PROJECTION-FREE APPROXIMATION OF GEOMETRICALLY CONSTRAINED PARTIAL DIFFERENTIAL EQUATIONS

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Abstract. We devise algorithms for the numerical approximation of partial differential equations involving a nonlinear, pointwise holonomic constraint. The elliptic, parabolic, and hyperbolic model equations are replaced by sequences of linear problems with a linear constraint. Stability and convergence holds unconditionally with respect to step sizes and triangulations. In the stationary situation a multilevel strategy is proposed that iteratively decreases the step size. Numerical experiments illustrate the accuracy of the approach.

1. Introduction

Partial differential equations with pointwise constraints have attracted considerable attention among pure and applied mathematicians in the last decades. Mathematically challenging problems like partial regularity, characterization of singularities, and occurrence of finite-time blow-up as well as modern applications in micromagnetics, geometry, continuum mechanics, and general relativity have motivated to develop and analyze numerical schemes for the approximate solution of this class of nonlinear partial differential equations. The nonlinear character of the problem and the lack of regularity of solutions cause that blackbox optimization routines perform poorly for this class of equations and necessitates the development of customized approximation schemes. Numerical methods that provide accurate numerical solutions and converge under restrictions on step sizes or conditions on underlying triangulations or require the solution of nonlinear systems of equations have been devised and analyzed in [LL89, Alo97, LW00, Alo08, Bar05, BBFP07, BP07, BFP08, BP08, Bar09b, Bar10, San12]. We aim at developing numerical schemes that are unconditionally stable and convergent, provide accurate approximations with a small number of degrees of freedom, and only require the solution of linear systems of equations.

Harmonic maps (into the sphere) are stationary points of the Dirichlet energy

$$I(u) = \frac{1}{2}\int_\Omega |\nabla u|^2 \,\mathrm{d}x$$

Date: August 20, 2013.

1991 *Mathematics Subject Classification.* 65N12 (65N15 65N30).

Key words and phrases. Finite elements, partial differential equations, pointwise constraints, harmonic maps, harmonic map heat flow, wave maps.

among vector fields $u : \Omega \to \mathbb{R}^m$ subject to the unit-length constraint $|u(x)| = 1$ for almost every $x \in \Omega$ and Dirichlet boundary conditions $u|_{\Gamma_{\rm D}} = u_{\rm D}$. The Euler-Lagrange equations characterize critical points and seek weak solutions of

$$-\Delta u = |\nabla u|^2 u, \qquad u|_{\Gamma_{\rm D}} = u_{\rm D},$$
$$|u|^2 = 1, \qquad \partial_\nu u|_{\Gamma_{\rm N}} = 0.$$

Here, $\Gamma_{\rm N} = \partial\Omega \setminus \Gamma_{\rm D}$ and $\partial_\nu u = \nabla u \cdot \nu$ is the outer normal derivative on $\partial\Omega$. The factor $\lambda = |\nabla u|^2$ on the right-hand side of the differential equation is the Lagrange-multiplier associated to the pointwise constraint. Gradient flows provide an attractive tool to find solutions of the Euler-Lagrange equations since these decrease the Dirichlet energy along trajectories. The simplest case corresponds to the L^2 gradient flow and reads

$$\partial_t u - \Delta u = |\nabla u|^2 u, \qquad u(t,\cdot)|_{\Gamma_{\rm D}} = u_{\rm D}, \qquad u(0) = u_0,$$
$$|u|^2 = 1, \qquad \partial_\nu u(t,\cdot)|_{\Gamma_{\rm N}} = 0.$$

This evolutionary partial differential equation called *harmonic map heat flow (into the sphere)* is of interest in its own right, in particular since it is closely related to the Landau-Lifshitz-Gilbert equation in micromagnetics. A hyperbolic variant specifies critical points of an action functional subject to the pointwise constraint and leads to the nonlinear wave equation

$$\partial_t^2 u - \Delta u = \big(|\nabla u|^2 - |\partial_t u|^2\big) u, \qquad u(t,\cdot)|_{\Gamma_{\rm D}} = u_{\rm D}, \qquad u(0) = u_0,$$
$$|u|^2 = 1, \qquad \partial_\nu u(t,\cdot)|_{\Gamma_{\rm N}} = 0, \qquad \partial_t u(0) = v_0.$$

Solutions of this nonlinear initial boundary value problem are called *wave maps (into the sphere)*.

The unit-length constraint in the equations enforces the vector fields to attain their pointwise values in the unit sphere. Various applications motivate to consider other submanifolds, e.g., given as the zero level set of a function $g : \mathbb{R}^m \to \mathbb{R}$, so that the pointwise constraint becomes $g(u(x)) = 0$ for almost every $x \in \Omega$ or $g(u(t,x)) = 0$ for almost every $(t,x) \in [0,T] \times \Omega$. We abbreviate these conditions by $g(u) = 0$.

The most general approach to the numerical solution of nonlinearly pointwise constrained partial differential equations is based on imposing the constraint at the nodes of an underlying triangulation in combination with predictor-corrector approaches that linearize the constraint to compute an update which is then projected onto the target manifold under consideration. To guarantee well posedness and stability of such methods restrictive conditions on the step size or properties of the underlying triangulation that permit to use monotonicity arguments need to be imposed. Alternatively, in highly symmetric situations as is provided by the case of the unit sphere equivalent reformulations of the nonlinear equations that are constraint preserving may be employed. Appropriate discretizations reflect this property but typically require the solution of nonlinear systems of equations.

In this paper we show that the projection step in predictor-corrector approaches can often be omitted. This leads to a violation of the constraint at the nodes of an underlying triangulation that is controlled by the step size independently of the number of iterations. Since it is in general impossible to satisfy the constraint almost everywhere in a numerical approximation scheme the additional error introduced by omitting the projection step does not seem to be relevant. This idea has previously been employed by the author in [Bar13] for the development of approximation schemes for large bending isometries.

We explain the main idea for a semi-discrete in time approximation of the harmonic map heat flow with $\Gamma_{\mathrm{D}} = \emptyset$. The unit-length constraint implies that we have $\partial_t u \cdot u = 0$ and if u^{k-1} is an approximation of $u(t_{k-1})$ and v^k of $\partial_t u(t_k)$ we may impose the orthogonality relation

$$v^k \cdot u^{k-1} = 0.$$

If u^{k-1} is given we compute v^k as the unique vector field in $H^1(\Omega;\mathbb{R}^m)$ with $v^k \cdot u^{k-1} = 0$ almost everywhere in Ω and

$$(v^k, w) + (\nabla[u^{k-1} + \tau v^k], \nabla w) = (|\nabla u^k|^2 u^{k-1}, w) = 0$$

for all $w \in H^1(\Omega;\mathbb{R}^m)$ with $w \cdot u^{k-1} = 0$ almost everywhere in Ω. Here, $\tau > 0$ is a time-step size and $(\cdot,\cdot)$ denotes the L^2 inner product. The existence and uniqueness of v^k is an immediate consequence of the Lax-Milgram lemma. Thus, we may define the new approximation

$$u^k = u^{k-1} + \tau v^k.$$

Even if u^{k-1} is a unit-length vector field the new approximation u^k will in general not satisfy the pointwise constraint. In fact, owing to the pointwise orthogonality of u^{k-1} and v^k we have for $\ell \geq 1$ that

$$|u^\ell|^2 = |u^{\ell-1} + \tau v^\ell|^2 = |u^{\ell-1}|^2 + \tau^2 |v^\ell|^2$$

and an inductive argument implies

$$|u^\ell|^2 = 1 + \tau^2 \sum_{k=1}^{\ell} |v^k|^2$$

provided that $|u^0| = 1$ almost everywhere in Ω. This yields that

$$\big\| |u^\ell|^2 - 1 \big\|_{L^1(\Omega)} \leq \tau^2 \sum_{k=1}^{\ell} \|v^k\|^2_{L^2(\Omega)}.$$

