Solving variational problems and partial differential equations mapping into general target manifolds

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Abstract

A framework for solving variational problems and partial differential equations that define maps onto a given generic manifold is introduced in this paper. We discuss the framework for arbitrary target manifolds, while the domain manifold problem was addressed in [J. Comput. Phys. 174(2) (2001) 759]. The key idea is to implicitly represent the target manifold as the level-set of a higher dimensional function, and then implement the equations in the Cartesian coordinate system where this embedding function is defined. In the case of variational problems, we restrict the search of the minimizing map to the class of maps whose target is the level-set of interest. In the case of partial differential equations, we re-write all the equation's geometric characteristics with respect to the embedding function. We then obtain a set of equations that, while defined on the whole Euclidean space, are intrinsic to the implicitly defined target manifold and map into it. This permits the use of classical numerical techniques in Cartesian grids, regardless of the geometry of the target manifold. The extension to open surfaces and submanifolds is addressed in this paper as well. In the latter case, the submanifold is defined as the intersection of two higher dimensional hypersurfaces, and all the computations are restricted to this intersection. Examples of the applications of the framework here described include harmonic maps in liquid crystals, where the target manifold is a hypersphere; probability maps, where the target manifold is a hyperplane; chroma enhancement; texture mapping; and general geometric mapping between high dimensional manifolds.
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1. Introduction

In a number of applications in mathematical physics, image processing, computer graphics, and medical imaging, we have to solve variational problems and partial differential equations defined on a general manifold $\mathcal{M}$ (*domain manifold*), which map the data onto another general manifold $\mathcal{N}$ (*target manifold*). That is, we deal with maps from $\mathcal{M}$ to $\mathcal{N}$. When these manifolds are for example three-dimensional

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surfaces, the implementation of the corresponding gradient descent flow or the given PDEs is considerably elaborate. In [5] we have shown how to address this problem for general domain manifolds, while restricting the target manifolds $\mathcal{N}$ to the trivial cases of the Euclidean space or hyperspheres (this framework has been followed for example in [2]). The key idea was to implicitly represent the domain surface as the (zero) level-set of a higher dimensional function ϕ, and then solve the PDE in the Cartesian coordinate system which contains the domain of this new embedding function. The technique was justified and demonstrated in [5]. It is the goal of this paper, [33], to show how to work with general target manifolds, and not just hyperplanes or hyperspheres as previously reported in the literature. Inspired by [5], we also embed the target manifold $\mathcal{N}$ as the (zero) level-set of a higher dimensional function ψ. That is, when solving the gradient descent flow (or in general, the PDE), we guarantee that the map receives its values on the zero level-set of ψ. The map is defined on the whole space, although it never receives values outside of this level-set. Examples of applications of this framework include harmonic maps in liquid crystals ($\mathcal{N}$ is a hypersphere) and three-dimensional surface warping [46]. In this last case, the basic idea is to find a smooth map between two given surfaces. Due to the lack of the new frameworks introduced here and in [5], this problem is generally addressed in the literature after an intermediate mapping of the surfaces onto the plane is performed (see also [27,49]). With these novel frameworks, direct three-dimensional maps can be computed without any intermediate mapping, thereby eliminating their corresponding geometric distortions [34]. For this application, as in [46], boundary conditions are needed, and how to add them to the frameworks introduced here and in [5] is addressed in [34].

To introduce the ideas, in this paper we concentrate on flat domain manifolds. [1] When combining this framework with the results in [5], we can of course work with general domains and then completely avoid other popular surface representations, like triangulated surfaces. We are then able to work with intrinsic equations, in Euclidean space and with classical numerics on Cartesian grids, regardless of the geometry of the involved domain and target manifolds. In addition to presenting the general theory, we also address the problem of target submanifolds and open hypersurfaces. A number of theoretical results complement the algorithmic framework here described.

For illustration purposes only, the proposed framework is presented for classical equations from the theory of harmonic maps. The technique can easily be extended to general equations, as it will be clear from the developments below.

1.1. Why implicit representations?

Let us conclude this introduction describing the main reasons and advantages of working with implicit representation when dealing with PDEs and variational problems.

The implicit representation of surfaces, here introduced for solving variational problems and PDEs, is inspired in part by the level-set work of Osher and Sethian [36]. This work, and those that followed it, showed the importance of representing deforming surfaces as level-sets of functions with higher dimensional domains, obtaining more robust and accurate numerical algorithms (and topological freedom). Note that, in contrast with the level-set approach of Osher and Sethian, our target manifold is fixed, what is "deforming" is the dataset being mapped onto it.

Solving PDEs and variational problems with polynomial meshes involves the non-trivial discretization of the equations in general polygonal grids, as well as the difficult numerical computation of other quantities like projections onto the discretized surface (when computing gradients and Laplacians for example). Although the use of triangulated surfaces is quite popular, there is still no consensus on how to

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[1] For completeness, we will present the general equations for both generic domain and target manifolds at the end of the paper. These equations are easily derived from [5] and the work presented in this paper.

compute simple differential characteristics such as tangents, normals, principal directions, and curvatures. On the other hand, it is commonly accepted that computing these objects for iso-surfaces (implicit representations) is simpler and more accurate and robust. This problem becomes even more significant when we not only have to compute these first and second order differential characteristics of the surface, but also have to use them to solve variational problems and PDEs for data defined on the surface. Very little work has been done on the formal analysis of finite difference schemes on non-Cartesian meshes. [2] Note also that working with polygonal representations is dimensionality dependent, and solving these equations for high dimensional (>2) surfaces becomes even more challenging and significantly less studied. The work here developed is valid for all dimensions of interest (we develop the computational and theoretical framework independently of the manifold dimension). Note that the computational cost of working with implicit representations is not higher than with meshes, since all the work is performed in a narrow band around the level-set(s) of interest.

Our framework of implicit representations enables us to perform all the computations on the Cartesian grid corresponding to the embedding function. These computations are, nevertheless, intrinsic to the surface. Advantages of using Cartesian grid instead of a triangulated mesh include the availability of well studied numerical techniques with accurate error measures and the topological flexibility of the surface, all leading to simple, accurate, robust and elegant implementations. The approach is general (applicable to PDEs and variational problems beyond those derived in this paper) and dimensionality independent as well. We should note of course that the computational framework here developed is only valid for manifolds which can be represented in implicit form or as intersection of implicit forms. As mentioned above, problems such as three-dimensional shape warping via PDEs could not be addressed (without intermediate projections) without the framework here proposed.

Numerical schemes that solve gradient descent flows and PDEs onto generic target manifolds $\mathcal{N}$ (and spheres or surfaces in particular) will, in general, move the points outside of $\mathcal{N}$ due to numerical errors. The points will then need to be projected back, [3] see for example [1,11] for the case of $\mathcal{N}$ being a sphere (where the projection is trivial, just a normalization). For general target manifolds, this projection means that for every point $p \in \mathbb{R}^d$ ($\mathcal{N} \subset \mathbb{R}^d$) we need to know the closest point to p in $\mathcal{N}$. This means knowing the distance from every point $p \in \mathbb{R}^d$ to $\mathcal{N}$ (or at least all points in a band of $\mathcal{N}$). This is nothing else than an implicit representation of the target $\mathcal{N}$, being the particular embedding in this case a distance function. This presents additional background for the framework here introduced, that is, if the embedding function for the surface has to be computed anyway for the projection, why not use it from the beginning if it helps in other steps in the computation?

In a number of applications, surfaces are already given in implicit form, e.g. [7], therefore, the framework introduced in this paper is not only simple and robust, but it is also natural in those applications. Moreover, in the state-of-the-art and most commonly used packages to obtain three-dimensional models from range data, the algorithms output an implicit (distance) function (see for example graphics.stanford.edu/projects/mich/). Therefore, it is very important, if nothing else for completeness, to have the computational framework here developed, so that the surface representation is dictated by the data and the application and not the other way around. On the other hand, not all surfaces (manifolds) are originally represented in implicit form. When the target manifold $\mathcal{N}$ is simple, like hyperspheres in the case of liquid crystals, the embedding process is trivial. For generic surfaces, we need to apply an algorithm that transforms the given explicit representation into an implicit one. Although this is still a very active area of research, many very

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[2] Very important work has been done for finite element approaches, e.g. by the group of Prof. M. Rumpf; as well as for particular equations on particular sub-division representations [3].

[3] For particular flat target manifolds as the whole space $\mathbb{R}^d$ or as those in [37], the projection is not needed. Other authors, e.g. [8,28], have avoided the projection step for particular cases, while in [51] the authors modify the given variational formulation, in some restricted cases, to include the projection step.

good algorithms have been developed, e.g. [16,20,29,48]. Note that this translation needs to be done only once for any surface. Note also that for rendering, the volumetric data can be used directly, without the need for an intermediate mesh representation.

Using the results described below and the basic "dictionary" provided in the Appendix, we can translate PDEs and variational problems, based on intrinsic characteristics of the manifold, into PDEs and variational problems that depend on the implicit manifold and the embedding space, and from there, use existent numerical schemes. This translation is done in a systematic and generic fashion.

2. The computational framework

From now on we assume that the target $d-1$-dimensional manifold $\mathcal{N}$ is given as the zero level set of a higher dimensional embedding function $\psi : \mathbb{R}^d \to \mathbb{R}$, which we consider to be a signed distance function (this mainly simplifies the notation). For the case where $\mathcal{N}$ is a surface in three-dimensional space for example, then $\psi : \mathbb{R}^3 \to \mathbb{R}$. We also assume that the domain manifold $\mathcal{M}$ is flat and open (as mentioned in Section 1, general domain manifolds were addressed in [5]). We illustrate the basic ideas with a functional from the theory of harmonic maps. This is just a particular example (and a very important one), and from this example it will be clear how the same arguments can be applied to any given variational problem and PDE. In particular, it can be applied to common Navier–Stokes flows used in brain warping [34].

2.1. The variational formulation and its Euler–Lagrange

We search for necessary conditions for the functional $E[\vec{u}]$, defined by

$$E[\vec{u}] \triangleq \int_{\mathcal{M}} e[\vec{u}] \, \mathrm{d}_{\mathcal{M}} v, \tag{1}$$

where

$$e[\vec{u}] \triangleq \frac{1}{2} \|\mathbf{J}_{\vec{u}}\|_{\mathscr{F}}^2 \tag{2}$$

to achieve a minimum. Here, $\| \cdot \|_{\mathscr{F}}^2 = \sum_{ij} (\cdot)_{ij}^2$ is the norm of Frobenius and $\mathbf{J}_{\vec{u}}$ is the Jacobian of the map $\vec{u} : \mathcal{M} \to \{\psi = 0\}$. Note that here we are already restricting the map to be onto the zero level-set of ψ, that is, onto the surface of interest $\mathcal{N}$ (the target manifold). This is what permits us to work with the embedding function and the whole space, while guaranteeing that the map will always be onto the target manifold, as desired. [4] Once again, this energy will be used throughout this paper to exemplify our framework. It will be clear after developing this example that the same arguments work for other variational formulations, as well as for generic PDEs defined onto generic surfaces.

Proposition 1. *The Euler–Lagrange of Eq.* (1), *with* (2), *is given by*

$$\Delta \vec{u} + \left(\sum_k \mathbf{H}_\psi \left[\frac{\partial \vec{u}}{\partial x_k}, \frac{\partial \vec{u}}{\partial x_k} \right] \right) \nabla \psi(\vec{u}) = 0, \tag{3}$$

where $\mathbf{H}_\psi$ *stands for the Hessian of the embedding function* ψ *(and we used the notation* $A[\vec{x}, \vec{y}] = \vec{y}^{\mathrm{T}} A \vec{x}$). *The solution to this equation is a map onto the zero level-set of* ψ.

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[4] We use $\vec{\cdot}$ to note that for the most general case, the function is vectorial.

Proof. The proof is based on adding to the classical techniques to compute Euler–Lagrange equations a projection step that guarantees that the perturbation keeps the map onto $\{\psi = 0\}$.

