

## CONSTRAINT PRESERVING IMPLICIT FINITE ELEMENT DISCRETIZATION OF HARMONIC MAP FLOW INTO SPHERES

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ABSTRACT. Discretization of the harmonic map flow into spheres often uses a penalization or projection strategy, where the first suffers from the proper choice of an additional parameter, and the latter from the lack of a discrete energy law, and restrictive mesh-constraints. We propose an implicit scheme that preserves the sphere constraint at every node, enjoys a discrete energy law, and unconditionally converges to weak solutions of the harmonic map heat flow.

### 1. INTRODUCTION

Critical points of the energy

$$(1.1) \quad E(\mathbf{u}) := \frac{1}{2} \int_{\Omega} |\nabla \mathbf{u}|^2 \, d\mathbf{x},$$

for maps  $\mathbf{u} : \Omega \rightarrow \mathbf{S}^2$ , where  $\Omega \subset \mathbf{R}^N$ ,  $N = 2, 3$ , is bounded and  $\mathbf{S}^2 \subset \mathbf{R}^3$  is the unit sphere, are known as harmonic maps into spheres. The above energy is prototypic for continuum models in ferromagnetics [14] and liquid crystal theory [1, 15], for example. At present, there are not many algorithms available for reliable approximation [1, 3]; main difficulties in the construction of convergent numerical methods are the nonconvexity of the constraint,  $|\mathbf{u}| = 1$  almost everywhere in  $\Omega$ , limited regularity and nonuniqueness of minimizers, as well as restricted flexibility of used Lagrange finite element functions.

An alternative strategy to study critical points of (1.1) is to consider long-time behavior of the harmonic map flow into spheres,

$$(1.2) \quad \mathbf{u}_t - \Delta \mathbf{u} = |\nabla \mathbf{u}|^2 \mathbf{u} \quad \text{on } \Omega_T, \quad \partial_{\mathbf{n}} \mathbf{u} = 0 \quad \text{on } \partial \Omega_T,$$

$$(1.3) \quad |\mathbf{u}| = 1 \quad \text{a.e. in } \Omega_T, \quad \mathbf{u}(0, \cdot) = \mathbf{u}_0 \quad \text{on } \Omega,$$

for any  $T > 0$ . Here,  $\Omega_T := (0, T) \times \Omega$  and  $\partial \Omega_T := (0, T) \times \partial \Omega$ , with  $\partial \Omega$  being the boundary of  $\Omega$  with outer unit normal  $\mathbf{n}$ . Problem (1.2)–(1.3) characterizes the  $L^2$ -gradient flow of (1.1), and solutions to this problem have been studied intensively over the last fifteen years [17, 7, 8, 11]; see [18] for a survey. Weak solutions to (1.2)–(1.3) satisfy (1.2) in a distributional sense, assume initial data in (1.3) in the

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sense of traces for  $\mathbf{u}_0 \in W^{1,2}(\Omega, \mathbf{S}^2)$ , and satisfy the following energy inequality (cf. [18]) for almost every  $T' \in (0, T)$ :

$$(1.4) \quad E(\mathbf{u}(T', \cdot)) + \int_0^{T'} \|\mathbf{u}_t(s, \cdot)\|_{L^2}^2 ds \leq E(\mathbf{u}_0).$$

It is well-known that there exists a subsequence  $\{t_{k'}\} \subset \{t_k\}$  with  $t_k \rightarrow \infty$ , such that  $\mathbf{u}^* = \lim_{k' \rightarrow \infty} \mathbf{u}(t_{k'}, \cdot)$  exists and is a harmonic map. In order to verify existence of weak solutions to (1.2)–(1.3), the problem is modified to first finding a solution  $\mathbf{u}^\varepsilon : \Omega_T \rightarrow \mathbf{R}^3$  of the following (nonconstrained) penalized formulation for  $\varepsilon > 0$  and  $T > 0$ :

$$(1.5) \quad \mathbf{u}_t^\varepsilon - \Delta \mathbf{u}^\varepsilon + \frac{1}{2\varepsilon} (|\mathbf{u}^\varepsilon|^2 - 1) \mathbf{u}^\varepsilon = 0 \quad \text{on } \Omega_T, \quad \partial_{\mathbf{n}} \mathbf{u}^\varepsilon = 0 \quad \text{on } \partial\Omega_T,$$

$$(1.6) \quad \mathbf{u}^\varepsilon(0, \cdot) = \mathbf{u}_0 \quad \text{on } \Omega;$$

cf. [7, 8]. Considering appropriate limits as  $\varepsilon \rightarrow 0$  for solutions to (1.5)–(1.6) then leads to weak solutions of (1.2)–(1.3), which satisfy (1.4). Apart from its use as an analytical tool, problem (1.5)–(1.6) is often the starting point to construct convergent numerical schemes for (1.2)–(1.3); however, the penalization parameter requires careful balancing with numerical parameters, and often leads to diffusive structures in practice.

From this background, we wish to design a convergent implicit discretization of (1.2)–(1.3) that uses a low order conforming finite element space, such that  $\mathbf{V}_h \subset W^{1,2}(\Omega; \mathbf{R}^3)$ , subordinate to a triangulation  $\mathcal{T}_h$  of  $\Omega$ , and a partition of  $(0, T)$  named  $I_k = \{t_j\}_{j \geq 0}$  of time-step size  $k > 0$ . Classical solutions to (1.2)–(1.3) satisfy  $|\mathbf{u}| = 1$  in  $\Omega_T$ , for  $|\mathbf{u}_0| = 1$  in  $\Omega$ ; this property is not valid any more for straightforward discretizations, due to damping character of most implicit temporal discretization schemes, and restricted flexibility of globally continuous, piecewise polynomial finite element functions. It is the idea of the following projection ansatz (cf. [16, 14]) to compensate for this shortcoming.

**Algorithm 1.1.** For  $j \geq 0$ , let  $\mathbf{U}^j \in \mathbf{V}_h$ . Then, determine  $\tilde{\mathbf{U}}^{j+1} \in \mathbf{V}_h$  from

$$(1.7) \quad (d_t \mathbf{U}^{j+1}, \Phi) + (\nabla \mathbf{U}^{j+1}, \nabla \Phi) = (|\nabla \mathbf{U}^j|^2 \mathbf{U}^{j+1}, \Phi) \quad \forall \Phi \in \mathbf{V}_h,$$

and define  $\mathbf{U}^{j+1} \in \mathbf{V}_h$  through

$$(1.8) \quad \mathbf{U}^{j+1}(\mathbf{z}) = \frac{\tilde{\mathbf{U}}^{j+1}(\mathbf{z})}{|\tilde{\mathbf{U}}^{j+1}(\mathbf{z})|}, \quad \text{for each node.}$$

*Remark 1.1.* Some modifications of the projection step are also studied in [16], where iterates  $\tilde{\mathbf{U}}^{j+1} \in \mathbf{V}_h$  are only shifted closer to the sphere, rather than projecting them back onto it.

In (1.7), we use  $d_t \varphi^j := k^{-1}(\varphi^j - \varphi^{j-1})$ , for  $j \geq 1$  and a sequence  $\{\varphi^j\}_{j \geq 0}$ . Problem (1.7)–(1.8) is computationally attractive, since staying on the sphere is decoupled from computing iterates from (1.7) in  $W^{1,2}(\Omega, \mathbf{R}^3)$ . The algorithm may be reinterpreted as a time-shifted penalization method, which is the starting point in [16, Chapter 4] for an error analysis: strong convergence (at optimal rates) may be established in canonical norms by an inductive argument, to compensate for the lack of a discrete energy law, and rests on existing (local) strong solutions to the problem (1.2)–(1.3). These arguments were extended to  $N = 3$  in [9]. However, reliability of long-time computation with Algorithm 1.1 remains an open question.

As is known from [6], existing weak solutions may show finite-time blow-up behavior even for  $N = 2$ , which thus leaves serious doubts on whether the efficient Algorithm 1.1 handles such situations reliably. In [5], and motivated by [2], an explicit fully discrete method which satisfies the side constraint at every spatial mesh-node is developed for the general  $p$ -harmonic flow, and convergence of iterates towards weak solutions of (1.2)–(1.3) is established under restrictive mesh-size conditions, which for (1.2)–(1.3) is  $k = o(h^2)$ .

The goal of this paper is to construct unconditionally convergent schemes for (1.2)–(1.3). A corresponding program was realized in [4] for the related Landau-Lifshitz-Gilbert equation; unfortunately, arguments there do not carry over to the present case, where in [4] the troublesome term  $-\mathbf{u} \times (\mathbf{u} \times \Delta \mathbf{u})$  in the Landau-Lifshitz formulation was deliberately exchanged by the damping term  $\mathbf{u} \times \mathbf{u}_t$  in the equivalent Gilbert formulation of the ferromagnetic problem.

