



Diffeomorphic Matching and Dynamic Deformable Surfaces with Applications in 3D Medical Imaging

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# **Diffeomorphic Matching and Dynamic Deformable Surfaces**

- Diffeomorphic matching in biomedical image processing
- Reproducing Kernel Hilbert Spaces (RKHS)
- Geometric surface matching distances
- Variational formulation of optimal diffeomorphic matching
- Discretization: Dirac measures and diffeomorphic point matching
- Numerical results: Matching snapshots of the mitral valve





# **Diffeomorphic Matching in Biomedical Image Processing**





# **Optimal Diffeomorphic Matching of 3D Curves and Surfaces**

Cardiovascular diseases often affect the mitral valve. Biomedical image processing provides the cardiologist with information about the degree of malfunctioning.







# **Optimal Matching of Biomedical 3D Movies**

<u>Biomedical Data:</u> Given a 3D movie of a deformable anatomical shape  $S(t) \subset \mathbb{R}^3$ ,  $t \in I := [0, T]$ , biomedical techniques enable the extraction of snapshots  $S_j := S(t_j)$  at specific time frames  $t_j$ ,  $0 \le j \le q$ .

Mathematical Task: Find a family  $F(\cdot,t)\in Diff(\mathbb{R}^3)$  ,  $t\in I,$  of time dependent  $\mathbb{R}^3\text{-diffeomorphisms}$ 

$$\mathbf{F}(\mathbf{S}_0; \mathbf{t}_0) \; = \; \mathbf{S}_0 \quad , \quad \mathbf{F}(\mathbf{S}_0; \mathbf{t}_j) \; = \; \mathbf{\hat{S}}_j \; , \; \mathbf{1} \leq j \leq q \; ,$$

which map the initial shape  $S_0$  onto shapes  $\hat{S}_j$  at the time frames  $t_j$  such that for all  $1 \leq j \leq q$  the shapes  $\hat{S}_j$  are as close to  $S_j$  as possible.





# Matching of Dynamic Deformable Surfaces: Previous Work

- Matching of two snapshots  $S_0$  and  $S_1$ ,
- Concepts based on diffeomorphic matching developed by Dupuis, Glaunès, Grenander, Miller, Mumford, Trouvè, Younes et al.,
- $F(\boldsymbol{\cdot},t)=F^{v_t}$  ,  $t\in I,$  generated by time dependent flow  $v_t$

 $\begin{array}{lll} \boldsymbol{\partial}_{\mathbf{t}} \mathbf{F}(\boldsymbol{\cdot},\mathbf{t}) \;=\; \mathbf{v}_{\mathbf{t}}(\mathbf{F}(\boldsymbol{\cdot},\mathbf{t})) \;,\; \; \mathbf{t} \in \mathbf{I} \;, \\ \mathbf{F}(\boldsymbol{\cdot},\mathbf{0}) \;=\; \mathbf{Id} \;, \end{array}$ 

- Rigid constraint  $F(S_0, t_1) = S_1$  replaced by soft constraint using suitably chosen geometric surface matching distances,
- Solution of the resulting optimization problem within a variational framework.





# Literature on Diffeomorphic Matching

U. Grenander and M.I. Miller; Computational anatomy: an emerging discipline. Quart. Appl. Math. 56, 617-694, 1998

M.I. Miller and L. Younes; Group action, diffeomorphism and matching: A general framework. Int. J. Comp. Vis. 41, 61-84, 2001

M.F. Beg, M.I. Miller, A, Trouvé, and L. Younes; Computing large deformations metric mappings via geodesic flows of diffeomorphisms. Int. J. Comp. Vision 61, 139-157, 2005

H. Guo, A. Rangarajan, and S. Joshi; Diffeomorphic point matching. In: Handbook of Mathematical Models in Computer Vision, Springer, Berlin-Heidelberg-New York, pp. 205-219, 2006

J. Glaunès, A. Qiu, M.I. Miller, and L. Younes; Large deformation diffeomorphic metric curve mapping. Int. J. Comp. Vision 80, 317-336, 2008





