## Department of Mathematics, University of Houston Institut für Mathematik, Universität Augsburg

## 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

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Diffeomorphic Matching in Biomedical Image Processing

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## 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.


Valve anatomy of the human heart (left) and anatomy of the mitral valve (right)

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## Optimal Matching of Biomedical 3D Movies

Biomedical Data: Given a 3D movie of a deformable anatomical shape $S(t) \subset \mathbb{R}^{3}$, $\mathrm{t} \in \mathrm{I}:=[0, \mathrm{~T}]$, biomedical techniques enable the extraction of snapshots $\mathrm{S}_{\mathrm{j}}:=\mathrm{S}\left(\mathrm{t}_{\mathrm{j}}\right)$ at specific time frames $\mathrm{t}_{\mathrm{j}}, 0 \leq \mathrm{j} \leq \mathrm{q}$.

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

$$
\mathrm{F}\left(\mathrm{~S}_{0} ; \mathrm{t}_{0}\right)=\mathrm{S}_{0} \quad, \quad \mathrm{~F}\left(\mathrm{~S}_{0} ; \mathrm{t}_{\mathrm{j}}\right)=\hat{\mathrm{S}}_{\mathrm{j}}, 1 \leq \mathrm{j} \leq \mathrm{q},
$$

which map the initial shape $S_{0}$ onto shapes $\hat{S}_{j}$ at the time frames $t_{j}$ such that for all $1 \leq \mathrm{j} \leq \mathrm{q}$ the shapes $\hat{\mathrm{S}}_{\mathrm{j}}$ are as close to $\mathrm{S}_{\mathrm{j}}$ as possible.

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## Matching of Dynamic Deformable Surfaces: Previous Work

- Matching of two snapshots $\mathrm{S}_{0}$ and $\mathrm{S}_{1}$,
- Concepts based on diffeomorphic matching developed by Dupuis, Glaunès, Grenander, Miller, Mumford, Trouvè, Younes et al.,
- $F(\cdot, t)=F^{v_{t}}, t \in I$, generated by time dependent flow $v_{t}$

$$
\begin{aligned}
\partial_{\mathrm{t}} \mathrm{~F}(\cdot, \mathrm{t}) & =\mathrm{v}_{\mathrm{t}}(\mathrm{~F}(\cdot, \mathrm{t})), \mathrm{t} \in \mathrm{I}, \\
\mathrm{~F}(\cdot, 0) & =\mathrm{Id},
\end{aligned}
$$

- Rigid constraint $\mathrm{F}\left(\mathrm{S}_{0}, \mathrm{t}_{1}\right)=\mathrm{S}_{1}$ 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-HeidelbergNew 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

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 Institut für Mathematik, Universität AugsburgGeneralization to Arbitrarily Many Intermediary Snapshots
Given $\mathrm{q}+1$ snapshots $\mathrm{S}_{\mathrm{j}}, 0 \leq \mathrm{j} \leq \mathrm{q}$, at time instants $\mathrm{t}_{\mathrm{j}} \in[0,1], 0=: \mathrm{t}_{0}<\mathrm{t}_{1}<\cdots<\mathrm{t}_{\mathrm{q}}:=1$, find a time dependent family of diffeomorphisms $F(\cdot, t) \in \operatorname{Diff}\left(\mathbb{R}^{3}\right), t \in[0,1]$, such that

$$
\sum_{\mathrm{j}=1}^{\mathrm{q}} \operatorname{dist}\left(\mathrm{~F}\left(\mathrm{~S}_{0}, \mathrm{t}_{\mathrm{j}}\right), \mathrm{S}_{\mathrm{j}}\right) \rightarrow \min
$$

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

$$
\begin{aligned}
\partial_{\mathrm{t}} \mathrm{~F}(\cdot, \mathrm{t}) & =\mathrm{v}_{\mathrm{t}}(\mathrm{~F}(\cdot, \mathrm{t})), \mathrm{t} \in \mathrm{I}, \\
\mathrm{~F}(\cdot, 0) & =\mathrm{Id} .
\end{aligned}
$$

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Reproducing Kernel Hilbert Spaces

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## Reproducing Kernel Hilbert Spaces I