An essential step in the development of our scheme is to restate (1.2)–(1.3), by using the vector identity  $\mathbf{a} \times (\mathbf{b} \times \mathbf{c}) = \langle \mathbf{a}, \mathbf{c} \rangle \mathbf{b} - \langle \mathbf{a}, \mathbf{b} \rangle \mathbf{c}$ , for all  $\mathbf{a}, \mathbf{b}, \mathbf{c} \in \mathbf{R}^3$ , together with (1.3)<sub>1</sub>, to derive

$$(1.9) \quad \mathbf{u}_t + \mathbf{u} \times (\mathbf{u} \times \Delta \mathbf{u}) = 0 \quad \text{in } \Omega_T.$$

Given the lowest order finite element space  $\mathbf{V}_h \subset W^{1,2}(\Omega; \mathbf{R}^3)$  subordinate to a triangulation  $\mathcal{T}_h$  of  $\Omega$  and a time-step size  $k > 0$ , our first approximation scheme reads as follows.

**Algorithm 1.2.** For  $j \geq 0$ , let  $\mathbf{U}^j \in \mathbf{V}_h$ , and determine  $\mathbf{U}^{j+1} \in \mathbf{V}_h$  from

$$(d_t \mathbf{U}^{j+1}, \Phi)_h + \left( \mathbf{U}^{j+1} \times (\mathbf{U}^{j+1} \times \tilde{\Delta}_h \mathbf{U}^{j+1}), \Phi \right)_h = 0 \quad \forall \Phi \in \mathbf{V}_h.$$

Here,  $(\cdot, \cdot)_h$  denotes a discrete version (reduced integration) of the inner product in  $L^2(\Omega; \mathbf{R}^3)$ ,  $\tilde{\Delta}_h : W^{1,2}(\Omega; \mathbf{R}^3) \rightarrow \mathbf{V}_h$  is a discrete version of the Laplacian, and we use  $d_t \varphi^j := k^{-1}(\varphi^j - \varphi^{j-1})$  for  $j \geq 1$ , for a sequence  $\{\varphi^j\}_{j \geq 0}$ ; we refer to Section 2 for details.

As will be shown in Lemma 3.1, solutions to this scheme satisfy an approximate discrete energy law and an approximate sphere constraint. Next, we propose a modified scheme, which satisfies both properties exactly, i.e., a discrete energy law and the sphere constraint at nodes of the triangulation; cf. Lemma 3.2. We denote  $\bar{\varphi}^{j+1/2} := \frac{1}{2}(\varphi^{j+1} + \varphi^j)$  for  $j \geq 0$ .

**Algorithm 1.3.** For  $j \geq 0$ , let  $\mathbf{U}^j \in \mathbf{V}_h$ , and determine  $\mathbf{U}^{j+1} \in \mathbf{V}_h$  from

$$(1.10) \quad (d_t \mathbf{U}^{j+1}, \Phi)_h + \left( \bar{\mathbf{U}}^{j+1/2} \times (\bar{\mathbf{U}}^{j+1/2} \times \tilde{\Delta}_h \bar{\mathbf{U}}^{j+1/2}), \Phi \right)_h = 0 \quad \forall \Phi \in \mathbf{V}_h.$$

It is well-known that strong solutions to (1.2)–(1.3) solve (1.9) in the distributional sense. In contrast, these relations need not hold for corresponding discretizations, due to competition of local and nonlocal aspects inherent to fully discrete finite-element based methods; cf. [4].

Our main result is unconditional convergence of Algorithm 1.3. For this purpose, let  $\mathbf{u}_{h,k} : \Omega_T \rightarrow \mathbf{R}^3$  be defined by ( $j \geq 0$ )

$$(1.11) \quad \mathbf{u}_{h,k}(t, \mathbf{x}) := \frac{t - t_j}{k} \mathbf{U}^{j+1}(\mathbf{x}) + \frac{t_{j+1} - t}{k} \mathbf{U}^j(\mathbf{x}) \quad \forall (t, \mathbf{x}) \in [t_j, t_{j+1}) \times \Omega.$$

**Theorem 1.1.** Let  $T > 0$ , and  $\mathcal{T}_h$  be a regular triangulation of  $\Omega$  with maximal mesh-size  $h > 0$ , and  $\mathbf{U}^0 \in \mathbf{V}_h$ , with  $|\mathbf{U}^0(\mathbf{z})| = 1$  for all  $\mathbf{z} \in \mathcal{N}_h$ . Let  $\{\mathbf{U}^j\}_{j \geq 0} \subset \mathbf{V}_h$

satisfy (1.10). Then  $|\mathbf{U}^j(\mathbf{z})| = 1$  for all  $\mathbf{z} \in \mathcal{N}_h$  and  $j \geq 0$ , and

$$E(\mathbf{U}^{j+1}) + k \sum_{\ell=0}^j \|\bar{\mathbf{U}}^{\ell+1/2} \times \tilde{\Delta}_h \bar{\mathbf{U}}^{\ell+1/2}\|_h^2 = E(\mathbf{U}^0).$$

Moreover, if  $\mathbf{U}^0 \rightarrow \mathbf{u}_0$  strongly in  $W^{1,2}(\Omega; \mathbf{R}^3)$  as  $(h, k) \rightarrow 0$ , there exists a subsequence of  $\{\mathbf{U}_{h,k}\}$  which converges weakly in  $\mathbf{W}^{1,2}(\Omega_T; \mathbf{R}^3)$  to a weak solution of (1.2)–(1.3).

The proof of Theorem 1.1 may be considered as an alternative way to construct weak solutions to (1.2)–(1.3).

The remainder of this paper is organized as follows: Preliminaries are stated in Section 2. Theorem 1.1 is verified in Section 3. A simple fixed-point iteration (Algorithm 4.1) for the solution of the nonlinear system in each step (1.10) is proposed in Section 4, and convergence is established under certain assumptions regarding  $h, k > 0$ , and the involved stopping criterion. Concluding remarks are stated in Section 5.

## 2. PRELIMINARIES

Let  $\Omega \subset \mathbf{R}^N$  be a bounded Lipschitz domain. We define the nonlinear Sobolev space

$$W^{1,2}(\Omega; \mathbf{S}^2) = \left\{ \mathbf{v} \in W^{1,2}(\Omega; \mathbf{R}^3) \mid \mathbf{v} \in \mathbf{S}^2 \text{ a.e. in } \Omega \right\},$$

which is equipped with the topology inherited from the one of  $W^{1,2}(\Omega; \mathbf{R}^3)$ . Critical points  $\mathbf{u} \in W^{1,2}(\Omega; \mathbf{S}^2)$  of  $E(\mathbf{u})$  may be characterized as solutions to the Euler-Lagrange equation

$$(2.1) \quad -\Delta \mathbf{u} = |\nabla \mathbf{u}|^2 \mathbf{u} \text{ on } \Omega, \quad \partial_{\mathbf{n}} \mathbf{u} = 0 \text{ on } \partial \Omega.$$

If a map  $\mathbf{u} \in W^{1,2}(\Omega, \mathbf{S}^2)$  satisfies (2.1) in the distributional sense, it is called a weakly harmonic map. We now make precise what we mean by a weak solution to (1.2)–(1.3).

**Definition 2.1.** Let  $\mathbf{u}_0 \in W^{1,2}(\Omega, \mathbf{S}^2)$ . Then  $\mathbf{u} : \Omega_T \rightarrow \mathbf{R}^3$  is a weak solution to (1.2)–(1.3), if

1.  $\mathbf{u} \in L^\infty(0, T; W^{1,2}(\Omega; \mathbf{R}^3)) \cap W^{1,2}(\Omega_T; \mathbf{R}^3)$  for all  $T > 0$ ,
2.  $|\mathbf{u}| = 1$  almost everywhere in  $\Omega_T$ ,
3.  $\mathbf{u}$  satisfies (1.4) for almost every  $T' \in (0, T)$ ,
4. for all  $\phi \in C^\infty(\bar{\Omega}_T; \mathbf{R}^3)$  there holds

$$(2.2) \quad \int_0^T \{(\mathbf{u}_t, \mathbf{u} \times \phi) + (\nabla \mathbf{u}, \nabla[\mathbf{u} \times \phi])\} dt = 0,$$

5. the initial condition holds in the sense of traces.

