Journal of Computational Mathematics, Vol.27, No.2-3, 2009, 170–183.

COMBINATION OF GLOBAL AND LOCAL APPROXIMATION SCHEMES FOR HARMONIC MAPS INTO SPHERES*

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Abstract

It is well understood that a good way to discretize a pointwise length constraint in partial differential equations or variational problems is to impose it at the nodes of a triangulation that defines a lowest order finite element space. This article pursues this approach and discusses the iterative solution of the resulting discrete nonlinear system of equations for a simple model problem which defines harmonic maps into spheres. An iterative scheme that is globally convergent and energy decreasing is combined with a locally rapidly convergent approximation scheme. An explicit example proves that the local approach alone may lead to ill-posed problems; numerical experiments show that it may diverge or lead to highly irregular solutions with large energy if the starting value is not chosen carefully. The combination of the global and local method defines a reliable algorithm that performs very efficiently in practice and provides numerical approximations with low energy.

Mathematics subject classification: 65N12, 65N30, 35J60.
Key words: Harmonic maps, Iterative methods, Pointwise constraint.

1. Introduction

We consider the simplest example of a geometric partial differential equation, namely, we study the problem of minimizing the Dirichlet energy among vector fields that satisfy boundary conditions and a pointwise unit length constraint. More precisely, given a bounded Lipschitz domain $\Omega \subset \mathbb{R}^d$, $d = 2, 3$, a positive integer m, and $u_{\rm D} \in H^{1/2}(\partial\Omega; \mathbb{R}^m)$ such that $|u_{\rm D}| = 1$ almost everywhere (a.e.) on $\partial\Omega$, we aim at finding (local) minimizers of the functional

$$E(u) := \frac{1}{2}\int_\Omega |\nabla u|^2 dx \tag{1.1}$$

among maps

$$u \in \mathcal{A}(u_{\rm D}) := \big\{ v \in H^1(\Omega; \mathbb{R}^m) : |v| = 1 \text{ a.e. in } \Omega,\ \ v|_{\partial\Omega} = u_{\rm D} \big\}.$$

The existence of (global) minimizers follows from the direct method in the calculus of variations provided that $\mathcal{A}(u_{\rm D}) \neq \emptyset$. Sufficient for this is that $u_{\rm D}$ is Lipschitz continuous on $\partial\Omega$, see [15]. Here, we restrict our attention to stationary points of E in $\mathcal{A}(u_{\rm D})$. These are the weak solutions of the Euler-Lagrange equations

$$-\Delta u = |\nabla u|^2 u \quad \text{in } \Omega, \quad |u| = 1 \quad \text{a.e. in } \Omega, \quad u|_{\partial\Omega} = u_{\rm D} \tag{1.2}$$

* Received January 2, 2008 / Revised version received April 24, 2008 / Accepted May 4, 2008 /

and are called *harmonic maps*. The nonlinear partial differential equation (1.2) occurs as a greatly simplified subproblem in ferromagnetics [14] and liquid crystal theory [15,21] and serves as a model problem for partial differential equations into manifolds. The main difficulties in the development of convergent numerical methods are the nonconvexity of the constraint $|u| = 1$ a.e. in Ω, limited regularity and nonuniqueness of solutions of (1.2), as well as restricted flexibility of standard finite element methods. These problems have successfully been addressed in [1,2]; the globally convergent iterative algorithm proposed and analyzed in those works realizes an H^1 gradient flow of E and computes stationary points of E in lowest order finite element spaces which satisfy the unit-length constraint at the nodes of the underlying triangulation. Weak subconvergence to a harmonic map and an energy decreasing property of the iteration are guaranteed if the underlying triangulations are weakly acute. The fact that the algorithm decreases the energy in each step is important, since it is known that harmonic maps may be discontinuous everywhere, cf. [18], whereas energy minimizing (or weakly stationary) harmonic maps are smooth away from a discrete set, cf. [10,19,20]; if $d = 2$ then harmonic maps are smooth [11] but may still fail to be unique. Although the algorithm of [1,2] is capable to deal with related difficulties, it suffers from extremely slow convergence. The presumably more efficient solution of the discrete formulation by means of a Newton iteration is critical for various reasons. First, the iteration matrix may become singular and second, by nonconvexity of the constraint, the iteration may fail to converge even if it is well-posed. Nevertheless, when a good initial value is available then the Newton iteration typically converges rapidly to a solution of the nonlinear system of equations. In order to benefit from the best properties of the global and the local scheme, we propose to alternatingly perform a few iterations of each scheme. This leads to a reliable iteration that converges faster than the global strategy in all of our numerical experiments. For other approaches to the computation of harmonic maps into spheres we refer the reader to [15,16]; for approximation results of harmonic maps into more general targets we refer to [3,17].

The outline of this article is as follows. Preliminaries and notation are introduced in Section 2. The discrete scheme and its properties are discussed in Section 3. In Section 4 we recall the global solver of [1,2] and define the local solution strategy which is based on a saddle point formulation with a separately convex augmented Lagrangian. The main contribution of this work is the combination of the global and local strategy and is stated in Section 5. Numerical experiments are reported in Section 6 and show that the global strategy is slowly convergent, that the local strategy may fail to converge at all, and that the combined strategy performs most efficiently in our examples.

2. Preliminaries

Throughout this paper we assume that $\mathcal{T}_h$ is a regular triangulation of the polygonal or polyhedral bounded Lipschitz domain $\Omega \subset \mathbb{R}^d$ into triangles or tetrahedra of maximal diameter h for $d = 2, 3$, respectively. The subscript h refers to the maximal mesh-size of $\mathcal{T}_h$, i.e., $h = \max_{T \in \mathcal{T}_h} \operatorname{diam}(T)$. When dealing with a sequence of triangulations, we assume that h belongs to a countable set of positive real numbers that accumulate at zero. We let $\mathcal{S}^1(\mathcal{T}_h) \subseteq H^1(\Omega)$ denote the lowest order finite element space on $\mathcal{T}_h$, i.e., $\phi_h \in \mathcal{S}^1(\mathcal{T}_h)$ if and only if $\phi_h \in C(\overline{\Omega})$ and $\phi_h|_T$ is affine for each $T \in \mathcal{T}_h$. The subset $\mathcal{S}^1_0(\mathcal{T}_h) \subset \mathcal{S}^1(\mathcal{T}_h)$ consists of all functions in $\mathcal{S}^1(\mathcal{T}_h)$ that vanish on $\partial\Omega$, i.e., $\mathcal{S}^1_0(\mathcal{T}_h) := \mathcal{S}^1(\mathcal{T}_h) \cap H^1_0(\Omega)$. Given the set of all nodes (or vertices) $\mathcal{N}_h$ in $\mathcal{T}_h$ and letting $\big(\varphi_z : z \in \mathcal{N}_h\big)$ denote the nodal basis in $\mathcal{S}^1(\mathcal{T}_h)$, we define the nodal interpolation operator $\mathcal{I}_h : C(\overline{\Omega}) \to \mathcal{S}^1(\mathcal{T}_h)$ by