Let H be a Hilbert space of functions on $\mathbb{R}^{\mathrm{d}}$ with inner product $(\cdot, \cdot)_{\mathrm{H}}$ and norm $\|\cdot\|_{\mathrm{H}}$. A function $K: \mathbb{R}^{\mathrm{d}} \times \mathbb{R}^{\mathrm{d}} \rightarrow \mathbb{C}$ is said to be a reproducing kernel of $H$, if the following two conditions hold true:
$(\mathrm{RK})_{1}$ For every $\mathrm{x} \in \mathbb{R}^{\mathrm{d}}$, we have $\mathrm{K}_{\mathrm{x}} \in \mathrm{H}$, where $\mathrm{K}_{\mathrm{x}}: \mathbb{R}^{\mathrm{d}} \rightarrow \mathbb{C}$ is given by

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

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

$$
\mathrm{f}(\mathrm{x})=\left(\mathrm{f}, \mathrm{~K}_{\mathrm{x}}\right)_{\mathrm{H}} \quad, \quad \mathrm{x} \in \mathbb{R}^{\mathrm{d}} .
$$

The kernel K is called Hermitian (positive definite), if for any finite set of points $\left\{\mathrm{y}_{1}, \cdots, \mathrm{y}_{\mathrm{n}}\right\} \subset \mathbb{R}^{\mathrm{d}}$ and any $\gamma_{\mathrm{i}} \in \mathbb{C}, 1 \leq \mathrm{i} \leq \mathrm{n}$, there holds

$$
\sum_{\mathrm{i}, \mathrm{j}=1}^{\mathrm{n}} \bar{\gamma}_{\mathrm{j}} \gamma_{\mathrm{i}} \mathrm{~K}\left(\mathrm{y}_{\mathrm{j}}, \mathrm{y}_{\mathrm{i}}\right) \in \mathbb{R}\left(\in \mathbb{R}_{+}\right) .
$$

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

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## Reproducing Kernel Hilbert Spaces II

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

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

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

$$
\mathrm{K}(\mathrm{x}, \mathrm{y})=\int_{\mathbb{R}^{\mathrm{d}}} \exp (\mathrm{i}(\mathrm{x}-\mathrm{y}) \cdot \mathrm{z}) \mathrm{d} \mu(\mathrm{z}) \quad, \quad \mathrm{x}, \mathrm{y} \in \mathbb{R}^{\mathrm{d}}
$$

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## Reproducing Kernel Hilbert Spaces III

A function $K: \mathbb{R}^{\mathrm{d}} \times \mathbb{R}^{\mathrm{d}} \rightarrow \mathbb{C}$ is called radial, if there exists a function r on $\mathbb{R}_{+}$such that

$$
\mathrm{K}(\mathrm{x}, \mathrm{y})=\mathrm{r}(|\mathrm{x}-\mathrm{y}|) \quad, \quad \mathrm{x}, \mathrm{y} \in \mathbb{R}^{\mathrm{d}} .
$$

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

$$
\mathrm{r}(\mathrm{t})=\int_{\mathbb{R}_{+}} \exp \left(-s \mathrm{t}^{2}\right) \mathrm{d} \mu(\mathrm{~s}) \quad, \quad \mathrm{t} \in \mathbb{R}_{+}
$$

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

$$
\|\operatorname{Df}\|_{\mathrm{F}} \leq \frac{\mathrm{d}}{\sigma}\|\mathrm{f}\|_{\mathrm{H}}
$$

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Geometric Surface Matching Distances

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## Geometric Matching Distances: Hausdorff Distance

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

$$
\mathrm{D}_{\mathrm{H}}\left(\mathrm{~S}, \mathrm{~S}^{\prime}\right):=\max \left(\mathrm{h}\left(\mathrm{~S}, \mathrm{~S}^{\prime}\right), \mathrm{h}\left(\mathbf{S}^{\prime}, \mathrm{S}\right)\right),
$$

where the Hausdorff disparity $h\left(S, S^{\prime}\right)$ is defined by means of

$$
\mathrm{h}\left(\mathrm{~S}, \mathrm{~S}^{\prime}\right):=\max _{\mathrm{x} \in \mathrm{~S}}\left(\min _{\mathrm{x}^{\prime} \in \mathrm{S}^{\prime}}\left|\mathrm{x}-\mathrm{x}^{\prime}\right|\right) .
$$

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

$$
\widetilde{\mathrm{D}}_{\mathrm{H}}\left(\mathbf{S}, \mathrm{~S}^{\prime}\right):=\mathrm{h}_{\mathrm{sm}}\left(\mathbf{S}, \mathrm{~S}^{\prime}\right)+\mathrm{h}_{\mathrm{sm}}\left(\mathbf{S}^{\prime}, \mathbf{S}\right),
$$

where $h_{s m}\left(S, S^{\prime}\right)$ refers to a smoothed Hausdorff disparity.