Upon choosing $w = v^k$ in the time-discrete evolution equation and employing the binomial formula $2(a+b)a = a^2 + ((a-b)^2 - b^2)$ we find

$$\|v^k\|^2 + \frac{\tau}{2}\|\nabla v^k\|^2 + \frac{1}{2\tau}\big(\|\nabla u^k\|^2 - \|\nabla u^{k-1}\|^2\big) = 0.$$

Multiplication by τ and summation over $k = 1, 2, ..., \ell$ lead to

$$I(u^k) + \tau \sum_{k=1}^{\ell} \|v^k\|^2 + \frac{\tau^2}{2} \sum_{k=1}^{\ell} \|\nabla v^k\|^2 = I(u^0).$$

A combination of the estimates thus implies for all $\ell \geq 1$ that

$$\big\| |u^\ell|^2 - 1 \big\|_{L^1(\Omega)} \leq \tau I(u^0).$$

This proves that the approximations satisfy the constraint in the limit $\tau \to 0$ and that the error in the approximation of the constraint is bounded independently of the number of time steps or the value of the time horizon.
The left plot of Figure 1 illustrates the numerical scheme. The corrections v^k are computed in the tangent spaces of the level surfaces of the function $g(p) = |p|^2 - 1$. The right plot of Figure 1 illustrates the numerical scheme augmented

by a projection step. Although the projection step is well defined its stability is critical in fully discrete schemes.

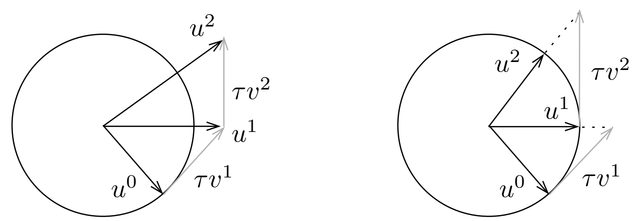

FIGURE 1. Omitting the projection step in the semi-implicit L^2 flow leads to approximations that violate the unit-length constraint but the corresponding error in $L^1(\Omega)$ is bounded independently of the number of iterations and controlled by the step size (left). A projection step leads to an accurate treatment of the constraint but requires restrictive conditions in fully discrete situations to guarantee stability (right).

We will apply the stategy that omits the projections to the fully discrete approximation of harmonic maps, the harmonic map heat flow, and wave maps into a large class of target manifolds characterized as the zero level set of a function $g \in C^2(\mathbb{R}^m)$. With the help of numerical experiments we will demonstrate that the method leads to accurate approximations.

2. Preliminaries

2.1. **Notation.** We use standard notation for Lebesgue and Sobolev spaces and abbreviate the norm in $L^2(\Omega;\mathbb{R}^\ell)$ by $\|\cdot\|$. We let $\lceil x \rceil = \min\{m \in \mathbb{Z} : m \geq x\}$ denote the smallest integer above a given number $x \in \mathbb{R}$. Throughout this article c stands for a generic positive constant that is independent of discretization parameters.

2.2. **Finite elemement spaces.** We assume that the bounded Lipschitz domain $\Omega \subset \mathbb{R}^d$, $d = 2, 3$, has a polyhedral boundary and let $\mathcal{T}_h$ be a regular triangulation of Ω into triangles or tetrahedra for $d = 2, 3$, respectively. If a nonempty, closed boundary part $\Gamma_{\mathrm{D}} \subset \partial\Omega$ is given we assume that it is resolved exactly by the edges or faces of the triangulation. The set of vertices or nodes of the triangulation is denoted by $\mathcal{N}_h$ and we let $(\varphi_z : z \in \mathcal{N}_h)$ be the nodal basis of the space

$$\mathcal{S}^1(\mathcal{T}_h) = \{w_h \in C(\overline{\Omega}) : w_h|_T \text{ affine for all } T \in \mathcal{T}_h\}$$

of continuous, elementwise affine functions. For $\Gamma_{\mathrm{D}} \subset \partial\Omega$ we let $H^1_{\mathrm{D}}(\Omega)$ be the set of Sobolev functions in $H^1(\Omega)$ that vanish on Γ_{D} and set

$$\mathcal{S}^1_{\mathrm{D}}(\mathcal{T}_h) = \mathcal{S}^1(\mathcal{T}_h) \cap H^1_{\mathrm{D}}(\Omega).$$

The nodal interpolation operator is denoted by $\mathcal{I}_h : C(\overline{\Omega}) \to \mathcal{S}^1(\mathcal{T}_h)$ and is applied componentwise to vector fields. The diameter of an element $T \in \mathcal{T}_h$ is given by the number h_T and we use the convention that the index h is up to a constant an upper bound for the maximal mesh-size in $\mathcal{T}_h$, i.e., $h_T \leq ch$ for all $T \in \mathcal{T}_h$. In this way we consider a sequence of triangulations $(\mathcal{T}_h)_{h>0}$, where $h > 0$ indicates a sequence of positive real numbers that accumulate at 0. The minimal mesh size is defined as $h_{\min} = \min_{T\in\mathcal{T}_h} h_T$. Letting $h_z = \operatorname{diam}(\omega_z)$ be the diameter of the node patch $\omega_z = \operatorname{supp}\varphi_z$ for every $z \in \mathcal{N}_h$ we have for all $1 \le r < \infty$ the norm equivalence

$$c^{-1}\|w_h\|_{L^r(\Omega)}^r \le \sum_{z\in\mathcal{N}_h} h_z^d |w_h(z)|^r \le c\|w_h\|_{L^r(\Omega)}^r \tag{2.1}$$

for all $w_h \in \mathcal{S}^1(\mathcal{T}_h)$. We say that $\mathcal{T}_h$ is weakly acute if $(\nabla\varphi_z, \nabla\varphi_y) \le 0$ for all distinct $z, y \in \mathcal{N}_h$. If $d = 3$ then sufficient for this is the restrictive condition that all angles between faces of tetrahedra are bounded by $\pi/2$.

2.3. **Difference quotients.** For the discretization of time-dependent problems we will employ backward difference quotients to approximate time derivatives. For a time-step size $\tau > 0$ and a sequence $(a^k)_{k=0,\dots,K}$ of real number, functions, or vector fields that are associated to the time steps $t_k = k\tau$, we denote

$$d_t a^k = \frac{1}{\tau}(a^k - a^{k-1}).$$

We note that for every $\theta \in [0, 1]$ we have the binomial identity

$$(a^{k-1} + \theta\tau d_t a^k)\cdot d_t a^k = \frac{d_t}{2}\|a^k\|^2 + \frac{\tau}{2}(2\theta - 1)\|d_t a^k\|^2.$$

We define the continuous interpolant $\widehat{a}_\tau$ of a sequence $(a^k)_{k=0,\dots,K}$ through

$$\widehat{a}_\tau(t) = \frac{t - t_{k-1}}{\tau} a^k - \frac{t - t_k}{\tau} a^{k-1}$$

for $t \in [t_{k-1}, t_k]$ and the piecewise constant interpolants

$$a_\tau^+(t) = a^k, \quad a_\tau^-(t) = a^{k-1}$$

for $t \in (t_{k-1}, t_k)$.

2.4. **Discrete constraint.** The following lemma shows that an approximate treatment of the equality constraint at the nodes of triangulations is sufficient to guarantee the validity of the constraint for cluster points of approximate solutions. We assume throughout that $g \in C^2(\mathbb{R}^m)$ and that there exist $c_1, c_2, c_3 > 0$ with

$$\begin{aligned}
|g(p) - g(q)| &\le c_1\big(1 + |g'(p)| + |g'(q)|\big)|p - q|,\\
|g'(p)| &\le c_2(1 + |p|),\\
|D^2 g(p)| &\le c_3
\end{aligned}$$

for all $p, q \in \mathbb{R}^m$, where we denote $g' = Dg$.