Assume that $\vec{u}$ is a map minimizing $E(\cdot)$. Given $t > 0$, we construct the variation

$$\vec{v}_t \triangleq \vec{u} + t\vec{r},$$

where $\vec{r}$ is a compact C^∞ map in $\mathcal{M}$. For an arbitrary $x \in \mathcal{M}$, we will in general not obtain that $\vec{v}_t(x) \in \{\psi = 0\}$ for all t and x. That is, $\psi(\vec{v}_t(x)) \neq 0$ at some (t, x). Therefore, this variation is not admissible. On the other hand, we can from it construct an admissible variation via

$$\vec{w}_t \triangleq \mathbf{\Pi}_{\{\psi=0\}}(\vec{v}_t),$$

where $\mathbf{\Pi}_{\{\psi=0\}} : R^d \rightarrow \{\psi = 0\}$ is the *projection operator* onto $\{\psi = 0\}$. Note that since ψ is a signed distance function, we can simply write this projection operator onto $\{\psi = 0\}$ as

$$\mathbf{\Pi}_{\{\psi=0\}}(\vec{\alpha}) = \vec{\alpha} - \psi(\vec{\alpha})\nabla\psi(\vec{\alpha}).$$

Let us now define

$$\mathscr{E}(t) \triangleq E[\vec{w}_t].$$

Since the energy achieves a minimum for $t = 0$,

$$\dot{\mathscr{E}}_0 \triangleq \frac{\mathrm{d}E(t)}{\mathrm{d}t}\bigg|_{(t=0)} = 0.$$

Let us compute this first variation. We have that

$$\dot{\mathscr{E}}_0 = \sum_{ij} \int_{\mathcal{M}} \left(\frac{\partial w_t^i}{\partial x_j} \frac{\mathrm{d}\left(\frac{\partial w_t^i}{\partial x_j}\right)}{\mathrm{d}t} \right)\Bigg|_{t=0} \mathrm{d}_{\mathcal{M}}v. \tag{4}$$

Moreover (recall that $\mathbf{H}_\psi$ stands for the Hessian of ψ),

$$\frac{\partial w_t}{\partial x_j} = \left(\frac{\partial\vec{u}}{\partial x_j} + t\frac{\partial\vec{r}}{\partial x_j} \right) - \left(\nabla\psi(\vec{w}_t) \cdot \left(\frac{\partial\vec{u}}{\partial x_j} + t\frac{\partial\vec{r}}{\partial x_j} \right) \right)\nabla\psi(\vec{w}_t) - \psi(\vec{w}_t)\mathbf{H}_\psi(\vec{w}_t)\left(\frac{\partial\vec{u}}{\partial x_j} + t\frac{\partial\vec{r}}{\partial x_j} \right) \tag{5}$$

and we observe that

$$\frac{\partial w_t}{\partial x_j}\bigg|_{(t=0)} = \frac{\partial\vec{u}}{\partial x_j} - \left(\nabla\psi(\vec{u}) \cdot \frac{\partial\vec{u}}{\partial x_j} \right)\nabla\psi(\vec{u})$$

since $\psi(\vec{u}) = 0$. We can further simplify this observing that $0 = \partial\psi(\vec{u})/\partial x_j = \nabla\psi(\vec{u}) \cdot \partial\vec{u}/\partial x_j$. Therefore,

$$\frac{\partial w_t}{\partial x_j}\bigg|_{(t=0)} = \frac{\partial\vec{u}}{\partial x_j}. \tag{6}$$

With a bit further work we can compute the additional derivative, $\mathrm{d}\left(\frac{\partial w_t^i}{\partial x_j}\right)/\mathrm{d}t = \partial\left(\frac{\mathrm{d}w_t^i}{\mathrm{d}t}\right)/\partial x_j$. This change in the order of derivatives is done in order to immediately evaluate the result at $t = 0$, thereby simplifying the following derivative. Following in an similar fashion, we obtain

$$\frac{\mathrm{d}w_t^i}{\mathrm{d}t} = \vec{r} - \left(\nabla\psi(\vec{w}_t) \cdot \vec{r}\right)\nabla\psi(\vec{w}_t) - \psi(\vec{w}_t)\mathbf{H}_\psi(\vec{w}_t)\vec{r} \tag{7}$$

and

$$\left.\frac{\mathrm{d}w_t^i}{\mathrm{d}t}\right|_{(t=0)} = \vec{r} - \left(\nabla\psi(\vec{u}) \cdot \vec{r}\right)\nabla\psi(\vec{u}). \tag{8}$$

Combining the above computations all together we obtain

$$\left.\frac{\mathrm{d}\left(\frac{\partial w_t^i}{\partial x_j}\right)}{\mathrm{d}t}\right|_{(t=0)} = \frac{\partial\left(\left.\frac{\mathrm{d}w_t^i}{\mathrm{d}t}\right|_{(t=0)}\right)}{\partial x_j}$$

$$= \frac{\partial\vec{r}}{\partial x_j} - \nabla\psi(\vec{u})\left\{\frac{\partial\vec{r}}{\partial x_j} \cdot \nabla\psi(\vec{u}) + \mathbf{H}_\psi\left(\vec{r},\frac{\partial\vec{u}}{\partial x_j}\right)\right\} - (\vec{r} \cdot \nabla\psi(\vec{u}))\left(\mathbf{H}_\psi\frac{\partial\vec{u}}{\partial x_j}\right). \tag{9}$$

Following from (4) we have that [5]

$$\dot{\mathscr{E}}_0 = \sum_j \int_{\mathscr{M}} \left.\left(\frac{\partial\vec{w}_t}{\partial x_j}\frac{\mathrm{d}\left(\frac{\partial\vec{w}_t}{\partial x_j}\right)}{\mathrm{d}t}\right)\right|_{t=0} \mathrm{d}_{\mathscr{M}}v = \sum_j \int_{\mathscr{M}} \left\{\frac{\partial\vec{r}}{\partial x_j} \cdot \frac{\partial\vec{u}}{\partial x_j} - (\vec{r} \cdot \nabla\psi(\vec{u}))\mathbf{H}_\psi\left[\frac{\partial\vec{u}}{\partial x_j},\frac{\partial\vec{u}}{\partial x_j}\right]\right\} \mathrm{d}_{\mathscr{M}}v. \tag{10}$$

Now, applying the divergence theorem we conclude the computation. We first write

$$\sum_{ij} \int_{\mathscr{M}} \frac{\partial\vec{r}}{\partial x_j} \cdot \frac{\partial\vec{u}}{\partial x_j} \, \mathrm{d}_{\mathscr{M}}v = \sum_i \int_{\mathscr{M}} \nabla r^i \cdot \nabla u^i \, \mathrm{d}_{\mathscr{M}}v$$

and then apply the fact $\nabla r^i \cdot \nabla u^i = \nabla \cdot (r^i \nabla u^i) - r^i \Delta u^i$, together with the divergence theorem, to obtain (**n** stands for the outward unit normal to $\partial\mathscr{M}$).

$$\sum_{ij} \int_{\mathscr{M}} \frac{\partial\vec{r}}{\partial x_j} \cdot \frac{\partial\vec{u}}{\partial x_j} \, \mathrm{d}_{\mathscr{M}}v = \sum_i \int_{\partial\mathscr{M}} r^i \frac{\partial u^i}{\partial\mathbf{n}} \, \mathrm{d}S - \int_{\mathscr{M}} r^i \Delta u^i \, \mathrm{d}_{\mathscr{M}}v \tag{11}$$

To conclude we put together this last expression with (9), and after some algebra we obtain that $\dot{\mathscr{E}}_0$ is equal to

$$\int_{\partial\mathscr{M}} \vec{r} \cdot \mathbf{J}_{\vec{u}}\mathbf{n} \, \mathrm{d}S - \int_{\mathscr{M}} \vec{r} \cdot \left\{\Delta\vec{u} + \left(\sum_k \mathbf{H}_\psi\left[\frac{\partial\vec{u}}{\partial x_k},\frac{\partial\vec{u}}{\partial x_k}\right]\right)\nabla\psi(\vec{u})\right\} \mathrm{d}_{\mathscr{M}}v. \tag{12}$$

The boundary condition is eliminated since the support of $\vec{r}$ is compactly included in $\mathscr{M}$. To eliminate the additional term for an arbitrary $\vec{r}$ we must impose

$$\Delta\vec{u} + \left(\sum_k \mathbf{H}_\psi\left[\frac{\partial\vec{u}}{\partial x_k},\frac{\partial\vec{u}}{\partial x_k}\right]\right)\nabla\psi(\vec{u}) = 0. \quad \square \tag{13}$$

Eq. (3) (or (13)) then gives the corresponding Euler–Lagrange for the given variational problem. Note, once again from our computations, that despite all the terms "live" in the Euclidean space where the target

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[5] We have used as before the notation $A[\vec{x},\vec{y}] = \vec{y}^{\mathrm{T}}A\vec{x}$.

manifold is embedded, $\vec{u}$ will always map onto the level-set of interest, $\{\psi = 0\}$, and, therefore, onto the surface of interest. This is guaranteed by this equation, no additional computations are needed. This is the beauty of the approach, while working freely on the Euclidean space (and, therefore, with Cartesian numerics), we can guarantee that the equations are intrinsic to the given surfaces of interest. We will further verify this in Section 2.3 to help the reader grasp the intuition behind this framework. In the same section we present a particular example of the above equation for a target surface given by a hypersphere.

2.1.1. The gradient-descent flow

The gradient descent corresponding to (13) is given by

$$\frac{\partial u^i}{\partial t} = \Delta u^i + \sum_{k=1}^{d} \mathbf{H}_\psi(\vec{u}) \left[\frac{\partial \vec{u}}{\partial x_k}, \frac{\partial \vec{u}}{\partial x_k} \right] \frac{\partial \psi}{\partial u^i}(\vec{u}), \tag{14}$$

where the initial datum $\vec{u}_0$ is given by the vector field we want to process, together with *Neumann* boundary conditions

$$\begin{cases} \vec{u}(x, 0) = \vec{u}_0(x), & x \in \mathcal{M}, \\ \mathbf{J}_{\vec{u}} \mathbf{n}|_{\partial \mathcal{M}} = \mathbf{0}. \end{cases} \tag{15}$$

To complete the picture, the use of *Neumann* boundary conditions needs to be justified. This is done in Appendix A.

2.2. Connections with harmonic maps

The goal of this section is to illustrate the connections of the equations above with the well-known theory of harmonic maps. As it is the case of the proof of Proposition 1, these connections are simple to derive, as we do below. Nevertheless, the derivations themselves present illustrative calculus with implicit surfaces and PDEs on them.

The expressions derived in previous sections come from the theory of harmonic maps, e.g. [6,9,13,15,17,18,22,25,38,41–43]. In general, harmonic maps are defined as those maps between two manifolds $(\mathcal{M}, g)$ and $(\mathcal{N}, h)$ which minimize the energy

$$E[\vec{u}] \triangleq \int_{\mathcal{M}} e[\vec{u}] \, dV_{\mathcal{M}}, \tag{16}$$

where, in local coordinates, the *energy density* $e[\vec{u}]$ is given by

$$e[\vec{u}](x) \triangleq \frac{1}{2} g^{pq}(x) h_{ij}(\vec{u}(x)) \frac{\partial u^i}{\partial x_p} \frac{\partial u^j}{\partial x_q}. \tag{17}$$

We have used Einstein's summation here, where repeated indices indicate summation with respect to this index, together with the usual notation for tensors. [6] When both the domain and target manifolds are represented explicitly, the classical case, the Euler–Lagrange equation corresponding to this energy is given by (see [41])

$$\Delta_{\mathcal{M}} u^l + \Gamma^l_{ij}(\vec{u}) g^{\alpha\beta} \frac{\partial u^i}{\partial x^\alpha} \frac{\partial u^j}{\partial x^\beta} = 0, \tag{18}$$

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[6] $(g^{-1})_{ij} \triangleq g^{ij}$.

where $\Delta_{\mathcal{M}}$ is the Laplace–Beltrami operator (reduced to the regular Laplacian for the case of flat domain manifolds) and $\Gamma^l_{ij}(\vec{u})$ stands for the Christoffel symbols of the target manifold, evaluated at $\vec{u}$. Note that the first component, the Laplace–Beltrami of u, addresses the domain manifold, whereas the second term addresses the target manifold. By embedding the target manifold, we are changing the Christoffel symbols (expressing them in implicit form, see below), [7] while the work in [5] changed the other terms, since the embedding was done to the domain manifold, see Section 4. The framework here introduced can then be seen as the re-writing of given PDEs mapping manifolds to manifolds in such a way that the intrinsic geometric characteristics of the equation are expressed using the embedding functions.

As an example, let us see what happens with the above energy for the Euclidean case. Since both metrics are proportional to the identity

$$e[\vec{u}](x) = \frac{K}{2} \sum_{ij} \left(\frac{\partial u^i}{\partial x_j} \right)^2$$

which is just a constant multiplying $\|\mathbf{J}_{\vec{u}}\|^2_{\mathscr{F}}$. Therefore, the energy defined in the previous case is just a particular case of harmonic maps. In general, this energy can be used in problems such as color image denoising and directions denoising [43,44], as a regularization term for ill-possed problems defined on general surfaces [19], for general denoising [40,47], for models of liquid crystals, and as a component of a system for surface mapping and matching [15,34,49].