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## Geometric Matching Distances: Borel Measure Distance

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

$$
\left\langle\mu, \mu^{\prime}\right\rangle_{\Gamma}:=\int_{\mathbb{R}^{3}} \int_{\mathbb{R}^{3}} \Gamma\left(\mathrm{x}, \mathrm{x}^{\prime}\right) \mathrm{d} \mu(\mathrm{x}) \mathrm{d} \mu^{\prime}\left(\mathrm{x}^{\prime}\right),
$$

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 $\mathrm{S} \subset \mathbb{R}^{3}$ with a measure $\mu_{\mathrm{S}} \in \mathrm{BM}\left(\mathbb{R}^{3}\right)$ induced on $S$ by the Lebesgue measure of $\mathbb{R}^{3}$.
- The distance between bounded Borel subsets $S, S^{\prime} \in \mathbb{R}^{3}$ is defined by means of

$$
\mathrm{D}_{\Gamma}^{2}\left(\mathrm{~S}, \mathrm{~S}^{\prime}\right):=\left\|\mu_{\mathrm{S}}-\mu_{\mathrm{S}^{\prime}}\right\|_{\Gamma}^{2}
$$

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Variational Formulation of the Optimal Matching Problem

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## Variational Formulation of the Optimal Matching Problem

Let $\mathcal{D}(\mathrm{I} ; \mathrm{V})$ be the space of all disparity functionals $\mathrm{D}: \mathrm{L}^{2}(\mathrm{I} ; \mathrm{V}) \rightarrow \mathbb{R}_{+}$of the form

$$
\mathrm{D}(\mathrm{v})=\Phi\left(\mathrm{F}^{\mathrm{v}}\left(\cdot, \mathrm{t}_{1}\right), \cdots . \mathrm{F}^{\mathrm{v}}\left(\cdot, \mathrm{t}_{\mathrm{q}}\right)\right),
$$

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

$$
\mathrm{E}(\mathrm{v})=\frac{1}{2} \int_{0}^{1}\left\|\mathrm{v}_{\mathrm{t}}\right\|_{\mathrm{V}}^{2} \mathrm{dt} .
$$

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

$$
(\mathrm{OP})_{1} \quad \mathrm{~J}\left(\mathrm{v}^{*}\right)=\inf _{\mathrm{v} \in \mathrm{~L}^{2}(\mathrm{I} ; \mathrm{V})} \mathrm{J}(\mathrm{v}), \quad \mathrm{J}(\mathrm{v}):=\mathrm{E}(\mathrm{v})+\lambda \mathrm{D}(\mathrm{v}),
$$

subject to

$$
\begin{aligned}
(\mathrm{OP})_{2} \quad \partial_{\mathrm{t}} \mathrm{~F}(\cdot, \mathrm{t}) & =\mathrm{v}_{\mathrm{t}}(\mathrm{~F}(\cdot, \mathrm{t})) \quad, \quad \mathrm{t} \in \mathrm{I}, \\
\mathrm{~F}(\cdot, 0) & =\mathrm{Id} .
\end{aligned}
$$

## Existence of a Minimizing Diffeomorphic Flow

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

$$
\liminf _{\mathrm{n} \rightarrow \infty}\left\|\mathrm{v}^{\mathrm{n}}\right\|_{\mathrm{L}^{2}(\mathrm{I} ; \mathrm{V})} \leq\left\|\mathrm{v}^{*}\right\|_{\mathrm{L}^{2}(\mathrm{I} ; \mathrm{V})} .
$$

Denoting by $\mathrm{F}^{\mathrm{n}}(\cdot, \mathrm{t}), \mathrm{F}^{*}(\cdot, \mathrm{t}) \in \operatorname{Diff}\left(\mathbb{R}^{3}\right), \mathrm{t} \in \mathrm{I}$, the unique flows solving $(\mathrm{OP})_{2} \mathrm{w} . r . \mathrm{t} . \mathrm{v}^{\mathrm{n}}, \mathrm{v}^{*}$, the main part of the proof is to show that

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

uniformly on bounded subsets of $\mathbb{R}^{3}$. This implies $\mathrm{D}\left(\mathrm{v}^{\mathrm{n}}\right) \rightarrow \mathrm{D}\left(\mathrm{v}^{*}\right)(\mathrm{n} \rightarrow \infty)$, and hence,

$$
\liminf _{\mathrm{n} \rightarrow \infty} \mathrm{~J}\left(\mathrm{v}^{\mathrm{n}}\right) \leq \lim _{\mathrm{n} \rightarrow \infty} \mathrm{D}\left(\mathrm{v}^{\mathrm{n}}\right)+\liminf _{\mathrm{n} \rightarrow \infty} \mathrm{E}\left(\mathrm{v}^{\mathrm{n}}\right) \leq \mathrm{D}\left(\mathrm{v}^{*}\right)+\mathrm{E}\left(\mathrm{v}^{*}\right)=\mathrm{J}\left(\mathrm{v}^{*}\right),
$$

which allows to conclude.