$$\mathcal{I}_h \psi := \sum_{z\in\mathcal{N}_h} \psi(z)\varphi_z$$

for $\psi \in C(\overline{\Omega})$. We write $(f,g) = \int_\Omega f\cdot g\,dx$ for $f,g \in L^2(\Omega;\mathbb{R}^m)$ and abbreviate $||f|| := ||f||_{L^2(\Omega)} = \big(f,f\big)^{1/2}$. For functions $\phi,\psi \in C(\overline{\Omega})$ a discrete inner product (also known as "numerical integration" or "mass lumping") is defined by

$$\big(\phi,\psi\big)_h := \int_\Omega \mathcal{I}_h[\phi\,\psi]\,dx = \sum_{z\in\mathcal{N}_h} \beta_z \phi(z)\,\psi(z),$$

where $\beta_z = \int_\Omega \varphi_z\,dx$ for all $z \in \mathcal{N}_h$. Notice that if $\psi \in C(\overline{\Omega})$ and $\big(\psi,\varrho_h\big)_h = 0$ for all $\varrho_h \in \mathcal{S}^1(\mathcal{T}_h)$ then $\psi(z) = 0$ for all $z \in \mathcal{N}_h$.

We say that the triangulation $\mathcal{T}_h$ of Ω is *weakly acute* if for all $z \in \mathcal{N}_h\backslash\partial\Omega$ and all $y \in \mathcal{N}_h\backslash\{z\}$ we have $\big(\nabla\varphi_z,\nabla\varphi_y\big) \le 0$. If $d = 2$ then a triangulation is weakly acute if and only if every sum of two angles opposite to an interior edge is bounded by π. For $d = 3$ a sufficient but not necessary condition is that every angle between two faces of a tetrahedron is bounded by $\pi/2$. For a detailed discussion about the construction of weakly acute triangulations of three-dimensional domains the reader is refered to [13]. An important consequence of the acute type property of a triangulation $\mathcal{T}_h$ is that if $v_h \in \mathcal{S}^1(\mathcal{T}_h)^m$ satisfies $|v_h(z)| \ge 1$ for all $z \in \mathcal{N}_h$ and $|v_h(z)| = 1$ for all $z \in \mathcal{N}_h \cap \partial\Omega$ then the function $Pv_h \in \mathcal{S}^1(\mathcal{T}_h)^m$ defined through

$$Pv_h(z) = \frac{v_h(z)}{|v_h(z)|}, \quad z \in \mathcal{N}_h,$$

satisfies, cf. [2],

$$\big\|\nabla P v_h\big\| \le ||\nabla v_h||. \tag{2.1}$$

The proof of (2.1) uses the fact that the finite element stiffness matrix is symmetric with non-positive off-diagonal entries (unless they correspond to a pair of nodal basis functions that are associated to two nodes on the boundary) and that the projection $\mathbb{R}^m \setminus B_1(0) \to \overline{B_1(0)}$, $x \mapsto x/|x|$, is Lipschitz continuous with constant 1, where $B_1(0) := \{x \in \mathbb{R}^m : |x| < 1\}$.

3. Discretization and Convergence to a Harmonic Map

Given a regular triangulation $\mathcal{T}_h$ of Ω and assuming that $u_{\rm D} \in C(\partial\Omega;\mathbb{R}^m)$, we set

$$\mathcal{A}_h(u_{\rm D}) := \big\{v_h \in \mathcal{S}^1(\mathcal{T}_h)^m : v_h(z) = u_{\rm D}(z) \text{ for all } z \in \mathcal{N}_h \cap \partial\Omega,\, |v_h(z)| = 1 \text{ for all } z \in \mathcal{N}_h\big\}.$$

We then consider the following discrete problem:

(P_h) Find a stationary point of $E(u_h)$ among $u_h \in \mathcal{A}_h(u_{\rm D})$.

Existing solutions of (P_h) will be called *discrete harmonic maps*. As proposed in [7] we may equivalently introduce a Lagrange multiplier and consider the following augmented problem:

$$(L_h) \qquad \begin{cases} \text{Find a saddle point } (u_h,\lambda_h) \in \mathcal{S}^1(\mathcal{T}_h)^m \times \mathcal{S}^1(\mathcal{T}_h) \\ \text{with } u_h(z) = u_{\rm D}(z) \text{ for all } z \in \mathcal{N}_h \cap \partial\Omega \text{ for} \\ L(u_h,\lambda_h) := \frac{1}{2}\int_\Omega |\nabla u_h|^2\,dx + \frac{1}{2}\big(\lambda_h, |u_h|^2 - 1\big)_h. \end{cases}$$

Remark 3.1. The scheme proposed originally in [7] is based on the functional

$$L(u_h,\lambda_h) := \frac{1}{2}\int_\Omega |\nabla u_h|^2\,dx + \frac{1}{2}\sum_{z\in\mathcal{N}_h} \lambda_h(z)\big(|u_h(z)|^2-1\big).$$

Even though this formulation is theoretically equivalent to (L_h), it corresponds to a strong penalization of the constraint and this may lead to instabilities for small mesh sizes.

The following assertions characterize solutions of (P_h) and (L_h) and are essential for the definition of the iterative schemes discussed below in Section 4.

Lemma 3.1. *A function $u_h \in \mathcal{S}^1(\mathcal{T}_h)^m$ is a discrete harmonic map if and only if $u_h(z) = u_{\rm D}(z)$ for all $z\in\mathcal{N}_h\cap\partial\Omega$ and one of the following equivalent conditions is satisfied:*
(a) we have $|u_h(z)|=1$ for all $z\in\mathcal{N}_h$ and

$$\big(\nabla u_h, \nabla v_h\big) = 0$$

for all $v_h\in\mathcal{S}^1_0(\mathcal{T}_h)^m$ such that $u_h(z)\cdot v_h(z)=0$ for all $z\in\mathcal{N}_h$;
(b) there exists $\lambda_h\in\mathcal{S}^1(\mathcal{T}_h)^m$ such that

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

for all $\big(v_h,\varrho_h\big)\in\mathcal{S}^1_0(\mathcal{T}_h)^m\times\mathcal{S}^1(\mathcal{T}_h)$.

