Metamorphoses of Functional Shapes in Sobolev Spaces

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Abstract In this paper, we describe in detail a model of geometric-functional variability between fshapes. These objects were introduced for the first time by Charlier et al. (J Found Comput Math, 2015. arXiv:1404.6039) and are basically the combination of classical deformable manifolds with additional scalar signal map. Building on the aforementioned work, this paper’s contributions are several. We first extend the original $L^2$ model in order to represent signals of higher regularity on their geometrical support with more regular Hilbert norms (typically Sobolev). We describe the bundle structure of such fshape spaces with their adequate geodesic distances, encompassing in one common framework usual shape comparison and image metamorphoses. We then propose a formulation of matching between any two fshapes from the optimal control perspective, study existence of optimal controls and derive Hamiltonian equations and conservation laws describing the dynamics of geodesics. Secondly, we tackle the discrete counterpart of these problems and equations through appropriate finite elements interpolation schemes on triangular meshes. At last, we show a few

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results of metamorphosis matchings on several synthetic and real data examples in order to highlight the key specificities of the approach.

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1 Introduction

Shape or pattern analysis is a long standing and still widely studied problem that has recently found many interesting connections with fields as varied as geometry mechanics, image processing, machine learning or computational anatomy. In its simplest form, it consists in estimating/quantifying deformations between geometric objects, typically a deformable template onto a target (registration) or multiple different subjects from a population group (atlas estimation).

There are already many existing deformation models under which registration problems may be formulated, [6,7,38,41] are examples among others where deformations belong to specific groups of diffeomorphisms. This paper falls in the context of the Large Deformation Diffeomorphic Metric Mapping (LDDMM) model [12,19,43] that has found quite a lot of attention over the past decade and triggered the development of diffeomorphometry, roughly speaking the analysis through a common Riemannian framework of the shape variability for many modalities of geometric objects including landmarks [29], images [12], unlabeled point clouds [23], curves and surfaces [17,20,24] or tensor fields [34].

Among numerous extensions of the original LDDMM model, several works have intended to enrich the pure diffeomorphic setting in order to account for shape variations that may not be retrieved solely by deformations. This was in particular the motivation behind the concept of metamorphosis introduced originally in [40]. Metamorphoses combine diffeomorphic transport with an additional dynamic evolution of the template and elegantly extends Riemannian metrics to these types of transformations. So far, metamorphoses have been defined and studied in the situation of landmarks, images and more recently on measures [37].

The main contribution of this paper is to construct a generalized metamorphosis framework and corresponding matching formulation for a class of objects coined as functional shapes in a recent article by the authors [15]. These functional shapes or fshapes are essentially scalar signals but, unlike images, supported on deformable shapes as curves, surfaces or more generally submanifolds of given dimension. In other words, they encompass mathematical objects like textured surfaces (Fig. 1); these are increasingly found in datasets issued from medical imaging, one common example being thickness maps estimated on anatomical membranes [32] or functional maps measured on cortical surfaces by fMRI.

One of the principal difficulty in analyzing the variability of fshapes in both their geometric and texture components is that it does not exactly fall in the standard approach of shape spaces and diffeomorphometry. In [15], a first tentative extension of LDDMM was introduced in place under the name of ’tangential model’ where transformations of functional shapes are basically split between a diffeomorphism of the support and an additive residual signal map living on the template coordinate system. This provides a fairly simple and easy-to-implement extension of the large deformation model. There are, however, several downsides to this approach. The main one is that signal evolution in this tangential model is static which results in a framework that lacks all the theoretical guarantees of a real metric setting like LDDMM.

A seemingly more adequate way is to adapt the idea of image metamorphosis to our situation of deformable geometric supports, which involves the introduction of a
dynamic model and metric for signal variations. This has been summarily proposed as the \textit{fshape metamorphosis} framework in \cite{15} where it was shown that this construction provides a Riemannian metric structure on metamorphoses, which in turn descends to a metric on fshape spaces. The former paper, however, restricted to the theoretical analysis of the model in the simplest case of signal functions in the $L^2$ space and did not study in depth the dynamics of geodesics. It also evidenced some significant limitations due to the lack of regularity in the signal part.

The present paper is meant as both a comprehensive extension and complement to \cite{15}. More specifically, we redefine functional shapes’ bundles and metamorphoses in the more general context of Sobolev spaces and show that we obtain again a complete metric space of fshapes. We then go further in formulating, in the infinite-dimensional setting, the natural generalization of registration for fshapes as a well-posed optimal control problem. Hamiltonian equations underlying the dynamics of the control system are also derived. This whole framework eventually includes within an integrated setting both large deformation registration of submanifolds as well as metamorphosis of classical images.

Based on these results, we formulate the equivalent discrete matching problem for fshapes represented as textured polyhedral meshes and deduce an fshape matching algorithm akin to geodesic shooting schemes. The algorithm is applied on a few synthetic as well as real data examples to illustrate, in the last section, the difference between metamorphosis and the simpler tangential model. These numerical experiments may also show the possible benefits of higher regularities for signal metrics in both models. It is important to stress that the metamorphosis and tangential models will typically generate different transformations. The relevance for actual applications of one particular model over the other will highly depend on the nature of the measured signal and the way that such signals are transformed by geometric deformations, and we leave this discussion for future study.

2 Functional Shape Spaces

2.1 Shape Spaces of Submanifolds

We start by recalling a few concepts and definitions about classical shape spaces that we borrow in part from \cite{4}. We shall consider shapes that are geometrical objects embedded into a given ambient vector space $\mathbb{R}^n$. More specifically, in the case of interest of this paper, these will be submanifolds (with or without boundary) $X$ in $\mathbb{R}^n$ of dimension $d$, for $1 \leq d \leq n$ and such that $X$ and the boundary $\partial X$ are of regularity $C^s$ with $s \geq 0$. Moreover, each $X$ carries a volume measure given by the restriction $\mathcal{H}^d \subset X$ of the $d$-dimensional Hausdorff measure in $\mathbb{R}^n$. Any such submanifold $X$ may be represented using a partition of unity and parametrization functions $q \in C^3(M, \mathbb{R}^n)$ where $M$ is some parameter space that we will take in all generality to be a $d$-dimensional submanifold with smooth boundary. This covers some of the typical situations in shape analysis literature where $M$ is, for instance, an open domain of $\mathbb{R}^d$ or the $d$-dimensional sphere $S^d$ (in the case of closed manifolds). Note, however, that the shape $X = q(M)$ itself is invariant to reparametrization of
the domain, i.e., to composing \( q \) on the right by any diffeomorphism of \( M \), and thus, shapes can be interpreted as equivalence classes of parametrization functions for this group action.

For all the rest of the paper, in the special case \( s = 0 \), we shall assume by convention that \( X \) is a \( d \)-dimensional bounded rectifiable subset of \( \mathbb{R}^n \) (c.f. [21] or [39] for more detailed definitions), in other words that there is a countable set of Lipschitz regular (and not just continuous) parametrization functions on \( \mathbb{R}^d \) that covers \( \mathcal{H}^d \)-almost all of \( X \). Rectifiable subsets include regular submanifolds as well as polyhedral meshes for instance and thus constitute a nice setting to model both discrete and continuous shapes.

As in classical shape space theory, geometrical shapes are acted on the left by groups of diffeomorphisms of the ambient space \( \mathbb{R}^n \). We will denote by \( \text{Diff}_p^p \text{Id} \) the group of \( C^p \)-diffeomorphisms of \( \mathbb{R}^n \) converging to \( \text{Id} \) at infinity. This is an open subset of the Banach affine space \( \text{Id} + C^p_0(\mathbb{R}^n, \mathbb{R}^n) \), with \( \Gamma^p_0(\mathbb{R}^n) = C^p_0(\mathbb{R}^n, \mathbb{R}^n) \) being the set of all \( C^p \) vector fields \( u \) of \( \mathbb{R}^n \) vanishing at infinity together with all its derivatives up to order \( p \), equipped with the norm

\[
\|u\|_{p, \infty} = \sum_{i=0}^{p} \sup \left\{ \left| \frac{\partial^i u}{\partial x_1^{i_1} \ldots \partial x_n^{i_n}}(x) \right| : x \in \mathbb{R}^n, (i_1, \ldots, i_n) \in \mathbb{N}^n, i_1 + \ldots + i_n = i \right\}.
\]

(1)

Now, \( \text{Diff}_p^p \text{Id} \) acts on a \( d \)-dimensional \( C^s \) submanifold \( X \) for any \( p \geq s \) by the simple transport equation:

\[
\phi \cdot X \mapsto \phi(X)
\]

for all \( \phi \in \text{Diff}_p^p \text{Id} \). If \( X \) is given through a parametrization \( q \in \mathcal{S} = \text{Emb}^s(M, \mathbb{R}^n) \) (assuming a unique parametrization domain to simplify), the set of \( C^s \) embeddings of \( M \) into \( \mathbb{R}^n \), then this action is equivalent to \( \phi \circ q \). It is also transitive on the set of all submanifolds given by these embeddings. When \( p \geq \max\{1, s\} \), the action has additional regularity properties as shown in [4]: in particular, for all \( q \in \text{Emb}^s(M, \mathbb{R}^n) \) the mapping \( R_q : \phi \mapsto \phi \circ q \) is differentiable and its differential, denoted by \( \xi_q : \Gamma^p(\mathbb{R}^n) \rightarrow C^s(M, \mathbb{R}^n), u \mapsto u \circ q \) is called the infinitesimal action of the group. In addition, for any time-dependent smooth velocity field \( v \in L^2([0, 1], \Gamma^p(\mathbb{R}^n)) \) that is square integrable in time, the flow equation \( \dot{q}(t) = \xi_{q(t)} v(t) \) with any initialization \( q(0) = q_0 \in \mathcal{S} \) has a unique solution \( q(\cdot) \in H^1([0, 1], \mathcal{S}) \), \( q(t) \) being the state at time \( t \).

### 2.2 Large Deformation Metrics and LDDMM Framework

Defining a metric on the previous shape space is done in a general way by constructing right-equivariant metrics on the acting group of diffeomorphisms [43]. This is addressed by the now well-studied Large Deformation Diffeomorphic Metric Mapping (LDDMM) model that constructs particular subgroups of \( \text{Diff}_p^p \text{Id} \) in which deformations are generated by flowing smooth vector fields. We give a brief summary in the following paragraphs.
One starts from an admissible space $V$, namely $V$ is assumed to be a Hilbert space that is continuously embedded into one of the previous space $\Gamma^p(\mathbb{R}^n)$. In that case, the metric on $V$ which we write $\|u\|_V$, is in particular controlled by the previous norm (1). We will also use in the rest of the paper the Riesz application that we write $K_V : V^* \to V$ defined by $(\tau | u) = \langle K_V \tau, u \rangle_V$ for all $\tau \in V^*$ and $u \in V$.

In most situations, and in particular for numerical applications of the LDDMM model, $V$ is constructed as a Reproducing Kernel Hilbert Space (RKHS) in which case $V$ is generated from a vector-valued kernel $K(x, y)$ of sufficient smoothness where for any $x, y \in \mathbb{R}^n$, $K(x, y)$ is an $n \times n$ matrix such that $K$ satisfies the usual positive-definiteness property:

$$\sum_{i, j} \alpha_i^T K(x_i, x_j) \alpha_j > 0$$

for all finite sets of distinct points $x_i$ and vectors $\alpha_i$ (not simultaneously vanishing). The central property of reproducing kernel spaces is that for any vector-valued distribution of the form $\alpha \otimes \delta_x : u \mapsto u(x) \cdot \alpha$, we have that $\alpha \otimes \delta_x \in V^*$ and $K_V(\alpha \otimes \delta_x)$ is the vector field of $V$ given by $K(x, \cdot) \alpha$.

Remark 1 An alternative but less elementary approach used to construct admissible RKHS of vector fields in the LDDMM framework is through differential operators. In that case, one starts with a differential operator $L$ defined on the space of smooth vector fields of $\mathbb{R}^n$. Under specific conditions on $L$, one can consider the Friedrich’s extension, which gives the existence of a Hilbert space $V$ and $\hat{L} : V \to V^*$ extending the initial operator $L$ such that the metric $\|\cdot\|_V$ writes:

$$\|u\|_V^2 = \left( \hat{L} u \bigg| u \right)_{L^2},$$

for smooth vector fields $u$. It can be then shown that $V$ is a reproducing kernel space and that the operators $K_V$ and $L$ are related by $K_V = \hat{L}^{-1}$. A comprehensive presentation of the construction and properties of kernel spaces in large deformation models can be found in [43] Chapter 13.

Now, if $V$ is simply assumed to be continuously embedded in $\Gamma^1(\mathbb{R}/line^n)$, the flow application of any time-dependent vector field $v \in L^2([0, 1], V)$ which is the mapping $\phi^v_t$ of $\mathbb{R}^n$ defined by:

$$\begin{cases}
\dot{\phi}^v_t = v_t \circ \phi^v_t \\
\phi^v_0 = \text{Id}
\end{cases}$$

exists at all times $t \in [0, 1]$ and $t \mapsto (\phi^v_t)$ defines a curve of diffeomorphisms in $H^1([0, 1], \text{Diff}_p^\infty)$. The set of all attainable flows at time 1, $G_V = \{ \phi^v_1 | v \in L^2([0, 1], V) \}$ is a subgroup of $\text{Diff}_p^\infty$. In addition, it can be equipped with a right-invariant distance defined as the minimal path length or action of all curves joining two given elements in $G_V$. In other words, for any $\phi \in G_V$:

$$d_{G_V}(\text{Id}, \phi) = \inf \left\{ \int_0^1 \| v_t \|_V^2 dt | v \in L^2([0, 1], V), \phi_1^v = \phi \right\}.$$
The distance $d_{GV}$ can be thought as a geodesic distance on the infinite-dimensional subgroup $G_V$ with the tangent space at identity identified with $V$ and the metric given by $\| \cdot \|_V$. Alternatively, this can be also interpreted within the framework of sub-Riemannian geometry, in which case the curves $\phi^v_t$ defined by (2) are horizontal curves in the full group $\text{Diff}^0_p$ for the subbundle and sub-Riemannian metric given by $V$ and $\| \cdot \|_V$: this is the point of view developed in [3, 5]. The dynamics of geodesics can be further described within a Hamiltonian formulation, which we shall detail later on.

The distance (3) on the deformation group $G_V$ induces in turn a distance between the shapes introduced in the previous subsection. For two $C^s$ submanifolds, $X_0$ (template) and $X_1$ (target) such that $X_1$ is in the orbit of $X_0$ for the action of $G_V$,

$$d_S(X_0, X_1) = \inf \left\{ \int_0^1 \| v_t \|^2_V dt \mid v \in L^2([0, 1], V), \phi^v_1(X_0) = X_1 \right\}. \quad (4)$$

Note that when $X_0$ and $X_1$ are parametrized by $q_0$ and $q_1$, then $X_t = \phi^v_t(X_0)$ is parametrized by $q(t) = \phi^v_t \circ q_0$ and by differentiating, we get back the state evolution equation $\dot{q}(t) = \xi q(t)v(t)$.

This way of quantifying shape variation is, however, only well defined within the orbit of a template shape $X_0$ under the action of $G_V$. In practice, the exact matching constraint $\phi^v_1(X_0) = X_1$ is not realizable, either because the group $G_V$ may not be big enough to account for all possible deformations or because shapes might not even be diffeomorphic due to noise perturbations. This issue can be resolved generically by considering instead a variational problem of the form:

$$\inf \left\{ \int_0^1 \| v_t \|^2_V dt + A(q(1)) \mid \dot{q}(t) = \xi q(t)v(t), \ v \in L^2([0, 1], V) \right\} \quad (5)$$

where $A$ is a data attachment term measuring the discrepancy between the approximate matched shape $q(1)$ with the actual target $q_1$. The minimization of (5) is exactly the formulation of registration between two shapes in the LDDMM model. This can be thought as an optimal control type of problem in infinite dimensions since the control is here given by the time-dependent velocity field $v$; this interpretation has been thoroughly studied in [4] and used in the rigorous derivation of Hamiltonian equations for the deformation dynamics, which we shall come back to in Sect. 3.

The actual construction of the discrepancy term $A$ in (5) in the situation of submanifolds is also a delicate issue. For instance, defining $A$ through the parametrization space like the $L^2$ metric $A(q(1)) = \int_M |q(1)(m) - q_1(m)|^2 dm$ is problematic in several respects, first because parametrizations are generally not available in practical situations where shapes are rather given as vertices with meshes and second because this type of discrepancy term is a metric between parametrizations but not necessarily between shapes, in the sense that it is not invariant to reparametrization.

A lot of work has been done in order to propose data attachment terms that are geometrical (invariant to reparametrization). We may cite, for example, the quotient Sobolev metrics on spaces of immersed curves presented in [9, 10]. An alternative path that has been actively investigated is the one of discrepancy terms obtained from...
geometric measure theory representations like measures [23], currents [24] and more recently varifolds [17,30]. These have the interesting advantage of being constructible for discrete and smooth shapes of all dimensions/codimensions while being fairly simple to compute numerically. We refer to the previous papers for more detailed discussions on this topic.

2.3 Functional Shapes

The general setting of shape spaces and large deformation models being summarized in the previous sections, we now turn to the main topic of this paper, which is about proposing a similar mathematical setting for functional shapes. In this section, we intend to set up formal definitions of functional shapes that extends the preliminary construction of [15] so as to treat signals with general Sobolev regularity.

Functional shapes are essentially objects that correspond to signals like images but defined on deformable geometries.

Definition 1 We say that the couple $(X, f)$ is a functional shape (or fshape) of regularity $s$ in $\mathbb{R}^n$, with $s \in \mathbb{N}$, if $X$ is a bounded $C^s$ submanifold of $\mathbb{R}^n$ and $f : X \to \mathbb{R}$ is a real-valued function on $X$ that belongs to $H^s(X)$, the set of Sobolev functions of order $s$ on $X$.

Typically, we will call $X$ the geometrical support of the fshape and $f$ the signal attached to this support. For $s = 0$, $H^0(X)$ is by convention the space $L^2(X)$ of square-integrable functions on $X$, i.e., of measurable functions $f$ such that

$$\|f\|_{L^2(X)}^2 = \int_X |f(x)|^2 d\mathcal{H}^d(x) < \infty.$$  

For $s \geq 1$, the Sobolev space $H^s(X)$ on the submanifold $X$ is defined in several equivalent ways in the literature. Following [8,25], it can be defined for instance as the completion of the space of smooth functions on $X$ for the norm:

$$\|f\|_{H^s(X)}^2 = \sum_{k=0}^s \|\nabla^k f\|_{L^2(X)}^2.$$  

These are all Hilbert spaces for the inner product defined by $\langle f_1, f_2 \rangle_{H^s(X)} = \sum_{k=0}^s \langle \nabla^k f_1, \nabla^k f_2 \rangle_{L^2(X)}$. We should precise here that for $s \geq 1$ we interpret the $s$ times covariant derivative $\nabla^s f$ of the function $f$ as a $(0, s)$ type tensor on the manifold $X$ and that $|\nabla^s f|$ denotes the trace norm of tensors given by $\sqrt{T^* T}$ where $T^*$ is the adjoint for the Riemannian metric on $X$. For example, if $s = 1$, $\nabla f \in T^* X$ and $|\nabla f|^2$ at each $x \in X$ turns out to be the usual norm of the tangential gradient vector for the Euclidean inner product on the ambient space $\mathbb{R}^n$.

Remark 2 Note that one may also define the $H^s$ norm on $X$ as follows

$$\|f\|_{H^s(X)}^2 = \sum_{k=0}^s \langle f, \Delta^k_X f \rangle_{L^2(X)}.$$
where $\Delta_X$ denotes the \textbf{Laplace–Beltrami operator} on $X$, i.e., minus the divergence of the tangential gradient on the manifold $X$. This gives a norm equivalent to (6) on the subspace $H^s_0(X)$, the completion of the space of smooth compactly supported function in the interior of $X$. For $s = 1$, (6) and (7) are in fact exactly equal on $H^1_0(X)$ thanks to Stokes formula.

We now seek a generalization of shape spaces presented in Sect. 2.1 to structure sets of fshapes and account for combined variations in geometry and signal. Using the notations and definitions recalled in Sect. 2.1, let $S$ be a shape space of $C^s$ submanifolds (for the action of a deformation group $G \subset \text{Diff}^p_{Id}$, $p \geq \max\{1, s\}$). We introduce the following definition

\textbf{Definition 2} The fshape bundle of regularity $s$ modeled on $S$ is the vector bundle:

$$\mathcal{F}^s_S = \{(X, f) | X \in S, f \in H^s(X)\}.$$ 

This is an extension to more general Sobolev spaces of the similar definition for $L^2$ that can be found in [15].

In the situations of interest for this paper, we will consider exclusively groups $G = G_V$ obtained as flows of time-dependent velocity fields modeled on an Hilbert space $V$ of vector fields with adequate regularity as explained in Sect. 2.2. In that case, shape spaces are generally taken as orbits for the action of $G_V$ of a particular bounded $C^s$ submanifold $X_0$ (called template), i.e., $S \doteq \{\phi(X_0) | \phi \in G_V\}$ which turns $S$ into a homogeneous space. The previous action extends naturally to $\mathcal{F}^s_S$ as follows:

$$\phi \cdot (X, f) \doteq (\phi(X), f \circ \phi^{-1}) \quad (8)$$

which corresponds to the idea of deforming the geometry by $\phi$ while pulling the signal back onto the deformed shape $\phi(X)$. This is well defined within our setting thanks to:

\textbf{Lemma 1} \textit{For all} $f \in H^s(X)$ \textit{and} $\phi \in \text{Diff}^s_{Id}$ \textit{with} $s' = \max\{s, 1\}$, $f \circ \phi^{-1} \in H^s(\phi(X))$.

This is a classical result for Sobolev spaces on compact manifolds (see, for example, [25] Chapter 2). Yet, for the rest of this paper, we shall also need some more precise control of $\|f \circ \phi^{-1}\|_{H^s(\phi(X))}$ \textit{with respect to} $\|f\|_{H^s(X)}$ \textit{and the deformation} $\phi$. The essential result is the following:

\textbf{Theorem 1} \textit{There exists a polynomial function} $P$ \textit{such that for any} $f \in H^s(X)$ \textit{and} $\phi \in \text{Diff}^s_{Id}$ \textit{we have}

$$\|f \circ \phi^{-1}\|_{H^s(\phi(X))} \leq P(\rho_{s'}(\phi))\|f\|_{H^s(X)}^2$$

\textit{where} $\rho_s(\phi) \doteq \sum_{k \leq s'} \|d^k(\phi - \text{Id})\|_\infty + \|d^k(\phi^{-1} - \text{Id})\|_\infty$ \textit{and} $d^k$ \textit{is the} $k$-\textit{times differential in} $\mathbb{R}^n$. 

\[\text{Springer}\]
The proof is slightly technical and requires passing in local coordinates with partition of unity. It is presented with full details in “Appendix A.”