2.2.1. An(other) informal calculation

We now present an additional computation that connects in a deep way the implicit framework with harmonic maps. We consider the harmonic energy density given in (17) for the planar domain manifold case ($g_{ij} = \delta_{ij}$). We can simplify things to obtain

$$e[\vec{u}](x) = \frac{1}{2} h_{ij}(\vec{u}(x)) \frac{\partial u^i}{\partial x_p} \frac{\partial u^j}{\partial x_p} = \frac{1}{2} \sum_p \mathbf{h}[\vec{u}_{x_p}, \vec{u}_{x_p}].$$

We know that $\mathbf{\Pi}_{\nabla\psi} = \mathbf{I} - \nabla\psi\nabla\psi^{\mathrm{T}}$ can be thought of as the inverse of the target manifold's *metric tensor*. But since $\nabla\psi$ is a zero eigenvalue eigenvector for $\mathbf{\Pi}_{\nabla\psi}$, it will be a ∞ eigenvalue eigenvector for $\mathbf{\Pi}^{-1}_{\nabla\psi}$. Then, we cannot use the identification $\mathbf{h} = (h_{ij}) \leftrightarrow \mathbf{\Pi}^{-1}_{\nabla\psi}$ in the above expression for the energy density. However, we can proceed as follows. Take $\epsilon > 1$ and define the metric [8]

$$\mathbf{h}^\epsilon \triangleq \left(\epsilon\mathbf{I} - \nabla\psi\nabla\psi^{\mathrm{T}} \right)^{-1}$$

one can then compute the inverse as (it is an elementary formula, see for example [26])

$$\mathbf{h}^\epsilon = \frac{1}{\epsilon} \left(\mathbf{I} + \frac{\nabla\psi\nabla\psi^{\mathrm{T}}}{\epsilon - 1} \right).$$

The energy density can be rewritten as (we will use a subindex ϵ)

$$e_\epsilon[\vec{u}](x) = \frac{1}{2\epsilon} \left(\sum_i \|\vec{u}_{x_i}\|^2 + \frac{1}{\epsilon - 1} \sum_i |\vec{u}_{x_i} \cdot \nabla\psi|^2 \right).$$

After computing the variational derivative for the functional $\int_{\mathcal{M}} e_\epsilon[\vec{u}](x)\, \mathrm{d}x$ we obtain that $\vec{u}$ must satisfy

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[7] Or alternatively, the second fundamental form of the target manifold.
[8] Since $\epsilon > 1$, all the eigenvalues are positive.

$$\Delta \vec{u} + \frac{1}{\epsilon - 1} \left(\sum_i \mathbf{H}_\psi [\vec{u}_{x_i}, \vec{u}_{x_i}] + \Delta \vec{u} \cdot \nabla \psi \right) \nabla \psi = 0.$$

By multiplying all the terms in the above equation by $\epsilon - 1$ and letting $\epsilon \to 1$ we find that the expression between brackets must vanish. As we will see in Section 2.3, what is between brackets is nothing but $\Delta v(x)$ where $v(x) = \psi(\vec{u}(x))$. So v is a harmonic function in $\mathcal{M}$. It is also evident that v satisfies Dirichlet boundary conditions if $\vec{u}$ does, and since we are trying to map things from $\mathcal{M}$ to $\mathcal{N}$, those boundary conditions for $\vec{u}$ must be such that $\mathrm{dist}(\vec{u}(x), \mathcal{N}) = 0$ for $x \in \mathcal{M}$, so $v|_{\partial \mathcal{M}} = 0$. Then, we conclude that v must be zero everywhere in $\mathcal{M}$.

2.3. Simple verifications

We now show that the Euler–Lagrange (13) and its corresponding gradient descent flow (14) are the extension for implicit targets of common equations derived in the literature for explicitly represented manifolds. We also explicitly show that the flow equation guarantees, as expected from the derivations above and in particular from the proof of Proposition 1, that if the initial datum is on the target manifold, it will remain on it. We also express the second fundamental form of a manifold that is implicitly represented. All these results will help to further illustrate the approach and verify its correctness.

2.3.1. Geodesics on implicit manifolds
It is well known, see [17,18,39], that arc-length parameterized geodesics on the manifold $\mathcal{N}$ satisfy the harmonic maps PDE, and, therefore, Eq. (3). If we assume isotropic and homogeneous metric over $\mathcal{N}$, from Eq. (3) we obtain that (arc-length parameterized) geodesics must satisfy

$$\ddot{\gamma} + \mathbf{H}_\psi \left[\dot{\gamma}, \dot{\gamma} \right] \nabla \psi(\gamma) = 0. \tag{19}$$

This important equation shows how to obtain geodesic curves on manifolds represented in implicit form.

2.3.2. Liquid crystals ($\mathcal{N} = S^{d-1}$, hypersphere)
One of the most popular examples of harmonic maps is given when the target manifold $\mathcal{N}$ is a hypersphere. That is, the map is onto S^{d-1}. In this case, the embedding (signed distance) function is simply $\psi(\vec{y}) = \|\vec{y}\| - 1$, $\vec{y} \in \mathbb{R}^d$. From this, $\nabla \psi(\vec{y}) = \vec{y}/\|\vec{y}\|$ and $(\mathbf{H}_\psi(\vec{y}))_{ij} = \delta_{ij}/\|\vec{y}\| - y_i y_j/\|\vec{y}\|^3$. We also have that

$$\mathbf{H}_\psi(\vec{u}(x)) \left[\frac{\partial \vec{u}}{\partial x_k}, \frac{\partial \vec{u}}{\partial x_k} \right] = \delta_{ij} \frac{\partial u^i}{\partial x_k} \frac{\partial u^j}{\partial x_k} - \frac{\partial u^i}{\partial x_k} \frac{\partial u^j}{\partial x_k} u_i u_j,$$

since $\|\vec{u}\| = 1$. In addition, $u^i(\partial u^i/\partial x_k) = 0$, fact simply obtained taking derivatives with respect to x_k. We then obtain that $(\partial u^i/\partial x_k)(\partial u^j/\partial x_k)u_i u_j = ((\partial u^i/\partial x_k)u_i)^2 = 0$, and $\sum_{k=1}^d \mathbf{H}_\psi(\vec{u}(x))[\frac{\partial \vec{u}}{\partial x_k}, \frac{\partial \vec{u}}{\partial x_k}] = \sum_{ik}(\frac{\partial u^i}{\partial x_k})^2 = \|\mathbf{J}_{\vec{u}}(x)\|_{\mathscr{F}}^2$. Therefore, the corresponding diffusion equation from (14) is

$$\frac{\partial \vec{u}}{\partial t} = \Delta \vec{u} + \|\mathbf{J}_{\vec{u}}\|_{\mathscr{F}}^2 \vec{u}$$

which is exactly the well known gradient descent flow for this case. We have then verified the correctness of the derivation in Proposition 1 for the case of unit spheres as target manifolds.

2.3.3. Diffusion of probabilities
In this case, $\mathcal{N} = \{x \in \mathbb{R}^d | x_i \geqslant 0, \sum_{i=1}^d x_i = 1\}$, which is not a closed manifold. However, by maximum principle arguments, if the initial datum is on $\mathcal{N}$, it will remain there for all time of smooth existence, see

Section 2.5.1 and [37]. Then, we can formally consider $\psi(x) = \sum_{i=1}^{d} x_i - 1/\sqrt{d}$, the signed distance from a point $x \in \mathbb{R}^d$ to the hyperplane $\{z \in \mathbb{R}^d \,|\, \sum_{i=1}^{d} z_i = 1\}$, where the sign was selected accordingly to our choice of $(1, \ldots, 1)/\sqrt{d}$ as the unit normal to the hyperplane. We then obviously obtain $\nabla\psi(x) = (1, \ldots, 1)/\sqrt{d}$ and $\mathbf{H}_\psi(x) = 0$ for all x. Consequently, the evolution equation for this case is

$$\vec{u}_t = \Delta\vec{u}$$

as expected [37].

2.3.4. Mapping restriction onto the zero level-set

We now explicitly show that if the initial datum belongs to the target surface given by the zero level-set of ψ, then the solution to the diffusion flow (14) also belongs to this level-set. This further shows the correctness of our approach.

Proposition 2. *A regular solution to Eq. (14) holds* $\psi(\vec{u}(x, t)) = 0 \ \forall x \in \mathcal{M}, \ \forall t \geqslant 0$ *of regularity.*

Proof. If the initial datum is on $\{\psi = 0\}$, then this property is true for $t = 0$. Let us define $v(x, t) = \psi(\vec{u}(x, t))$. Then, [9]

$$\frac{\partial v}{\partial t} = \nabla\psi(\vec{u}) \cdot \frac{\partial\vec{u}}{\partial t} = \Delta\vec{u} \cdot \nabla\psi(\vec{u}) + \sum_{k=1}^{d} \mathbf{H}_\psi(\vec{u}) \left[\frac{\partial\vec{u}}{\partial x_k}, \frac{\partial\vec{u}}{\partial x_k} \right]$$

since ψ is a distance function. In addition, $\partial v/\partial x_i = \nabla\psi(\vec{u}) \cdot \partial\vec{u}/\partial x_i$, and then

$$\frac{\partial^2 v}{\partial x_i^2} = \left(\mathbf{H}_\psi(\vec{u}) \frac{\partial\vec{u}}{\partial x_i} \right) \cdot \frac{\partial\vec{u}}{\partial x_i} + \nabla\psi(\vec{u}) \cdot \frac{\partial^2\vec{u}}{\partial x_i^2}.$$

Adding on $i = 1, \ldots, d$, it follows that $\partial v/\partial t = \Delta v$, meaning that v verifies the heat flow. In addition to this, $(\partial v/\partial\mathbf{n})|_{\partial\mathcal{M}} = \nabla_x(\psi(\vec{u}(x, t))) \cdot \mathbf{n} = \mathbf{J}_{\vec{u}}^{\mathrm{T}}\nabla\psi(\vec{u}) \cdot \mathbf{n} = (\nabla\psi(\vec{u}))^{\mathrm{T}}\mathbf{J}_{\vec{u}}\mathbf{n} = (\nabla\psi(\vec{u}))^{\mathrm{T}}\mathbf{0} = 0$, due to the boundary conditions on the evolution of $\vec{u}$.

We have then obtained that v verifies the heat flow with *Neumann* boundary conditions and with zero initial data. From the uniqueness of the solution, it follows that $v(x, t) = 0 \ \forall x \in \mathcal{M}, \ \forall t \geqslant 0$. $\square$

2.3.5. Second fundamental form for implicit surfaces

If we compare the gradient descent flow (and Euler–Lagrange equation) we have obtained with the classical one from harmonic maps, we see that the main difference is that Christoffel symbols for the target manifold term appearing in the classical formulation have been replaced by a new term that includes the Hessian of the embedding function. We obtained this by first embedding the target manifold and then restricting the search for the minimizing map to the class of maps onto the zero level-set of the embedding function. This approach can be followed to apply this framework to any related variational problem. We now show how the same equation can be obtained by simply substituting the second fundamental form of the explicit target manifold by the corresponding expression for an implicit target manifold. This will illustrate how to apply our framework to more general PDEs, not necessarily gradient descent flow. The basic idea is just to replace all the PDE components concerning the target manifold by their counterparts for implicit representations.

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[9] The calculations that follow in the proof do not take into account that ψ might fail to be differentiable at some points. This could be simply addressed by a regularization argument. Moreover, we use the fact that there exists $T > 0$ such that $\vec{u}$ is regular in $[0, T)$.

In [30] (p. 150) it is shown that the *scalar second fundamental form h* at a point p of a hypersurface $\mathscr{S}$ can be written in the form

$$h(p)(V, W) = \frac{\mathbf{H}_\psi(p)[V, W]}{\|\nabla\psi\|^2}$$

for $V, W \in T_p\mathscr{S}$. According to [30] (p. 139) the *vectorial second fundamental form* is given by

$$II(p)(V, W) = h(p)(V, W)\frac{\nabla\psi}{\|\nabla\psi\|}$$

From (18) and what we have just seen it is obvious that the *implicit* version of the *harmonic map* Euler–Lagrange is (13).

As stated before, the implicit representation of the target surface permits then to compute the second fundamental form using differences on Cartesian grids, without the need to develop new numerical techniques on polygonal grids.

From the result just presented, in order to transform a given PDE into its counterpart when the target manifold is represented in implicit form, all that needs to be done is to re-write all the characteristics of the PDE, concerning this target manifold, in implicit form. For completeness, in Appendix B we present basic facts on calculus on implicitly represented hypersurfaces.

2.4. Explicit derivation of the diffusion flow

Here, we first proceed in a naïve way to obtain an equivalent formulation of the gradient descent flow that will help in the numerical implementation. We assume we have a family $\{\vec{u}(\vec{x}, t)\}_t$ of mappings from Ω to $\mathscr{N}$. For each t we define the *harmonic energy* of a member of the family as

$$E(t) = \frac{1}{2}\int_\Omega \|\mathbf{J}_{\vec{u}(\vec{x}, t)}\|_F^2 \, \mathrm{d}x.$$

We then find a variation of the family such that $E(t)$ decreases. To accomplish this we formally differentiate the energy with respect to t. A simple computation yields

$$\dot{E}(t) = -\int_\Omega \vec{u}_t \cdot \Delta\vec{u} \, \mathrm{d}x.$$

Now, since $\vec{u}(\vec{x}, t) \in \mathscr{N} \; \forall\vec{x} \in \Omega$ and $\forall t$ of smooth existence, one must have $\vec{u}_t(\vec{x}, t) \in T_{\vec{u}(\vec{x}, t)}\mathscr{N}$. An appropriate choice for $\vec{u}_t$ would be

$$\vec{u}_t = \mathbf{\Pi}_{T_{\vec{u}(\vec{x}, t)}\mathscr{N}}(\Delta\vec{u}) \tag{20}$$

since this makes $\dot{E}(t) = -\int_\Omega \|\vec{u}_t\|^2 \, \mathrm{d}x \leqslant 0$.

The projection operator in (20), as we already know (see Appendix B), can be expressed in a very simple form using ψ (the signed distance function to $\mathscr{N}$),

$$\mathbf{\Pi}_{T_{\vec{p}}\mathscr{N}}(\vec{v}) = \vec{v} - \vec{v} \cdot \nabla\psi(p)\nabla\psi(p). \tag{21}$$

Now, it should happen that (20) is *equivalent* to (14). We show this in Section 5.

