PFAFFIAN EQUATIONS: A VARIATIONAL PERSPECTIVE

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Abstract. Pfaffian equations are part of a classic area well-established in Differential Geometry. From a more analytical viewpoint, it has been traditionally treated in textbooks dealing with Differential Equations focusing on analytical techniques to understand and, eventually, find solutions. The success of those methods are however limited to explicit situations where computations can be carried out to the end. There are some general existence and uniqueness results as well. Yet the numerical approximation of such solutions has not been, to the best of our knowledge, treated. By means of a variational approach based on a true vector variational problem, we propose a mechanism to examine and numerically approximate such solutions, explore its remarkable properties, and test its practical performance in a number of explicit examples. The method can be implemented in situations where the underlying field defining the Pfaffian equation is not known exactly, but may be part of a broader approximation scheme.

1. Introduction

The field of Pfaffian differential equations, though a very classical area, is, to a good extent, somewhat unknown these days, at least in Analysis. It is however something well established in Differential Geometry or Algebra. Although formally formulated by Pfaff ([26]), the problem was already known to Euler ([12]). It has been treated in classic texts of differential equations ([15], [21], [25], [27]) at the conceptual level, and its significance and relationship to PDEs is known too. Yet its competition with standard differential systems (ODEs), or even PDEs, has always been in favor of the latter, since in most of those texts, once its meaning and the basic techniques to find solutions in well-prepared exercises is explored, the focus turns to standard ODEs and/or PDEs.

The relevance of Pfaffian equations in Differential Geometry and Algebra looks, on the other hand, very well-known and very solidly studied in a number of sources: [2], [7], [8], [17]. The more recent survey [11] is a good summary of the most important facts. Some of this literature is only available in Russian or French. From the point of view of Analysis, there are also some interesting and very classical papers as well as some more recent ones: in addition to those already mentioned, [10], [14], [20], [23]. There is even a specialized contribution to the history of this kind of differential equations [18]. Since it is not part of the program in standard courses in Analysis or Geometry at the undergraduate level, some times it serves as a nice subject for projects for interested students [1].

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A Pfaffian differential equation is an expression of the form

$$\omega \equiv \sum_{i=1}^{N} u_i(\mathbf{x})\, dx_i = 0, \quad \mathbf{x} = (x_1, x_2, \dots, x_N), \tag{1.1}$$

for N functions $u_i(\mathbf{x})$. In vector notation, we also write

$$\omega = \mathbf{u}(\mathbf{x}) \cdot d\mathbf{x}, \quad \mathbf{u} = (u_1, u_2, \dots, u_N), d\mathbf{x} = (dx_1, dx_2, \dots, dx_N). \tag{1.2}$$

A $\mathcal{C}^1$-manifold $\mathcal{M}$ of dimension $k \geq 1$ is called an integral manifold of (1.1) if the differential 1-form ω identically vanishes on $\mathcal{M}$. The Pfaffian equation (1.1) is said to be completely integrable if there is a unique integral manifold of the highest possible dimension $N-1$ through each point $\mathbf{x}_0 \in \mathbb{R}^N$. All of these concepts can be considered in a N-dimensional ambient manifold instead of in the euclidean space $\mathbb{R}^N$.

We see that the emphasis is placed on the solution manifold $\mathcal{M}$ of co-dimension one, solution of (1.1) through each point $\mathbf{x}_0 \in \mathbb{R}^N$. From a more practical viewpoint, such manifold, at least locally, is sought through some unknown parametrization

$$\mathbf{x}(\mathbf{t}) : \mathbf{Q} \subset \mathbb{R}^{N-1} \to \mathbb{R}^N, \quad \mathbf{0} \in \mathbf{Q}, \mathbf{x}(\mathbf{0}) = \mathbf{x}_0, \mathbf{t} = (t_1, t_2, \dots, t_{N-1}),$$

in such a way that

$$\mathbf{u}(\mathbf{x}) \cdot \frac{\partial \mathbf{x}}{\partial t_i} = 0, \quad i = 1, 2, \dots, N-1, \quad \mathbf{x}(\mathbf{0}) = \mathbf{x}_0. \tag{1.3}$$

In this way, (1.3) can be regarded as a very special system of first-order PDEs. However, there is, from the outset, a tremendous lack of uniqueness of solutions as a given manifold admits infinitely many such parameterizations. This is again a way to stress that the true solution of the Pfaff equation (1.1) is the manifold $\mathcal{M}$ itself through $\mathbf{x}_0$.

Possibly, the most general existence theorem for solutions of (1.3) is the one in [3] where both existence and uniqueness of solutions is shown under continuity and Lipschitzianity, respectively, of the functions involved. Traditionally, smoothness was required, and this general hypothesis of smoothness is taken for granted here. In addition, a more general integrability condition than (1.6) below is proposed in [3], and a numerical method of resolution based on the polygonal line of Euler is proposed. There are more recent works by these same authors refining these results, but unfortunately they are available only in russian ([4], [5]).

Though analytically, some fundamental facts are known about this kind of problems as we have just stated, as far as we can tell there is no attempt in the literature to approximate numerically the manifold-solutions of (1.1). This was our main motivation. Our proposal is variational in nature, as we focus on minimizing an error functional of the form

$$E(\mathbf{x}) = \int_{\mathbf{Q}} \frac{1}{2} \sum_i \left(\mathbf{u}(\mathbf{x}) \cdot \frac{\partial \mathbf{x}}{\partial t_i} \right)^2 d\mathbf{t}$$

under the constraint $\mathbf{x}(\mathbf{0}) = \mathbf{x}_0$, for a given point $\mathbf{x}_0 \in \mathbb{R}^N$. For definiteness, we will focus on the first situation of interest $N = 3$, so that we can be more explicit about main ingredients of the problem

$$\mathbf{x}(\mathbf{t}) : \mathbf{Q} \subset \mathbb{R}^2 \to \mathbb{R}^3, \quad \mathbf{x} = (x_1, x_2, x_3), \mathbf{t} = (t_1, t_2);$$

$\mathbf{Q}$ is taken to be the unit disk in the plane, and for a fixed point $\mathbf{x}_0$ where our vector field $\mathbf{u}$ does not vanish, we seek to minimize the error functional

$$E(\mathbf{x}) = \int_{\mathbf{Q}} \frac{1}{2} |\mathbf{u}(\mathbf{x}(\mathbf{t}))\nabla\mathbf{x}(\mathbf{t})|^2 \, d\mathbf{t}, \tag{1.4}$$

under $\mathbf{x}(\mathbf{0}) = \mathbf{x}_0$. Note that the functional $E(\mathbf{x})$ can be given in an intrinsic form

$$E(\mathbf{x}) = \frac{1}{2} \int_{\mathbf{x}(\mathbf{Q})} |\Pi_{\mathbb{T}_X}(\mathbf{u}(X))|^2 \, dX,$$

where X is a generic point in the parametrized, embedded manifold $\mathbf{x}(\mathbf{Q})$, $\mathbb{T}_X$ is the tangent plane at X, and $\Pi_{\mathbb{T}_X}$ is the orthogonal projection onto $\mathbb{T}_X$. The form given in (1.4) is however better suited for calculations and numerical approximation.

Even though, our goal is to explore an approximation procedure of solutions, the underlying variational problem as described is quite appealing for various reasons:

- it is an explicit example of a vector variational problem for vector functions $\mathbf{x}$ between euclidean spaces where the dimension of the target space is strictly greater than the dimension of the starting space, and there are not many of these in the literature;
- that the point-constraint $\mathbf{x}(\mathbf{0})$ be preassigned is also peculiar, and have not been considered before;
- the integrand

$$W(\mathbf{x}, \mathbf{X}) = \frac{1}{2} |\mathbf{u}(\mathbf{x})\mathbf{X}|^2, \quad \mathbf{x} \in \mathbb{R}^3, \mathbf{X} \in \mathbb{R}^{3\times 2}, \tag{1.5}$$

  for our functional enjoys the fundamental property of convexity with respect to the gradient variable $\mathbf{X}$, but it is non-convex in joint pairs $(\mathbf{x}, \mathbf{X})$, and non-coercive in $\mathbf{X}$;
- a fundamental danger to avoid is that the two tangent vectors $\partial\mathbf{x}/\partial t_i$ be dependent somewhere, i.e. the rank of $\nabla\mathbf{x}$ be one.

Despite these important difficulties, the nature of our error functional $E(\mathbf{x})$ leads to a very clear certificate of convergence: a good approximation of a true solution of maximal dimension of the Pfaffian equation (1.1) is found whenever $E(\mathbf{x})$ is sufficiently small, and the rank of $\nabla\mathbf{x}$ is two everywhere. This is elementary to realize, but important from a practical viewpoint.

In addition to exploring the one-dimensional case in arbitrary dimension (solutions of co-dimension one for $N = 2$, and of no maximal dimension for $N > 2$), we focus on the case $N = 3$ and look for pieces of surfaces as local solutions of (1.1) around a point $\mathbf{x}_0 \in \mathbb{R}^3$ where $\mathbf{u}(\mathbf{x}_0) \neq \mathbf{0}$. The difficulties described above keep us from showing existence of minimizers for (1.4), but we establish two important results with a clear significance for the numerical approximation.

For the first, we examine the variational problem associated with the perturbed functional

$$E_\epsilon(\mathbf{x}) = \int_{\mathbf{Q}} \left(\frac{1}{2} |\mathbf{u}(\mathbf{x}(\mathbf{t}))\nabla\mathbf{x}(\mathbf{t})|^2 + \frac{\epsilon}{2} |\nabla\mathbf{x}(\mathbf{t})|^2 + \frac{\epsilon}{2} |\mathbf{x}(\mathbf{t})|^2 \right) d\mathbf{t}, \quad \epsilon > 0,$$

under the same constraint $\mathbf{x}(\mathbf{0}) = \mathbf{x}_0$, and show that there are minimizers $\mathbf{x}_\epsilon$, for which the family $\{\mathbf{x}_\epsilon\}$ is a minimizing sequence for the unperturbed functional $E \equiv E_0$. The main trouble here is to discard the possibility that a family of minimizers $\{\mathbf{x}_\epsilon\}$ for E_ϵ should converge to the trivial solution $\mathbf{x} \equiv \mathbf{x}_0$. We will

avoid this difficulty by enforcing a unilateral boundary condition of place, although we have not observed this singular behavior in our numerical experiments.

