L}^2(\Omega)$, and pointwise a.e. in
 823 Ω . Moreover, weak H^1 -convergence guarantees attainment of traces, namely $s = g$
 824 and $\mathbf{u} = \tilde{\mathbf{u}} = \mathbf{r}$ on Γ_D . To see this, note that $g_h = I_h[g] \rightarrow g$ in $W^{1,p}(\Omega)$ for $p > d$,
 825 according to (6.3), and so in $H^1(\Omega)$. Therefore $s_h - g_h \in H_0^1(\Omega)$ satisfies

$$826 \quad s_h - g_h \rightharpoonup s - g \in H_0^1(\Omega),$$

827 because $H_0^1(\Omega)$ is closed under weak convergence. Hence $s = g$ on Γ_D in the sense
 828 of traces, as asserted. Dealing with \mathbf{u}_h and $\tilde{\mathbf{u}}_h$ is identical. Since $\mathbf{u}_h = I_h[s_h \mathbf{n}_h]$,
 829 interpolation and inverse estimates, yield

$$830 \quad \begin{aligned} \|\mathbf{u}_h - s_h \mathbf{n}_h\|_{\mathbf{L}^2(\Omega)}^2 &\lesssim \sum_{K \in \mathcal{T}_h} h_K^4 \|D^2(s_h \mathbf{n}_h)\|_{\mathbf{L}^2(K)}^2 \\ &\lesssim \sum_{K \in \mathcal{T}_h} h_K^2 \|\nabla(s_h \mathbf{n}_h)\|_{\mathbf{L}^2(K)}^2 \lesssim h^2 E_1^h[s_h, \mathbf{n}_h] \leq Ch^2. \end{aligned}$$

831 This shows that $s_h \mathbf{n}_h$ and \mathbf{u}_h converge strongly in $\mathbf{L}^2(\Omega)$ towards the same limit i.e.,
 832 $\tilde{\mathbf{u}} = \mathbf{u}$. Moreover, $s_h \mathbf{n}_h$ converges to \mathbf{u} weakly in $\mathbf{H}^1(\Omega)$ and pointwise a.e. in Ω .

833 *Step 2: $|s| = |\mathbf{u}|$ a.e. in Ω .* The triangle inequality yields

$$834 \quad \begin{aligned} \|\mathbf{u}_h|^2 - |s_h|^2\|_{L^1(\Omega)} &\leq \| |\mathbf{u}_h|^2 - I_h[|\mathbf{u}_h|^2] \|_{L^1(\Omega)} \\ &\quad + \| I_h[|\mathbf{u}_h|^2] - |s_h|^2 \|_{L^1(\Omega)} + \| |s_h|^2 - I_h[|s_h|^2] \|_{L^1(\Omega)}. \end{aligned}$$

835 For the first and third terms on the right-hand side, standard interpolation estimates
 836 yield

$$837 \quad \| |s_h|^2 - I_h[|s_h|^2] \|_{L^1(\Omega)} \lesssim h^2 \|\nabla s_h\|_{\mathbf{L}^2(\Omega)}^2, \quad \| |\mathbf{u}_h|^2 - I_h[|\mathbf{u}_h|^2] \|_{L^1(\Omega)} \lesssim h^2 \|\nabla \mathbf{u}_h\|_{\mathbf{L}^2(\Omega)}^2.$$

839 On the other hand, since $\{s_h\}$ is uniformly bounded in $L^\infty(\Omega)$, we infer that

$$840 \quad \begin{aligned} \| I_h[|\mathbf{u}_h|^2] - |s_h|^2 \|_{L^1(\Omega)} &= \| I_h[|s_h|^2(|\mathbf{n}_h|^2 - 1)] \|_{L^1(\Omega)} \\ &\leq \| s_h \|_{L^\infty(\Omega)}^2 \| I_h[|\mathbf{n}_h|^2 - 1] \|_{L^1(\Omega)} \leq \varepsilon \| s_h \|_{L^\infty(\Omega)}^2 \rightarrow 0, \end{aligned}$$

841 as $\varepsilon \rightarrow 0$. As $|s_h| \rightarrow |s|$ and $|\mathbf{u}_h| \rightarrow |\mathbf{u}|$ a.e. in Ω , we conclude that $|s| = |\mathbf{u}|$ a.e. in Ω .