We refer to [17, 18] for a verification of its existence and qualitative analyses. By choosing (a regularization of)  $\phi = \mathbf{u} \times \psi$  in (2.2) one checks with the properties of the vector product and with  $|\mathbf{u}| = 1$  almost everywhere in  $\Omega_T$  that the weak solution of (1.2)–(1.3) satisfies for all  $\psi \in C_0^\infty(\Omega_T; \mathbf{R}^3)$

$$\int_0^T \{(\mathbf{u}_t, \psi) + (\nabla \mathbf{u}, \nabla \psi) - (|\nabla \mathbf{u}|^2 \mathbf{u}, \psi)\} dt = 0.$$

Throughout this paper we assume that  $\mathcal{T}_h$  is a quasiuniform regular triangulation of the polygonal or polyhedral bounded Lipschitz domain  $\Omega \subset \mathbf{R}^N$  into triangles or tetrahedra for  $N = 2, 3$ , respectively. We use the lowest order finite element space  $\mathbf{V}_h \subset W^{1,2}(\Omega; \mathbf{R}^3)$ ,

$$\mathbf{V}_h = \left\{ \Phi \in C(\bar{\Omega}; \mathbf{R}^3) : \Phi|_K \in \mathcal{P}_1(K; \mathbf{R}^3) \quad \forall K \in \mathcal{T}_h \right\},$$

where  $\mathcal{P}_1(K; \mathbf{R}^3)$  denotes the set of polynomials of total degree less than or equal to one if restricted to the element  $K \in \mathcal{T}_h$ . Given the set of nodes (or vertices)  $\mathcal{N}_h$  in  $\mathcal{T}_h$ , and letting  $\{\varphi_{\mathbf{z}} : \mathbf{z} \in \mathcal{N}_h\}$  denote the nodal basis in  $V_h$ , we define the nodal interpolation operator  $\mathcal{I}_h : C(\bar{\Omega}; \mathbf{R}^3) \rightarrow \mathbf{V}_h$  by  $\mathcal{I}_h \psi := \sum_{\mathbf{z} \in \mathcal{N}_h} \psi(\mathbf{z}) \varphi_{\mathbf{z}}$ , for  $\psi \in C(\bar{\Omega}; \mathbf{R}^3)$ . For  $\mathbf{f}, \mathbf{g} \in L^2(\Omega; \mathbf{R}^3)$ , and  $\langle \cdot, \cdot \rangle$  the inner product in  $\mathbf{R}^3$ , let

$$(\mathbf{f}, \mathbf{g}) = \int_{\Omega} \langle \mathbf{f}, \mathbf{g} \rangle \, dx.$$

For functions  $\phi, \psi \in C(\bar{\Omega}; \mathbf{R}^3)$  we use

$$(\phi, \psi)_h = \int_{\Omega} \mathcal{I}_h(\langle \phi, \psi \rangle) \, dx = \sum_{\mathbf{z} \in \mathcal{N}_h} \beta_{\mathbf{z}} \langle \phi(\mathbf{z}), \psi(\mathbf{z}) \rangle,$$

where  $\beta_{\mathbf{z}} = \int_{\Omega} \varphi_{\mathbf{z}} \, dx$ , and  $\mathbf{z} \in \mathcal{N}_h$ . We define  $\|\Phi\|_h^2 = (\Phi, \Phi)_h$ , and have for all  $\Phi, \Psi \in \mathbf{V}_h$ ,

$$(2.3) \quad \|\Phi\|_{L^2} \leq \|\Phi\|_h \leq (N+2)^{1/2} \|\Phi\|_{L^2},$$

$$(2.4) \quad \left| (\Phi, \Psi)_h - (\Phi, \Psi) \right| \leq Ch \|\Phi\|_{L^2} \|\nabla \Psi\|_{L^2},$$

where  $h$  is the maximal mesh-size of  $\mathcal{T}_h$ . Here and throughout the paper,  $C > 0$  denotes an  $(h, k)$ -independent constant. We define the discrete Laplacian  $\tilde{\Delta}_h : W^{1,2}(\Omega; \mathbf{R}^3) \rightarrow \mathbf{V}_h$  via

$$(2.5) \quad -(\tilde{\Delta}_h \phi, \Psi)_h = (\nabla \phi, \nabla \Psi) \quad \forall \Psi \in \mathbf{V}_h.$$

If  $\mathcal{T}_h$  is a quasiuniform triangulation of  $\Omega$ , then there exists a constant  $C > 0$  such that for all  $\Phi \in \mathbf{V}_h$  there hold

$$(2.6) \quad \|\tilde{\Delta}_h \Phi\|_h \leq Ch^{-2} \|\Phi\|_h \quad \text{and} \quad \|\tilde{\Delta}_h \Phi\|_{L^\infty} \leq Ch^{-2} \|\Phi\|_{L^\infty}.$$

The proof of the first estimate in (2.6) follows directly from the inverse estimate  $\|\nabla \Phi\| \leq Ch^{-1} \|\Phi\|$ . In order to verify the second estimate, let  $\mathbf{z} \in \mathcal{N}_h$  be such that  $\|\tilde{\Delta}_h \Phi\|_{L^\infty} = |\tilde{\Delta}_h \Phi(\mathbf{z})|$ . Choosing  $\Psi = \tilde{\Delta}_h \Phi(\mathbf{z}) \varphi_{\mathbf{z}}$  in (2.5) yields that

$$\begin{aligned} |\tilde{\Delta}_h \Phi(\mathbf{z})|^2 &= \beta_{\mathbf{z}}^{-1} (\tilde{\Delta}_h \Phi, \Psi)_h \\ &\leq |\tilde{\Delta}_h \Phi(\mathbf{z})| \beta_{\mathbf{z}}^{-1} \sum_{\mathbf{y} \in \mathcal{N}_h} |\Phi(\mathbf{y})| |\langle \nabla \varphi_{\mathbf{y}}, \nabla \varphi_{\mathbf{z}} \rangle| \leq C |\tilde{\Delta}_h \Phi(\mathbf{z})| \beta_{\mathbf{z}}^{-1} \|\Phi\|_{L^\infty} \|\nabla \varphi_{\mathbf{z}}\|_{L^2}^2 \\ &\leq C |\tilde{\Delta}_h \Phi(\mathbf{z})| \beta_{\mathbf{z}}^{-1} \|\Phi\|_{L^\infty} h^{-2} \|\varphi_{\mathbf{z}}\|_{L^2}^2 \leq C |\tilde{\Delta}_h \Phi(\mathbf{z})| h^{-2} \|\Phi\|_{L^\infty}, \end{aligned}$$

where we have used the fact that the number of nodes  $\mathbf{y} \in \mathcal{N}_h$  such that  $\langle \nabla \varphi_{\mathbf{y}}, \nabla \varphi_{\mathbf{z}} \rangle \neq 0$  is bounded  $h$ -independently,  $\|\nabla \varphi_{\mathbf{y}}\| \leq C \|\nabla \varphi_{\mathbf{z}}\|$  for such  $\mathbf{y}$ , and  $\beta_{\mathbf{z}}^{-1} \|\varphi_{\mathbf{z}}\|^2 \leq C$ .

3. PROOF OF THEOREM 1.1

The first lemma outlines properties of iterates from Algorithm 1.2.

**Lemma 3.1.** *For Algorithm 1.2, suppose  $|\mathbf{U}^0(\mathbf{z})| = 1$  for all  $\mathbf{z} \in \mathcal{N}_h$ . Then the sequence  $\{\mathbf{U}^j\}_{j \geq 0}$  satisfies for all  $j \geq 0$*

- (i)  $|\mathbf{U}^{j+1}(\mathbf{z})|^2 + k^2 \sum_{\ell=0}^j |d_t \mathbf{U}^{\ell+1}(\mathbf{z})|^2 = 1 \quad \forall \mathbf{z} \in \mathcal{N}_h,$
- (ii)  $\frac{1}{2} \|\nabla \mathbf{U}^{j+1}\|_{L^2}^2 + k \sum_{\ell=0}^j \left[ \frac{k}{2} \|\nabla d_t \mathbf{U}^{\ell+1}\|_{L^2}^2 + \left\| \mathbf{U}^{j+1} \times \tilde{\Delta}_h \mathbf{U}^{j+1} \right\|_h^2 \right]$   
 $= \frac{1}{2} \|\nabla \mathbf{U}^0\|_{L^2}^2,$
- (iii)  $k \sum_{\ell=0}^j \|d_t \mathbf{U}^{\ell+1}\|_h^2 \leq \frac{1}{2} \|\nabla \mathbf{U}^0\|_{L^2}^2.$