Lemma 2.1 (Constraint approximation)**.** *Assume that $h \le c h_{\min}^{d/2-1}[\log(h_{\min}^{-1})]^{-1/2}$. If $(u_h)_{h>0}$ is a bounded sequence in $H^1(\Omega;\mathbb{R}^m)$ such that $u_h \in \mathcal{S}^1(\mathcal{T}_h)^m$ for all $h > 0$, $u_h \to u$ in $L^2(\Omega;\mathbb{R}^m)$ for some $u \in H^1(\Omega;\mathbb{R}^m)$ as $h \to 0$, and*

$$\|\mathcal{I}_h g(u_h)\|_{L^1(\Omega)} \to 0$$

as $h \to 0$ then we have $g(u) = 0$ almost everywhere in Ω.

Proof. Two applications of the triangle inequality show that

$$\|g(u_h)\|_{L^1(\Omega)} \le \|g(u) - g(u_h)\|_{L^1(\Omega)} + \|g(u_h) - \mathcal{I}_h g(u_h)\|_{L^1(\Omega)} + \|\mathcal{I}_h g(u_h)\|_{L^1(\Omega)}.$$

Owing to the assumptions of the lemma we have that the third term on the right-hand side tends to zero as $h \to 0$. The assumptions on g imply that

$$\|g(u) - g(u_h)\|_{L^1(\Omega)} \le c\|u - u_h\|$$

so that also the first term on the right-hand side vanishes as $h \to 0$. We use an elementwise interpolation estimate in $L^2(\Omega;\mathbb{R}^m)$ to verify

$$\begin{aligned}\|g(u_h) - \mathcal{I}_h g(u_h)\|_{L^1(\Omega)}^2 &\le c \sum_{T\in\mathcal{T}_h} h_T^4 \|D^2[g(u_h)]\|_{L^2(T)}^2 \\ &\le c\|D^2 g(u_h)\|_{L^\infty(\Omega)}^2 \sum_{T\in\mathcal{T}_h} h_T^4 \|\nabla u_h\|_{L^4(T)}^4 \\ &\le c\|D^2 g(u_h)\|_{L^\infty(\Omega)}^2 \sum_{T\in\mathcal{T}_h} h_T^4 \|\nabla u_h\|_{L^2(T)}^2 \|\nabla u_h\|_{L^\infty(T)}^2.\end{aligned}$$

With the unform boundedness of $D^2 g$ and the inverse estimate $\|\nabla u_h\|_{L^\infty(T)} \le c h_T^{-1} \|u_h\|_{L^\infty(T)}$ we deduce that

$$\|g(u_h) - \mathcal{I}_h g(u_h)\|_{L^1(\Omega)}^2 \le c h^2 \|u_h\|_{L^\infty(\Omega)}^2 \|\nabla u_h\|^2.$$

Finally, the estimate $\|u_h\|_{L^\infty(\Omega)} \le c h_{\min}^{1-d/2} \log(h_{\min}^{-1}) \|u_h\|_{H^1(\Omega)}$ which follows from inverse estimates and the Sobolev inequality $\|v\|_{L^s(\Omega)} \le c(d-r)^{-1}\|v\|_{W^{1,r}(\Omega)}$ for $1 \le r < d$ and $s = dr/(d-r)$ yields that

$$\|g(u_h) - \mathcal{I}_h g(u_h)\|_{L^1(\Omega)}^2 \le c h^2 h_{\min}^{2-d} \log(h_{\min}^{-1}) \|u_h\|_{H^1(\Omega)}^4$$

Hence, as $h \to 0$ we find $g(u_h) \to 0$ in $L^1(\Omega)$. For an appropriate subsequence $h' > 0$ we have $u_{h'} \to u$ and $g(u_{h'}) \to 0$ almost everywhere in Ω and hence $g(u) = 0$. □

Remarks 2.1. *(i) The condition $h \le c h_{\min}^{d/2-1} [\log(h_{\min}^{-1})]^{-1/2}$ is a mild restriction on the strength of the grading of a triangulation. For quasiuniform triangulations we have $h_{\min} \ge ch$ and the condition is satisfied.*
(ii) The boundedness of the sequence $(u_h)_{h>0}$ in $H^1(\Omega;\mathbb{R}^m)$ implies the existence of a weakly convergent subsequence which converges strongly in $L^2(\Omega;\mathbb{R}^m)$.

2.5. **Projection estimates.** The renormalization of a finite element function increases its Dirichlet energy in general. The following lemma shows for the case of the unit sphere that this increase is uniformly bounded.

Lemma 2.2 (Projection)**.** *There exists $c_\Pi > 0$ that only depends on the geometry of the triangulation $\mathcal{T}_h$ such that for all $\phi_h \in \mathcal{S}^1(\mathcal{T}_h)^m$ with $|\phi_h(z)| \ge 1$ for all $z \in \mathcal{N}_h$ we have*

$$\|\nabla \Pi_h \phi_h\| \le c_\Pi \|\nabla \phi_h\|$$

with $\Pi_h\phi_h \in \mathcal{S}^1(\mathcal{T}_h)^m$ defined by

$$\Pi_h \phi_h(z) = \frac{\phi_h(z)}{|\phi_h(z)|}$$

for all $z \in \mathcal{N}_h$, i.e., $\Pi_h\phi_h = \mathcal{I}_h[\phi_h/|\phi_h|]$.

Proof. We prove the estimate for every element $T \in \mathcal{T}_h$ which implies the global statement by summation. For $T = \mathrm{conv}\{z_0, z_1, ..., z_d\}$ we let $\Phi_T : T \to \widehat{T}$ denote the affine linear mapping to the standard simplex $\widehat{T} = \mathrm{conv}\{0, e_1, ..., e_d\}$ with $\Phi_T(z_j) = e_j$ for $j = 1, 2, ..., d$ and $\Phi_T(z_0) = 0$. Setting $\widehat{\phi}_h = \phi_h \circ \Phi_T^{-1}$ and $\widehat{\Pi_h\phi_h} = (\Pi_h\phi_h) \circ \Phi_T^{-1}$ we have by Lipschitz continuity of the mapping $p \mapsto p/\max\{1, |p|\}$ for $p \in \mathbb{R}^m$ with constant 1 that

$$\Big|\frac{\partial \widehat{\Pi_h\phi_h}}{\partial \widehat{x}_j}\Big| = \Big|\frac{\phi_h(z_j)}{|\phi_h(z_j)|} - \frac{\phi_h(z_0)}{|\phi_h(z_0)|}\Big| \le \big|\phi_h(z_j) - \phi_h(z_0)\big| = \Big|\frac{\partial \widehat{\phi}_h}{\partial \widehat{x}_j}\Big|$$

for $j = 1, 2, ..., d$, i.e., $\|\widehat{\nabla}\widehat{\Pi_h \phi_h}\|_{L^2(\widehat{T})} \le \|\widehat{\nabla}\widehat{\phi}_h\|_{L^2(\widehat{T})}$. The equivalence $h_T^{d/2-1}\|\widehat{\nabla}\widehat{w}_h\|_{L^2(\widehat{T})} \sim \|\nabla w_h\|_{L^2(T)}$ for all $w_h \in \mathcal{S}^1(\mathcal{T}_h)$, cf., e.g., [Ran08], implies that $\|\nabla \Pi_h \phi_h\|_{L^2(T)} \le c_T \|\nabla \phi_h\|_{L^2(T)}$ with a constant $c_T > 0$ that depends on the geometry of T but not on its diameter. □

Remark 2.1. *If $\mathcal{T}_h$ is weakly acute then the estimate holds with $c_\Pi = 1$, cf.* [Bar05].