### Generalization to Arbitrarily Many Intermediary Snapshots

Given q+1 snapshots  $S_j, 0 \le j \le q$ , at time instants  $t_j \in [0,1], 0 =: t_0 < t_1 < \cdots < t_q := 1$ , find a time dependent family of diffeomorphisms  $F(\cdot, t) \in Diff(\mathbb{R}^3), t \in [0,1]$ , such that

$$\sum_{j=1}^{q} dist(\mathbf{F}(\mathbf{S}_{0},\mathbf{t}_{j}),\mathbf{S}_{j}) \ \rightarrow min \ ,$$

where  $dist(\cdot, \cdot)$  is a geometric surface matching distance, and  $F(\cdot, t) = F^{v_t}, t \in [0, 1]$ , is generated by a time dependent flow  $v_t$  according to

 $\begin{array}{lll} \boldsymbol{\partial}_{\mathbf{t}} \mathbf{F}(\boldsymbol{\cdot},\mathbf{t}) \;=\; \mathbf{v}_{\mathbf{t}}(\mathbf{F}(\boldsymbol{\cdot},\mathbf{t})) \;,\; \; \mathbf{t} \in \mathbf{I} \;, \\ \mathbf{F}(\boldsymbol{\cdot},\mathbf{0}) \;=\; \mathbf{Id} \;. \end{array}$ 





# **Reproducing Kernel Hilbert Spaces**





# **Reproducing Kernel Hilbert Spaces I**

Let H be a Hilbert space of functions on  $\mathbb{R}^d$  with inner product  $(\cdot, \cdot)_H$  and norm  $\|\cdot\|_H$ . A function  $K : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{C}$  is said to be a reproducing kernel of H, if the following two conditions hold true:

 $(RK)_1 \ \ \text{For every} \ x \in \mathbb{R}^d,$  we have  $K_x \in H,$  where  $K_x : \mathbb{R}^d \to \mathbb{C}$  is given by

 $\mathbf{K}_{\mathbf{x}}(\mathbf{y}) = \mathbf{K}(\mathbf{y}, \mathbf{x}) \quad , \quad \mathbf{y} \in \mathbb{R}^{\mathbf{d}} \; .$ 

 $(\mathbf{R}\mathbf{K})_{\mathbf{2}}~~\mathbf{For}~\mathbf{every}~\mathbf{x}\in\mathbb{R}^{d}$  and every  $\mathbf{f}\in\mathbf{H}$  there holds

 $\mathbf{f}(\mathbf{x}) \;=\; (\mathbf{f}, \mathbf{K}_{\mathbf{x}})_{\mathbf{H}} \quad,\quad \mathbf{x} \in \mathbb{R}^d \ .$ 

The kernel K is called Hermitian (positive definite), if for any finite set of points  $\{y_1, \cdots, y_n\} \subset \mathbb{R}^d$  and any  $\gamma_i \in \mathbb{C}, 1 \leq i \leq n$ , there holds  $\sum_{i,j=1}^n \bar{\gamma}_j \gamma_i \ K(y_j, y_i) \in \mathbb{R} \ (\in \mathbb{R}_+) \ .$ 

The Hilbert space H is said to be a Reproducing Kernel Hilbert space (RKHS), if there exists a reproducing kernel on H.





# **Reproducing Kernel Hilbert Spaces II**

Proposition 2 [Aronszajn] For any positive definite kernel  $K : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{C}$  there exists a uniquely determined RKHS H of functions on  $\mathbb{R}^d$  with reproducing kernel K. Any RKHS H with a positive definite kernel K is a Hilbert space of functions on  $\mathbb{R}^d$ for which pointwise evaluations are continuous linear functionals.

A kernel K is said to be translation invariant, if for all  $a \in \mathbb{R}^d$ 

 $\mathbf{K}(\mathbf{x}-\mathbf{a},\mathbf{y}-\mathbf{a}) \ = \ \mathbf{K}(\mathbf{x},\mathbf{y}) \quad, \quad \mathbf{x},\mathbf{y}\in \mathbb{R}^d \ .$ 

Proposition 3 [Bochner] A kernel  $K : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{C}$  is a continuous positive definite translation invariant kernel, iff there exists a finite positive Borel measure  $\mu$  on  $\mathbb{R}^d$  such that

$$\mathbf{K}(\mathbf{x},\mathbf{y}) \;=\; \int\limits_{\mathbb{R}^d} \mathbf{exp}(\mathbf{i}(\mathbf{x}-\mathbf{y}){\boldsymbol{\cdot}}\mathbf{z}) \; \, \mathbf{d} oldsymbol{\mu}(\mathbf{z}) \quad, \quad \mathbf{x},\mathbf{y} \in \mathbb{R}^d \;.$$





#### **Reproducing Kernel Hilbert Spaces III**

A function  $\mathbf{K} : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{C}$  is called radial, if there exists a function  $\mathbf{r}$  on  $\mathbb{R}_+$  such that  $\mathbf{K}(\mathbf{x}, \mathbf{y}) = \mathbf{r}(|\mathbf{x} - \mathbf{y}|)$ ,  $\mathbf{x}, \mathbf{y} \in \mathbb{R}^d$ .

