QUASI-OPTIMAL ERROR ESTIMATES FOR THE APPROXIMATION OF STABLE HARMONIC MAPS

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Abstract. Based on a quantitative version of the inverse function theorem and an appropriate saddle-point formulation we derive a quasi-optimal error estimate for the finite element approximation of harmonic maps into spheres with a nodal discretization of the unit-length constraint. The estimate holds under natural regularity requirements and appropriate geometric stability conditions on solutions. Extensions to other target manifolds including boundaries of ellipsoids are discussed.

1. Introduction

Harmonic maps into spheres are stationary configurations for the Dirichlet energy

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

among vector fields $u : \Omega \to \mathbb{R}^m$, $\Omega \subset \mathbb{R}^d$, satisfying prescribed boundary conditions $u|_{\Gamma_\mathrm{D}} = u_\mathrm{D}$ and the pointwise sphere constraint

$$u(x) \in S^{m-1} \quad \Longleftrightarrow \quad |u(x)|^2 - 1 = 0$$

for almost every $x \in \Omega$. The existence of global minimizers is an immediate consequence of the direct method in the calculus of variations provided that the admissible set is non-empty. More generally, stationary points satisfy the Euler–Lagrange equations

$$-\Delta u = |\nabla u|^2 u, \quad u|_{\Gamma_\mathrm{D}} = u_\mathrm{D}, \quad \partial_n u|_{\Gamma_\mathrm{N}} = 0, \quad |u|^2 = 1, \tag{1}$$

where $\Gamma_\mathrm{N} = \partial\Omega \setminus \Gamma_\mathrm{D}$. Since the right-hand side in the partial differential equation may only belongs to $L^1(\Omega;\mathbb{R}^m)$ regularity of solutions cannot be expected in general and in fact solutions that are everywhere discontinuous exist, cf. [22, 20].

Motivated by related models and applications in micromagnetics, liquid crystal devices, and nonlinear bending, cf., e.g., [16, 8, 6] and references therein, the numerical approximation of pointwise constrained variational problems has received considerable attention in the last decades. Various discretizations and iterative schemes have been devised and analyzed in [18,

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1, 5, 3, 12]. To avoid unjustified regularity assumptions, the convergence of numerical methods has often been based on weak compactness results for the Euler–Lagrange equations which shows that weak accumulation points of approximations are harmonic maps. To fully justify the methods it is important to prove their optimal convergence in the case of sufficiently regular solutions, and only a few results in this direction are available, cf. [10, 13, 12].

An attractive and flexible approach to deriving error estimates for numerical schemes has been identified in [13] and it is our aim to address its validity for three-dimensional domains Ω and higher-dimensional target manifolds. Their approach is based on the Lagrange functional

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

that imposes the constraint via a Lagrange multiplier λ. A suitable functional analytical framework interprets the constraint term in a weaker sense and seeks stationary pairs (u,λ) in the affine space

$$\mathcal{A} = (u_{\mathrm{D}}, 0) + X,$$

with the product space

$$X = H^1_{\mathrm{D}}(\Omega;\mathbb{R}^m) \cap L^\infty(\Omega;\mathbb{R}^m) \times H^{-1}(\Omega),$$

where $H^{-1}(\Omega)$ is the topological dual of the Sobolev space $H^1_{\mathrm{D}}(\Omega)$. To derive error estimates in a neighborhood of a solution (u,λ) the mapping properties of the second variation of L are releavant. Its stable invertibility can be analyzed in terms of a saddle-point problem which seeks for a given functional $(f,g) \in X'$ a solution $(v,\mu) \in X$ such that

$$\begin{aligned}
(\nabla v, \nabla w) + \langle \lambda, v\cdot w\rangle + \langle \mu, u\cdot w\rangle &= \langle f, w\rangle,\\
\langle \eta, u\cdot v\rangle &= \langle g, \eta\rangle,
\end{aligned}$$

for all $(w,\eta)\in X$. Well established theories for saddle-point problems assert that the problem has a unique and stable solution if and only if the bilinar form

$$b_u(\mu, v) = \langle \mu, u\cdot v\rangle$$

is bounded and satisfies an inf-sup condition, and the bilinear form

$$a_\lambda(v,w) = (\nabla v, \nabla w) + (\lambda, v\cdot w),$$

with $\lambda = -|\nabla u|^2$, is bounded and defines an invertible operator on the kernel of b_u with respect to the second argument. The inf-sup condition is obtained by choosing for given $\mu \in H^{-1}(\Omega)$ the function $v = \phi u$, where $\phi \in H^1_{\mathrm{D}}(\Omega)$ satisfies $\langle \mu, \phi\rangle = \|\mu\|_{H^{-1}}$. The kernel of b_u consists of tangential vector fields $v \in T_u$ with

$$T_u = \big\{ v \in H^1_{\mathrm{D}}(\Omega;\mathbb{R}^m) \cap L^\infty(\Omega;\mathbb{R}^m) : v\cdot u = 0 \text{ a.e.}\big\}.$$

We say that u is a stable harmonic map, if a_λ is H^1 coercive on T_u. Besides the special case $|\nabla u| < c_P^{-1}$ with the Poincaré constant $c_P > 0$ a coercivity result holds if the one-dimensional sphere is considered as a target manifold, i.e., $m = 2$ and $u : \Omega \to S^1$. In this case tangential vector fields are given by

$$v = \alpha u^\perp,$$

with $\alpha \in H^1_{\rm D}(\Omega)$ and the rotation $u^\perp$ of u by $\pi/2$. We then have the coercivity property

$$a_\lambda(v,v) = \int_\Omega |\nabla \alpha|^2 \,{\rm d}x \ge (1 + \|\nabla u\|^2_{L^\infty} c_P^2)^{-1} \|\nabla v\|^2,$$

whenever the harmonic map u satisfies $u \in W^{1,\infty}(\Omega;\mathbb{R}^2)$. Remarkably, this stability property fails if the (same) harmonic map u is allowed to attain values in the two-dimensional sphere. Indeed, by embedding the image of u into S^2 via $\widetilde{u} = [u,0]^\mathsf{T}$, and considering $v = \alpha e_3 \in T_{\widetilde{u}}$ we find that

$$a_\lambda(v,v) = \int_\Omega |\nabla \alpha|^2 - |\nabla u|^2 \alpha^2 \,{\rm d}x.$$

The right-hand side can only be positive for all $\alpha \in H^1_{\rm D}(\Omega)$ if $|\nabla u|$ is sufficiently small.

Only a few results are available concerning the uniqueness and stability of harmonic maps into higher-dimensional spheres, cf., e.g., [15, 14]. In particular, if a cut-locus condition is satisfied, e.g., if the image of a harmonic map is strictly contained in a hemisphere, then [15, Theorem B] states that the only Jacobi field along a harmonic map u, i.e., a field $v \in T_u$ with $a_\lambda(v,v) = 0$, is the trivial one. If $u \in \mathcal{A}$ is an absolute minimizer for I then we have that a_λ is semi-definite and if, e.g., $u \in W^{1,\infty}(\Omega;\mathbb{R}^m)$ a contradiction argument implies that a_λ is coercive on T_u. In view of limited regularity properties, cf. [21, 17, 20] and nonuniqueness properties, cf., e.g., [4], a more general theory cannot be expected.