3. Harmonic maps

Given a closed subset $\Gamma_D \subset \partial\Omega$ of positive surface measure and $u_D = \widetilde{u}_D|_{\Gamma_D}$ for some $\widetilde{u}_D \in C(\overline{\Omega};\mathbb{R}^m) \cap H^1(\Omega;\mathbb{R}^m)$ with $g(\widetilde{u}_D) = 0$ in Ω we aim at approximating critical points for

$$I(u) = \frac{1}{2}\int_\Omega |\nabla u|^2 \,\mathrm{d}x \quad \text{subject to } g(u) = 0.$$

The direct method of the calculus of variations implies the existence of solutions and these are characterized by

$$(\nabla u, \nabla w) = 0$$

for all $w \in H^1_D(\Omega;\mathbb{R}^m)$ with $w \cdot g'(u) = 0$ in Ω. The following algorithm iteratively computes approximate solutions for this problem.

Algorithm 1 (Harmonic maps)**.** *Let $u_h^0 \in \mathcal{S}^1(\mathcal{T}_h)^m$ with $u_h^0(z) = u_D(z)$ for all $z \in \mathcal{N}_h \cap \Gamma_D$ and $g\big(u_h^0(z)\big) = 0$ for all $z \in \mathcal{N}_h$. Choose $\tau, \varepsilon_{\mathrm{stop}} > 0$ and set $k = 1$.*
(1) Compute $v_h^k \in \mathcal{S}^1_D(\mathcal{T}_h)^m$ such that $v_h^k(z) \cdot g'\big(u_h^{k-1}(z)\big) = 0$ for all $z \in \mathcal{N}_h$ and

$$(\nabla v_h^k, \nabla w_h) + (\nabla[u_h^{k-1} + \tau v_h^k], \nabla w_h) = 0$$

for all $w_h \in \mathcal{S}^1_D(\mathcal{T}_h)^m$ with $w_h(z) \cdot g'\big(u_h^{k-1}(z)\big) = 0$ for all $z \in \mathcal{N}_h$.
(2) Set $u_h^k = u_h^{k-1} + \tau v_h^k$ and stop if $\|\nabla v_h^k\| \le \varepsilon_{\mathrm{stop}}$. Otherwise increase $k \to k+1$ and continue with (1).

The algorithm terminates within a finite number of iterations and provides an approximate harmonic map in the sense of the following proposition.

Proposition 3.1 (Termination)**.** *Algorithm 1 terminates within a finite number of iterations and provides a function $u_h^* = u_h^K \in \mathcal{S}^1(\mathcal{T}_h)^m$ for some $K \in \mathbb{N}$ such that $u_h^*(z) = u_D(z)$ for all $z \in \mathcal{N}_h \cap \Gamma_D$ and*

$$(\nabla u_h^*, \nabla w_h) = \mathcal{R}_h(w_h)$$

for all $w_h \in \mathcal{S}^1_D(\mathcal{T}_h)^m$ with $\mathcal{I}_h[w_h \cdot g'(u_h^*)] = 0$ and a bounded linear functional $\mathcal{R}_h : H^1_D(\Omega;\mathbb{R}^m) \to \mathbb{R}$ satisfying $\|\mathcal{R}_h\|_{H^1_D(\Omega)'} \le \varepsilon_{\mathrm{stop}}$. Moreover, we have

$$\|\mathcal{I}_h g(u_h^*)\|_{L^1(\Omega)} \le c\tau I(u_h^0)$$

and $I(u_h^*) \le I(u_h^0)$.

Proof. Given $u_h^{k-1} \in \mathcal{S}^1(\mathcal{T}_h)^m$ the set

$$\mathcal{F}_h[u_h^{k-1}] = \{w_h \in \mathcal{S}^1_D(\mathcal{T}_h)^m : w_h(z) \cdot g'\big(u_h^{k-1}(z)\big) = 0 \text{ for all } z \in \mathcal{N}_h\}$$

is a closed subspace of $\mathcal{S}^1_D(\mathcal{T}_h)^m$ so that the Lax-Milgram lemma implies the existence of a unique solution $v_h^k \in \mathcal{F}_h[u_h^{k-1}]$ in every iteration. Choosing $w_h = v_h^k =$

$d_t u_h^k$, incorporating the binomial formula $2(a+b)a = a^2 + ((a+b)^2 - b^2)$, and noting $u_h^k = u_h^{k-1} + \tau v_h^k$ lead to

$$\|\nabla v_h^k\|^2 + \frac{1}{2\tau}\big(\|\nabla u_h^k\|^2 - \|\nabla u_h^{k-1}\|^2\big) + \frac{\tau}{2}\|\nabla v_h^k\|^2 = 0.$$

Multiplication by τ and summation over $k = 1, 2, ..., \ell$ show

$$\frac{1}{2}\|\nabla u_h^\ell\|^2 + \tau\big(1 + \frac{\tau}{2}\big)\sum_{k=1}^{\ell}\|\nabla v_h^k\|^2 = \frac{1}{2}\|\nabla u_h^0\|^2.$$

This implies $\|\nabla v_h^k\| \to 0$ as $k \to \infty$ and hence the convergence of the iteration and the estimate $\|\nabla u_h^\ell\| \le \|\nabla u_h^0\|$ for all $\ell \ge 0$. At termination with some $K \in \mathbb{N}$ we have for $u_h^* = u_h^K = u_h^{K-1} + \tau v_h^K$ that

$$(\nabla u_h^*, \nabla w_h) = (\nabla v_h^K, \nabla w_h)$$

for all $w_h \in \mathcal{S}^1_{\rm D}(\mathcal{T}_h)^m$ with $w_h(z)\cdot g'\big(u_h^*(z)\big) = 0$ for all $z \in \mathcal{N}_h$. Since $\|\nabla v_h^K\| \le \varepsilon_{\rm stop}$ this implies the asserted identity. For every node $z \in \mathcal{N}_h$ and $\ell \ge 1$ we have by a Taylor expansion with some $\xi_z \in \mathbb{R}^m$ that

$$\begin{aligned} g\big(u_h^\ell(z)\big) &= g\big(u_h^{\ell-1}(z) + \tau v_h^\ell(z)\big) \\ &= g\big(u_h^{\ell-1}(z)\big) + \tau g'\big(u_h^{\ell-1}(z)\big)\cdot v_h^\ell(z) + \frac{\tau^2}{2}D^2 g(\xi_z)[v_h^\ell(z), v_h^\ell(z)] \\ &= g\big(u_h^{\ell-1}(z)\big) + \frac{\tau^2}{2}D^2 g(\xi_z)[v_h^\ell(z), v_h^\ell(z)]. \end{aligned}$$

Recalling that $D^2 g$ is uniformly bounded it follows that

$$|g\big(u_h^K(z)\big)| \le \|D^2 g\|_{L^\infty(\mathbb{R}^m)}\frac{\tau^2}{2}\sum_{\ell=1}^{K}|v_h^\ell(z)|^2.$$

Multiplication by h_z^d and summation over $z \in \mathcal{N}_h$ together with the norm equivalences (2.1) and Poincaré's inequality imply the asserted estimate. □

Remarks 3.1. *(i) If $M = g^{-1}(\{0\})$ is the boundary of a convex set, i.e., $M = \partial\mathcal{C}$ for a convex set $\mathcal{C} \subset \mathbb{R}^m$, and if $\mathcal{T}_h$ is weakly acute then one may define the update u_h^k via*

$$u_h^k(z) = \Pi_{\mathcal{C}}\big(u_h^{k-1}(z) + \tau v_h^k(z)\big)$$

for all $z \in \mathcal{N}_h$ with the orthogonal projection $\Pi_{\mathcal{C}}$ onto $\mathcal{C}$. Since $u_h^{k-1}(z) + \tau v_h^k(z) \notin \operatorname{int}(\mathcal{C})$ we then have $u_h^k(z) \in M = \partial\mathcal{C}$ and the Lipschitz continuity of $\Pi_{\mathcal{C}}$ with constant 1 implies

$$\|\nabla u_h^k\| \le \|\nabla[u_h^{k-1} + \tau v_h^k]\| \le \|\nabla u_h^{k-1}\|.$$

This allows to devise an algorithm whose iterates satisfy the constraint at the nodes exactly and converges with $\tau = 1$, cf. [Alo97, Bar05, Bar10]. *Weak acuteness is a restrictive condition if $d = 3$ and if the triangulation is not weakly acute the step size restriction $\tau = \mathcal{O}(h)$ has to be imposed to guarantee stability when the projection step is included, cf.* [Bar10].
(ii) The proposition proves global convergence of Algorithm 1. Newton iterations are in general only locally convergent but can be combined with Algorithm 1 as in [Bar09a].
(iii) Convergence of approximations as $(h, \tau, \varepsilon_{\rm stop}) \to 0$ for the case $g(p) = |p|^2 - 1$ can be shown with the help of Lemma 2.1 and weak compactness arguments,

cf. [Alo97, Bar05]. *The case of target manifolds different from the unit sphere is difficult in general owing to the lack of related compactness results, cf.* [Bar10] *for certain convergence results if* $d = 2$.