2.5. Remarks on the solutions of the diffusion flow

In previous subsections we have derived novel equations for PDEs mapping into target manifolds. We complete the work of this section with relevant results from the literature on the mathematical correctness of these equations.

The well-posedness of these diffusion problem with *Neumann* boundary conditions is addressed in [24,35], where the following results are obtained, here included for completeness.

Theorem 1. *For a given C^∞ mapping $\vec{u}_0 : \mathscr{M} \to \mathscr{N} \subset \mathbb{R}^{n+1}$ with $\partial \vec{u}_0 / \partial \mathbf{n} = 0$ on $\partial \mathscr{M}$ and for every $2 + \dim(\mathscr{M}) < p < +\infty$ there exists an $\epsilon > 0$ (depending on $\vec{u}_0$) and a mapping $\vec{u} : \mathscr{M} \to \mathscr{N}$ of class $\mathbf{L}_2^p(\mathscr{M} \times [0, \epsilon], \mathbb{R}^{n+1})$.* [10] *Moreover, $\vec{u}$ is unique and C^∞ except at the corner $\partial \mathscr{M} \times \{0\}$.*

Theorem 2. *Let $(\mathscr{M}, g)$ and $(\mathscr{N}, h)$ be compact Riemmanian Manifolds with convex boundary. Let $\vec{u} : \mathscr{M} \times [0, \omega) \to \mathscr{N}$ be a maximal solution of the diffusion problem with initial value a C^∞ mapping $\vec{u}_0$,* [11] *with $\chi_0 \triangleq \|e[\vec{u}_0]\|_{\mathbf{L}^\infty} > 0$. Let $r \in \mathbb{R}$ be such that $Ric_{\mathscr{M}} \geqslant -\frac{r}{2} g$,* [12] *and $R \geqslant 0$ such that all sectional curvatures of $\mathscr{N}$ are not greater than $R/4$. Then,*
1. *In the case $r + R\chi_0 > 0$*
   (a) if $R > 0$ then

$$\begin{cases} \omega \geqslant \frac{1}{r} \log(1 + \frac{r}{R\chi_0}) & \text{when } r \neq 0, \\ \omega \geqslant \frac{1}{R\chi_0} & \text{when } r = 0 \end{cases}$$

   (b) if $R = 0$ then $\omega = +\infty$.
2. *In the case $r + R\chi_0 \leqslant 0$, $\omega = +\infty$.*

2.5.1. Maps into open surfaces

So far, we have only addressed the case when the target surface is closed (zero level-set). We now briefly deal with open surfaces. We show, following classical results, that when the map $\vec{u}$ is evolving according to the flow in Section 2.1.1, the set $\mathscr{C}(t) \triangleq \{\vec{u}(x, t), x \in \mathscr{M}\}$ remains inside the initial *convex-hull* of $\mathscr{C}_0 \triangleq \{\vec{u}_0(x), x \in \mathscr{M}\} \, \forall t \geqslant 0$. This property is basically a consequence of the maximum principle. In the actual computations, this might of course be violated due to numerical errors, and we will later discuss how to correct for this as well.

Let us first motivate the general result presented below for the planar case. Assume that the target manifold $\mathscr{N}$ is flat, for example R^k (we still assume that the domain manifold $\mathscr{M}$ is flat). Let $\vec{u}(x, t)$ solve $\partial \vec{u} / \partial t = \Delta \vec{u}$ for $x \in \mathscr{M}$ and $t \geqslant 0$, and $(\partial \vec{u} / \partial \mathbf{n})|_{\partial \mathscr{M}} = 0$. Let $\varXi$ be a convex set of R^k with smooth boundary (this guarantees that the distance function is also smooth almost everywhere, see [39] for a formal statement), and ξ the signed distance function to this set (positive outside and negative inside). Define $g(x, t) \triangleq \xi(\vec{u}(x, t))$. Then, it follows that $\partial g / \partial t - \Delta g = -\sum_{i=1}^{k} \mathbf{H}_\xi(\partial \vec{u} / \partial x_k, \partial \vec{u} / \partial x_k)$. [13] Since $\varXi$ is convex, so it is ξ. Then, the *Hessian* of ξ is *positive semi-definite*, meaning that $\partial g / \partial t - \Delta g \leqslant 0$. Following the scalar

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[10] $\mathbf{L}_2^p(\mathscr{M} \times [0, \epsilon], \mathbb{R}^{n+1})$ is the space of functions $f : \mathscr{M} \to \mathbb{R}^{n+1}$ such that for every $i = 1, \dots, n+1$, $\nabla_{\mathscr{M}} f^i$, $\mathbf{H}_{f^i}^{\mathscr{M}}$ and $\frac{\partial f^i}{\partial t}$ are all in $\mathbf{L}^2(\mathscr{M} \times [0, \epsilon])$.

[11] A solution $\vec{u} : \mathscr{M} \times [0, \omega) \to \mathscr{N}$ of the diffusion problem is *maximal* if it cannot be extended to be a solution on $\mathscr{M} \times [0, \omega + \epsilon)$ for any $\epsilon > 0$ or if $\omega = +\infty$.

[12] $Ric_{\mathscr{M}}$ stands for the Ricci curvature tensor of $\mathscr{M}$.

[13] Note once again that we are omitting details regarding the correct handling of the distance function, since it is not everywhere differentiable. However, by a regularization argument, the same conclusion holds.

maximum principle, $\max_{\{x \in \mathcal{M}, t \geqslant 0\}} g(x, t) = \max_{\{x \in \mathcal{M}\}} g(x, 0)$. If $\{\vec{u}_0(x), x \in \mathcal{M}\} \subseteq \Xi$, which is equivalent to $0 \geqslant \xi(\vec{u}_0(x)) = g(x, 0)$, we obtain that $g(x, t) \leqslant 0$, and $\vec{u}(x, t) \in \Xi$ for all $x \in \mathcal{M}$ y $t \geqslant 0$.

The general result now presented is from [24]. We quote it here for completeness. [14]

Theorem 3. *Let $\vec{u}(x, t)$ be the solution of* (14) *at time t. Let us assume that for $t \leqslant T$ this solution remains smooth. Let $I_0 = \vec{u}_0(\Omega)$, and $\mathscr{I}_0$ be the convex hull of I_0. Then, for $(x, t) \in \Omega \times [0, T]$, $\vec{u}(x, t) \in \mathscr{I}_0$.*

3. Maps into implicit submanifolds

Here, we present a modification to the diffusion flow introduced above, which is well suited to diffuse data that belongs to a certain *submanifold* $\mathscr{C}$ of $\mathscr{N} = \{\psi = 0\}$. We specify this submanifold by $\mathscr{C} = \{\psi = 0\} \cap \{\Phi = 0\}$, where we select $\Phi : \mathbb{R}^N \to R$ to be the signed *intrinsic* (to $\mathscr{N}$) distance function to $\{\Phi = 0\}$, satisfying (see Appendix B for the notation)

$$1 = \|\nabla_\psi \Phi\| = \sqrt{\|\nabla \Phi\|^2 - |\nabla \psi \cdot \nabla \Phi|^2}. \tag{22}$$

In addition we specify the condition

$$\Phi(p) = 0 \quad \text{for } p \in \mathscr{K}_{\mathscr{C}},$$

where

$$\mathscr{K}_{\mathscr{C}} = \{x \in \mathbb{R}^N | x = p + \alpha \nabla \psi(p) \text{ with } p \in \mathscr{C}, \ \alpha \in \mathbb{R}\}$$

is the *cone* intersecting $\{\psi = 0\}$ at $\mathscr{C}$ and director rays normal also to $\{\psi = 0\}$.

The reason for specifying the submanifold this way is that we cannot proceed as before, simply specifying the submanifold as the zero level set of its Euclidean distance function. This is because such function would be singular precisely on the submanifold.

As we show in Appendix B, the Hessian of Φ, *intrinsic* to $\mathscr{N}$ evaluated at the point p, and restricted to act on vectors that belong to $T_p \mathscr{N}$, can be written in the form

$$\mathbf{H}_\Phi^{\mathscr{N}}(p) = \mathbf{H}_\Phi(p) - \Lambda(p)\mathbf{H}_\psi(p), \tag{23}$$

where $\Lambda(p) = \nabla \Phi(p) \cdot \nabla \psi(p)$. This expression will be used below.

We now derive the Euler–Lagrange corresponding to this additional mapping restriction. For this, we use a technique slightly different that the one in Section 2.1.

Proposition 3. *The Euler–Lagrange of the functional* (1), *when the solution is restricted to the implicitly represented submanifold $\mathscr{C}$ defined above, is given by*

$$\Delta \vec{u} + \left(\sum_k \mathbf{H}_\psi(\vec{u}) \left[\frac{\partial \vec{u}}{\partial x_k}, \frac{\partial \vec{u}}{\partial x_k} \right] \right) \nabla \psi(\vec{u}) + \left(\sum_k \mathbf{H}_\Phi^{\mathscr{N}}(\vec{u}) \left[\frac{\partial \vec{u}}{\partial x_k}, \frac{\partial \vec{u}}{\partial x_k} \right] \right) \nabla_\psi \Phi(\vec{u}) = 0. \tag{24}$$

Proof. Let us assume that $\vec{u}$ achieves a minimum of the energy functional (1). We must build a variation of $\vec{u}$ that belongs to $\mathscr{C}$, the intersection of the zero level-sets of two embedding functions (and not just of ψ as before). It is clear that one such variation would be

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[14] The proof of this result has a lot of interest in itself since it can be carried out within the implicit framework introduced in this paper.

$$\vec{w}_\lambda = \mathbf{\Pi}_\mathscr{C}\left(\vec{u} + \lambda\vec{v}\right).$$

We are interested only on those terms of $e[\vec{w}_\lambda]$ that do not vanish after the $\sum_{i=1}^N (\partial/\partial x_i)(\cdot)|_{\lambda=0}$ operation, namely those linear in λ. Therefore, we only preserve those terms in $\vec{w}_\lambda$ which are constant or linear in λ:

$$\vec{w}_\lambda \simeq \vec{u} + \lambda\mathbf{\Pi}_{T_{\vec{u}}\mathscr{C}}(\vec{v}).$$

We write

$$\mathbf{\Pi}_{T_{\vec{u}}\mathscr{C}}(\vec{v}) = \mathbf{\Pi}_{T_{\vec{u}}\{\psi=0\}}\left\{\vec{v} - \left(\vec{v}\cdot\nabla_\psi\Phi(\vec{u})\right)\nabla_\psi\Phi(\vec{u})\right\} = \vec{v} - \left(\vec{v}\cdot\nabla_\psi\Phi(\vec{u})\right)\nabla_\psi\Phi(\vec{u}) - (\vec{v}\cdot\nabla\psi(\vec{u}))\nabla\psi(\vec{u}),$$

where $\nabla_\psi\Phi(\vec{u}) = \nabla\Phi(\vec{u}) - \Lambda(\vec{u})\nabla\psi(\vec{u})$ is the gradient of Φ *intrinsic* to $\{\psi = 0\}$. In this way we find that (up to a first order in λ)

$$
\begin{aligned}
e[\vec{w}_\lambda] \simeq e[\vec{u}] + \lambda\sum_{i=1}^N \vec{u}_{x_i}\cdot\Bigg[& \vec{v}_{x_i} - \vec{v}_{x_i}\cdot\nabla_\psi\Phi(\vec{u})\nabla_\psi\Phi(\vec{u}) - \vec{v}\cdot\frac{\partial\nabla_\psi\Phi(\vec{u})}{\partial x_i}\nabla_\psi\Phi(\vec{u}) \\
& - \vec{v}\cdot\nabla_\psi\Phi(\vec{u})\frac{\partial\nabla_\psi\Phi(\vec{u})}{\partial x_i} - \vec{v}_{x_i}\cdot\nabla\psi(\vec{u})\nabla\psi(\vec{u}) - \vec{v}\cdot\frac{\partial\nabla\psi(\vec{u})}{\partial x_i}\nabla\psi(\vec{u}) - \vec{v}\cdot\nabla\psi(\vec{u})\frac{\partial\nabla\psi(\vec{u})}{\partial x_i}\Bigg].
\end{aligned}
\tag{25}
$$

Since $\Phi(\vec{u}) = \psi(\vec{u}) = 0$, differentiating with respect to x_i we obtain that $\nabla\Phi(\vec{u})\cdot\vec{u}_{x_i} = \nabla\psi(\vec{u})\cdot\vec{u}_{x_i} = 0$, and therefore

$$\nabla_\psi\Phi(\vec{u})\cdot\vec{u}_{x_i} = 0.$$

The expression (25) can be simplified to obtain

$$e[\vec{w}_\lambda] \simeq e[\vec{u}] + \lambda\sum_{i=1}^N \vec{u}_{x_i}\cdot\left[\vec{v}_{x_i} - \vec{v}\cdot\nabla_\psi\Phi(\vec{u})\frac{\partial\nabla_\psi\Phi(\vec{u})}{\partial x_i} - \vec{v}\cdot\nabla\psi(\vec{u})\frac{\partial\nabla\psi(\vec{u})}{\partial x_i}\right].$$