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## Necessary Optimality Conditions

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

$$
\begin{array}{ll}
(\mathrm{OP})_{3} & -\partial_{\mathrm{t}} \mathrm{p}_{\mathrm{t}}^{*}-\mathrm{b}_{\mathrm{v}^{*}, \mathrm{t}_{\mathrm{t}}^{*}}^{*}=0 \quad, \quad \mathrm{t} \in\left(\mathrm{t}_{\mathrm{j}-1}, \mathrm{t}_{\mathrm{j}}\right), \\
& \mathrm{p}_{\mathrm{t}_{\mathrm{q}}^{+}}^{*}=0, \mathrm{p}_{\mathrm{t}_{\mathrm{j}}^{-}}^{*}=\mathrm{p}_{\mathrm{t}_{\mathrm{j}}^{+}}^{*}+\lambda \partial_{\mathrm{j}} \Phi\left(\mathrm{~F}^{*}\left(\cdot, \mathrm{t}_{\mathrm{j}}\right)\right), 1 \leq \mathrm{j} \leq \mathrm{q} . \\
(\mathrm{OP})_{4} \quad & \mathrm{p}_{\mathrm{t}}^{*}+\rho_{\mathrm{t}, \mathrm{v}^{*}}=0 \quad, \quad \mathrm{t} \in \mathrm{I},
\end{array}
$$

Here, $\mathrm{b}_{\mathrm{v}, \mathrm{t}}$ is a Borel function of $\mathrm{D}_{\mathrm{v}} \mathrm{v}_{\mathrm{t}}\left(\mathrm{F}^{\mathrm{v}}(\cdot, \mathrm{t})\right)$, and $\rho_{\mathrm{t}, \mathrm{v}}$ is a vector valued Borel measure with density $\mathrm{Kv}_{\mathrm{t}}$.

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Discretization: Dirac Measures and Diffeomorphic Point Matching

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## Discretization: Dirac Measures and Diffeomorphic Point Matching

- We discretize the snapshots $\mathrm{S}_{\mathrm{j}}, 0 \leq \mathrm{j} \leq \mathrm{q}$, and the dynamically deformed surfaces $\hat{S}_{j}=\mathrm{F}^{\mathrm{v}}\left(\mathrm{S}_{0}, \mathrm{t}_{\mathrm{j}}\right)$ by point sets

$$
\mathrm{X}_{\mathrm{j}}=\left\{\mathrm{x}_{1}^{\mathrm{j}}, \cdots, \mathrm{x}_{\mathrm{N}_{\mathrm{j}}}^{\mathrm{j}}\right\} \quad, \quad \hat{\mathrm{X}}_{\mathrm{j}}=\mathrm{F}^{\mathrm{v}}\left(\mathrm{X}_{0}, \mathrm{t}_{\mathrm{j}}\right)=\left\{\mathrm{F}^{\mathrm{v}}\left(\mathrm{x}_{1}^{0}, \mathrm{t}_{1}\right), \cdots, \mathrm{F}^{\mathrm{v}}\left(\mathrm{x}_{\mathrm{N}_{0}}^{0}, \mathrm{t}_{\mathrm{j}}\right)\right\} .
$$

- We denote by $\mathrm{x}_{\mathrm{n}}(\mathrm{t})=\mathrm{F}^{\mathrm{v}}\left(\mathrm{x}_{\mathrm{n}}^{0}, \mathrm{t}_{\mathrm{j}}\right), \mathrm{x}_{\mathrm{n}}(0)=\mathrm{x}_{\mathrm{n}}^{0}, 1 \leq \mathrm{n} \leq \mathrm{N}_{0}$, the trajectories emanating from $x_{n}^{0}$, i.e., the solutions of the initial value problems

$$
\frac{\mathrm{d}}{\mathrm{dt}} \mathrm{x}_{\mathrm{n}}(\mathrm{t})=\mathrm{v}_{\mathrm{t}}\left(\mathrm{x}_{\mathrm{n}}(\mathrm{t})\right), \mathrm{t} \in[0,1] \quad, \quad \mathrm{x}_{\mathrm{n}}(0)=\mathrm{x}_{\mathrm{n}}^{0}
$$