In the case of the unit sphere, i.e., $g(p) = |p|^2 - 1$, we have $|u_h^k(z)| \geq 1$ for all $z \in \mathcal{N}_h$ and $k \geq 0$. The renormalization is thus well-defined and this motivates the following multilevel strategy that starts with a large step size and stopping criterion, carries out the iteration of Algorithm 1, renormalizes the output, decreases the step size, and repeats these steps until a prescribed step size and stopping criterion is attained.

Algorithm 2 (Multilevel strategy)**.** *Let* $u_h^0 \in \mathcal{S}^1(\mathcal{T}_h)^m$ *with* $u_h^0(z) = u_{\rm D}(z)$ *for all* $z \in \mathcal{N}_h \cap \Gamma_{\rm D}$ *and* $|u_h^0(z)|^2 = 1$ *for all* $z \in \mathcal{N}_h$ *and choose* $\tau, \varepsilon_{\rm stop} > 0$, *and* $L \geq 0$. *Set* $\widetilde{\varepsilon}_{\rm stop} = 2^L \varepsilon_{\rm stop}$, $\widetilde{\tau} = 2^L \tau$, $\ell = 0$, $k = 1$, *and* $u_h^{\ell,0} = u_h^0$.
(1) Compute $v_h^{\ell,k} \in \mathcal{S}^1_{\rm D}(\mathcal{T}_h)^m$ *such that* $v_h^{\ell,k}(z) \cdot u_h^{\ell,k-1}(z) = 0$ *for all* $z \in \mathcal{N}_h$ *and*

$$(\nabla v_h^{\ell,k}, \nabla w_h) + (\nabla [u_h^{\ell,k-1} + \widetilde{\tau} v_h^{\ell,k}], \nabla w_h) = 0$$

for all $w_h \in \mathcal{S}^1_{\rm D}(\mathcal{T}_h)^m$ *with* $w_h(z) \cdot u_h^{\ell,k-1}(z) = 0$ *for all* $z \in \mathcal{N}_h$.
(2) Set $u_h^{\ell,k} = u_h^{\ell,k-1} + \widetilde{\tau} v_h^{\ell,k}$. *If* $\|\nabla v_h^{\ell,k}\| > \widetilde{\varepsilon}_{\rm stop}$ *increase* $k \to k+1$ *and continue with (1).*
(3) Stop if $\ell = L$. *Otherwise, increase* $\ell \to \ell + 1$, *decrease* $\widetilde{\tau} \to \widetilde{\tau}/2$, $\widetilde{\varepsilon}_{\rm stop} \to \widetilde{\varepsilon}_{\rm stop}/2$, *define* $u_h^{\ell,0} \in \mathcal{S}^1(\mathcal{T}_h)^m$ *by*

$$u_h^{\ell,0}(z) = \frac{u_h^{\ell-1,k}(z)}{|u_h^{\ell-1,k}(z)|}$$

for all $z \in \mathcal{N}_h$, *set* $k = 1$, *and continue with (1).*

With the arguments of the proof of Proposition 3.1 we obtain the following result.

Proposition 3.2 (Multilevel convergence)**.** *Algorithm 2 is well defined, terminates within a finite number of iterations, and provides a function* $u_h^* \in \mathcal{S}^1(\mathcal{T}_h)^m$ *such that* $u_h^*(z) = u_{\rm D}(z)$ *for all* $z \in \mathcal{N}_h \cap \Gamma_{\rm D}$ *and*

$$(\nabla u_h^*, \nabla w_h) = \mathcal{R}_h(w_h)$$

for all $w_h \in \mathcal{S}^1_{\rm D}(\mathcal{T}_h)^m$ *with* $\mathcal{I}_h[w_h \cdot u_h^*] = 0$ *and a bounded linear functional* $\mathcal{R}_h : H^1_{\rm D}(\Omega; \mathbb{R}^m) \to \mathbb{R}$ *satisfying* $\|\mathcal{R}_h\|_{H^1_{\rm D}(\Omega)'} \leq \varepsilon_{\rm stop}$. *Moreover, with* $c_\Pi > 0$ *such that*

$$\|\nabla \phi_h\| \leq c_\Pi \Big\| \nabla \mathcal{I}_h \Big[\frac{\phi_h}{|\phi_h|} \Big] \Big\|$$

for all $\phi_h \in \mathcal{S}^1(\mathcal{T}_h)^m$ *with* $|\phi_h(z)| \geq 1$ *for all* $z \in \mathcal{N}_h$ *we have*

$$\|\mathcal{I}_h |u_h^*|^2 - 1\|_{L^1(\Omega)} \leq \tau c_\Pi^L I(u_h^0).$$

Proof. The proof follows from a repeated application of Proposition 3.1 and noting that

$$\|\nabla u_h^{\ell,0}\| \leq c_\Pi \|\nabla u_h^{\ell-1,k}\|$$

for $\ell = 1, 2, ...L$. □

Remarks 3.2. *(i) If the underlying triangulation is weakly acute then we have* $c_\Pi = 1$ *and* $I(u_h^*) \leq I(u_h^0)$.
(ii) The upper bound for the error in the approximation of the constraint can be replaced by $\tau I(u_h^{L,0})$ *which is expected to be a sharper bound for the error* $\|\mathcal{I}_h |u_h^*|^2 - 1\|_{L^1(\Omega)}$ *since the Dirichlet energy is decreased on every level.*

4. Harmonic map heat flow

The iterative scheme devised and analyzed in the previous section computes approximations of harmonic maps with the help of the corresponding H^1 gradient flow. The related L^2 gradient flow is the harmonic map heat flow into $M = g^{-1}(\{0\})$ defined through

$$(\partial_t u, w) + (\nabla u, \nabla w) = 0, \quad g(u) = 0, \quad u(0) = u_0,$$

for almost every $t \in [0,T]$ and all $w \in H^1_{\mathrm{D}}(\Omega;\mathbb{R}^m)$ with $w \cdot g'\big(u(t,\cdot)\big) = 0$ together with the boundary conditions

$$u(t,\cdot)|_{\Gamma_{\mathrm{D}}} = u_{\mathrm{D}}, \quad \partial_\nu u(t,\cdot)|_{\Gamma_{\mathrm{N}}} = 0.$$

Here, the case $\Gamma_{\mathrm{D}} = \emptyset$ is not excluded. This initial boundary value problem can be approximately solved by changing the inner product used in Algorithm 1. We incorporate a parameter $\theta \in [0,1]$ that allows to analyze a class of midpoint schemes. We assume that the initial data $u_0 \in H^1(\Omega;\mathbb{R}^m)$ is continuous and satisfies $u_0|_{\Gamma_{\mathrm{D}}} = u_{\mathrm{D}}$ and $g(u_0) = 0$ in Ω.