For diffeomorphisms belonging to a group $G_V$, Theorem 1 implies the following bound:

**Corollary 1** If the Hilbert space $V$ is continuously embedded into $\Gamma^s$, then there exists constants $C, \kappa \geq 0$ such that for all $\phi \in G_V$ and $f \in H^s(X)$, we have

$$\|f \circ \phi^{-1}\|_{H^s(\phi(X))}^2 \leq C \exp(\kappa d_{G_V}(\text{Id}, \phi)) \|f\|_{H^s(X)}^2.$$

**Proof** This is essentially a consequence of some properties of flows detailed in [43] Chapter 8, in particular, that when $V \hookrightarrow \Gamma^s$, for all $t \in [0, 1]$:}

$$\sum_{k \leq s} \|d^k (\phi - \text{Id})\|_{\infty} \leq \alpha e^{\beta} \int_0^1 \|v_t\|_V^2 dt,'$$

$$\sum_{k \leq s} \|d^k (\phi^{-1} - \text{Id})\|_{\infty} \leq \alpha e^{\beta} \int_0^1 \|v_t\|_V^2 dt,'$$

where $\alpha$ and $\beta$ are two positive constants independent of $v$. In addition, using the fact that if $\phi \in G_V$, there exists $v \in L^2([0, 1], V)$ such that $\phi = \phi_v^1$ and $d_{G_V}(\text{Id}, \phi)^2 = \int_0^1 \|v_t\|_V^2 dt$, we obtain directly the result thanks to Theorem 1. □

The action of $G_V$ on the fshape bundle considered so far only accounts for the geometrical part of fshape variability, or in other words for horizontal motions in the fshape bundle. To complete it, we also need to introduce vertical motions in $\mathcal{F}_S^s$ which are essentially variations of signal functions within a given fiber. Thus, we shall consider fshape transformations as combinations of a geometrical deformation $\phi \in G_V$ and addition of a residual signal function $\zeta$ on the signal part of the fshape. Namely, if $(X, f) \in \mathcal{F}_S^s$ and $(\phi, \zeta) \in G_V \times H^s(X)$, we shall consider the 'action':

$$(\phi, \zeta) \cdot (X, f) \doteq (\phi(X), (f + \zeta) \circ \phi^{-1}). \quad (9)$$

Note that unlike the classical setting of shape spaces, without further assumptions, this can be no longer considered as an actual group action since the set of all transformations $(\phi, h)$ in $\mathcal{F}_S^s$ is not even a group but should be rather thought as a section of the bundle $G_V \times \mathcal{F}_S^s$. Yet, the previous notions together with Eq. (9) provides a fairly natural generalization to fshapes. It is for instance easy to verify that we now recover a transitivity property extending the one on $S$, in the sense that for any fshapes $(X_1, f_1)$ and $(X_2, f_2) \in \mathcal{F}_S^s$, there exists $\phi \in G_V$, $h \in H^s(X_1)$ such that $(\phi, \zeta) \cdot (X_1, f_1) = (X_2, f_2)$.

### 2.4 Metamorphoses

The question we now address is to extend the LDDMM metrics on the shape space $S$ defined as in Eq. (4) to a Sobolev fshape bundle $\mathcal{F}_S^s$ constructed over $S$. The
metrics we shall consider rely on the model of metamorphosis. Metamorphoses were first introduced in the case of $L^2$ images and landmarks in [40] and regularly completed from the theoretical and numerical perspective thereafter. Among other references, one can quote the works of [27] extending the Euler–Poincaré equations on diffeomorphisms to metamorphoses, or more recently [36] studying metamorphoses in spaces of discrete measures. In what follows, we will build on the preliminary results of [15] for the case of fshapes with $s = 0$.

As we recalled previously, in the standard LDDMM model, distances on shape spaces are obtained by induction from right-invariant distances $d_{G_V}$ on the acting group of diffeomorphisms or equivalently from the infinitesimal metric $\| \cdot \|_V$ on the tangent space $V$ to $G_V$ at Id. In order to provide a similar sub-Riemannian structure on geometric-functional transformations, we start by introducing a dynamic model for those transformations that we shall name fshape metamorphosis.

Let $\mathcal{F}^S_f$ be a fshape bundle. If $(X, f)$ is a specific fshape in $\mathcal{F}^S_f$, we define a metamorphosis of $(X, f)$ as a couple of a time-varying infinitesimal deformation $v \in L^2([0, 1], V)$ and infinitesimal signal variation $h \in L^2([0, 1], H^s(X))$. The time integration of $(v, h) \in L^2([0, 1], V \times H^s(X))$ parametrizes an fshape transformation path $(\phi^v_t, \zeta^h_t)$ with $\phi^v_t \in G_V$ and $\zeta^h_t \in H^s(X)$ through the dynamical equations:

$$\begin{align*}
\phi^v_t &= v_t \circ \phi^v_0 \\
\zeta^h_t &= h_t \\
\phi^v_0 &= \text{Id}, \quad \zeta^h_0 = 0
\end{align*}$$

We then define the infinitesimal metric on $V \times H^s(X)$ by

$$\| (v, h) \|_{(X, f)}^2 = \frac{\gamma_V}{2} \| v \|_V^2 + \frac{\gamma_f}{2} \| h \|_{H^s(X)}^2$$

where $\gamma_V, \gamma_f > 0$ are weighting parameters. In integrated form, this gives the following energy of the path $(\phi^v_t, \zeta^h_t)$:

$$E_X(v, h) = \frac{\gamma_V}{2} \int_0^1 \| v_t \|_V^2 \, dt + \frac{\gamma_f}{2} \int_0^1 \| h_t \circ (\phi^v_t)^{-1} \|_{H^s(X)}^2 \, dt$$

(10)

with $X_t \equiv \phi^v_t(X)$. Note that the penalty on the signal variation $h_t$ at each time is measured on the deformed submanifold $X_t$ with respect to the metric $\| \cdot \|_{H^s(X_t)}$. The framework presented in [15] as tangential model is obtained by precisely neglecting those metric changes and taking the approximation $\| h_t \|_{H^s(X_t)}^2$ instead. We first remark that $\| h_t \circ (\phi^v_t)^{-1} \|_{H^s(X_t)}$ is well defined since thanks to Lemma 1 and Corollary 1, we know that $h_t \circ (\phi^v_t)^{-1} \in H^s(X_t)$ and in addition we have for all $t \in [0, 1]$,

$$\| h_t \circ (\phi^v_t)^{-1} \|_{H^s(X_t)}^2 \leq C \exp(\kappa d_{G_V}(\text{Id}, \phi^v_t)) \| f \|_{H^s(X)}^2 \leq C \exp \left( \kappa t \left( \int_0^t \| v_r \|_V^2 \, dr \right)^{1/2} \right) \| f \|_{H^s(X)}^2$$
which gives that \( f_0^1 \| h_t \circ (\phi_t^v)^{-1}\|_{H^s(X_t)}^2 \) is finite thanks to the assumptions on \( v \) and \( h \).

Mimicking the previous setting on shape space, we can define a distance between two given fsheps (\( X, f \)) and (\( X', f' \)) in the bundle \( F_S^x \):

\[
d_{F_S^x}((X, f), (X', f'))^2 = \inf \{ E(v, h) \mid (\phi_v^X, \zeta_h^X) \cdot (X, f) = (X', f') \}
\]

This is a direct extension to fsheps of Eq. (4) in the sense that it is easy to verify that if \( f \) and \( f' \) are both constant and equal signals on \( X \) and \( X' \), then we have exactly \( d_{F_S^x}((X, f), (X', f')) = d_S(X, X') \).

**Theorem 2** \( d_{F_S^x} \) is a distance on the fshape bundle \( F_S^x \) and for all \((X, f)\) and \((X', f')\) there exists a geodesic path \((v, h) \in L^2([0, 1], V \times H^s(X))\), i.e., such that \( d_{F_S^x}((X, f), (X', f'))^2 = E_X(v, h) \).

**Proof** The case \( s = 0 \) is treated by Theorems 1 and 2 of [15]. A few steps of the proof generalize straightforwardly to all Sobolev metrics. This is the case for the symmetry of \( d_{F_S^x} \), triangular inequality and the finiteness of \( d_{F_S^x}((X, f), (X', f')) \) for all fsheps \((X, f), (X', f')\) in the bundle \( F_S^x \). We do not repeat the proof of those steps for the sake of concision but instead focus on the ones more specific to general \( s \).

- We first show that given \((X, f), (X', f') \in F_S^x\) there exists \((v, h) \in L^2([0, 1], V \times H^s(X))\) such that \( d_{F_S^x}((X, f), (X', f')) = E_X(v, h)^{1/2} \). From the definition and finiteness of the distance, we know that there exists a sequence \((v^n, h^n) \in (L^2([0, 1], V \times H^s(X)))^\mathbb{N}\) such that \( E_X(v^n, h^n)^{1/2} \to d_{F_S^x}((X, f), (X', f')) < \infty \). This implies that the sequence \((v^n)\) is bounded in \( L^2([0, 1], V) \). Therefore, up to an extraction, we can assume that \( v^n \rightharpoonup v \) where \( \rightharpoonup \) denotes the weak convergence. Now, \( v^n \rightharpoonup v \) in \( L^2([0, 1], V) \) implies that \( \phi_t^{v^n} \) converges to \( \phi_t^{v} \) as well as all derivatives up to order \( s \) uniformly on \( t \in [0, 1] \) and on \( x \) in any compact subset of \( \mathbb{R}^n \) (c.f. [43] Theorem 8.11), and thus uniformly on \( X \). Now for the second part of the energy, we have that the sequence

\[
\int_0^1 \| h_t^n \circ (\phi_t^{v^n})^{-1}\|_{H^s(X_t^n)}^2 dt
\]

with \( X_t^n \doteq \phi_t^{v^n}(X) \) is bounded. Applying Theorem 1 with \( \phi_t^{v} \circ (\phi_t^{v^n})^{-1} \) and using the previous uniform convergence of the \( \phi_t^{v^n} \), we can see that \( (h^n) \) is also bounded for the metric defined by:

\[
\| h \|_{L^2([0, 1], H^s(X^{\phi_t^v}))} = \int_0^1 \| h_t \|_{H^s(X^{\phi_t^v}_t)}^2 dt = \int_0^1 \| h_t \circ (\phi_t^{v^n})^{-1}\|_{H^s(X_t^n)}^2 dt
\]
with $X_t^\infty \doteq \phi_t^{\infty}(X)$. Therefore, up to a second extraction we can assume that there exists $h^\infty_n \in L^2([0, 1], H^s(X))$ such that $h^n \rightharpoonup h^\infty$ weakly for the above metric. The next thing to show is that the functional $(v, h) \mapsto E_X(v, h)$ is lower (semi-)continuous for these topologies on $v$ and $h$. For the velocity field $v$, it is clear that $v \mapsto \int_0^1 \|v_t\|^2 dt$ is lower semicontinuous. As for the second term, we have, using the weak semicontinuity with respect to the metric $L^2([0, 1], H^s, \phi^\infty)$,

$$
\int_0^1 \|h_t^\infty \circ (\phi_t^{\infty})^{-1}\|^2_{H^s(X_t^\infty)} dt \leq \liminf_{n \to +\infty} \int_0^1 \|h_t^n \circ (\phi_t^{\infty})^{-1}\|^2_{H^s(X_t^n)} dt.
$$

(12)

Next, since $(\phi_t^{\infty})$ converges to $\phi_t^\infty$ uniformly on every compact as well as all derivatives up to order $s$, with Lemma 6 in “Appendix A,” we have for any $h \in L^2([0, 1], H^s(X))$ and $t \in [0, 1]$,

$$
\|h_t \circ (\phi_t^{\infty})^{-1}\|_{H^s(X_t^\infty)} = \|h_t\|_{H^s, \phi_t^\infty} = \lim_{n \to +\infty} \|h_t\|_{H^s, \phi_t^n}.
$$

(13)

It results from (12) and (13) that:

$$
\int_0^1 \|h_t^\infty \circ (\phi_t^{\infty})^{-1}\|^2_{H^s(X_t^\infty)} dt \leq \liminf_{n \to +\infty} \int_0^1 \|h_t^n \circ (\phi_t^{\infty})^{-1}\|^2_{H^s(X_t^n)} dt
$$

and consequently

$$
d_{\mathcal{F}^S_\delta}((X, f), (X', f')) \leq E_X(v^\infty, h^\infty) \leq \lim_{n \to +\infty} E_X(v^n, h^n) = d_{\mathcal{F}^S_\delta}((X, f), (X', f'))
$$

leading to the result.

- Finally, we can prove that $d_{\mathcal{F}^S_\delta}((X, f), (X', f')) = 0$ implies that $X = X'$ and $f = f'$. This is because, with the previous point, there exists $(v, h) \in L^2([0, 1], V \times H^s(X))$ such that $d_{\mathcal{F}^S_\delta}((X, f), (X', f')) = E_X(v, h)_{1/2} = 0$. Then, $v = 0$ and $h = 0$ which leads to $\phi_t^\infty = \text{Id}$, $\xi_t^h = 0$ and gives the desired result.\hfill \Box

The fact that we eventually obtain a distance on the fshape bundle is in no way trivial and precisely originates from the dynamical evolution model and the associated energy that was defined. In contrast, the simpler “tangential” model for fshape transformations that was detailed and exploited in [15] does not provide a real distance nor even a pseudo-distance. We can add to Theorem 2 a few other properties of the spaces $\mathcal{F}^S_\delta$, in particular:

**Property 1** The space $\mathcal{F}^S_\delta$ equipped with its distance (11) is a complete metric space.

**Proof** Consider a Cauchy sequence $(X^n, f^n)_{n \in \mathbb{N}}$ in $\mathcal{F}^S_\delta$. We can assume that up to the extraction of a subsequence, we have $d_{\mathcal{F}^S_\delta}((X^{n-1}, f^{n-1}), (X^n, f^n)) \leq 2^{-(n-1)/2}$. Thanks to Theorem 2, we can write $X^n = \phi_1^{\infty-1}(X^{n-1})$ and $f^n = (f^{n-1} + \xi_1^{h^{n-1}}) \circ (\phi_1^{\infty})^{-1}$ with $E_X(v^n, h^n) \leq 2^{-n}$. This implies in particular that $\int_0^1 \|v_t^n\|^2 dt \leq 2^{-n}$.
and consequently $\psi^n = \phi_1^n \circ \phi_1^{n-2} \circ \ldots \circ \phi_1^0$ is a Cauchy sequence in the group $G_V$. It was shown (Theorem 8.15 in [43]) that $G_V$ is itself a complete metric space; therefore, $\psi^n$ converges to $\psi$. Let’s write $X_\infty \doteq \psi_\infty(X_0)$. On the other hand, we have that $\xi^n = \zeta_1^n \circ \psi^{n-1} + \ldots + \zeta_1^0 \in H^s(X_0)$ thanks to Lemma 1. Now for all $n \in \mathbb{N}$,

$$
\|\xi^n - \xi^{n-1}\|^2_{H^s(X_0)} = \|\xi_1^{n-1} \circ \psi^{n-1}\|^2_{H^s(X_0)}
\leq \int_0^1 \|h_t^{n-1} \circ \psi^{n-1}\|^2_{H^s(X_0)} \, dt
\leq \int_0^1 \|h_t^{n-1} \circ (\phi_t^{n-1})^{-1} \circ (\phi_t^{n-1} \circ \psi^{n-1})\|^2_{H^s(X_0)} \, dt
\leq \int_0^1 C \exp(\kappa d_{G_V}(\text{Id}, \phi_t^{n-1} \circ \psi^{n-1})) \|h_t^{n-1} \circ (\phi_t^{n-1})^{-1}\|^2_{H^s(\phi_t^{n-1}(X_{n-1}))} \, dt
$$

(14)

by using the bound of Corollary 1. Now

$$
d_{G_V}(\text{Id}, \phi_t^{n-1} \circ \psi^{n-1}) \leq d_{G_V}(\text{Id}, \psi^{n-1}) + d_{G_V}(\psi^{n-1}, \phi_t^{n-1} \circ \psi^{n-1})
\leq d_{G_V}(\text{Id}, \psi^{n-1}) + d_{G_V}(\text{Id}, \phi_t^{n-1})
$$

thanks to the right-invariance of $d_{G_V}$, and we know that $d_{G_V}(\text{Id}, \psi^{n-1})$ converges to $d_{G_V}(\text{Id}, \psi_\infty)$ as $n \to \infty$ while $d_{G_V}(\text{Id}, \phi_t^{n-1}) \leq 2^{n-1}$ so the first term on the right of inequality (14) is bounded. It gives eventually that there exists some constants $C, C' > 0$:

$$
\|\xi^n - \xi^{n-1}\|^2_{H^s(X_0)} \leq C \int_0^1 \|h_t^{n-1} \circ (\phi_t^{n-1})^{-1}\|^2_{H^s(\phi_t^{n-1}(X_{n-1}))} \, dt \leq C' 2^{n-1}.
$$

This shows that $\xi^n$ is also a Cauchy sequence in $H^s(X_0)$ and therefore $\xi^n \to \xi_\infty \in H^s(X_0)$. We write $f_\infty \doteq (f_0 + \xi_\infty) \circ (\psi_\infty)^{-1} \in H^s(X_\infty)$.

The previous points show that $(X_\infty, f_\infty) \in F_S$ and we only need to verify that $(X^n, f^n)$ indeed converges to $(X_\infty, f_\infty)$ for the metric $d_{F_S}$. To do so, we construct a path parametrized by a certain $(v, h)$ connecting $(X^n, f^n)$ to $(X_\infty, f_\infty)$. It is defined on dyadic intervals $[i^k, i^{k+1}]$ with $t_k \doteq \sum_{j=1}^{i^{k+1}} 2^{-j}$ by:

$$
v_t = 2^{k+1} v_{2^{k+1}(t-i^k)},
$$
$$
h_t = 2^{k+1} \left(h_{2^{k+1}(t-i^k)} \circ \psi_{n+k} \circ (\psi^n)^{-1}\right).
$$

One can check that $v \in L^2([0, 1], V)$, $h \in L^2([0, 1], H^s(X^n))$ and that the flow of $(v, h)$ on the interval $[i^k, i^{k+1}]$ is given by $t \mapsto (\phi_{\beta_k(t)}^{n+k} \circ \psi_{n+k} \circ (\psi^n)^{-1}, \zeta_{\beta_k(t)}^{n+k} \circ \psi_{n+k} \circ (\psi^n)^{-1})$ with $\beta_k(t) = 2^{k+1}(t-i^k)$. It results that for all $k \in \mathbb{N}$, $\phi_k v(X^n) = X^{n+k}$,
\[(f^n + \zeta^h) \circ (\phi_1^n)^{-1} = f^{n+k}.\] Moreover, \(\phi_1^n(X^n) = X^\infty\) and \((f^n + \zeta^h) \circ (\phi_1^n)^{-1} = f^\infty\) using the convergence shown before. From the definition of the distance, we have that

\[
d_{F_S}((X^n, f^n), (X^\infty, f^\infty))^2 \leq E_{X^n}(v, h)^2 \leq 2^{-(n-1)}
\]

which completes the proof of Property 1. \(\square\)

### 2.5 Parametrized fshapes

All previous notions of functional shapes and metamorphoses may be transposed to the representation of shapes as parametrizations, which will be essential in particular for the theoretical derivations of the following section. Namely, we can represent any geometrical support \(X\) by a \(C^{s'}\)-regular embedding (\(s' = \max\{s, 1\}\)) \(q \in \text{Emb}^{s'}(M, \mathbb{R}^n)\) where \(M\) is the parameter set which is typically a compact manifold (possibly with boundary) of dimension \(d\) and regularity at least \(s'\), for example an open subset of \(\mathbb{R}^d\) in the simplest situation. To stay consistent with the notations of “Appendix A,” in all the following, we will write \(\nabla\) for the covariant derivative on the parameter manifold \(M\).

In this embedded setting, a functional shape may be represented by a couple \((q, \tilde{f})\) with \(\tilde{f} = f \circ q : M \to \mathbb{R}\), which we will call a parametrized fshape. We give an illustration of an fshape and one parametric version in Fig. 1. The Sobolev metric of Eq. (6) can be also expressed in the parameter space \(M\) based on the pullback metric and covariant derivatives of tensors. Specifically, for \(q \in \text{Emb}^{s'}(M, \mathbb{R}^n)\) and a signal \(\tilde{f} \in H^s(M)\) the pullback \(H^s\) norm on \(M\) that we denote \(\|\cdot\|_{H^s_q}\) can be expressed as follows:

\[
\|\tilde{f}\|_{H^s_q} \doteq \|\tilde{f} \circ q^{-1}\|_{H^{s'}(X)} = \sum_{k=0}^s \int_M g^0_k(\nabla^k \tilde{f}, \nabla^k \tilde{f}) \text{vol}(g) \quad (15)
\]

with \(\nabla^k\) being a shortcut for \(\nabla^{k,q}\), the \(k\) times covariant derivative induced on \(M\) by the embedding \(q\), \(g^0_k\) the induced product metric on \((0, k)\)-tensors of \(M\) and \(\text{vol}(g)\) the corresponding volume density as previously. Note that (15) is by construction invariant to reparametrizations of \(M\). For a more detailed exposition of these operators and notations, we refer the interested reader to [11]. To be a little more concrete, in the simple case \(s = 1\) and \(M = \Omega \subset \mathbb{R}^d\) an open subset, the norm (15) can be rewritten...
Fig. 1  Example of functional shape from computational anatomy: a cortical surface with thickness estimations (left) and a corresponding spherical parametrization (right)

based on $\nabla$ (which is simply the gradient of functions on $\Omega$ in that case):

$$
\| \tilde{f} \|_{H^1_0(M)}^2 = \frac{1}{2} \left( \int_{\Omega} \tilde{f}(m)^2 |G_q(m)|^{1/2} dm 
+ \int_{\Omega} (\nabla \tilde{f}(m))^T G_q(m)^{-1} \nabla \tilde{f}(m)|G_q(m)|^{1/2} dm \right)
$$

where $G_q(m)$ is the $d \times d$ matrix $G_q(m) = (\partial_i q(m) \cdot \partial_j q(m))_{i,j=1,...,d}$, and the induced volume density is the square root of its determinant $|G_q(m)|^{1/2}$.