The second one is even more surprising: under the well-known integrability condition

$$\mathbf{u} \cdot (\nabla \wedge \mathbf{u}) = 0 \tag{1.6}$$

(see next section), equilibrium solution $\mathbf{x}$ for E in (1.4) are necessarily solutions of (1.1) with $E(\mathbf{x}) = 0$. Said differently, in spite of lack of joint convexity on pairs $(\mathbf{x}, \mathbf{X})$ of the integrand (1.5), the only critical solutions for E are global minimizers with $E(\mathbf{x}) = 0$. This unexpected fact ensures that typical numerical procedures (steepest descent, conjugate gradient, Newton-Raphson) to minimize E can only converge, when they do, to regular solutions of (1.1). This is exactly what we have found in our numerical experiments (see the final section below). If the above integrability condition does not hold, our suspicion is that an approximation minimizing procedure will also furnish $E(\mathbf{x}) = 0$ but the underlying surface is singular: the rank of $\nabla \mathbf{x}$ is one in a non-negligible subset. We have confirmed this in practice with some examples.

After reviewing some basic material concerning this kind of equations, we focus on the one-dimensional case looking for solutions of (1.1) of dimension one. This one-dimensional feature makes the analysis much easier and complete. The case of two-dimensional manifolds in $\mathbb{R}^3$ is, however, much more involved, as it requires a fundamental integrability condition (1.6) to ensure existence of local solutions around points $\mathbf{x}_0 \in \mathbb{R}^3$ where the vector field $\mathbf{u}(\mathbf{x}_0) \neq \mathbf{0}$ does not vanish. Finally, we work the numerical approximation for a number of selected examples. We use a typical conjugate gradient method to iteratively approximate minimizers (minimizing sequence) of (1.4). As indicated earlier, there is a principal practical danger to be avoided as the trivial solution $\mathbf{x} \equiv \mathbf{x}_0$ is definitely a minimizer for functional E. Our experiments never led to such singular solution, and confirm the apparent non-existence of local minima. See more details below.

2. Some preliminaries

Typically, (1.1) is considered for $N \geq 3$, since the case $N = 2$ corresponds to a standard differential equation in the plane

$$u_1(x_1, x_2)\, dx_1 + u_2(x_1, x_2)\, dx_2 = 0,$$

written usually as

$$P(x, y)\, dx + Q(x, y)\, dy = 0. \tag{2.1}$$

This system is equivalent (except for a common factor that does not change integral curves) to

$$x'(t) = -Q(x, y), \quad y'(t) = P(x, y), \tag{2.2}$$

and in this way, it is clear that solutions to Pfaffian equation (2.1) are the same as the ones for the differential ODE system (2.2).

The case $N = 3$ is, for this reason, studied explicitly most of the time as it amounts to exploring situations other than standard ODE systems. It reads in explicit form

$$P(x, y, z)\, dx + Q(x, y, z)\, dy + R(x, y, z)\, dz = 0. \tag{2.3}$$

A 2-dimensional manifold embedded in $\mathbb{R}^3$ is an integral solution of this equation if the normal to the tangent plane to it in every point is given by the vector field (P, Q, R). Yet note that (1.1) may accept one-dimensional solutions of the form

$$\mathbf{x}(t) : J \to \mathbb{R}^N, \quad \mathbf{u}(\mathbf{x}(t)) \cdot \mathbf{x}'(t) = 0 \text{ in } J, \tag{2.4}$$

and higher-dimensional solutions may be searched for by assembling in a suitable way a whole continuum of such one-dimensional solutions. This is a typical method of solving first-order PDEs (method of characteristic, Lagrange-Charpit method, etc). Those higher-dimensional solutions are not the ones we are concerned about here.

We know that the existence of (local) solutions for (2.4) does not require any particular restrictive condition on the field $\mathbf{u}$. However, two dimensional solutions $z = z(x, y)$ of (2.3) does ask for the integrability constraint

$$\mathbf{u} \cdot (\nabla \wedge \mathbf{u}) = 0. \tag{2.5}$$

This was known from the very beginning. Even Euler knew about this condition. Note how this differential constraint is somewhat complementary to

$$\mathbf{u} \wedge (\nabla \wedge \mathbf{u}) = \mathbf{0}.$$

This last condition determines the so-called Beltrami fields that play a relevant role in fluid dynamics ([22]). Differential restriction (2.5) on the field $\mathbf{u}$ essentially amounts to the fact that equation (2.3) admits an integrating factor, so that a suitable (non-constant) multiple of $\mathbf{u} = (P, Q, R)$ becomes the gradient of a scalar function $f(x, y, z)$ whose level sets

$$f(x, y, z) = f(x_0, y_0, z_0), \quad \mathbf{x}_0 = (x_0, y_0, z_0),$$

are precisely the solutions of (2.3). If condition (2.5) does not hold, then there are no regular, 2-dimensional solutions.

Though Pfaffian equations are not part of the contents of most popular books on differential equations, it has been examined at the conceptual level in various classic textbooks as indicated in the Introduction. The treatment reduces, as with first-order equations or systems, to some understanding of potential analytical methods of finding solutions that can only be worked out in selected, well-prepared examples. Nothing about the numerical approximation is never intended or pursued.

In the Differential Geometry arena, by contrast, Pfaffian equations are more fully understood in connection with symplectic and contact structures. Possibly, the most recent, complete and accessible account is [11] where the relevance and significance of these equations is explored in a number of physical systems.

The following is a typical (local) existence result for the particular case of two-dimensional manifolds in $\mathbb{R}^3$ ([3]).

Proposition 2.1. *Let*

$$\mathbf{u}(\mathbf{x}) : \Omega \subset \mathbb{R}^3 \to \mathbb{R}^3$$

be a smooth, non-vanishing vector field. For every $\mathbf{x}_0 \in \Omega$, there is a local, regular, parametrized, two-dimensional manifold $\mathcal{M}$ solution of (2.3) *through $\mathbf{x}_0$ if and only if $\mathbf{u}$ verifies the integrability condition* (2.5).

Our goal is to look at (2.3) from a purely variational perspective, and, in particular, provide a mechanism to numerically approximate the local solutions implied by this proposition.

3. The one-dimensional case

Suppose a smooth vector field $\mathbf{u} : \mathbb{R}^N \to \mathbb{R}^N$ is given. Instead of looking for integral curves solutions of the differential system

$$\mathbf{x}'(t) = \mathbf{u}(\mathbf{x}(t)), \quad t \in \mathbb{R},$$

as it is the main concern for ODEs, we are instead interested about the orthogonal families of curves

$$\mathbf{x}'(t) \cdot \mathbf{u}(\mathbf{x}(t)) = 0 \text{ in } \mathbb{R}. \tag{3.1}$$

It is obvious that the way to deal with this last differential condition is by looking at the orthogonal differential system

$$\mathbf{x}'(t) = \mathbf{u}^{\perp}(\mathbf{x}(t)), \tag{3.2}$$

being aware that a reparametrization and a possible change of orientation may be involved. Since this procedure, or we should rather say, because this procedure of passing from a vector field $\mathbf{u}(\mathbf{x}) : \mathbb{R}^N \to \mathbb{R}^N$ to one which is orthogonal in dimension higher than two is not cannonical or unique in any way, we will rather stick to the form (3.1), and see to what extent we can enforce such a condition for full families of curves in $\mathbb{R}^N$. Notice that equation (3.1) is independent of the size of the vector field $\mathbf{u}(\mathbf{x})$.

As far as we can tell, there is no standard method to tackle solution curves $\mathbf{x}(t) : \mathbb{R} \to \mathbb{R}^N$ of (3.1) other than passing to (3.2). Since we are not willing to resort to the orthogonal vector field $\mathbf{u}^{\perp}$ to setup a differential system since, as indicated, this process is not canonical in higher-dimension, we will adopt a variational approach. This does not mean that we would like to avoid orthogonal fields $\mathbf{u}^{\perp}$ for other purposes as necessary or convenient. We will explore the optimization problem

$$\text{Minimize in } \mathbf{x}(t) : \quad E(\mathbf{x}) = \int_{-1}^{1} \frac{1}{2}(\mathbf{x}'(t) \cdot \mathbf{u}(\mathbf{x}(t))^2 \, dt \tag{3.3}$$

among all curves $\mathbf{x}(t) \in H^1(-1, 1; \mathbb{R}^N)$ such that $\mathbf{x}(0) = \mathbf{x}_0$, and $\mathbf{x}_0 \in \mathbb{R}^N$ is a fixed vector. The trivial, constant solution $\mathbf{x} \equiv \mathbf{x}_0$ is definitely a minimizer, but we are interested in finding non-trivial minimizers. To this end, consider the family of perturbed variational problems

$$\text{Minimize in } \mathbf{x}(t) : \quad E_\epsilon(\mathbf{x}) = \int_{-1}^{1} [\frac{1}{2\epsilon}(\mathbf{x}'(t) \cdot \mathbf{u}(\mathbf{x}(t)))^2 + \frac{1}{2}|\mathbf{x}'(t) - \mathbf{u}^{\perp}(\mathbf{x}_0)|^2] \, dt \tag{3.4}$$

for $\epsilon > 0$, under the same conditions as before, namely,

$$\mathbf{x}(t) \in H^1(-1, 1; \mathbb{R}^N), \quad \mathbf{x}(0) = \mathbf{x}_0.$$

The constant vector $\mathbf{u}^{\perp}(\mathbf{x}_0)$ can be taken to be in any way as long as it is orthogonal to $\mathbf{u}(\mathbf{x}_0)$. It can be chosen of unit length for normalization. It is clear that there is a unique minimizer $\mathbf{x}_\epsilon$ for such a problem, for each fixed, positive ϵ. This is standard. Since the end-point values at $\{-1, 1\}$ are not restricted in any way, such minimizer should comply with the transversality condition at both end-points. Because of the strict convexity of the integrand, this optimality condition at both end-points can be formulated by saying that $\mathbf{x}'_\epsilon(a)$, $a = \pm 1$, is the unique optimal solution $\mathbf{U} = \mathbf{x}'_\epsilon(a)$ of the mathematical program

$$\text{Minimize in } \mathbf{U} \in \mathbb{R}^2 : \quad \frac{1}{2\epsilon}(\mathbf{U} \cdot \mathbf{u}(\mathbf{x}_\epsilon(a)))^2 + \frac{1}{2}|\mathbf{U} - \mathbf{u}^{\perp}(\mathbf{x}_0)|^2 \tag{3.5}$$

In fact, this mathematical program plays an important role in our analysis in this section.