Proposition 4 [Schönberg] A radial function K with a continuous function r is a continuous positive definite translation invariant kernel, iff there exists a positive Borel measure  $\mu$  on  $\mathbb{R}_+$  such that

$$\mathbf{r}(\mathbf{t}) \;=\; \int\limits_{\mathbb{R}_+} \mathbf{exp}(-\mathbf{st}^2) \; \mathbf{d} oldsymbol{\mu}(\mathbf{s}) \quad, \quad \mathbf{t} \in \mathbb{R}_+ \;.$$

Proposition 5 [Schönberg] Let H be an RKHS of vector valued functions on  $\mathbb{R}^d$ with Gaussian kernel K, i.e.,  $\mathbf{r}(\mathbf{t}) = (2\pi)^{-d/2} \exp(-\mathbf{t}^2/(2\sigma^2))$ . If  $\mathbf{f} \in \mathbf{H}$  with Jacobian  $\mathbf{D}\mathbf{f} \in \mathbb{R}^{d \times d}$ , then there holds

$$\|\mathrm{D} \mathbf{f}\|_\mathrm{F} \ \le \ rac{\mathrm{d}}{\sigma} \ \|\mathbf{f}\|_\mathrm{H} \ .$$





# **Geometric Surface Matching Distances**





#### Geometric Matching Distances: Hausdorff Distance

The Hausdorff distance between two bounded subsets  $\mathbf{S},\mathbf{S}'\in\mathbb{R}^3$  is given by

$$\mathbf{D}_{\mathbf{H}}(\mathbf{S},\mathbf{S}') \; := \; \mathbf{max}\Big(\mathbf{h}(\mathbf{S},\mathbf{S}'),\mathbf{h}(\mathbf{S}',\mathbf{S})\Big)$$

where the Hausdorff disparity  $\mathbf{h}(\mathbf{S},\mathbf{S}')$  is defined by means of

$$\mathbf{h}(\mathbf{S},\mathbf{S}') := \max_{\mathbf{X} \in \mathbf{S}} \left( \min_{\mathbf{X}' \in \mathbf{S}'} |\mathbf{x} - \mathbf{x}'| 
ight).$$

**Remark:** The Hausdorff distance is not smooth. Instead, we use

$$\widetilde{\mathbf{D}}_{\mathbf{H}}(\mathbf{S},\mathbf{S}') \ := \ \mathbf{h}_{\mathbf{sm}}(\mathbf{S},\mathbf{S}') + \mathbf{h}_{\mathbf{sm}}(\mathbf{S}',\mathbf{S}) \ ,$$

where  $h_{sm}(S, S')$  refers to a smoothed Hausdorff disparity.





#### Geometric Matching Distances: Borel Measure Distance

- We denote by  $BM(\mathbb{R}^3)$  the linear space of bounded Borel measures on  $\mathbb{R}^3$  equipped with the inner product

$$\langle oldsymbol{\mu},oldsymbol{\mu}' 
angle_{oldsymbol{\Gamma}} \; := \; \int\limits_{\mathbb{R}^3} \int\limits_{\mathbb{R}^3} \Gamma(\mathbf{x},\mathbf{x}') \; \mathbf{d}oldsymbol{\mu}(\mathbf{x}) \; \mathbf{d}oldsymbol{\mu}'(\mathbf{x}') \; ,$$

where  $\Gamma(\cdot, \cdot)$  is a smooth, symmetric, and translation-invariant bounded positive definite kernel on  $\mathbb{R}^3 \times \mathbb{R}^3$ .