Moreover, since

$$\frac{\partial\nabla_\psi\Phi(\vec{u})}{\partial x_i} = \mathbf{H}_\Phi\vec{u}_{x_i} - \frac{\partial\Lambda}{\partial x_i}(\vec{u})\nabla\psi(\vec{u}) - \Lambda(\vec{u})\mathbf{H}_\psi\vec{u}_{x_i}$$

we have

$$\frac{\partial\nabla_\psi\Phi(\vec{u})}{\partial x_i}\cdot\vec{u}_{x_i} = \mathbf{H}_\Phi^\mathscr{N}[\vec{u}_{x_i}, \vec{u}_{x_i}].$$

With all this in mind we find that (again, up to first order in λ)

$$e[\vec{w}_\lambda] \simeq e[\vec{u}] + \lambda\sum_{i=1}^N \vec{u}_{x_i}\cdot\left[\vec{v}_{x_i} - \vec{v}\cdot\nabla_\psi\Phi(\vec{u})\mathbf{H}_\Phi^\mathscr{N}[\vec{u}_{x_i}, \vec{u}_{x_i}] - \vec{v}\cdot\nabla\psi(\vec{u})\mathbf{H}_\psi(\vec{u})[\vec{u}_{x_i}, \vec{u}_{x_i}]\right].$$

Using this expression, after imposing that $(\partial/\partial\lambda)|_{\lambda=0}\int_\Omega e[\vec{w}_\lambda]\,dv = 0$ for every $\vec{v}$, we find that the Euler–Lagrange is

$$\Delta\vec{u} + \left(\sum_k \mathbf{H}_\psi\left[\frac{\partial\vec{u}}{\partial x_k}, \frac{\partial\vec{u}}{\partial x_k}\right]\right)\nabla\psi(\vec{u}) + \left(\sum_k \mathbf{H}_\Phi^\mathscr{N}\left[\frac{\partial\vec{u}}{\partial x_k}, \frac{\partial\vec{u}}{\partial x_k}\right]\right)\nabla_\psi\Phi(\vec{u}) = 0.
\tag{26}$$

an expression utterly predictable. $\square$

3.1. Simple verification

As for the case of closed manifolds, we now verify that in fact the gradient descent corresponding to the Euler–Lagrange (26) keeps $\vec{u}$ in $\{\psi = 0\} \cap \{\Phi = 0\}$.

Proposition 4. *If $\vec{u}$ is a solution to the gradient descent flow corresponding to Eq. (26), then $\vec{u}$ maps into the submanifold $\{\psi = 0\} \cap \{\Phi = 0\}$.*

Proof. We just need to show that both $v(x, t) \triangleq \psi(\vec{u}(x, t))$ and $\mu(x, t) \triangleq \Phi(\vec{u}(x, t))$ are always zero. The idea is the same one we used in Section 2.3, it is enough to show that both v and μ satisfy the *heat equation* with adiabatic *boundary conditions*:

[ψ] We have

$$v_t = \nabla\psi \cdot \Delta\vec{u} + \sum_k \mathbf{H}_\psi \left[\frac{\partial\vec{u}}{\partial x_k}, \frac{\partial\vec{u}}{\partial x_k} \right]$$

since $\nabla\psi \perp \nabla_\psi\Phi$. Also

$$\Delta v = \nabla\psi \cdot \Delta\vec{u} + \sum_k \mathbf{H}_\psi \left[\frac{\partial\vec{u}}{\partial x_k}, \frac{\partial\vec{u}}{\partial x_k} \right]$$

and

$$v_t = \Delta v.$$

[Φ] We have

$$\mu_t = \nabla\Phi \cdot \Delta\vec{u} + \nabla\Phi \cdot \nabla_\psi\Phi \left(\sum_k \mathbf{H}_\Phi^{\mathscr{N}} \left[\frac{\partial\vec{u}}{\partial x_k}, \frac{\partial\vec{u}}{\partial x_k} \right] \right) + \Lambda \left(\sum_k \mathbf{H}_\psi \left[\frac{\partial\vec{u}}{\partial x_k}, \frac{\partial\vec{u}}{\partial x_k} \right] \right).$$

From $\nabla\Phi \cdot \nabla_\psi\Phi = \nabla_\psi\Phi \cdot \nabla_\psi\Phi = \|\nabla_\psi\Phi\|^2 = 1$, the above equation continues as

$$= \nabla\Phi \cdot \Delta\vec{u} + \left(\sum_k \mathbf{H}_\Phi^{\mathscr{N}} \left[\frac{\partial\vec{u}}{\partial x_k}, \frac{\partial\vec{u}}{\partial x_k} \right] \right) + \Lambda \left(\sum_k \mathbf{H}_\psi \left[\frac{\partial\vec{u}}{\partial x_k}, \frac{\partial\vec{u}}{\partial x_k} \right] \right)$$

$$= \nabla\Phi \cdot \Delta\vec{u} + \left(\sum_k \mathbf{H}_\Phi \left[\frac{\partial\vec{u}}{\partial x_k}, \frac{\partial\vec{u}}{\partial x_k} \right] \right).$$

Also

$$\Delta\mu = \nabla\Phi \cdot \Delta\vec{u} + \left(\sum_k \mathbf{H}_\Phi \left[\frac{\partial\vec{u}}{\partial x_k}, \frac{\partial\vec{u}}{\partial x_k} \right] \right)$$

and then

$$\mu_t = \Delta\mu$$

Finally, it is easy to see that both v and μ satisfy *Neumann boundary conditions*. Since at $t = 0$ both functions are zero, we must have that they are identically zero. □

3.2. Example

We now present an example of the evolution corresponding to the above equation, where the target manifold is the circle $S^1 \subset \mathbb{R}^3$. We will prove, by direct calculation, that the evolution PDE corresponding to (26) reduces to the expected one from the classical theory of harmonic maps (liquid crystals).

Let $\mathscr{C} = \{(x,y,z) \in \mathbb{R}^3 | x^2 + y^2 = 1, z = 0\}$. We will then choose the representation $\mathscr{C} = \{(x,y,z) \in \mathbb{R}^3 | z = 0\} \cap \{(x,y,z) | x^2 + y^2 = 1\}$. We select $\mathcal{N} = \{(x,y,z) \in \mathbb{R}^3 | z = 0\}$, that is, $\psi(x,y,z) = z$ and therefore $\nabla \psi = \vec{e}_3 = (0,0,1)$. The set $\mathscr{K}_{\mathscr{C}}$ is then given by $\{(x,y,z) | x^2 + y^2 = 1\}$. In Fig. 1 we depict this situation. Now we solve (22) with the condition $\Phi|_{\mathscr{K}_{\mathscr{C}}} = 0$. Observe that $\nabla_\psi \Phi = (\Phi_x, \Phi_y, 0)$. Then, the PDE we must solve reads $\Phi_x^2 + \Phi_y^2 = 1$, and the solution that satisfies the boundary condition above is $\Phi(x,y,z) = \sqrt{x^2 + y^2} - 1$. Let $\rho = \sqrt{x^2 + y^2}$. One computes that $\nabla \Phi(x,y,z) = (x,y,0)\rho^{-1}$. We can now find the components of $\mathbf{H}_\Phi$, the Hessian matrix of Φ at the point (x,y,z), to obtain $\Phi_{xx} = \rho^{-1} - x^2\rho^{-3}$, $\Phi_{yy} = \rho^{-1} - y^2\rho^{-3}$, $\Phi_{xy} = \Phi_{yx} = -xy\rho^{-3}$, and $\Phi_{zx} = \Phi_{xz} = \Phi_{zy} = \Phi_{yz} = \Phi_{zz} = 0$. Since $\mathbf{H}_\psi = 0$ we obtain $\mathbf{H}_\Phi^{\mathcal{N}}(x,y,z) = \mathbf{H}_\Phi(x,y,z)$.

The next step is to write Eq. (26) in this specific case. The first observation is that, again, since $\mathbf{H}_\psi = 0$, the time evolution corresponding to (26) simplifies to

$$\vec{u}_t = \Delta \vec{u} + \left(\sum_k \mathbf{H}_\Phi(\vec{u}) \left[\vec{u}_{x_k}, \vec{u}_{x_k} \right] \right) \nabla \Phi(\vec{u}).$$

For any vector $\vec{v} = (v_x, v_y, v_z) \in \mathbb{R}^3$, one has at the point (x,y,z), $\mathbf{H}_\Phi[\vec{v}, \vec{v}] = v_x^2(1 - x^2) + v_x^2(1 - x^2) - 2xyv_xv_y = v_x^2 + v_y^2 - (xv_x + yv_y)^2$.

It is also of great help knowing, from Section 3.1, that along the time evolution, both $\psi(\vec{u}) = 0$ and $\Phi(\vec{u}) = 0$ if the initial datum is on $\mathscr{C}$. This translates into $\rho = 1$ everywhere in our expressions for $\mathbf{H}_\Phi$ and $\nabla \Phi$. Let us write $\vec{u} = (U, V, W)$. Then, since $U^2 + V^2 = 1$, differentiating with respect to x_k we find $UU_{x_k} + VV_{x_k} = 0$. We also have $W = 0$.

Hence, $\mathbf{H}_\Phi(\vec{u})[\vec{u}_{x_k}, \vec{u}_{x_k}] = U_{x_k}^2 + V_{x_k}^2 - (UU_{x_k} + VV_{x_k})^2 = U_{x_k}^2 + V_{x_k}^2$, and the time evolution equation reads

$$\begin{cases} U_t = \Delta U + (\|\nabla U\|^2 + \|\nabla V\|^2)U, \\ V_t = \Delta V + (\|\nabla U\|^2 + \|\nabla V\|^2)V, \\ W = 0, \end{cases} \tag{27}$$
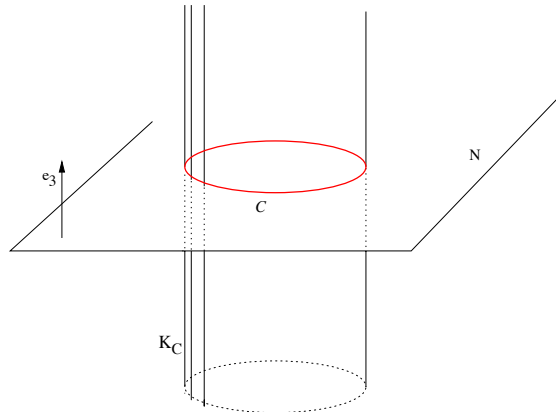

Fig. 1. Example of a mapping into $S^1 \subset \mathbb{R}^3$.

which we immediately recognize as the one corresponding to diffusion of maps into S^1 ($\subset \mathbb{R}^2$, if we discard the superfluous component W), see for example Appendix A, Eq. (A.2).

4. Implicit domain manifolds and *p*-harmonic maps

For completeness, we present now the formulas corresponding to the case where both the domain and target manifolds are represented in implicit form (with the embedding functions being the corresponding signed distance ones). Deriving these formulas is straightforward using the framework here presented when combined with the work in [5]. We also show the corresponding flows for *p*-harmonic maps.

4.1. p-Harmonic maps

We still assume $\mathcal{M}$ to be planar. The energy density (2) (but not the dependence of the energy on its density) is redefined as follows. For every $p \in [1, +\infty)$ let

$$e_p[\vec{u}] \triangleq \frac{1}{p} \|\mathbf{J}_{\vec{u}}\|_{\mathcal{F}}^p.$$

A simple application of variational calculus leads to conclude that [15]

$$\vec{u}_t = p^{1-\frac{2}{p}} \mathbf{\Pi}_{\nabla \psi(\vec{u})} \left(\nabla \cdot \left((e_p[\vec{u}])^{1-\frac{2}{p}} \mathbf{J}_{\vec{u}}^T \right) \right). \tag{28}$$

Note that if $p < 2$ difficulties are expected to arise, see [43] and the references therein.

4.2. Generic (implicit) domain manifolds

Let $\mathcal{M} = \{x \in \mathbb{R}^m : \phi(x) = 0\}$, where $\phi(\cdot)$ is the signed distance function to $\mathcal{M}$. Then the diffusion is given by

$$\vec{u}_t = \nabla \cdot \left(\mathbf{\Pi}_{\nabla \phi} \mathbf{J}_{\vec{u}}^T \right) + \left(\sum_{k,r} \mathbf{H}_\psi [\vec{u}_{x_r}, \vec{u}_{x_k}] \left(\mathbf{\Pi}_{\nabla \phi} \right)_{kr} \right) \nabla \psi. \tag{29}$$

The whole deduction rests upon the redefinition of the energy (1) and its density (2). Now we should define the energy density to be

$$e_\phi[\vec{u}] \triangleq \frac{1}{2} \|\mathbf{J}_{\vec{u}}^\phi\|_{\mathcal{F}}^2,$$

where the *intrinsic Jacobian* of $\vec{u}$ can be written as (see Appendix B for more details) $\mathbf{J}_{\vec{u}}^\phi = \mathbf{J}_{\vec{u}} \mathbf{\Pi}_{\nabla \phi}$.
The new definition for the energy should be [16]

$$E[\vec{u}] \triangleq \int_{\mathbb{R}^m} e_\phi[\vec{u}] \delta(\phi(x)) \, dx. \tag{30}$$

---

[15] The divergence operator convention (for a matrix A) we have used is $\nabla \cdot A = (\nabla \cdot \vec{A}_{v_1} | \cdots | \nabla \cdot \vec{A}_{v_r})$, where $\vec{A}_{v_i}$ stands for the *i*th column of A. That is, we apply a columnwise divergence.