Lemma 3.1. *Let*

$$\mathbf{w}_\epsilon, \mathbf{w}_0 \neq \mathbf{0}, \mathbf{v} \in \mathbb{R}^N, \quad \mathbf{w}_\epsilon \to \mathbf{w}_0 \text{ as } \epsilon \to 0,$$

and consider the two mathematical programs

$$\text{Minimize in } \mathbf{u} \in \mathbb{R}^N : \quad \frac{1}{2}|\mathbf{u}-\mathbf{v}|^2 + \frac{1}{2\epsilon}(\mathbf{u}\cdot\mathbf{w}_\epsilon)^2,$$
$$\text{Minimize in } \mathbf{u} \in \mathbb{R}^N : \quad \frac{1}{2}|\mathbf{u}-\mathbf{v}|^2 \text{ under } \mathbf{u}\cdot\mathbf{w}_0 = 0.$$

Let $\mathbf{u}_\epsilon$, for each fixed $\epsilon > 0$, be the unique minimizer of the first, and $\mathbf{u}_0$, the unique minimizer of the second. Then $\mathbf{u}_\epsilon \to \mathbf{u}_0$ as $\epsilon \to 0$.

Proof. It is evident that

$$\frac{1}{2}|\mathbf{u}_\epsilon-\mathbf{v}|^2 + \frac{1}{2\epsilon}(\mathbf{u}_\epsilon\cdot\mathbf{w}_\epsilon)^2 \leq \frac{1}{2}|\mathbf{v}|^2$$

because $\mathbf{u}_\epsilon$ is the minimizer of the corresponding problem. This inequality implies, on the one hand, that $\mathbf{u}_\epsilon \to \tilde{\mathbf{u}}_0$, possibly along a certain sequence of values of ϵ which we do not care to relabel, and some $\tilde{\mathbf{u}}_0 \in \mathbb{R}^N$. On the other hand, $\mathbf{u}_\epsilon \cdot \mathbf{w}_\epsilon \to 0$, for otherwise the previous upper bound could not hold as $\epsilon \to 0$. In particular, $\tilde{\mathbf{u}}_0 \cdot \mathbf{w}_0 = 0$. We claim that in fact, $\tilde{\mathbf{u}}_0 = \mathbf{u}_0$.

Let $\mathbf{u}$ be feasible for the second problem, i.e. $\mathbf{u}\cdot\mathbf{w}_0 = 0$, and take $\tilde{\mathbf{u}}_\epsilon$ such that

$$\tilde{\mathbf{u}}_\epsilon \cdot \mathbf{w}_\epsilon = 0, \quad \tilde{\mathbf{u}}_\epsilon \to \mathbf{u}.$$

This is always possible provided $\mathbf{w}_0$ is not the null vector. Then

$$\frac{1}{2}|\mathbf{u}_\epsilon-\mathbf{v}|^2 \leq \frac{1}{2}|\mathbf{u}_\epsilon-\mathbf{v}|^2 + \frac{1}{2\epsilon}(\mathbf{u}_\epsilon\cdot\mathbf{w}_\epsilon)^2 \leq \frac{1}{2}|\tilde{\mathbf{u}}_\epsilon-\mathbf{v}|^2$$

again because of the fact that $\mathbf{u}_\epsilon$ is the minimizer for the first problem in the statement. As $\epsilon \to 0$, we see that

$$\frac{1}{2}|\tilde{\mathbf{u}}_0-\mathbf{v}|^2 \leq \frac{1}{2}|\mathbf{u}-\mathbf{v}|^2.$$

The arbitrariness of $\mathbf{u}$ implies that $\tilde{\mathbf{u}}_0$ is the minimizer of the second mathematical program in the statement, and by the uniqueness of such a minimizer, we conclude that

$$\mathbf{u}_\epsilon \to \tilde{\mathbf{u}}_0 = \mathbf{u}_0.$$

□

Our existence result for the one-dimensional case is the following.

Proposition 3.2. *Suppose $\mathbf{u}$ is a smooth vector field with $\mathbf{u}(\mathbf{x}_0)$ not null. Take any non-null, orthogonal vector $\mathbf{u}^\perp(\mathbf{x}_0)$ to it. Then problem* (3.3) *admits non-trivial minimizers $\mathbf{x} \in H^1(-1,1;\mathbb{R}^N)$ such that*

$$\mathbf{x}'(t)\cdot\mathbf{u}(\mathbf{x}(t)) = 0 \text{ for a.e. } t \in (-1,1), \quad \mathbf{x}(0) = \mathbf{x}_0, \mathbf{x}'(0) = \mathbf{u}^\perp(\mathbf{x}_0).$$

Proof. Recall that $\mathbf{x}_\epsilon$ is the unique minimizer for E_ϵ according to our above discussion. By considering the trivial feasible path $\mathbf{y}_\epsilon \equiv \mathbf{x}_0$, we see that

$$\int_{-1}^{1} [\frac{1}{2\epsilon}(\mathbf{x}_\epsilon'(t)\cdot\mathbf{u}(\mathbf{x}_\epsilon(t)))^2 + \frac{1}{2}|\mathbf{x}_\epsilon'(t) - \mathbf{u}^\perp(\mathbf{x}_0)|^2]\, dt = E_\epsilon(\mathbf{x}_\epsilon) \leq E_\epsilon(\mathbf{y}_\epsilon) = 1, \tag{3.6}$$

for all positive ϵ. Recall that we have taken

$$|\mathbf{u}^\perp(\mathbf{x}_0)| = 1.$$

Since the two terms in the functional E_ϵ are non-negative, this uniform upper bound implies that

$$\|\mathbf{x}'_\epsilon\|_{L^2(-1,1;\mathbb{R}^2)}$$

is bounded, and

$$\mathbf{x}'_\epsilon \cdot \mathbf{u}(\mathbf{x}_\epsilon) \to 0 \text{ in } L^2(-1,1).$$

In particular, there is a feasible weak limit $\mathbf{x}$,

$$\mathbf{x}_\epsilon \rightharpoonup \mathbf{x} \text{ in } H^1(-1,1;\mathbb{R}^2), \quad \mathbf{x}(0) = \mathbf{x}_0,$$

and, since the convergence of $\mathbf{x}_\epsilon$ to $\mathbf{x}$ is strong in $L^2(-1,1;\mathbb{R}^2)$, we can conclude that $\mathbf{x}'(t) \cdot \mathbf{u}(\mathbf{x}(t)) = 0$ for a.e. $t \in (-1,1)$. We would like to discard the possibility that this limit $\mathbf{x}$ be the trivial solution $\mathbf{x} \equiv \mathbf{x}_0$.

We go back to (3.6), to conclude that, because of the non-negativeness of the first term, and developing the square,

$$\int_{-1}^{1} \frac{1}{2}|\mathbf{x}'_\epsilon(t)|^2 \, dt - (\mathbf{x}_\epsilon(1) - \mathbf{x}_\epsilon(-1)) \cdot \mathbf{u}^\perp(\mathbf{x}_0) \le 0,$$

or

$$\|\mathbf{x}'_\epsilon\|^2_{L^2(-1,1;\mathbb{R}^2)} \le 2|\mathbf{x}_\epsilon(1) - \mathbf{x}_\epsilon(-1)|.$$

If the sequence of non-negative numbers on the left-hand side is uniformly away from zero, we can discard that the limit $\mathbf{x}$ be the constant, trivial path, because the limit of the right-hand side is $2|\mathbf{x}(1) - \mathbf{x}(-1)|$.

Suppose, then, that in fact

$$\|\mathbf{x}'_\epsilon\|^2_{L^2(-1,1;\mathbb{R}^2)} \to 0, \quad \mathbf{x}_\epsilon \to \mathbf{x}_0 \text{ in } L^\infty(-1,1;\mathbb{R}^2). \tag{3.7}$$

and hence

$$\mathbf{x}'_\epsilon \to \mathbf{0} \text{ in } L^2(-1,1;\mathbb{R}^2).$$

According to our above discussion concerning transversality, $\mathbf{x}'_\epsilon(a)$ is the unique solution of the mathematical program (3.5), and, after Lemma 3.1, it converges to the unique solution of

$$\text{Minimize in } \mathbf{U} \in \mathbb{R}^2 : \quad \frac{1}{2}|\mathbf{U} - \mathbf{u}^\perp(\mathbf{x}_0)|^2 \text{ subject to } \mathbf{U} \cdot \mathbf{u}(\mathbf{x}(a)) = 0,$$

which is given through the equation

$$\mathbf{U} - \mathbf{u}^\perp(\mathbf{x}_0) + \lambda \mathbf{u}(\mathbf{x}(a)) = \mathbf{0}, \quad \lambda = \frac{\mathbf{u}^\perp(\mathbf{x}_0) \cdot \mathbf{u}(\mathbf{x}(a))}{|\mathbf{u}(\mathbf{x}(a))|^2}.$$

If we assume that $\mathbf{x}(a) = \mathbf{x}_0$ for some a different from zero, then $\lambda = 0$, and

$$\mathbf{x}'_\epsilon(a) \to \mathbf{U}, \quad \mathbf{U} - \mathbf{u}^\perp(\mathbf{x}_0) = \mathbf{0}.$$

By taking into account that we can redo everything in the interval $(-a, a)$ with $0 < a < 1$ arbitrary, we reach a contradiction with (3.7) since $\mathbf{u}^\perp(\mathbf{x}_0)$ is not the null vector. □

There is another remarkable fact concerning the functional in (3.3).