- We identify a bounded Borel subset  $S \subset \mathbb{R}^3$  with a measure  $\mu_S \in BM(\mathbb{R}^3)$ induced on S by the Lebesgue measure of  $\mathbb{R}^3$ .
- The distance between bounded Borel subsets  $\mathbf{S},\mathbf{S}'\in\mathbb{R}^3$  is defined by means of

$$\mathrm{D}_{\Gamma}^2(\mathrm{S},\mathrm{S}') \;:=\; \| \mu_{\mathrm{S}} - \mu_{\mathrm{S}'} \|_{\Gamma}^2 \;.$$





# Variational Formulation of the Optimal Matching Problem





## Variational Formulation of the Optimal Matching Problem

Let  $\mathcal{D}(\mathbf{I}; \mathbf{V})$  be the space of all disparity functionals  $\mathbf{D} : \mathbf{L}^2(\mathbf{I}; \mathbf{V}) \to \mathbb{R}_+$  of the form  $\mathbf{D}(\mathbf{v}) = \Phi(\mathbf{F}^{\mathbf{v}}(\cdot, \mathbf{t}_1), \cdots, \mathbf{F}^{\mathbf{v}}(\cdot, \mathbf{t}_q))$ ,

where  $\Phi : Diff(\mathbb{R}^3)^q \to \mathbb{R}_+$  is a continuous function, and let  $E : L^2(I; V) \to \mathbb{R}_+$  be the energy functional

$${f E}({f v}) \;=\; {1\over 2} \int\limits_0^{\hat{}} \|{f v}_t\|_V^2 \;dt \;.$$

Optimization Problem: For  $D \in \mathcal{D}(I; V)$ , find  $v^* \in L^2(I; V)$  such that

$$\begin{array}{rcl} (OP)_1 & J(v^*) \ = \ \inf_{v \ \in \ L^2(I; \ V)} J(v) &, \quad J(v) \ := \ E(v) + \lambda D(v) \ , \\ subject \ to \\ & (OP)_2 & \partial_t F(\cdot, t) \ = \ v_t(F(\cdot, t)) &, \quad t \in I \ , \\ & F(\cdot, 0) \ = \ Id \ . \end{array}$$





## Existence of a Minimizing Diffeomorphic Flow

Theorem 1. Assume that the embedding  $V \subset W^{s,2}(\mathbb{R}^3)$ , s > 5/2, is continuous. Then, the optimal diffeomorphic matching problem  $(OP)_1, (OP)_2$  has a solution  $v^* \in L^2(I; V)$ . Proof. Let  $\{v^n\}_{\mathbb{N}}$  be a minimizing sequence. Due to the boundedness of  $\{v^n\}_{\mathbb{N}}$ , there exist  $\mathbb{N}' \subset \mathbb{N}$  and  $v^* \in L^2(I; V)$  such that

 $\lim_{n\,\to\,\infty} \inf_{\infty}\, \|v^n\|_{L^2(I;V)} \ \le \ \|v^*\|_{L^2(I;V)} \ .$ 

Denoting by  $F^n(\cdot, t), F^*(\cdot, t) \in Diff(\mathbb{R}^3), t \in I$ , the unique flows solving  $(OP)_2$  w.r.t.  $v^n, v^*$ , the main part of the proof is to show that

 $\mathbf{F}^{\mathbf{n}}(\mathbf{\cdot},\mathbf{t}) \to \mathbf{F}^{*}(\mathbf{\cdot},\mathbf{t}) \quad (\mathbf{n} \to \infty) \ , \ \mathbf{t} \in \mathbf{I} \ ,$ 

uniformly on bounded subsets of  $\mathbb{R}^3$ . This implies  $\mathbf{D}(\mathbf{v}^n) \to \mathbf{D}(\mathbf{v}^*) \ (\mathbf{n} \to \infty)$ , and hence,  $\lim_{n \to \infty} \inf_{\mathbf{x}} \mathbf{J}(\mathbf{v}^n) \leq \lim_{n \to \infty} \mathbf{D}(\mathbf{v}^n) + \lim_{n \to \infty} \inf_{\mathbf{x}} \mathbf{E}(\mathbf{v}^n) \leq \mathbf{D}(\mathbf{v}^*) + \mathbf{E}(\mathbf{v}^*) = \mathbf{J}(\mathbf{v}^*) ,$ 

which allows to conclude.