Algorithm 3 (Harmonic map heat flow)**.** *Let $u_h^0 \in \mathcal{S}^1(\mathcal{T}_h)^m$ be defined through $u_h^0(z) = u_0(z)$ for all $z \in \mathcal{N}_h$ and set $k = 1$.*
(1) Compute $v_h^k \in \mathcal{S}^1_{\mathrm{D}}(\mathcal{T}_h)^m$ such that $v_h^k(z) \cdot g'\big(u_h^{k-1}(z)\big) = 0$ for all $z \in \mathcal{N}_h$ and

$$(v_h^k, w_h) + (\nabla[u_h^{k-1} + \theta\tau v_h^k], \nabla w_h) = 0$$

for all $w_h \in \mathcal{S}^1_{\mathrm{D}}(\mathcal{T}_h)^m$ with $w_h(z) \cdot g'\big(u_h^{k-1}(z)\big) = 0$ for all $z \in \mathcal{N}_h$.
(2) Set $u_h^k = u_h^{k-1} + \tau v_h^k$ and stop if $k \geq K = \lceil T/\tau \rceil$. Otherwise increase $k \to k+1$ and continue with (1).

The properties of Algorithm 3 are similar to those of Algorithm 1.

Proposition 4.1 (Stability)**.** *Algorithm 3 computes a sequence of functions $(u_h^k)_{k=0,\dots,K} \subset \mathcal{S}^1(\mathcal{T}_h)^m$ such that $u_h^k(z) = u_{\mathrm{D}}(z)$ for all $z \in \mathcal{N}_h \cap \Gamma_{\mathrm{D}}$ and $k = 0,1,\dots,K$, and*

$$I(u_h^\ell) + \tau \sum_{k=1}^{\ell} \|v_h^k\|^2 + (2\theta - 1)\frac{\tau^2}{2} \sum_{k=1}^{\ell} \|\nabla v_h^k\|^2 = I(u_h^0)$$

for all $\ell = 1,2,\dots,K$. With the interpolants $\widehat{u}_{h,\tau}, u_{h,\tau}^-, u_{h,\tau}^+ : [0,T] \times \Omega \to \mathbb{R}^m$ of the sequence $(u_h^k)_{k=0,\dots,K}$ we have

$$(\partial_t \widehat{u}_{h,\tau}, w_h) + (\nabla[(1-\theta)u_{h,\tau}^- + \theta u_{h,\tau}^+], \nabla w_h) = 0$$

for almost every $t \in [0,T]$ and all $w_h \in \mathcal{S}^1_{\mathrm{D}}(\mathcal{T}_h)^m$ with $\mathcal{I}_h\big[w_h \cdot g'\big(u_{h,\tau}^-(t)\big)\big] = 0$ in Ω and if $\theta \geq 1/2$ then

$$\|\mathcal{I}_h g(u_h^+(t,\cdot))\|_{L^1(\Omega)} \leq c\tau I(u_h^0).$$

Proof. Choosing $w_h = v_h^k = d_t u_h^k$ in the equation of Algorithm 3 the proof follows the lines of the proof of Proposition 3.1. $\square$

Remarks 4.1. *(i) A projection step can be included if the target manifold is the boundary of a convex set. Stability of the iteration then requires that $\mathcal{T}_h$ is weakly acute or that $\tau = \mathcal{O}(h^2)$.*
(ii) Unconditional convergence to solutions of subsequences of numerical approximations as $(h,\tau) \to 0$ in the case $g(p) = |p|^2 - 1$ and $\theta \geq 1/2$ follows with the

techniques from [BBFP07, Alo08]. *If $\theta < 1/2$ then the condition $\tau \le ch_{\min}^2$ needs to be imposed.*
(iii) If $m = 3$ and $g(p) = |p|^2 - 1$ then the harmonic map heat flow into the unit sphere can equivalently be defined through the equation

$$\partial_t u + u \times (u \times \Delta u) = 0$$

together with initial and homogeneous Neumann boundary conditions. The Landau-Lifshitz-Gilbert equation seeks a mapping $u : [0,T] \times \Omega \to \mathbb{R}^3$ with $|u(t,x)| = 1$ in $[0,T] \times \Omega$ and

$$\partial_t u + \alpha u \times (u \times \Delta u) - u \times \Delta u = 0$$

with a small damping parameter $\alpha > 0$. The discretization of this equation is analogous to the discretization of the harmonic map heat flow, cf. [AJ06, Alo08]. *In particular, projection steps can be omitted.*

5. Wave maps

The partial differential equation that defines wave maps reads

$$(\partial_t^2 u, w) + (\nabla u, \nabla w) = 0, \quad g(u) = 0, \quad u(0) = u_0, \quad \partial_t u(0) = v_0,$$

for all $w \in H^1_{\mathrm{D}}(\Omega; \mathbb{R}^m)$ with $w \cdot g'(u) = 0$ together with the boundary conditions

$$u(t, \cdot)|_{\Gamma_{\mathrm{D}}} = u_{\mathrm{D}}, \quad \partial_\nu u(t, \cdot)|_{\Gamma_{\mathrm{N}}} = 0,$$

where $\Gamma_{\mathrm{D}} = \emptyset$ is admissible. We assume that the data functions $u_0 \in H^1(\Omega; \mathbb{R}^m)$ and $v_0 \in L^2(\Omega; \mathbb{R}^m)$ are continuous and compatible and employ the following algorithm to approximate solutions.

Algorithm 4 (Wave maps)**.** *Let $u_h^0, v_h^0 \in \mathcal{S}^1(\mathcal{T}_h)^m$ be defined through $u_h^0(z) = u_0(z)$ and $v_h^0(z) = v_0(z)$ for all $z \in \mathcal{N}_h$ and set $k = 1$.*
(1) Compute $v_h^k \in \mathcal{S}^1_{\mathrm{D}}(\mathcal{T}_h)^m$ such that $v_h^k(z) \cdot g'\big(u_h^{k-1}(z)\big) = 0$ for all $z \in \mathcal{N}_h$ and

$$(d_t v_h^k, w_h) + (\nabla [u_h^{k-1} + \theta \tau v_h^k], \nabla w_h) = 0$$

for all $w_h \in \mathcal{S}^1_{\mathrm{D}}(\mathcal{T}_h)^m$ with $w_h(z) \cdot g'\big(u_h^{k-1}(z)\big) = 0$ for all $z \in \mathcal{N}_h$.
(2) Set $u_h^k = u_h^{k-1} + \tau v_h^k$ and stop if $k \ge K = \lceil T/\tau \rceil$. Otherwise increase $k \to k+1$ and continue with (1).

Proposition 5.1 (Stability)**.** *Algorithm 4 computes sequences of functions $(u_h^k)_{k=0,\dots,K}, (v_h^k)_{k=0,\dots,K} \subset \mathcal{S}^1(\mathcal{T}_h)^m$ such that $u_h^k(z) = u_{\mathrm{D}}(z)$ for all $z \in \mathcal{N}_h \cap \Gamma_{\mathrm{D}}$ and $k = 0, 1, \dots, K$ and*

$$\frac{1}{2}\|v_h^\ell\|^2 + \frac{1}{2}\|\nabla u_h^\ell\|^2 + \frac{\tau^2}{2}\sum_{k=1}^{\ell} \|d_t v_h^k\|^2 + (2\theta - 1)\frac{\tau^2}{2}\sum_{k=1}^{\ell} \|\nabla v_h^k\|^2 = \frac{1}{2}\|v_h^0\|^2 + \frac{1}{2}\|\nabla u_h^0\|^2.$$

for all $\ell = 1, 2, \dots, K$. With the interpolants $\widehat{v}_{h,\tau}, \widehat{u}_{h,\tau}, u_{h,\tau}^-, u_{h,\tau}^+ : [0,T] \times \Omega \to \mathbb{R}^m$ of the sequences we have

$$(\partial_t \widehat{v}_{h,\tau}, w_h) + (\nabla [(1-\theta) u_{h,\tau}^- + \theta u_{h,\tau}^+], \nabla w_h) = 0$$

for almost every $t \in [0,T]$ and all $w_h \in \mathcal{S}^1_{\mathrm{D}}(\mathcal{T}_h)^m$ with $w_h \cdot \mathcal{I}_h g'\big(u_{h,\tau}^-(t)\big) = 0$ in Ω and if $\theta \ge 1/2$ then

$$\|\mathcal{I}_h g(u_{h,\tau}^+(t, \cdot))\|_{L^1(\Omega)} \le c\tau(t+1)(\|v_h^0\|^2 + \|\nabla u_h^0\|^2).$$