Proposition 3.3. *Equilibria for* (3.3)*, and not just minimizers, not passing through a singularity of* $\mathbf{u}$ *and such that*

$$\mathbf{x}(0) = \mathbf{x}_0, \quad \mathbf{x}'(0) \cdot \mathbf{u}(\mathbf{x}_0) = 0,$$

are always solutions of (3.1)*.*

Proof. Once we know that there are minimizers $\mathbf{x}$ for (3.3), it is legitimate to investigate the form of optimality conditions. This is so for minimizers $\mathbf{x}$ not going through a singularity of $\mathbf{u}$, because otherwise $\mathbf{u}$ is assumed to be smooth, and $\mathbf{x}$ is absolutely continuous.

For the sake of notation, put

$$\gamma(t) = \mathbf{x}'(t) \cdot \mathbf{u}(\mathbf{x}(t))$$

for such a equilibria $\mathbf{x}(t)$. Optimality conditions read

$$-[\gamma \mathbf{u}(\mathbf{x})]' + \gamma \mathbf{x}' \nabla \mathbf{u}(\mathbf{x}) = \mathbf{0} \text{ in } (0,1), \quad \gamma(0) = 0.$$

Since $\mathbf{u}(\mathbf{x})$ is differentiable, the previous equations ensure that so is γ, and then

$$\gamma' \mathbf{u}(\mathbf{x}) + \gamma[\nabla \mathbf{u}(\mathbf{x})\mathbf{x}' - \mathbf{x}' \nabla \mathbf{u}(\mathbf{x})] = \mathbf{0} \text{ in } (0,1), \quad \gamma(0) = 0.$$

This is a collection of linear problems for γ having the trivial solution as the unique solution, i.e.

$$\mathbf{x}'(t) \cdot \mathbf{u}(\mathbf{x}(t)) \equiv 0 \text{ in } (0,1),$$

as desired. □

4. The two-dimensional case in $\mathbb{R}^3$

As usual, some ingredients for the passage to higher dimension may be just a generalization of the techniques in the previous section while others may require new ideas. In our situation, the most fundamental change is that we have to deal with surfaces and these are objects that depend on two independent variables. We have to deal with partial derivatives and ordinary differential equations become partial differential equations of some sort.

Surfaces are parametrized by vector mappings

$$\mathbf{x}(\mathbf{t}) : \mathbf{Q} \subset \mathbb{R}^2 \to \mathbb{R}^3, \quad \mathbf{t} = (t_1, t_2), \mathbf{x} = (x_1, x_2, x_3),$$

where $\mathbf{Q}$ is the unit square or the unit disk. The differential $\nabla \mathbf{x}(\mathbf{t})$ is a 3×2-matrix at every $\mathbf{t}$. We are also given a smooth vector field $\mathbf{u}(\mathbf{x}) : \mathbb{R}^3 \to \mathbb{R}^3$ with an isolated set of equilibria, in such a way that we may assume, if convenient, that it is a unitary vector field except in an isolated set of points where it is not defined. We also put

$$\mathbf{u}^\perp(\mathbf{x}) : \mathbb{R}^3 \to \mathbb{R}^{3\times 2}, \quad \mathbf{u}\mathbf{u}^\perp = \mathbf{0} \in \mathbb{R}^2, \text{rank}(\mathbf{u}^\perp(\mathbf{x})) = 2,$$

so that $\{\mathbf{u}(\mathbf{x}), \mathbf{u}^\perp(\mathbf{x})\}$ is a orthonormal basis of $\mathbb{R}^3$, except in those points where $\mathbf{u}$ is not defined. Fix a point $\mathbf{x}_0 \in \mathbb{R}^3$ where $\mathbf{u}$ does not vanish $\mathbf{u}(\mathbf{x}_0) \neq \mathbf{0}$.

Problem 4.1. *Find non-singular maps* $\mathbf{x}(\mathbf{t})$*, for which the rank of the matrix* $\nabla \mathbf{x}(\mathbf{t})$ *is* 2 *for a.e.* $\mathbf{t} \in \mathbf{Q}$*, such that*

$$\mathbf{u}(\mathbf{x}(\mathbf{t}))\nabla \mathbf{x}(\mathbf{t}) = \mathbf{0} \text{ in } \mathbf{Q}, \quad \mathbf{x}(\mathbf{0}) = \mathbf{x}_0. \tag{4.1}$$

Note that if we put

$$\mathbf{x} = (x, y, z), \quad \mathbf{u}(\mathbf{x}) = (P(x, y, z), Q(x, y, z), R(x, y, z))$$

then (4.1) becomes exactly the Pfaff equation (2.3).

To understand better the structure of such equations or systems, we become interested in the variational problem

$$\text{Minimize in } \mathbf{x}(\mathbf{t}): \quad E(\mathbf{x}) = \int_{\mathbf{Q}} \frac{1}{2} |\mathbf{u}(\mathbf{x}(\mathbf{t}))\nabla\mathbf{x}(\mathbf{t})|^2 \, d\mathbf{t} \tag{4.2}$$

where maps $\mathbf{x}(\mathbf{t}) \in H^1(\mathbf{Q}; \mathbb{R}^3)$ and

$$\mathbf{x}(\mathbf{0}) = \mathbf{x}_0 \in \mathbb{R}^3, \quad \nabla\mathbf{x}(\mathbf{0}) = \mathbf{u}^{\perp}(\mathbf{x}_0).$$

Intuitively, we suspect that this situation is much more delicate that its two-dimensional counterparts. Indeed, we can explicitly indicate the following fundamental differences, possibly among others:

(1) As far as we can tell, the main point in the one-dimensional situation to escape from the trivial, singular solution $\mathbf{x} \equiv \mathbf{x}_0$ cannot be valid in this case. Note that transversality conditions at end-points $\{-1, 1\}$ played a crucial role in that endeavor. This cannot be generalized to the higher-dimensional framework because natural boundary conditions now involve the vanishing of the normal derivative, but, in principle, not the full derivative. This is a main trouble.

(2) Another issue was coercivity. The role of the second term in (3.4) was to overcome this difficulty. Something similar will have to be implemented in the higher dimensional case.

(3) As we have seen in the preceding section, and indicated in the Introduction, there is no structural condition to be demanded on the field $\mathbf{u}$ for the one-dimensional case. However, this is not the case in the higher-dimensional situation. The differential constraint (2.5)

$$\mathbf{u} \cdot (\nabla \wedge \mathbf{u}) = 0$$

must play a crucial role in showing the existence of a solution for Problem 4.1.

(4) There is also the issue of orientation. We well know that orientation is also a fundamental feature to bear in mind when dealing with surfaces in $\mathbb{R}^3$, just as the orientation preserving condition is fundamental in non-linear hyperelasticity ([6], [9]). In this scenario, one could specify the constraint

$$\det \begin{vmatrix} \mathbf{u}(\mathbf{x}) \\ \nabla\mathbf{x} \end{vmatrix} > 0 \text{ in } \mathbf{Q},$$

to be held by competing mappings. Since we know from hyperelasticity and geometry that this is a rather delicate property to deal with, we will overlook it here.

Our proposal ought to incorporate a way to get around all of these difficulties, at least the first three. As stated, we will ignore the fourth one mainly because our computations did not show any particular difficulty with it.

For the first issue, to discard the constant trivial solution, we adopt a unilateral boundary condition of place ([9]) of the form

$$\Psi(\mathbf{x}) \leq 0 \text{ on } \partial\mathbf{Q}, \quad \Psi(\mathbf{x}) = R^2 - |\mathbf{x}|^2 \tag{4.3}$$

for some fixed $R > 0$, to be suitably chosen. Note that the trivial, constant map $\mathbf{x} \equiv \mathbf{x}_0$ violates such a condition, and so it is banished from our consideration from the very beginning. The planar mapping

$$\mathbf{X}_0(\mathbf{t}) = \mathbf{x}_0 + \mathbf{u}(\mathbf{x}_0)^\perp \mathbf{t},$$

where $\mathbf{u}(\mathbf{x}_0)^\perp$ is a selected basis of the plane passing through $\mathbf{x}_0$, as indicated earlier, and with normal vector $\mathbf{u}(\mathbf{x}_0)$, will also be important. As a matter of fact, R in (4.3) is chosen in such a way that $\mathbf{X}_0$ is feasible, i.e.

$$\Psi(\mathbf{X}_0) \leq 0 \text{ on } \partial\mathbf{Q}.$$

This is always possible.

To enforce coercivity, we will add to the functional in (4.2) the standard quadratic term

$$\int_{\mathbf{Q}} \frac{\epsilon}{2}(|\nabla \mathbf{x}(\mathbf{t})|^2 + |\mathbf{x}(\mathbf{t})|^2)\, d\mathbf{t}$$

as a small perturbation to it.

Concerning the central third point, we will examine the relevance of the differential integrability condition (2.5) when looking at optimality. If this condition holds, then we will check that every equilibrium solution $\mathbf{x}$ will be a solution of Problem 4.1, thus excluding the possibility that in approximating minimizers in (4.2) iterates may get stuck in local minima. This is a major advantage for our numerical treatment of solutions.