Provided that the harmonic map u is regular, i.e., we have that $u \in H^2(\Omega;\mathbb{R}^m) \cap W^{1,\infty}(\Omega;\mathbb{R}^m)$, and stable, i.e., the bilinear form a_λ is H^1 coercive on T_u, we derive the quasi-optimal error estimate

$$\|\nabla(u - u_h)\| + \|\lambda - \lambda_h\|_{H^{-1}} \le c_u h,$$

for a canonical discretization of the Lagrange functional and the unique finite element solution $(u_h, \lambda_h) \in \mathcal{S}^1(\mathcal{T}_h)^m \times \mathcal{S}^1_{\rm D}(\mathcal{T}_h)$ in an appropriate neighborhood of u. Our analysis thus shows that the arguments of [13] also apply to higher-dimensional domains and targets under appropriate and meaningful conditions. Some restrictions arise from the simpler functional analytical framework in the discrete setting and the resulting use of inverse estimates to control L^∞ norms.

The outline of the article is as follows. Some preliminaries are stated in Section 2. The main error estimate is derived in Section 3 by verifying the conditions of the inverse function theorem. The application of the analysis to other target manifolds is addressed in Section 4. Numerical experiments that confirm the theoretical results are reported in Section 5.

2. Preliminaries

We use standard notation to denote Lebesgue and Sobolev spaces. The integration domain is often omitted in norms and we abbreviate the inner product and norm in $L^2(\Omega;\mathbb{R}^\ell)$ by $(\cdot,\cdot)$ and $\|\cdot\|$, respectively. Throughout the article $c>0$ denotes a factor that may depend on regularity properties of a fixed solution u but not on the mesh-sizes of a sequence of triangulations; the dependence on u is occasionally indicated via a subindex. We let $c_P>0$ denote the smallest positive number with $\|v\| \le c_P\|\nabla v\|$ for all $v\in H^1_{\rm D}(\Omega)$; we remark that $c_P \le d_\Omega/\pi$ if $\Gamma_{\rm D} = \partial\Omega$ and Ω is a convex domain with diameter d_Ω, cf. [19].

2.1. Finite element functions.

For a regular and quasi-uniform triangulation $\mathcal{T}_h$ of the simplicial domain $\Omega\subset\mathbb{R}^d$ with mesh-size $h>0$ we denote the C^0 conforming finite element space by $\mathcal{S}^1(\mathcal{T}_h)$ of elementwise linear functions. We denote the subspace of functions vanishing on $\Gamma_{\rm D}$ by

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

We let $\mathcal{N}_h$ be the set of vertices of elements and denote the nodal interpolation operator applied to scalar or vector-valued functions by

$$\mathcal{I}_h : C(\overline{\Omega};\mathbb{R}^\ell)\to \mathcal{S}^1(\mathcal{T}_h)^\ell, \quad \mathcal{I}_h v = \sum_{z\in\mathcal{N}_h} v(z)\varphi_z,$$

where $(\varphi_z : z\in\mathcal{N}_h)$ is the scalar nodal basis for $\mathcal{S}^1(\mathcal{T}_h)$. We note that we have the nodal interpolation estimate for $v\in H^1_{\rm D}(\Omega;\mathbb{R}^\ell)$ with $v|_T\in H^2(T)$ for all $T\in\mathcal{T}_h$ that

$$\|v-\mathcal{I}_h v\| + h\|\nabla(v-\mathcal{I}_h v)\| \le ch^2\|D_h^2 v\|,$$

where D_h^2 denotes the elementwise application of the Hessian. For an elementwise poynomial function $\phi_h\in H^1(\Omega)$ we have

$$\|\phi_h - \mathcal{I}_h\phi_h\|_{L^1} \le ch^2\|D_h^2\phi_h\|_{L^1}.$$

We make repeated use of inverse estimates, which read for $v_h\in\mathcal{S}^1_{\rm D}(\mathcal{T}_h)$

$$\|\nabla v_h\|_{L^p} \le ch^{-1}\|v_h\|_{L^p} \tag{2}$$

and, using Sobelev inequalities, with $\gamma_{\rm inv}(h) = 1, 1+|\log h|, h^{-1/2}$ for $d = 1,2,3$, respectively, we moreover have that

$$\|v_h\|_{L^\infty} \le c\gamma_{\rm inv}(h)\|\nabla v_h\|. \tag{3}$$

The estimate can be deduced from elementary local norm equivalences and Sobolev inequalities, i.e.,

$$\|v_h\|_{L^\infty} \le ch^{-d/p}\|v_h\|_{L^p} \le ch^{-d/p}\|\nabla v_h\|$$

with $p\le\infty$, $p<\infty$, and $p\le 2d$, for $d=1,2,3$, respectivly. A precise characterization of the Sobolev embedding is needed if $d=2$, cf. [4], a weaker result for $d = 2$ is obtained with $p = d/\varepsilon$ for fixed $\varepsilon > 0$. A discrete inner product is for $v, w \in C(\overline{\Omega})$ defined via

$$(v, w)_h = \int_\Omega \mathcal{I}_h(v \cdot w)\,\mathrm{d}x = \sum_{z \in \mathcal{N}_h} \beta_z v(z) \cdot w(z),$$

where $\beta_z = \int_\Omega \varphi_z \,\mathrm{d}x$ is positive. For $v_h \in \mathcal{S}^1(\mathcal{T}_h)$ we have $\|v_h\|_h \le \|v_h\| \le c\|v_h\|_h$. We frequently use the following estimate.

Lemma 2.1 (Quadrature control)**.** *For $\psi_h \in \mathcal{S}^1_{\mathrm{D}}(\mathcal{T}_h)$ and $\phi \in C(\overline{\Omega})$ with $\phi|_T \in H^2(T)$ for all $T \in \mathcal{T}_h$ we have*

$$\big|(\psi_h, \phi)_h - (\psi_h, \phi)\big| \le ch^2\big(\|\nabla \psi_h\|\|\nabla \mathcal{I}_h \phi\| + \|\psi_h\|\|D_h^2 \phi\|\big).$$

In case of an elementwise polynomial function $\phi_h \in C(\overline{\Omega})$ we have

$$\big|(\psi_h, \phi_h)_h - (\psi_h, \phi_h)\big| \le ch\|\psi_h\|\|\nabla \phi_h\|.$$

Proof. We have that

$$(\psi_h, \phi)_h - (\psi_h, \phi) = \int_\Omega \mathcal{I}_h(\psi_h \phi) - \psi_h \mathcal{I}_h \phi \,\mathrm{d}x + \int_\Omega \psi_h(\mathcal{I}_h \phi - \phi)\,\mathrm{d}x,$$

and the two terms on the right-hand side are controlled with the L^1 and L^2 nodal interpolation estimates stated above. The second estimate follows from the first one by using the inverse estimate (2) (generalized to elementwise polynomial functions) twice and the H^1 stability of $\mathcal{I}_h$ on elementwise polynomial functions. □

We let $\Pi_h : L^2(\Omega) \to \mathcal{S}^1_{\mathrm{D}}(\mathcal{T}_h)$ denote the L^2 projection onto $\mathcal{S}^1_{\mathrm{D}}(\mathcal{T}_h)$ and by $\widetilde{\Pi}_h : L^2(\Omega) \to \mathcal{S}^1_{\mathrm{D}}(\mathcal{T}_h)$ the modified version given by

$$(\widetilde{\Pi}_h v, \phi_h)_h = (v, \phi_h)$$

for all $\phi_h \in \mathcal{S}^1_{\mathrm{D}}(\mathcal{T}_h)$. We note that Π_h is H^1 stable on quasi-uniform triangulations. The modified projection has similar properties as Π_h.