Proof. Choosing $w_h = v_h^k = d_t u_h^k$ in the equation of Algorithm 4 leads to

$$\frac{d_t}{2}\|v_h^k\|^2 + \frac{\tau}{2}\|d_t v_h^k\|^2 + \frac{d_t}{2}\|\nabla u_h^k\|^2 + (2\theta-1)\frac{\tau^2}{2}\|\nabla v_h^k\|^2 = 0.$$

Summation over $k = 1, 2, ..., \ell$ and multiplication by τ imply the first asserted identity. If $\theta \geq 1/2$ then we have $\|v_h^k\| \leq c$ for all $k = 0, 1, ..., K$ and with the arguments of the proof of Proposition 3.1 we deduce the asserted bound for $\|\mathcal{I}_h g(u_{h,\tau}^+(t,\cdot))\|_{L^1(\Omega)}$. □

Remarks 5.1. *(i) The linearized treatment of the constraint prohibits the use of the test function $w_h = (u_h^{k-1} + u_h^k)/2$ which would be desirable in the case $\theta = 1/2$ to verify whether the scheme is dissipation-free.*
(ii) Unconditional convergence to solutions of subsequences of approximations as $(h,\tau) \to 0$ in the case $g(p) = |p|^2 - 1$ can be shown for $\theta \geq 1/2$ as in [BFP08, Bar09b]. *If $\theta < 1/2$ then the condition $\tau \leq ch_{\min}^2$ needs to be imposed.*

6. Numerical experiments

We report in this section the practical performance of the projection-free approximation schemes for two- and three-dimensional settings. The implementations were realized in Matlab with a direct solution of linear systems of equations. The employed triangulations were obtained by uniform red-refinements of coarse triangulations of $\Omega = (-1/2, 1/2)^d$ with mesh size $h \sim 1$. We will refer to the triangulation that is obtained by ℓ successive uniform refinements through the mesh-size $h = 2^{-\ell}$.

6.1. **Harmonic maps.** We tested Algorithms 1 and 2 in an example that leads to the singular solution $u(x) = x/|x|$, $x \in \Omega$, if $d = 3$ and a smooth solution if $d = 2$.

Example 6.1. *Let $m = 3$, and $g(p) = |p|^2 - 1$ for $p \in \mathbb{R}^3$, $\Omega = (-1/2, 1/2)^d$ for $d = 2, 3$, $\Gamma_{\mathrm{D}} = \partial\Omega$, $\Gamma_{\mathrm{N}} = \emptyset$, and $u_{\mathrm{D}}(x) = x/|x|$ for $x \in \Gamma_{\mathrm{D}}$.*

In Tables 1 and 2 we displayed the error in the approximation of the constraint with respect to the L^1 and L^∞ norm, the initial energy, and the number of iterations of Algorithm 1 for different mesh-sizes with $d = 2$ and $d = 3$, respectively. We employed different mesh-sizes $h = 2^{-\ell}$ for $\ell = 3, 4, 5, 6$ and $\ell = 2, 3, 4, 5$ for $d = 2$ and $d = 3$, respectively, and the parameters

$$\tau = h, \quad \varepsilon_{\mathrm{stop}} = h.$$

The algorithm was initialized with vector fields defined through

$$u_h^0(z) = \begin{cases} u_{\mathrm{D}}(z) & \text{for } z \in \mathcal{N}_h \cap \Gamma_{\mathrm{D}}, \\ \xi_z/|\xi_z| & \text{for } z \in \mathcal{N}_h \setminus \Gamma_{\mathrm{D}}, \end{cases}$$

where $\xi_z \in [-1/2, 1/2]^3$ denotes for every $z \in \mathcal{N}_h$ a random vector. The initial energy $I(u_h^0)$ is thus strongly mesh-dependent and grows like h^{-2} which is suboptimal in view of the bound for the approximation error for the constraint of Proposition 3.1. Nevertheless, we observe an experimental convergence of the approximation error in the constraint as $h \to 0$. The analysis of Algorithm 1 shows that the number of iterations depends on the value of the initial energy and for the suboptimal choice of u_h^0 in this experiment and the stopping criterion $\varepsilon_{\mathrm{stop}} = h$ we see that the number of iterations increases like h^{-2}.
Table 3 illustrates the performance of the multilevel iteration defined by Algorithm 2 with different numbers of levels L and for fixed $d = 2$, $h = 2^{-5}$, $\tau = \varepsilon_{\mathrm{stop}} = h$. We

h	$\|\mathcal{I}_h\|u_h^*\|^2 - 1\|_{L^1}$	$\|\mathcal{I}_h\|u_h^*\|^2 - 1\|_{L^\infty}$	$I(u_h^0)$	K_{iter}
2^{-3}	0.0854	0.1192	109.61	86
2^{-4}	0.0640	0.0997	472.99	194
2^{-5}	0.0467	0.0848	1972.40	569
2^{-6}	0.0292	0.0545	7997.41	2425

Table 1. Error in the constraint approximation in different norms, initial energy, and iteration numbers for Algorithm 1 in Example 6.1 with $d = 2$, $h = 2^{-\ell}$, $\ell = 3, 4, 5, 6$, and $\tau = \varepsilon_{\text{stop}} = h$.

h	$\|\mathcal{I}_h\|u_h^*\|^2 - 1\|_{L^1}$	$\|\mathcal{I}_h\|u_h^*\|^2 - 1\|_{L^\infty}$	$I(u_h^0)$	K_{iter}
2^{-2}	0.0634	0.1483	30.53	25
2^{-3}	0.0763	0.1546	168.67	206
2^{-4}	0.0560	0.1168	811.78	790
2^{-5}	0.0186	0.0878	3577.04	856

Table 2. Error in the constraint approximation in different norms, initial energy, and iteration numbers for Algorithm 1 in Example 6.1 with $d = 3$, $h = 2^{-\ell}$, $\ell = 3, 4, 5, 6$, and $\tau = \varepsilon_{\text{stop}} = h$.

L	$\|\mathcal{I}_h\|u_h^*\|^2 - 1\|_{L^1}$	$\|\mathcal{I}_h\|u_h^*\|^2 - 1\|_{L^\infty}$	K_{iter}
0	0.04668170	0.08484197	569
1	0.00000827	0.00002337	353
2	0.00000346	0.00000903	233
3	0.00000404	0.00001005	185
4	0.00000397	0.00000994	162
5	0.00000397	0.00000994	162

Table 3. Error in the constraint approximation and (total) iteration numbers for the multilevel iteration of Algorithm 2 in Example 6.1 with $d = 2$, $h = 2^{-5}$, $\tau = \varepsilon_{\text{stop}} = h$, and number of levels $L = 0, 1, ..., 5$.