[16] We have already taken into account that $\|\nabla \phi\| = 1$.

Comparing (29) with (18), we can infer the implicit form of the Christoffel symbols [17]

$$\mathbf{\Gamma}_{ij}^l(\vec{u}) = \frac{\partial^2 \psi}{\partial u^i \, \partial u^j}(\vec{u}) \frac{\partial \psi}{\partial u^l}(\vec{u}).$$

4.3. Generic (implicit) domain manifold and p-harmonic maps

Using both generalizations presented above, we arrive at the following formula with a bit more computational effort

$$\vec{u}_t = p^{1-\frac{2}{p}} \mathbf{\Pi}_{\nabla\psi(\vec{u})}\left(\nabla \cdot \left((e_{\phi,p}[\vec{u}])^{1-\frac{2}{p}} \mathbf{\Pi}_{\nabla\phi} \mathbf{J}_{\vec{u}}^{\mathrm{T}}\right)\right),\tag{31}$$

where

$$e_{\phi,p}[\vec{u}] \triangleq \frac{1}{p}\|\mathbf{J}_{\vec{u}}^{\phi}\|_{\mathscr{F}}^p.$$

4.4. Diffusion of tangent and normal directions

Throughout this section we will assume $\dim(\mathscr{M}) = \dim(\mathscr{N})$. Assume we want to diffuse intrinsic vectorial data constrained to be a direction (unit norm) and to be either normal or tangent to the domain manifold, e.g. [5]. This is an extremely important case, for example to denoise principal directions and normal vectors. We now derive these equations, which to the best of our knowledge have not been reported before even for explicit manifolds.

To achieve this goal, we minimize the functional (30) taking a variation of the form (assume $\vec{u}$ minimizes the energy functional while satisfying both $\|\vec{u}\| = 1$ and $\Pi(\vec{u}) = \vec{u}$)

$$\vec{u}_\lambda(x) \triangleq \frac{\vec{u} + \lambda\Pi(\vec{v})}{\|\vec{u} + \lambda\Pi(\vec{v})\|},$$

where $\vec{v} : \mathscr{M} \to \mathbb{R}^d$ is smooth and Π is either $\mathbf{\Pi}_{T_x\mathscr{M}}$ or $\mathbf{\Pi}_{N_x\mathscr{M}}$ (projection onto the tangent or normal space, respectively). Let $\vec{w} = \Pi(\vec{v})$. Then it follows easily that

$$\frac{\mathrm{d}E[\vec{u}_\lambda]}{\mathrm{d}t}\bigg|_{\lambda=0} = -\int_{\mathbb{R}^m} \left\{\Delta_\phi\vec{u} + 2e_\phi[\vec{u}]\vec{u}\right\} \cdot \vec{w}\delta(\phi(x)) \, \mathrm{d}x.$$

Imposing $(\mathrm{d}E[\vec{u}_\lambda]/\mathrm{d}t)|_{\lambda=0} = 0$ for all v implies

$$\Pi\left(\Delta_\phi\vec{u} + 2e_\phi[\vec{u}]\vec{u}\right) = \Pi\left(\Delta_\phi\vec{u}\right) + 2e_\phi[\vec{u}]\vec{u} = 0$$

Finally, the diffusion flow obtained is

$$\frac{\partial\vec{u}}{\partial t}(x,t) = \Pi_x\left(\Delta_\phi\vec{u}(x,t)\right) + 2e_\phi[\vec{u}](x,t)\vec{u}(x,t).\tag{32}$$

---

[17] Of course $g^{ij} = (\mathbf{\Pi}_{\nabla\phi})_{ij}(= g_{ij}^{-1})$. Then, it is nice to observe (although formally incorrect) that since $\mathbf{\Pi}_{\nabla\phi}\nabla\phi = 0$, then the metric $g : \mathbb{R}^d \to \mathbb{R}^{d\times d}$ has eigenvalue $+\infty$ in the direction given by $\nabla\phi$ thus prohibiting intermingling of information between adjacent level sets of ϕ.

Note that if the PDE (32) admits a smooth solution until time T, [18] and if (for instance) we are dealing with tangent directions diffusion, the function $f(x,t) \triangleq \nabla\phi(x) \cdot \vec{u}(x,t)$ satisfies $f_t(x,t) = 2e_\phi[\vec{u}]f(x,t)$. Therefore,

$$f(x,t) = f(x,0)\,e^{2\int_0^t e[\vec{u}](x,t)\,\mathrm{d}t}$$

thus verifying that if $\nabla\phi(x) \cdot \vec{u}(x,0) = 0$ then $\nabla\phi(x) \cdot \vec{u}(x,t) = 0$ for $t \leqslant T$. We also want to check whether $\|\vec{u}(x,t)\| = 1 \; \forall(x,t)$. Let

$$F_\phi[\vec{u}](t) \triangleq \frac{1}{2} \int_{\mathbb{R}^d} \|\mathbf{J}_{\vec{u}}\|_{\mathscr{F}}^2 \delta(\phi(x))\,\mathrm{d}x.$$

Then $\dot{F}_\phi[\vec{u}](t) = -\int_{\mathbb{R}^d} \vec{u}_t \cdot \Delta_\phi \vec{u}\delta(\phi(x))\,\mathrm{d}x$. Since both $\|\vec{u}\| = 1$ and $\Pi(\vec{u}) = \vec{u}$ (so $\Pi(\vec{u}_t) = \vec{u}_t$ since Π does not depend on t) must hold, and in order to make $\dot{F}_\phi[\vec{u}](t)$ non-positive we choose

$$\vec{u}_t = \Pi\mathbf{\Pi}_{T_{\vec{u}}\{\|\vec{u}\|=c\}}\Delta_\phi\vec{u}, \tag{33}$$

where $\mathbf{\Pi}_{T_{\vec{u}}\{\|\vec{u}\|=c\}} = \mathbf{I} - \vec{u}/\|\vec{u}\|\,\vec{u}^{\mathrm{T}}/\|\vec{u}\|$ for any $c > 0$.

Note that the above evolution indeed forces $\vec{u}(x,t)$ to satisfy both imposed conditions. Let $\vec{v} : \mathbb{R}^d \to \mathbb{R}^d$ be such that $\Pi(\vec{v}) = \vec{0}$. Then $(\vec{v} \cdot \vec{u})_t = \vec{v} \cdot \vec{u}_t = \vec{v} \cdot \Pi\mathbf{\Pi}_{T_{\vec{u}}S^{d-1}}\Delta_\phi\vec{u} = \Pi^{\mathrm{T}}\vec{v} \cdot \mathbf{\Pi}_{T_{\vec{u}}\{\|\vec{u}\|=c\}}\Delta_\phi\vec{u} = 0$, since the projection matrix is symmetric, and just using this we have $((1/2)\|\vec{u}\|^2)_t = \vec{u} \cdot \vec{u}_t = \vec{u} \cdot \mathbf{\Pi}_{T_{\vec{u}}\{\|\vec{u}\|=c\}} = 0$ trivially. Finally, using $\|\vec{u}\| = 1$ and carrying out some computations in a way similar to Section 5, [19] one can prove that (33) reduces to (32).

5. Numerical implementation and examples

We now discuss the numerical implementation of the flows previously introduced. Since the target manifold is now implicitly represented, we can basically use classical, well studied, numerical techniques on Cartesian grids. In other words, the framework here introduced permits the use of already existing numerical techniques, thereby enjoying their available analysis results. This is a key concept, instead of working on the development of new numerical schemes for meshes, the use of implicit representations following our framework brings us back to classical schemes. Moreover, examples like those in Fig. 5 have not been reported in the literature yet, since prior to our approach all PDEs for mapping three-dimensional meshes used projections as intermediate steps. Therefore, the work here proposed, when combined with [5], not only permits to use classical numerical schemes to solve PDEs and variational problems for surfaces, it is also an enabling technology for general maps.

Note that although the flows derived in this paper guarantee that the map remains on the target (submanifold), numerical errors can move it away from it, requiring a simple projection step (see the projection equations presented before in this paper). In particular, when dealing with submanifolds, although the evolution equations also guarantee that the solution will remain inside the convex hull, due to numerical discretization, $\vec{u}$ could be taken outside of it during the evolution. In order to numerically project it back, we need to have a distance function to this convex hull defined on the implicitly defined target manifold. In [32] we have shown how to computationally optimal compute such a distance function on implicitly defined manifolds, and this is the technique used for this projection into the convex hull.

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[18] Note that we might be subject to the topological obstruction given by the Hairy Ball Theorem when $\dim(\mathscr{M}) = \dim(\mathscr{N})$ is odd.
[19] The main difference is that now one must take into account the Laplace–Beltrami expressed "implicitly", see Appendix B for more details on intrinsic differential operators within the implicit framework.

An explicit scheme can be devised to implement (29) (recall that this is the extension, for general domain manifolds, of the Eq. (14) derived in Section 2). However, following [14], it turns out that it is more convenient to implement the *mathematically equivalent* evolution derived in Section 2.4. More specifically, the *equivalent* evolution is (see Eq. (21))

$$\frac{\partial u}{\partial t} = \Delta u - (\Delta u \cdot \nabla \psi) \nabla \psi. \tag{34}$$

That both evolutions are equivalent is easy to see.

Proposition 5. *Eq.* (34) *is equivalent to the mapping into implicit surfaces flow* (14).

Proof. One has that $f(x, t) \triangleq \psi(\vec{u}(x, t)) = 0 \; \forall (x, t) \in \Omega \times \mathbb{R}^+ \cup \{0\}$ for $\vec{u}(\cdot, \cdot)$ satisfying (14). Now, differentiating f with respect to x_i we obtain

$$\nabla \psi(\vec{u}) \cdot \vec{u}_{x_i} = 0.$$

Differentiating again with respect to x_i,

$$\mathbf{H}_\psi[\vec{u}_{x_i}, \vec{u}_{x_i}] + \nabla \psi \cdot \vec{u}_{x_i x_i} = 0.$$

Summing for all i,

$$\sum_i \mathbf{H}_\psi[\vec{u}_{x_i}, \vec{u}_{x_i}] + \nabla \psi \cdot \Delta \vec{u} = 0$$

and using the previous expression we derive (34) from (14). $\square$

5.1. Numerical scheme

All the coding was done using Flujos as the main core (see [21]) and VTK (see [52]) for visualization purposes. Note that for visualization purposes only, the surfaces are triangulated at the end, via marching cubes as implemented in [52]. This is not at all an intrinsic component of our framework, and many applications (e.g. brain warping and regularization problems) are interested in the values of the solution $\vec{u}$, without the need for visualization of the target surface.

All the examples below were carried based in Eq. (31). Once again, the numerical implementation is straightforward (at least when $p = 2$), since it is basic Cartesian numerics, and full details and analysis can be found in the standard literature in numerical analysis. We select a particular efficient scheme from the literature, while others (including implicit or semi-implicit schemes) could be used as well.

We use forward time discretization (explicit scheme), and for the spatial discretization, we used the following well-known recipe. To spatially discretize

$$f_t(x, t) = \nabla \cdot (\mathbf{K}(x) \nabla f(x, t)) \tag{35}$$

($\mathbf{K}(x)$ is a symmetric positive semi-definite matrix), we consider *backward* approximation of the divergence and a *forward* approximation of the gradient. Let us explain how this applies in our situation, and for that we assume $p = 2$ in (31). Then, the equation we have to implement is

$$\vec{u}_t(x, t) = \mathbf{\Pi}_{\nabla \psi(\vec{u}(x, t))} \left(\nabla \cdot \left(\mathbf{\Pi}_{\nabla \phi(x)} \left(\mathbf{J}_{\vec{u}}^{\mathrm{T}}(x, t) \right) \right) \right). \tag{36}$$

If we do not take into account the outer projection matrix, every coordinate of $\vec{u}$ evolves according to

$$u_t^i(x, t) = \nabla \cdot \left(\mathbf{\Pi}_{\nabla \phi(x)} \nabla u^i(x, t) \right)$$

Fig. 2. Diffusion of a noisy texture map (left) onto an implicit sphere (right). (This is a color figure. See the journal web page for the color version.)

having for each component the same structure than the model evolution (35). We then borrow the above discretization for our evolution. If we consider the coupling among different u^i's imposed by the projection matrix $\mathbf{\Pi}_{\nabla\psi(\cdot)}$, we see that we still preserve numerical stability since this matrix is positive semidefinite and has spectral radius not greater than 1. [20] In more detail, it can be shown after some calculations (see [23,45]) that for the scheme (p now denotes a position over the grid)

$$\vec{v}_p^{n+1} = \vec{v}_p^n + \Delta t \mathbf{P}(\vec{v}_p^n)\left(\nabla^- \cdot \left(\mathbf{Q}(p)\nabla^+ \vec{v}_p^n\right)\right)$$

the stability condition is of the form ($\lambda = \Delta t/(\Delta x)^2$)

$$\lambda \leqslant \min_{p,u} \frac{S(p)}{\rho(\mathbf{P}(u)) \max\{S^2(p), D^2(p)\}}$$

or

$$\lambda \leqslant \frac{1}{\max_u \rho(\mathbf{P}(u))} \min_p \left\{\frac{S(p)}{\max\{S^2(p), D^2(p)\}}\right\},$$

where $\rho(\mathbf{P}(p))$ stands for the spectral radius of the matrix $\mathbf{P}(p)$, $S(p) = \sum_{ij}(q_{ij}(p) + q_{ij}(p - \Delta x\vec{e}_i))$, and $D(p) = \sum_{ij}(q_{ij}(p) - q_{ij}(p - \Delta x\vec{e}_i))$. In our case we may admit $D(\cdot)$ to be small compared with $S(\cdot)$ (given the identification $\mathbf{Q} \leftrightarrow \mathbf{\Pi}_{\nabla\phi}$) when Δx is small. This can be easily related to the curvatures of $\{\phi = 0\}$ giving a condition on the sampling of the distance function (ϕ) representing the domain manifold. This condition mainly means that we require a fine enough sampling as to guarantee that the change in the normals to the level surfaces of ϕ is small between adjacent grid points. This condition is obviated when the domain manifold is planar. So the stability condition becomes

$$\lambda \leqslant \frac{1}{\max_u \rho(\mathbf{P}(u)) \max_p S(p)}.$$

---

[20] Note that $\|\vec{v}\|^2 \geqslant \mathbf{\Pi}_{\nabla\psi}[\vec{v}, \vec{v}] = \|v\|^2 - |\nabla\psi \cdot \vec{v}|^2 \geqslant 0$ for all $\vec{v}$. We have used that ϕ is a distance function.