Proof. It is clear that (b) implies (a). Suppose that (a) is satisfied and let $\lambda_h\in\mathcal{S}^1(\mathcal{T}_h)$ be defined through

$$\lambda_h(z) := -\beta_z^{-1}\big(\nabla u_h, \nabla(u_h(z)\varphi_z)\big)$$

for all $z\in\mathcal{N}_h$. Given any $v_h\in\mathcal{S}^1_0(\mathcal{T}_h)^m$ there exist $v_h^\perp, v_h^{||}\in\mathcal{S}^1_0(\mathcal{T}_h)^m$ and $\alpha_z\in\mathbb{R}$, $z\in\mathcal{N}_h\setminus\partial\Omega$, such that $v_h = v_h^\perp + v_h^{||}$, $v_h^\perp(z)\cdot u_h(z)=0$, and $v_h^{||}(z)=\alpha_z u_h(z)$ for all $z\in\mathcal{N}_h\setminus\partial\Omega$. Then, since $\big(\nabla u_h,\nabla v_h^\perp\big)=0$ and $|u_h(z)|=1$ for all $z\in\mathcal{N}_h$, we deduce with the definition of the coefficients β_z that

$$\begin{aligned}\big(\nabla u_h,\nabla v_h\big) &= \big(\nabla u_h, \nabla v_h^{||}\big)\\ &= \sum_{z\in\mathcal{N}_h\setminus\partial\Omega}\alpha_z\big(\nabla u_h,\nabla(u_h(z)\varphi_z)\big)\\ &= -\sum_{z\in\mathcal{N}_h\setminus\partial\Omega}\alpha_z\beta_z\lambda_h(z)\big|u_h(z)\big|^2\\ &= -\sum_{z\in\mathcal{N}_h\setminus\partial\Omega}\beta_z\lambda_h(z)u_h(z)\cdot v_h(z)\\ &= -\big(\lambda_h, u_h\cdot v_h\big)_h.\end{aligned}$$

This is the first identity in (b). Since $|u_h(z)|=1$ for all $z\in\mathcal{N}_h$, the second identity in (b) is also satisfied. It remains to show that (a) and (b) are equivalent definitions of discrete harmonic maps. Assume that u_h is a solution of (P_h) respectively (L_h). Then, one immediately verifies that (b) is satisfied.

Conversely, suppose that one of the equivalent conditions (a) and (b) holds. Given $\varepsilon>0$ and a continuously differentiable path $(-\varepsilon,\varepsilon)\to\mathcal{A}_h(u_{\rm D})$, $t\mapsto w_h^t$ which satisfies $w_h^0 = u_h$, we have to show that $\frac{d}{dt}E(w_h^t)\big|_{t=0} = 0$. For every $z \in \mathcal{N}_h$ we have, using $|w_h^t(z)| = 1$ for all $t \in (-\varepsilon, \varepsilon)$, that

$$0 = \frac{d}{dt}|w_h^t(z)|^2\big|_{t=0} = u_h(z) \cdot v_h(z),$$

where $v_h(z) := \frac{d}{dt}w_h^t(z)\big|_{t=0}$. Owing to (a), we deduce that

$$\frac{d}{dt}E(w_h^t)\big|_{t=0} = \big(\nabla u_h, \nabla v_h\big) = 0$$

and this shows that u_h is a discrete harmonic map. □

To show that a sequence of solutions of (P_h) related to a sequence of triangulations of maximal mesh-size $h > 0$ converges to a harmonic map as $h \to 0$, we employ the following lemma which we state here only for $m = 3$. We remark that the assertions of the lemma and the subsequent theorem can also be generalized to the case $m \neq 3$ by making an appropriate use of the wedge product. We include a short proof for the sake of completeness.

Lemma 3.2. [6] *Let $m = 3$. A function $u \in \mathcal{A}(u_{\rm D})$ is a harmonic map, i.e., it is a weak solution of* (1.2), *if and only if*

$$\big(\nabla u, u \times \nabla\phi\big) = 0 \tag{3.1}$$

for all $\phi \in H_0^1(\Omega;\mathbb{R}^3) \cap L^\infty(\Omega;\mathbb{R}^3)$.

Proof. Let u be a weak solution of (1.2). Then, testing (1.2) with $v = u \times \phi$ and employing properties of the cross product, we verify

$$\begin{aligned} 0 &= \sum_{j=1}^d \big(\partial_j u, \partial_j(u \times \phi)\big) \\ &= \sum_{j=1}^d \big\{\big(\partial_j u, \partial_j u \times \phi\big) + \big(\partial_j u, u \times \partial_j\phi\big)\big\} \\ &= \sum_{j=1}^d \big(\partial_j u, u \times \partial_j\phi\big) = \big(\nabla u, u \times \nabla\phi\big). \end{aligned}$$

Conversely, suppose that (3.1) is satisfied. Then, let $v \in H_0^1(\Omega;\mathbb{R}^3) \cap L^\infty(\Omega;\mathbb{R}^3)$, choose $\phi = u \times v$, recall $a \times (b \times c) = (a \cdot c)b - (a \cdot b)c$ for $a, b, c \in \mathbb{R}^3$, and notice $u \cdot \partial_j u = 0$ a.e. in Ω for $j = 1, 2, ..., d$ to deduce that

$$\begin{aligned} 0 &= \sum_{j=1}^d \big(\partial_j u, u \times \partial_j\phi\big) \\ &= \sum_{j=1}^d \big\{\big(\partial_j u, u \times (\partial_j u \times v)\big) + \big(\partial_j u, u \times (u \times \partial_j v)\big)\big\} \\ &= \sum_{j=1}^d \big\{\big(\partial_j u, (u \cdot v)\partial_j u\big) - \big(\partial_j u, (u \cdot \partial_j u)v\big)\big\} + \sum_{j=1}^d \big\{\big(\partial_j u, (u \cdot \partial_j v)u\big) - \big(\partial_j u, |u|^2\partial_j v\big)\big\} \\ &= \sum_{j=1}^d \big\{\big(|\partial_j u|^2, u \cdot v)\big) - \big(\partial_j u, \partial_j v\big)\big\}, \end{aligned}$$

which is the weak formulation of (1.2). □

Provided that a sequence of discrete harmonic maps is bounded in H^1 it weakly accumulates at harmonic maps. Like the previous lemma, the following assertion can also be established for $m \neq 3$.

Theorem 3.1. *Let $m = 3$. Suppose that $u_D \in C(\partial\Omega; \mathbb{R}^3)$ and $u_D|_E \in H^1(E; \mathbb{R}^3)$ for each edge or face $E \subseteq \partial\Omega$ if $d = 2$ or $d = 3$, respectively. Let $(u_h)_{h>0}$ be a sequence of discrete harmonic maps such that $u_h \in \mathcal{S}^1(\mathcal{T}_h)^3$ and*

$$||\nabla u_h|| \leq C \text{ for all } h > 0.$$

Then, every weak accumulation point of the sequence $(u_h)_{h>0}$ is a harmonic map satisfying $u|_{\partial\Omega} = u_D$.