With a given $q \in \text{Emb}^s(M, \mathbb{R}^n)$, the equivalence between $f$ and the parametric representation $\tilde{f}$ is justified by:

Lemma 2  The application $f \mapsto f \circ q$ is an isomorphism between $H^s(X)$ and $H^s(M)$. In addition, there exists a constant $C \geq 0$ (depending on $q$) such that for all $f \in H^s(X)$:

$$
\frac{1}{C} \| f \|_{H^s(M)} \leq \| f \|_{H^s(X)} = \| \tilde{f} \|_{H^s_0(M)} \leq C \| \tilde{f} \|_{H^s(M)}.
$$

Proof  The proof may be adapted using similar elements as in the proof of Theorem 1 in “Appendix A.” We will just indicate the main lines here. The first part of the statement is a consequence of Proposition 2.2 in [25]. If $\tilde{g}$ and $g$ denote, respectively, the original Riemannian metric on $M$ and the one induced on $M$ from the restriction of the Euclidean metric on the submanifold $X$ by the embedding $q$, we know from, e.g., [25] that there exists a constant $\tilde{C} > 0$ depending on the bounds of $q$ and its first-order derivatives on the compact manifold $M$ such that:

$$
\frac{1}{\tilde{C}} \tilde{g} \leq g \leq \tilde{C} \tilde{g}
$$

in the sense of bilinear forms, and similarly for the cometrics. Now, given a coordinate system on a certain neighborhood $K \subset M$, following the same reasoning as in Lemma 5, we can show an equivalent equality equation (41) between coordinate
derivatives of \( f \) and the covariant derivatives with respect to the metric \( g \) where coefficients are all bounded from above on \( K \) by a certain constant (dependent on \( q \) and its derivatives up to order \( k \)). Then, we can invoke the same arguments as in the end of the proof of Theorem 1 and thus obtain successively constants \( C' \) and \( C'' \) such that:

\[
\sum_{k=0}^{s} \int_{K} g_{k}^{0}(\nabla^{k} \tilde{f}, \nabla^{k} \tilde{f}) \, \text{vol}(g) \leq C' \sum_{k=0}^{s} \int_{K} |\partial^{k} \tilde{f}|^{2} \, dx \\
\leq C'C'' \int_{K} \bar{g}_{k}^{0}(\nabla^{k} \tilde{f}, \nabla^{k} \tilde{f}) \, \text{vol}(\bar{g})
\]

and thus \( \| \tilde{f} \|_{H^{s}_{\tilde{f}}} \leq C \| \tilde{f} \|_{H^{s}(\bar{M})}^{2} \). A reverse inequality is obtained by simply redoing the previous reasoning with \( q^{-1} : X \to M. \)

Following these lines, we can then basically identify the previous bundle \( \mathcal{F}_{S}^{s} \) with the product space \( \text{Emb}^{s}(M, \mathbb{R}^{n}) \times H^{s}(M) \). Any fshape transformation \( (\phi, \bar{\zeta}) \) becomes, in the parametrized setting, an element \( (\phi, \bar{\zeta}) \) of \( \mathcal{G}_{V} \times H^{s}(M) \) that acts on \( (q, \tilde{f}) \) by:

\[
(\phi, \bar{\zeta}) \cdot (q, \tilde{f}) = (\phi \circ q, \tilde{f} + \bar{\zeta}).
\]

It is then quite clear that this is now a group action of the direct product group \( G_{V} \times H^{s}(M) \) on \( \text{Emb}^{s}(M, \mathbb{R}^{n}) \times H^{s}(M) \) and that the action is transitive, which turns the set of parametrized fshapes into a more usual shape space [3] but for an extended group of transformations.

The dynamics of a metamorphosis of a parametrized fshape \( (q_{0}, \tilde{f}_{0}) \) writes:

\[
\begin{align*}
\dot{q}_{t} &= v_{t} \circ q_{t} \\
\dot{\tilde{f}}_{t} &= h_{t}
\end{align*}
\]

with \( v \in L^{2}([0, 1], V) \) and \( h \in L^{2}([0, 1], H^{s}(M)) \). The energy of \( (v, h) \) corresponding to (10) becomes:

\[
E_{q_{0}}(v, \tilde{h}) = \frac{\nu}{2} \int_{0}^{1} \| v_{t} \|_{V}^{2} \, dt + \frac{\nu}{2} \int_{0}^{1} \| \tilde{h}_{t} \circ q_{t}^{-1} \|_{H^{s}(q_{t}(M))}^{2} \, dt \\
= \frac{\nu}{2} \int_{0}^{1} \| v_{t} \|_{V}^{2} \, dt + \frac{\nu}{2} \sum_{k=0}^{s} \int_{M} g_{t,k}^{0}(\nabla^{k} \tilde{f}_{t}, \nabla^{k} \tilde{f}_{t}) \, \text{vol}(g_{t}) \, dt
\]

where we use the shortcut notation \( g_{t} \) for the metric on \( M \) obtained by pullback from the embedding \( q_{t} \), and \( V \), unless stated otherwise, denote the covariant derivative for that metric.

This representation of shapes and fshapes through embeddings gives us a fixed functional space in which to formulate variational problems like matching: this is critical to the theoretical analysis we develop in the next section. However, it is important to emphasize that it does not directly embody the fundamental invariance of the
objects and metrics to the group of reparametrizations of $M$. The consequences of this additional invariance will be addressed separately in Sect. 3.3.2.

3 Matching Between fshapes: Optimal Control Formulation

3.1 Inexact Matching

With our previous construction, the distance $d_{\mathcal{FS}}$ is only well defined between two fshapes belonging to the same bundle. In that case, computing the distance between them amounts in finding a geodesic path mapping the first fshape exactly on the second one. As already discussed at the end of Sect. 2.2, this is only achievable if the geometric supports are themselves equivalent up to a diffeomorphism in the group $G_V$.

Exact registration under the previous framework is generally not relevant either because actual deformations of the geometric supports in a population of fshapes are not entirely modeled by diffeomorphisms in $G_V$ and Sobolev signal variations or because it is essential to regularize the estimated transformations to obtain more significant results from the point of view of statistical analysis. Thus, it is common to instead solve inexact matching problems that involve an additional data attachment (or dissimilarity) term.

In the context of functional shapes with the metamorphosis setting that was introduced above, given parametrized template fshape $(q_0, \tilde{f}_0)$ and a target fshape $(q_{\text{tar}}, \tilde{f}_{\text{tar}})$ both in $\text{Emb}^s(M, \mathbb{R}^n) \times H^s(M)$, we will focus on variational problems that have the general form:

\[
\begin{align*}
(v^*, \tilde{h}^*) = & \text{arginf} \left\{ E_{q_0}(v, \tilde{h}) + A(q_1, \tilde{f}_1) \mid v \in L^2([0, 1], V), \tilde{h} \in L^2([0, 1], H^s(M)) \right\} \\
\dot{q}_t &= v_t \circ q_t = \xi_{q_t} v_t \\
\dot{\tilde{f}}_t &= \tilde{h}_t
\end{align*}
\]

(16)

where $A$ is the data attachment term between the transformed fshape $(q_1, \tilde{f}_1)$ and the target, therefore measuring the registration mismatch. In other words, while $(q_1, \tilde{f}_1)$ belongs to the same bundle as the template by construction, $A$ can be thought as a cross-bundle term that accounts for possible variability outside the bundle. We shall keep this term as general as it can be for now but specific choices will be discussed below.

Equation (16) is once again an optimal control problem, this time with two controls given by the deformation field $v_t$ and the variable $\tilde{h}_t$ of signal transformation. The fundamental questions that are addressed in the following sections deal with the existence of such optimal controls as well as their characterization in terms of Hamiltonian dynamics that will be later exploited for the design of matching algorithms.
3.2 Existence of Solutions

3.2.1 A General Result

The existence of solutions to the problem of Eq. (16) depends on the properties of the data attachment term $A$. Using classical arguments of functional analysis, we have that:

**Theorem 3** If the functional $(v, \tilde{h}) \mapsto A(q_1, \tilde{f}_1) = A(\phi_{t}^{0} \circ q_0, \tilde{f}_0 + \xi \tilde{h})$ is weakly lower semicontinuous in $L^2([0,1], V \times H^s(M))$, then there exists at least one solution to the optimal control problem in Eq. (16).

**Proof** Let $(v^n, \tilde{h}^n)$ be a minimizing sequence. Then, it is clear that $(v^n)$ must be bounded in $L^2([0,1], V)$ which, up to an extraction, implies that $v^n \rightharpoonup v^*$ and $\phi_t^n \rightharpoonup \phi_t^*$ converges to $\phi_t^* \doteq \phi_t^{v^*}$ uniformly on every compact set and for all $t \in [0,1]$ as well as all derivatives of order at most $s$. In addition, the quantity

$$
\int_0^1 \|\hat{h}_t^n \circ (q_t^n)^{-1}\|^2_{H^s(q_t^n(M))} \, dt = \int_0^1 \|h_t^n \circ (\phi_t^n)^{-1}\|^2_{H^s(\phi_t^n \circ q(M))} \, dt
$$

is also bounded. Applying Theorem 1 with $\phi_t^* \circ (\phi_t^n)^{-1}$ and the previous uniform convergence of the $\phi_t^n$, we obtain that the sequence $(h^n)$ is bounded for the metric:

$$
\|h\|_{L^2([0,1], H^s, \phi^*)}^2 = \int_0^1 \|h_t^n \circ (\phi_t^n)^{-1}\|^2_{H^s(\phi_t^n \circ q(M))} \, dt
$$

It results that we can assume, up to another extraction, that $(h^n)$ weakly converges to a certain $h^*$ in $L^2([0,1], H^s, \phi^*)$. In addition, once again with Corollary 1 applied to $(\phi_t^n)^{-1}$, we get that there exists a constant $C$ (depending on $\phi^*$) such that for all $\tilde{h} \in L^2([0,1], H^s_0(M))$:

$$
\|\tilde{h}\|_{L^2([0,1], H^s_0(M))} \leq C \|h\|_{L^2([0,1], H^s, \phi^*)}
$$

and adding the result of Lemma 2, there is a constant $C'$ (depending on $\phi^*$ and $q = q_0$) such that $\|\tilde{h}\|_{L^2([0,1], H^s_0(M))} \leq C' \|h\|_{L^2([0,1], H^s, \phi^*)}$. Therefore, since the sequence $(h^n)$ is weakly converging to $h^*$ in $L^2([0,1], H^s, \phi^*)$, we also have that $(\tilde{h}^n)$ is weakly converging to $\tilde{h}^*$ in $L^2([0,1], H^s(M))$. Now, repeating the same reasoning as in the proof of Theorem 2, we have, on the one hand, $E_{q_0}(v^*, \tilde{h}^*) \leq \liminf_{n \to +\infty} E_{q_0}(v^n, \tilde{h}^n)$ using the weak convergence in $L^2([0,1], H^s, \phi^*)$ and, on the other hand, that

$$
A(q_1^*, \tilde{f}_0 + \xi \tilde{h}^*) \leq \liminf_{n \to +\infty} A(q_1^n, \tilde{f}_0 + \xi \tilde{h}^n)
$$

since $\tilde{h}^n \rightharpoonup \tilde{h}^*$ in $L^2([0,1], H^s(M))$. We conclude that $(v^*, h^*)$ is a minimizer of (16). □
The easiest choice for fshape parametrizations would be quite naturally:

\[ A(q_1, \tilde{f}_1) = \int_M |q_1(m) - q^{\text{tar}}(m)|^2 d\mathcal{H}^d(m) + \int_M (\tilde{f}_1(m) - \tilde{f}^{\text{tar}}(m))^2 d\mathcal{H}^d(m). \]  

(17)

This is a simple squared \( L^2 \) distance of the functions’ couple \((q, \tilde{f})\). It is not difficult to verify that this choice of \( A \) leads to the desired weak semicontinuity property and thus to existence of solutions for the control problem. The fundamental issue is that such terms are comparing the parametric functions \( q \) and \( \tilde{f} \) provided such parametrizations are even obtainable in practice, and more importantly they do not compare the fshapes represented by these parametrizations. If signals \( \tilde{f}_1 \) and \( \tilde{f}^{\text{tar}} \) are both constants on \( M \), we end up again with the term of the end of Sect. 2.2, which is not invariant through reparametrizations. The general assumption of Theorem 3 is unfortunately not verified for some other choices of functional shapes’ data attachment terms, in particular the parametrization-invariant ones that are discussed in the following.

3.2.2 Functional Varifold Fidelity Terms

For purely geometric shapes, as mentioned above, there are different frameworks constructing parametrization-invariant data attachment terms. However, the adjunction of signal functions on the shapes can make some of these frameworks rather difficult to extend. The viewpoint of geometric measure theory and representation of shapes by currents or varifolds has the advantage of being fairly easy to adapt to the situation of fshapes. This has been done, respectively, in [15,16,18]. In the following paragraphs, we give a very brief recap on the essential definitions and properties of the functional varifold setting that is otherwise described more thoroughly in [15,18].

The key idea is to again embed fshapes in certain functional spaces but in a different way than with the previous parametrization representation. These are essentially spaces of generalized distributions which are called functional varifolds (fvarifold). Specifically, a \( d \)-dimensional functional varifold \( \mu \) is distribution on the product \( \mathbb{R}^n \times G_d(\mathbb{R}^n) \times \mathbb{R} \), where \( G_d(\mathbb{R}^n) \) is the Grassmannian of the \( d \)-dimensional linear subspaces in \( \mathbb{R}^n \). In other words, \( \mu \) belongs to the dual space \( \mathcal{D}^* \) of continuous test functions on \( \mathbb{R}^n \times G_d(\mathbb{R}^n) \times \mathbb{R} \), i.e., \( \mathcal{D} = C_0(\mathbb{R}^n \times G_d(\mathbb{R}^n) \times \mathbb{R}) \). Now, any fshape \((X, f)\) with regularity \( s \in \mathbb{N} \) can be associated with the functional varifold \( \mu_{(X,f)} \) defined for all \( \omega \in W \) by:

\[ \mu_{(X,f)}(\omega) = \int_X \omega(x, T_x X, f(x)) d\mathcal{H}^d(x) \]

where \( T_x X \) is the tangent space to \( X \) at \( x \) viewed as an element of \( G_d(\mathbb{R}^n) \). Similarly, a parametrized fshape \((q, \tilde{f})\) can be represented by the fvarifold \( \tilde{\mu}_{(q,\tilde{f})} \):

\[ \tilde{\mu}_{(q,\tilde{f})}(\omega) = \int_M \omega(q(m), T_q(m), \tilde{f}(m)) \text{vol}(g^q) \]
with \( T_q(m) \) being the space spanned by the vectors \( \partial_1 q(m), \ldots, \partial_d q(m) \). This distribution is invariant to reparametrization as we have \( \mu_{(q, \tilde{f})} = \mu_{(q(M), \tilde{f} \circ q^{-1})} \).

With the previous definitions, it appears relevant to define a fidelity term between fshapes by induction from a metric constructed on the dual space \( W^* \). Such metrics may even lead to closed form expressions if \( W \) is taken as a RKHS of functions on \( \mathbb{R}^n \times G_d(\mathbb{R}^n) \times \mathbb{R} \). We consider positive definite kernels of the form \( k = k_p \otimes k_t \otimes k_f \) where \( k_p, k_t \) and \( k_f \) are three positive definite kernels, respectively, on \( \mathbb{R}^n, G_d(\mathbb{R}^n) \) and \( \mathbb{R} \), and take \( W \) the unique RKHS corresponding to the kernel \( k \). Results of [15] can be summarized as follows:

**Property 2** If all kernels \( k_p, k_t \) and \( k_f \) are continuous on their respective spaces and \( k_p(x, \cdot), k_f(s, \cdot) \) vanish at infinity for all \( (x, s) \in \mathbb{R}^n \times \mathbb{R} \), then the RKHS \( W \) associated with \( k \) is continuously embedded in \( D \). It results that for any fshape \( (X, f) \) (resp. parametrized fshape \( (q, \tilde{f}) \)), one has \( \mu_{(X, f)} \in W^* \) (resp. \( \mu_{(q, \tilde{f})} \in W^* \)). In addition, the dual RKHS metric on \( W^* \) satisfies:

\[
\|\mu_{(q, \tilde{f})}\|_{W^*} = \int_{\mathcal{M} \times \mathcal{M}} k_p(q(m), q(m')) k_f(\tilde{f}(m), \tilde{f}(m')) k_t(Tq(m), Tq(m')) \frac{\text{vol}(g^q)(m) \text{vol}(g^q)(m')}{\text{vol}(g^q)(m')}. 
\]

Now, with the notations of the previous sections, we may define data attachment terms as:

\[
A(q_1, \tilde{f}_1) = \|\mu_{(q_1, \tilde{f}_1)} - \mu_{(q_{\text{tar}}, \tilde{f}_{\text{tar}})}\|_{W^*}^2 \\
= \int_{\mathcal{M} \times \mathcal{M}} k_p(q_1(m), q_1(m')) k_f(\tilde{f}_1(m), \tilde{f}_1(m')) k_t(Tq_1(m), Tq_1(m')) \frac{\text{vol}(g^{q_1})(m) \text{vol}(g^{q_1})(m')}{\text{vol}(g^{q_1})} \\
- 2 \int_{\mathcal{M} \times \mathcal{M}} k_p(q_{\text{tar}}(m), q_{\text{tar}}(m')) k_f(\tilde{f}_{\text{tar}}(m), \tilde{f}_{\text{tar}}(m')) k_t(Tq_{\text{tar}}(m), Tq_{\text{tar}}(m')) \frac{\text{vol}(g^{q_{\text{tar}}})(m) \text{vol}(g^{q_{\text{tar}}})(m')}{\text{vol}(g^{q_{\text{tar}}})} \\
+ \int_{\mathcal{M} \times \mathcal{M}} k_p(q_{\text{tar}}(m), q_{\text{tar}}(m')) k_f(\tilde{f}_{\text{tar}}(m), \tilde{f}_{\text{tar}}(m')) k_t(Tq_{\text{tar}}(m), Tq_{\text{tar}}(m')) \frac{\text{vol}(g^{q_{\text{tar}}})(m) \text{vol}(g^{q_{\text{tar}}})(m')}{\text{vol}(g^{q_{\text{tar}}})}. 
\]

As opposed to (17), \( A \) is now by construction invariant to reparametrization and measures proximity between the fshapes based on the relative positions of their points, tangent spaces and functional values through the three kernels \( k_p, k_t, k_f \).

**Remark 3** It is important to point out that with the sole conditions of Property 2, Formula (18) might only define a pseudo-metric between fshapes as the association \( (X, f) \mapsto \mu_{(X, f)} \) is not necessarily injective. While having a true distance for \( A \) is not absolutely fundamental since it is here just used as a relaxation term in the control problem, it is still possible to recover an actual metric by adding a few simple assumptions on the choice of kernels. These questions are thoroughly treated in [17] for standard shapes and [15] for functional shapes.
At this point, we are interested in the problem of existence of solutions to (16) when \( A \) is given by a fvarifold fidelity term (18). The case of metamorphoses in \( L^2 \) (i.e., for \( s = 0 \)) was treated extensively in [15] Section 5. In that case, Theorem 3 does not apply because fvarifold terms are generally not lower semicontinuous for the weak convergence in \( L^2([0, 1], L^2(M)) \). Instead, the proof was derived from the standard approach of geometric measure theory. Without repeating the entire argument for the sake of brevity, the result proven in Theorem 7 of [15] translates to our formulation as follows:

**Theorem 4** In addition to the assumptions of Property 2, if all kernels \( k_e, k_f, k_t \) are \( C^2 \) regular and if \( \gamma_V \) and \( \gamma_f \) are large enough, there exists a solution in \( L^2([0, 1], V \times L^2(M)) \) of the control problem (16) with \( s = 0 \).

This result shows the important restriction that occurs when doing fshape metamorphoses in the space \( L^2 \); the existence of solutions only holds when the weight of the energy term relative to the data attachment one is large enough. This condition may also be crucial in numerical applications from a stability perspective, as evidenced in Section 9 of [15].

This is one of the motivation to extend the framework to higher regularity norms. Indeed, in the Sobolev case for \( s \geq 1 \), one can recover a stronger existence result using weak continuity arguments. The important result on the data attachment term that is needed is the following:

**Lemma 3** Assuming that kernels are chosen as in Property 2 with in addition \( k_f \) of regularity \( C^1 \) with all its derivatives vanishing at infinity, if \( \tilde{f}^n \to \tilde{f}^* \) in \( L^2(M) \), then \( A(q, \tilde{f}^n) \to A(q, \tilde{f}^*) \) for any \( q \in C^1(M, \mathbb{R}^n) \).

**Proof** A similar result was proved in the slightly different setting of functional currents in Proposition 3 of [18] or [16]. We give a more direct proof in our setting for completeness. It suffices to show that for any \( \omega \in W, \mu(q, \tilde{f}^n)(\omega) \to \mu(q, \tilde{f}^*) (\omega) \) as \( n \to \infty \). Indeed taking \( \omega = K_W \mu(q_{tar}, \tilde{f}_{tar}) \) with \( K_W : W^* \to W \) the usual Riesz duality application, this would imply that \( (\mu(q, \tilde{f}^n), \mu(q_{tar}, \tilde{f}_{tar}))_{W^*} \to (\mu(q, \tilde{f}^*), \mu(q_{tar}, \tilde{f}_{tar}))_{W^*} \) for any parametrized fshape \( (q_{tar}, \tilde{f}_{tar}) \) and thus the claimed result by bilinearity. Now, one has by definition:

\[
\begin{align*}
(\mu(q, \tilde{f}^n) - \mu(q, \tilde{f}^*)) (\omega) &= \int_M (\omega(q(m), T_q(m), \tilde{f}^n(m)) \\
&\quad - \omega(q(m), T_q(m), \tilde{f}^*(m))) \, \text{vol}(g).
\end{align*}
\]

Consequently, there exists some constants \( C > 0 \) (whose values may change from line to line) such that

\[
| (\mu(q, \tilde{f}^n) - \mu(q, \tilde{f}^*)) (\omega) | \leq \int_M | \omega(q(m), T_q(m), \tilde{f}^n(m)) \\
&\quad - \omega(q(m), T_q(m), \tilde{f}^*(m)) | \, \text{vol}(g^q) \\
&\leq C \int_M | \tilde{f}^n(m) - \tilde{f}^*(m) | \, \text{vol}(g^q)
\]
\[ \leq C \| \hat{f}^n - \hat{f}^* \|_{L^2(M)} \xrightarrow{n \to \infty} 0 \]

where the second inequality results from the fact that, with the assumptions on kernels, \( \omega \in W \) is \( C^1 \) in its last variable with bounded derivatives, and the last inequality follows from the compactness of \( M \).