Fig. 3. Diffusion of a noisy texture map onto an implicit teapot. We show two different views (noisy on the top and regularized on the bottom). (This is a color figure. See the journal web page for the color version.)

Since by Cauchy–Schwartz's inequality (and the aforementioned assumption on the change of $\nabla\phi$ between adjacent grid points) $2d$ (in practise) upper-bounds $S(p)$, remembering the fact that $\rho(\mathbf{P}(p)) \leqslant 1$, we arrive at $\lambda \leqslant 1/2d$. Note that if a more careful implementation is desired, good choices are ADI or AOS schemes, see [53].

All derivatives in $\mathbf{\Pi}_{\nabla\psi(\cdot)}$ and $\mathbf{\Pi}_{\nabla\phi(\cdot)}$ were approximated by central differences. An interpolation scheme had to be used since the evaluations of $\mathbf{\Pi}_{\nabla\psi(\cdot)}$ in the above equation are at positions given by $\vec{u}(x,t)$, positions not necessarily on the underlying grid. We used linear interpolation for this purpose.

Note that as done in [5], when the domain manifold is also implicitly represented, the values of the map on it are, from time to time (every 5 iterations, for example), extended to its surrounding offset due to stability considerations, we call this process "extension evolution". This process is well known in the area of implicit surfaces. Also, as explained before, due to numerical discretization, the discretely computed solution map can be taken out of the target manifold during the evolution. In this paper, we simply project it
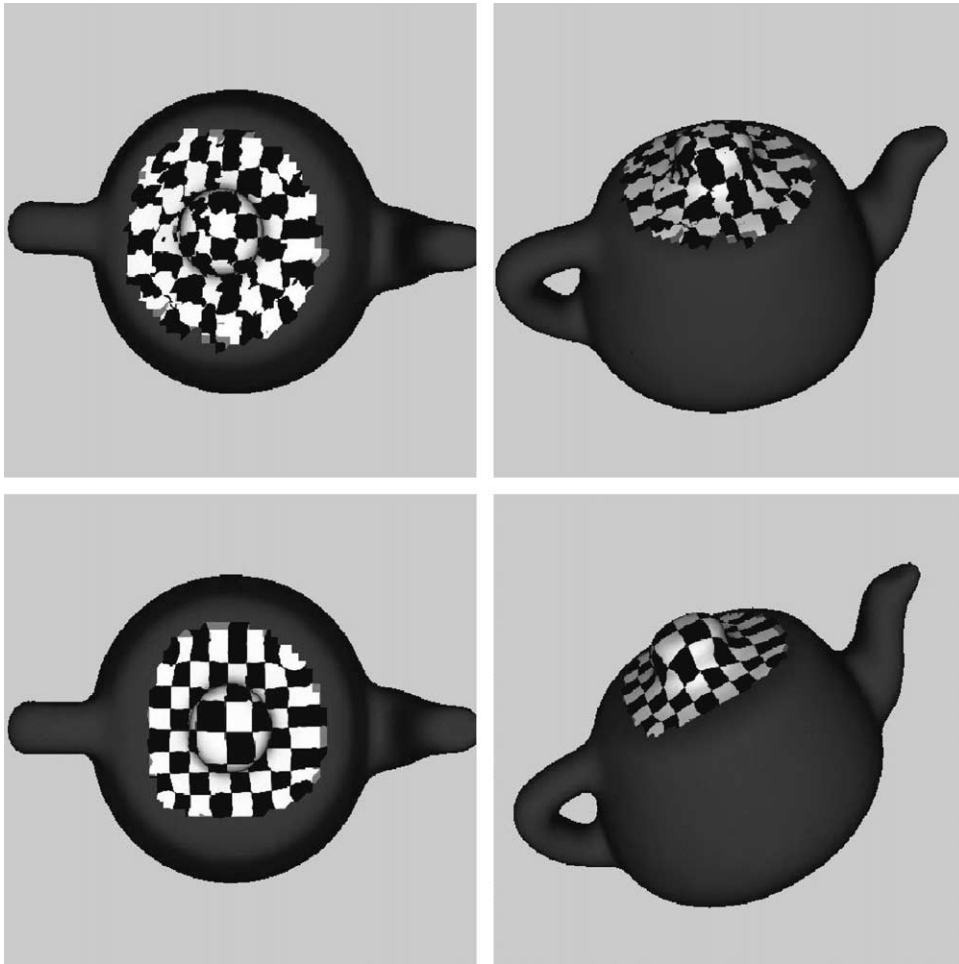
Fig. 4. Diffusion of a texture map for an implicit teapot (noisy on the top and regularized on the bottom). A chess board texture is mapped.

back at every iteration. We have seen that this projection is a trivial step due to the fact that the embedding is a distance function. It is quite straightforward to show that the results reported in [1] can be extended for our equations as well, at least for convex hypersurfaces (additional numerical work in this area has been performed by E and Wang [14]). This guarantees then that the projection step does not introduce numerical problems. Further analysis of this projection step will be reported elsewhere.

This provides the whole numerical scheme for this particular equation using our framework. To resume, we implement (36) with simple finite differences schemes (central, forward, and backward differences). At every numerical iteration, the values of $\vec{u}$ are projected to the zero level-set to correct for possible numerical errors (projection which becomes trivial since the embedding function is a distance function). If the domain manifold is not planar, every k ($k = 5$ in our experiments) iterations we run a certain number of iterations of the extension evolution, [5]. When needed, we interpolate the values of the grid onto the underlying surface by simple linear interpolation. All these steps are classical, simple to implement, based on well known numerical schemes, and are generic and not designed just for a particular flow.
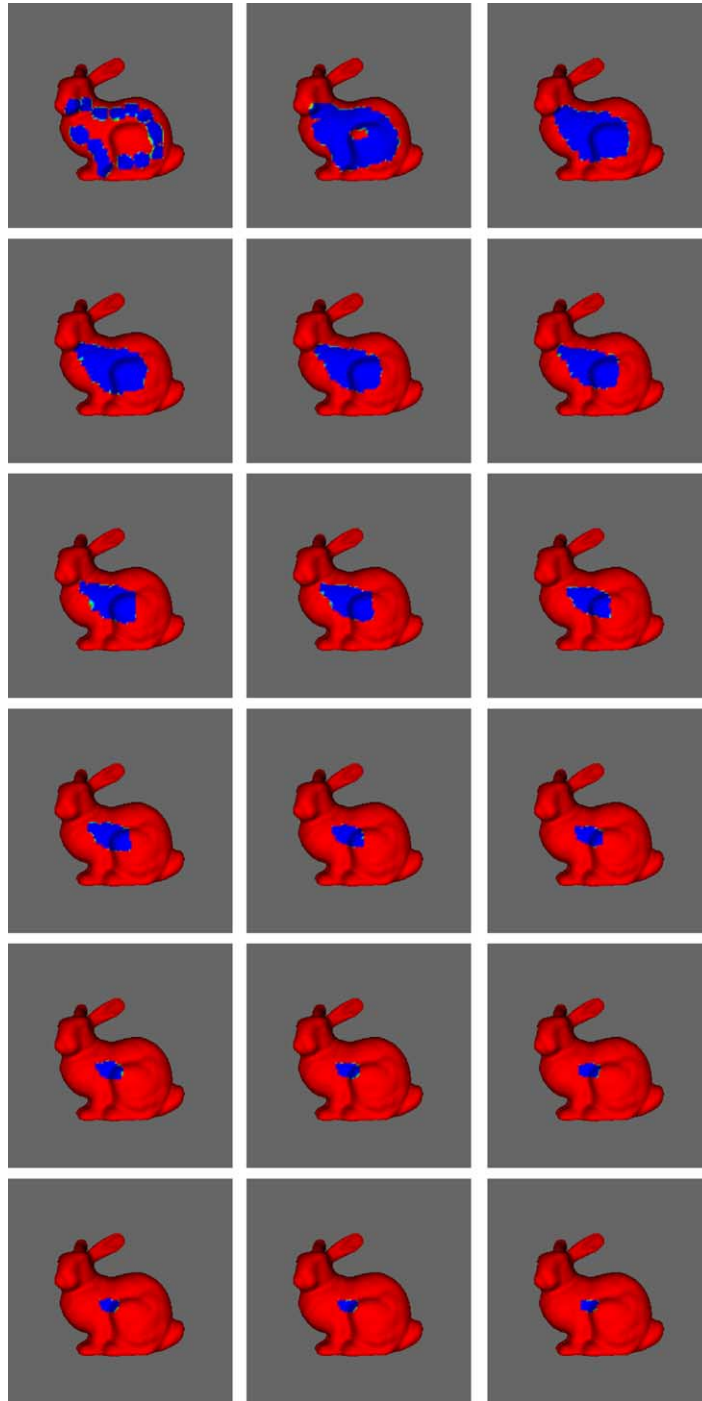
Fig. 5. Diffusion of a random map from an implicit torus to the implicit bunny. In blue are marked those points of the bunny's surface pointed by the map at every instant. Different figures correspond to increasing instances of the evolution, from top to bottom and left to tight. We show the map at 17 of 100 iterations performed to the initial map with a time step of .01. We used the 2-harmonic heat flow with adiabatic conditions. (This is a color figure. See the journal web page for the color version.)

5.2. Examples

In all the examples below, the domain manifold $\mathscr{M}$ is either the Euclidean space $\mathbb{R}^2$ or an implicit torus. The target manifold $\mathscr{N}$ is an implicit surface in $\mathbb{R}^3$, that is, the zero level-set of $\psi : \mathbb{R}^3 \rightarrow \mathbb{R}$, ψ being a signed distance function (this is of course also the case when the surface is a sphere, ψ being as in Section 2.3).

In order to present interesting examples we construct texture maps, add noise to them, and then diffuse them using our framework. Let $\mathscr{S}$ be the surface onto which we want to map a given (planar) image defined in a subset $D \subset \mathbb{R}^2$. Then, the *texture map* is a map $\vec{T} : \mathscr{S} \rightarrow D$. Once the map is known, we inverted it to find a map $\vec{u}_0 : D \rightarrow \mathscr{S}$. Then, we built up the noisy map $\vec{u} : D \rightarrow \mathscr{S}$ defined by

$$\vec{u}(x) = \mathbf{\Pi}_{\mathscr{S}} \Big(\vec{u}_0(x) + \vec{\mathbf{n}}(x) \Big),$$

where $\vec{\mathbf{n}} : D \rightarrow \mathscr{S}$ is random map with small prescribed power σ. We then feed the evolution (14) with $\vec{u}$ as initial condition, and Neumann boundary conditions. After a certain number of steps, we stop the evolution, invert the resulting map, and use it as a texture map to paint the surface with a certain texture. [21]

As a means of finding a suitable $\vec{T}$ we have implemented the work in [50] (a multidimensional scaling approach), combined with the technique developed in [32] for computing distances on implicit surfaces. In all the steps just described there are some minor implementation details, mainly regarding interpolation tasks, that we omit for the sake of clarity.

In Figs. 2–4 we then denoise vectors from the plane $\mathbb{R}^2$ to a three-dimensional surface defined as the zero level-set of $\psi : \mathbb{R}^3 \rightarrow \mathbb{R}$ and map a texture image to the surface using the obtained map. Note that the map is the one being processed, not the image itself.