*Proof.* Assertion (i) follows from choosing  $\Phi = \mathbf{U}^{j+1}(\mathbf{z})\varphi_{\mathbf{z}} \in \mathbf{V}_h$ , for  $\mathbf{z} \in \mathcal{N}_h$  in Algorithm 1.2, binomial formula, and assumption for initial data. In order to verify (ii), choose  $\Phi = -\tilde{\Delta}_h \mathbf{U}^{j+1}$  and find

$$\frac{1}{2} d_t \|\nabla \mathbf{U}^{j+1}\|_{L^2}^2 + \frac{k}{2} \|\nabla d_t \mathbf{U}^{j+1}\|_{L^2}^2 + \left( \mathbf{U}^{j+1} \times (\mathbf{U}^{j+1} \times \tilde{\Delta}_h \mathbf{U}^{j+1}), -\tilde{\Delta}_h \mathbf{U}^{j+1} \right)_h = 0.$$

Thanks to  $(\mathbf{a} \times \mathbf{b}, \mathbf{c}) := -(\mathbf{a} \times \mathbf{c}, \mathbf{b})$  for all  $\mathbf{a}, \mathbf{b}, \mathbf{c} \in \mathbf{R}^3$ , this verifies (ii). The estimate (iii) now follows from (i)–(ii), by setting  $\Phi = d_t \mathbf{U}^{j+1}$  and using Young’s inequality.  $\square$

Next, we ask for corresponding stability properties for Algorithm 1.3. As will be clear in Section 4, it is useful to consider an extended version of (1.10) for this purpose. Let  $\{\mathbf{R}^{j+1}\} \subset \mathbf{V}_h$  be given, and let  $\|\mathbf{R}^{j+1}\|_h \leq \varepsilon$ , for all  $j \geq 0$ , and some  $\varepsilon > 0$ . For  $j \geq 0$ , let  $\mathbf{U}^j \in \mathbf{V}_h$ , and find  $\mathbf{U}^{j+1} \in \mathbf{V}_h$  such that

$$(3.1) \quad \begin{aligned} & (d_t \mathbf{U}^{j+1}, \Phi)_h + \left( \bar{\mathbf{U}}^{j+1/2} \times (\bar{\mathbf{U}}^{j+1/2} \times \tilde{\Delta}_h \bar{\mathbf{U}}^{j+1/2}), \Phi \right)_h \\ & = (\bar{\mathbf{U}}^{j+1/2} \times \mathbf{R}^{j+1}, \Phi)_h \quad \forall \Phi \in \mathbf{V}_h. \end{aligned}$$

The following lemma provides discrete counterparts of items 1 and 4 in Definition 2.1 for iterates  $\{\mathbf{U}^j\}$  which satisfy (3.1).

**Lemma 3.2.** *Let  $0 \leq \varepsilon < 1$ , and  $|\mathbf{U}^0(\mathbf{z})| = 1$  for all  $\mathbf{z} \in \mathcal{N}_h$ . Suppose that  $\{\mathbf{U}^j\}, \{\mathbf{R}^{j+1}\} \subset \mathbf{V}_h$  satisfy (3.1). Then, for all  $j \geq 0$ ,*

- (i)  $|\mathbf{U}^{j+1}(\mathbf{z})| = 1 \quad \forall \mathbf{z} \in \mathcal{N}_h,$
- (ii)  $\frac{1}{2} \|\nabla \mathbf{U}^{j+1}\|_{L^2}^2 + (1 - \varepsilon) k \sum_{\ell=0}^j \left\| \bar{\mathbf{U}}^{\ell+1/2} \times \tilde{\Delta}_h \bar{\mathbf{U}}^{\ell+1/2} \right\|_h^2$   
 $\leq \frac{1}{2} \|\nabla \mathbf{U}^0\|_{L^2}^2 + \varepsilon t_{j+1},$
- (iii)  $k \sum_{\ell=0}^j \|d_t \mathbf{U}^{\ell+1}\|_h^2 \leq \frac{1}{2} \|\nabla \mathbf{U}^0\|_{L^2}^2 + \frac{5\varepsilon}{4} t_j.$

*Proof.* Choose  $\Phi = \bar{\mathbf{U}}^{j+1/2}(\mathbf{z})\varphi_{\mathbf{z}}$ , for  $\mathbf{z} \in \mathcal{N}_h$  to verify assertion (i). To verify (ii), set  $\Phi = -\tilde{\Delta}_h \bar{\mathbf{U}}^{j+1/2}$  in (3.1) and deduce

$$\begin{aligned} & \frac{1}{2}d_t\|\nabla\mathbf{U}^{j+1}\|^2 + \|\bar{\mathbf{U}}^{j+1/2} \times \tilde{\Delta}_h \bar{\mathbf{U}}^{j+1/2}\|_h^2 \\ &= -(d_t\mathbf{U}^{j+1}, \tilde{\Delta}_h \bar{\mathbf{U}}^{j+1/2})_h - \left(\bar{\mathbf{U}}^{j+1/2} \times (\bar{\mathbf{U}}^{j+1/2} \times \tilde{\Delta}_h \bar{\mathbf{U}}^{j+1/2}), \tilde{\Delta}_h \bar{\mathbf{U}}^{j+1/2}\right)_h \\ &= -(\bar{\mathbf{U}}^{j+1/2} \times \mathbf{R}^{j+1}, \tilde{\Delta}_h \bar{\mathbf{U}}^{j+1/2})_h \leq \frac{1}{4\varepsilon}\|\mathbf{R}^{j+1}\|_h^2 + \varepsilon\|\bar{\mathbf{U}}^{j+1/2} \times \tilde{\Delta}_h \bar{\mathbf{U}}^{j+1/2}\|_h^2, \end{aligned}$$

from which we infer assertion (ii) after summation. For (iii), we set  $\Phi = d_t\mathbf{U}^{j+1}$  in (3.1), the bound  $\|\bar{\mathbf{U}}^{j+1/2}\|_{L^\infty} \leq 1$ , and Young’s inequality to conclude

$$\begin{aligned} \|d_t\mathbf{U}^{j+1}\|_h^2 &= \left(\bar{\mathbf{U}}^{j+1/2} \times \tilde{\Delta}_h \bar{\mathbf{U}}^{j+1/2}, \bar{\mathbf{U}}^{j+1/2} \times d_t\mathbf{U}^{j+1}\right)_h \\ &\quad + (\bar{\mathbf{U}}^{j+1/2} \times \mathbf{R}^{j+1}, d_t\mathbf{U}^{j+1})_h \\ &\leq \|\bar{\mathbf{U}}^{j+1/2} \times \tilde{\Delta}_h \bar{\mathbf{U}}^{j+1/2}\|_h \|\bar{\mathbf{U}}^{j+1/2}\|_{L^\infty} \|d_t\mathbf{U}^{j+1}\|_h \\ &\quad + \|\bar{\mathbf{U}}^{j+1/2}\|_{L^\infty} \|d_t\mathbf{U}^{j+1}\|_h \|\mathbf{R}^{j+1}\|_h \\ &\leq \frac{1}{2}\|\bar{\mathbf{U}}^{j+1/2} \times \tilde{\Delta}_h \bar{\mathbf{U}}^{j+1/2}\|_h^2 + \frac{1}{2\varepsilon}\|\mathbf{R}^{j+1}\|_h^2 + \frac{1}{2}(1 + \varepsilon)\|d_t\mathbf{U}^{j+1}\|_h^2. \end{aligned}$$

Thanks to (ii), this verifies assertion (iii). □

Existence of sequences  $\{\mathbf{U}^j\}_{j \geq 0} \subset \mathbf{V}_h$  which solve Algorithm 1.2, resp. (3.1), follows from Brouwer’s fixed point theorem: for given  $\{\mathbf{R}^{j+1}\} \subset \mathbf{V}_h$ , consider the continuous mapping  $\mathbf{F} : \mathbf{V}_h \rightarrow \mathbf{V}_h$ , where for all  $j \geq 0$ ,

$$\mathbf{F}(\Phi) = \frac{2}{k}(\Phi - \mathbf{U}^j) + \mathcal{I}_h[\Phi \times (\Phi \times \tilde{\Delta}_h \Phi) - (\Phi \times \mathbf{R}^{j+1})].$$

For all  $\Phi \in \mathbf{V}_h$  such that  $\|\Phi\|_h \geq \|\mathbf{U}^j\|_h$  we have

$$(\mathbf{F}(\Phi), \Phi)_h = \frac{2}{k}(\|\Phi\|_h^2 - (\mathbf{U}^j, \Phi)_h) \geq \frac{2}{k}\|\Phi\|_h(\|\Phi\|_h - \|\mathbf{U}^j\|_h) \geq 0.$$

Brouwer’s theorem implies the existence of  $\Phi^* \in \mathbf{V}_h$  such that  $\mathbf{F}(\Phi^*) = 0$  (cf. e.g. [12, Corollary 1.1, p. 279]). Then  $\mathbf{U}^{j+1} := 2\Phi^* - \mathbf{U}^j$  solves (3.1). The following result immediately implies Theorem 1.1.