We will then focus on the perturbed functional

$$E_\epsilon(\mathbf{x}) = \int_{\mathbf{Q}} \left(\frac{1}{2}|\mathbf{u}(\mathbf{x}(\mathbf{t}))\nabla \mathbf{x}(\mathbf{t})|^2 + \frac{\epsilon}{2}|\nabla \mathbf{x}(\mathbf{t})|^2 + \frac{\epsilon}{2}|\mathbf{x}(\mathbf{t})|^2 \right) d\mathbf{t}, \quad \epsilon \geq 0, \tag{4.4}$$

and look for minimizers $\mathbf{x}_\epsilon \in H^1(\mathbf{Q}; \mathbb{R}^3)$ under the conditions

$$\mathbf{x}(\mathbf{0}) = \mathbf{x}_0, \quad \Psi(\mathbf{x}) \leq 0 \text{ on a fixed neighborhood of } \partial\mathbf{Q}. \tag{4.5}$$

As noticed above, the plane map $\mathbf{X}_0$ is feasible, and so this variational problem is well-posed. We will simply say, for the sake of simplicity, that $\Psi(\mathbf{x}) \leq 0$ on $\partial\mathbf{Q}$, but we actually mean (4.5).

Proposition 4.2. *Let*

$$\mathbf{u}(\mathbf{x}) : \mathbf{B}_r(\mathbf{x}_0) \subset \mathbb{R}^3 \to \mathbb{R}^3, \quad r > R,$$

be a smooth, non-vanishing vector field.

1. *For each $\epsilon > 0$, there is a minimizer $\mathbf{x}_\epsilon \in H^1(\mathbf{Q}; \mathbb{R}^3)$ for (4.4).*
2. *The family $\{\mathbf{x}_\epsilon\}$ is minimizing for the unperturbed functional E_0.*

Proof. For each $\epsilon > 0$, the integrand of E_ϵ is coercive and convex (in $\nabla \mathbf{x}$) and so (1) holds. Note that if $\{\mathbf{x}_{\epsilon,j}\}$ is a minimizing sequence such that

$$\mathbf{x}_{\epsilon,j} \rightharpoonup \mathbf{x}_\epsilon \text{ in } H^1(\mathbf{Q}; \mathbb{R}^3), \quad \Psi(\mathbf{x}_{\epsilon,j}) \leq 0 \text{ on } \partial\mathbf{Q}$$

then $\mathbf{x}_{\epsilon,j} \to \mathbf{x}_\epsilon$ in $L^2(\mathbf{Q})$, and so

$$\Psi(\mathbf{x}_\epsilon) \leq 0 \text{ on } \partial\mathbf{Q}.$$

To prove (2), let $\{\mathbf{x}_\epsilon\}$ be a minimizer of the functional $E_\epsilon(\mathbf{x})$, for each $\epsilon > 0$ and put

$$E_0(\mathbf{x}) = E_\epsilon(\mathbf{x})|_{\epsilon=0} (= E(\mathbf{x})).$$

From

$$E_\epsilon(\mathbf{x}_\epsilon) \leq E_\epsilon(\mathbf{x}) = E_0(\mathbf{x}) + \int_{\mathbf{Q}} \left(\frac{\epsilon}{2} |\nabla \mathbf{x}(\mathbf{t})|^2 + \frac{\epsilon}{2} |\mathbf{x}(\mathbf{t})|^2 \right) \, d\mathbf{t}$$

for all admissible $\mathbf{x}$ and $\epsilon > 0$; and

$$E_0(\mathbf{x}_\epsilon) \leq E_0(\mathbf{x}_\epsilon) + \int_{\mathbf{Q}} \left(\frac{\epsilon}{2} |\nabla \mathbf{x}_\epsilon(\mathbf{t})|^2 + \frac{\epsilon}{2} |\mathbf{x}_\epsilon(\mathbf{t})|^2 \right) \, d\mathbf{t} = E_\epsilon(\mathbf{x}_\epsilon),$$

it then follows

$$\liminf_{\epsilon \to 0} E_0(\mathbf{x}_\epsilon) \leq E_0(\mathbf{x}),$$

which, from the arbitrariness of admissible $\mathbf{x}$, completes the proof. □

In general, there cannot be a way to show that this family of minimizers $\{\mathbf{x}_\epsilon\}$ may admit a sequence converging to anything in $H^1(\mathbf{Q}; \mathbb{R}^3)$, since we know that this is impossible unless we have the integrability condition (2.5). As we know, if such condition $\mathbf{u} \cdot (\nabla \wedge \mathbf{u}) = 0$ does hold, then

$$\mathbf{u}(\mathbf{x}) = \lambda(\mathbf{x}) \nabla U(\mathbf{x}), \quad U : \mathbf{B}_r(\mathbf{x}_0) \subset \mathbb{R}^3 \to \mathbb{R},$$

for some scalar, smooth, non-vanishing functions $\lambda(\mathbf{x})$ and $U(\mathbf{x})$. It is then elementary to argue that feasible maps $\mathbf{x}$ with $U(\mathbf{x}) = U(\mathbf{x}_0)$ will be minimizers of E_0. By the way, note that in the two-dimensional situation there is always (al least locally) an integrating factor $\lambda(\mathbf{x})$ for every field $\mathbf{u}(\mathbf{x})$ transforming it into a gradient field. Alternatively, one can invoke the local existence theorem in [3] under the same integrability condition.

5. Optimality conditions

We would like to explore optimality conditions for the Pfaffian functional $E_0 \equiv E$ given explicitly by

$$E(\mathbf{x}) = \frac{1}{2} \int_Q \left(\mathbf{u}(\mathbf{x}(\mathbf{t})) \cdot \mathbf{x}_{t_1}(\mathbf{t})^2 + \mathbf{u}(\mathbf{x}(\mathbf{t})) \cdot \mathbf{x}_{t_2}(\mathbf{t})^2 \right) \, d\mathbf{t} \tag{5.1}$$

where $\mathbf{x}_{t_i}$ means differentiation of $\mathbf{x}$ with respect to the variable t_i, $i = 1, 2$, and defined for the same class of embedded surfaces as before. The integrand is given explicitly by

$$F(\mathbf{y}, \mathbf{z}) = \frac{1}{2} (\mathbf{u}(\mathbf{y}) \cdot \mathbf{z}_1)^2 + \frac{1}{2} (\mathbf{u}(\mathbf{y}) \cdot \mathbf{z}_2)^2, \quad \mathbf{z} = \begin{pmatrix} \mathbf{z}_1 \\ \mathbf{z}_2 \end{pmatrix}.$$

It is easy to find the optimality system for E, and to derive some interesting consequences.

Proposition 5.1. *Let the mapping* $\mathbf{x}$ *be a smooth, critical map for the Pfaffian functional* (5.1).

(1) *If the condition*

$$\mathbf{u} \cdot (\nabla \wedge \mathbf{u}) = 0$$

holds, then $\mathbf{x}(Q)$ *is a non-singular, embedded, surface (with boundary) which is a solution of the corresponding Pfaffian system*

$$\mathbf{u} \cdot d\mathbf{x} = 0. \tag{5.2}$$

(2) *At any rate, we must always have*

$$(\mathbf{u}(\mathbf{x})\cdot\mathbf{x}_{t_1})_{t_1}+(\mathbf{u}(\mathbf{x})\cdot\mathbf{x}_{t_2})_{t_2}=0,$$

and then, for almost every $\mathbf{x}_0$ *determining the critical map* $\mathbf{x}(0)=\mathbf{x}_0$*, either the Pfaffian functional* E *does not vanish, or else the surface* $\mathbf{x}(Q)$ *is singular with the two tangent vectors* $\mathbf{x}_{t_i}$ *being dependent.*

Proof. For each $i=1,2$, the optimality system incorporates two terms of the form

$$-[\mathbf{u}(\mathbf{x})\cdot\mathbf{x}_{t_i}\,\mathbf{u}(\mathbf{x})]_{t_i}+\mathbf{u}(\mathbf{x})\cdot\mathbf{x}_{t_i}\,\mathbf{x}_{t_i}\nabla\mathbf{u}(\mathbf{x}).$$

Taking into account the identity

$$\mathbf{v}\nabla\mathbf{u}-\nabla\mathbf{u}\mathbf{v}=\mathbf{v}\wedge(\nabla\wedge\mathbf{u})$$

valid for three-dimensional vectors, this sum can be rewritten as

$$-[\mathbf{u}(\mathbf{x})\cdot\mathbf{x}_{t_i}]_{t_i}\mathbf{u}(\mathbf{x})+\mathbf{u}(\mathbf{x})\cdot\mathbf{x}_{t_i}\,\mathbf{x}_{t_i}\wedge(\nabla\wedge\mathbf{u}(\mathbf{x})).$$

Note that $\nabla\wedge\mathbf{u}$ is the curl of the vector field $\mathbf{u}$. Altogether, we find that the Euler-Lagrange system can be cast in the form

$$\begin{aligned}-[(\mathbf{u}(\mathbf{x})\cdot\mathbf{x}_{t_1})_{t_1}+(\mathbf{u}(\mathbf{x})\cdot\mathbf{x}_{t_2})_{t_2}]\mathbf{u}(\mathbf{x})\\ +[(\mathbf{u}(\mathbf{x})\cdot\mathbf{x}_{t_1})\mathbf{x}_{t_1}+(\mathbf{u}(\mathbf{x})\cdot\mathbf{x}_{t_2})\mathbf{x}_{t_2}]\wedge(\nabla\wedge\mathbf{u}(\mathbf{x}))=\mathbf{0}.\end{aligned}$$

The vector field

$$\Pi\mathbf{u}\equiv[(\mathbf{u}(\mathbf{x})\cdot\mathbf{x}_{t_1})\mathbf{x}_{t_1}+(\mathbf{u}(\mathbf{x})\cdot\mathbf{x}_{t_2})\mathbf{x}_{t_2}]$$

belongs to the tangent space spanned by the two basic tangent vectors $\mathbf{x}_{t_1}$ and $\mathbf{x}_{t_2}$. It would be the orthogonal projection onto it, if $\{\mathbf{x}_{t_1},\mathbf{x}_{t_2}\}$ is a orthonormal basis. We write the optimality system in the compact form

$$-\operatorname{Div}(\mathbf{u}(\mathbf{x})\nabla\mathbf{x})\,\mathbf{u}+\Pi\mathbf{u}\wedge(\nabla\wedge\mathbf{u})=\mathbf{0}, \tag{5.3}$$

where

$$\operatorname{Div}(\mathbf{u}(\mathbf{x})\nabla\mathbf{x})\equiv(\mathbf{u}(\mathbf{x})\cdot\mathbf{x}_{t_1})_{t_1}+(\mathbf{u}(\mathbf{x})\cdot\mathbf{x}_{t_2})_{t_2}.$$

It is instructive to realize that the inner product $\mathbf{u}\cdot\Pi\mathbf{u}$ is exactly, except for a constant, the integrand of the Pfaffian functional E.