Lemma 2.2 (Modified L^2 projection)**.** *The projection $\widetilde{\Pi}_h$ satisfies for all $v \in H^1_{\mathrm{D}}(\Omega)$*

$$\|\nabla \widetilde{\Pi} v\| + h^{-1}\|\widetilde{\Pi} v - v\| \le c\|\nabla v\|.$$

Proof. With the standard L^2 projection Π_h onto V_h, define $\delta_h = \widetilde{\Pi} v - \Pi_h v$. We then have

$$\|\delta_h\|^2 \le \|\delta_h\|_h^2 = (\delta_h, \widetilde{\Pi} v - \Pi_h v)_h = (\delta_h, \Pi_h v) - (\delta_h, \Pi_h v)_h.$$

Therefore, using Lemma 2.1, estimate (2), and the H^1-stability of Π_h we find that

$$\|\delta_h\|^2 \le ch^2\|D_h^2(\delta_h \cdot \Pi_h v)\|_{L^1} = ch^2\|\nabla \delta_h\|\|\nabla \Pi_h v\| \le ch\|\delta_h\|\|\nabla v\|.$$

Hence $\|\delta_h\| \le ch\|\nabla v\|$ and another application of an inverse estimate yields $\|\nabla \delta_h\| \le c\|\nabla v\|$. We therefore get

$$\|\nabla \widetilde{\Pi} v\| \le \|\nabla \Pi_h v\| + \|\nabla \delta_h\| \le c\|\nabla v\|.$$

The error estimate follows from a related estimate for Π_h. □

We often use the dual space $H^{-1}(\Omega) = (H^1_{\rm D}(\Omega))'$ which is equipped with the operator norm

$$\|\mu\|_{H^{-1}} = \sup_{\phi \in H^1_{\rm D}(\Omega)\setminus\{0\}} \frac{\langle \mu, \phi\rangle}{\|\nabla \phi\|}.$$

We have the inverse estimate

$$\|\mu_h\| \le c h^{-1} \|\mu_h\|_{H^{-1}}$$

for all $\mu_h \in \mathcal{S}^1_{\rm D}(\mathcal{T}_h)$. The Clément quasi-interpolation operator $\mathcal{J}_h : L^1(\Omega) \to \mathcal{S}^1(\mathcal{T}_h)$ is with the sets $\omega_z = \operatorname{supp} \varphi_z$, $z \in \mathcal{N}_h$, defined via

$$\mathcal{J}_h \alpha = \sum_{z\in\mathcal{N}_h} \alpha_z \varphi_z, \quad \alpha_z = |\omega_z|^{-1} \int_{\omega_z} \alpha \,{\rm d}x.$$

The variant $\mathcal{J}_{h,{\rm D}} : L^1(\Omega) \to \mathcal{S}^1_{\rm D}(\mathcal{T}_h)$ is obtained by setting $\alpha_z = 0$ for all $z \in \mathcal{N}_h \cap \Gamma_{\rm D}$. We remark that we have

$$(\mathcal{J}_{h,{\rm D}}\alpha, v)_h = (\mathcal{J}_h \alpha, v)_h$$

for $v \in C(\overline{\Omega})$ with $v|_{\Gamma_{\rm D}} = 0$. For $\alpha \in H^1(\Omega)$ we have

$$\|\alpha - \mathcal{J}_h\alpha\| \le ch\|\nabla\alpha\|.$$

A similar estimate holds for $\alpha \in H^1_{\rm D}(\Omega)$ and $\mathcal{J}_{h,{\rm D}}\alpha$, cf., e.g., [4].

2.2. **Inverse function theorem.**

As in [11, 13] we use the following quantitative version of the inverse function theorem to derive a local error estimate.

Theorem 2.3 (Inverse function theorem)**.** *Suppose that $F : X \to X'$ is continuous and assume that $\widetilde{x} \in X$ satisfies $\|F(\widetilde{x})\|_{X'} \le \kappa$. If there exist $c'_L, c_{\rm inv}, \varepsilon > 0$ such that F is Fréchet differentiable in $B_\varepsilon(\widetilde{x})$, with $DF(\widetilde{x})$ invertible, and*

$$\|DF(\widetilde{x})^{-1}\|_{L(X',X)} \le c_{\rm inv},$$
$$\|DF(x_1) - DF(x_2)\|_{L(X,X')} \le c'_L \|x_1 - x_2\|_X$$

for all $x_1, x_2 \in B_\varepsilon(\widetilde{x})$ with $\varepsilon > 0$ so that $c'_L c_{\rm inv}\varepsilon \le 1/2$ and $\kappa \le \varepsilon/(2c_{\rm inv})$, then there exists a unique $x \in B_\varepsilon(\widetilde{x})$ such that $F(x) = 0$.

Proof. The result is an immediate conseqence of the proof of [7, Thm. 3.1.5, p. 113]. □

We remark that if F is defined on an affine space $\mathcal{A} = x_{\rm D} + X$ then the theorem can be applied to $\widetilde{F}(x) = F(x_{\rm D} + x)$. The theorem also implies the superlinear convergence of the Newton-type iteration $x^{k+1} = x^k - DF(\widetilde{x})^{-1}F(x^k)$ and of the classical Newton iteration if a bound on the the inverse of the Jacobian holds in $B_\varepsilon(\widetilde{x})$. For quadratic convergence, a bound on the second variation of F is required.

3. Error estimate

We recall that harmonic maps into spheres are defined as stationary pairs $(u, \lambda) \in \mathcal{A}$ for the functional

$$L(u, \lambda) = \frac{1}{2}\int_\Omega |\nabla u|^2 \,\mathrm{d}x + \frac{1}{2}\langle \lambda, |u|^2 - 1\rangle$$

An optimal pair satisfies the Euler–Lagrange equations (1) with

$$\lambda = -|\nabla u|^2.$$

A finite element approximation is sought in the space of admissible pairs

$$\mathcal{A}_h = (u_{\mathrm{D},h}, 0) + X_h,$$

with $u_{\mathrm{D},h} = \mathcal{I}_h \widetilde{u}_{\mathrm{D}}$ for a continuous extension $\widetilde{u}_{\mathrm{D}}$ of u_{D} and the homogeneous space X_h defined via

$$X_h = \mathcal{S}^1_{\mathrm{D}}(\mathcal{T}_h)^m \times \mathcal{S}^1_{\mathrm{D}}(\mathcal{T}_h) \subset H^1_{\mathrm{D}}(\Omega; \mathbb{R}^m) \times H^{-1}(\Omega).$$

Here, no uniform bounds are included in the definition of X_h in order to have a Hilbert space structure. Discrete harmonic maps are stationary configurations for the functional

$$L_h(u_h, \lambda_h) = \frac{1}{2}\int_\Omega |\nabla u_h|^2 \,\mathrm{d}x + \frac{1}{2}\int_\Omega \mathcal{I}_h\big[\lambda_h(|u_h|^2 - 1)\big] \,\mathrm{d}x.$$

Discrete harmonic maps $(u_h, \lambda_h) \in \mathcal{A}_h$ satisfy, cf. [13, 4],

$$\begin{aligned}(\nabla u_h, \nabla v_h) + (\lambda_h, u_h \cdot v_h)_h &= 0,\\ (\mu_h, |u_h|^2 - 1)_h &= 0,\end{aligned}$$

for all $(v_h, \mu_h) \in X_h$. The saddle-point system can be formulated as a nonlinear equation with a mapping $F_h : \mathcal{A}_h \to X_h'$ via

$$F_h(u_h, \lambda_h)[(v_h, \mu_h)] = (\nabla u_h, \nabla v_h) + (\lambda_h, u_h \cdot v_h)_h + (\mu_h, |u_h|^2 - 1)_h.$$

The variational derivative of F_h is given by

$$\begin{aligned}DF_h(u_h, \lambda_h)[(v_h, \mu_h),(w_h, \eta_h)] &= (\nabla v_h, \nabla w_h)\\ &\quad + (\lambda_h, w_h \cdot v_h)_h + (\mu_h, u_h \cdot w_h)_h + (\eta_h, u_h \cdot v_h).\end{aligned}$$