Proof. Owing to the boundedness of $(u_h)_{h>0}$ in $H^1(\Omega; \mathbb{R}^3)$ there exist weak accumulation points. Let $u \in H^1(\Omega; \mathbb{R}^3)$ be such a point and let $(u_{h'})_{h'>0}$ be a subsequence such that $u_{h'} \rightharpoonup u$ weakly in $H^1(\Omega; \mathbb{R}^3)$. In the following we do not employ the relabeling of the subsequence. By interpolation estimates and $|u_h| \leq 1$ a.e. in Ω we have

$$\big\||u_h|^2 - 1\big\| \leq Ch \,\big\|D\big[|u_h|^2\big]\big\| \leq 2Ch\,||\nabla u_h||.$$

Hence, $|u_h|^2 \to 1$ in $L^2(\Omega)$ and in particular $|u| = 1$ a.e. in Ω. If $d = 1$ then $u_h = u_D$ on $\partial\Omega$ for all $h > 0$. If $d = 2$ or $d = 3$ then for each edge or face $E \subseteq \partial\Omega$ we have

$$||u_h - u_D||_{L^2(E)} \leq Ch\,||\partial u_D/\partial s||_{L^2(E)}.$$

This implies that $u_h|_{\partial\Omega} \to u_D$ in $L^2(\partial\Omega)$ and the weak continuity of the trace operator leads to $u|_{\partial\Omega} = u_D$ in the sense of traces. Let $\phi \in C^\infty(\overline{\Omega}; \mathbb{R}^3) \cap H^1_0(\Omega; \mathbb{R}^3)$ and set $v_h := \mathcal{I}_h[u_h \times \phi] \in \mathcal{S}^1_0(\mathcal{T}_h)^3$. Then $u_h(z) \cdot v_h(z) = 0$ for all $z \in \mathcal{N}_h$. Moreover, for each $T \in \mathcal{T}_h$ we have, since $D^2 u_h|_T \equiv 0$ and $|u_h| \leq 1$ a.e. in Ω,

$$\begin{aligned} ||\nabla(v_h - u_h \times \phi)||_{L^2(T)} &\leq Ch\,||D^2[u_h \times \phi]||_{L^2(T)} \\ &\leq Ch\left(||\nabla\phi||_{L^\infty(T)}\,||\nabla u_h||_{L^2(T)} + ||D^2\phi||_{L^2(T)}\right) \end{aligned}$$

as $h \to 0$. Hence, $\nabla(v_h - u_h \times \phi) \to 0$ in $L^2(\Omega)$. Arguing as in the proof of Lemma 3.2 we infer

$$\begin{aligned} \big(\nabla u_h, \nabla(u_h \times \phi)\big) &= \sum_{j=1}^d \big(\partial_j u_h, \partial_j(u_h \times \phi)\big) \\ &= \sum_{j=1}^d \big(\partial_j u_h, (\partial_j u_h) \times \phi\big) + \big(\partial_j u_h, u_h \times (\partial_j \phi)\big) \\ &= \sum_{j=1}^d \big(\partial_j u_h, u_h \times (\partial_j \phi)\big) = \big(\nabla u_h, u_h \times \nabla\phi\big). \end{aligned}$$

A combination of these estimates and identities with the fact that $u_h \to u$ strongly in $L^2(\Omega; \mathbb{R}^3)$ and $u_h \rightharpoonup u$ weakly in $H^1(\Omega; \mathbb{R}^3)$ leads to

$$\begin{aligned} 0 &= \big(\nabla u_h, \nabla v_h\big) \\ &= \big(\nabla u_h, \nabla\{\mathcal{I}_h[u_h \times \phi] - u_h \times \phi\}\big) + \big(\nabla u_h, \nabla\{u_h \times \phi\}\big) \\ &= \big(\nabla u_h, \nabla\{\mathcal{I}_h[u_h \times \phi] - u_h \times \phi\}\big) + \big(\nabla u_h, u_h \times \nabla\phi\big) \\ &\to \big(\nabla u, u \times \nabla\phi\big) \end{aligned}$$

as $h \to 0$. Lemma 3.2 implies that u is a harmonic map. □

Remark 3.2. If (1.2) admits a unique solution u then the entire sequence $(u_h)_{h>0}$ converges to u.

4. Iterative Strategies for the Solution of (P_h)

In this section we discuss two iterative schemes for the practical solution of the equivalent nonlinear discrete formulations stated in Lemma 3.1.

4.1. H^1 gradient flow approach

The iterative strategy due to [1] realizes an H^1 gradient flow approach and linearizes the constraint $|u_h|^2 = 1$ about an approximation u_h^j. This results in the iterative solution of elliptic problems on appropriate tangent spaces to define the corrections.

Algorithm ($\mathbf{A}^{\mathbf{global}}$). *Let $\varepsilon > 0$ and $u_h^0 \in \mathcal{A}_h(u_{\mathrm{D}})$. Set $j := 0$.*
(1) Compute $w_h^j \in \mathcal{S}_0^1(\mathcal{T}_h)^m$ such that $u_h^j(z) \cdot w_h^j(z) = 0$ for all $z \in \mathcal{N}_h$ and

$$\big(\nabla\big[u_h^j - w_h^j\big], \nabla v_h\big) = 0$$

for all $v_h \in \mathcal{S}_0^1(\mathcal{T}_h)^m$ such that $u_h^j(z) \cdot v_h(z) = 0$ for all $z \in \mathcal{N}_h$.
(2) Let $u_h^{j+1} \in \mathcal{S}^1(\mathcal{T}_h)^m$ be defined through

$$u_h^{j+1}(z) = \frac{u_h^j(z) - w_h^j(z)}{|u_h^j(z) - w_h^j(z)|}$$

for all $z \in \mathcal{N}_h$.
(3) Stop if $||\nabla w_h^j|| \le \varepsilon$; set $j := j + 1$ and go to (1) otherwise.

Remark 4.1. (i) Notice that Step (1) is the minimization of $E(u_h^j - w_h)$ among $w_h \in \mathcal{S}_0^1(\mathcal{T}_h)^m$ satisfying $u_h^j(z) \cdot w_h(z) = 0$ for all $z \in \mathcal{N}_h$ and admits a unique solution.
(ii) Since $|u_h^j(z) - w_h^j(z)|^2 = 1 + |w_h^j(z)|^2 \ge 1$ for all $z \in \mathcal{N}_h$, the normalization in Step (2) is well defined.
(iii) Step (1) can equivalently be written as: Find $(w_h^j, \lambda_h^j) \in \mathcal{S}_0^1(\mathcal{T}_h)^m \times \mathcal{S}_0^1(\mathcal{T}_h)$ such that

$$\begin{aligned} -\big(\nabla\big[u_h^j - w_h^j\big], \nabla v_h\big) + \big(\lambda_h^j, u_h^j \cdot v_h\big)_h &= 0, \\ \big(\varrho_h, u_h^j \cdot w_h^j\big)_h &= 0, \end{aligned}$$

for all $(v_h, \varrho_h) \in \mathcal{S}_0^1(\mathcal{T}_h)^m \times \mathcal{S}_0^1(\mathcal{T}_h)$. This is a well-posed discrete saddle-point formulation. However, the *inf-sup condition* (cf., e.g., [5]) only seems to hold with an h-dependent constant.