We claim that the function $\operatorname{Div}(\mathbf{u}(\mathbf{x})\nabla\mathbf{x})$ ought to vanish identically always. Otherwise, if it does not, assuming that $\mathbf{u}$ is never the null vector and multiplying (5.3) by $\Pi\mathbf{u}$ and $\nabla\wedge\mathbf{u}$, we would have that

$$\mathbf{u}\cdot(\nabla\wedge\mathbf{u})=\mathbf{u}\cdot\Pi\mathbf{u}=\mathbf{0},$$

and $\mathbf{x}$ would become a global minimizer of E in such a region, i.e. $\mathbf{u}(\mathbf{x})\nabla\mathbf{x}\equiv 0$. But if this is so, then $\operatorname{Div}(\mathbf{u}(\mathbf{x})\nabla\mathbf{x})$ identically vanishes as well.

Once we know that $\operatorname{Div}(\mathbf{u}(\mathbf{x})\nabla\mathbf{x})$ identically vanishes, the optimality system (5.3) then leads to $\Pi\mathbf{u}\wedge(\nabla\wedge\mathbf{u})=\mathbf{0}$, and

$$\Pi\mathbf{u}=\lambda(\nabla\wedge\mathbf{u}),\ \text{some scalar function }\lambda.$$

If the integrability condition $\mathbf{u}\cdot(\nabla\wedge\mathbf{u})=0$ holds, then we deduce immediately that $\Pi\mathbf{u}\cdot\mathbf{u}$ vanishes and the regular surface with parameterization $\mathbf{x}$ becomes a solution of the associated Pfaffian equation. If, on the other hand, the integrability condition does not hold, then either $\Pi\mathbf{u}\cdot\mathbf{u}$ is not zero; or if it is, the scalar function λ identically vanishes. In this last situation, $\Pi\mathbf{u}$ vanishes and so does $\Pi\mathbf{u}\cdot\mathbf{u}$, hence the solution of the Pfaffian equation cannot be regular (having dimension two) for almost every point $\mathbf{x}_0$ because that would imply the integrability condition according to the equivalence in Proposition 2.1. □

It is not clear, in the situation where the integrability condition does not hold, how the non-vanishing field $\mathbf{u} \cdot (\nabla \wedge \mathbf{u})$ determines the non-vanishing value of the Pfaffian functional E.

The principal feature of our numerical method based on the minimization of the Pfaffian functional is the following corollary.

Corollary 5.2. *Let $\mathbf{u} : \Omega \subset \mathbb{R}^3 \to \mathbb{R}^3$ be a no-where vanishing, smooth vector field. If the integrability condition $\mathbf{u} \cdot (\nabla \wedge \mathbf{u}) = 0$ holds, then every stationary map $\mathbf{x} : Q \to \mathbb{R}^3$ of the Pfaffian functional E in (5.1) is a solution of the Pfaffian equation (5.2).*

The significance of this fact implies that a numerical method to approximate stationary maps for the functional E can never get stuck in local minima or other kinds of equilibrium maps, if the integrability condition holds. The functional E is systematically pushed to zero. This is a fundamental certificate of convergence of our variational approach.

6. Approximation

6.1. **Numerical approach.** We explore numerically the approximating global minimizers of (4.2):

$$\text{Minimize in } \mathbf{x}(\mathbf{t}) : \quad E(\mathbf{x}) = \int_{\mathbf{Q}} \frac{1}{2} |\mathbf{u}(\mathbf{x}(\mathbf{t}))\nabla\mathbf{x}(\mathbf{t})|^2 \, d\mathbf{t}$$

where maps $\mathbf{x}(\mathbf{t}) \in H^1(\mathbf{Q}; \mathbb{R}^3)$ and

$$\mathbf{x}(\mathbf{0}) = \mathbf{x}_0 \in \mathbb{R}^3, \quad \nabla\mathbf{x}(\mathbf{0}) = \mathbf{u}^{\perp}(\mathbf{x}_0),$$

furnishing approximated local solutions to Problem 4.1, through typical descent methods. We would like to stress again the two fundamental features of our variational approach in action when utilized for approximation:

(1) There is no danger of local minima or other types of equilibrium solutions, provided the given field $\mathbf{u}$ complies with the integrability condition $\mathbf{u} \cdot (\nabla \wedge \mathbf{u}) = 0$ (Corollary 5.2);
(2) the fact that functional E goes down to zero is taken as a certificate of convergence to a true solution, since $E = 0$ means

$$\mathbf{u}(\mathbf{x}) \cdot \frac{\partial \mathbf{x}}{\partial t_1} = \mathbf{u}(\mathbf{x}) \cdot \frac{\partial \mathbf{x}}{\partial t_2} = 0, \quad \mathbf{t} = (t_1, t_2); \text{ and}$$

(3) there has not been any need to implement the unilateral boundary condition of place (4.3) as our approximations have never gone to the singular solution.

We applied a Conjugate Gradient (CG) type scheme with Fletcher and Reeves update formula [13] (among several other different possibilities, see e.g. [16]) with a simple, yet effective, line search which will be explained in detail below. Our numerical experiments have been implemented using the free software FreeFem++ v4.11 (available at http://www.freefem.org/; see also [19]) and for the visualization of the surfaces we have used Paraview 5.11.0 (available at https://www.kitware.com/open-source/# paraview), which is also free. We have considered other numerical methods for the numerical approximation of the solution of the problem under analysis, beside the CG scheme. We have also explored an Gradient Descent (GD) and also

Newton-Rapshon (NR) algorithms, for the functional E above, in order to approximate its optimal solutions. In our computations, CG performed better than GD, both with the same type of line search. The main reasons why we have opted for CG over NR was, on the one hand because the former performed quite well, while on the other, we wanted to deliberately avoid the known sensitivity to initial conditions of NR type schemes since we always use as initial condition a plane which only has to comply with the only constraint of our problem, that is $\mathbf{x}(\mathbf{0}) = \mathbf{x}_0$.
The Conjugate Gradient is as follows: given $\mathbf{x}^0 \in H^1(\mathbf{Q}, \mathbb{R}^3)$, $\overline{\alpha} > 0$ and $c \in (0, 1)$,

- $\mathbf{p}^0 := -\nabla E(\mathbf{x}^0)$
- $\mathbf{x}^1 := \mathbf{x}^0 + \alpha^0 \mathbf{p}^0$

until $E(\mathbf{x}^k) < tol$ or $\frac{||\nabla E(\mathbf{x}^k)||_\infty}{||\mathbf{x}^k||_\infty} < tol$:

- $\nabla E(\mathbf{x}^k)$
- $\beta^k := \frac{||\nabla E(\mathbf{x}^k)||^2_{L^2}}{||\nabla E(\mathbf{x}^{k-1})||^2_{L^2}}$
- $\mathbf{p}^k := -\nabla E(\mathbf{x}^k) + \beta^k \mathbf{p}^{k-1}$
- $\mathbf{x}^{k+1} := \mathbf{x}^k + \alpha^k \mathbf{p}^k$.

We set the tolerance $tol = 1. \times 10^{-6}$ for our computations. To calculate α^k, in each step, we do not perform an exact line search, mainly due to its computational cost; instead, to determine the step size, we make a standard simple approximation, which can be found in [24], that will give us a second order approximation of the optimal value: for a fixed $\overline{\alpha} > 0$ given, we select

$$\alpha^k = \frac{1}{2} \frac{\overline{\alpha}^2 \langle \nabla E(\mathbf{x}^k), \mathbf{p}^k \rangle_{H^1}}{E(\mathbf{x}^k + \overline{\alpha}\mathbf{p}^k) - E(\mathbf{x}^k) + \overline{\alpha} \langle \nabla E(\mathbf{x}^k), \mathbf{p}^k \rangle_{H^1}},$$

if

$$E(\mathbf{x}^k + \overline{\alpha}\mathbf{p}^k) - E(\mathbf{x}^k) + c\,\overline{\alpha} \langle \nabla E(\mathbf{x}^k), \mathbf{p}^k \rangle_{H^1} > 0,$$

for a certain pre-chosen $c \in (0, 1)$. Otherwise we simply select $\alpha^k = \overline{\alpha}$. To compute $\nabla E(\mathbf{x})$, we use the equality

$$\delta E(\mathbf{x}, \mathbf{v}) = \langle \nabla E(\mathbf{x}), \mathbf{v} \rangle_{H^1}, \tag{6.1}$$

for every $\mathbf{v} \in H^1(\mathbf{Q}, \mathbb{R}^3))$, where $\delta E(\mathbf{x}, \mathbf{v})$ is the Gateaux derivative

$$\begin{aligned} \delta E(\mathbf{x}, \mathbf{v}) = \int_{\mathbf{Q}} & \mathbf{u}(\mathbf{x}) \cdot \mathbf{x}_{t_1} \left[(\nabla \mathbf{u}(\mathbf{x})\, \mathbf{v}) \cdot \mathbf{x}_{t_1} + \mathbf{u}(\mathbf{x}) \cdot \mathbf{v}_{t_1} \right] \\ & + \mathbf{u}(\mathbf{x}) \cdot \mathbf{x}_{t_2} \left[(\nabla \mathbf{u}(\mathbf{x})\, \mathbf{v}) \cdot \mathbf{x}_{t_2} + \mathbf{u}(\mathbf{x}) \cdot \mathbf{v}_{t_2} \right] d\mathbf{t}, \ \mathbf{t} = (t_1, t_2). \end{aligned}$$