Note that the conclusion does **not** hold if we only have weak and not strong convergence in \( L^2(M) \). Now, the consequence is the following existence theorem:

**Theorem 5** With the same assumptions on \( k_e, k_f, k_t \) as in Lemma 3, if \( \gamma_V, \gamma_f > 0 \), there exists a solution \((v^*, h^*) \in L^2([0, 1], V \times H^s(M)) \) of the control problem (16) with \( s \geq 1 \).

**Proof** Let \((v^n, h^n)\) be a minimizing sequence for (16) with data attachment term of the form (18). Then, since \( \gamma_V, \gamma_f > 0 \), both sequences:

\[
\int_0^1 \| v^n_t \|_V^2 \, dt
\]

and with \( q^n_t := \phi v^n_t \circ q \)

\[
\int_0^1 \| \tilde{h}^n_t \circ (q^n_t)^{-1} \|_{H^s(q^n_t(M))}^2 \, dt
\]

are bounded. In particular, since \( v^n \) is bounded in \( L^2([0, 1], V) \), we can assume up to an extraction that \( v^n \rightharpoonup v^* \) which implies that for all \( t \in [0, 1] \), \( \phi v^n_t \) and its derivatives up to order \( s \) converge uniformly on every compact toward \( \phi^* = \phi v^* \). Following the same steps and notations as in the proof of Theorem 3, we can assume that \( h^n = \tilde{h}^n \circ q^{-1} \) converges to \( h^* \) weakly in \( L^2([0, 1], H^s(M)) \) which implies that \( E_{q_0}(v^*, \tilde{h}^n) \leq \liminf_{n \to +\infty} E_{q_0}(v^n, \tilde{h}^n) \). We also have that \( \tilde{h}^n \) is bounded in the space \( L^2([0, 1], H^s(M)) \) and converges weakly to \( h^* \) in \( L^2([0, 1], H^s(M)) \). Now, since \( \zeta_1 \tilde{h}^n = \int_0^1 \tilde{h}^n_t \, dt \), we deduce that:

\[
\| \zeta_1 \tilde{h}^n \|_{H^s(M)} \leq \int_0^1 \| \tilde{h}^n_t \|_{H^s(M)}^2 \, dt
\]

and consequently \( \zeta_1 \tilde{h}^n \) is bounded in \( H^s(M) \). As \( s \geq 1 \), from Rellich–Kondrachov theorem (Theorem 10.1 in [25]), we deduce that \( \zeta_1 \tilde{h}^n \) converges (strongly) to a certain \( \zeta \in L^2(M) \) up to another extraction. Moreover, for any \( v \in L^2(M) \), using the weak convergence of \( \tilde{h}^n \rightharpoonup \tilde{h}^* \) we have

\[
\langle v, \zeta_1 \tilde{h}^n \rangle_{L^2(M)} = \int_0^1 \langle v, h^n_t \rangle_{L^2(M)} \, dt \xrightarrow{n \to \infty} \int_0^1 \langle v, h^*_t \rangle_{L^2(M)} \, dt = \langle v, \zeta_1 h^* \rangle_{L^2(M)}.
\]
Since we also have \( \zeta_1 \rightarrow \zeta_\infty \) strongly in \( L^2(M) \), it must hold that \( \zeta_\infty = \zeta_1^* \). With the result of Lemma 3, it results that \( A(q_1, \tilde{f}_0 + \tilde{\zeta}^n) \xrightarrow{n \to \infty} A(q_1, \tilde{f}_0 + \tilde{\zeta}^n) \) and eventually

\[
E_{q_0}(v^*, \tilde{h}^*) + A(q_1, \tilde{f}_0 + \tilde{\zeta}^n) \leq \liminf_{n \to +\infty} E_{q_0}(v^n, \tilde{h}^n) + A(q_1, \tilde{f}_0 + \tilde{\zeta}^n)
\]

leading to the fact that \((v^*, \tilde{h}^*)\) is a minimizer of (16). \( \square \)

A last element that will be needed in the derivations of the following sections is the first variation of fvarifold fidelity terms, namely the differential of \( A(q, \tilde{f}) \) with respect to variations of the parametrized fshape \((q, \tilde{f})\). This was computed in the purely geometrical situation in [17,33] and generalized to the functional case in [15]. In this paper, we will in fact only be relying on the qualitative form of this first variation. Thus, to keep the exposition brief, we will just recall the following: if we assume that all kernels \( k_p, k_i, k_f \) are \( C^1 \) and \( q \in C^2(M, \mathbb{R}^n) \), \( \tilde{f} \in C^1(M) \), then \( q \mapsto A(q, \tilde{f}) \) and \( \tilde{f} \mapsto A(q, \tilde{f}) \) are Fréchet differentiable and the differential take the form

\[
(\partial q A|\delta q) = \int_M \left[ \left\langle \alpha, (\delta q)^\perp \right\rangle + \left( \beta (dq^{-1})^* (\nabla \tilde{f})(\delta q)^\top \right) \right] \text{vol}(g) + \int_{\partial M} \langle \eta, \delta q \rangle \text{dl} \\
(\partial \tilde{f} A|\delta \tilde{f}) = \int_M \gamma \delta \tilde{f} \text{vol}(g)
\]

where \( \alpha \) is a normal vector field, \( \beta, \gamma \) are scalar functions on \( M \), \( \eta \) is defined on the boundary \( \partial M \) and is a vector field normal to the boundary of the submanifold, \( (\delta q)^\perp, (\delta q)^\top \) are, respectively, the tangential and orthogonal components of \( \delta q \) to the submanifold parametrized by \( q \) and \((dq^{-1})^* : T^*M \to T^*X \) is the adjoint map of the tangent of the inverse application \( q^{-1} \).

### 3.3 Hamiltonian Equations

#### 3.3.1 PMP and General Equations

Following the existence of solutions, we are now interested in their characterization. For shape matching, this is traditionally done invoking the Pontryagin Maximum Principle (PMP) in order to derive Hamiltonian equations of optimal solutions’ dynamics [5,33]. We extend this approach to fshape metamorphoses and the optimal control problem given by Eq. (16). Here we have two state variables \( \tilde{f} \in H^s(M) \) and the immersion \( q \) that we take in the space \( C^s(M, \mathbb{R}^n) \) with \( s' = \max(s, 1) \), and two time-dependent controls \( v_i \in V \) and \( \tilde{h}_i \in H^s(M) \). We introduce two additional co-state variables \( p \in C^{s'}(M, \mathbb{R}^n)^* \) and \( p^{\tilde{f}} \in H^s(M)^* \) that we call, respectively, the geometric and functional momenta, and the following Hamiltonian

\[
H(q, \tilde{f}, p, p^{\tilde{f}}, v, \tilde{h}) \doteqdot (p|\xi_q v) + (p^{\tilde{f}}|\tilde{h}) - \frac{\gamma_v}{2} \|v\|_V^2 - \frac{\gamma_{\tilde{h}}}{2} \|\tilde{h}\|_{H^s}^2
\]

with

\[
\frac{\partial H}{\partial \tilde{f}} = \frac{\partial H}{\partial p^{\tilde{f}}} = \frac{\partial H}{\partial v} = 0
\]

\[
\frac{\partial H}{\partial p} = \xi_q v \quad \frac{\partial H}{\partial p^{\tilde{f}}} = \tilde{h}
\]

\[
\frac{\partial H}{\partial \xi_q} = \frac{\partial H}{\partial \xi} = \frac{\partial H}{\partial \tilde{h}} = \frac{\partial H}{\partial \tilde{h}} = 0
\]
where we remind that $\xi_q v = v \circ q$ is the infinitesimal action of $v$ on $q$ and $(p|\xi_q v)$, $(p^f|\hat{h})$ are shortcuts notations for the duality brackets in $C^{s'}(M, \mathbb{R}^n)$ and $H^s(M)$, respectively, and $\| \cdot \|_{H^s}$ is given by Eq. (15).

Assuming additional regularity for vector fields of $V$, we obtain the following Hamiltonian equations along optimal solutions:

**Theorem 6** We assume that $V$ is continuously embedded into $\Gamma^{s'+1}$. If $(v, \tilde{h})$ is an optimal solution for (16), there exists time-dependent co-states $p \in H^1([0, 1], C^{s'}(M, \mathbb{R}^n)^*)$ and $p^f \in H^1([0, 1], H^s(M)^*)$ such that:

$$
\begin{cases}
    \dot{q}_t = -\partial_p H(q_t, \tilde{f}_t, p_t, p^f_t, v_t, \tilde{h}_t) \\
    \dot{f}_t = -\partial_p f H(q_t, \tilde{f}_t, p_t, p^f_t, v_t, \tilde{h}_t) \\
    \dot{p}_t = -\partial_q H(q_t, \tilde{f}_t, p_t, p^f_t, v_t, \tilde{h}_t) \\
    \dot{p}^f_t = -\partial_{f^*} H(q_t, \tilde{f}_t, p_t, p^f_t, v_t, \tilde{h}_t) = 0 \\
    \partial_v H(q_t, \tilde{f}_t, p_t, p^f_t, v_t, \tilde{h}_t) = 0, \quad \partial_{\tilde{h}} H(q_t, \tilde{f}_t, p_t, p^f_t, v_t, \tilde{h}_t) = 0
\end{cases}
$$

(21)

with the endpoint conditions

$$
p_1 = -\partial_q A(q_1, \tilde{f}_1), \quad p^f_1 = -\partial_{\tilde{f}} A(q_1, \tilde{f}_1).
$$

(22)

The proof is detailed in “Appendix B.”

We can go a little further by expressing the last two conditions on the controls in the previous Hamiltonian equations and get the so-called **reduced Hamiltonian equations**.

**Corollary 2** If $(v, \tilde{h})$ is an optimal solution for (16), there exists co-states $p \in H^1([0, 1], C^{s'}(M, \mathbb{R}^n)^*)$ and $p^f \in H^1([0, 1], H^s(M)^*)$ such that:

$$
v_t = \frac{1}{\gamma_V} K_V \xi_{q_t} p_t, \quad \tilde{h}_t = \frac{1}{\gamma_f} F^s_{q_t} p^f_t
$$

and the state variables evolution is described by the following reduced Hamiltonian equations

$$
\begin{cases}
    \dot{q}_t = \partial_{\tilde{f}} H_r(q_t, \tilde{f}_t, p_t, p^f_t) \\
    \dot{f}_t = \partial_p f H_r(q_t, \tilde{f}_t, p_t, p^f_t) \\
    \dot{p}_t = -\partial_q H_r(q_t, \tilde{f}_t, p_t, p^f_t) \\
    \dot{p}^f_t = -\partial_{\tilde{f}} H_r(q_t, \tilde{f}_t, p_t, p^f_t) = 0
\end{cases}
$$

(23)

with $p_1 = -\partial_q A(q_1, \tilde{f}_1), p^f_1 = -\partial_{\tilde{f}} A(q_1, \tilde{f}_1)$ and

$$
H_r(q, \tilde{f}, p, p^f) \equiv \frac{1}{2\gamma_V} (p|K_q p) + \frac{1}{2\gamma_f} \| F^s_{q} p^f \|_{H^s(M)}^2.
$$

**Proof** The optimal $v$ must satisfy for almost all $t \in [0, 1], (\partial_v H(q_t, \tilde{f}_t, p_t, p^f_t, v_t, \tilde{h}_t))|_{\delta v} = 0$ for all $\delta v \in V$. Introducing the dual application of the infinitesimal action
\( \xi_q^* : C^{s'}(M, \mathbb{R})^* \rightarrow V^* \), this gives:

\[
(\xi_q^*, p_t | \delta v)_V = 0 \Rightarrow v_t = \frac{1}{\gamma_V} K_V \xi_q^*, p_t
\]

where we recall that \( K_V : V^* \rightarrow V \) is the Riesz duality operator of \( V \). On the other hand, \( (\partial^*_h H(q_t, \tilde{f}_t, p_t, p_{f\tilde{t}}, v_t, \tilde{h}_t) | \delta \tilde{h}) = 0 \) for all \( \delta \tilde{h} \in H^s(M) \) leading to:

\[
(p_{f\tilde{t}} | \delta \tilde{h}) - \gamma_f (v_t, \delta \tilde{h})_{H^s_0(M)} = 0.
\]

Note that the previous equation involves the duality in \( H^s(M) \) for the left term and the duality in \( H^s(M) \) for the right one. The two Hilbert norms being equivalent on \( H^s(M) \) (Lemma 2), we can introduce the linear mapping \( F_q^s : H^s(M)^* \rightarrow H^s(M) \) defined by the property:

\[
(F_q^s p | \tilde{h})_{H^s_0(M)} = (p | \tilde{h})
\]

for all \( p, \tilde{h} \in H^s(M) \). This leads to

\[
\tilde{h}_t = \frac{1}{\gamma_f} F_q^s p_{f\tilde{t}}.
\]

Now, plugging the expressions of the optimal \( v \) and \( \tilde{h} \) in (20), we obtain the so-called reduced Hamiltonian of the problem:

\[
H_r(q, \tilde{f}, p, p_{f\tilde{t}}) = \frac{1}{\gamma_V} (p | \xi_q^* K_V \xi_q^* p) + \frac{1}{2\gamma_V} (K_V \xi_q^* p, K_V \xi_q^* p)_V - \frac{1}{2\gamma_f} \| F_q^s p_{f\tilde{t}} \|_{H^s}^2
\]

\[
= \frac{1}{2\gamma_V} (p | \xi_q^* K_V \xi_q^* p) + \frac{1}{2\gamma_f} \| F_q^s p_{f\tilde{t}} \|_{H^s}^2
\]

with \( K_q : C^{s'}(M, \mathbb{R}^n)^* \rightarrow C^{s'}(M, \mathbb{R}^n), \ p \mapsto \xi_q^* K_V \xi_q^* p, \) as well as the reduced Hamiltonian equations (23). We notice that the reduced Hamiltonian does not depend on the variable \( \tilde{f} \) giving once again \( \dot{p}_{f\tilde{t}} = \partial^*_f H_r(q_t, \tilde{f}_t, p_t, p_{f\tilde{t}}) = 0. \)

The operator \( K_q \) in the expression of \( H_r \) can be also written based on the expression of the kernel \( K_V \): for \( p \in C^{s'}(M, \mathbb{R}^n)^* \) associated with the vector-valued measure \( dp \) on \( M \), \( K_q p \) is the vectors field given by

\[
K_q p(\omega) = \int_M K_V (q(\omega), q(\omega')) dp(\omega').
\]
it explicitly in the case $s = 0$ (c.f. Sect. 3.3.4 below) or implicitly with the adequate elliptic operator as in the proof of Property 3.

### 3.3.2 Conservation Laws

There are still additional symmetries that can be uncovered from the particular form of the Hamiltonian and the intrinsic invariance of the system to reparametrizations of $M$. Indeed, in the case of fshape metamorphoses, we recall the expression of the Hamiltonian:

$$H(q, \tilde{f}, p, p^f, v, \tilde{h}) \doteq (p|\xi_q v) + (p_f|\tilde{h}) - \frac{\gamma}{2} \|v\|_V^2 - \frac{\gamma_f}{2} \|\tilde{h}\|_{H^2_{\text{eq}}}^2.$$  

We can again consider the right group action on the state variables by the reparametrization group $\text{Diff}^s(M)$ defined for all $\tau \in \text{Diff}^s(M)$:

$$\tau \cdot (q, f) = (q \circ \tau, f \circ \tau)$$

On the other hand, defining the action on the co-states $(p, p^f)$ as the following push-forward operations:

$$(\tau^* p|\delta q) \doteq (p|\delta q \circ \tau^{-1}), \quad (\tau^* p^f|\delta f) \doteq (p^f|\delta f \circ \tau^{-1})$$

we observe that the Hamiltonian is then invariant to the action in the sense that:

$$H(q \circ \tau, \tilde{f} \circ \tau, \tau^* p, \tau^* p^f, v, \tilde{h} \circ \tau) = H(q, f, p, p^f, v, \tilde{h})$$

This can be checked easily by using the equivariance of the norm $\|\cdot\|_{H^2_{\text{eq}}}$, i.e., that $\|\tilde{h} \circ \tau\|_{H^2_{\text{eq}}} = \|\tilde{h}\|_{H^2_{\text{eq}}}$. Denoting $\mathcal{X}(M)$ the space of continuous vector fields on $M$ that are tangential to the boundary $\partial M$, this leads to the following conservation law:

**Theorem 7** Along each optimal trajectory $t \mapsto (q_t, \tilde{f}_t)$ such that $\tilde{f}_t \in H^{s+1}(M)$, we have that the following $\mu_t \in \mathcal{X}(M)^*$:

$$\mu_t \doteq dq_t^* p_t + d\tilde{f}_t^* p^f_t = 0 \quad (25)$$

for all $t \in [0, 1]$.

**Proof** We introduce a one-parameter group of diffeomorphic reparametrizations of $M$, $z \mapsto \tau_z$, $z \in [-\epsilon, \epsilon]$, with $\tau_z \in \text{Diff}(M)$, $\tau_0 = \text{Id}_M$ and $\dot{\tau}_0 = u$ with $u$ a $C^1$ vector field on $M$. Since $\tau_z(M) = M$ for all $z$, it implies that the normal component of $u$ along the boundary of the domain vanishes and so $u \in \mathcal{X}(M)$. With the actions introduced above, we have seen that for all $z \in [-\epsilon, \epsilon]$

$$H(\tau_z \cdot q, \tau_z \cdot \tilde{f}, \tau_z^* p, \tau_z^* p^f, v, \tau_z \cdot \tilde{h}) = H(q, \tilde{f}, p, p^f, v, \tilde{h}).$$
With the assumptions made, we have $\dot{f}_t \in H^{s+1}(M)$ and thus $\dot{h}_t \in H^{s+1}(M)$ for all $t$, and differentiating the previous expression at $z = 0$ leads eventually to:

$$0 = (\partial_q H|dq(0)) + \left. \frac{d}{dz} \right|_{z=0} (\partial_{p_f} H|\tau^*_z p) + \left. \frac{d}{dz} \right|_{z=0} (\partial_{p_f} H|\tau^*_z p^f) + (\partial_q H|\nabla \dot{h} \cdot u)$$

$$= (\partial_q H|dq(0)) - (p|dq \circ q(dq(0))) - \gamma_f(\dot{h}, \nabla \dot{h} \cdot u)|_{H_q^s}$$

$$= (\partial_q H|dq(0)) - (p|dq \circ q(dq(0))) - (F_q^s p^f, \nabla \dot{h} \cdot u)|_{H_q^s} = 0$$

which, by the definition of $F_q^s$, gives

$$0 = (\partial_q H|dq(0)) - (p|dq \circ q(dq(0))) - (p^f|\nabla \dot{h} \cdot u). \quad (26)$$

Now, defining $\mu_t$ as in Eq. (25), if $(q_t, \dot{f}_t, p_t, p^f_t)$ satisfies the Hamiltonian equations (21), we obtain:

$$(\dot{\mu}_t|u) = \frac{d}{dt} \left[ (p_t|dq_t(u)) + (p^f_t|d\dot{h}_t(u)) \right]$$

$$= (p_t|dq_t(u)) + (p_t|dq \circ q_t(dq_t(u))) + (p^f_t|d\dot{h}_t(u))$$

$$= (\partial_{p_f} H|dq_t(u)) + (p_t|dq \circ q_t(dq_t(u))) + (p^f_t|\nabla \dot{h}_t \cdot u).$$

Using Eq. (26) at $(q_t, \dot{f}_t, p_t, p^f_t)$, we find that for any $u$ and thus the conservation of $\mu_t$. In addition, we have with (22) the endpoint conditions $p_1 = -\partial_q A(q_1, \dot{f}_1), p^f = -\partial_f A(q_1, f_1)$. Since varifold data attachment terms are invariant to reparametrization, i.e., $A(q \circ \tau_z, \tilde{f} \circ \tau_z) = A(q, f)$ for all $z \in [-\epsilon, \epsilon]$ we obtain by differentiating with respect to $z$ that for all $u$:

$$(\partial_q A(q_1, \dot{f}_1)|dq_1 \cdot u) + (\partial_{f_1} A(q_1, \dot{f}_1)|\nabla \dot{f}_1 \cdot u) = - (p_1|dq_1 \cdot u) - (p^f|\nabla \dot{f}_1 \cdot u) = 0$$

or, in other words:

$$dq_1^* p_1 + d \dot{f}_1^* p^f = 0.$$

With the previous conservation of $\mu_t$, we get the result claimed in Theorem 7. \hfill \Box

This conservation law leads in particular to some properties of orthogonality for the momentum $p_t$. Indeed, since for any vector field $u \in X(M)$,

$$(p_t|dq_t \cdot u) = -(p^f|\nabla \dot{f}_t \cdot u)$$

we can see that $p_t$ vanishes for all tangent vector fields to $q_t(M)$ that satisfy $\nabla \dot{f}_t \cdot u$, i.e., that are tangential to the level lines of the signal $f_t$.

The only non-trivial assumption in Theorem 7 is the $H^{s+1}$ regularity of the signal $\dot{f}_t$ (or equivalently $\dot{h}_t$) along the entire trajectory. In lack of a more general result, we provide at least a sufficient condition (when $M$ has no boundary) in the property below:
Property 3 Assume that $M$ is a manifold without boundary. Provided the kernels defining the fidelity term in (18) are sufficiently regular, if $V$ is continuously embedded into the space $C^{2s'}(\mathbb{R}^n, \mathbb{R}^n)$ with $s' = \min\{s, 1\}$, and $q_1 \in C^{2s'}(M, \mathbb{R}^n)$, $\tilde{f}_1 \in H^{s+1}(M)$, then optimal solutions of (16) satisfy for all $t \in [0, 1]$, $q_t \in C^{2s'}(M, \mathbb{R}^n)$ and $\tilde{f}_t \in H^{s+1}(M)$.