842 *Step 3: Convergence of $\{\mathbf{n}_h\}$.* We now define $\mathbf{n} : \Omega \rightarrow \mathbb{R}^3$ as $\mathbf{n} := s^{-1} \mathbf{u}$ in
 843 $\Omega \setminus \Sigma$ and as an arbitrary unit vector in Σ . Step 2 implies, by construction, that
 844 $|\mathbf{n}| = 1$ a.e. in Ω . This shows that $(s, \mathbf{n}, \mathbf{u})$ satisfies the structural condition (2.6),
 845 i.e., $(s, \mathbf{n}, \mathbf{u}) \in \mathcal{A}$.

846 We now observe that $s(x) \neq 0$ for a.e. $x \in \Omega \setminus \Sigma$ by definition of Σ . Since
 847 $s_h(x) \rightarrow s(x)$ as $h \rightarrow 0$, if h is sufficiently small (depending on x), then $s_h(x) \neq 0$ is

848 valid. Consequently,

$$849 \quad \mathbf{n}_h(x) = \frac{s_h(x)\mathbf{n}_h(x)}{s_h(x)} \rightarrow \frac{\mathbf{u}(x)}{s(x)} = \mathbf{n}(x),$$

850 i.e., $\mathbf{n}_h \rightarrow \mathbf{n}$ pointwise a.e. in $\Omega \setminus \Sigma$. Since $\{\mathbf{n}_h\}$ is uniformly bounded in $\mathbf{L}^\infty(\Omega)$, the
851 Lebesgue dominated convergence theorem yields $\mathbf{n}_h \rightarrow \mathbf{n}$ strongly in $\mathbf{L}^2(\Omega \setminus \Sigma)$.

852 Finally, the L^2 -differentiability of \mathbf{n} and the orthogonal decomposition of $\nabla \mathbf{u}$,
853 both valid a.e. in $\Omega \setminus \Sigma$, follow from [Proposition 2.1](#) (orthogonal decomposition). This
854 concludes the proof. \square

855 We are now in the position to prove the lim-inf inequality.

856 *Proof of [Theorem 3.1](#)(ii).* The sequence $\{(s_h, \mathbf{n}_h, \mathbf{u}_h)\} \subset \mathcal{A}_{h,\varepsilon}(g_h, \mathbf{r}_h)$ satisfies
857 the assumptions of [Lemma 6.5](#) (characterization of limits). Hence, we can apply it
858 to obtain subsequences (not relabeled) converging to the respective limits $(s, \mathbf{n}, \mathbf{u}) \in$
859 $\mathcal{A}(g, \mathbf{r})$. Moreover, since also the sequences $\{\mathbf{n}_h \otimes \nabla s_h\}$ and $\{s_h \nabla \mathbf{n}_h\}$ are uniformly
860 bounded in $\mathbf{L}^2(\Omega)$, there exist subsequences (not relabeled) and functions \mathbf{M}, \mathbf{N} in
861 $\mathbf{L}^2(\Omega)$ such that $\mathbf{n}_h \otimes \nabla s_h \rightharpoonup \mathbf{M}$ and $s_h \nabla \mathbf{n}_h \rightharpoonup \mathbf{N}$ weakly in $\mathbf{L}^2(\Omega)$. Combining the
862 equality $s_h \nabla \mathbf{n}_h = \nabla(s_h \mathbf{n}_h) - \mathbf{n}_h \otimes \nabla s_h$, which is valid in every element of \mathcal{T}_h , with
863 $s_h \mathbf{n}_h \rightharpoonup \mathbf{u}$ weakly in $\mathbf{H}^1(\Omega)$, helps identify the limits $\mathbf{N} = \nabla \mathbf{u} - \mathbf{M}$.