And so, to get the desired gradient, we have to solve the linear, coupled PDE system in (6.1). Our reference domain will be

$$\mathbf{Q} = \{(t_1, t_2) \in \mathbb{R}^2 : 0.0001 < t_1^2 + t_2^2 < 1\}$$

and the mesh we use has 11365 vertices (with 3 of them on the inner boundary in which we will impose $\mathbf{v} \equiv 0$) and 22377 triangles, see Figure 1. We made this choice instead of the more standard one

$$\mathbf{Q}' = \{(t_1, t_2) \in \mathbb{R}^2 : t_1^2 + t_2^2 < 1\}$$

because with $\mathbf{Q}$ we have a very simple and yet effective way of imposing the condition $\mathbf{x}(\mathbf{0}) = \mathbf{x}_0$ in FreeFem++ to the whole family of approximate solutions. We use P_2-Lagrange finite element approximations for the solutions $\mathbf{x}$, in order to have sharp approximations. As mentioned before, we wanted a method which can be

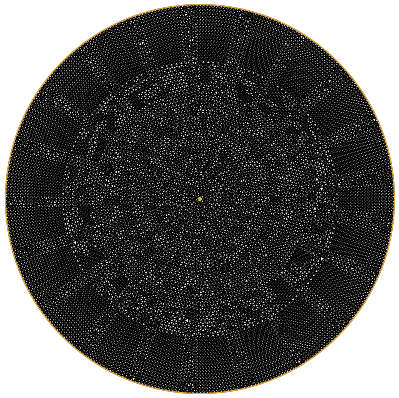


FIGURE 1. Mesh for the domain $\mathbf{Q}$.

implemented in the more interesting situations, that is, the ones for which we don't have any clue about the solution of the Pfaffian equation; and so one important aspect is to have a procedure for which a general, simple initialization like a plane passing through $\mathbf{x}(\mathbf{0}) = \mathbf{x}_0$ and orthogonal to $\mathbf{u}(\mathbf{x}_0)$ will suffice. Note that the local convergence character of the NR method would force us to select an initialization sufficiently close to a solution, which in general will be not known a priori.
We have explored, numerically, different explicit examples, which will be detailed in the following section.

6.2. **Some examples.**

Example 1. *The case of spheres. In this case we have*

$$\mathbf{u}(x_1, x_2, x_3) = (2x_1, 2x_2, 2x_3),\ \mathbf{x}(\mathbf{0}) = (0, 0, 1)$$

and so we can use the plane $\mathbf{x}^0 = (t_1, t_2, 1)$ *as initialization. From the numerical point of view, we observe that, for our simulations, the CG method is very quick, since with 8 iterations we attain the value*

$$E(\mathbf{x}^8) = 2.31923 \times 10^{-7}.$$

The evolution of the log *cost of* $E(\mathbf{x}^k)$ *can be seen in Figure 2b, while the plot of* $\mathbf{x}^8$ *can be seen in Figure 2a. The exact solution in this case is known a priori,* $\mathbf{x} \equiv x_1^2 + x_2^2 + x_3^2 = 1$*, and so we can estimate the error in* L^2 *norm over the domain* $\mathbf{Q}$*, which is*

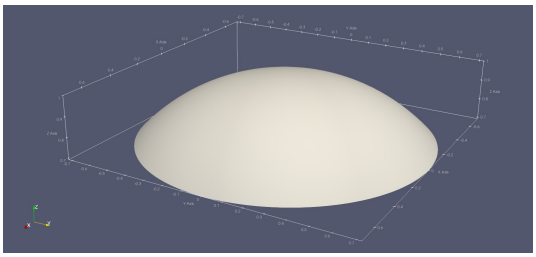
$$||\mathbf{x}^8 - \mathbf{x}||_{L^2} = 7.98085 \times 10^{-4}.$$

In order to test the robustness of our approximations, we have also added some small perturbation to the initial data

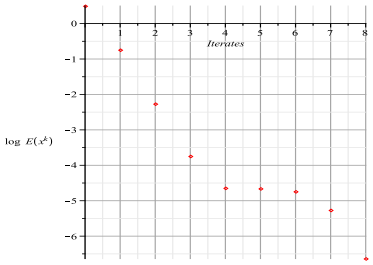
$$\mathbf{x}^0 = (t_1 + 0.001(t_1^2 + t_2^2), t_2 - 0.001(t_1^2 + t_2^2), 1 + 0.002(t_1^2 + t_2^2))$$

and then run the computations again. We attained the tolerance, again with 8 iterations, with the values

$$E(\mathbf{x}^8) = 1.46309 \times 10^{-7},$$
$$||\mathbf{x}^8 - \mathbf{x}||_{L^2} = 5.93937 \times 10^{-4}$$

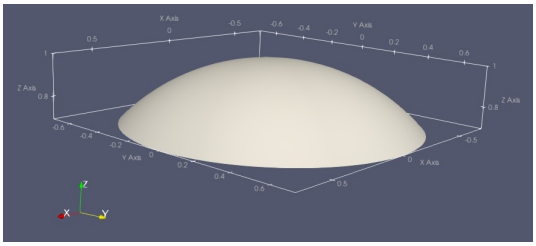


(A) Plot of $\mathbf{x}^8$

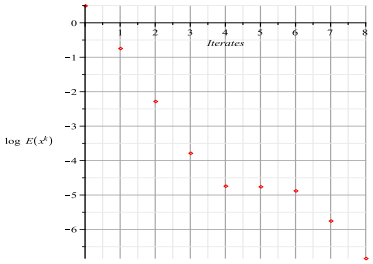


(B) Evolution of log cost

FIGURE 2. Approximate solution for $\mathbf{u}(x_1, x_2, x_3) = (2x_1, 2x_2, 2x_3)$, with $\mathbf{x}(\mathbf{0}) = (0, 0, 1)$, using initialization $\mathbf{x}^0 = (t_1, t_2, 1)$.



(A) Plot of $\mathbf{x}^8$



(B) Evolution of log cost

FIGURE 3. Approximate solution for $\mathbf{u}(x_1, x_2, x_3) = (2x_1, 2x_2, 2x_3)$, with $\mathbf{x}(\mathbf{0}) = (0, 0, 1)$, using the perturbed data $\mathbf{x}^0 = (t_1 + 0.001(t_1^2 + t_2^2), t_2 - 0.001(t_1^2 + t_2^2), 1 + 0.002(t_1^2 + t_2^2))$.

Figures 3a and 3b complete the evidenced robustness to perturbation of initial data.
One is not obliged to use the plane which is orthogonal to $\mathbf{x}(\mathbf{0})$ *for initialization: in fact, if we set* $\mathbf{x}^0 = (0.25t_1, 0.75t_2, 1)$ *as the new initialization (notice that for this plane we also have the value* $(0, 0, 1)$ *for* $(t_1, t_2) = (0, 0)$*, in order to comply with the constraint* $\mathbf{x}(\mathbf{0}) = \mathbf{x}_0$*; it is straightforward to solve the system for another initial point* $\mathbf{x}_0$*), we reach the tolerance with 6 iterations (see also Figure 4b):*

$$E(\mathbf{x}^6) = 5.15129 \times 10^{-7},$$

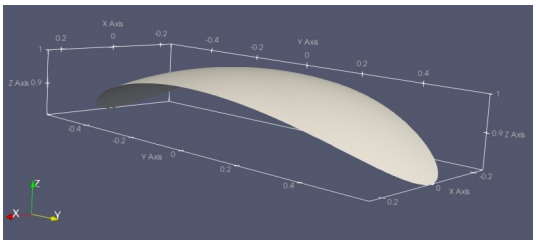
this time with the error

$$||\mathbf{x}^6 - \mathbf{x}||_{L^2} = 2.29167 \times 10^{-4},$$

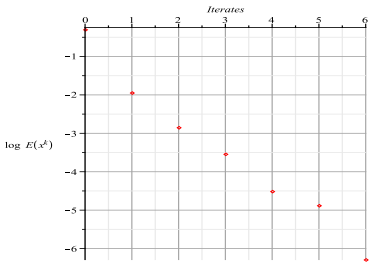
despite the fact that the graph (Figure 4a) could somehow mislead us is this case since the solution is a different piece of the sphere.

Example 2. *The case of hyperbolic paraboloids. We set*

$$\mathbf{u}(x_1, x_2, x_3) = (2x_1, -2x_2, 1), \ \mathbf{x}(\mathbf{0}) = (0, 0, 1).$$

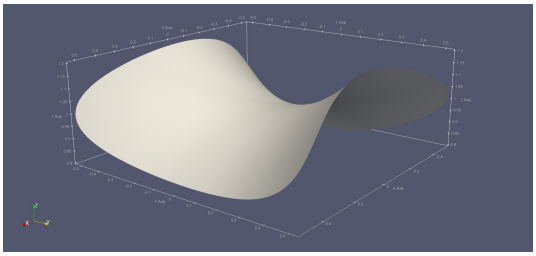


(A) Plot of $\mathbf{x}^6$

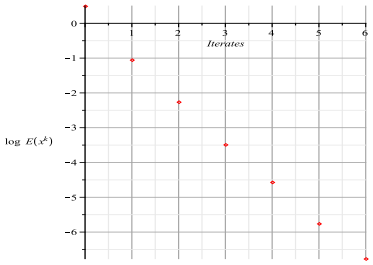


(B) Evolution of log cost

FIGURE 4. Approximate solution for $\mathbf{u}(x_1, x_2, x_3) = (2x_1, 2x_2, 2x_3)$, with $\mathbf{x}(\mathbf{0}) = (0, 0, 1)$, using initialization $\mathbf{x}^0 = (0.25t_1, 0.75t_2, 1)$.