To investigate the invertibility of the linear operator $DF_h(\widetilde{u}_h, \widetilde{\lambda}_h) : X_h \to X_h'$ we resort to established theories for linear saddle-point problems on Hilbert spaces and define for a given pair $(\widetilde{u}_h, \widetilde{\lambda}_h)$ the bilinear forms

$$\begin{aligned}a_{\widetilde{\lambda}_h}(v_h, w_h) &= (\nabla v_h, \nabla w_h) + (\widetilde{\lambda}_h, w_h \cdot v_h)_h,\\ b_{\widetilde{u}_h}(\mu_h, v_h) &= (\mu_h, \widetilde{u}_h \cdot v_h)_h,\end{aligned} \tag{4}$$

for all $v_h, w_h \in \mathcal{S}^1_{\mathrm{D}}(\mathcal{T}_h)^m$ and $\mu_h \in \mathcal{S}^1_{\mathrm{D}}(\mathcal{T}_h)$. The invertibility is equivalent to the existence of a unique solution $(v_h, \mu_h) \in X_h$ for every right-hand side $(f_h, g_h) \in X_h'$ such that

$$\begin{aligned}a_{\widetilde{\lambda}_h}(v_h, w_h) + b_{\widetilde{u}_h}(\mu_h, w_h) &= (f_h, w_h),\\ b_{\widetilde{u}_h}(\eta_h, v_h) &= (g_h, \eta_h),\end{aligned}$$

for all $(w_h,\eta_h)\in X_h$. Sufficient for this is that $a_{\widetilde{\lambda}_h}$ is coercive on the kernel of $b_{\widetilde{u}_h}$ and that $b_{\widetilde{u}_h}$ satisfies an inf-sup condition, cf. [2, 9].

Lemma 3.1 (Invertibility)**.** *(i) For every $\widetilde{u}_h\in\mathcal{S}^1(\mathcal{T}_h)^m$ the bilinear form $b_{\widetilde{u}_h}$ satisfies the inf-sup condition*

$$\sup_{v_h\in\mathcal{S}^1_{\rm D}(\mathcal{T}_h)^m\setminus\{0\}}\frac{b_{\widetilde{u}_h}(\mu_h,v_h)}{\|\nabla v_h\|}\ge c\|\widetilde{u}_h\|^{-1}_{W^{1,\infty}}\|\mu_h\|_{H^{-1}}$$

for all $\mu_h\in\mathcal{S}^1_{\rm D}(\mathcal{T}_h)$. Moreover $b_{\widetilde{u}_h}$ is continuous with bound $c\|\widetilde{u}_h\|_{W^{1,\infty}}$.
(ii) Assume that the the pair $(u,\lambda)\in\mathcal{A}$ satisfies

$$u\in H^2(\Omega;\mathbb{R}^m)\cap W^{1,\infty}(\Omega;\mathbb{R}^m),\quad \lambda\in H^1(\Omega)\cap L^\infty(\Omega), \tag{5}$$

and that there exists $c_a>0$ such that

$$a_\lambda(v,v)\ge c_a\|\nabla v\|^2\quad\text{for all } v\in T_u. \tag{6}$$

Define $(\widetilde{u}_h,\widetilde{\lambda}_h)\in\mathcal{A}_h$ via

$$\widetilde{u}_h=\mathcal{I}_hu,\quad \widetilde{\lambda}_h=\mathcal{J}_{h,\rm D}\lambda.$$

Then for h sufficiently small we have

$$a_{\widetilde{\lambda}_h}(v_h,v_h)\ge(c_a/2)\|\nabla v_h\|^2$$

for all $v_h\in\mathcal{S}^1_{\rm D}(\mathcal{T}_h)^m)$ with $\mathcal{I}_h(v_h\cdot\widetilde{u}_h)=0$. Moreover, $a_{\widetilde{\lambda}_h}$ is continuous with bound $c\|\widetilde{\lambda}_h\|$.
(iii) Under the conditions of (ii) the operator $DF_h(\widetilde{u}_h,\widetilde{\lambda}_h)$ is invertible with $\|DF_h(\widetilde{u}_h,\widetilde{\lambda}_h)\|_{L(X_h',X_h)}\le c_{\rm inv}$ for a constant $c_{\rm inv}>0$ that depends on $\|u\|_{W^{1,\infty}}$, $\|\lambda\|$, and c_a. The smallness condition on h additionally depends on $\|\nabla\lambda\|$ and $\|D^2u\|$.

Proof. (i) To verify the inf-sup condition for $b_{\widetilde{\lambda}_h}$ we follow [13] and note that the Hahn–Banach theorem implies that for given $\mu_h\in\mathcal{S}^1_{\rm D}(\mathcal{T}_h)$ there exists $\phi\in H^1_{\rm D}(\Omega)$ with $\|\nabla\phi\|=1$ and

$$(\mu_h,\phi)=\|\mu_h\|_{H^{-1}}.$$

With the modified L^2 projection $\widetilde{\Pi}_h$ we define

$$v_h=\mathcal{I}_h((\widetilde{\Pi}_h\phi)\widetilde{u}_h).$$

Since $|\widetilde{u}_h(z)|^2=1$ for all $z\in\mathcal{N}_h$ this choice implies that we have

$$b_{\widetilde{u}_h}(\mu_h,v_h)=(\mu_h,(\widetilde{\Pi}_h\phi)\widetilde{u}_h\cdot\widetilde{u}_h)_h=(\mu_h,\widetilde{\Pi}_h\phi)_h=(\mu_h,\phi)=\|\mu_h\|_{H^{-1}}.$$

Using the H^1-stability of $\mathcal{I}_h$ on elementwise polynomials and the H^1 stability of $\widetilde{\Pi}_h$ on quasi-uniform meshes, we find that

$$\|\nabla v_h\|\le c\|\nabla((\widetilde{\Pi}_h\phi)\widetilde{u}_h)\|\le c\|\nabla\widetilde{\Pi}_h\phi\|\|\widetilde{u}_h\|_{W^{1,\infty}}\le c\|\nabla\phi\|\|\widetilde{u}_h\|_{W^{1,\infty}},$$

i.e., $\|\nabla v_h\|\|\widetilde{u}_h\|^{-1}_{W^{1,\infty}}\le c$. Combining the last two estimates leads to

$$b_{\widetilde{u}_h}(\mu_h,v_h)\ge c\|\widetilde{u}_h\|^{-1}_{W^{1,\infty}}\|\nabla v_h\|\|\mu_h\|_{H^{-1}},$$

which is the asserted inf-sup property. Using Lemma 2.1 and an inverse estimate, we verify the boundedness of $b_{\widetilde{u}_h}$, i.e.,

$$\begin{aligned} |b_{\widetilde{u}_h}(\mu_h, v_h)| &\le |(\mu_h, \widetilde{u}_h \cdot v_h)| + ch\|\mu_h\|\|\nabla(\widetilde{u}_h \cdot v_h)\| \\ &\le \|\mu_h\|_{H^{-1}}\|\widetilde{u}_h\|_{W^{1,\infty}}\|\nabla v_h\|, \end{aligned}$$

(ii) Given $v_h \in \mathcal{S}^1_{\mathrm{D}}(\mathcal{T}_h)^m$ with $\mathcal{I}_h(v_h \cdot \widetilde{u}_h) = 0$ the function

$$\widetilde{v}^h = v_h - (v_h \cdot u)u$$

satisfies $\widetilde{v}^h \in T_u$ and hence we have $a_\lambda(\widetilde{v}^h, \widetilde{v}^h) \ge c_a\|\nabla \widetilde{v}^h\|^2$. Using that we may replace $\widetilde{\lambda}_h$ by $\mathcal{J}_h\lambda$ in $a_{\widetilde{\lambda}_h}$, Lemma 2.1 and (3) lead to

$$\big|(\widetilde{\lambda}_h, |v_h|^2)_h - (\mathcal{J}_h\lambda, |v_h|^2)\big| \le ch\gamma_{\mathrm{inv}}(h)\|\mathcal{J}_h\lambda\|\|\nabla v_h\|^2.$$