Proof With the equation $\dot{q}_t = v_t \circ q_t$, it is clear that with $q_1 \in C^{2s'}(M, \mathbb{R}^n)$ and $v_t \in C^{2s'}(\mathbb{R}^n, \mathbb{R}^n)$ for all $t$, we get $q_t \in C^{2s'}(M, \mathbb{R}^n)$ for all $t$. On the other hand, the evolution of $\tilde{f}$ is governed by the equation $\dot{\tilde{f}}_t = h_t = \frac{1}{\gamma_f} F_{q_t} p^\tilde{f}$. Since $q_1 \in C^{2s'}(M, \mathbb{R}^n)$ and $\tilde{f}_1 \in H^{s+1}(M)$ and with the regularity assumptions on the kernels defining the fidelity term, it can be seen from (18) and (19) that

$$(p^\tilde{f} | h) = - (\partial_f A(q_1, \tilde{f}_1)) h) = - \int_M \gamma h \, \text{vol}(g)$$

where $\gamma$ is a function which we can assume to belong to $H^1(M)$ with appropriate regularity of kernels (and since $\tilde{f}_1 \in H^{s+1}(M) \subset H^1(M)$). Now we examine the two cases:

- $s = 0$: in that case, as shall be detailed in Sect. 3.3.4, $F_{q_t} p^\tilde{f} = - |g_t|^{-1/2} \gamma$ where $|g_t|^{-1/2}$ is the volume density induced on $M$ by the embedding $q_t$. Since $q_t \in C^2(M, \mathbb{R}^n)$, we have $h_t = \frac{1}{\gamma_f} F_{q_t} p^\tilde{f} \in H^1(M)$ for all $t \in [0, 1]$ and therefore $\tilde{f}_t \in H^1(M)$.

- $s \geq 1$: then $s' = s$ and we can introduce the operators $A_{g_t} \doteq \sum_{k=0}^s (\nabla^*)^k (\nabla)^s$ where once again $\nabla$ is the covariant derivative operator associated with the metric $g_t$ and $\nabla^*$ its adjoint for that metric. As such, $A_{g_t}$ is an elliptic self-adjoint positive differential operator on $M$ of order $2s$ and from the results of [28] Theorem 19.2.1, $A_{g_t}$ is a Fredholm operator from $H^{2s}(M)$ to $L^2(M)$ and since it is self-adjoint the index of the operator vanishes. Moreover, $A_{g_t}$ being positive and thus injective, it results that it is also surjective. Consequently, there exists $u \in H^{2s}(M)$ such that $A_{g_t} u = \gamma$ and by definition of $A_{g_t}$, we deduce that $\tilde{h}_t = \frac{1}{\gamma_f} F_{q_t} p^\tilde{f} = - \frac{1}{\gamma_f} u \in H^{2s}(M) \subset H^{s+1}(M)$. Now, with $\tilde{f}_1 \in H^{s+1}(M)$, we obtain eventually $\tilde{f}_t \in H^{s+1}(M)$ for all $t$.

\[\square\]

3.3.3 Link to Image Metamorphosis

As presented so far, the model of fshape metamorphoses generalizes submanifold diffeomorphic registration, which corresponds to the limit case of $\gamma_f \to +\infty$ in the expression of the energy (10) and $k_f \equiv 1$ in the fidelity term (18).

But it can be also viewed as extending metamorphoses of classical images studied in previous works like [27,37,40]. In the fshape perspective, this is the situation where $M = \Omega$ is a bounded domain of $\mathbb{R}^d$ and all geometrical shapes are fixed to $X = q(\Omega) = \Omega$. In other words, keeping the notation $\Omega \subset \mathbb{R}^n$ for the image domain itself, we take $V$ to be embedded into $C^{s+2}_0(\Omega)$, the space of velocity fields of class $C^{s+2}$ on $\Omega$ such that, together with all derivatives of order $\leq s$, vanish on the boundary of $\Omega$.  

\[\square\]
We then obtain paths $t \mapsto q_t \in C^{s+2}(\Omega, \Omega)$ with $q_0 = \text{Id}_\Omega$ and $\dot{q}_t = v_t \circ q_t$. In that particular setting, this implies that for all $t$, $q_t$ identifies to the deformation $\phi_t$ itself and is in that case a $C^{s+2}$-diffeomorphism of $\Omega$. We can then introduce the change of variable $\tilde{h} = \zeta \circ \phi \iff \zeta = \tilde{h} \circ \phi^{-1}$, and the Hamiltonian of (20) becomes:

$$H(\phi, \tilde{f}, p, p^f, v, \zeta) = (p|v \circ \phi) + (p^f|\zeta \circ \phi) - \frac{\gamma}{2} \|v\|_{H^q}^2 - \frac{\gamma}{2} \|\zeta \circ \phi\|_{H^q}^2$$

$$= (p|v \circ \phi) + (p^f|\zeta \circ \phi) - \frac{\gamma}{2} \|v\|_{H^s(\Omega)}^2 - \frac{\gamma}{2} \|\zeta\|_{H^s(\Omega)}^2$$

(27)

With $q = \phi$ and $\zeta = \tilde{h} \circ \phi^{-1}$ and introducing the application $\tilde{\xi}_\phi : H^s(\Omega) \to H^s(\Omega)$, $\zeta \mapsto \zeta \circ \phi$ and the Riesz isometry $K_{H^s} : H^s(\Omega)^* \to H^s(\Omega)$, Hamiltonian equations (21) and (23) may be rewritten as:

$$\begin{align*}
\dot{\phi} &= v \circ \phi \\
\dot{\tilde{f}} &= \zeta \circ \phi \\
\dot{p} &= -\partial_{\phi}(p|v \circ \phi) - \partial_{\phi}(p^f|\zeta \circ \phi) \\
\dot{p^f} &= 0 \\
v &= \frac{1}{\gamma} K_V \xi_{\phi}^* p, \quad \zeta = \frac{1}{\gamma_f} (F_q^s p^f) \circ \phi^{-1} = \frac{1}{\gamma} K_{H^s} \left(\tilde{\xi}_{\phi}^* p^f\right)
\end{align*}$$

(28)

the last equality resulting from the fact that $F_q^s p^f = K_{H^s} \left(\tilde{\xi}_{\phi}^* p^f\right) \circ \phi$ since for all $u \in H^s(\Omega)$

$$\left(K_{H^s} \tilde{\xi}_{\phi}^* p^f\right) \circ \phi, u\right|_{H^s_q} = \left(K_{H^s} \tilde{\xi}_{\phi}^* p^f, u \circ \phi^{-1}\right)_{H^s(\Omega)}$$

$$= \left(\tilde{\xi}_{\phi}^* p^f | u \circ \phi^{-1}\right)$$

$$= \left(p^f | \tilde{\xi}_{\phi} (u \circ \phi^{-1})\right)$$

$$= \left(p^f | u\right).$$

Thus, eventually, the Hamiltonian of (27), the Hamiltonian evolution equations (28) and the conservation law of Theorem 7 are precisely the ones of image metamorphosis given in Section 2 of [37] (in the case of Sobolev metrics) which, as expected, can be treated theoretically as a special case of the functional shape setting presented here.

### 3.3.4 The Particular Case $s = 0$

We now give a more specific and explicit expression for the evolution equations in the simplest case $s = 0$ that corresponds to the continuous form of the discrete $L^2$ metamorphosis equations presented in [15]. In particular, we will be able to give a more precise description of the nature of the geometric and functional momenta $p$ and $p^f$.

We make the additional regularity assumptions of Theorem 7, that is $q \in C^2(M, \mathbb{R}^n)$ and $\tilde{f}_1 \in H^1(M)$. We can also identify $p^f$ as the $L^2$ function on $M$
given by Riesz representation theorem. The operator $F_0^q$ can be then expressed easily since:

$$\langle p f, \tilde{h} \rangle_{L^2(M)} = \int_M p f(m) \tilde{h}(m) d\mathcal{H}^d(m)$$

$$= \int_M |g|^{-1/2}(m) p f(m) \tilde{h}(m) \text{vol}(g)$$

$$= \langle |g|^{-1/2} p f, \tilde{h} \rangle_{L^2_q}.$$

where we write as previously $g$ for the pullback metric induced by $q$ and $|g|^{1/2}$ the corresponding volume density. This gives $F_0^q p f = |g|^{1/2} p f$ and the reduced Hamiltonian

$$H_r(q, \dot{f}, p, p f) = \frac{1}{2} g_t^f (p | K_q p |) + \frac{1}{2} \int_M (p f)^2 |g|^{-1/2} d\mathcal{H}^d.$$

The two first equations in the Hamiltonian system then write:

$$\begin{cases}
\dot{q}_t = \frac{1}{2g} K_q p_t \\
\dot{f}_t = \frac{1}{2f} |g_t|^{-1/2} p f
\end{cases}$$

where $p f$ is a shortcut for $p f^f = p f_t$. With the assumptions made, $p f$ is a $H^1$ function on $M$ and the previous equation implies that for all $t$, $\dot{f}_t$ is also in $H^1(M)$. Writing in short $g_t$ for the metric induced by $q_t$, the evolution of geometric momentum $p_t$ is described by:

$$\left( \dot{p}_t | \delta q \right) = -\frac{1}{2g} \left( \partial_q (p_t | K_q p_t) | \delta q \right) - \frac{1}{2f} \left( \partial_q \int_M (p f)^2 |g|^{-1/2} d\mathcal{H}^d | \delta q \right).$$

The previous expression involves the variation of the volume density $|g|^{-1/2}$ with respect to $q$. This is given, for example, in [11] and leads to:

$$\left( \dot{p}_t | \delta q \right) = -\frac{1}{2g} \left( \partial_q (p_t | K_q p_t) | \delta q \right) - \frac{1}{2f} \int_M (p f)^2 |g|^{-1/2} \left[ \text{div}_{g_t}(\delta q^\top) - H_{g_t} \cdot \delta q \right] d\mathcal{H}^d$$

(29)

where $\delta q = \delta q^\top + \delta q^\perp$ is the decomposition of $\delta q$ in its tangential and normal components to the immersion $q_t$, $\text{div}_{g_t}(\delta q)$ is by definition the tangential divergence of the vector field $\delta q^\top$ and $H_{g_t}$ the mean curvature vector for the metric $g_t$. The previous equation involves two terms, the first of which is the same one appearing in Hamiltonian equations of pure geometric shape registration, while the second one induces retro action of signal on geometric evolution.

Momentum $p$ belongs a priori to the very large space of distributions $C^1(M, \mathbb{R}^n)^*$. However, with the previous assumptions, its general form can be in fact described more
accurately as a vector field on $M$ plus a singular term on the boundary. Moreover, $p_t$ is orthogonal to the shape at time $t$ at all points located in the interior of a level set of $\tilde{f}_t \circ q_t^{-1} = f_t$ and tangential components in $p_t$ only appears at boundaries of the level sets of these signals, as illustrated in Fig. 2. This is justified by the following result:

**Property 4** For all $t \in [0,1]$, we have:

$$p_t = p_t^{in} + p_t^{bo}$$

where $p_t^{in}$ is a vector field in $L^2(M, \mathbb{R}^n)$ and $p_t^{bo} = \int_{\partial M} \delta_s \otimes w_t(s) d\mathcal{H}^{d-1}(s)$ a vector-valued distribution supported on $\partial M$. Moreover, the tangential part of vector field $p_t^{in}$ lies in the vector bundle generated by the vector field $\nabla f_t$.

**Proof** As already noted before in Eq. (19), the boundary condition $p_1 = -\partial_q A(q_1, \tilde{f}_1)$ implies that $p_1$ decomposes as $p_1 = p_1^{in} + p_1^{bo}$ where $p_1^{in} \in L^2(M, \mathbb{R}^n)$ and $p_1^{bo}$ is a singular vector distribution supported on the boundary $\partial M$ of the form $p_1^{bo} = \int_{\partial M} \delta_s \otimes w_1(s) d\mathcal{H}^{d-1}(s)$ with $w_1$ a vector field on $\partial M$. In addition, the time derivative of $p_t$ in Eq. (29) can be rewritten using the divergence theorem and regularity of $q$ and $p f$ as:

$$\dot{(p_t | \delta q)} = -\frac{1}{2\gamma f} (\partial_q (p_t | K_{q_t} p_t) | \delta q) + \frac{1}{2\gamma f} \int_M \nabla (|g_t|^{-1}(p_f)^2) \cdot \delta q^\top |g_t|^{1/2} d\mathcal{H}^d$$

$$- \frac{1}{2\gamma f} \int_M (p_f)^2 |g_t|^{-1/2} H_{q_t} \cdot \delta q^\top d\mathcal{H}^d + \frac{1}{2\gamma f} \int_{\partial M} |g_t|^{-1}(p_f)^2 \delta q^\top \cdot N_{q_t} d\mathcal{H}^{d-1}$$

where once again $\nabla$ denotes the pullback covariant derivative by the embedding $q_t$, $N_{q_t}$ the unit outward normal vector field on the boundary. Moreover, for any vector field $p^{in} \in L^2(M, \mathbb{R}^n)$, the expression of $K_q$ in (24) becomes:

$$K_q p^{in} = \int_M K_V(q(\cdot), q(m)) p^{in}(m) d\mathcal{H}^d(m)$$
and therefore

\[(p^\text{in}|K_q p^\text{in}) = \iint_{M \times M} p^\text{in}(m) \cdot K_V(q(m), q(m')) p^\text{in}(m') d\mathcal{H}^d(m) d\mathcal{H}^d(m')\]

leading to a variation in \(L^2(M, \mathbb{R}^n)\)

\[\partial_q(p^\text{in}|K_q p^\text{in})(m) = \int_M p^\text{in}(m) \cdot \partial_1 K_V(q(m), q(m')) p^\text{in}(m') d\mathcal{H}^d(m').\]

On the other hand, if \(p^\text{bo}\) is any singular vector-valued measure on \(\partial M\) of the form \(p^\text{bo} = \int_{\partial M} \delta_s \otimes w(s) d\mathcal{H}^{d\!-\!1}(s)\) with \(w(s) \in \mathbb{R}^n\) for all \(s\) then:

\[K_q p^\text{bo} = \int_{\partial M} K_V(q(\cdot), q(s)) w(s) d\mathcal{H}^{d\!-\!1}(s).\]

As previously, we obtain that the different terms \(\partial_q(p^\text{in}|K_q p^\text{bo})\), \(\partial_q(p^\text{bo}|K_q p^\text{in})\), \(\partial_q(p^\text{bo}|K_q p^\text{bo})\) can be expressed either as \(L^2\) vector fields or vector-valued distributions on \(\partial M\). Thus, writing \(\dot{p}_t = F(p_t, q_t)\), we see that the application \(F\) restricted to distributions of the form \(p = p^\text{in} + p^\text{bo}\) decomposes as \(F(p^\text{in} + p^\text{bo}, q) = F_1(p^\text{in}, q) + F_2(p^\text{bo}, q)\) where \(F_1(\cdot, q)\) and \(F_2(\cdot, q)\) are \(C^1\) applications, respectively, from the space of \(L^2\) vector fields into itself and the space of singular vector measures on \(\partial M\) into itself. With the condition on \(p\) at \(t = 1\), we deduce that at all \(t\), \(p_t\) is a distribution of the same form.

The last statement in the property follows from the conservation law of Theorem 7. Indeed we have, for all vector field \(u \in \mathcal{X}(M)\) vanishing on the boundary of \(M\),

\[(p^\text{in}_t|dq_t(u)) = -(p^f_t|\nabla \tilde{f}_t \cdot u).\]

We deduce that \((p^\text{in}_t|dq_t(u))\) vanishes for any \(u\) orthogonal to the (vector) \(\nabla \tilde{f}_t\) giving that the component of \(p^\text{in}_t\) tangential to \(q_t\) must live in the space generated by \(\nabla (\tilde{f}_t \circ q_t^{-1}) = \nabla f_t\).

\[\square\]

### 3.3.5 An Example of Geodesic Trajectories

As an explicit example of joint evolution of geometry and signal under the previous metamorphosis model in \(L^2\) (\(s = 0\)), we consider the very simple case of centered 2-dimensional spheres in \(\mathbb{R}^3\) with constant signals. Denote by \(q_t : S^2 \to \mathbb{R}^3\) the parametrization of the sphere of radius \(r_t\), i.e., \(q_t(m) = r_t m\) and with constant signals \(f_t\) on \(S^2\). Considering only trajectories governed by constant normal momentum field \(p_0 = \rho_0 m\), constant functional momentum \(p^f\) and a translation/rotation invariant kernel for deformations of the form \(K_V(x, y) = k_V(|x - y|^2)Id_{3 \times 3}\), it is clear that geodesic trajectories from the metamorphosis equations of previous subsection can only lead to spherical shapes with constant signals and at all times \(p_t = \rho_t m\). We can thus describe geodesic trajectories by the evolution of the radius \(r_t\) and the signal value \(f_t\), which we will deduce from the previous reduced Hamiltonian equations.
In this specific case, we have $|g_t|^{1/2} = r_t^2$ and consequently:

$$\dot{f}_t = \frac{p_f}{\gamma_f r_t^2}$$

Secondly, the velocity field $v_t \circ q_t = \gamma_V^{-1} K_{q_t} p_t$ is such that:

$$K_{q_t} p_t (m) = \left( \int_{\mathbb{S}^2} k_V (r_t^2 |m - m'|^2) m' d\mathcal{H}^2(m') \right) \rho_t$$

$$= \left( \int_{\mathbb{S}^2} k_V (2r_t^2 [1 - \langle m, m' \rangle]) m' d\mathcal{H}^2(m') \right) \rho_t$$

which leads to the following evolution on the sphere radius $r_t$:

$$\dot{r}_t = \frac{1}{\gamma_V} \left( \int_{\mathbb{S}^2} k_V (2r_t^2 [1 - \langle m, m' \rangle]) \langle m, m' \rangle d\mathcal{H}^2(m') \right) \rho_t$$

Using the Funk–Hecke formula, we can rewrite the previous as:

$$\dot{r}_t = \frac{1}{\gamma_V} 4\pi \left( \int_{-1}^{1} u k_V (2r_t^2 [1 - u]) du \right) \rho_t$$

Finally, the ODE on $p_t$ translates to the following one on $\rho_t$:

$$\dot{\rho}_t = -\frac{1}{2\gamma_V} \chi'(r_t) \rho_t^2 + \frac{(p_f)^2}{\gamma_f r_t^3}$$

Eventually, we have obtained that the time evolution of fshapes in this situation is governed by the following three differential equations:

$$\begin{cases} 
    \dot{f}_t = \frac{p_f}{\gamma_f r_t^2} \\
    \dot{r}_t = \frac{1}{\gamma_V} \chi(r_t) \rho_t \\
    \dot{\rho}_t = -\frac{1}{2\gamma_V} \chi'(r_t) \rho_t^2 + \frac{(p_f)^2}{\gamma_f r_t^3}
\end{cases}$$

(30)

There are several remarks to be made on the previous equations. First, we see that the speed of signal evolution is proportional to the inverse of the squared radius; thus, $f_t$ will vary faster at times when the sphere is smaller in size. Secondly, the equations governing the radius evolution are identical to the pure LDDMM equations except for the additional recall term $(p_f)^2/(\gamma_f r_t^3)$ in the momentum dynamics. This term may 'bend' the usual trajectories of classical shape evolution as evidenced in the plots of
Fig. 3. Sphere case: examples of evolutions of the radius and signals along geodesic trajectories for different initial momenta $\rho_0$ and $p_f$ and Gaussian kernel ($\sigma = 0.5$, $\gamma_V = 1$, $\gamma_f = 5$ and $f_0 = r_0 = 0.5$).

The left hand figures for instance show that under certain combinations of parameters and initial conditions, the sphere may contract (while signal variation accelerates) before expanding, which is a very different behavior compared to the case of pure geometric shapes or to the 'tangential' model for fshapes developed in [15].

4 Discrete Model

The model of fshape metamorphosis described so far may be rewritten in a totally discrete setting, which is the essential step toward an actual matching algorithm solving numerically the minimization problem of Eq. (16). Discretization schemes have already been developed in previous articles for simpler or less general models. In [35], the authors partly address the important issue of $\Gamma$-convergence of the discrete solutions. The discrete framework, the notations and the definitions in the rest of this section closely follow the ones of [15].

4.1 Discrete fshapes

We assume that a continuous fshape $(X, f)$ of dimension $d$ embedded in $\mathbb{R}^n$ is only known through a finite set of $P \geq (d + 1)$ points with their attached signal and connectivity relations between vertices. We assume that every cells of the graph are
simplexes of dimension $d$. In practice, there may be an uncertainty in the acquisition process and the coordinates of the points may be noisy (i.e., the vertices may be close to $X$ but not necessarily on $X$). Note also that the value of the signal is usually only known at the vertices as this is measurements made during the acquisition process. It means that, in order to evaluate the signal inside a cell, an interpolation method (on the discrete fshape) should be defined.

An important example that motivates this work is the case of functional surface ($d = 2$) coming from 3D medical imaging ($n = 3$). This kind of data usually comes from a complex pipeline ranging from image acquisition to segmentation and surface extraction. In this context, the ideal underlying continuous functional surface $(X, f)$ is unknown and is approximated by a textured triangular mesh typically containing several thousands of points ($P \approx 10^4$).

In the discrete setting, an fshape is therefore described by a triplet of objects $(x, f, C)$ where

- $x = (x_k)_{k=1,...,P}$ is the $P \times n$ matrix of the $P$ vertex coordinates $x_k \in \mathbb{R}^n$.
- $f = (f_k)_{k=1,...,P} \in \mathbb{R}^{P \times 1}$ is a column vector containing the signal values $f_k \in \mathbb{R}$ attached to the vertex of coordinates $x_k$ (i.e., signal is stored in Lagrangian coordinates).
- $C \in \{1, \ldots, P\}^{T \times (d+1)}$ is a $T \times (d+1)$ connectivity matrix composed by $T > 0$ simplices of dimension $d$ so that the $\ell$th row of $C$ contains the indices of the $d+1$ vertices of the cell $\ell \in \{1, \ldots, T\}$.

In exact translation of the continuous transport equations (9), the transformation of a discrete fshape by a deformation $\phi$ and functional residual $\zeta \in \mathbb{R}^{P \times 1}$ is the discrete fshape given by $\phi \cdot x \doteq \phi(x) = (\phi(x_k))_{k=1,...,P}$, $f + \zeta = (f_k + \zeta_k)_{k=1,...,P}$ and the same connectivity matrix $C$.