864 Let $\Phi \in C_c^\infty(\Omega \setminus \Sigma)$ be an arbitrary $d \times d$ tensor field. We can thus write

$$865 \quad \langle \mathbf{n}_h \otimes \nabla s_h - \mathbf{n} \otimes \nabla s, \Phi \rangle_{\Omega \setminus \Sigma} = \langle (\mathbf{n}_h - \mathbf{n}) \otimes \nabla s_h, \Phi \rangle_{\Omega \setminus \Sigma} + \langle \mathbf{n} \otimes (\nabla s_h - \nabla s), \Phi \rangle_{\Omega \setminus \Sigma}.$$

866 We note that $\mathbf{n}_h \rightarrow \mathbf{n}$ strongly in $L^2(\Omega \setminus \Sigma)$ implies

$$867 \quad \langle (\mathbf{n}_h - \mathbf{n}) \otimes \nabla s_h, \Phi \rangle_{\Omega \setminus \Sigma} \leq \|\mathbf{n}_h - \mathbf{n}\|_{\mathbf{L}^2(\Omega \setminus \Sigma)} \|\nabla s_h\|_{\mathbf{L}^2(\Omega)} \|\Phi\|_{\mathbf{L}^\infty(\Omega \setminus \Sigma)} \rightarrow 0,$$

868 whereas $s_h \rightarrow s$ weakly in $H^1(\Omega)$ yields $\langle \mathbf{n} \otimes (\nabla s_h - \nabla s), \Phi \rangle_{\Omega \setminus \Sigma} \rightarrow 0$. Hence, we
869 infer that $\langle \mathbf{n}_h \otimes \nabla s_h - \mathbf{n} \otimes \nabla s, \Phi \rangle_{\Omega \setminus \Sigma} \rightarrow 0$, whence $\mathbf{n}_h \otimes \nabla s_h \rightharpoonup \mathbf{n} \otimes \nabla s$ weakly
870 in $\mathbf{L}^2(\Omega \setminus \Sigma)$. This in turn identifies the limit $\mathbf{M} = \mathbf{n} \otimes \nabla s$, and gives thus the
871 identity $\mathbf{N} = \nabla \mathbf{u} - \mathbf{n} \otimes \nabla s$ a.e. in $\Omega \setminus \Sigma$. We deduce that $\nabla \mathbf{n} = \mathbf{N}/s$, where $\nabla \mathbf{n}$
872 is understood in the L^2 -sense according to [Proposition 2.1](#). Exploiting the fact that
873 norms are weakly lower semicontinuous, along with $|\mathbf{n} \otimes \nabla s|^2 = |\nabla s|^2$ a.e. in $\Omega \setminus \Sigma$,
874 and $\nabla s = \mathbf{0}$ a.e. in Σ , it holds that

$$\begin{aligned} \liminf_{h \rightarrow 0} E_1^h[s_h, \mathbf{n}_h] &= \liminf_{h \rightarrow 0} \left\{ \frac{\kappa}{2} \|\mathbf{n}_h \otimes \nabla s_h\|_{\mathbf{L}^2(\Omega)}^2 + \frac{1}{2} \|s_h \nabla \mathbf{n}_h\|_{\mathbf{L}^2(\Omega)}^2 \right\} \\ 875 \quad &\geq \liminf_{h \rightarrow 0} \left\{ \frac{\kappa}{2} \|\mathbf{n}_h \otimes \nabla s_h\|_{\mathbf{L}^2(\Omega \setminus \Sigma)}^2 + \frac{1}{2} \|s_h \nabla \mathbf{n}_h\|_{\mathbf{L}^2(\Omega \setminus \Sigma)}^2 \right\} \\ &\geq \frac{\kappa}{2} \|\mathbf{n} \otimes \nabla s\|_{\mathbf{L}^2(\Omega \setminus \Sigma)}^2 + \frac{1}{2} \|s \nabla \mathbf{n}\|_{\mathbf{L}^2(\Omega \setminus \Sigma)}^2 = E_1[s, \mathbf{n}]. \end{aligned}$$

876 Since $s_h \rightarrow s$ a.e. in Ω and ψ is continuous, $\psi(s_h) \rightarrow \psi(s)$ a.e. in Ω . The Fatou lemma
877 yields

$$878 \quad E_2[s] = \int_{\Omega} \psi(s) = \int_{\Omega} \lim_{h \rightarrow 0} \psi(s_h) \leq \liminf_{h \rightarrow 0} \int_{\Omega} \psi(s_h) = \liminf_{h \rightarrow 0} E_2^h[s].$$

879 Altogether, we thus obtain the lim-inf inequality [\(3.6\)](#). This finishes the proof. \square

880 **6.4. Properties of the numerical scheme.** To start with, we prove well-
881 posedness and stability of [Algorithm 4.1](#).