**Theorem 3.3.** *Suppose that the assumptions of Lemma 3.2 are valid, and  $\{\mathbf{U}^j\}, \{\mathbf{R}^j\}$  solve (3.1). Let  $\mathbf{u}_{h,k,\varepsilon} : \Omega_T \rightarrow \mathbf{R}^3$ , as in (1.11). For  $\mathbf{U}^0 \rightarrow \mathbf{u}_0$  strongly in  $W^{1,2}(\Omega, \mathbf{R}^3)$  as  $h \rightarrow 0$ , there exists a subsequence of  $\{\mathbf{u}_{h,k,\varepsilon}\}$  which converges weakly in  $W^{1,2}(\Omega_T, \mathbf{R}^3)$  as  $(h, k, \varepsilon) \rightarrow 0$  to a weak solution of (1.2)–(1.3).*

The verification of this result is given in the remainder of this section. Next, we drop sub-indices of  $\mathbf{u}_{h,k,\varepsilon}$ , and also introduce

$$\mathbf{u}^-(t, \cdot) := \mathbf{U}^j, \quad \mathbf{u}^+(t, \cdot) := \mathbf{U}^{j+1}, \quad \bar{\mathbf{u}}(t, \cdot) := \bar{\mathbf{U}}^{j+1/2} \quad t \in [t_j, t_{j+1}).$$

Now, the bounds of Lemma 3.2 and relations between  $\mathbf{u}, \mathbf{u}^+, \bar{\mathbf{u}}$  yield the existence of  $\mathbf{u} \in W^{1,2}(\Omega_T, \mathbf{R}^3)$  such that as  $(h, k, \varepsilon) \rightarrow 0$ ,

$$\begin{aligned} (3.2) \quad & \mathbf{u}, \mathbf{u}^+, \bar{\mathbf{u}} \xrightarrow{*} \mathbf{u} \quad \text{in } L^\infty(0, T, W^{1,2}(\Omega, \mathbf{R}^3)), \\ & \mathbf{u}, \mathbf{u}^+, \bar{\mathbf{u}} \rightarrow \mathbf{u} \quad \text{in } L^2(\Omega_T, \mathbf{R}^3), \\ & \partial_t \mathbf{u} \rightarrow \partial_t \mathbf{u} \quad \text{in } L^2(\Omega_T, \mathbf{R}^3). \end{aligned}$$

Since  $|\mathbf{u}^+| = 1$  for all  $\mathbf{z} \in \mathcal{N}_h$  and almost all  $t \in (0, T)$ , there holds that  $\mathcal{I}_h[|\mathbf{u}^+|^2] = 1$  for almost all  $\mathbf{x} \in \Omega$  and  $t \in (0, T)$ , and hence we deduce with standard results for nodal interpolation

$$\begin{aligned} \|\mathbf{u}^+ - 1\|_{L^2(K)} &\leq Ch \|\nabla[|\mathbf{u}^+|^2 - 1]\|_{L^2(K)} \\ &\leq Ch \|(\mathbf{u}^+)^T \nabla \mathbf{u}^+\|_{L^2(K)}^2 \leq Ch \|\nabla \mathbf{u}^+\|_{L^2(K)}^2, \end{aligned}$$

for all  $K \in \mathcal{T}_h$  that  $|\mathbf{u}| \rightarrow 1$  almost everywhere in  $\Omega_T$ , and hence  $|\mathbf{u}| = 1$  almost everywhere.

We use weak lower semicontinuity of norms and the fact that  $\mathbf{U}^0 \rightarrow \mathbf{u}_0$  in assertion (ii) of Lemma 3.2 to verify that  $\mathbf{u}$  satisfies (1.4). Since the trace operator is bounded and linear, it is weakly continuous as an operator from  $W^{1,2}(\Omega_T, \mathbf{R}^3)$  into  $L^2(\Omega, \mathbf{R}^3)$ , and we deduce that  $\mathbf{u}(0, \cdot) = \mathbf{u}_0$  in the sense of traces. Lemma 3.4 states that the missing property 4 of Definition 2.1 for  $\mathbf{u}$  to be a weak solution of (1.2)–(1.3) is valid as well.

**Lemma 3.4.** *For  $\mathbf{u} : \Omega_T \rightarrow \mathbf{R}^3$  as in (3.2) and all  $\boldsymbol{\psi} \in C^\infty(\overline{\Omega}_T, \mathbf{R}^3)$ , then the following identity is satisfied:*

$$\int_0^T \{(\partial_t \mathbf{u}, \mathbf{u} \times \boldsymbol{\psi}) + (\nabla \mathbf{u}, \nabla[\mathbf{u} \times \boldsymbol{\psi}])\} dt = 0.$$

*Proof.* For  $t \in (0, T)$  let  $\boldsymbol{\Psi}(t, \cdot) = \mathcal{I}_h \boldsymbol{\psi}(t, \cdot)$ , where  $\boldsymbol{\psi} \in C^\infty(\overline{\Omega}_T, \mathbf{R}^3)$ . Then

$$\begin{aligned} (\partial_t \mathbf{u}, \overline{\mathbf{u}} \times \boldsymbol{\Psi})_h - (\partial_t \mathbf{u}, \mathbf{u} \times \boldsymbol{\psi}) &= \left[ (\partial_t \mathbf{u}, \mathcal{I}_h[\overline{\mathbf{u}} \times \boldsymbol{\Psi}])_h - (\partial_t \mathbf{u}, \mathcal{I}_h[\overline{\mathbf{u}} \times \boldsymbol{\Psi}]) \right] \\ &\quad + (\partial_t \mathbf{u}, \mathcal{I}_h[\overline{\mathbf{u}} \times \boldsymbol{\Psi}] - \overline{\mathbf{u}} \times \boldsymbol{\Psi}) + (\partial_t \mathbf{u}, \overline{\mathbf{u}} \times [\boldsymbol{\Psi} - \boldsymbol{\psi}]) \\ &\quad + (\partial_t \mathbf{u}, [\overline{\mathbf{u}} - \mathbf{u}] \times \boldsymbol{\psi}) + (\partial_t \mathbf{u} - \partial_t \mathbf{u}, \mathbf{u} \times \boldsymbol{\psi}). \end{aligned}$$

The properties of  $(\cdot, \cdot)_h$ ,  $W^{1,2}$ -stability of  $\mathcal{I}_h$ , and  $\|\overline{\mathbf{u}}\|_{L^\infty} \leq 1$  yield

$$\begin{aligned} &\left| (\partial_t \mathbf{u}, \mathcal{I}_h[\overline{\mathbf{u}} \times \boldsymbol{\Psi}])_h - (\partial_t \mathbf{u}, \mathcal{I}_h[\overline{\mathbf{u}} \times \boldsymbol{\Psi}]) \right| \\ &\leq Ch \|\partial_t \mathbf{u}\|_{L^2} \|\nabla \mathcal{I}_h[\overline{\mathbf{u}} \times \boldsymbol{\Psi}]\|_{L^2} \leq Ch \|\partial_t \mathbf{u}\|_{L^2} (\|\nabla \overline{\mathbf{u}}\|_{L^2} + 1) \|\boldsymbol{\psi}\|_{W^{1,\infty}}. \end{aligned}$$

A similar argumentation shows

$$\left| (\partial_t \mathbf{u}, \mathcal{I}_h[\overline{\mathbf{u}} \times \boldsymbol{\Psi}] - \overline{\mathbf{u}} \times \boldsymbol{\Psi}) \right| + \left| (\partial_t \mathbf{u}, \overline{\mathbf{u}} \times [\boldsymbol{\Psi} - \boldsymbol{\psi}]) \right| \leq Ch \|\partial_t \mathbf{u}\|_{L^2} (\|\nabla \overline{\mathbf{u}}\|_{L^2} + 1) \|\boldsymbol{\psi}\|_{W^{1,\infty}}.$$

A combination of the last three equations yields

$$\begin{aligned} I &:= \left| \int_0^T (\partial_t \mathbf{u}, \overline{\mathbf{u}} \times \boldsymbol{\Psi})_h - (\partial_t \mathbf{u}, \mathbf{u} \times \boldsymbol{\psi}) dt \right| \\ &\leq Ch \|\partial_t \mathbf{u}\|_{L^2(\Omega_T)} (\|\nabla \overline{\mathbf{u}}\|_{L^2(\Omega_T)} + 1 + \|\overline{\mathbf{u}} - \mathbf{u}\|_{L^2(\Omega_T)}) \|\boldsymbol{\psi}\|_{L^\infty(0,T;W^{1,\infty})} \\ &\quad + \left| \int_0^T (\partial_t \mathbf{u} - \partial_t \mathbf{u}, \mathbf{u} \times \boldsymbol{\psi}) dt \right|. \end{aligned}$$