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

$$
\mu_{\mathrm{S}_{\mathrm{j}}}=\sum_{\mathrm{m}=1}^{\mathrm{N}_{\mathrm{j}}} \mathrm{~b}_{\mathrm{m}}^{\mathrm{j}} \delta_{\mathrm{x}_{\mathrm{m}}^{\mathrm{j}}}, \quad \mu_{\hat{\mathrm{S}}_{\mathrm{j}}}=\sum_{\mathrm{n}=1}^{\mathrm{N}_{0}} \mathrm{a}_{\mathrm{n}} \delta_{\mathrm{x}_{\mathrm{n}}\left(\mathrm{t}_{\mathrm{j}}\right)} \quad, \quad 1 \leq \mathrm{j} \leq \mathrm{q} .
$$

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## Discretization: Dirac Measures and Diffeomorphic Point Matching

- Setting $\mathrm{x}(\mathrm{t})=\left(\mathrm{x}_{1}(\mathrm{t}), \cdots, \mathrm{x}_{\mathrm{N}_{0}}(\mathrm{t})\right)^{\mathrm{T}}, \mathrm{t} \in(0,1)$, the disparity cost funtional reads

$$
\mathrm{D}(\mathrm{v})=\sum_{\mathrm{j}=1}^{\mathrm{q}} \lambda_{\mathrm{j}} \mathrm{D}_{\mathrm{j}}\left(\mathrm{x}\left(\mathrm{t}_{\mathrm{j}}\right)\right) \quad, \quad \mathrm{D}_{\mathrm{j}}\left(\mathrm{x}\left(\mathrm{t}_{\mathrm{j}}\right)\right):=\left\|\mu_{\mathrm{S}_{\mathrm{j}}}-\mu_{\hat{\mathrm{S}}_{\mathrm{j}}}\right\|_{\mathrm{K}_{\sigma_{\mathrm{j}}}}^{2},
$$

where $\mathrm{K}_{\sigma_{\mathrm{j}}}, 1 \leq \mathrm{j} \leq \mathrm{q}$, are appropriately chosen radial Gaussian kernels.

- We approximate the flow $\mathrm{v}_{\mathrm{t}}$ by a linear combination of $\mathrm{K}_{\mathrm{x}_{\mathrm{n}}(\mathrm{t})}, 1 \leq \mathrm{n} \leq \mathrm{N}_{0}$,

$$
\mathrm{v}_{\mathrm{t}}(\mathrm{x})=\sum_{\mathrm{n}=1}^{\mathrm{N}_{0}} \mathrm{~K}_{\sigma_{0}}\left(\mathrm{x}_{\mathrm{n}}(\mathrm{t}), \mathrm{x}\right) \alpha_{\mathrm{n}}(\mathrm{t}) \quad, \quad \mathrm{x} \in \mathbb{R}^{3} .
$$

It follows that

$$
\left\|\mathrm{v}_{\mathrm{t}}\right\|_{\mathrm{V}}^{2}=\sum_{\mathrm{n}=1}^{\mathrm{N}_{0}} \sum_{\mathrm{n}^{\prime}=1}^{\mathrm{N}_{0}} \mathrm{~K}_{\sigma_{0}}\left(\mathrm{x}_{\mathrm{n}}(\mathrm{t}), \mathrm{x}_{\mathrm{n}^{\prime}}(\mathrm{t})\right) \alpha_{\mathrm{n}}^{\mathrm{T}}(\mathrm{t}) \alpha_{\mathrm{n}}(\mathrm{t}) \quad, \quad \mathrm{t} \in[0,1] .
$$

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## The Discrete Optimization Problem

Setting $\alpha(\mathrm{t})=\left(\alpha_{1}(\mathrm{t}), \cdots, \alpha_{\mathrm{N}_{0}}(\mathrm{t})\right)^{\mathrm{T}} \in \mathbb{R}^{\mathrm{d} \mathrm{N}_{0}}, \mathrm{t} \in(0,1)$, and

$$
\mathrm{A}(\mathrm{x}(\mathrm{t})):=\left(\mathrm{K}_{\sigma_{0}}\left(\mathrm{x}_{\mathrm{n}}(\mathrm{t}), \mathrm{x}_{\mathrm{n}^{\prime}}(\mathrm{t})\right) \mathrm{I}_{\mathrm{d}}\right)_{\mathrm{n}, \mathrm{n}^{\prime}=1}^{\mathrm{N}_{0}} \in \mathbb{R}^{\mathrm{dN} \mathrm{~N}_{0} \times \mathrm{dN}_{0}}
$$