882 *Proof of Proposition 4.1.* Let $i \in \mathbb{N}_0$ and $\ell \in \mathbb{N}_0$. For fixed $s_h^i \in V_h$ (resp.,
 883 $\mathbf{n}_h^{i+1} \in \mathbf{V}_h$), the left-hand side of (4.1) (resp., of (4.3)) is a coercive and continuous
 884 bilinear form on $\mathbf{V}_{h,D}$ (resp., on $V_{h,D}$). Therefore, the variational problem admits a
 885 unique solution $\mathbf{t}_h^{i,\ell} \in \mathcal{K}_h[\mathbf{n}_h^{i,\ell}]$ (resp., $s_h^{i+1} \in V_h$) by the Lax–Milgram theorem. This
 886 shows part (i) and (iii) of Proposition 4.1.

887 Choosing the test function $\phi_h = \tau_n \mathbf{t}_h^{i,\ell} = \mathbf{n}_h^{i,\ell+1} - \mathbf{n}_h^{i,\ell} \in \mathcal{K}_h[\mathbf{n}_h^{i,\ell}]$ in (4.1) yields

$$888 \quad \tau_n \|\mathbf{t}_h^{i,\ell}\|_*^2 + \kappa \langle \mathbf{n}_h^{i,\ell+1} \otimes \nabla s_h^i, (\mathbf{n}_h^{i,\ell+1} - \mathbf{n}_h^{i,\ell}) \otimes \nabla s_h^i \rangle_\Omega$$

$$889 \quad + \langle s_h^i \nabla \mathbf{n}_h^{i,\ell+1}, s_h^i \nabla (\mathbf{n}_h^{i,\ell+1} - \mathbf{n}_h^{i,\ell}) \rangle_\Omega = 0.$$

892 Using the identity $2a(a-b) = a^2 - b^2 + (a-b)^2$, valid for all $a, b \in \mathbb{R}$, we obtain

$$893 \quad (6.7) \quad E_1^h[s_h^i, \mathbf{n}_h^{i,\ell+1}] - E_1^h[s_h^i, \mathbf{n}_h^{i,\ell}] + \tau_n \|\mathbf{t}_h^{i,\ell}\|_*^2 + \tau_n^2 E_1^h[s_h^i, \mathbf{t}_h^{i,\ell}] = 0.$$

894 In particular, $E_1^h[s_h^i, \mathbf{n}_h^{i,\ell+1}] \leq E_1^h[s_h^i, \mathbf{n}_h^{i,\ell}]$ is valid. Since $E_1^h[s_h^i, \mathbf{n}_h^{i,\ell}] \geq 0$ for all
 895 $i \in \mathbb{N}_0$, the sequence $\{E_1^h[s_h^i, \mathbf{n}_h^{i,\ell}]\}_{\ell \in \mathbb{N}_0}$ is convergent (as it is monotonically decreasing
 896 and bounded from below). In particular, it is a Cauchy sequence, which entails that
 897 the stopping criterion (4.2) is met in a finite number of iterations. This shows part (ii)
 898 of the proposition.

899 Let $\ell_i \in \mathbb{N}_0$ be the smallest integer for which the stopping criterion (4.2) is
 900 satisfied. Recall that $\mathbf{n}_h^{i+1} = \mathbf{n}_h^{i,\ell_i+1}$ and $\mathbf{n}_h^i = \mathbf{n}_h^{i,0}$. Summation of (6.7) over $\ell =$
 901 $0, \dots, \ell_i$ yields

$$902 \quad (6.8) \quad E_1^h[s_h^i, \mathbf{n}_h^{i+1}] - E_1^h[s_h^i, \mathbf{n}_h^i] + \tau_n \sum_{\ell=0}^{\ell_i} \|\mathbf{t}_h^{i,\ell}\|_*^2 + \tau_n^2 \sum_{\ell=0}^{\ell_i} E_1^h[s_h^i, \mathbf{t}_h^{i,\ell}] = 0.$$