Since  $\overline{\mathbf{u}} \rightarrow \mathbf{u}$  in  $L^2(\Omega_T, \mathbf{R}^3)$  and  $\partial_t \mathbf{u} \rightarrow \partial_t \mathbf{u}$  in  $L^2(\Omega_T, \mathbf{R}^3)$ , we infer that  $I \rightarrow 0$  for  $(h, k, \varepsilon) \rightarrow 0$ . We have, using that  $\langle \nabla \mathbf{u}, \nabla[\mathbf{u} \times \boldsymbol{\psi}] \rangle = \langle \nabla \mathbf{u}, [\mathbf{u} \times \nabla \boldsymbol{\psi}] \rangle$  and  $\langle \nabla \overline{\mathbf{u}}, \nabla[\overline{\mathbf{u}} \times \boldsymbol{\Psi}] \rangle = \langle \nabla \overline{\mathbf{u}}, [\overline{\mathbf{u}} \times \nabla \boldsymbol{\Psi}] \rangle$ ,

$$\begin{aligned} (\nabla \overline{\mathbf{u}}, \nabla \mathcal{I}_h[\overline{\mathbf{u}} \times \boldsymbol{\Psi}]) - (\nabla \mathbf{u}, \nabla[\mathbf{u} \times \boldsymbol{\psi}]) &= (\nabla \overline{\mathbf{u}}, \nabla\{\mathcal{I}_h[\overline{\mathbf{u}} \times \boldsymbol{\Psi}] - \overline{\mathbf{u}} \times \boldsymbol{\Psi}\}) \\ &\quad + (\nabla \overline{\mathbf{u}}, \overline{\mathbf{u}} \times \nabla[\boldsymbol{\Psi} - \boldsymbol{\psi}]) + (\nabla \overline{\mathbf{u}}, [\overline{\mathbf{u}} - \mathbf{u}] \times \nabla \boldsymbol{\psi}) + (\nabla[\overline{\mathbf{u}} - \mathbf{u}], \mathbf{u} \times \nabla \boldsymbol{\psi}). \end{aligned}$$



Interpolation estimates and  $D^2\bar{\mathbf{u}}|_K = 0$  for all  $K \in \mathcal{T}$  imply that

$$\begin{aligned} & \left| \left( \nabla \bar{\mathbf{u}}, \nabla \{ \mathcal{I}_h \bar{\mathbf{u}} \times \Psi \} - \bar{\mathbf{u}} \times \Psi \right) \right| + \left| \left( \nabla \bar{\mathbf{u}}, \bar{\mathbf{u}} \times \nabla [\Psi - \psi] \right) \right| \\ & \leq Ch \|\nabla \bar{\mathbf{u}}\|_{L^2} (\|\nabla \bar{\mathbf{u}}\|_{L^2} + 1) \|\psi\|_{W^{2,\infty}}. \end{aligned}$$

We combine the previous two equations to verify that

$$\begin{aligned} II & := \left| \int_0^T \left( \nabla \bar{\mathbf{u}}, \nabla \mathcal{I}_h \bar{\mathbf{u}} \times \Psi \right) - \left( \nabla \mathbf{u}, \nabla [\mathbf{u} \times \psi] \right) dt \right| \\ & \leq Ch \|\nabla \bar{\mathbf{u}}\|_{L^2(\Omega_T)} (\|\nabla \bar{\mathbf{u}}\|_{L^2(\Omega_T)} + 1) \|\psi\|_{L^\infty(0,T;W^{2,\infty})} \\ & \quad + \|\nabla \bar{\mathbf{u}}\|_{L^2(\Omega_T)} \|\bar{\mathbf{u}} - \mathbf{u}\|_{L^2(\Omega_T)} \|\psi\|_{L^\infty(0,T;W^{1,\infty})} + \left| \int_0^T \left( \nabla [\bar{\mathbf{u}} - \mathbf{u}], \mathbf{u} \times \nabla \psi \right) dt \right|. \end{aligned}$$

Using that  $\bar{\mathbf{u}} \rightarrow \mathbf{u}$  in  $L^2(\Omega_T, \mathbf{R}^3)$  and  $\nabla \bar{\mathbf{u}} \rightarrow \nabla \mathbf{u}$  in  $L^2(\Omega_T, \mathbf{R}^{3N})$  we deduce that  $II \rightarrow 0$  as  $(h, k, \varepsilon) \rightarrow 0$ . Using  $\|\mathcal{R}^+\|_h \leq \varepsilon$  for almost all  $t \in (0, T)$  we verify that  $\|\mathcal{R}^+\|_h \leq \varepsilon$  for almost all  $t \in (0, T)$  and that

$$III := \left| \int_0^T \left( \bar{\mathbf{u}} \times \mathcal{R}^+, \bar{\mathbf{u}} \times \Psi \right)_h dt \right| \leq \|\mathcal{R}^+\|_{L^2(\Omega_T)} \|\psi\|_{L^2(\Omega_T)} \leq T^{1/2} \varepsilon \|\psi\|_{L^2(\Omega_T)}.$$

Noting that

$$\left( [1 - |\bar{\mathbf{u}}|^2] \tilde{\Delta}_h \bar{\mathbf{u}}, \bar{\mathbf{u}} \times \Psi \right)_h \leq \|\bar{\mathbf{u}} \times \tilde{\Delta}_h \bar{\mathbf{u}}\|_h \|1 - |\bar{\mathbf{u}}|^2\|_h \|\psi\|_{L^\infty}$$

and using that  $|1 - |\bar{\mathbf{u}}|^2| = |\langle \mathbf{u} - \bar{\mathbf{u}}, \mathbf{u} + \bar{\mathbf{u}} \rangle| \leq 2|\mathbf{u} - \bar{\mathbf{u}}|$  we deduce

$$\begin{aligned} IV & := \left| \int_0^T \left( [1 - |\bar{\mathbf{u}}|^2] \tilde{\Delta}_h \bar{\mathbf{u}}, \bar{\mathbf{u}} \times \Psi \right)_h dt \right| \\ & \leq C \|\bar{\mathbf{u}} \times \tilde{\Delta}_h \bar{\mathbf{u}}\|_{L^2(\Omega_T)} \|\psi\|_{L^\infty(\Omega_T)} \|\mathbf{u} - \bar{\mathbf{u}}\|_{L^2(\Omega_T)}. \end{aligned}$$

With the bounds of Lemma 3.2 and since  $\bar{\mathbf{u}} \rightarrow \mathbf{u}$  in  $L^2(\Omega_T, \mathbf{R}^3)$  we verify that  $IV \rightarrow 0$  as  $(h, k, \varepsilon) \rightarrow 0$ . In order to verify the assertion of the lemma we rewrite (3.1) as

$$\left( \partial_t \mathbf{u}, \Phi \right)_h + \left( \bar{\mathbf{u}} \times (\bar{\mathbf{u}} \times \tilde{\Delta}_h \bar{\mathbf{u}}), \Phi \right)_h = \left( \bar{\mathbf{u}} \times \mathcal{R}^+, \Phi \right)_h,$$

for  $\Phi \in \mathbf{V}_h$  and almost all  $t \in (0, T)$ . The choice  $\Phi(t, \cdot) = \mathcal{I}_h [(\bar{\mathbf{u}} \times \Psi)(t, \cdot)]$  leads to

$$\left( \partial_t \mathbf{u}, \bar{\mathbf{u}} \times \Psi \right)_h + \left( \bar{\mathbf{u}} \times (\bar{\mathbf{u}} \times \tilde{\Delta}_h \bar{\mathbf{u}}), \bar{\mathbf{u}} \times \Psi \right)_h = \left( \bar{\mathbf{u}} \times \mathcal{R}^+, \bar{\mathbf{u}} \times \Psi \right)_h.$$

The vector product identity

$$\langle \mathbf{a} \times \mathbf{b}, \mathbf{c} \times \mathbf{d} \rangle = \langle \mathbf{a}, \mathbf{c} \rangle \langle \mathbf{b}, \mathbf{d} \rangle - \langle \mathbf{b}, \mathbf{c} \rangle \langle \mathbf{a}, \mathbf{d} \rangle \quad \forall \mathbf{a}, \mathbf{b}, \mathbf{c}, \mathbf{d} \in \mathbf{R}^3,$$

and the definition of  $\tilde{\Delta}_h$  imply that

$$\left( \partial_t \mathbf{u}, \bar{\mathbf{u}} \times \Psi \right)_h + \left( \nabla \bar{\mathbf{u}}, \nabla \mathcal{I}_h \bar{\mathbf{u}} \times \Psi \right) = \left( \bar{\mathbf{u}} \times \mathcal{R}^+, \bar{\mathbf{u}} \times \Psi \right)_h + \left( [1 - |\bar{\mathbf{u}}|^2] \tilde{\Delta}_h \bar{\mathbf{u}}, \bar{\mathbf{u}} \times \Psi \right)_h.$$