### 4.2 Discrete Functional Norm

At this stage, a continuous fshape $(X, f)$ is approximated by a discrete fshape $(x, f, C)$ which is nothing but a graph of simplices with a signal attached at each vertex. From this graph, we define a piecewise polyhedral domain $T$ of $\mathbb{R}^n$ made of $d$-dimensional simplices whose vertices and edges are stored in $x$ and $C$. Now let $\tilde{f} : T \to \mathbb{R}$ be a function satisfying $\tilde{f}(x_k) = f_k$. The $H^s$ norm of $\tilde{f}$ on $T$ is denoted $\|f\|_{H^s(x)}$ (we drop the dependency of $\tilde{f}$) and can be written in all generality as

$$\|f\|^2_{H^s(x)} = f^T D_s(x) f$$

(31)

where $D_s(x)$ is a symmetric positive definite $P \times P$ matrix whose entries depend on the connectivity structure stored in $C$ and the interpolation formula chosen to define $\tilde{f}$ on $T$. The entry of $D_s(x)$ may be computed from the matrices $x$ and $C$, and $D_s(x)$ is generally sparse. In the following subsections, we will examine the most useful cases in practice: $d = 1$ where $T$ is the union of piecewise linear segments and $d = 2$ where $T$ is the union of piecewise triangular cells.
Fig. 4 An illustration of two different interpolations to defined \( \tilde{f} \) on \( T \) composed by a single triangle. The graph of \( \tilde{f} \) is in green. \( a \) Mass lumping: piecewise constant interpolation and \( b \) finite element of order 1

4.2.1 Mass Lumping (\( s = 0 \))

We discuss how to compute the \( L^2 \) norm (i.e., the \( H^s \) norm with \( s = 0 \)) of a signal interpolated by a piecewise constant function \( \tilde{f} \) on \( T \) such as in Fig. 4a. The idea is to choose an interpolation scheme that gives a diagonal weight matrix. We let

\[
D_0(x) = \text{Diag} \left[ \left( \frac{1}{d+1} \sum_{\tau \ni x_k} r_\tau \right)_{k=1, \ldots, P} \right]
\]

where \( r_\tau \) is the \( d \)-volume of simplex \( \tau \). The \( L^2 \) norm of the discrete signal may then be computed by using \( D_0 \) of Eq. (32) in Formula (31). If \( T \) is triangular mesh (\( d = 2 \)), it means that the \( k \)th diagonal entry of \( D_0(x) \) is computed by performing a sum of the areas of all triangles \( \tau \in T \) containing the \( k \)th vertex (of coordinate vector \( x_k \)).

4.2.2 Exact Formula for P1 Finite Elements (\( s = 1 \))

We now discuss how to compute the \( H^1 \) norm of a signal \( f \) interpolated with P1 finite elements. We first introduce some notations. Let \( (\psi^{(0)}_\tau)_{\tau \in T} \) be the canonical basis for the finite elements of order 0 (i.e., \( \psi^{(0)}_\tau : T \rightarrow \mathbb{R} \) is equal to 1 on the cell \( \tau \) and 0 everywhere else) and \( (\psi^{(1)}_k)_{k=1, \ldots, P} \) be the canonical basis for the finite elements of order 1 (i.e., \( \psi^{(1)}_k : T \rightarrow \mathbb{R} \) is continuous piecewise linear such that \( \psi^{(1)}_k(x_\ell) = 1 \) if \( k = \ell \) and 0 if \( k \neq \ell \).

Let \( \tilde{f} = \sum_{k=1}^P f_k \psi_k^{(1)} \) be the function defined on \( T \) by piecewise linear interpolation of the \( f_k \)'s with P1 finite elements. Using standard numerical integration formula as in [1], p. 178 we have
\[ \| \tilde{f} \|_{L^2(T)}^2 = \| f \|_{L^2(x)}^2 = \begin{cases} \sum_{\tau \in T} \frac{r_{\tau}}{6} \left( (f_{\tau}^{(1)})^2 + 4(f_{\tau}^{(12)})^2 + (f_{\tau}^{(2)})^2 \right), & \text{if } d = 1 \\ \sum_{\tau \in T} \frac{r_{\tau}}{3} \left( (f_{\tau}^{(12)})^2 + (f_{\tau}^{(21)})^2 + (f_{\tau}^{(31)})^2 \right), & \text{if } d = 2 \end{cases} \]

where \( f_{\tau}^{(ij)} = \frac{1}{2}(f_i^{(j)} + f_j^{(i)}) \) is the value of \( \tilde{f} \) at the center of the edge linking vertices \( i \) and \( j \) in cell \( \tau \). We can then define the matrix \( D_0(x) \in \mathbb{R}^{P \times P} \) (corresponding to the P1 interpolation) as the symmetric matrix of the following quadratic form

\[ f \mapsto f^T D_0(x) f = \| f \|_{L^2(x)}^2. \quad (33) \]

Formula (33) may be used as an alternative to Eq. (32) to compute \( L^2 \) norm. We emphasize that matrix \( D_0 \) in Eq. (33) is sparse but no longer diagonal and that the computation is exact on finite elements of order 1.

For the computation of the \( H^1 \) norm of \( \tilde{f} \), note that the gradient of \( \tilde{f} \) is defined almost everywhere on \( T \) and is constant on the interior of each cell. We thus introduce the function \( g = \sum_{\tau \in T} c_{\tau} \psi_{\tau}^{(0)} \) with \( c_{\tau} = \| \nabla \tilde{f}_{\tau} \|_{\mathbb{R}^d} \) and we use the simple integration formula exact on finite elements of order 0 to get

\[ \| \nabla \tilde{f} \|_{L^2(T)}^2 = \| g \|_{L^2(x)}^2 = \sum_{\tau \in T} r_{\tau} c_{\tau}^2. \]

Finally, \( D_1(x) \in \mathbb{R}^{P \times P} \) is the symmetric matrix of the quadratic form defined by

\[ f \mapsto f^T D_1(x) f = \| f \|_{L^2(x)}^2 + \| \nabla f \|_{L^2(x)}^2. \]

4.2.3 General Cases \((s > 1)\)

In our implementation and simulations, we did not consider \( H^s \) norms with \( s > 1 \) mostly because the data at hand are not suited for higher-order finite element interpolation. Our assumption is indeed that the signal \( f \) defined on \( X \) is a priori only known or measured at the vertices \( x \) of \( T \), which is a quite common situation in data resulting from segmentation of biomedical images. In such case, there is no canonical way to interpolate the discrete signal \( f \) on \( T \) with finite elements of order \( s \) greater than 1. In addition, as we show with the examples of Sect. 5, using \( H^1 \) norm is sufficient in practice to avoid most of the oscillating effects appearing in the \( L^2 \) case.

We point out that, in principle, higher-order Sobolev norms could be implemented either by (1) considering different interpolation methods than finite elements or (2) extending the model of discrete functional shapes of Sect. 4.1 to situations where the vector \( f \) includes values of the signal at additional points inside each face of the mesh and in such a way that higher-order finite element methods could be used. The rest of our proposed framework and matching algorithm then adapts naturally, although the numerical cost could increase quite significantly as a result.
4.3 Deformation on Discrete fshapes

4.3.1 Discrete Hamiltonian Equations

We can now derive a discrete fshape metamorphosis model along the same lines as the continuous one of previous sections. If we fix $M$ as the template polyhedral manifold $X_0$ itself and consider signals that are obtained with a given finite element interpolation of the values at the vertices, then the state variables in this discrete setting are the two vectors $x$ and $f$ and a metamorphosis is determined by a couple $(v_t, h_t)$ with $v \in L^2([0, 1], V)$ and $h_t = (h_{k,t}) \in \mathbb{R}^{P \times 1}$ such that we have the finite-dimensional evolution equations:

\[
\begin{align*}
\dot{x}_{k,t} &= v_t(x_{k,t}) \\
\dot{f}_{k,t} &= h_{k,t}
\end{align*}
\]

The energy (10) becomes:

\[
E_x(v, h) = \frac{\gamma}{2} \int_0^1 \|v_t\|^2_V dt + \frac{\gamma f}{2} \int_0^1 h^T_t D_s(x_t) h_t dt
\]

The Hamiltonian corresponding to the minimization problem with this discrete energy also takes the form:

\[
H(x_t, f_t, p_t, p^f_t, v_t, h_t) = (p_t | v_t(x)) + (p^f_t | h_t) - \frac{\gamma}{2} \|v_t\|^2_V - \frac{\gamma f}{2} h^T_t D_s(x_t) h_t
\]

where $p \in \mathbb{R}^{P \times n}$ and $p^f \in \mathbb{R}^{P \times 1}$ are the discrete co-state variables. Denoting $K$ the vector kernel associated with the RKHS $V$, the optimality conditions along geodesics $\partial_v H(x_t, f_t, p_t, p^f_t, v_t, h_t) = 0$ and $\partial_h H(x_t, f_t, p_t, p^f_t, v_t, h_t) = 0$ from the PMP lead to the following expressions of the optimal controls:

\[
\begin{align*}
v_t &= \frac{1}{\gamma v} \sum_{\ell=1}^P K(x_{\ell,t}, \cdot) p_{\ell,t} \\
\end{align*}
\]

\[
\begin{align*}
h_t &= \frac{1}{\gamma f} D_s^{-1}(x_t) p^f_t
\end{align*}
\]

As usual for the LDDMM model, optimal velocity fields $v_t$ are entirely parametrized by the finite-dimensional momenta vectors $p_{k,t}$ attached to each vertex position. It results in the following discrete reduced Hamiltonian:

\[
H_r(x_t, f_t, p_t, p^f_t) = \frac{1}{2\gamma v} p^T_t K_{x_t,x_t} p_t + \frac{1}{2\gamma f} (p^f_t)^T D_s^{-1}(x_t) p^f_t
\]

where $p^T_t K_{x_t,x_t} p_t = \sum_{k,\ell=1}^P p^T_{k,t} K(x_{k,t}, x_{\ell,t}) p_{\ell,t}$. 
4.3.2 _Forward Equations_

From Eq. (23), we obtain the discrete equivalent of the Hamiltonian evolution equations:

\[
\begin{pmatrix}
\dot{x}_t \\
\dot{f}_t \\
\dot{p}_t \\
\dot{p}_f^t
\end{pmatrix}
= \begin{pmatrix}
\partial_p H_r(x_t, f_t, p_t, p_f^t) \\
\partial_{p_f} H_r(x_t, f_t, p_t, p_f^t) \\
-\partial_x H_r(x_t, f_t, p_t, p_f^t) \\
-\partial_{f_r} H_r(x_t, f_t, p_t, p_f^t)
\end{pmatrix}
= F(x_t, f_t, p_t, p_f^t).
\]

(36)

It may be written in an explicit way by using Formula (35) and we have

\[
F(x_t, f_t, p_t, p_f^t) = \begin{pmatrix}
\frac{1}{\gamma} V K_{x_t, x_t} p_t \\
\frac{1}{\gamma} D_s^{-1}(x_t) p_f^t \\
-\frac{1}{2\gamma} p_f^T \partial_{x_t} K_{x_t, x_t} p_t + \frac{1}{2\gamma} (D_s^{-1}(x_t) p_f^t)^T \partial_{x_t} D_s(x_t) (D_s^{-1}(x_t) p_f^t) \\
0
\end{pmatrix}.
\]

Some remarks can be made about the system of forward equations (36). First, we recover the fact that the momentum \( p_f^t \) is constant over the time (see Theorem 6) and for that reason we have dropped the subscript \( t \) in writing \( p_f \equiv p_f^t \). We also point out that Formula (36) contains new terms (i.e., compared to the 'tangential' algorithm of [15]) related to the evolution of the signal. In particular, \( \dot{p}_t \) now depends on the functional momentum \( p_f \) meaning that a variation in the signal induces a variation in the geometry (see Sect. 3.3.5 for an illustration). Finally, these new terms involve in particular the inverse of the sparse matrix \( D_s(x_t) \in \mathbb{R}^{P \times P} \) used in the computation of the functional norms (see Eq. (31)). Each time step thus requires solving the sparse (but still large) linear system \( D_s(x_t) h = p_f^t \) which may be numerically costly. We use MATLAB linear sparse solver to perform that operation. Yet, this can result in a typically 5–10 times slower algorithm compared to the 'tangential' one for fsshapes having in the range of ten thousand vertices.

4.3.3 _Data Attachment Term_

We now briefly describe the discretization of the fvarifold fidelity terms of Sect. 3.2.2 (more details are found in [15] and [17]). As previously, let us consider a discrete fsshape \((x, f, C)\) made of the \( d\)-dimensional distinct and non-degenerate simplices \( S_1, \ldots, S_T \) each obtained from the rows of matrix \( C \). The corresponding fvarifold then equals \( \mu(x, f) = \sum_{i=1}^{T} \mu_{S_i} \) and by bilinearity of the fvarifold metric:

\[
\|\mu(x, f)\|^2_{W_*} = \sum_{i=1}^{T} \sum_{j=1}^{T} \langle \mu_{S_i}, \mu_{S_j} \rangle_{W_*}
\]

For each \( i \in \{1, \ldots, T\} \), \( T_i S_i \) for \( x \in S_i \) is a constant element of \( G_d(\mathbb{R}^n) \) corresponding to the unique \( d\)-dimensional subspace that contains \( S_i \): we will write it \( V_i \). We
also choose the simple constant interpolation of the signal function inside each of the simplex; namely we write \( f(x) = \bar{f}_i \) for \( x \in S_i \) where \( \bar{f}_i \) is by definition the average of the function values at the vertices of \( S_i \). This leads to:

\[
\| \mu(x, f) \|_{W^*}^2 = \sum_{i=1}^{T} \sum_{j=1}^{T} k_t(V_i, V_j).k_f(\bar{f}_i, \bar{f}_j) \int S_i \times S_j k_p(x, x') d\text{vol}_S(x) d\text{vol}_S(x').
\]

Since the remaining integral has no general closed form expression except for simple polynomial kernels, we make the additional approximation \( k_p(x, x') \approx k_p(\bar{x}_i, \bar{x}_j) \) for all \( x \in S_i \) and \( x' \in S_j \) where for all \( i \), \( \bar{x}_i \) is the center of mass of simplex \( S_i \) (i.e., the average of the positions of vertices in \( S_i \)). Thus, finally, we obtain the approximation:

\[
\| \mu(x, f) \|_{W^*}^2 \approx \sum_{i=1}^{T} \sum_{j=1}^{T} k_p(\bar{x}_i, \bar{x}_j) k_t(V_i, V_j) k_f(\bar{f}_i, \bar{f}_j) \text{vol}(S_i) \text{vol}(S_j). \quad (37)
\]

Note that (37) can be also interpreted as the metric resulting from approximating each simplex of a discrete fshape as a single Dirac varifold.

It is then straightforward to deduce a similar formula for the computation of the fidelity term \( g(x_1, f_1) = \| \mu(x_1, f_1) - \mu(x_{\text{tar}}, f_{\text{tar}}) \|_{W^*}^2 \). The resulting formula has a complexity in \( O(T^2) \) which is similar to the cost of integrating the Hamiltonian systems in the algorithm we present in the next section. In terms of numerical precision, the approximation error in (37) can be shown to be of the order of \( O(\delta) \) where \( \delta \) is the maximum diameter of the simplices for signal functions that are at least continuous. Moreover, assuming that all three kernels \( k_p, k_t \) and \( k_f \) are differentiable, one obtains directly the derivatives of (37) with respect to the intermediate variables \( (\bar{x}_i), (V_i) \) and \( (\bar{f}_i) \) and recovers the derivatives with respect to the original vertex and signal coordinates \( x \) and \( f \) by the chain rule.

**Remark 4** We just point out that the construction and numerical evaluation of kernel \( k_t \) on the Grassmannian \( G_d(\mathbb{R}^n) \) requires particular care and we refer to [17] for a treatment of the general case. In the specific applications of this paper focusing on curves and surfaces in \( \mathbb{R}^2 \) or \( \mathbb{R}^3 \), the \( V_i \)'s can be represented by a single unit vector (tangent or normal) modulo orientation and the kernel \( k_t \) can be then built quite simply as a kernel on the unit sphere with an additional property of antipodal symmetry.

### 4.3.4 Geodesic Shooting Algorithm

The discrete equivalent of fshape registration equation (16) can be eventually cast as a finite dimensional optimization problem on the initial momenta variables \( p_0 = p_{t|t=0} \in \mathbb{R}^{P \times 3} \) and \( p^f \in \mathbb{R}^{P \times 1} \) that writes:

\[
\min_{p_0, p^f} J(p_0, p^f) = \frac{1}{2\gamma_v} p_0^T K_{x,x} p_0 + \frac{1}{2\gamma_f} (p^f)^T D_s^{-1}(x_0) p^f + \gamma \mathcal{W}g(x_1, f_1) \quad (38)
\]
subject to the dynamics described by Eq. (36). Due to the intricate dependency of final states \( x_1 \) and \( f_1 \) in the variables \( p_0 \) and \( p^f \) as well as the possible non-convexity of \( g \), this is typically a non-convex problem and thus, at best, we aim at finding a (not necessarily unique) minimum. The formulation of Eq. (38) suggests a geodesic shooting scheme for solving the minimization generalizing widely used similar frameworks in diffeomorphic shape matching, as the ones presented, for example, in [2, 42].

In the case of our problem, this amounts essentially in a gradient descent on the initial momenta variables \( (p_0, p^f) \). The gradients of the two first terms in Eq. (38) are easily computed, only the last term \( g(x_1, f_1) \) that involves final states is slightly more involved. It may be tackled by integrating backward the so-called adjoint linearized system of equations (see, for instance, Section 4 of [4]):

\[
\begin{pmatrix}
\dot{X}_t \\
\dot{F}_t \\
\dot{P}_t \\
\dot{P}^f_t
\end{pmatrix} = (dF(x_t, f_t, p_t, p^f_t))^T
\begin{pmatrix}
X_t \\
F_t \\
P_t \\
P^f_t
\end{pmatrix}
\tag{39}
\]

with the adjoint variables \( X_t \in \mathbb{R}^{P \times n}, F_t \in \mathbb{R}^{P \times 1}, P_t \in \mathbb{R}^{P \times n}, P^f_t \in \mathbb{R}^{P \times 1} \) and the endpoint conditions \( X_1 = \partial_x g(x_1, f_1), F_1 = \partial_f g(x_1, f_1), P_1 = \partial_p g(x_1, f_1) = 0 \) and \( P^f_1 = \partial_p^f g(x_1, f_1) = 0 \). The system of Eq. (39) which may be explicitly written with

\[
dF^T = \begin{pmatrix}
(\partial_x \partial_p H_r)^T & (\partial_x \partial_p^f H_r)^T & - (\partial_x \partial_x H_r)^T & 0 \\
0 & 0 & 0 & 0 \\
(\partial_p \partial_p H_r)^T & 0 & - (\partial_p \partial_x H_r)^T & 0 \\
0 & (\partial_p^f \partial_p^f H_r)^T & - (\partial_p^f \partial_x H_r)^T & 0
\end{pmatrix}
\]

is in practice tedious to implement. In our codes, we use instead the finite difference trick presented in [4] (Section 4.1 just before Proposition 9). This method has several advantages: it is rather general as it can be used for various Hamiltonian systems and it greatly simplifies the implementation as it avoids computing the second order derivatives of \( H_r \). To integrate the adjoint system (39), we only need to compute a single directional derivative at each time step with a finite difference method. Namely, for a well chosen \( h > 0 \) we have,

\[
\begin{pmatrix}
\dot{X}_t \\
\dot{F}_t \\
\dot{P}_t \\
\dot{P}^f_t
\end{pmatrix} \approx \frac{1}{2h} \begin{pmatrix}
\partial_x H_r(x_t - h P_t, f_t, p_t + h X_t, p^f_t + h F_t) \\
\partial_p H_r(x_t - h P_t, f_t, p_t + h X_t, p^f_t + h F_t) \\
\partial_p^f H_r(x_t - h P_t, f_t, p_t + h X_t, p^f_t + h F_t) \\
0
\end{pmatrix}
\begin{pmatrix}
\partial_x H_r(x_t + h P_t, f_t, p_t - h X_t, p^f_t - h F_t) \\
\partial_p H_r(x_t + h P_t, f_t, p_t - h X_t, p^f_t - h F_t) \\
\partial_p^f H_r(x_t + h P_t, f_t, p_t - h X_t, p^f_t - h F_t) \\
0
\end{pmatrix}.
\]
We use here a central finite difference scheme which requires two evaluations of the gradient of $H_r$. The numerical cost of the backward integration is then twice the price of the forward system of Eq. (36). It is also possible to use a forward finite difference scheme. In that case, to save some computational time, one may re-use the values of the gradient of $H_r$ evaluated during the forward integration. This latter method allows to compute the backward integration at the same computational cost than the forward system but with an extra cost of storage and lesser numerical precision.

In summary, the gradient of the objective functional with respect to $p_0$ and $p^f$ is obtained by the following forward–backward scheme:

1. Compute $(x_t, f_t, p_t, p^f_t)$ by integrating equation (36) forward with initial conditions $(x_0, f_0, p_0, p^f_0)$.
2. Compute the gradients of $g(x_1, f_1)$ with respect to $f$ and $x$.
3. Transport the gradients to $t = 0$ by integrating backward equation (39) with final conditions $X_1 = \partial_x g(x_1, f_1)$, $F_1 = \partial_f g(x_1, f_1)$, $P_1 = 0$, $P^f_1 = 0$.
4. Set $\nabla p_0 J = \frac{1}{\gamma} V K x, x p_0 + P_0$ and $\nabla p^f J = D_0(x_0)(\frac{1}{\gamma_f} D_{s}^{-1}(x_0) p^f + \gamma W P^f_0)$

We point out that the gradient with respect to the functional momentum $p^f$ at step (4) is computed with respect to the $L^2$ metric on $X_0$ instead of the Euclidean metric, which adds the extra weight matrix $D_0(x_0)$. This can be crucial, for example, when the mesh $X_0$ is not regular but contains triangles of very different areas. The updates on $p^f$ obtained from the gradient computed with respect to this metric ensure that the signal variations $\dot{f} = D_{s}^{-1}(x) p^f$ will not be too much affected by the quality of the initial mesh.