903 Choosing the test function $w_h = \tau_s d_t s_h^{i+1} = s_h^{i+1} - s_h^i \in V_{h,D}$ in (4.3) and performing
 904 the same algebraic computation as above, we arrive at

$$906 \quad E_1^h[s_h^{i+1}, \mathbf{n}_h^{i+1}] - E_1^h[s_h^i, \mathbf{n}_h^{i+1}] + \tau_s \|d_t s_h^{i+1}\|_{L^2(\Omega)}^2 + \tau_s^2 E_1^h[d_t s_h^{i+1}, \mathbf{n}_h^{i+1}]$$

$$907 \quad + \langle \psi'_c(s_h^{i+1}) - \psi'_c(s_h^i), s_h^{i+1} - s_h^i \rangle_\Omega = 0.$$

909 Applying [23, Lemma 4.1], which yields the inequality

$$910 \quad E_2^h[s_h^{i+1}] - E_2^h[s_h^i] \leq \langle \psi'_c(s_h^{i+1}) - \psi'_c(s_h^i), s_h^{i+1} - s_h^i \rangle_\Omega,$$

911 we obtain

$$913 \quad E_1^h[s_h^{i+1}, \mathbf{n}_h^{i+1}] - E_1^h[s_h^i, \mathbf{n}_h^{i+1}] + \tau_s \|d_t s_h^{i+1}\|_{L^2(\Omega)}^2 + \tau_s^2 E_1^h[d_t s_h^{i+1}, \mathbf{n}_h^{i+1}]$$

$$914 \quad + E_2^h[s_h^{i+1}] - E_2^h[s_h^i] \leq 0.$$

916 Adding the latter with (6.8), and exploiting cancellation of $E_1^h[s_h^i, \mathbf{n}_h^{i+1}]$, we deduce

$$917 \quad (6.9) \quad E^h[s_h^{i+1}, \mathbf{n}_h^{i+1}] - E^h[s_h^i, \mathbf{n}_h^i] \leq -\tau_n \sum_{\ell=0}^{\ell_i} \|\mathbf{t}_h^{i,\ell}\|_*^2 - \tau_n^2 \sum_{\ell=0}^{\ell_i} E_1^h[s_h^i, \mathbf{t}_h^{i,\ell}]$$

$$- \tau_s \|d_t s_h^{i+1}\|_{L^2(\Omega)}^2 - \tau_s^2 E_1^h[d_t s_h^{i+1}, \mathbf{n}_h^{i+1}] \leq 0.$$

918 This shows (4.6) and concludes the proof. \square

919 We recall that [Algorithm 4.1](#) does not enforce the unit-length constraint of the
 920 director field \mathbf{n}_h^j . We finish this paper with a proof that violation of such constraint is
 921 controlled by τ_n and that $\|\mathbf{n}_h^j\|_{L^\infty(\Omega)}$ is uniformly bounded provided the parameters
 922 h and τ_n are suitably chosen.

923 *Proof of [Proposition 4.3](#).* Let $j \geq 1$. Summation of [\(6.9\)](#) over $i = 0, \dots, j-1$
 924 yields

$$925 \quad (6.10) \quad E^h[s_h^j, \mathbf{n}_h^j] + \tau_n \sum_{i=0}^{j-1} \sum_{\ell=0}^{\ell_i} \|\mathbf{t}_h^{i,\ell}\|_*^2 \leq E^h[s_h^0, \mathbf{n}_h^0].$$

926 Moreover, the tangential update $\mathbf{t}_h^{i,\ell}(z)$ is perpendicular to $\mathbf{n}_h^{i,\ell}(z)$ for all $z \in \mathcal{N}_h$,
 927 whence $\mathbf{n}_h^{i,\ell+1}(z) = \mathbf{n}_h^{i,\ell}(z) + \tau_n \mathbf{t}_h^{i,\ell}(z)$ satisfies $|\mathbf{n}_h^{i,\ell+1}(z)|^2 = |\mathbf{n}_h^{i,\ell}(z)|^2 + \tau_n^2 |\mathbf{t}_h^{i,\ell}(z)|^2$.
 928 Iterating in ℓ and i gives

$$929 \quad |\mathbf{n}_h^j(z)|^2 = |\mathbf{n}_h^0(z)|^2 + \tau_n^2 \sum_{i=0}^{j-1} \sum_{\ell=0}^{\ell_i} |\mathbf{t}_h^{i,\ell}(z)|^2 = 1 + \tau_n^2 \sum_{i=0}^{j-1} \sum_{\ell=0}^{\ell_i} |\mathbf{t}_h^{i,\ell}(z)|^2 \geq 1.$$