# **Necessary Optimality Conditions**

Theorem 2. In addition to the assumptions of Theorem 1 suppose that the functional  $\Phi : C(\mathbb{R}^3)^q \to \mathbb{R}$  has Gâteaux derivatives  $\partial_j \Phi \in M(\mathbb{R}^3), 1 \leq j \leq q$ . If  $\mathbf{v}^* \in L^2(\mathbf{I}; \mathbf{V})$  is a solution of  $(OP)_1, (OP)_2$ , then there exists a family  $\mathbf{p}^* = \mathbf{p}_t^*, t \in \mathbf{I}$ , of vector valued Borel measures on  $\mathbf{I} \times \mathbb{R}^3$  satisfying the jump process

 $(OP)_4 p_t^* + \rho_{t,v^*} = 0 , t \in I ,$ 

Here,  $b_{v,t}$  is a Borel function of  $D_v v_t(F^v(\cdot,t))$ , and  $\rho_{t,v}$  is a vector valued Borel measure with density  $Kv_t$ .





Discretization: Dirac Measures and Diffeomorphic Point Matching





#### **Discretization: Dirac Measures and Diffeomorphic Point Matching**

• We discretize the snapshots  $S_j, 0 \leq j \leq q,$  and the dynamically deformed surfaces  $\hat{S}_j = F^v(S_0,t_j)$  by point sets

$$X_j \ = \ \{x_1^j, \cdots, x_{N_j}^j\} \quad, \quad \hat{X}_j \ = \ F^v(X_0, t_j) \ = \ \{F^v(x_1^0, t_1), \cdots, F^v(x_{N_0}^0, t_j)\}$$

• We denote by  $x_n(t)=F^v(x_n^0,t_j)$ ,  $x_n(0)=x_n^0, 1\leq n\leq N_0$ , the trajectories emanating from  $x_n^0$ , i.e., the solutions of the initial value problems

$$\frac{d}{dt} \, \, \mathbf{x}_n(t) \; = \; \mathbf{v}_t(\mathbf{x}_n(t)) \ , \ t \in [0,1] \quad , \quad \mathbf{x}_n(0) \; = \; \mathbf{x}_n^0 \ .$$

- We approximate the Borel measures associated with  $S_j$  and  $\hat{S}_j$  by weighted sums of Dirac measures

$$\mu_{S_j} \ = \ \sum_{m=1}^{N_j} b_m^j \ \delta_{x_m^j} \quad , \quad \mu_{\hat{S}_j} \ = \ \sum_{n=1}^{N_0} a_n \ \delta_{x_n(t_j)} \quad , \quad 1 \leq j \leq q \ .$$





#### **Discretization: Dirac Measures and Diffeomorphic Point Matching**

• Setting  $\mathbf{x}(t) = (\mathbf{x}_1(t), \cdots, \mathbf{x}_{N_0}(t))^T, t \in (0, 1)$ , the disparity cost functional reads  $\mathbf{D}(\mathbf{v}) = \sum_{j=1}^q \lambda_j \mathbf{D}_j(\mathbf{x}(t_j)) \quad , \quad \mathbf{D}_j(\mathbf{x}(t_j)) := \|\boldsymbol{\mu}_{S_j} - \boldsymbol{\mu}_{\hat{S}_j}\|_{K_{\sigma_j}}^2,$ 

where  $K_{\sigma_j}, 1 \leq j \leq q$ , are appropriately chosen radial Gaussian kernels.

 $\bullet \ \ \text{We approximate the flow } v_t \ \text{by a linear combination of } K_{x_n(t)}, 1 \leq n \leq N_0,$ 

$$\mathbf{v}_t(\mathbf{x}) \;=\; \sum_{n=1}^{N_0} \mathbf{K}_{\sigma_0}(\mathbf{x}_n(t),\mathbf{x}) \; \alpha_n(t) \quad, \quad \mathbf{x} \in \mathbb{R}^3 \;.$$

It follows that

$$\|\mathbf{v}_t\|_V^2 \ = \ \sum_{n=1}^{N_0} \sum_{n'=1}^{N_0} K_{\sigma_0}(\mathbf{x}_n(t), \mathbf{x}_{n'}(t)) \ \alpha_n^T(t) \alpha_n(t) \quad , \quad t \in [0, 1] \ .$$





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#### The Discrete Optimization Problem

$$\begin{array}{ll} \textbf{Setting } \boldsymbol{\alpha}(t) = (\boldsymbol{\alpha}_1(t), \cdots, \boldsymbol{\alpha}_{N_0}(t))^T \in \mathbb{R}^{dN_0}, t \in (0,1), \ \textbf{and} \\ \\ \textbf{A}(\textbf{x}(t)) \ \coloneqq \ \left(\textbf{K}_{\sigma_0}(\textbf{x}_n(t), \textbf{x}_{n'}(t)) \textbf{I}_d\right)_{n,n'=1}^{N_0} \in \mathbb{R}^{dN_0 \times dN_0} \end{array}$$

the discrete optimization problem reads:

Discrete Optimization Problem: Find  $\alpha^* \in L^2(I; \mathbb{R}^{dN_0})$  and  $x^*(t)$  such that





#### **Existence of a Solution and Necessary Optimality Conditions**

Theorem 3. The discrete optimization problem  $(DOP)_1, (DOP)_2$  has a solution  $\alpha^* = \alpha^*(t), t \in I$ . If  $x^* = x^*(t), t \in I$ , is the associated trajectory, there exists a function  $p^* = p^*(t), t \in I$ , which solves the final time problem

$$\begin{split} (DOP)_3 & -\frac{d}{dt} \; p^*(t) \; = \; B(\mathbf{x}^*(t), \boldsymbol{\alpha}^*(t))^T \; \left( p^*(t) + \frac{1}{2} \; \boldsymbol{\alpha}^*(t) \right) \; , \; t \in (t_{j-1}, t_j) \; , \\ p^*(t_q^+) = 0 \; , \; p^*(t_j^-) = p^*(t_j^+) + \lambda_j \; \boldsymbol{\nabla} D_j(\mathbf{x}^*(t_j)) \; , \; 1 \leq j \leq q \; , \end{split}$$

 $(DOP)_4 \qquad A(x^*(t))(\alpha^*(t) + p^*(t)) = 0 , t \in I ,$ 

where the matrix  $B(\mathbf{x}^*(\mathbf{t}), \boldsymbol{\alpha}^*(\mathbf{t})) \in \mathbb{R}^{dN_0 \times dN_0}$  is given by

 $\mathbf{B}(\mathbf{x}^*(\mathbf{t}), \boldsymbol{lpha}^*(\mathbf{t})) = \boldsymbol{\nabla}_{\mathbf{x}}(\mathbf{A}(\mathbf{x}^*(\mathbf{t}), \boldsymbol{lpha}^*(\mathbf{t})))$ .





# **Fully Discrete Optimization Problem**





**Fully Discrete Optimal Diffeomorphic Matching Problem I** For the discretization in time of the optimality system  $(DOP)_2 - (DOP)_4$  we introduce  $\Delta_{I} := \left\{ \begin{array}{c} \left| \Delta_{I_{i}} \right|, \ \Delta_{I_{i}} \end{array} \right\} := \left\{ t_{j-1} =: t^{L_{j-1}} < t^{L_{j-1}+1} < \cdots < t^{L_{j}} := t_{j} \right\},$ where  $\Delta_{I_j}, 1 \leq j \leq q$ , are subpartitions of  $I_j := [t_{j-1}, t_j]$ . Setting  $\Delta t^{\ell} := t^{\ell+1} - t^{\ell}, 0 =: L_0 \leq \ell \leq L := L_q$ , the discretized optimality system reads  $\frac{\mathbf{x}^{\boldsymbol{\ell}+1}-\mathbf{x}^{\boldsymbol{\ell}}}{\boldsymbol{\boldsymbol{\lambda}}+\boldsymbol{\boldsymbol{\ell}}} \;=\; \mathbf{A}(\mathbf{x}^{\boldsymbol{\ell}}\boldsymbol{\alpha}^{\boldsymbol{\ell}}\;,\; \mathbf{L}_0 \leq \boldsymbol{\ell} \leq \mathbf{L}\;,$  $(\mathbf{DOC})_1$  $\mathbf{x}^{\mathbf{0}} = \mathbf{x}^{(\mathbf{0})}$  ,  $\frac{p^{(\ell-1)^+} - p^{\ell^-}}{\Delta + \ell - 1} = B(x^{\ell}, \alpha^{\ell})^T (p^{\ell^-} + \alpha^{\ell}/2) , \ \ell = L_j, \cdots, L_{j-1} + 1 ,$  $(\mathbf{DOC})_2$  $\mathbf{p}^{\mathbf{L}_{\mathbf{q}}^{+}} = \mathbf{0} \;,\; \mathbf{p}^{\mathbf{L}_{\mathbf{j}}^{-}} = \mathbf{p}^{\mathbf{L}_{\mathbf{j}}^{+}} + \lambda_{\mathbf{i}} \mathbf{
abla} \mathbf{D}_{\mathbf{i}}(\mathbf{x}^{\mathbf{L}_{\mathbf{j}}}) \;,\; 1 \leq \mathbf{j} \leq \mathbf{q} \;,$  $\mathbf{A}(\mathbf{x}^{\boldsymbol{\ell}})(\boldsymbol{\alpha}^{\boldsymbol{\ell}} + \mathbf{p}^{\boldsymbol{\ell}^+}) , \ \mathbf{L}_0 \leq \boldsymbol{\ell} \leq \mathbf{L} - 1 .$  $(\mathbf{DOC})_3$ 