The iteration of Algorithm (A^{global}) converges unconditionally on triangulations that are weakly acute.

Proposition 4.1. *Suppose that $\mathcal{T}_h$ is weakly acute. Then, for every $j \ge 0$ we have*

$$||\nabla u_h^{j+1}|| \le ||\nabla u_h^j||$$

and $||\nabla w_h^j|| \to 0$ as $j \to \infty$. Moreover, the sequence $(u_h^j)_{j\ge 0}$ accumulates at discrete harmonic maps.

Proof. Owing to the definition of w_h^j, we have

$$||\nabla(u_h^j - w_h^j)||^2 = \big(\nabla\big[u_h^j - w_h^j\big], \nabla u_h^j\big) \leq ||\nabla(u_h^j - w_h^j)||\,||\nabla u_h^j||.$$

Since $\big|\big(u_h^j - w_h^j\big)(z)\big| \geq 1$ and since $\mathcal{T}_h$ is weakly acute we infer with (2.1) and the definition of u_h^{j+1} that

$$||\nabla u_h^{j+1}|| \leq ||\nabla(u_h^j - w_h^j)||.$$

Thus, we have

$$||\nabla u_j^{j+1}|| \leq ||\nabla u_h^j||.$$

Since $\big(\nabla u_h^j, \nabla w_h^j\big) = ||\nabla w_h^j||^2$ we infer that

$$||\nabla u_h^{j+1}||^2 \leq ||\nabla(u_h^j - w_h^j)||^2 = ||\nabla u_h^j||^2 - ||\nabla w_h^{j+1}||^2$$

and a summation over $j = 0, 1, 2, ...$ implies

$$\sum_{j=0}^{\infty} \|\nabla w_h^{j+1}\|^2 \leq \|\nabla u_h^0\|^2,$$

i.e., $||\nabla w_h^j|| \to 0$ as $j \to \infty$. The fact that every convergent subsequence of $(u_h^j)_{j\geq 0}$ converges to a discrete harmonic map then follows immediately with Lemma 3.1. □

4.2. Newton iteration for the solution of (L_h)

The numerical solution of (P_h) respectively (L_h) with a Newton iteration leads to a different scheme. We define $X_h := \mathcal{S}_0^1(\mathcal{T}_h)^m \times \mathcal{S}_0^1(\mathcal{T}_h)$ and recast (b) of Lemma 3.1 as: Find $x_h = (\widetilde{u}_h, \lambda_h) \in X_h$ such that for all $y_h = (v_h, \varrho_h) \in X_h$ we have

$$\begin{aligned} F(x_h)[y_h] :=& \big(\nabla[\widetilde{u}_h + u_{\mathrm{D},h}], \nabla v_h\big) + \big(\lambda_h, [\widetilde{u}_h + u_{\mathrm{D},h}] \cdot v_h\big)_h \\ &+ \frac{1}{2}\big(\varrho_h, |[\widetilde{u}_h + u_{\mathrm{D},h}]|^2 - 1)_h = 0, \end{aligned}$$

where $u_{\mathrm{D},h} \in \mathcal{S}^1(\mathcal{T}_h)^m$ satisfies $u_{\mathrm{D},h}(z) = u_{\mathrm{D}}(z)$ for all $z \in \mathcal{N}_h \cap \partial\Omega$. Given some $x_h^j \in X_h$, a Newton iteration computes in each step a correction $c_h^j \in X_h$ such that for all $y_h \in X_h$ we have

$$DF(x_h^j)(c_h^j)[y_h] = -F(x_h^j)[y_h]$$

and defines the new iterate $x_h^{j+1} := x_h^j + c_h^j$. Replacing $\widetilde{u}_h + u_{\mathrm{D},h}$ by u_h, the scheme may be written as follows.

Algorithm ($\mathbf{A}^{\mathbf{local}}$). *Let $\varepsilon > 0$. Choose $u_h^0 \in \mathcal{S}^1(\mathcal{T}_h)^m$ and $\lambda_h^0 \in \mathcal{S}_0^1(\mathcal{T}_h)$ such that $u_h^0(z) = u_{\mathrm{D}}(z)$ for all $z \in \mathcal{N}_h \cap \partial\Omega$. Set $j := 0$.*
(1) Compute $(w_h^j, \mu_h^j) \in X_h$ such that

$$\begin{aligned} \big(\nabla w_h^j, \nabla v_h\big) + \big(\lambda_h^j, w_h^j \cdot v_h\big)_h + \big(\mu_h^j, u_h^j \cdot v_h\big)_h &= -\big(\nabla u_h^j; \nabla v_h\big) - \big(\lambda_h^j, u_h^j \cdot v_h\big)_h, \\ \big(\varrho_h, u_h^j \cdot w_h^j\big)_h &= -\frac{1}{2}\big(\varrho_h, |u_h^j|^2 - 1\big)_h, \end{aligned}$$

for all $(v_h, \varrho_h) \in X_h$.
(2) Set $(u_h^{j+1}, \lambda_h^{j+1}) := (u_h^j + w_h^j, \lambda_h^j + \mu_h^j)$.
(3) Stop if $||\nabla w_h^j|| \leq \varepsilon$. Otherwise, set $j := j + 1$, and go to (1).