With this estimate we find that

$$\begin{aligned} &\big|a_{\widetilde{\lambda}_h}(v_h,v_h) - a_\lambda(\widetilde{v}^h, \widetilde{v}^h)\big| \\ &\quad\le \|\nabla(v_h - \widetilde{v}^h)\|\big(\|\nabla v_h\| + \|\nabla \widetilde{v}^h\|\big) + ch\gamma_{\mathrm{inv}}(h)\|\mathcal{J}_h\lambda\|\|\nabla v_h\|^2 \\ &\qquad + \|\mathcal{J}_h\lambda\|\|v_h - \widetilde{v}_h\|_{L^4}\big(\|v_h\|_{L^4} + \|\widetilde{v}^h\|_{L^4} + \|\mathcal{J}_h\lambda - \lambda\|\|\widetilde{v}^h\|^2_{L^4}\big). \end{aligned}$$

To bound the terms on the right-hand side we note that $\mathcal{I}_h((v_h \cdot u)u) = 0$ and hence

$$\begin{aligned} \|\nabla(v_h - \widetilde{v}^h)\| &\le ch\|D^2_h((v_h \cdot u)u)\| \\ &\le ch\big(\|\nabla v_h\|\|\nabla u\|_{L^\infty} + \|v_h\|_{L^\infty}(\|D^2 u\| + \|\nabla u\|^2_{L^\infty})\big) \\ &\le ch\gamma_{\mathrm{inv}}(h)\|\nabla v_h\|. \end{aligned}$$

A Sobolev embedding and a Poincaré inequality show that the same bound applies to $\|v_h - \widetilde{v}^h\|_{L^4}$. Moreover, we have that

$$\|\widetilde{v}^h\| + \|\nabla \widetilde{v}^h\| + \|\widetilde{v}^h\|_{L^4} + \|v_h\|_{L^4} \le c\|\nabla v_h\|.$$

Noting stability and approximation properties of the Clément quasi-interpolant, the combination of the estimates implies that

$$a_{\widetilde{\lambda}_h}(v_h, v_h) \ge a_\lambda(\widetilde{v}^h, \widetilde{v}^h) - ch\gamma_{\mathrm{inv}}(h)\|\nabla v_h\|^2,$$

which is the asserted coercivity property. Finally, as a consequence of Lemma 2.1 and inverse estimates, $a_{\widetilde{\lambda}_h}$ satisfies the bound

$$\begin{aligned} |a_{\widetilde{\lambda}_h}(v_h, w_h)| &\le \|\nabla v_h\|\|\nabla w_h\| + |(\widetilde{\lambda}_h, v_h \cdot w_h)| + ch\|\widetilde{\lambda}_h\|\|\nabla(v_h \cdot w_h)\| \\ &\le (1 + ch\gamma_{\mathrm{inv}}(h))\|\widetilde{\lambda}_h\|\|\nabla v_h\|\|\nabla w_h\|. \end{aligned}$$

(iii) The inf-sup condition for $b_{\widetilde{u}_h}$ and the coercivity of $a_{\widetilde{\lambda}_h}$ on the kernel of $b_{\widetilde{u}_h}$, which is given by $\ker b_{\widetilde{u}_h} = \{v_h \in \mathcal{S}^1_{\mathrm{D}}(\mathcal{T}_h)^m : \mathcal{I}_h(v_h \cdot \widetilde{u}_h) = 0\}$ imply the invertibility of $DF(\widetilde{u}_h, \widetilde{\lambda}_h)$, cf. [2, 9]. The $W^{1,\infty}$ stability of $\mathcal{I}_h$ and the L^2 stability of $\mathcal{J}_h$ imply that the bounds on $DF(\widetilde{u}_h, \widetilde{\lambda}_h)$ depend on $\|u\|_{W^{1,\infty}}$ and $\|\lambda\|$. □

The second auxiliary result bounds the operator norm of $F(\widetilde{u}_h, \widetilde{\lambda}_h)$ for interpolants of a regular harmonic map (u, λ).

Lemma 3.2 (Residual of interpolants)**.** *Assume that a harmonic map $(u, \lambda) \in \mathcal{A}$ satisfies* (5) *and define $(\widetilde{u}_h, \widetilde{\lambda}_h) \in \mathcal{A}_h$ via $\widetilde{u}_h = \mathcal{I}_h u$ and $\widetilde{\lambda}_h = \mathcal{J}_{h,\mathrm{D}} \lambda$. We then have that*

$$\big|F_h(\widetilde{u}_h, \widetilde{\lambda}_h)[(v_h, \mu_h)]\big| \le ch \|(v_h, \mu_h)\|_{X_h},$$

where c depends on $\|D^2 u\|$ and $\|u\|_{W^{1,\infty}}$.

Proof. The pair (u, λ) satisfies for all $(v, \mu) \in X$ the identity $F(u, \lambda)[(v, \mu)] = 0$, where

$$F(u, \lambda)[(v, \mu)] = (\nabla u, \nabla v) + (\lambda, u \cdot v) + (\mu, |u|^2 - 1).$$

Since $X_h \subset X$ we thus have that

$$\begin{aligned}
\big|F_h(\widetilde{u}_h, \widetilde{\lambda}_h)[(v_h, \mu_h)]\big| &= \big|F_h(\widetilde{u}_h, \widetilde{\lambda}_h)[(v_h, \mu_h)] - F(u, \lambda)[(v_h, \mu_h)]\big| \\
&\le \big|(\nabla[\widetilde{u}_h - u], \nabla v_h)\big| + \big|(\widetilde{\lambda}_h, \widetilde{u}_h \cdot v_h)_h - (\lambda, u \cdot v_h)\big| = I + II,
\end{aligned}$$

where we used that $|u|^2 = \mathcal{I}_h |\widetilde{u}_h|^2 = 1$, so that contributions involving μ_h vanish. For the first term we deduce with nodal interpolation estimates that

$$I \le ch \|D^2 u\| \|\nabla v_h\|.$$

To bound the second term we first note that $\widetilde{u}_h \cdot v_h|_{\Gamma_\mathrm{D}} = 0$ so that we may replace $\widetilde{\lambda}_h$ by $\mathcal{J}_h \lambda$. With Lemma 2.1, inverse estimates, and $\widetilde{u}_h = \mathcal{I}_h u$, we find that

$$\begin{aligned}
II &\le \big|(\mathcal{J}_h \lambda, \widetilde{u}_h \cdot v_h)_h - (\mathcal{J}_h \lambda, u \cdot v_h)\big| + \big|(\mathcal{J}_h \lambda, u \cdot v_h)) - (\lambda, u \cdot v_h)\big| \\
&\le ch^2 \big(\|\nabla \mathcal{J}_h \lambda\| \|\nabla \mathcal{I}_h (u \cdot v_h)\| + \|\mathcal{J}_h \lambda\| \|D_h^2 (u \cdot v_h)\|\big) + ch \|\nabla \lambda\| \|u \cdot v_h\| \\
&\le ch \|\nabla v_h\| \|\lambda\|_{H^1} \big(\|u\|_{W^{1,\infty}} + \|D^2 u\|\big).
\end{aligned}$$

The combination of the estimates implies the result. ☐

To derive an error estimate using the inverse function theorem a local Lipschitz continuity property for DF_h is required.