930 Then, using the equivalence of the L^p -norm of a discrete function with the weighted
 931 ℓ^p -norm of the vector collecting its nodal values (see, e.g., [\[8, Lemma 3.4\]](#)), for h_z
 932 being the diameter of the nodal patch associated with $z \in \mathcal{N}_h$, we see that

$$\begin{aligned} 933 \quad \|I_h[|\mathbf{n}_h^j|^2] - 1\|_{L^1(\Omega)} &\lesssim \sum_{z \in \mathcal{N}_h} h_z^d (|\mathbf{n}_h^j(z)|^2 - 1) \leq \tau_n^2 \sum_{z \in \mathcal{N}_h} h_z^d \sum_{i=0}^{j-1} \sum_{\ell=0}^{\ell_i} |\mathbf{t}_h^{i,\ell}(z)|^2 \\ &\lesssim \tau_n^2 \sum_{i=0}^{j-1} \sum_{\ell=0}^{\ell_i} \|\mathbf{t}_h^{i,\ell}\|_{L^2(\Omega)}^2. \end{aligned}$$

934 Combining [\(4.8\)](#) with [\(6.10\)](#) leads to

$$935 \quad \|I_h[|\mathbf{n}_h^j|^2] - 1\|_{L^1(\Omega)} \lesssim C_* \tau_n^2 \sum_{i=0}^{j-1} \sum_{\ell=0}^{\ell_i} \|\mathbf{t}_h^{i,\ell}\|_*^2 \leq C_* \tau_n E^h[s_h^0, \mathbf{n}_h^0],$$

936 which turns out to be [\(4.9\)](#).

937 It remains to estimate $\|\mathbf{n}_h^j\|_{L^\infty(\Omega)}$. Let us consider first the weighted H^1 -metric
 938 in [\(4.5\)](#). Using a global inverse estimate (see, e.g., [\[8, Remark 3.8\]](#)) and the Poincaré
 939 inequality, we obtain

$$\begin{aligned} \|\mathbf{n}_h^j\|_{L^\infty(\Omega)}^2 - 1 &= \max_{z \in \mathcal{N}_h} |\mathbf{n}_h^j(z)|^2 - 1 \leq \tau_n^2 \sum_{i=0}^{j-1} \sum_{\ell=0}^{\ell_i} \max_{z \in \mathcal{N}_h} |\mathbf{t}_h^{i,\ell}(z)|^2 \\ 940 \quad &\lesssim \tau_n^2 \sum_{i=0}^{j-1} \sum_{\ell=0}^{\ell_i} \|\mathbf{t}_h^{i,\ell}\|_{L^\infty(\Omega)}^2 \lesssim \tau_n^2 h_{\min}^{2-d} |\log h_{\min}|^2 \sum_{i=0}^{j-1} \sum_{\ell=0}^{\ell_i} \|\mathbf{t}_h^{i,\ell}\|_{\mathbf{H}^1(\Omega)}^2 \\ &\lesssim \tau_n^2 h_{\min}^{2-d-\alpha} |\log h_{\min}|^2 \sum_{i=0}^{j-1} \sum_{\ell=0}^{\ell_i} \|h^{\alpha/2} \nabla \mathbf{t}_h^{i,\ell}\|_{L^2(\Omega)}^2 \\ &\leq \tau_n h_{\min}^{2-d-\alpha} |\log h_{\min}|^2 E^h[s_h^0, \mathbf{n}_h^0]. \end{aligned}$$

941 Therefore, [\(4.11\)](#) is satisfied if $\tau_n h_{\min}^{2-d-\alpha} |\log h_{\min}|^2 \leq C^*$ with C^* arbitrary. For the
 942 L^2 -metric [\(4.4\)](#), the result follows analogously, provided that $\tau_n h_{\min}^{-d} \leq C^*$. \square

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