Remark 4.2. (i) If $\big(w_h^j,\mu_h^j\big)$ with $w_h^j\equiv 0$ is a solution of (1) then u_h^j is a discrete harmonic map.
(ii) Notice that Step (1) admits no solution if, e.g., $u_h^j(z)=0$ for some $z\in\mathcal{N}_h\setminus\partial\Omega$, since in this case the choice $\varrho_h=\varphi_z$ leads to

$$\big(\varphi_z,u_h^j\cdot w_h^j\big)_h=0\neq\frac{1}{2}\beta_z=-\frac{1}{2}\big(\varphi_z,|u_h^j|^2-1\big)_h$$

for all $w_h^j\in\mathcal{S}_0^1(\mathcal{T}_h)^m$. Therefore, global well-posedness and convergence of Algorithm (A^{local}) is false in general.
(iii) In case of termination of the iteration, the output u_h^* need not satisfy $|u_h^*(z)|=1$ exactly for all $z\in\mathcal{N}_h$.
(iv) Assuming that $|u_h^j(z)|=1$ for all $z\in\mathcal{N}_h$ and defining

$$X_h^{\tan}[u_h^j]:=\big\{v_h\in\mathcal{S}_0^1(\mathcal{T}_h)^m: v_h(z)\cdot u_h^j(z)=1 \text{ for all } z\in\mathcal{N}_h\big\},$$

Step (2) is equivalent to finding $w_h^j\in X_h^{\tan}[u_h^j]$ such that

$$\big(\nabla w_h^j,\nabla v_h\big)+\big(\lambda_h^j,u_h^j\cdot v_h\big)_h=-\big(\nabla u_h^j,\nabla v_h\big),$$

for all $v_h\in X_h^{\tan}[u_h^j]$. Notice that up to the second term on the left-hand side this is the iteration of Algorithm (A^{global}). Hence, Algorithm (A^{global}) may be regarded as a simplified Newton iteration.
(v) A one-dimensional optimization along the correction vector can be incorporated to improve the stability of the scheme.
(vi) Homogeneous Dirichlet boundary conditions have been included for λ_h to avoid non-definiteness of the problem in Step (2).

Standard results (see, e.g., [8]) assert that the Newton iteration converges if, there exists $x_h^*\in X_h$ such that $F(x_h^*)=0$, $DF(x_h^*)$ is regular, and x_h^0 is sufficiently close to x_h^*. In the following example we show that in general, the derivative DF is singular, i.e., Step (1) of Algorithm (A^{local}) may fail to admit a unique solution. We note however that the following example obeys symmetry properties and may therefore be an exceptional case. Such cases cannot occur if the so called cut-locus condition of [12] is satisfied. Notice that a (continuous) harmonic map satisfies $\Delta u-\lambda u=0$ with the Lagrange multiplier given by $\lambda=-|\nabla u|^2$.

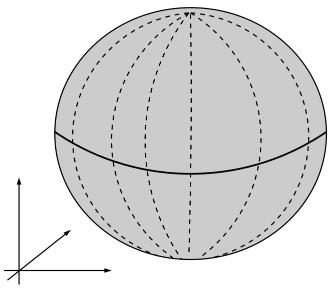

Fig. 4.1. Every unit speed geodesic connecting north and south pole defines a harmonic map in Example 4.1 (a)

Example 4.1. (a) Let $u : (0,1) \to \mathbb{R}^3$ be a harmonic map satisfying, $u(0) = -u(1) = (0,0,1)$, i.e., $u \in H^1(0,1)^3$ satisfies $|u| = 1$ a.e. in $(0,1)$,

$$u'' + |u'|^2 u = 0 \text{ in weak sense,}$$

and $u(0) = -u(1) = (0,0,1)$. Then, for each $\phi \in (-\pi,\pi)$ the map

$$u_\phi := R_\phi u := \begin{pmatrix} \cos\phi & \sin\phi & 0 \\ -\sin\phi & \cos\phi & 0 \\ 0 & 0 & 1 \end{pmatrix} u$$

is a harmonic map subject to the same boundary conditions, i.e., it satisfies $|u_\phi| = 1$ a.e. in $(0,1)$, $u_\phi(0) = -u_\phi(1) = (0,0,1)$, and

$$u_\phi'' + |u_\phi'|^2 u_\phi = 0 \text{ in weak sense.}$$

The function

$$w := \frac{d}{d\phi}\Big|_{\phi=0} u_\phi = R_0 u := \begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} u$$

satisfies $w \neq 0$, $w(0) = w(1) = 0$, $w \cdot u = 0$ a.e. in $(0,1)$, and

$$w'' + |u'|^2 w = R_0 u'' + |u'|^2 R_0 u = R_0\big(u'' + |u'|^2 u\big) = 0,$$

in particular, we have $w \in H_0^1(0,1)^3$, $u \cdot w = 0$ a.e. in $(0,1)$, and, with $\lambda = -|u'|^2$,

$$(w', v') + (\lambda, w \cdot v) = 0$$

for all $v \in H_0^1(0,1)^3$ such that $u \cdot v = 0$ a.e. in $(0,1)$.
(b) The same example can be constructed in a discrete setting: let $\mathcal{T}_h$ be a partition of the interval $(0,1)$ and $u_h \in \mathcal{S}^1(\mathcal{T}_h)^3$ such that $|u_h(z)| = 1$ for all $z \in \mathcal{N}_h$, $u_h(0) = -u_h(1) = (0,0,1)$, and suppose that there exists $\lambda_h \in \mathcal{S}^1(\mathcal{T}_h)$ so that

$$\big(u_h', v_h'\big) + \big(\lambda_h, u_h \cdot v_h\big) = 0$$

for all $v_h \in \mathcal{S}^1(\mathcal{T}_h)^3$. Arguing as in (a) we find that the vector field $w_h := R_0 u_h \in \mathcal{S}_0^1(\mathcal{T}_h)^3$ is non-trivial, satisfies $w_h(z) \cdot u_h(z) = 0$ for all $z \in \mathcal{N}_h$, and

$$\big(w_h', v_h'\big) + \big(\lambda_h, w_h \cdot v_h\big) = 0.$$

for all $v_h \in \mathcal{S}_0^1(\mathcal{T}_h)^3$ with $v_h(z) \cdot u_h(z) = 0$ for all $z \in \mathcal{N}_h$. Defining $\mu_h \in \mathcal{S}_0^1(\mathcal{T}_h)$ such that

$$\big(\mu_h, \varphi_z\big)_h = -\big(w_h', \varphi_z'\big) - \big(\lambda_h, w_h \cdot \varphi_z\big)_h$$

for all $z \in \mathcal{N}_h \setminus \partial\Omega$ we see that $\big(w_h, \mu_h\big) \in X_h$ is a non-trivial solution of the system in Step (1) of Algorithm (A^{local}).

5. Combined Algorithm

The following algorithm alternatingly iterates the global and the local strategy. Notice that if the local strategy does not converge within a prescribed number of iterations, the last iterate of the global strategy is used to proceed further with the global strategy. The algorithm reduces to Algorithm (A^{global}) or (A^{local}) if either $N_{global} = 0$ or $N_{local} = 0$. Figure 5.1 provides a schematic description of the Algorithm.