Lemma 3.3 (Lipschitz estimate)**.** *For all $(u_h, \lambda_h), (\widetilde{u}_h, \widetilde{\lambda}_h) \in \mathcal{A}_h$ we have*

$$\begin{aligned}
&\big|DF_h(u_h, \lambda_h)[(v_h, \mu_h), (w_h, \eta_h)] - DF_h(\widetilde{u}_h, \widetilde{\lambda}_h)[(v_h, \mu_h), (w_h, \eta_h)]\big| \\
&\quad \le c \gamma_{\mathrm{inv}}(h) \|(u_h - \widetilde{u}_h, \lambda_h - \widetilde{\lambda}_h)\|_{X_h} \|(v_h, \mu_h)\|_{X_h} \|(w_h, \eta_h)\|_{X_h}.
\end{aligned}$$

Proof. We have

$$\begin{aligned}
&\big|DF_h(u_h, \lambda_h)[(v_h, \mu_h), (w_h, \eta_h)] - DF_h(\widetilde{u}_h, \widetilde{\lambda}_h)[(v_h, \mu_h), (w_h, \eta_h)]\big| \\
&\quad \le \big|(\lambda_h - \widetilde{\lambda}_h, w_h \cdot v_h)_h\big| + \big|(\mu_h, [u_h - \widetilde{u}_h] \cdot w_h)_h\big| + \big|(\eta_h, [u_h - \widetilde{u}_h] \cdot v_h)_h\big|.
\end{aligned}$$

To estimate the terms on the right-hand side we consider the first term and use Lemma 2.1 and inverse estimates to deduce that

$$\begin{aligned}\big|(\lambda_h - \widetilde{\lambda}_h, w_h \cdot v_h)_h\big| &\le \big|(\lambda_h - \widetilde{\lambda}_h, w_h \cdot v_h)\big| + ch\|(\lambda_h - \widetilde{\lambda}_h)\|\|\nabla(w_h \cdot v_h)\| \\ &\le c\|\lambda_h - \widetilde{\lambda}_h\|_{H^{-1}}\|\nabla(w_h \cdot v_h)\| \\ &\le c\gamma_{\rm inv}(h)\|\lambda_h - \widetilde{\lambda}_h\|_{H^{-1}}\|\nabla w_h\|\|\nabla v_h\|.\end{aligned}$$

The other terms are estimated analogously. □

The quasi-optimal error estimate results from an application of the inverse function theorem, cf. Theorem 2.3.

Theorem 3.4 (Error estimate)**.** *Let $u \in H^1(\Omega;\mathbb{R}^m)$ be a harmonic map such that with $\lambda = -|\nabla u|^2$ the pair $(u,\lambda) \in \mathcal{A}$ satisfies (5) and (6). Then, for h sufficiently small, there exists a unique solution $(u_h,\lambda_h) \in \mathcal{A}_h$ for $F_h(u_h,\lambda_h) = 0$ in a neighborhood $B_\varepsilon(u,\lambda)$ with $\varepsilon = c\gamma_{\rm inv}(h)^{-1}$ that satisfies*

$$\|\nabla(u - u_h)\| + \|\lambda - \lambda_h\|_{H^{-1}} \le c_u h.$$

Proof. (i) We verify the conditions of the inverse function theorem. Letting $(\widetilde{u}_h, \widetilde{\lambda}_h) = (\mathcal{I}_h u, \mathcal{J}_{h,\mathrm{D}}\lambda)$ we have the smallness result from Lemma 3.2 with $\kappa = c_u h$, the Lipschitz estimate from Lemma 3.3 with $c_L = c_u\gamma_{\rm inv}(h)$, the invertibility result from Lemma 3.1 with $c_{\rm inv} = c_u$. Hence, within $B_\varepsilon(\widetilde{u}_h, \widetilde{\lambda}_h)$ for every $\varepsilon > 0$ with $c_u h \le \varepsilon \le c'_u\gamma_{\rm inv}(h)^{-1}$ there exists a unique solution $(u_h,\lambda_h) \in X_h$ with $F_h(u_h,\lambda_h) = 0$.
(ii) To derive the error estimate we first note that we may choose $\varepsilon = c_h h$ so that

$$\|\nabla(u_h - \widetilde{u}_h)\| + \|\lambda_h - \widetilde{\lambda}_h\|_{H^{-1}} \le ch.$$

We have $\|\nabla(u - \widetilde{u}_h)\| \le ch$. To bound the quasi-interpolation error $\|\lambda - \widetilde{\lambda}_h\|_{H^{-1}}$ we define $\delta_h = \mathcal{J}_{h,\mathrm{D}}\lambda - \mathcal{J}_h\lambda$ and note that

$$(\delta_h, \phi) = (\delta_h, \phi - \mathcal{J}_{h,\mathrm{D}}\phi) + (\delta_h, \mathcal{J}_{h,\mathrm{D}}\phi) - (\delta_h, \mathcal{J}_{h,\mathrm{D}}\phi)_h,$$

where we used that the last term vanishes. With estimates for the Clément quasi-interpolant and Lemma 2.1 we deduce that

$$|(\delta_h, \phi)| \le ch\|\delta_h\|\|\nabla\phi\| + ch\|\delta_h\|\|\nabla\mathcal{J}_{h,\mathrm{D}}\phi\|.$$

Inverse estimates and H^1 and L^2 stability properties of the Clément quasi-interpolant $\mathcal{J}_{h,\mathrm{D}}$ thus imply that

$$\|\delta_h\|_{-1} \le ch\|\delta_h\| \le ch\|\lambda\|.$$

Noting $\|\lambda - \mathcal{J}_h\lambda\| \le ch\|\nabla\lambda\|$ we find that $\|\lambda - \mathcal{J}_{h,\mathrm{D}}\lambda\|_{H^{-1}} \le ch$, which implies the error estimate. □

4. Other target manifolds

To discuss the validity of the theory in case of other target manifolds we consider a hypersurface $\mathcal{M} \subset \mathbb{R}^m$ given as the zero level set of a twice continuously differentiable function $g : \mathbb{R}^m \to \mathbb{R}$, i.e.,

$$\mathcal{M} = \{s \in \mathbb{R}^m : g(s) = 0\}.$$

We assume that Dg is nonvanishing on $\mathcal{M}$; the kernel of Dg defines the tangent space of $\mathcal{M}$. Harmonic maps into $\mathcal{M}$ are then defined as stationary configurations $(u, \lambda) \in \mathcal{A}$ for the Lagrange functional

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

where the last term is interpreted as the application of λ to $g(u)$. Stationary points (u, λ) satisfy $F(u, \lambda) = 0$, where

$$F(u, \lambda)[(v, \mu)] = (\nabla u, \nabla v) + (\lambda, Dg(u) \cdot v) + \langle \mu, g(u) \rangle.$$

Crucial for the application of the inverse function theorem are the invertibility and continuity properties of the second variation of I given by

$$\begin{aligned} DF(u, \lambda)[(v, \mu), (w, \eta)] = (\nabla v, \nabla w) &+ (\lambda, D^2 g(u)[v, w]) \\ &+ \langle \mu, Dg(u) \cdot w \rangle + \langle \eta, Dg(u) \cdot v \rangle. \end{aligned}$$

The invertibility of DF can be analyzed as in the case of the unit sphere using $v_h = \mathcal{I}_h((\widetilde{\Pi}_h \phi)|Dg(u)|^{-2} Dg(u))$ to establish the inf-sup condition. A local Lipschitz continuity property requires bounding the difference

$$\begin{aligned} &\big|\langle \lambda, D^2 g(u)[v, w] \rangle - \langle \widetilde{\lambda}, D^2 g(\widetilde{u})[v, w] \rangle\big| \\ &\qquad \le \|\lambda - \widetilde{\lambda}\|_{H^{-1}} \|\nabla (D^2 g(u)[v, w])\| \\ &\qquad\quad + \|\widetilde{\lambda}\|_{H^{-1}} \|\nabla ((D^2 g(u) - D^2 g(\widetilde{u}))[v, w])\|. \end{aligned} \tag{7}$$