**Fully Discrete Optimal Diffeomorphic Matching Problem II** Theorem 4. Let  $J_{\Delta_{\tau}}$  be the discrete objective functional  $\mathbf{J}_{\boldsymbol{\Delta}_{\mathrm{I}}}(\boldsymbol{\alpha}) \; = \; \frac{1}{2} \; \sum_{\ell=1}^{\mathrm{L}-1} \boldsymbol{\Delta} \mathbf{t}^{\boldsymbol{\ell}} \; (\boldsymbol{\alpha}^{\boldsymbol{\ell}})^{\mathrm{T}} \mathbf{A}(\mathbf{x}^{\boldsymbol{\ell}}) \boldsymbol{\alpha}^{\boldsymbol{\ell}} \; + \; \sum_{\mathrm{i}=1}^{\mathrm{q}} \lambda_{\mathrm{j}} \mathbf{D}_{\mathrm{j}}(\mathbf{x}^{\mathrm{L}_{\mathrm{j}}}) \; .$ The discrete optimality system  $(DOC)_1 - (DOC)_3$  represents the first order necessary optimality conditions for the discrete optimization problem 
$$\begin{split} & \underset{\boldsymbol{\alpha}}{\min} \; J_{\boldsymbol{\Delta}_{I}}(\boldsymbol{\alpha}) \;, \\ \frac{x^{\boldsymbol{\ell}+1}-x^{\boldsymbol{\ell}}}{\Delta t^{\boldsymbol{\ell}}} \; = \; A(x^{\boldsymbol{\ell}}) \boldsymbol{\alpha}^{\boldsymbol{\ell}} \;\;, \quad L_{0} \leq \boldsymbol{\ell} \leq L-1 \;, \end{split}$$
subject to  $x^0 = x^{(0)}$ Corollary. Let  $(\mathbf{x}^*, \mathbf{p}^*, \boldsymbol{\alpha}^*)$  with  $\mathbf{x}^* = \{\mathbf{x}^{\boldsymbol{\ell}}_*\}_{\boldsymbol{\ell}=0}^{L}$  etc. satisfy  $(\text{DOC})_1 - (\text{DOC})_3$ . Then, we have  $\mathbf{0} = \nabla \mathbf{J}_{\Delta_{\mathbf{I}}}(\boldsymbol{\alpha}^*) = \{\mathbf{g}^{\boldsymbol{\ell}}\}_{\boldsymbol{\ell}=\mathbf{0}}^{\mathbf{L}-1} \quad , \quad \mathbf{g}^{\boldsymbol{\ell}} = \mathbf{A}(\mathbf{x}^{\boldsymbol{\ell}}_*)(\boldsymbol{\alpha}^{\boldsymbol{\ell}}_* + \mathbf{p}^{\boldsymbol{\ell}}_*) \; .$ 





### Matching Algorithm: Continuation in the Regularization Parameter

Role of the regularization parameters: For simplicity, we assume  $\lambda_j = \lambda > 0, 1 \le j \le q$ . The regularization parameter provides a balance between the matching quality and the regularizing kinetic energy. The larger  $\lambda$ , the more emphasis is on the matching quality.

**Problem:** The gradient method does not converge for large  $\lambda$ , in particular, if the initial iterate is not close to a local minimum.

Remedy: Continuation in the regularization parameter. This results in an inner/outer iteration with outer iterations in  $\lambda$  and inner iterations featuring the gradient method with Armijo line search. A termination criterion for the outer iterations is

$$D_j \ := \ \kappa \Big( \sum_{n=1}^{N_0} (d_n^j)^2 \Big)^{1/2} < \vartheta \quad , \quad d_n^j \ := \ \min_{1 \, \leq \, m \, \leq \, N_j} \ |x_n(t_j) - x_m(t_j)| \ ,$$

where  $\vartheta > 0$  is a given threshold and  $0 < \kappa \le 1$  (e.g.,  $\kappa = 0.9$ ).