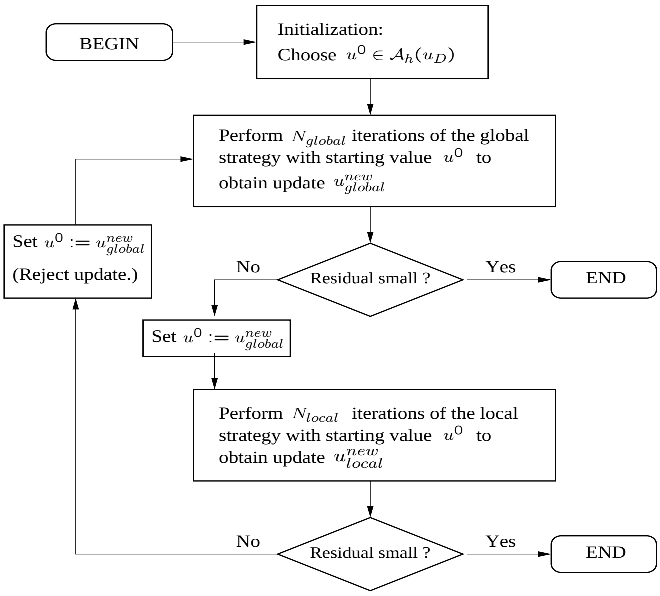

Fig. 5.1. Schematic description of the combination of the local and global approximation schemes in Algorithm ($A^{combined}$)

Algorithm ($\mathbf{A^{combined}}$). *Let $\varepsilon > 0$ and let N_{global}, N_{local} be non-negative integers such that $\max\{N_{global}, N_{local}\} > 0$. Choose $u_h^0 \in \mathcal{A}_h(u_D)$ and set $j = j_{global} := 0$.*

(G0) If $j_{global} = N_{global}$ then set $j_{local} := 0$ and go to (II).

(G1) Compute $w_h^j \in \mathcal{S}_0^1(\mathcal{T}_h)^m$ such that $u_h^j(z) \cdot w_h^j(z) = 0$ for all $z \in \mathcal{N}_h$ and

$$\big(\nabla\big[u_h^j - w_h^j\big], \nabla v_h\big) = 0$$

for all $v_h \in \mathcal{S}_0^1(\mathcal{T}_h)^m$ such that $u_h(z) \cdot v_h(z) = 0$ for all $z \in \mathcal{N}_h$.

(G2) Define $u_h^{j+1} \in \mathcal{S}^1(\mathcal{T}_h)^m$ through

$$u_h^{j+1}(z) = \frac{u_h^j(z) - w_h^j(z)}{|u_h^j(z) - w_h^j(z)|}$$

for all $z \in \mathcal{N}_h$.

(G3) Stop if $\|\nabla w_h^j\|_{L^2(\Omega)} \le \varepsilon$; set $j := j+1$, $j_{global} := j_{global} + 1$, and go to (G0) otherwise.

(II) Set $u_h^{old} := u_h^j$ and choose $\lambda_h^j \in \mathcal{S}_0^1(\mathcal{T}_h)$.

(L0) If $j_{local} = N_{local}$ then set $u_h^j := u_h^{old}$, $j_{global} := 0$, and go to (G0) .

(L1) Compute $(w_h^j, \mu_h^j) \in X_h$ such that

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

for all $(v_h, \varrho_h) \in X_h$. If no solution exists then set $j := j+1$, $j_{local} := N_{local}$, and go to (L0).

(L2) Set $(u_h^{j+1}, \lambda_h^{j+1}) = (u_h^j + w_h^j, \lambda_h^j + \mu_h^j)$.

(L3) Stop if $\|\nabla w_h^j\|_{L^2(\Omega)} \le \varepsilon$; set $j := j+1$, $j_{local} := j_{local} + 1$, and go to (L0) otherwise.

Remark 5.1. (i) The constraint $u_h^j(z) \cdot w_h^j(z) = 0$, $z \in \mathcal{N}_h$, provides a Lagrange multiplier which may be used to define an initial value λ_h^j in Step (II) for the initialization of the local strategy, cf. Remark 4.1 (iii).
(ii) Another useful stopping criterion for the (temporary) termination of the global strategy can also be based on a small decrease of the Dirichlet energy.

The following proposition is an immediate consequence of the fact that Algorithm ($A^{combined}$) reduces to Algorithm (A^{global}) if the local scheme always fails to converge.

Proposition 5.1. *Suppose that* $N_{global} > 0$. *Then Algorithm* ($A^{combined}$) *converges within a finite number of iterations.*

6. Numerical Experiments

The numerical experiments reported in this section were obtained with a MATLAB implementation of Algorithm ($A^{combined}$). All systems of linear equations were solved with the backslash operator which performed satisfactory.

For a uniform triangulation $\mathcal{T}_h$ of $\Omega := (-1/2, 1/2)^2$ into 2048 triangles of diameter $h = \sqrt{2}\, 2^{-5}$ we defined a function $u_h^0 \in \mathcal{S}^1(\mathcal{T}_h)^3$ through

$$u_h^0(z) = \begin{cases} u_D(z) = \big(z/|z|, 0\big) & \text{for } z \in \mathcal{N}_h \cap \partial\Omega, \\ \xi_h(z) & \text{for } z \in \mathcal{N}_h \setminus \partial\Omega, \end{cases}$$

where for each $z \in \mathcal{N}_h \setminus \partial\Omega$, $\xi_h(z)$ is a random unit vector in $\mathbb{R}^3$, cf. the left plot in Figure 6.1.

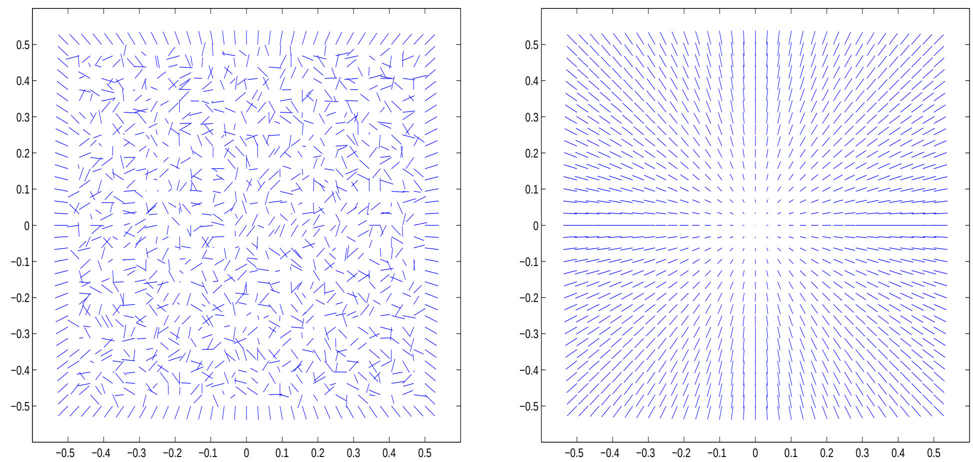

Fig. 6.1. First two components of the initial vector field $u_h^0 \in \mathcal{S}^1(\mathcal{T}_h)^3$ (left) and output $u_h^{19} \in \mathcal{S}^1(\mathcal{T}_h)^3$ of Algorithm ($A^{combined}$) with $\varepsilon = 10^{-9}$, $N_{global} = N_{local} = 5$ (vectors are scaled for presentational purposes)