the discrete optimization problem reads:
Discrete Optimization Problem: Find $\alpha^{*} \in \mathrm{~L}^{2}\left(\mathbf{I} ; \mathbb{R}^{\mathrm{dN}}\right)$ and $\mathrm{x}^{*}(\mathrm{t})$ such that
$(\mathrm{DOP})_{1} \quad \mathrm{~J}\left(\alpha^{*}\right)=\inf _{\alpha} \mathrm{J}(\alpha), \mathrm{J}(\alpha):=\frac{1}{2} \int_{0}^{1} \alpha(\mathrm{t})^{\mathrm{T}} \mathrm{A}(\mathrm{x}(\mathrm{t})) \alpha(\mathrm{t}) \mathrm{dt}+\sum_{\mathrm{j}=1}^{\mathrm{q}} \lambda_{\mathrm{j}} \mathrm{D}_{\mathrm{j}}\left(\mathrm{x}\left(\mathrm{t}_{\mathrm{j}}\right)\right)$,
subject to

$$
\begin{aligned}
\frac{\mathrm{d}}{\mathrm{dt}} \mathrm{x}^{*}(\mathrm{t}) & =\mathrm{A}\left(\mathrm{x}^{*}(\mathrm{t})\right) \alpha^{*}(\mathrm{t}) \quad, \quad \mathrm{t} \in \mathrm{I}, \\
\mathrm{x}^{*}(0) & =\mathrm{x}^{0}
\end{aligned}
$$

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 Institut für Mathematik, Universität AugsburgExistence of a Solution and Necessary Optimality Conditions
Theorem 3. The discrete optimization problem $(\mathrm{DOP})_{1},(\mathrm{DOP})_{2}$ has a solution $\alpha^{*}=\alpha^{*}(\mathrm{t}), \mathrm{t} \in \mathrm{I}$. If $\mathrm{x}^{*}=\mathrm{x}^{*}(\mathrm{t}), \mathrm{t} \in \mathrm{I}$, is the associated trajectory, there exists a function $\mathrm{p}^{*}=\mathrm{p}^{*}(\mathrm{t}), \mathrm{t} \in \mathrm{I}$, which solves the final time problem

$$
\begin{aligned}
&(\mathrm{DOP})_{3} \quad-\frac{\mathrm{d}}{\mathrm{dt}} \mathrm{p}^{*}(\mathrm{t})=\mathrm{B}\left(\mathrm{x}^{*}(\mathrm{t}), \alpha^{*}(\mathrm{t})\right)^{\mathrm{T}}\left(\mathrm{p}^{*}(\mathrm{t})+\frac{1}{2} \alpha^{*}(\mathrm{t})\right), \mathrm{t} \in\left(\mathrm{t}_{\mathrm{j}-1}, \mathrm{t}_{\mathrm{j}}\right), \\
& \mathrm{p}^{*}\left(\mathrm{t}_{\mathrm{q}}^{+}\right)=0, \mathrm{p}^{*}\left(\mathrm{t}_{\mathrm{j}}^{-}\right)=\mathrm{p}^{*}\left(\mathrm{t}_{\mathrm{j}}^{+}\right)+\lambda_{\mathrm{j}} \nabla \mathrm{D}_{\mathrm{j}}\left(\mathrm{x}^{*}\left(\mathrm{t}_{\mathrm{j}}\right)\right), 1 \leq \mathrm{j} \leq \mathrm{q}, \\
&(\mathrm{DOP})_{4} \quad \mathrm{~A}\left(\mathrm{x}^{*}(\mathrm{t})\right)\left(\alpha^{*}(\mathrm{t})+\mathrm{p}^{*}(\mathrm{t})\right)=0, \mathrm{t} \in \mathrm{I},
\end{aligned}
$$

where the matrix $B\left(x^{*}(t), \alpha^{*}(t)\right) \in \mathbb{R}^{d N_{0}} \times \mathrm{dN}_{0}$ is given by

$$
\mathrm{B}\left(\mathrm{x}^{*}(\mathrm{t}), \alpha^{*}(\mathrm{t})\right)=\nabla_{\mathrm{x}}\left(\mathrm{~A}\left(\mathrm{x}^{*}(\mathrm{t}), \alpha^{*}(\mathrm{t})\right)\right) .
$$

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## Fully Discrete Optimization Problem

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## Fully Discrete Optimal Diffeomorphic Matching Problem I