We have, e.g.,

$$\begin{aligned} \|\nabla (D^2 g(u)[v, w])\| \le \|D^3 g(u)\|_{L^\infty} &\|\nabla u\| \|v\|_{L^\infty} \|w\|_{L^\infty} \\ &+ c\|D^2 g(u)\|_{L^\infty} \|\nabla v\| \|\nabla w\|. \end{aligned}$$

Bounding the first term on the right-hand side in a discrete setting using the H^1_{D} norms of v and w requires applying the inverse estimate (3) twice, which leads to $c_L' \le c\gamma_{\mathrm{inv}}(h)^2$. If $d = 1$ or $d = 2$ this still allows us to apply the inverse function theorem, cf. [13], while if $d = 3$ it is in general not guaranteed that $2c_{\mathrm{inv}}\kappa \le 1/(2c_{\mathrm{inv}} c_L')$ as both, $\gamma_{\mathrm{inv}}(h)^{-2}$ and κ, are of order $O(h)$. A positive case corresponds to boundaries of ellipsoids for which g can be chosen as a quadratic function so that $D^2 g$ is constant and the right-hand side in (7) simplifies. Slightly more general, it suffices to require that $D^3 g$ is sufficiently small and assuming that we have the additional regularity property $u \in W^{2,\infty}(\Omega; \mathbb{R}^m)$.

5. Numerical experiments

In this section we experimentally investigate the validity of the error estimate and the related aspect of the convergence properties of the Newton scheme for nonsingular S^2-valued harmonic maps in two- and three-dimensional settings. The first example is obtained from the stereographic projection.

Example 5.1 (Inverse stereographic projection). *Let $d = 2$ and $\Omega = (-1/2, 1/2)^2$, $\Gamma_{\mathrm{D}} = \partial\Omega$, and $u_{\mathrm{D}} = \pi_{\mathrm{st}}^{-1}|_{\partial\Omega}$ with the inverse stereographic projection $\pi_{\mathrm{st}}^{-1} : \Omega \to S^2$ given for $x \in \Omega$ by*

$$\pi_{\mathrm{st}}^{-1}(x) = (|x|^2 + 1)^{-1} \begin{bmatrix} 2x \\ 1 - |x|^2 \end{bmatrix}.$$

Then $u = \pi_{\mathrm{st}}^{-1}$ is a harmonic map with $u|_{\partial\Omega} = u_{\mathrm{D}}$.

The second example considers the prototypical harmonic map $x \mapsto x/|x|$, $x \in \mathbb{R}^3$, away from the origin to avoid a singular solution.

Example 5.2 (Radial projection). *Let $d = 3$, $\Omega = (-1/2, 1/2)^3$, $\Gamma_{\mathrm{D}} = \partial\Omega$, and for $s = 0.9e_3$ and and $x \in \partial\Omega$*

$$u_{\mathrm{D}}(x) = \frac{x - s}{|x - s|}.$$

Then $u(x) = (x - s)/|x - s|$ is a harmonic map with $u|_{\partial\Omega} = u_{\mathrm{D}}$.

The sufficient condition for global H^1 coercivity $|\nabla u| < c_P^{-1} \le \pi$ is satisfied in the first and violated in the second example. Visualizations of numerical solutions for the examples are displayed in Figure 1; they illustrate that the cut-locus condition is satisfied in both cases. To iteratively compute discrete harmonic maps, we use the Newton scheme which computes for an initial pair $(u_h^0, \lambda_h^0) \in \mathcal{A}_h$ the iterates $(u_h^k, \lambda_h^k) \in \mathcal{A}_h$ via the corrections $(d_h^k, \delta_h^k) \in X_h$ that solve

$$DF_h(u_h^k, \lambda_h^k)[(v_h, \mu_h), (d_h^k, \delta_h^k)] = -F_h(u_h^k, \lambda_h^k)[v_h, \mu_h]$$

for all $(v_h, \mu_h) \in X_h$ and the update

$$(u_h^{k+1}, \lambda_h^{k+1}) = (u_h^k, \lambda_h^k) + (d_h^k, \delta_h^k),$$

until $\|\nabla d_h^k\| + \|\delta_h^k\| \le \varepsilon_{\mathrm{stop}}$. We always use $\varepsilon_{\mathrm{stop}} = 10^{-10}$ and denote the final output by (u_h, λ_h).

5.1. **Experimental convergence rates.** We use sequences of uniformly refined triangulations of the domains $\Omega = (-1/2, 1/2)^d$ into triangles or tetrahedra obtained from ℓ uniform refinements and with maximal mesh sizes h_ℓ comparable to $2^{-\ell}$. We refer to these triangulations and quantities related to it via an index ℓ instead of h_ℓ. We computed approximate solutions in Examples 5.1 and 5.2 and determined the discrete approximation errors

$$\|e_\ell\|_X = \|\nabla(u_\ell - \mathcal{I}_\ell u)\| + \|\lambda_\ell - \mathcal{I}_{\ell,\mathrm{D}}\lambda\|_{H_h^{-1}},$$

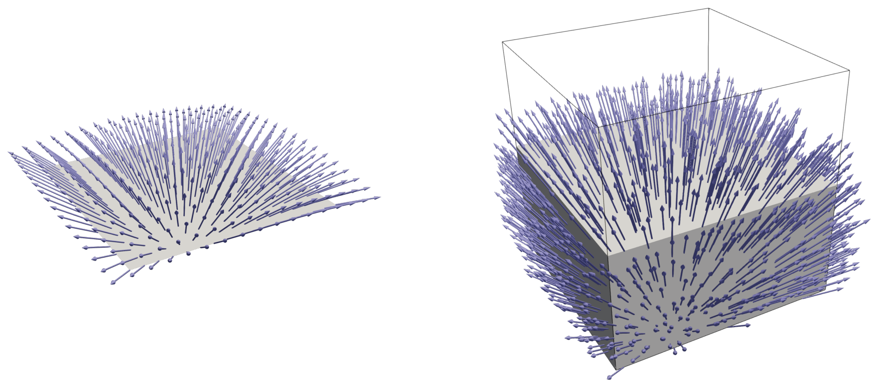

FIGURE 1. Numerical solutions in Examples 5.1 (left) and 5.2 (right).

as well as the approximation errors of the Lagrange multiplier in L^2 and H^{-1} norms, i.e.,

$$\|e_\ell^\lambda\| = \|\lambda_\ell - \mathcal{I}_{\ell,\mathrm{D}}\lambda\|, \quad \|e_\ell^\lambda\|_{H^{-1}} = \|\lambda_\ell - \mathcal{I}_{\ell,\mathrm{D}}\lambda\|_{H_h^{-1}}.$$

Here, $\mathcal{I}_{\ell,\mathrm{D}}$ denotes the nodal interpolant with vanishing nodal values on Γ_D. We approximated the H^{-1} norm of a finite element function $\mu_h \in \mathcal{S}^1_\mathrm{D}(\mathcal{T}_h)$ by the equivalent quantity $\|\mu_h\|_{H_h^{-1}} = \|\nabla(-\Delta_{h,\mathrm{D}})^{-1}\mu_h\|$ with the finite element approximation $(-\Delta_{h,\mathrm{D}})^{-1}$ of the inverse of the negative Laplace operator subject to homogeneous Dirichlet boundary conditions on Γ_D. Experimental convergence rates for an error quantity δ_ℓ were determined via the logarithmic slopes given by

$$\mathrm{eoc}(\delta_\ell) = \frac{\log\big(\delta_\ell/\delta_{\ell-1}\big)}{\log(h_\ell/h_{\ell-1})}.$$

For sequences of uniform triangulations in two dimensions obtained from red refinements of the triangles we have $h_\ell/h_{\ell-1} = 1/2$. Table 1 displays the full approximation errors for a sequence of uniform triangulations with nodes $\mathcal{N}_\ell$ and the experimental convergence rates for different error quantities. We observe a superconvergence phenomenon in the form of a quadratic rate for the full approximation error. The discrete Lagrange multipliers converge with respect to the L^2 norm with the suboptimal experimental rate approximately 0.5. The same quantities were computed on a sequence of uniformly refined triangulations with reduced symmetry properties. These were obtained by randomly perturbing the midpoints of edges that define the vertices of new triangles. The results shown in Table 2 reveal that this eliminates the superconvergence phenomenon. Because of the higher complexity of three-dimensional triangulations and the lack of symmetry properties of the exact solution a larger preasymptotic range is expected in the three-dimensional setting of Example 5.2. The results shown in Table 3 indicate a tendency to a linear convergence behavior on the employed sequence of unperturbed uniform triangulations; the Lagrange multipliers appear to converge at optimal rates in H^{-1} as well as in L^2.