L	$\|\mathcal{I}_h\|u_h^*\|^2 - 1\|_{L^1}$	$\|\mathcal{I}_h\|u_h^*\|^2 - 1\|_{L^\infty}$	K_{iter}
0	0.05599896	0.11684442	790
1	0.00001268	0.00096441	449
2	0.00001317	0.00119701	400
3	0.00001328	0.00144665	386
4	0.00001328	0.00144665	386

Table 4. Error in the constraint approximation and (total) iteration numbers for the multilevel iteration of Algorithm 2 in Example 6.1 with $d = 3$, $h = 2^{-4}$, $\tau = \varepsilon_{\text{stop}} = h$, and number of levels $L = 0, 1, ..., 4$.

see that the increasing number of levels decreases the total number of iterations compared to the single level iteration corresponding to $L = 0$. Moreover, the approximation of the constraint is significantly improved which is in agreement with Remark 3.2. Since the triangulation is weakly acute Algorithm 1 with step size $\tau = 1$ and a projection step may be used in this example. In this case the scheme terminated after 35 iterations. Table 4 shows the corresponding results for the three-dimensional situation with $h = 2^{-4}$. Again we observe a significant decrease of the total number of iterations compared to the iteration with a fixed step size. Our triangulations of the unit cube in $\mathbb{R}^3$ are not weakly acute so that the projection scheme with step size $\tau = 1$ cannot be applied in this situation.

6.2. **Harmonic map heat flow.** It is well understood that the harmonic map heat flow can develop singularities from smooth initial data. The following example from [CDY92] leads to such a situation and provides a worst-case scenario for numerical approximation schemes.

Example 6.2. *Let $d = 2$, $T = 1$, $\Omega = (-1/2, 1/2)^2$, $\Gamma_{\rm D} = \partial\Omega$, $\Gamma_{\rm N} = \emptyset$, $m = 3$, $g(p) = |p|^2 - 1$, and*

$$u_0(x) = \frac{1}{|x|}\big(x_1 \sin\phi(2|x|), x_2 \sin\phi(2|x|), |x|\cos\phi(2|x|)\big)^\top$$

for $x = (x_1, x_2) \in \Omega$ and $\phi(s) = (3\pi/2)\min\{s^2, 1\}$.

We approximated the nonlinear evolution problem specified by Example 6.2 with Algorithm 3 and the discretization parameters $\theta = 1$, $h = 2^{-\ell}$, $\ell = 6, 7, 8, 9$, and $\tau = h$. Figure 2 visualizes the development of the approximation error $\|\mathcal{I}_h|u_h^k|^2 - \|_{L^1(\Omega)}$ in dependence of the number of time steps $k = 0, 1, ..., K$ and the mesh-size h. Initially this error increases rapidly but then attains a constant value when the evolution becomes almost stationary. The experimental error decays only nearly linearly with the step size $\tau = h$ within the considered time interval and does not show the full linear convergence proved in Proposition 4.1. This is expected to be related to the global character in time of the estimate. The approximation error appears large compared to the values of the employed step sizes which reflects the influence of the large initial energy $I(u_0) \approx 72.16$.

6.3. **Wave maps.** The partial regularity properties and occurrence of singularities in wave maps is less well understood than for the harmonic map heat flow. Although finite-time blow-up is known to occur [KST08] no explicit examples seem to be available. The initial data defined in the following example leads to maximal, unbounded gradients in numerical experiments.

Example 6.3. *Let $d = 2$, $T = 1$, $\Omega = (-1/2, 1/2)^2$, $\Gamma_{\rm D} = \emptyset$, $\Gamma_{\rm N} = \partial\Omega$, $m = 3$, $g(p) = |p|^2 - 1$, $v_0 = 0$, and*

$$u_0(x) = \begin{cases} \big(2a(|x|)x_1, 2a(|x|)x_2, a(|x|)^2 - |x|^2\big)^\top / \big(a(|x|)^2 + |x|^2\big) & \text{for } |x| \le 1/2, \\ (0, 0, -1)^\top & \text{for } |x| \ge 1/2, \end{cases}$$

for $x = (x_1, x_2) \in \Omega$ and $a(s) = (1 - 2s)^4$.

We ran Algorithm 4 with $\theta = 1$, $h = 2^{-\ell}$ for $\ell = 5, 6, 7, 8$, $\tau = h/4$, and the discrete initial data functions $u_h^0 = \mathcal{I}_h u_0$ and $v_h^0 = \mathcal{I}_h v_0 = 0$. Figure 3 shows the temporal development of the constraint violation, i.e., the sequence

$$\|\mathcal{I}_h|u_h^k|^2 - 1\|_{L^1(\Omega)}$$

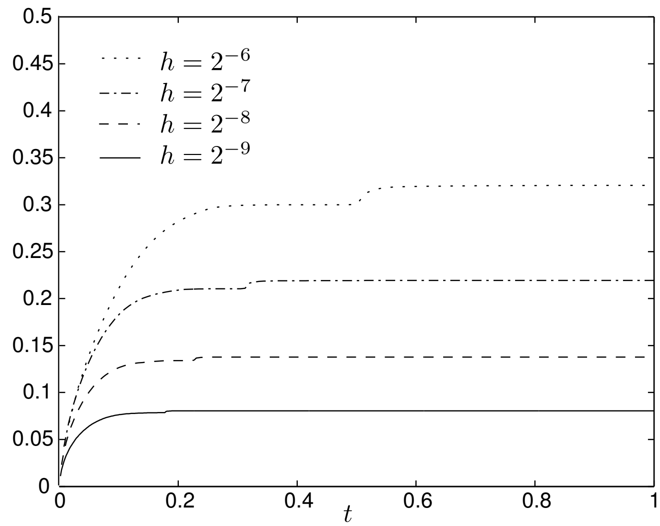

FIGURE 2. Development of the constraint approximation error $\|\mathcal{I}_h|u_{h,\tau}^+(t)|^2 - 1\|_{L^1}$ for different mesh-sizes $h = 2^{-\ell}$, $\ell = 6, 7, 8, 9$, and $\tau = h$ in the approximation of the harmonic map heat flow specified in Example 6.2 with Algorithm 3. The error grows rapidly in an initial time interval and then remains nearly constant. It decays nearly linearly with the step size $\tau = h$.

for $k = 0, 1, ..., K$ with $K = \lceil T/\tau \rceil$. We note that for the initial data defined in Example 6.3 we have that the quantity

$$\frac{1}{2}\big(\|v_h^0\|^2 + \|\nabla u_h^0\|^2\big)$$

is uniformly bounded and this is reflected in the decay of the approximation error of the constraint, i.e., we observe experimentally a linear decay of the approximation error $\|\mathcal{I}_h|u_h^k|^2 - \|_{L^1(\Omega)}$ as $h = \tau \to 0$ at fixed times t_k. The error increases in time proportionally to t which is in agreement with the error bound derived in Proposition 5.1.

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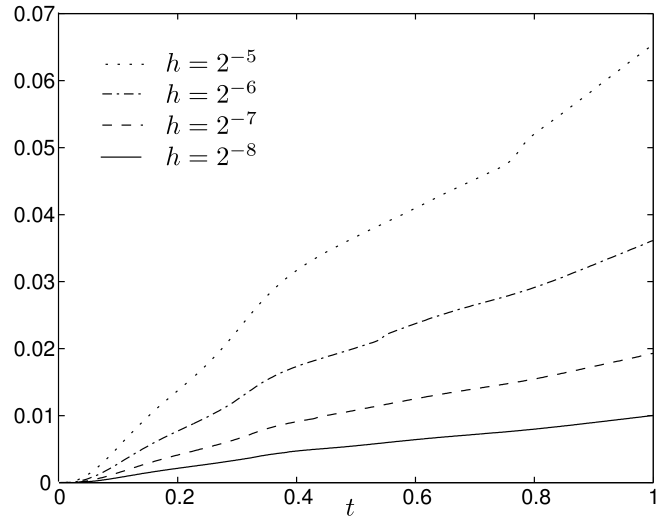

FIGURE 3. Development of the constraint approximation error $\|\mathcal{I}_h|u^+_{h,\tau}(t)|^2 - 1\|_{L^1}$ for different mesh-sizes $h = 2^{-\ell}$, $\ell = 5, 6, 7, 8$, and $\tau = h$ in the approximation of a wave map evolution specified in Example 6.3 with Algorithm 4. The error grows linearly in time and decays linearly with the step size $\tau = h/4$.

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