For the discretization in time of the optimality system $(\mathrm{DOP})_{2}-(\mathrm{DOP})_{4}$ we introduce

$$
\Delta_{\mathrm{I}}:=\bigcup_{\mathrm{j}=1}^{\mathrm{q}} \Delta_{\mathrm{I}_{\mathrm{j}}}, \Delta_{\mathrm{I}_{\mathrm{j}}}:=\left\{\mathrm{t}_{\mathrm{j}-1}=: \mathrm{t}^{\mathrm{L}_{\mathrm{j}-1}}<\mathrm{t}^{\mathrm{L}_{\mathrm{j}-1}+1}<\cdots<\mathrm{t}^{\mathrm{L}_{\mathrm{j}}}:=\mathrm{t}_{\mathrm{j}}\right\},
$$

where $\Delta_{\mathrm{I}_{\mathrm{j}}}, 1 \leq \mathrm{j} \leq \mathrm{q}$, are subpartitions of $\mathrm{I}_{\mathrm{j}}:=\left[\mathrm{t}_{\mathrm{j}-1}, \mathrm{t}_{\mathrm{j}}\right]$.
Setting $\Delta \mathrm{t}^{\ell}:=\mathrm{t}^{{ }^{\ell}+1}-\mathrm{t}^{\ell}, 0=: \mathrm{L}_{0} \leq \ell \leq \mathrm{L}:=\mathrm{L}_{\mathrm{q}}$, the discretized optimality system reads

$$
\begin{array}{ll}
(\mathrm{DOC})_{1} & \frac{\mathrm{x}^{\ell+1}-\mathrm{x}^{\ell}}{\Delta \mathrm{t}^{\ell}}=\mathrm{A}\left(\mathrm{x}^{\ell} \alpha^{\ell}, \mathrm{L}_{0} \leq \ell \leq \mathrm{L},\right. \\
\mathrm{x}^{0}=\mathrm{x}^{(0)}, \\
(\mathrm{DOC})_{2} \quad & \frac{\mathrm{p}^{(\ell-1)^{+}}-\mathrm{p}^{\ell^{-}}}{\Delta \mathrm{t}^{\ell-1}}=\mathrm{B}\left(\mathrm{x}^{\ell}, \alpha^{\ell}\right)^{\mathrm{T}}\left(\mathrm{p}^{\ell^{-}}+\alpha^{\ell} / \mathbf{2}\right), \ell=\mathrm{L}_{\mathrm{j}}, \cdots, \mathrm{~L}_{\mathrm{j}-1}+1, \\
& \mathrm{p}^{\mathrm{L}_{\mathrm{q}}^{+}}=0, \mathrm{p}^{\mathrm{L}_{\mathrm{j}}^{-}}=\mathrm{p}^{\mathrm{L}_{\mathrm{j}}^{+}}+\lambda_{\mathrm{j}} \nabla \mathrm{D}_{\mathrm{j}}\left(\mathrm{x}^{\mathrm{L}_{\mathrm{j}}}\right), 1 \leq \mathrm{j} \leq \mathrm{q}, \\
(\mathrm{DOC})_{3} \quad & \mathrm{~A}\left(\mathrm{x}^{\ell}\right)\left(\alpha^{\ell}+\mathrm{p}^{\ell^{+}}\right), \mathrm{L}_{0} \leq \ell \leq \mathrm{L}-1 .
\end{array}
$$

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## Fully Discrete Optimal Diffeomorphic Matching Problem II

Theorem 4. Let $\mathrm{J}_{\Delta_{\mathrm{I}}}$ be the discrete objective functional

$$
\mathrm{J}_{\Delta_{\mathrm{I}}}(\alpha)=\frac{1}{2} \sum_{\ell=0}^{\mathrm{L}-1} \Delta^{\ell} \mathrm{t}^{\ell}\left(\alpha^{\ell}\right)^{\mathrm{T}} \mathrm{~A}\left(\mathrm{x}^{\ell}\right) \alpha^{\ell}+\sum_{\mathrm{j}=1}^{\mathrm{q}} \lambda_{\mathrm{j}} \mathrm{D}_{\mathrm{j}}\left(\mathrm{x}^{\mathrm{L}_{\mathrm{j}}}\right) .
$$

The discrete optimality system $(\mathrm{DOC})_{1}-(\mathrm{DOC})_{3}$ represents the first order necessary optimality conditions for the discrete optimization problem

$$
\min _{\alpha} \mathrm{J}_{\Delta_{\mathrm{I}}}(\alpha),
$$

subject to

$$
\begin{aligned}
\frac{\mathrm{x}^{\ell+1}-\mathrm{x}^{\ell}}{\Delta \mathrm{t} \ell} & =\mathrm{A}\left(\mathrm{x}^{\ell}\right) \alpha^{\ell} \quad, \quad \mathrm{L}_{0} \leq \ell \leq \mathrm{L}-1 \\
\mathrm{x}^{0} & =\mathrm{x}^{(0)} .
\end{aligned}
$$