Thereby we verify that for  $(h, k, \varepsilon) \rightarrow 0$ ,

$$\left| \int_0^T \left( \partial_t \mathbf{u}, \mathbf{u} \times \psi \right) + \left( \nabla \mathbf{u}, \nabla [\mathbf{u} \times \psi] \right) dt \right| \leq I + II + III + IV \rightarrow 0.$$

This finishes the proof of Theorem 3.3, which reduces to Theorem 1.1 for  $\varepsilon = 0$ .  $\square$

4. FIXED POINT METHOD FOR ALGORITHM 1.3

A fully practical version of Algorithm 1.3 requires an iterative solution of the nonlinear system of equations in each step. The subsequent method is motivated by the substitution  $kd_t \mathbf{U}^{j+1} = 2\mathbf{W}^{j+1} - 2\mathbf{U}^j$ , for  $\mathbf{W}^{j+1} = \bar{\mathbf{U}}^{j+1/2}$ , such that (1.10) takes the form

$$(4.1) \quad \begin{aligned} & \frac{2}{k} (\mathbf{W}^{j+1}, \Phi)_h + \left( \mathbf{W}^{j+1} \times (\mathbf{W}^{j+1} \times \tilde{\Delta}_h \mathbf{W}^{j+1}), \Phi \right)_h \\ & = \frac{2}{k} (\mathbf{U}^j, \Phi)_h \quad \forall \Phi \in \mathbf{V}_h. \end{aligned}$$

A suitable stopping criterion is stated to assure convergence of the following fully practical scheme. Inputs are the time-step size  $k > 0$ , a positive integer  $J$ , a regular triangulation  $\mathcal{T}_h$  of  $\Omega \subset \mathbf{R}^N$ , a parameter  $\varepsilon > 0$ , initial data  $\mathbf{U}^0 \in \mathbf{V}_h$  such that  $|\mathbf{U}^0(\mathbf{z})| = 1$  for all  $\mathbf{z} \in \mathcal{N}_h$ , and  $\mathbf{R}^0 = \mathbf{0}$ . Outputs of the subsequent algorithm are sequences  $\{\mathbf{U}^j\}$  and  $\{\mathbf{R}^j\}$ .

**Algorithm 4.1.** 1. For  $j \geq 0$ , set  $\mathbf{W}^{j+1,0} := \mathbf{U}^j$ , and  $\ell := 0$ .  
 2. Compute  $\mathbf{W}^{j+1,\ell+1} \in \mathbf{V}_h$ , such that for all  $\Phi \in \mathbf{V}_h$

$$(4.2) \quad \frac{2}{k} (\mathbf{W}^{j+1,\ell+1}, \Phi)_h + \left( \mathbf{W}^{j+1,\ell+1} \times (\mathbf{W}^{j+1,\ell} \times \tilde{\Delta}_h \mathbf{W}^{j+1,\ell}), \Phi \right)_h = \frac{2}{k} (\mathbf{U}^j, \Phi)_h.$$

3. Set  $\mathbf{E}^{j+1,\ell+1} := \mathbf{W}^{j+1,\ell+1} - \mathbf{W}^{j+1,\ell}$ , and

$$\mathbf{R}^{j+1} = \mathbf{W}^{j+1,\ell+1} \times \tilde{\Delta}_h \mathbf{E}^{j+1,\ell+1} + \mathbf{E}^{j+1,\ell+1} \times \tilde{\Delta}_h \mathbf{W}^{j+1,\ell}.$$

Stop if  $\|\mathbf{R}^{j+1}\| \leq \varepsilon$ , and set  $\mathbf{U}^{j+1} := 2\mathbf{W}^{j+1,\ell+1} - \mathbf{U}^j$ , and go to 1; set  $\ell = \ell + 1$  and continue with 2 otherwise.

4. Stop if  $j + 1 = J$ ; set  $j = j + 1$  and go to 1 otherwise.

The following theorem shows that all steps in Algorithm 4.1 are well-defined, that the algorithm terminates, and that iterates converge to weak solutions of (1.2)–(1.3) if  $k = \mathcal{O}(h^2)$ . The key tool for its verification is Theorem 3.3.

**Theorem 4.1.** Suppose that  $\mathcal{T}_h$  is quasiuniform. Let  $0 \leq j \leq J - 1$  and  $\mathbf{U}^j \in \mathbf{V}_h$  such that  $|\mathbf{U}^j(\mathbf{z})| = 1$  for all  $\mathbf{z} \in \mathcal{N}_h$ . Then, for all  $\ell \geq 0$ , (4.2) has a unique solution  $\mathbf{W}^{j+1,\ell+1} \in \mathbf{V}_h$  such that  $|\mathbf{W}^{j+1,\ell+1}(\mathbf{z})| \leq 1$ , and  $|\left[2\mathbf{W}^{j+1,\ell+1} - \mathbf{U}^j\right](\mathbf{z})| = 1$  for all  $\mathbf{z} \in \mathcal{N}_h$ . Moreover, there holds for some  $\tilde{C} > 0$

$$(4.3) \quad \|\mathbf{E}^{j+1,\ell+1}\|_h \leq \tilde{C}kh^{-2}\|\mathbf{E}^{j+1,\ell}\|_h.$$

For  $k$  such that  $\tilde{C}kh^{-2} < 1$ , there holds (3.1), and hence iterates  $\{\mathbf{U}^j\}$  of Algorithm 4.1 subconverge to a weak solution of (1.2)–(1.3) in the sense which is made precise in Theorem 3.3 for  $(h, k, \varepsilon) \rightarrow 0$ .

*Remark 4.1.* By Banach fixed point theorem, contraction property (4.3) for  $\Gamma = \tilde{C}kh^{-2}$  implies existence of a unique  $\mathbf{W}^{j+1} \in \mathbf{V}_h$  which solves (4.1) for given  $\mathbf{U}^j$ , and satisfies for all  $\ell \geq 1$ ,

$$\begin{aligned} \text{i)} \quad & \|\mathbf{W}^{j+1} - \mathbf{W}^{j+1,\ell+1}\|_h \leq \frac{\Gamma^\ell}{1 - \Gamma} \|\mathbf{W}^{j+1,1} - \mathbf{U}^j\|_h, \\ \text{ii)} \quad & \|\mathbf{W}^{j+1} - \mathbf{W}^{j+1,\ell+1}\|_h \leq \frac{\Gamma}{1 - \Gamma} \|\mathbf{W}^{j+1,\ell} - \mathbf{W}^{j+1,\ell+1}\|_h. \end{aligned}$$

*Proof. Step 1: Well-posedness and discrete sphere constraint.* The left-hand side in (4.2) defines a continuous bilinear form  $a(\mathbf{W}^{j+1,\ell+1}, \boldsymbol{\phi}_h)$  on  $[\mathbf{V}_h]^2$ . The choice  $\boldsymbol{\Phi} = \mathbf{W}^{j+1,\ell+1}$  shows that  $a$  is elliptic. Hence, there exists a unique solution  $\mathbf{W}^{j+1,\ell+1}$  in (4.2). On choosing  $\boldsymbol{\Phi} = \mathbf{W}^{j+1,\ell+1}(\mathbf{z})\varphi_{\mathbf{z}}$  for  $\mathbf{z} \in \mathcal{N}_h$  we verify that  $|\mathbf{W}^{j+1,\ell+1}(\mathbf{z})| \leq |\mathbf{U}^j(\mathbf{z})| = 1$ . Defining  $\tilde{\mathbf{U}}^{j+1} = 2\mathbf{W}^{j+1,\ell+1} - \mathbf{U}^j$ , (4.2) implies for all  $\boldsymbol{\Phi} \in \mathbf{V}_h$  that

$$\frac{1}{k}(\tilde{\mathbf{U}}^{j+1} - \mathbf{U}^j, \boldsymbol{\Phi})_h + \left( \mathbf{W}^{j+1,\ell+1} \times (\mathbf{W}^{j+1,\ell} \times \tilde{\Delta}_h \mathbf{W}^{j+1,\ell}), \boldsymbol{\Phi} \right)_h = 0.$$

Choosing  $\boldsymbol{\Phi} = \mathbf{W}^{j+1,\ell+1}(\mathbf{z})\varphi_{\mathbf{z}}$  for  $\mathbf{z} \in \mathcal{N}_h$  in (4.2) and noting that  $\mathbf{W}^{j+1,\ell+1} = \frac{1}{2}[\tilde{\mathbf{U}}_h^{j+1} + \mathbf{U}^j]$  yields that  $|\tilde{\mathbf{U}}_h^{j+1}(\mathbf{z})|^2 = |\mathbf{U}^j(\mathbf{z})|^2 = 1$ .