The rest of the fshape matching algorithm consists in an adaptive step gradient descent simultaneously on $p_0$ and $p^f$. The architecture of the code is in MATLAB with time-consuming segments (computation of kernel sums for the most part) externalized in CUDA. The whole code is available upon request to the authors as part of the FshapesTk software [14].

5 Results and Discussion

In this section, we show a few results of the fshape matching algorithm presented in Sect. 4.3.4. We will first focus on some simple examples to illustrate certain aspects of the method in particular the influence of the norm regularity. Following these, we evaluate qualitatively the output of the algorithm on a few examples of functional shapes originating from medical imaging. All experiments were performed on a server machine equipped with a Nvidia GTX 555 graphics card.

5.1 Synthetic Data

5.1.1 Digits

We first evaluate the algorithm on an example mimicking the situation of gray level images as in Sect. 3.3.3. Here, the geometrical part of both the source and target
Fig. 5  Digits: source fshape (left) and target fshape (right)

Fig. 6  Estimated metamorphoses of fshapes with a signal representing handwritten digits. The meshes are plotted in wireframe representation to clearly see the deformations. Three experiments for different parameters in the energy are shown: $\gamma_V/\gamma_f = 1$ (first row), $\gamma_V/\gamma_f = 20$ (second row) and $\gamma_V/\gamma_f = 100$ (third row)

fshapes is the flat square $[-1, 1] \times [-1, 1] \times \{0\} \subset \mathbb{R}^3$. These two distinct triangular meshes were created with a standard Delaunay triangulation method and contain 4900 vertices each as shown in Fig. 5. The signal part represents two handwritten digits with value ranging from 0 (red) to 0.6 (blue).

Figure 6 shows an example of metamorphoses in $L^2$ with varying penalty coefficients on the functional momentum part of the energy $\gamma_f$ and $\gamma_V$. Results are consistent with the expected behavior: the smaller $\gamma_f$, the more the transformation is performed in the photometric component instead of deforming the image by the diffeomorphism. We chose for the kernel $K$ defining $\| \cdot \|_V$ a sum of two radial scalar Gaussian [13] with (small) widths 0.2 and 0.1 (the square having an edge of size 2). The optimization is performed with a coarse to fine strategy (as described in [15]), and the final kernels...
Fig. 7 Similar example of metamorphosis as Fig. 6 using different mesh sampling: 4900 vertices (first row), 2457 vertices (second row) and 1241 vertices (third row)

$k_p$ and $k_f$ are taken Gaussian as well with, respectively, $\sigma_p = 0.05$ and $\sigma_f = 0.7$. We also show, with Fig. 7, the effect of mesh precision on the estimated metamorphosis: although local differences can be observed, the overall dynamics remain quite similar in the three cases.

Note that the size and shape of triangles can vary quite substantially with the deformation as opposed to using a fixed grid with an Eulerian approach as in the image metamorphosis model of [40]. This may in turn affect the quality of the discrete approximations of the signal part although those mesh distortions still remain controlled through the diffeomorphism energy constraint. It would be interesting, in future work, to combine our approach with local remeshing strategies on the template shape in order to better limit the errors in the signal discretization.

5.1.2 Stanford Bunny

Secondly, we examine the effect of increasing the metric regularity in the functional dynamics’ penalty. The example in Fig. 8 is a metamorphosis of a sphere (with 10,242 vertices) onto the Stanford bunny surface (with 2581 vertices) with a fairly smooth signal function. Results from metamorphosis in $H^1$ display nice regular evolution throughout time and a resulting transformation very consistent with the target despite the difference of sampling between the two meshes. On the other hand, the equivalent result in $L^2$ (with the same parameters) shows some residual oscillatory patterns in the recovered signal unlike the target one, appearing mostly in areas where the transformation is not as close to the target. The qualitative comparison is shown in Fig. 9 with several views. This effect is particularly obvious on the below part of the
mesh where some holes are present in the target. Such oscillations had been noticed already and studied in simpler settings as in [35]. They are in a sense numerical manifestations of the conditions on the existence of solutions to the problem with $L^2$ and the absence of weak continuity in $L^2$ of the varifold terms. Note that oscillations may be still alleviated if one increases the penalty weight $\gamma_f$; however, this would also result in less overall accuracy in the signal matching. Another classical advantage of $H^1$ metamorphosis over $L^2$ is the robustness to signal noise: resulting metamorphoses in $L^2$ are much more affected by the presence of noise or outliers in signal values than higher regularity metrics. In terms of running time, however, the $L^2$ metamorphosis scheme with the mass lumping discretization described in Sect. 4.2.1 only involves inversion of diagonal linear systems in the signal dynamics, resulting in an algorithm running in 45 min which is about 6 times faster compared to the finite elements scheme of the $H^1$ case.

5.1.3 Tangential versus Metamorphosis Model

In order to prolong the discussion of Sect. 3.3.5, we give a second illustration, in a simulated situation, of the difference of dynamics between the metamorphosis model and the previous simpler tangential framework presented in [15,35]. In the latter case, the optimization problem is the same except that the energy (34) of the fshape transformation is replaced by:

$$E^{\text{tan}}_{x}(v, h) = \frac{\gamma V}{2} \int_{0}^{1} ||v_t||^2_V dt + \frac{\gamma_f}{2} \int_{0}^{1} h_t^T D_s(x_0) h_t dt.$$
In other words, the energy of the functional variation is measured with respect to the metric on the fixed template shape \( x_0 \). As explained in [15], it implies that for optimal paths, \( \mathbf{h}_t \) is stationary with respect to \( t \) and therefore that the evolution of the signal at each given point is linear in time. This allows in turn to simplify quite substantially the optimization algorithm.

In this experiment, we consider two planar curves from the Surrey fish database with artificial signals plotted as heat color maps in Fig. 10. We then compute solutions to the matching problem between the 1D template and target shape using a common fixed set of kernel size and balancing weight parameters both for the \( H^1 \) metamorphosis model and the \( H^1 \) tangential model. In Fig. 11, some intermediate time points along the optimal matching paths obtained for each method. Although the end time shape matches closely the target for both approaches, it is important to notice the difference in the evolution from \( t = 0 \) to \( t = 1 \) that reflects the intrinsically distinct properties of the two.

To emphasize this, in Fig. 12, we look more precisely into the geometric and functional components of the shape transformations. It is first obvious that the
deformations resulting from the optimal vector fields $v$ differ quite a bit: in the metamorphosis case, we observe a stronger horizontal component in the trajectories that tends to favor matching between portions of the template and target curves with closer signal values. The figures on the right allow to visualize the evolution of the functional components across the time steps. Once again, the two models produce different dynamics: if the signal evolution speed in the tangential case is constant (c.f. previous remark), for metamorphosis we can see that the variations of signals are faster near $t = 0$ and slower near $t = 1$ while the expansion rate of the curve has the opposite behavior. This is consistent with the observations of Sect. 3.3.5 since the template has smaller length and needs to be enlarged to match the target.

5.2 Real Data

The algorithm is also tested on some functional shapes occurring in medical imaging. In the following, we present a couple of qualitative results on these datasets mostly to try the behavior and robustness of the method on potentially more involved situations than the previous synthetic cases. Nevertheless, the experiments of this section are
Fig. 12  Closer look at the comparison between tangential and metamorphosis matching models. The left figures show the geometric evolution of the fshapes (trajectories of vertices are plotted in blue), while the right column depicts the signal dynamics by superimposing all consecutive time steps. At convergence, both methods achieve small and comparable values of the fidelity term. However, the balance between the geometric and functional parts of the final energies differs: these are, respectively, $p_0^T K_{x,x} p_0 = 0.94$ and $(pf)^T D_s^{-1}(x_0)p_f = 4.31$ in the tangential model, $p_0^T K_{x,x} p_0 = 0.97$ and $(pf)^T D_s^{-1}(x_0)p_f = 1.68$ in the metamorphosis case.

presented as illustrations but clearly not as actual applications of the method for specific anatomical studies.

5.2.1 Thickness Maps

We first examine the output of metamorphosis matching (with $H^1$ norm) on anatomical surfaces with estimation of the membrane thickness at each vertex. The first example in Fig. 13 is from a dataset of Nerve Fiber Layer (NFL) membranes in the retina with estimated measurements of thickness. The example corresponds to two age-matched subjects, one control and one affected by glaucoma. Each surface has 5000 vertices, and the algorithm is run for 220 iterations in a total time of about 3.3 h. We show the output metamorphosis together with the magnitude of the geometric momentum and the functional momentum. The deformation is mostly concentrated along the optical nerve opening while the functional momentum shows the overall decrease in thickness, particularly in a typical crescent region around the opening. Although illustrated here on two particular subjects, such anatomical effects have been analyzed and confirmed statistically in [32].

5.2.2 Heart Pressure

As a last example, we consider the epicardium surfaces of an heart (between the initial and final states of the cardiac cycle) with signals corresponding to simulated pressure maps on the membrane (see Fig. 14). We show the time evolution obtained...
Fig. 13  Metamorphosis between two subjects of the Nerve Fiber Layer dataset (data courtesy of S. Lee, M. Sarunic, F. Beg, Simon Fraser University)

Fig. 14  Valves dataset: epicardium surfaces with simulated pressure (data courtesy of C. Chnafa, S. Mendez and F. Nicoud, University of Montpellier). a Source and b target (Color figure online)

from the $H^1$ metamorphosis matching algorithm in Fig. 15 second row. Surfaces have approximately 26,000 vertices, and the algorithm took on the order of 5 h to reach convergence. As a comparison, the results for the simplified tangential model mentioned previously, and which algorithm is detailed in [15], is shown Fig. 15 first row. In terms of numerical cost, the tangential model avoids the cost of solving linear
systems of equations at each time step and results in a total run time, for this example, of 20 min.

5.3 Conclusion and Discussion

We have presented a new model for the representation and registration of fshapes, i.e., objects combining a deformable geometric support with a photometric component. From a theoretical standpoint, this model extends the existing idea of metamorphosis on flat images and, unlike earlier approaches like the tangential model of [15], leads to a well-defined complete metric space structure when restricting to fshape bundles. In addition, the framework was derived for the class of signals of higher Sobolev regularity on the manifolds which we showed is necessary in certain instances.

This was then cast into a formulation for geometric-functional matching between two given fshapes, combining metamorphosis energy with data attachment terms based
on functional varifolds. We have shown that it is a well-posed optimal control problem (with some conditions on energy weights in the case \( s = 0 \)) and investigated carefully the Hamiltonian dynamics of minimizers as well as the equivalent of the EP-diff conservation equation for that model. We have also derived the corresponding discrete model and algorithm to numerically solve the matching problem in the cases \( s = 0 \) and \( s = 1 \). Similar discretization schemes for higher-order Sobolev spaces is left for future study. Other important questions regarding the \( \Gamma \)-convergence of the discrete to the continuous models were also not addressed here, although a significant step was made in that direction with the results of [35]. Still, numerical simulations show the ability of this approach to recover joint geometric and photometric variations between a given template and target shape at the price of extra parameters in the model and extra numerical cost compared to a pure diffeomorphic registration.

The approach was restricted to the problem of matching between two subjects, the direct follow-up being to extend the model and algorithm to atlas estimation on populations, following the footsteps of [15,32]. One advantage to expect from it is that the metric framework we obtain from metamorphosis would provide a more theoretically suitable setting to statistical analysis on those geometric-functional transformations.

A second clear restriction of the paper comes from the very nature of signals and the definition of geometric action in Eq. (8) that was considered here. The model was indeed built on standard image deformation action and is therefore not necessarily adapted to all types of functional maps. Other typical cases could involve densities, vector fields, tensor fields on shapes for which the transport equations could significantly differ from Eq. (8) and so would the associated Hamiltonian dynamics and the behavior of geodesics. We postulate, however, that a very similar approach to the one developed here could be undertaken with other signal spaces or group actions and lead to interesting extensions of the present work. This work and possible future extensions could also find interesting connections with complex fluid dynamics [22,26] appearing, for example, in the modeling of liquid crystals, as it typically involves combined spatial and orientational dynamics.

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### A Proof of Theorem 1

Before the actual proof of Theorem 1, we shall introduce a few definitions and intermediate results. Let \( s \geq 0 \) and \( s' = \max(s, 1) \) and we recall that \( X \) is a compact submanifold of \( \mathbb{R}^n \) of dimension \( d \) and class \( C^s \) and that \( V \hookrightarrow C^s_0(\mathbb{R}^n, \mathbb{R}^n) \). For a given coordinate system \( (x^i)_{1 \leq i \leq d} \), we will denote by \( (\partial_i) \) and \( (dx^i) \) the corresponding frame and coframe, respectively. We introduce the following class of sections over the \((a, b)\) tensor bundle:

**Definition 3** We say that \( A \in \Gamma_{pol}^{p,s}(T_b^a(U)) \) with \( a, b, p, s \in \mathbb{N}, a, b \leq s \) and \( p < s' \) if there exists a coordinate system \( (x^i)_{1 \leq i \leq d} \) on \( U \) such that for any \( (\phi, u) \in \text{Diff}^s_0(\mathbb{R}^n) \times U \)
\[ A(\phi, u) = A^\alpha_\beta(\phi, u) \partial^\alpha_x \otimes dx^\beta \]

where for any compact \( K \subset U \) there exists two polynomials \( P \) and \( Q \) such that for any multi-indices \( \alpha, \beta \) and for any \( \phi, \phi' \in \text{Diff}^s_0 \) we have

\[
u \mapsto A^\alpha_\beta(\phi, u) \in C^p(U, \mathbb{R}), \quad \sup_{K, k \leq p} | \partial^k A^\alpha_\beta(\phi, u) | \leq P(\rho_s(\phi)),
\]

and

\[
\sup_{K, k \leq p} | \partial^k A^\alpha_\beta(\phi, u) - \partial^k A^\alpha_\beta(\phi', u) | \leq \rho_s(\phi' \circ \phi^{-1}) Q(\rho_s(\phi), \rho_s(\phi'))
\]

with the notation \( \rho_s(\psi) \doteq \sum_{k \leq s} \| d^k (\psi - \text{Id}) \|_\infty + \| d^k (\psi^{-1} - \text{Id}) \|_\infty \) for any \( \psi \in \text{Diff}^s_0(\mathbb{R}^n) \).

In the previous, we point out that \( \alpha \) and \( \beta \) are multi-indices of integers between 1 and \( d \) such that \( |\alpha| = a, |\beta| = b \). When \( a = b = 0 \), the space \( \Gamma^{p,s}_\text{pol}(T^a_b(U)) \) will be denoted \( C^{p,s}_\text{pol}(U) \).

**Remark 5** A first important remark is that the definition is not dependent on the choice of the coordinate system. Indeed, if \( s = 0 \), we have \( a = b = p = 0 \) and the definition does not depend on any coordinate system. If \( s = 1 \) then \( p = 0 \) and if \( (y_1, \ldots, y^d) \) is another coordinate system, it is sufficient to notice that \( \frac{\partial}{\partial y^i} = \frac{\partial}{\partial x^i} \frac{\partial}{\partial y^j} \) and \( dx^i = \frac{\partial y^i}{\partial x^j} dy^j \) where the mappings \( \frac{\partial y^i}{\partial x^j} \) and \( \frac{\partial x^i}{\partial y^j} \) are continuous and bounded on \( K \). Last, if \( s \geq 2 \), we get \( A^\alpha_\beta(\phi, u) \frac{\partial^a}{\partial y^a} \otimes dy^\beta = A^\alpha_\beta(\phi, u) \frac{\partial^a}{\partial x^a} \otimes dx^\beta \) for \( \tilde{A}^\alpha_\beta(\phi, u) = A^\alpha_\beta(\phi, u) \frac{\partial y^\alpha}{\partial x^\beta} \frac{\partial x^\beta}{\partial y^\alpha} \) with \( \frac{\partial y^\alpha}{\partial x^i} = \prod_{i=1}^a \frac{\partial y^\alpha}{\partial x^i} \in C^{s-1}(U, \mathbb{R}) \) and \( \frac{\partial x^\beta}{\partial y^i} = \prod_{i=1}^b \frac{\partial x^\beta}{\partial y^i} \in C^{s-1}(U, \mathbb{R}) \). Since \( p \leq s - 1 \), we deduce that \( \tilde{A}^\alpha_\beta(\phi, u) \in C^p(U, \mathbb{R}) \) for any \( (\tilde{\alpha}, \tilde{\beta}) \) and satisfies the needed polynomial controls in the coordinate system \( (y^1, \ldots, y^d) \) thanks to the Faà di Bruno Formula.

A second useful remark is that \( C^{p,s}_\text{pol}(U) \) is an algebra over the field \( \mathbb{R} \).

**Lemma 4** Assume here that \( s \geq 2 \). For any coordinate system \( (x^i)_{1 \leq i \leq d} \) on an open set \( U \subset X \), we have for any \( 1 \leq i \leq d \) that

\[
\nabla \partial_i \in T^{s-2,s}_1(T^1_0(U)) \text{ and } \nabla dx^i \in T^{s-2,s}_0(T^0_2(U))
\]

where for \( \phi \in \text{Diff}^s_0(\mathbb{R}^n) \), \( \nabla = \nabla^\phi \) is the Levi–Civita covariant derivative associated with the pullback metric \( g = g^\phi \) on \( X \) of the induced metric \( g^{\phi(X)} \) on \( Y = \phi(X) \) by the Euclidean metric on \( \mathbb{R}^n \).

**Proof** First we have \( \nabla \partial_j = \Gamma^{ij}_k \partial_i \otimes dx^j \) where the \( \Gamma^{ij}_k \) are the Christoffel symbols of second kind so that it is sufficient to prove that \( \Gamma^{ik}_j \in C^{s-2,s}_\text{pol}(U) \). For given \( \phi \in G_V \), as a function of \( u \in U \) we have \( g_{ij} = \langle d\phi, \partial_i, d\phi, \partial_j \rangle \in C^{s-1}(U, \mathbb{R}) \). Using the chain

\[
\begin{array}{c}
\end{array}
\]
Lemma 5

Let \( g \) exist a polynomial of degree \( 1 \) and where \( \phi \) deduce immediately that \( g \in C^{s-1,\infty}_{\text{pol}}(U) \).

We need now a similar control for the cometric \( g_{ij} \). Denoting \( g = (g_{ij})_{1 \leq i, j \leq d} \), we have \( g^{-1} = (g^{-1})_{1 \leq i, j \leq d} \) and \( g^{-1} = \text{com}(g)^T / \det(g) \) where \( \text{com}(g) \) is the comatrix of the matrix \( g \). Since \( \text{com}(g)^T \) is a polynomial expression in the coefficients \( g_{ij} \), we get, using the algebra structure property of Remark 5, that all the coefficients of \( \text{com}(g) \) are in \( C^{s-1,\infty}_{\text{pol}}(U) \). Similarly, \( \det(g) \in C^{s-1,\infty}_{\text{pol}}(U) \) so that, in order to get \( \det(g)^{-1} \in C^{s-1,\infty}_{\text{pol}}(U) \), it is sufficient to prove that for any compact \( K \subset U \), there exists a polynomial \( P \) such that

\[
\det(g)^{-1} \leq P(\rho_s(\phi)). \tag{40}
\]

However, since \( T_{\phi(u)} Y = \text{Span}\{d\phi(u) \cdot \partial_i, 1 \leq i \leq d\} \) where \( Y = \phi(X) \), then for \( (e_1, \ldots, e_d) \) an orthonormal basis of \( T_{\phi(u)} Y \), we have \( \det(g)^{-1} = \det(\langle d\phi^{-1}(\phi(u)) \cdot e_i, d\phi^{-1}(\phi(u)) \cdot e_j \rangle) \leq ||d\phi^{-1}||^2 \). Using the fact that \( \Gamma^k_{ij} = \frac{1}{2}(\partial_i g_{mj} + \partial_j g_{mi} - \partial_m g_{ij})g^{mk} \) we get immediately that \( \Gamma^k_{ij} \in C^{s-2,\infty}_{\text{pol}}(U) \) and \( \nabla \rho_i \in C^{s-2,\infty}_{\text{pol}}(T_1^1(U)) \). Now since \( 0 = \nabla(dx^i(\partial_j)) = \nabla dx^i(\partial_j) + dx^j(\nabla \partial_j) \) we get \( \nabla dx^i(\partial_j) = -\Gamma^k_{ij} dx^l \) and \( \nabla dx^i = -\Gamma^l_{ij} dx^l \otimes dx^l \). Since we have just proved that \( \Gamma^k_{ij} \in C^{s-2,\infty}_{\text{pol}}(U) \), we get the result. \( \square \)

Lemma 5 Let \( \mathcal{I} = \{ (\alpha, \beta) | \alpha \in [1, d]^a, \beta \in [1, d]^b, 1 \leq a < b \leq s \} \) and \( (x^i)_{1 \leq i \leq d} \) be a coordinate system defined on an open set \( U \subset X \).