Corollary. Let $\left(\mathrm{x}^{*}, \mathrm{p}^{*}, \alpha^{*}\right)$ with $\mathrm{x}^{*}=\left\{\mathrm{x}_{*}^{\ell}\right\}_{\ell=0}^{\mathrm{L}}$ etc. satisfy $(\mathrm{DOC})_{1}-(\mathrm{DOC})_{3}$. Then, we have

$$
0=\nabla \mathrm{J}_{\Delta_{\mathrm{I}}}\left(\alpha^{*}\right)=\left\{\mathrm{g}^{\ell}\right\}_{\ell=0}^{\mathrm{L}-1} \quad, \quad \mathrm{~g}^{\ell}=\mathrm{A}\left(\mathrm{x}_{*}^{\ell}\right)\left(\alpha_{*}^{\ell}+\mathrm{p}_{*}^{\ell}\right)
$$

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## Matching Algorithm: Continuation in the Regularization Parameter

Role of the regularization parameters: For simplicity, we assume $\lambda_{j}=\lambda>0,1 \leq \mathrm{j} \leq \mathrm{q}$. 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

$$
\mathrm{D}_{\mathrm{j}}:=\kappa\left(\sum_{\mathrm{n}=1}^{\mathrm{N}_{0}}\left(\mathrm{~d}_{\mathrm{n}}^{\mathrm{j}}\right)^{2}\right)^{1 / 2}<\vartheta \quad, \quad \mathrm{d}_{\mathrm{n}}^{\mathrm{j}}:=\min _{1 \leq \mathrm{m} \leq \mathrm{N}_{\mathrm{j}}}\left|\mathrm{x}_{\mathrm{n}}\left(\mathrm{t}_{\mathrm{j}}\right)-\mathrm{x}_{\mathrm{m}}\left(\mathrm{t}_{\mathrm{j}}\right)\right|,
$$

where $\vartheta>0$ is a given threshold and $0<\kappa \leq 1$ (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 $\left|\nabla \mathrm{J}\left(\alpha_{\nu}^{(\mu)}\right)\right|<\theta\left|\nabla \mathrm{J}\left(\alpha_{\nu}^{(0)}\right)\right|$ is satisfied, go to Step 5. Otherwise, go to Step 4.1.
Step 5: Termination of the outer iteration
If the termination criterion $\mathrm{D}_{\mathrm{j}}<\vartheta, 1 \leq \mathrm{j} \leq \mathrm{q}$, 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.

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Matching Mitral Annulus Snapshots

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Diffeomorphic Matching of Multiple Annulus Snapshots


Matching Multiple Snapshots of the Mitral Annulus at $\mathrm{t}=1,3,5,7,10$

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 Institut für Mathematik, Universität AugsburgDiffeomorphic Matching of Multiple Annulus Snapshots: Hausdorff Matching



Convergence history: Accuracy indicators (1.) and Hausdorff disparities (r.)

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Diffeomorphic Matching of Multiple Annulus Snapshots: Hausdorff Matching



Pareto frontiers: Accuracy indicators (1.) and Hausdorff disparities (r.)

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Diffeomorphic Matching of Multiple Annulus Snapshots: Measure Matching


Convergence history: Accuracy indicators

(1.) and measure matching disp. (r.)

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Diffeomorphic Matching of Multiple Annulus Snapshots: Measure Matching


Pareto frontiers: Accuracy indicators (1.) and measure matching disp. (r.)

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Matching Anterior Leaflet Snapshots

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

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Diffeomorphic Matching of Multiple Anterior Leaflet Snapshots


Matching errors between computed deformations and snapshots

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## Diffeomorphic Matching of Multiple Anterior Leaflet Snapshots




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

## Diffeomorphic Matching of Multiple Anterior Leaflet Snapshots




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

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Pareto frontiers: max. distances to snapshots (1.), $90 \%$ of max. dist. (r.)

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Numerical Results:<br>Matching Posterior Leaflet Snapshots

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

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Diffeomorphic Matching of Multiple Posterior Leaflet Snapshots



Approximation error at $t_{3}$


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.)

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Diffeomorphic Matching of Multiple Posterior Leaflet Snapshots



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

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Diffeomorphic Matching of Multiple Posterior Leaflet Snapshots



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