*Step 2: Property (4.3).* Subtract two subsequent equations in (4.2) and choose  $\boldsymbol{\Phi} = \mathbf{E}_h^{j+1,\ell+1}$  to verify that for  $\ell \geq 1$  there holds

$$\begin{aligned} \frac{2}{k} \|\mathbf{E}^{j+1,\ell+1}\|_h^2 &= - \left( \mathbf{W}^{j+1,\ell} \times (\mathbf{E}^{j+1,\ell} \times \tilde{\Delta}_h \mathbf{W}^{j+1,\ell}), \mathbf{E}^{j+1,\ell+1} \right)_h \\ &\quad - \left( \mathbf{W}^{j+1,\ell} \times (\mathbf{W}^{j+1,\ell-1} \times \tilde{\Delta}_h \mathbf{E}^{j+1,\ell}), \mathbf{E}^{j+1,\ell+1} \right)_h \\ &\leq \|\mathbf{W}^{j+1,\ell}\|_{L^\infty} \|\mathbf{E}^{j+1,\ell}\|_h \|\tilde{\Delta}_h \mathbf{W}^{j+1,\ell}\|_{L^\infty} \|\mathbf{E}^{j+1,\ell+1}\|_h \\ &\quad + \|\mathbf{W}^{j+1,\ell}\|_{L^\infty} \|\mathbf{W}^{j+1,\ell-1}\|_{L^\infty} \|\tilde{\Delta}_h \mathbf{E}^{j+1,\ell}\|_h \|\mathbf{E}^{j+1,\ell+1}\|_h. \end{aligned}$$

We employ the estimates in (2.6) and use  $\|\mathbf{W}^{j+1,\ell}\|_{L^\infty} \leq 1$  to deduce (4.3).

*Step 3: Convergence towards weak solutions of (1.2)–(1.3).* Suppose that for some  $\ell \geq 0$  we have  $\mathbf{U}^{j+1} = 2\mathbf{W}^{j+1,\ell+1} - \mathbf{U}^j$ , in particular  $\mathbf{U}^{j+1/2} = \mathbf{W}^{j+1,\ell+1}$ . Then, the system in (4.2) implies that for all  $\boldsymbol{\phi}_h \in \mathbf{V}_h$  there holds

$$\begin{aligned} &(d_t \mathbf{U}^{j+1}, \boldsymbol{\Phi})_h + \left( \mathbf{U}^{j+1/2} \times (\mathbf{U}^{j+1/2} \times \tilde{\Delta}_h \mathbf{U}^{j+1/2}), \boldsymbol{\Phi} \right)_h \\ &= \left( \mathbf{U}^{j+1/2} \times (\mathbf{W}^{j+1,\ell+1} \times \tilde{\Delta}_h \mathbf{W}^{j+1,\ell+1}), \boldsymbol{\Phi} \right)_h \\ &\quad - \left( \mathbf{U}^{j+1/2} \times (\mathbf{W}^{j+1,\ell} \times \tilde{\Delta}_h \mathbf{W}^{j+1,\ell}), \boldsymbol{\Phi} \right)_h \\ &= \left( \mathbf{U}^{j+1/2} \times (\mathbf{E}^{j+1,\ell+1} \times \tilde{\Delta}_h \mathbf{W}^{j+1,\ell+1}), \boldsymbol{\Phi} \right)_h \\ &\quad + \left( \mathbf{U}^{j+1/2} \times (\mathbf{W}^{j+1,\ell} \times \tilde{\Delta}_h \mathbf{E}^{j+1,\ell+1}), \boldsymbol{\Phi} \right)_h \\ &= (\mathbf{U}^{j+1/2} \times \mathbf{R}^{j+1}, \boldsymbol{\Phi})_h. \end{aligned}$$

Hence, (3.1) is valid, and Theorem 3.3 implies convergence of iterates towards weak solutions of (1.2)–(1.3) for  $(h, k, \varepsilon) \rightarrow 0$ . This finishes the proof of the theorem.  $\square$

*Remark 4.2.* Newton schemes for the approximate solution of (1.10) do in general not fit into the form (3.1). Suppose that  $\tilde{\mathbf{U}}^j \in \mathbf{V}_h$  is given. Then, in order to compute an approximation of  $\mathbf{U}^{j+1/2}$ , one is led to finding  $\mathbf{W}^* \in \mathbf{V}_h$  such that  $F(\mathbf{W}^*) = 0$ , where

$$F(\mathbf{W}) = \frac{2}{k}(\mathbf{W} - \tilde{\mathbf{U}}^j) + \mathcal{I}_h[\mathbf{W} \times (\mathbf{W} \times \tilde{\Delta}_h \mathbf{W})].$$

Given an iterate  $\mathbf{W}^\ell$  (e.g. with  $\mathbf{W}^0 = \tilde{\mathbf{U}}^j$ ), the correction  $\mathbf{C} \in \mathbf{V}_h$  in the update  $\mathbf{W}^{\ell+1} = \mathbf{W}^\ell - \mathbf{C}$  is the solution of  $DF(\mathbf{W}^\ell)[\mathbf{C}] = F(\mathbf{W}^\ell)$ , i.e.,  $\mathbf{C}$  satisfies

$$\begin{aligned} \frac{2}{k}(\mathbf{C}, \Phi)_h + \left( \mathbf{C} \times (\mathbf{W}^\ell \times \tilde{\Delta}_h \mathbf{W}^\ell), \Phi \right)_h + \left( \mathbf{W}^\ell \times (\mathbf{C} \times \tilde{\Delta}_h \mathbf{W}^\ell), \Phi \right)_h \\ + \left( \mathbf{W}^\ell \times (\mathbf{W}^\ell \times \tilde{\Delta}_h \mathbf{C}), \Phi \right)_h = \frac{2}{k}(\mathbf{W}^\ell - \tilde{\mathbf{U}}^j, \Phi)_h + \left( \mathbf{W}^\ell \times (\mathbf{W}^\ell \times \tilde{\Delta}_h \mathbf{W}^\ell), \Phi \right)_h, \end{aligned}$$

for all  $\Phi_h \in \mathbf{V}_h$ . Setting  $\tilde{\mathbf{U}}^{j+1} := 2\mathbf{W}^{\ell+1} - \tilde{\mathbf{U}}^j$ , i.e.,  $\tilde{\mathbf{U}}^{j+1/2} = \mathbf{W}^{\ell+1}$ , the equation may be rewritten as

$$\begin{aligned} (d_t \tilde{\mathbf{U}}^{j+1}, \Phi)_h + \left( \tilde{\mathbf{U}}^{j+1/2} \times (\tilde{\mathbf{U}}^{j+1/2} \times \tilde{\Delta}_h \tilde{\mathbf{U}}^{j+1/2}), \Phi \right)_h \\ = \left( \mathbf{C} \times (\mathbf{W}^\ell \times \tilde{\Delta}_h \mathbf{C}), \Phi \right)_h + \left( \mathbf{C} \times (\mathbf{C} \times \tilde{\Delta}_h \mathbf{W}^\ell), \Phi \right)_h \\ + \left( \mathbf{W}^\ell \times (\mathbf{C} \times \tilde{\Delta}_h \mathbf{C}), \Phi \right)_h - \left( \mathbf{C} \times (\mathbf{C} \times \tilde{\Delta}_h \mathbf{C}), \Phi \right)_h, \end{aligned}$$

which is not of the form (3.1).

## 5. CONCLUDING REMARKS

We proposed a constraint preserving, implicit discretization (i.e., Algorithm 1.3) of the harmonic map flow into spheres (1.2)–(1.3); reduced spatial integration, trapezoidal rule, as well as projected discrete Laplacian are main tools to overcome stiffness of used (lowest order) finite elements and show unconditional convergence towards weak solutions of (1.2)–(1.3) — as opposed to former schemes in the literature. Analytical studies for a simple, linear fixed point method (Algorithm 4.1) which preserves (discrete) sphere constraint elaborate necessary mesh-size constraints to validate a contraction property at each time-step, and evidence need of a careful selection of a stopping criterion and a corresponding parameter to achieve overall convergence towards weak solutions of (1.2)–(1.3). The studies in Section 4 motivate higher order fixed point methods for improved flexibility with respect to both, mesh-size constraints and stopping criterion, which is left to future work.

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