We also show an example of diffusion of random maps from an implicit torus to the implicit bunny model, see Fig. 5. As expected from the theory, when evolving this set with the harmonic flow, the set converges to a unique point. This particular example of mapping a given three-dimensional surface to another one was previously addressed via artificial, distortion introducing, projections to the plane or sphere when the surface was represented as meshes [46].

6. Conclusions

In this paper we have shown how to implement variational problems and partial differential equations onto general target surfaces. We have also addressed the case of open target surfaces and sub-manifolds. The key concept is to represent the target (sub-)manifolds in implicit form, and then implement the equations in the corresponding embedding space. This framework completes the work with general domain manifolds reported in [5], thereby providing a complete solution to the computation of maps between generic manifolds.

We are currently using this framework to map two generic surfaces for warping (without intermediate projections onto the plane), and to develop numerical techniques for high order flows on and onto surfaces. To complete the general computational framework here introduced, a detailed numerical analysis on comparison with mesh based techniques is to be performed. For the work on implicit domain manifolds introduced in [5], some of this analysis was recently performed in [2]. We plan to perform similar tests for implicit target manifolds and results will be reported elsewhere.

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[21] Note that we are not proposing this as a complete texture mapping alternative, it is just to provide an illustrative example.

Acknowledgements

Appendix A. Boundary conditions for the gradient descent flow

We now justify the use of Neumann boundary conditions for the gradient descent flow in Section 2.1.1. In the scalar case, one has the evolution problem

$$\begin{cases} I_t(x,t) = \Delta I(x,t), & x \in \mathscr{M}, \ t \geqslant 0, \\ I(x,0) = I_0(x), & x \in \mathscr{M}, \\ \nabla I \cdot \mathbf{n}|_{\partial \mathscr{M}} = \mathbf{0}. \end{cases} \tag{A.1}$$

We observe that the quantity $\sigma(t) \triangleq \int_{\mathscr{M}} I(x,t) \, \mathrm{d}_{\mathscr{M}} v$ remains constant,

$$\dot{\sigma}(t) = \int_{\mathscr{M}} I_t(x,t) \, \mathrm{d}_{\mathscr{M}} v = \int_{\mathscr{M}} \Delta I(x,t) \, \mathrm{d}_{\mathscr{M}} v = \int_{\mathscr{M}} \nabla \cdot (\nabla I) \, \mathrm{d}_{\mathscr{M}} v = \int_{\partial \mathscr{M}} \nabla I \cdot \mathbf{n} \, \mathrm{d}_{\mathscr{M}} s = 0$$

thereby imposing the boundary conditions.

One wonders which quantity is preserved thru time by the flow in the general case, when imposing the boundary condition (15). We illustrate this for the particular case of $\mathscr{N} = S^1$. In this case, the evolution equations are given by (see also Section 2.3)

$$\begin{cases} X_t = \Delta X + (\|\nabla X\|^2 + \|\nabla Y\|^2) X, \\ Y_t = \Delta Y + (\|\nabla X\|^2 + \|\nabla Y\|^2) Y. \end{cases} \tag{A.2}$$

The Neumann boundary conditions for this case are written as

$$\nabla X \cdot \mathbf{n} = \nabla Y \cdot \mathbf{n} = 0 \quad \text{in } \partial \mathscr{M}.$$

Transforming to polar coordinates (ρ, θ) one finds that the evolution equations (for smooth initial data, and at least for some time) are (see also [38])

$$\begin{cases} \theta_t = \Delta \theta, \\ \rho_t = 0 \end{cases} \tag{A.3}$$

with boundary conditions

$$\nabla \theta \cdot \mathbf{n} = 0 \quad \text{in } \partial \mathscr{M}.$$

Again one finds that $\int_{\mathscr{M}} \theta(x,t) \, \mathrm{d}_{\mathscr{M}} v$ is *constant*.

In the most general case, when the target manifold is arbitrary, one might guess that the *intrinsic barycenter* [22] of the map is preserved through time, since that's exactly what the particular cases given

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[22] The intrinsic barycenter G of the map $\vec{u} : \Omega \to \mathscr{N}$ is defined by $G = \operatorname{argmin}_{p \in \mathscr{N}} (1/2) \int_{\Omega} \mathrm{d}_{\mathscr{N}}^2(p, \vec{u}(x)) \, \mathrm{d}x$. See [12] for more details on the barycenter.

above show us. However, to the best of our knowledge, there is not such a result in the literature of harmonic maps, and the conservation of the barycenter is only obtained when constraints are added. The examples discussed above still motivate the use of Neumann boundary conditions.

Appendix B. Implicit calculus

We now present basic facts about differential calculus on implicitly represented surfaces. For more information see for example [4,10,31].

We have a smooth scalar function $f : \mathbb{R}^d \to \mathbb{R}$, and a smooth vector field $\vec{\lambda} : \mathbb{R}^d \to \mathbb{R}^D$ (d and D are not necessarily equal). The manifold onto which the calculus is to be done is represented as $\mathscr{S} = \{\psi = 0\}$, for $\psi(\cdot)$ the signed distance function to $\mathscr{S}$.

All the ideas of differentiation can be obtained from simple considerations related to the restriction of the function to a geodesic curve living in the manifold. We consider an arc-length parameterized geodesic curve $\gamma : [-\epsilon, \epsilon] \to \mathscr{S}$ such that $\gamma(0) = p$ is a given point of $\mathscr{S}$. We denote $F(t) = f(\gamma(t))$ and $\vec{\Lambda}(t) = \vec{\lambda}(\gamma(t))$.

B.1. Implicit gradient

We differentiate once $F(t)$ to obtain $\dot{F}(0) = \nabla f(p) \cdot \dot{\gamma}(0)$. Since $\dot{\gamma}(0) \in T_p\mathscr{S}$ (the tangent plane), we find the implicit gradient of f at p to be $\nabla_{\mathscr{S}} f(p) = \nabla f(p) - \nabla f(p) \cdot \vec{n}(p)\vec{n}(p)$, where $\vec{n}(p)$ stands for the normal to the manifold at p. Since we can also write $\vec{n}(p) = \nabla \psi(p)$, we obtain

$$\nabla_{\mathscr{S}} f(p) \triangleq \nabla f(p) - (\nabla f(p) \cdot \nabla \psi(p))\nabla \psi(p).$$

We often use the alternative notation $\nabla_\psi f$ since the definition can be applied to any level set of ψ. Note that we can write $\nabla_\psi f = \mathbf{\Pi}_{\nabla \psi} \nabla f$, where

$$\mathbf{\Pi}_{\nabla \psi} \triangleq \mathbf{I} - \nabla \psi \nabla \psi^{\mathrm{T}}.$$

B.2. Implicit Hessian

If we compute the second derivative of F we find that $\ddot{F}(0) = \nabla f(p) \cdot \ddot{\gamma}(0) + \mathbf{H}_f[\dot{\gamma}(0), \dot{\gamma}(0)]$. Now, we know that an arc-length parameterized geodesic curve of $\mathscr{S}$ must satisfy the *harmonic maps* differential equation

$$\ddot{\gamma} + \mathbf{H}_\psi(\gamma)[\dot{\gamma}, \dot{\gamma}]\nabla \psi(\gamma) = 0.$$

We then find that $\ddot{F}(0) = (\mathbf{H}_f(p) - \nabla f(p) \cdot \nabla \psi(p)\mathbf{H}_\psi(p))[\dot{\gamma}, \dot{\gamma}]$. Again we have that $\dot{\gamma} \in T_p\mathscr{S}$, and we find the implicit Hessian of f at p to be

$$\mathbf{H}_f^{\mathscr{S}}(p) \triangleq \mathbf{\Pi}_\psi \mathbf{h}_f \mathbf{\Pi}_\psi,$$

where

$$\mathbf{h}_f \triangleq \mathbf{H}_f(p) - \nabla f(p) \cdot \nabla \psi(p)\mathbf{H}_\psi(p).$$

We will frequently use the alternative notation $\mathbf{H}_f^\psi(p)$.

B.3. Implicit Laplacian

From the previous computation it is an easy exercise to compute the implicit Laplacian or Laplace–Beltrami of f since by definition $\Delta_{\mathscr{S}} f = \mathrm{trace}\{\mathbf{H}_f^{\mathscr{S}}\}$.

For any pair of symmetric matrices $\mathbf{A}$ and $\mathbf{B}$ one has that $\text{trace}\{\mathbf{ABA}\} = \sum_i \sum_j \sum_k a_{ij}a_{ik}b_{jk}$ and $\text{trace}\{\mathbf{AB}\} = \sum_i \sum_j a_{ij}b_{ij}$. Now we have that $\mathbf{\Pi}_\psi B \mathbf{\Pi}_\psi = \mathbf{B} + \nabla\psi\nabla\psi^{\mathrm{T}}\mathbf{B}\nabla\psi\nabla\psi^{\mathrm{T}} - \nabla\psi\nabla\psi^{\mathrm{T}}\mathbf{B} - \mathbf{B}\nabla\psi\nabla\psi^{\mathrm{T}}$. We then obtain

$$\text{trace}\{\mathbf{\Pi}_\psi B \mathbf{\Pi}_\psi\} = \text{trace}\{\mathbf{B}\} + \sum_i \sum_j \sum_k \psi_{x_i}\psi_{x_j}\psi_{x_i}\psi_{x_k}b_{jk} - 2\sum_i \sum_j \psi_{x_i}\psi_{x_j}b_{ij}$$

Recalling that $\psi(\cdot)$ is a *distance function*, so that it satisfies $\|\nabla\psi\| = 1$, we find

$$\text{trace}\{\mathbf{\Pi}_\psi B \mathbf{\Pi}_\psi\} = \text{trace}\{\mathbf{B}\} - \sum_i \sum_j \psi_{x_i}\psi_{x_j}b_{ij} = \text{trace}\{\mathbf{B}\} - \mathbf{B}[\nabla\psi, \nabla\psi].$$

We conclude the reasoning by taking $\mathbf{B} = \mathbf{h}_f$

$$\text{trace}\{\mathbf{H}_f^{\mathscr{S}}\} = \text{trace}\{\mathbf{h}_f\} - \mathbf{h}_f[\nabla\psi, \nabla\psi] = \text{trace}\{\mathbf{h}_f\} - \mathbf{H}_f[\nabla\psi, \nabla\psi]$$

since $\mathbf{H}_\psi[\nabla\psi, \nabla\psi] = 0$. Since $\text{trace}\{\mathbf{H}_f\} = \Delta f - (\nabla f \cdot \nabla\psi)\Delta\psi$, we find that

$$\Delta_{\mathscr{S}} f = \Delta f - (\nabla f \cdot \nabla\psi)\Delta\psi - \mathbf{H}_f[\nabla\psi, \nabla\psi].$$

It is interesting to observe how the expression just found for $\Delta_{\mathscr{S}} f$ coincides with the one obtained by minimizing the *intrinsic Dirichlet integral*, [23]

$$D(f) \triangleq \frac{1}{2}\int_{\mathbb{R}^d} \|\nabla_{\mathscr{S}} f\|^2 \delta(\psi)\,\mathrm{d}v$$

as is done in [5]. The authors showed that a smooth function f extremizing $D(f)$ must satisfy

$$\nabla \cdot (\nabla f - (\nabla f \cdot \nabla\psi)\nabla\psi) = 0.$$

We should verify that this definition coincides with ours. This is accomplished as follows

$$\begin{aligned}\nabla \cdot (\nabla f - (\nabla f \cdot \nabla\psi)\nabla\psi) &= \Delta f - (\nabla f \cdot \nabla\psi)\Delta\psi - \nabla(\nabla f \cdot \nabla\psi) \cdot \nabla\psi \\ &= \Delta f - (\nabla f \cdot \nabla\psi)\Delta\psi - \mathbf{H}_f[\nabla\psi, \nabla\psi] - \mathbf{H}_\psi[\nabla f, \nabla\psi] \\ &= \Delta f - (\nabla f \cdot \nabla\psi)\Delta\psi - \mathbf{H}_f[\nabla\psi, \nabla\psi] = \Delta_{\mathscr{S}} f \text{ (according to our definition)},\end{aligned}$$

since $\mathbf{H}_\psi[\nabla\psi, \cdot] = 0$.

B.4. Vector calculus

- *Implicit Jacobian*: With the ideas developed before, we easily find (differentiating $\vec{\Lambda}(t)$) that

$$\mathbf{J}_{\vec{\lambda}}^{\mathscr{S}} \triangleq J_{\vec{\lambda}}\mathbf{\Pi}_\psi.$$

- *Implicit Divergence*: Using the expression for the intrinsic Jacobian we write

$$\nabla_{\mathscr{S}} \cdot \vec{\lambda} \triangleq \text{trace}(\mathbf{J}_{\vec{\lambda}}\mathbf{\Pi}_\psi)$$

  and

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[23] As one expects since this is the definition of *harmonic functions*.

$$\nabla_{\mathscr{S}} \cdot \vec{\lambda} \triangleq \nabla \cdot \vec{\lambda} - \mathbf{J}_{\vec{\lambda}}[\nabla\psi, \nabla\psi].$$

It is useful to observe that $\nabla_{\mathscr{S}} \cdot \vec{\lambda} = \nabla \cdot \vec{\lambda}$ when $\vec{\lambda}(x) \in T_x\{\psi = 0\}$.

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