There exists a family of functions \( (c^\alpha_{\beta})_{(\alpha, \beta) \in \mathcal{I}} \) such that

1. for any \( (\alpha, \beta) \in \mathcal{I} \), we have \( c^\alpha_{\beta} \in C^{s-1(1+|\beta|-|\alpha|),\infty}_{\text{pol}}(U) \subset C^{0,\infty}_{\text{pol}}(U) \)
2. for any \( 0 \leq k \leq s \) any \( \phi \in H^1_{\text{loc}}(U) \) and any \( \beta \in [1, d]^k \), we have (a.e.) on \( U \)

\[
\partial^k_{\beta} f = \nabla^k_{\beta} f + \sum_{l=1}^{k-1} \sum_{|\alpha|=l} c^\alpha_{\beta} \nabla^l_{\alpha} f \tag{41}
\]

where for \( s \geq 1 \) and \( \phi \in \text{Diff}^1_0(\mathbb{R}^n) \), \( \nabla = \nabla^\phi \) is Levi–Civita covariant derivative associated with the pullback metric \( g = g^\phi \) on \( X \) on the Euclidean metric on \( \phi(X) \) and where \( \partial^k_{\beta} f = \partial^k_{\beta} f(\partial^k_{\beta}) \) and \( \nabla^l_{\alpha} f = \nabla^l f(\partial^l_{\alpha}) \).
Proof For $k = 0$ or $k = 1$ the result is trivial. Let consider a proof by induction for $k \geq 1$. We have for $\beta \in [1, d]^k$ and $\tilde{\beta} = (i, \beta)$ that

$$\partial^{k+1}_{\tilde{\beta}} f = \partial_i (\partial^k_{\tilde{\beta}} f) = \partial_i \left[ \nabla^k_{\tilde{\beta}} f + \sum_{l=1}^{k-1} \sum_{\alpha, |\alpha| = l} c^\alpha_{\tilde{\beta}} \nabla^l_{\alpha} f \right].$$

However, $\partial_i (\nabla^k_{\tilde{\beta}} f) = \nabla^{k+1}_{\tilde{\beta}} f + \nabla^k f (\nabla_i \partial^k_{\tilde{\beta}})$. Moreover, since we have

$$\nabla_i \partial^k_{\tilde{\beta}} = \sum_{l=1}^k \mathcal{S}_{i j=1} \partial_i \otimes \nabla_i \partial_i \otimes \mathcal{S}_{j=l+1} \partial_{\beta_j} = \sum_{l=1}^k \Gamma^m_{i j} \mathcal{S}_{j=1}^{l-1} \partial_{\beta_j} \otimes \partial_m \otimes \mathcal{S}_{j=l+1} \partial_{\beta_j}$$

we get that $\nabla_i \partial^k_{\tilde{\beta}} \in \Gamma^s_{\alpha \beta} (T^0_k (U))$ and $\nabla^k f (\nabla_i \partial^k_{\tilde{\beta}})$ can be written as $\sum_{\alpha, |\alpha| = k} c^\alpha_{\tilde{\beta}} \nabla^k f$ for functions $c^\alpha_{\tilde{\beta}} \in C^s_{\alpha \beta} (U)$. Similarly, we have for $1 \leq l \leq k$ and $\alpha \in [1, d]^l$ that

$$\partial_i (c^\alpha_{\tilde{\beta}} \nabla^l_{\alpha} f) = \partial_i (c^\alpha_{\tilde{\beta}}) \nabla^l_{\alpha} f + c^\alpha_{\tilde{\beta}} \nabla^{l+1}_{i (\alpha, \alpha)} f + c^\alpha_{\tilde{\beta}} \nabla^{l}_{\alpha} (\nabla_i \partial^l_{\alpha}).$$

Denoting $c^\alpha_{\tilde{\beta}, 1} = \partial_i (c^\alpha_{\tilde{\beta}}) \in C^s_{\alpha \beta} (U)$, $c^\alpha_{\tilde{\beta}, 2} = c^\alpha_{\tilde{\beta}} \in C^s_{\alpha \beta} (U)$ and since $\nabla_i \partial^l_{\alpha} \in \Gamma^s_{\alpha \beta} (T^0_{l+1} (U))$, $c^\alpha_{\tilde{\beta}, 3} = c^\alpha_{\tilde{\beta}} \chi (\nabla_i \partial^l_{\alpha}) \in C^s_{\alpha \beta} (U) \subseteq C^s_{\alpha \beta} (U)$ we get that $\partial_i (c^\alpha_{\tilde{\beta}} \nabla^l_{\alpha} f)$ can be written as

$$\sum_{m=1}^{l+1} \sum_{|\gamma| = m} c^\gamma_{\tilde{\beta}} \nabla^m_{\gamma} f$$

for some appropriate functions $c^\gamma_{\tilde{\beta}} \in C^s_{\alpha \beta} (U)$ and decomposition (41) holds for the rank $k + 1$.

We finally get to the main result itself.

Proof of Theorem 1 The starting point is to recast the Sobolev norm on $Y = \phi (X)$ as an integral on $X$ through the pullback metric and pullback covariant derivative. Up to the introduction of a finite partition of unity $(\chi_l)$ subordinated to finite covering of $X$ with charts $(U_l, \psi_l)$, we can restrict to one open set $U = U_l$ and show that for $\chi = \chi_l$ and $K = \text{supp}(\rho)$, there exists a polynomial $P$ such that

$$\sum_{k=0}^{s} \int_K \chi \, g^0_k (\nabla^k f, \nabla^k f) \, \text{vol}(g) \leq P (\rho_s (\phi)) \sum_{k=0}^{s} \int_K \chi \, \bar{g}^0_k (\nabla^k f, \nabla^k f) \, \text{vol}(\bar{g}) \quad (42)$$

where $\bar{g} = g^{\text{Id}}$ and $\nabla = \nabla^{\text{Id}}$. For $s = 0$ the results comes from the inequalities (40). Let assume that $s \geq 1$ (and thus $s' = s$). From Lemma 5, there exists universal functions $c^\alpha_{\tilde{\beta}} \in C^0_{\alpha \beta} (U)$ for any pair $(\alpha, \beta) \in \mathcal{I}$ such that $\partial^k_{\beta} f = \nabla^k_{\beta} f + \sum_{l=1}^{k-1} \sum_{|\alpha| = l} c^\alpha_{\tilde{\beta}} \nabla^l_{\alpha} f$.

In particular, if we denote $\mathcal{J} = \{(k, \gamma) \mid 0 \leq k \leq d, \gamma \in [1, d]^k\}$, $f = (\partial^k_{\beta} f)_{(k, \gamma) \in \mathcal{J}}$ and $\tilde{f} = (\nabla^k f)_{(k, \gamma) \in \mathcal{J}}$, then there exists $M \in C^0_{\alpha \beta} (U, L (\mathcal{J}, \mathcal{J}))$ (invertible since triangular with ones on the diagonal) with coefficients in $C^0_{\alpha \beta} (U)$ such that $f = M \tilde{f}$.
Moreover, since $\sum_{k=0}^{s} s_k^0 (\nabla^k f, \nabla^k f) \text{vol}(g)$ can be rewritten as $q(\tilde{f})$ where $q$ is a non-degenerate positive quadratic form continuously depending on the location $u \in U$ and coefficients in $C_p^{s-1, s}(U) \subset C_p^{0, s}(U)$, we get that there exists a polynomial $\tilde{P}$ such that $q(\tilde{f}) = q(M^{-1} f) \leq P(\rho_s(\phi))|f|^2$ so that

$$\sum_{k=0}^{s} \int_K \chi \cdot s_k^0 (\nabla^k f, \nabla^k f) \text{vol}(g) \leq \tilde{P}(\rho_s(\phi)) \sum_{k=0}^{s} \int_K \chi \cdot |\partial^k f|^2 \text{d}x.$$  

Furthermore, considering $M$ for $\phi = \text{Id}$ there exists a constant $R \geq 0$ such that we have $\sum_{k=0}^{s} \int_K \chi \cdot |\partial^k f|^2 \text{d}x \leq R \sum_{k=0}^{s} \int_K \chi \cdot s_k^0 (\nabla^k f, \nabla^k f) \text{vol}(g)$ so that (42) holds with $P = R \tilde{P}$ and we have obtained Theorem 1. $\square$

We conclude this appendix by adding an extra property of continuity with respect to $\phi$ of the pullback $H^s$ metrics, which is used in the proof of Theorem 2. From the previous developments, we get that for any chart $(U, \varphi)$ on $X$ associated with a coordinate system $(x^1, \ldots, x^d)$ on $U$ there exists a family of functions $c_{\beta}^\alpha$ such that for any $f \in H^s_{loc}(U)$

$$\partial_{\beta}^k f = \nabla_{\beta}^k f + \sum_{l=1}^{k-1} \sum_{|\alpha| = |l|} c_{\beta}^\alpha \nabla_{\alpha}^l f. \tag{43}$$

Let us denote $E = \bigoplus_{k=0}^{s} (\otimes T^k X)$, $E$ is a $C^{s-1}$ vector bundle over $X$. For any local chart $(U, \varphi)$ with coordinate functions $(x^1, \ldots, x^d)$, $(q_k(d\varphi))_{\beta \in [1, d]^k, 1 \leq k \leq d}$ is a local frame of $E$ over $U$ where $q_k : \otimes T^k X \rightarrow E$ denotes the canonical embedding. We will also consider $\text{End}(E) \rightarrow X$ the endomorphism vector bundle where $\text{End}(E)_x \cong \text{End}(E_x)$.

**Definition 4** We say that $M \in \Gamma^{0, s}(\text{End}(E))$ where $M : \text{Diff}_0^s(\mathbb{R}^n) \rightarrow \Gamma^0(\text{End}(E))$ if for any coordinate system $(x^1, \ldots, x^d)$ defined on an open set $U \subset M$, all the coefficients of $M$ in the local frame $(d\varphi^\beta)_{\beta}$ are in $C_p^{0, s}(U)$.

**Definition 5** We say that $G \in \Gamma^{0, s}(E^* \otimes E^*)$ where $G : \text{Diff}_0^s(\mathbb{R}^n) \rightarrow \Gamma^0(E^* \otimes E^*)$ if for any coordinate system $(x^1, \ldots, x^d)$ defined on an open set $U \subset M$, all the coefficients of $G$ in the local frame $(q_k(\partial^{k}_{\alpha} \otimes q_{k'}(\partial^{k'}_{\alpha'})))$ for $0 \leq k, k' \leq s$ and $(\alpha, \alpha') \in [1, d]^k \times [1, d]^{k'}$ are in $C_p^{0, s}(U)$, where $q_k : \otimes T M \rightarrow E^*$ is the canonical embedding.

Now, writing

$$\|f\|_{H^s, \varphi(X)} \doteq \|f \circ \varphi^{-1}\|_{H^s(\varphi(X))}$$

as the pullback $H^s$ metric on $X$ induced by $\phi \in \text{Diff}_0^s(\mathbb{R}^n)$, we have the following property:

**Lemma 6** For any $f \in H^s(X)$, the application $\text{Diff}_0^s(\mathbb{R}^n) \rightarrow \mathbb{R}_+$, $\phi \mapsto \|f\|_{H^s, \varphi(X)}$ is continuous.
Proof Let us introduce \( p_E : \text{Diff}^s_0(\mathbb{R}^n) \times H^s(X) \to L^2(X, E) \) such that

\[
p_E(\phi, f) \equiv \bigoplus_{k=0}^s q_k(\nabla^k f)
\]

where \( \nabla = \nabla^\phi \) for \( \phi \in \text{Diff}^s_0(\mathbb{R}^n) \) as well as the pullback of the metric \( g_E(\phi) = \bigoplus_{k=0}^s g^k \) with once again \( g = g^\phi \). Then, we have by definition

\[
\|f\|_{H^s,\phi(X)}^2 = \int_X g_E(\phi)(p_E(\phi, f), p_E(\phi, f)) \text{vol}(g^\phi).
\]

Now, with (43), we see that there exists \( M \in \Gamma^{0,s}(\text{End}(E)) \) such that \( p_E(\phi, f) = M(\phi) \cdot p_E(\text{Id}, f) \). Similarly, thanks to the previously derived expressions of the metric \( g^\phi \), we have \( g_E \in \Gamma^{0,s}(E^* \otimes E^*) \) and thus there exists \( S \in \Gamma^{0,s}(\text{End}(E)) \) such that

\[
\int_X g_E(\phi)(p_E(\phi, f), p_E(\phi, f)) \text{vol}(g^\phi) = \int_X \bar{g}_E \left( \Lambda(\phi) \cdot p_E(f), p_E(f) \right) \text{vol}(g)
\]

with \( \Lambda \in \Gamma^{0,s}(\text{End}(E)) \) and \( \bar{g}_E = g_E(\text{Id}) \), \( \bar{g}_E(f) = p_E(\text{Id}, f) \). Since the coefficients of \( \Lambda \) in a local frame belong to \( C_\text{pol}^{0,s} \), they are in particular continuous with respect to \( \phi \) for the norm of uniform convergence of \( \phi \) and its derivatives up to order \( s \) on the compact \( X \). As a consequence, if \( \phi^n \to \phi \), then \( \Lambda(\phi^n) \to \Lambda(\phi) \) in \( \Gamma^0(\text{End}(E)) \) and:

\[
\|f\|_{H^s,\phi^n(X)}^2 \xrightarrow{n \to \infty} \int_X \bar{g}_E \left( \Lambda(\phi) \cdot p_E(f), p_E(f) \right) \text{vol}(g) = \|f\|_{H^s,\phi(X)}^2
\]

which completes the proof. \( \square \)

B Proof of Theorem 6

The proof follows similar steps as the pure diffeomorphic case derived in [5]. Let us introduce the total cost functional:

\[
J(q, \tilde{f}, v, \tilde{h}) = \int_0^1 \left[ \frac{\nu^0}{2} \|v_t\|_{V_t}^2 + \frac{\nu^1}{2} \|\tilde{h}_t\|_{H^s_{\tilde{h}_t}}^2 \right] \, dt + g(q_1, \tilde{f}_1)
\]

\[
= \int_0^1 L(q_t, v_t, \tilde{h}_t) \, dt + g(q_1, \tilde{f}_1)
\]
where $L$ is by definition the Lagrangian function. It is differentiable with respect to $v \in V, \tilde{h} \in H^s(M)$ as well as $q \in C^s(M, \mathbb{R}^n)$ since $s' \geq s$. The variation of $J$ writes:

$$
\begin{align*}
\delta J(q, \tilde{f}, v, \tilde{h}) &= \int_0^1 \left[ \left( \partial_q L(q_t, v, \tilde{h}_t) \right| \delta q_t + \left( \partial_v L(q_t, v_t, \tilde{h}_t) \right| \delta v_t + \left( \partial_{\tilde{h}} L(q_t, v_t, \tilde{h}_t) \right| \delta \tilde{h}_t \right] \, dt \\
&\quad + \left( \partial_q g(q_1, \tilde{f}_1) \right| \delta q_1 + \left( \partial_{\tilde{f}} g(q_1, \tilde{f}_1) \right| \delta \tilde{f}_1
\end{align*}
$$

Note that the previous expression involves different duality brackets, in $(C^s(M, \mathbb{R}^n)^*, C^s(M, \mathbb{R}^n))$ for variation with respect to $\delta q$, in $(V^*, V)$ for the variation with respect to $\delta v$ and in $(H^s(M)^*, H^s(M))$ for the variation with respect to $\delta \tilde{h}$ and $\delta \tilde{f}$. Formally, the optimality of solutions $(q_t, \tilde{f}_t, v_t, \tilde{h}_t)$ means that $\delta J$ should vanish under variations satisfying the control evolutions $\dot{q}_t = \xi_q v_t$ and $\dot{\tilde{f}}_t = \tilde{h}_t$.

Let $H^1_{(q_0, \tilde{h}_0)}(\mathbb{R}^1, C^s(M, \mathbb{R}^n) \times H^s(M))$ be the space of time-dependent states with $H^1$ regularity in time and initial conditions $(q_0, \tilde{f}_0)$. We define the constraint application

$$
\mathcal{Y} : H^1_{(q_0, \tilde{h}_0)}(\mathbb{R}^1, C^s(M, \mathbb{R}^n) \times H^s(M)) \times L^2([0, 1], V \times H^s(M))
$$

by $\mathcal{Y}(q, \tilde{f}, v, \tilde{h}) = (q - \xi_q v, \tilde{f} - \tilde{h})$. It is clearly differentiable with respect to $\tilde{f}, v$ and $\tilde{h}$. Now, since it is assumed that $V \hookrightarrow \Gamma^{s+1}$, the application $q \mapsto \xi_q v = v \circ q$ is differentiable with respect to $q \in C^s(M, \mathbb{R}^n)$ and equal to $(\partial_q \xi_q v | \delta q) = d_q v(\delta q)$. It results that $\mathcal{Y}$ is differentiable with respect to $q$ as well.

With these notations, we are considering minimizers of $J$ in the constraint set $\mathcal{Y}^{-1}_1(\{0\})$. In order to invoke Lagrange multipliers theorem in this infinite-dimensional setting (Theorem 4.1 in [31]), it needs to be checked that $d_{(q, f, v, \tilde{h})} \mathcal{Y}$ is surjective for all $(q, \tilde{f}, v, \tilde{h})$. Writing $\mathcal{Y}_1(q, v) = \tilde{q} = \xi_q v$ and $\mathcal{Y}_2(\tilde{f}, \tilde{h}) = \tilde{f} - \tilde{h}$, we have from Lemma 3 of [5] that $d_{(q, v)} \mathcal{Y}_1$ is surjective and it is straightforward to verify that so is $d_{(f, \tilde{h})} \mathcal{Y}_2$.

We deduce the existence of Lagrange multipliers $p \in L^2([0, 1], C^s(M, \mathbb{R}^n))^*$ and $p\tilde{f} \in L^2([0, 1], H^s(M))^*$ such that:

$$
0 = \left( d_{(q, f, v, \tilde{h})} J + (d_{(q, f, v, \tilde{h})} \mathcal{Y})^*(p, p\tilde{f}) \left| (\delta q, \delta \tilde{f}, \delta v, \delta \tilde{h}) \right. \right)
$$

$$
= (p | \delta q) - (p | \partial_q \xi_q v \delta q) - (p | \xi_q v \delta v) + (p | \delta \tilde{f}) - (p | \delta \tilde{h})
$$

$$
+ \int_0^1 \left[ \left( \partial_q L(q_t, v_t, \tilde{h}_t) \right| \delta q_t + \left( \partial_v L(q_t, v_t, \tilde{h}_t) \right| \delta v_t + \left( \partial_{\tilde{h}} L(q_t, v_t, \tilde{h}_t) \right| \delta \tilde{h}_t \right] \, dt
$$

$$
+ \left( \partial_q g(q_1, \tilde{f}_1) \right| \delta q_1 + \left( \partial_{\tilde{f}} g(q_1, \tilde{f}_1) \right| \delta \tilde{f}_1
$$

\[ (44) \]
Moreover, as $H^s(M)$ is reflexive, it satisfies the Radon–Nikodym property and we have $L^2([0, 1], H^s(M))^* = L^2([0, 1], H^s(M)^*)$ which allows to identify $p^f$ as a square-integrable function in $H^s(M)^*$. The case of the geometric momentum $p$ is, however, slightly more involved but was addressed separately in Lemma 4 of [5], leading to an equivalent identification $p \in L^2([0, 1], C^s(M, \mathbb{R}^n)^*)$. It is then straightforward from the expression of the Hamiltonian in (20) that $\dot{q}_t = \xi_{q_t} v_t = \partial_p H(q_t, \tilde{f}_t, p_t, p^f_t, v_t, \tilde{h}_t)$ and $\tilde{f} = \tilde{h}_t = \partial_{p^f} H(q_t, \tilde{f}_t, p_t, p^f_t, v_t, \tilde{h}_t)$.

Considering the variation on $\delta q$ only (i.e., with $\delta v = 0, \delta \tilde{f} = 0$ and $\delta \tilde{h} = 0$) in (44), we obtain for all $\delta q \in C^s(M, \mathbb{R}^n)$:

$$
(p | \delta q) = (p | \partial_q \xi_{q} v, \delta q) - \int_0^1 (\partial_q L(q_t, v_t, \tilde{h}_t)|\delta q_t) dt - (\partial_q g(q_1, \tilde{f}_1)|\delta q_1)
$$

$$
= \int_0^1 (p_t | (\partial_q \xi_{q_t} v_t)(\delta q_t)) dt - \int_0^1 (\partial_q L(q_t, v_t, \tilde{h}_t)|\delta q_t) dt - (\partial_q g(q_1, \tilde{f}_1)|\delta q_1)
$$

$$
= \int_0^1 ((\partial_q \xi_{q_t} v_t)^* p_t - \partial_q L(q_t, v_t, \tilde{h}_t)|\delta q_t) dt - (\partial_q g(q_1, \tilde{f}_1)|\delta q_1)
$$

(45)

Let’s denote $r_t = \delta q_t$ so that $\delta q_t = \int_0^t r_s ds$ and:

$$
\int_0^1 (\partial_q \xi_{q} v, r_t)|\delta q_t) dt = \int_0^1 \int_0^t (\partial_q \xi_{q} v, r_s)|\delta q_t) dt
$$

$$
= \int_0^1 \left( \int_s^t (\partial_q \xi_{q} v, r_t)|\delta q_t) dt \right) ds
$$

This together with (45) shows that $p_t = \int_0^t \alpha_s ds - \partial_q g(q_1, \tilde{f}_1)$ for almost all $t \in [0, 1]$. Now since $\alpha \in L^2([0, 1], C^s(M, \mathbb{R}^n)^*) \subset L^1([0, 1], C^s(M, \mathbb{R}^n)^*)$, it results that $p \in H^1([0, 1], C^s(M, \mathbb{R}^n)^*)$ and:

$$
\dot{p}_t = -\partial_q L(q_t, v_t, \tilde{h}_t) - (\partial_q \xi_{q_t} v_t)^* p_t = -\partial_q H(q_t, \tilde{f}_t, p_t, p^f_t, v_t, \tilde{h}_t)
$$

with the endpoint condition $p_1 = -\partial_q g(q_1, \tilde{f}_1)$.

Similarly, the variation with respect to $\delta \tilde{f}$ in (44) leads to:

$$
(p^f | \delta \tilde{f}) + \partial_f g(q_1, \tilde{f}_1)|\delta \tilde{f}_1) = 0
$$

If we write $\rho_t = \delta \tilde{f}_t$, we obtain:

$$
\int_0^1 (p^f + \partial_f g(q_1, \tilde{f}_1)|\rho_t) dt = 0
$$
which thus holds for all $\rho \in L^2([0, 1], H^s(M))$. It results that for almost all $t \in [0, 1]$, $p_t^f = -\partial f g(q_t, \tilde{f}_t)$ or in other words $p_t^f \in H^1([0, 1], H^s(M)^*)$ and:

$$\dot{p}_t^f = 0 = -\partial \tilde{f} H(q_t, \tilde{f}_t, p_t^f, v_t, \tilde{h}_t)$$

Finally, the variations with respect to $v$ and $\tilde{h}$ give:

$$\int_0^1 \left( \xi_{q_t}^* p_t - (\partial_v L(q_t, v_t, \tilde{h}_t)) \delta v_t \right) dt = 0$$

for all $\delta v \in L^2([0, 1], V)$, $\delta \tilde{h} \in L^2([0, 1], H^s(M))$. Therefore

$$\dot{\xi}_{q_t}^* p_t - (\partial_v L(q_t, v_t, \tilde{h}_t)) = \partial_{v} H(q_t, \tilde{f}_t, p_t^f, v_t, \tilde{h}_t) = 0$$

$$p_t^f = \partial_{\tilde{h}} L(q_t, v_t, \tilde{h}_t) = \partial_{\tilde{h}} H(q_t, \tilde{f}_t, p_t^f, v_t, \tilde{h}_t) = 0$$

and the proof of Theorem 6 is complete.

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