We ran Algorithm ($A^{combined}$) with $\varepsilon = 10^{-9}$ and (i) $N_{global} = 1$ and $N_{local} = 0$, i.e., using only the global strategy, (ii) $N_{global} = 0$ and $N_{local} = 1$, i.e., using only the local strategy, and (iii) $N_{global} = 5$ and $N_{local} = 5$, i.e., using a combination of the local and global straetegies. Figure 6.2 displays for each of these choices the H^1 norm of the correction vectors w_h^j as a function of the number of iterations j in a semi-logarithmic scaling. We observe that the local strategy alone does not converge within 60 iterations, the global strategy reaches a residual less than ε within 50 iterations, and the combined strategy terminates after only 19 iterations. We deduce that the initial value obtained by 5 iterations of the global strategy does not lead to a convergent local scheme, while the one obtained with 10 iterations does indeed lead to rapid convergence. The first two components of the output obtained with the combined strategy are displayed in the right plot of Figure 6.1; the algorithm computes a smooth vector field.

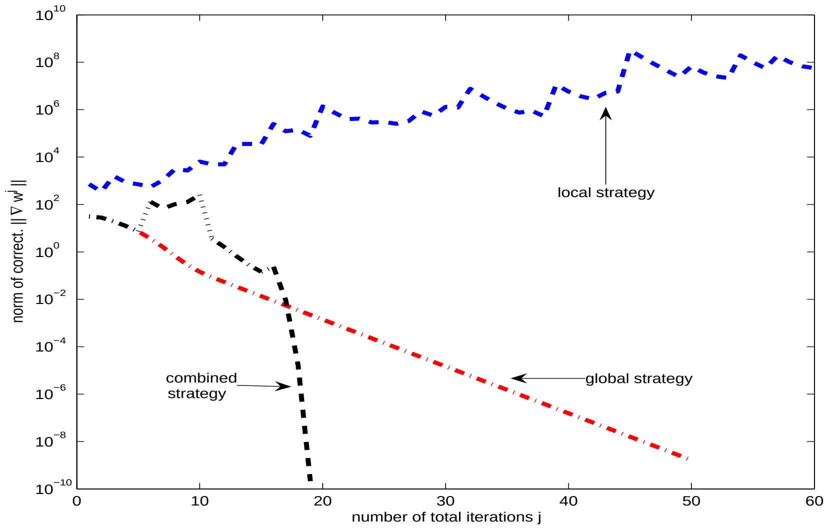

Fig. 6.2. Norm $||\nabla w_h^j||$ of corrections w_h^j in Algorithm $(A^{combined})$ versus number of total iterations for local, global, and combined iteration strategy. The combined iteration is defined through $N_{local} = N_{global} = 5$

Acknowledgments. Supported by Deutsche Forschungsgemeinschaft through the DFG Research Center MATHEON 'Mathematics for key technologies' in Berlin. The authors wish to thank C. Melcher for pointing out the Example 4.1.

References

[1] F. Alouges, A new algorithm for computing liquid crystal stable configurations: the harmonic mapping case, *SIAM J. Numer. Anal.*, **34** (1997), 1708-1726.

[2] S. Bartels, Stability and convergence of finite element approximation schemes for harmonic maps, *SIAM J. Numer. Anal.*, **43**, (2005), 220-238.

[3] S. Bartels, Finite Element Approximation of Harmonic Maps Between Surfaces, Habilitation Thesis (submitted), 2008.

[4] S. Bartels, A. Prohl, Implicit finite element method for harmonic map heat flow into spheres, *Math. Comput.*, **76** (2007), 1847-1859.

[5] D. Braess, Finite elements. Theory, Fast Solvers, and Applications in Solid Mechanics, 2nd edition. Cambridge University Press, Cambridge, 2001.

[6] Y. Chen, The weak solutions to the evolution problem of harmonic maps, *Math. Z.*, **201** (1989), 69-74.

[7] U. Clarenz, G. Dziuk, Numerical methods for conformally parametrized surfaces, Interphase 2003: Numerical Methods for Free Boundary Problems, Cambridge, UK, 2003.

[8] P. Deuflhard, Newton Methods for Nonlinear Problems, Springer-Verlag, Berlin, 2004.

[9] L.C. Evans, Weak Convergence Methods for nonlinear Partial Differential Equations, *CBMS Regional Conf. Series in Mathematics*, **74** (1990), Providence.

[10] L.C. Evans, Partial regularity for stationary harmonic maps into spheres, *Arch. Ration. Mech. An.*, **116** (1991), 101-113.

[11] F. Hélein, Régularité des applications faiblement harmoniques entre une surface et une variété riemannienne, *C.R. Acad. Sci. Paris Sér. I Math.* **312** (1991), 591-596.

[12] W. Jäger, H. Kaul, Uniqueness and stability of harmonic maps and their Jacobi fields, *Manuscripta Math.*, **28** (1979), 269-291.

[13] S. Korotov, M. Křížek, Acute type refinements of tetrahedral partitions of polyhedral domains, *SIAM J. Numer. Anal.*, **39** (2001), 724-733.

[14] M. Kružík, A. Prohl, Recent Developments in modeling, analysis and numerics of ferromagnetism, *SIAM Rev.*, **48** (2006), 439-483.

[15] S.Y. Lin, M. Luskin, Relaxation methods for liquid crystal problems, *SIAM J. Numer. Anal.*, **26** (1989), 1310-1324.

[16] P. Morgan, Newton and conjugate gradient for harmonic maps from the disc into the sphere, *ESAIM Contr. Optim. Ca.*, **10** (2004), 142-167.

[17] S. Müller, M. Struwe, V. Šverák, Harmonic maps on planar lattices, *Ann. Scuola Norm. Sup. Pisa Cl. Sci.*, **25**:4 (1997), 713-730.

[18] T. Rivière, Everywhere discontinuous harmonic maps into spheres, *Acta Math.*, **175** (1995), 197-226.

[19] R. Schoen, K. Uhlenbeck, A regularity theory for harmonic maps, *J. Diff. Geom.*, **17** (1982), 307-355.

[20] L. Simon, Theorems on Regularity and Singularity of Energy Minimizing Harmonic Maps, Lecture Notes in Mathematics ETH Zürich, Birkhäuser, 1996.

[21] E.G. Virga, Variational Theories for Liquid Crystals. Applied Mathematics and Mathematical Computation **8**, Chapman & Hall, London, 1994.