(A) Plot of $\mathbf{x}^6$



(B) Evolution of log cost

FIGURE 5. Approximate solution for $\mathbf{u}(x_1, x_2, x_3) = (2x_1, -2x_2, 1)$, with $\mathbf{x}(\mathbf{0}) = (0, 0, 1)$, using initialization $\mathbf{x}^0 = (t_1, t_2, 1)$.

In this case we use again, as initialization, the plane $\mathbf{x}^0 = (t_1, t_2, 1)$. *With only 6 iterations we obtain*

$$E(\mathbf{x}^6) = 1.71941 \times 10^{-7}.$$

The exact solution is also known in this case: $\mathbf{x} \equiv x_1^2 - x_2^2 + x_3 = 1$, *and so we can estimate the error obtained by our approximation in* L^2 *norm over the domain* $\mathbf{Q}$, *which is*

$$||\mathbf{x}^6 - \mathbf{x}||_{L^2} = 5.32093 \times 10^{-5}.$$

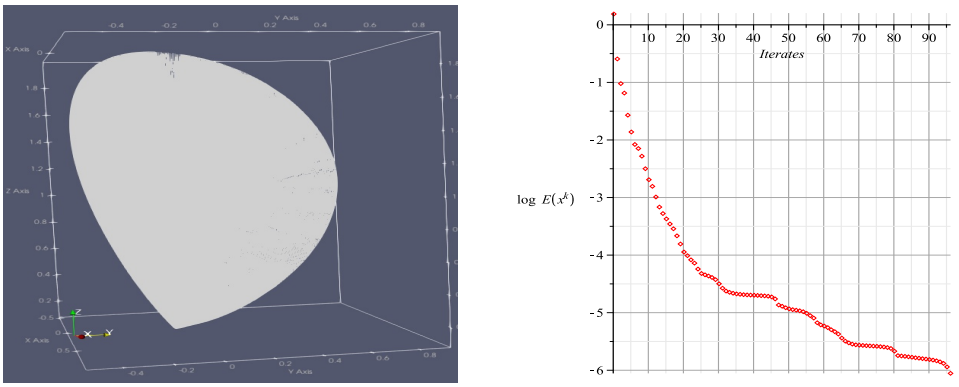
The plot of $\mathbf{x}^6$ *can be seen in Figure 5a while the evolution of* log *cost of* $E(\mathbf{x}^k)$ *can be seen in Figure 5b.*

Example 3. *The case of a two sheets hyberboloid. With*

$$\mathbf{u}(x_1, x_2, x_3) = (x_2 + x_3, x_1 + x_3, x_1 + x_2), \mathbf{x}(\mathbf{0}) = (1, 0, 0),$$

we use as initialization, the plane $\mathbf{x}^0 = (t_1 + 1, t_2, 0)$. *In this case we go below the tolerance after 93 iterations:*

$$E(\mathbf{x}^{93}) = 9.15743 \times 10^{-7}.$$



(A) Plot of $\mathbf{x}^{93}$ (B) Evolution of log cost

FIGURE 6. Approximate solution for $\mathbf{u}(x_1, x_2, x_3) = (x_2 + x_3, x_1 + x_3, x_1 + x_2)$, with $\mathbf{x}(\mathbf{0}) = (1, 0, 0)$, using initialization $\mathbf{x}^0 = (t_1 + 1, t_2, 0)$.

which is still quite reasonable. The exact solution in this case is $\mathbf{x} \equiv x_1x_2 + x_1x_3 + x_2x_3 = 0$*, which enables us to estimate the error obtained by our approximation in* L^2 *norm over the domain* $\mathbf{Q}$*, which is*

$$||\mathbf{x}^{93} - \mathbf{x}||_{L^2} = 7.46709 \times 10^{-4}.$$

The plot of approximate solution and the evolution of log *cost of* $E(\mathbf{x}^k)$ *can be seen, respectively, in Figures 6a and 6b.*

Example 4. *A non-integrable case. In this example, we put*

$$\mathbf{u}(x_1, x_2, x_3) = (x_2, x_3, x_1), \ \mathbf{x}(\mathbf{0}) = (1, 1, 0)$$

and use as initialization the plane $\mathbf{x}^0 = (t_2 + 1, t_1 + 1, -t_2)$*. It is straightforward to see that the integrability condition* (2.5) *is not satisfied, so there does not exists any (even non-constant) multiple of* $\mathbf{u}$ *such that it becomes the gradient of some scalar function* $f(x_1, x_2, x_3)$*. As condition* (2.5) *does not hold, if the system possesses a solution, it cannot be a regular, 2-dimensional solution. In fact, we can see in Figure 7a that the initial plane collapses into a curve in the space.*
After 1100 iterations, we attain the fixed threshold, obtaining

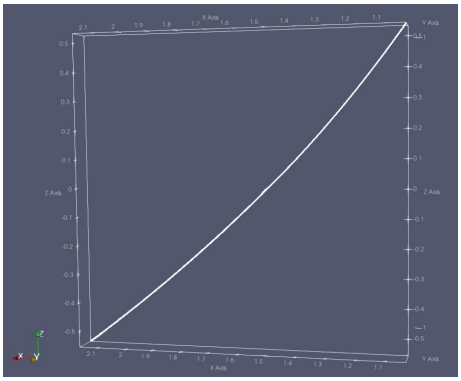
$$E(\mathbf{x}^{1100}) = 9.999582067 \times 10^{-7}.$$

From the graph of the evolution of log *cost of* $E(\mathbf{x}^k)$ *(Figure 7b) one can observe that we only need less than 150 iterations (in fact, exactly 138 iterations are needed) to go below* $1. \times 10^{-5}$*.*

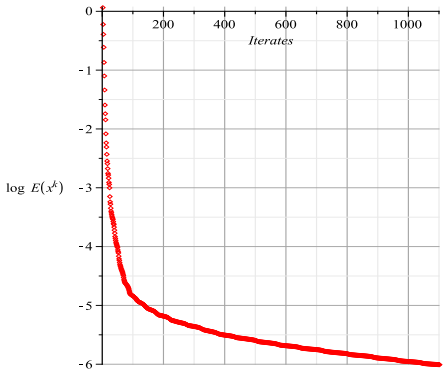
Example 5. *An integrable case where we don't know a priori the solution. We set*

$$\mathbf{u}(x_1, x_2, x_3) = (-x_2, x_1, x_1^2x_3), \ \mathbf{x}(\mathbf{0}) = (0.8, -1, 0).$$

It is clear that this (nonlinear) vector function is not a gradient of some scalar function $f(x_1, x_2, x_3)$ *but, as it verifies the integrability condition* (2.5)*, there must exist some function* $\lambda(x_1, x_2, x_3)$ *such that* $\lambda\mathbf{u}$ *is the gradient of such* f*.*

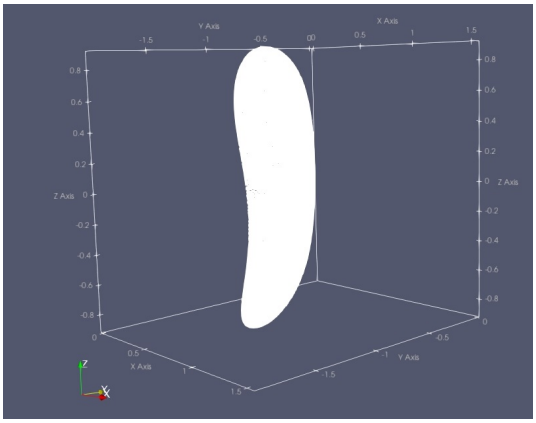


(A) Plot of $\mathbf{x}^{1100}$

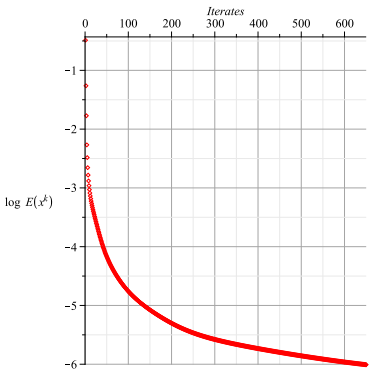


(B) Evolution of log cost

FIGURE 7. Approximate solution for $\mathbf{u}(x_1, x_2, x_3) = (x_2, x_3, x_1)$, with $\mathbf{x}(\mathbf{0}) = (1, 1, 0)$, using initialization $\mathbf{x}^0 = (t_2 + 1, t_1 + 1, -t_2)$.



(A) Plot of $\mathbf{x}^{649}$



(B) Evolution of log cost

FIGURE 8. Approximate solution for $\mathbf{u}(x_1, x_2, x_3) = (-x_2, x_1, x_1^2 x_3)$, with $\mathbf{x}(\mathbf{0}) = (0.8, -1, 0)$, using initialization $\mathbf{x}^0 = (0.8(t_1 + 1), -(t_1 + 1), t_2)$.

In this example we have used the plane $\mathbf{x}^0 = (0.8(t_1 + 1), -(t_1 + 1), t_2)$ *as the initialization. To achieve the desired tolerance, one needs now 649 iterations:*

$$E(\mathbf{x}^{649}) = 9.99875 \times 10^{-7}.$$

Similarly to the previous example, if we set the tolerance to be $1. \times 10^{-5}$*, one will only need 137 iterations to go reach it.*

One interesting feature is that with very few iterations the solution appears, from a qualitative viewpoint, to be very close to the surface which is the solution of the problem in each one of the above examples.

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