ℓ	$\#\mathcal{N}_\ell$	$\|e_\ell\|_X$	eoc($\|e_\ell^\lambda\|$)	eoc($\|e_\ell^\lambda\|_{H_h^{-1}}$)	eoc($\|e_\ell\|_X$)
1	9	2.000e−1	0.	0.	0.
2	25	6.632e−2	4.150e−1	1.916	1.593
3	81	1.726e−2	4.643e−1	1.960	1.942
4	289	4.360e−3	4.840e−1	1.990	1.985
5	1089	1.093e−3	4.925e−1	1.997	1.996
6	4225	2.734e−4	4.964e−1	1.999	1.999
7	16641	6.835e−5	4.983e−1	2.000	2.000

Table 1. Approximation errors and experimental convergence rates in Example 5.1 on a sequence of uniformly refined triangulations consisting of right-angled triangles. A superconvergence phenomenon is observed for the full approximation error, suboptimal convergence occurs for the Lagrange multiplier in L^2.

ℓ	$\#\mathcal{N}_\ell$	$\|e_\ell\|_X$	eoc($\|e_\ell^\lambda\|$)	eoc($\|e_\ell^\lambda\|_{H_h^{-1}}$)	eoc($\|e_\ell\|_X$)
1	9	2.242e−1	0.	0.	0.
2	25	5.963e−2	4.724e−1	3.057	2.228
3	81	2.498e−2	5.244e−1	1.151	1.392
4	289	1.068e−2	4.914e−1	1.361	1.319
5	1089	5.363e−3	5.333e−1	1.173	1.176
6	4225	2.967e−3	5.298e−1	9.452e−1	9.128e−1
7	16641	1.427e−3	5.178e−1	1.182	1.190

Table 2. Approximation errors and experimental convergence rates in Example 5.1 on a sequence of uniformly refined triangulations consisting of perturbed right-angled triangles. No superconvergence phenomenon occurs and the theoretically predicted rates are confirmed, suboptimal convergence occurs for the Lagrange multiplier in L^2.

ℓ	$\#\mathcal{N}_\ell$	$\|e_\ell\|_X$	eoc($\|e_\ell^\lambda\|$)	eoc($\|e_\ell^\lambda\|_{H_h^{-1}}$)	eoc($\|e_\ell\|_X$)
1	27	1.241e−1	0.	0.	0.
2	125	1.424e−1	3.616e−1	−9.108e−1	−2.807e−1
3	729	1.452e−1	1.690e−1	2.700e−1	−4.193e−2
4	4913	1.095e−1	−6.774e−1	7.368e−1	8.583e−1
5	35937	7.788e−2	−7.586e−1	6.733e−1	7.197e−1

Table 3. Approximation errors and experimental convergence rates in the three-dimensional setting of Example 5.2 on a sequence of uniformly refined triangulations.

5.2. **Iteration convergence.** The conditions of the inverse function theorem imply the superlinear convergence of Newton type iterations provided that the starting value is sufficiently close to the solution. In order to experimentally determine the size of this neighborhood and to quantify the convergence speed, we use oscillating perturbations of the nodal interpolants of the exact solutions as starting values, i.e.,

$$u_h^0 = \mathcal{I}_h u + \xi_h, \quad \lambda_h^0 = \mathcal{I}_{h,\mathrm{D}}\lambda + \zeta_h.$$

The vectorial and scalar perturbations are given by

$$\xi_h = n_{f,\varrho}(x)[1,\dots,1]^\mathsf{T}, \quad \zeta_h = n_{f,\varrho}(x),$$

where for a given frequency f and strength $\varrho \geq 0$ the noise function $n_{f,\varrho}$ is given by

$$n_{f,\varrho}(x) = \varrho\sin(2\pi f x_1)\dots\sin(2\pi f x_d).$$

We experimentally investigated the experimental convergence behavior of the Newton iteration by representing the residual $F_h(u_h^k, \lambda_h^k)$ in the nodal basis of the finite element spaces and computing its Euclidean norm. Table 4 displays the decay of the residuals and indicates a superlinear but non-quadratic convergence behavior in the two-dimensional settting of Example 5.1 with a perturbed triangulation $\mathcal{T}_7$. The perturbation parameters were chosen as $f = 10$ and $\varrho = h_\ell$.

step k	time (s)	res_{k-1}	$\mathrm{res}_{k-2}/\mathrm{res}_{k-1}$
0	4.291e−1	1.000	0
1	1.153e2	8.128	8.128
2	1.337e3	1.448e−3	1.781e−4
3	1.500e3	1.897e−5	1.311e−2
4	3.470e3	5.329e−7	2.809e−2
5	5.463e3	9.428e−10	1.769e−3
6	7.513e3	3.867e−12	4.102e−3

TABLE 4. Iterations of the Newton iteration on the perturbed triangulation $\mathcal{T}_7$ in Example 5.1 with norms of resdiuals $\mathrm{res}_k \simeq F_h(u_h^k, \lambda_h^k)$. Their quotients indicate a superlinear, non-quadratic convergence behavior.

To experimentally determine the convergence area of the Newton iteration as neighborhoods of the interpolants $x_h = (\mathcal{I}_h u, \mathcal{I}_{h,\mathrm{D}}\lambda)$ we used perturbations of x_h of increasing size, i.e.,

$$f = 10, \quad \varrho = h,\, h^{3/4},\, h^{1/2},\, h^{1/4},\, h^0.$$

Tables 5 and 6 display the iteration numbers required to achieve the stopping criterion on the fixed triangulations $\mathcal{T}_7$ and $\mathcal{T}_5$ for Examples 5.1 and 5.2, respectively. A hyphen indicates that the criterion was not satisfied within 25 iterations.

ℓ	$\varrho = 0$	h	$h^{3/4}$	$h^{1/2}$	$h^{1/4}$	h^0
1	2	2	3	3	2	3
2	2	4	2	5	5	5
3	2	5	5	8	8	—
4	2	4	5	6	—	—
5	2	5	5	6	—	—
6	2	5	5	6	—	—
7	3	6	6	6	—	—

TABLE 5. Iteration numbers for the Newton method in the two-dimensional Example 5.1 for different perturbations of strength ϱ of the nodal interpolants as starting value.

ℓ	$\varrho = 0$	h	$h^{3/4}$	$h^{1/2}$	$h^{1/4}$	h^0
1	3	3	3	3	3	3
2	3	3	3	3	3	3
3	3	11	11	—	—	—
4	3	9	12	—	—	—
5	4	6	8	—	—	—

TABLE 6. Iteration numbers for the Newton method in the three-dimensional Example 5.2 for different perturbations of strength ϱ of the nodal interpolants as starting value.

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