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### Matching Algorithm: Inner/Outer Iterative Scheme

Step 1: Initialization

Choose thresholds  $\theta > 0, \vartheta > 0$ , as well as  $\gamma > 1$  for continuation and  $0 < \kappa \leq 1$ .

Step 2: Initialization of the outer iteration

Choose initial value  $\lambda_0$  and set  $\nu := 0$ .

Step 3: Initialization of the inner iteration

Compute  $\alpha_{\nu}^{(0)}$  by an appropriate initialization and set  $\mu := 0$ .

Step 4: Gradient method with Armijo line search

Step 4.1: Set  $\mu := \mu + 1$  and compute  $\alpha_{\nu}^{(\mu)}$  by gradient descent with Armijo line search. Step 4.2: If the termination criterion  $|\nabla J(\alpha_{\nu}^{(\mu)})| < \theta |\nabla J(\alpha_{\nu}^{(0)})|$  is satisfied, go to Step 5. Otherwise, go to Step 4.1.

Step 5: Termination of the outer iteration

If the termination criterion  $D_j < \vartheta$ ,  $1 \le j \le q$ , is satisfied, stop the algorithm. Otherwise, set  $\nu := \nu + 1$ ,  $\alpha_{\nu}^{(0)} := \alpha_{\nu-1}^{(\mu)}$ ,  $\lambda_{\nu} := \gamma \lambda_{\nu-1}$ , and go to Step 4.





Numerical Results: Matching Mitral Annulus Snapshots





#### Diffeomorphic Matching of Multiple Annulus Snapshots



#### Matching Multiple Snapshots of the Mitral Annulus at t = 1,3,5,7,10





# Diffeomorphic Matching of Multiple Annulus Snapshots: Hausdorff Matching



Convergence history: Accuracy indicators (l.) and Hausdorff disparities (r.)





#### Diffeomorphic Matching of Multiple Annulus Snapshots: Hausdorff Matching



Pareto frontiers: Accuracy indicators (l.) and Hausdorff disparities (r.)





### Diffeomorphic Matching of Multiple Annulus Snapshots: Measure Matching



Convergence history: Accuracy indicators (l.) and measure matching disp. (r.)





#### Diffeomorphic Matching of Multiple Annulus Snapshots: Measure Matching



Pareto frontiers: Accuracy indicators (l.) and measure matching disp. (r.)





Numerical Results: Matching Anterior Leaflet Snapshots





# Diffeomorphic Matching of Multiple Anterior Leaflet Snapshots



Matching four snapshots of the anterior leaflet at instants 0,1,5,10





#### Diffeomorphic Matching of Multiple Anterior Leaflet Snapshots



Matching errors between computed deformations and snapshots





### **Diffeomorphic Matching of Multiple Anterior Leaflet Snapshots**



Matching the anterior leaflet boundary: Instants 0,1 (l.) and 1,5,10 (r.)





## **Diffeomorphic Matching of Multiple Anterior Leaflet Snapshots**



Pareto frontiers: separate Hausdorff disparities (l.), global Hausdorff disp. (r.)





### **Diffeomorphic Matching of Multiple Anterior Leaflet Snapshots**



Pareto frontiers: max. distances to snapshots (l.), 90 % of max. dist. (r.)





Numerical Results: Matching Posterior Leaflet Snapshots





# **Diffeomorphic Matching of Multiple Posterior Leaflet Snapshots**



Matching four snapshots of the posterior leaflet at instants 0,1,5,10





### Diffeomorphic Matching of Multiple Posterior Leaflet Snapshots



Matching errors between computed deformations and snapshots





### **Diffeomorphic Matching of Multiple Posterior Leaflet Snapshots**



Matching the posterior leaflet boundary: Instants 0,1 (l.) and 1,5,10 (r.)





**Diffeomorphic Matching of Multiple Posterior Leaflet Snapshots** 



Geometric accuracy (l.), Pareto frontiers (r.) for equally chosen weights





## **Diffeomorphic Matching of Multiple Posterior Leaflet Snapshots**



Geometric accuracy (l.), Pareto frontiers (r.) for dynamically adjusted weights