Diffeomorphic Density Matching by Optimal Information Transport

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Joint work with:
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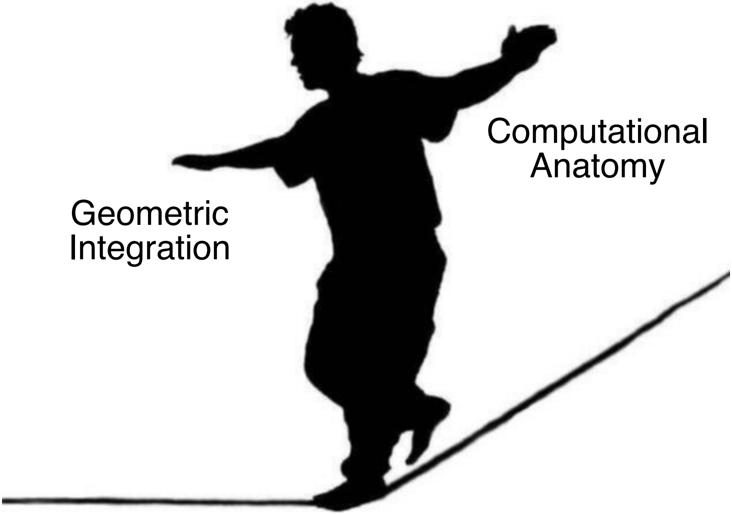
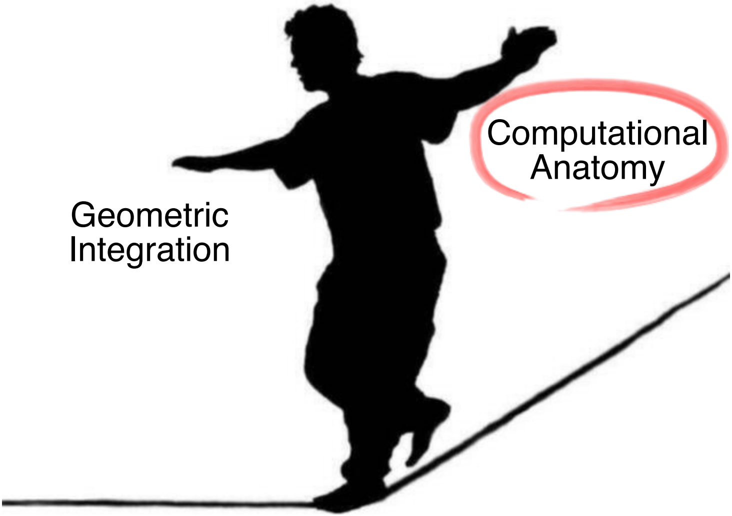

Geometric
Integration
Computational
Anatomy


Computational
Anatomy
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Outline of talk

1. What is computational anatomy?

2. Diffeomorphic density matching
   - Optimal mass transport
   - Optimal information transport

3. Examples

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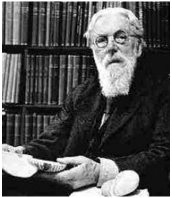
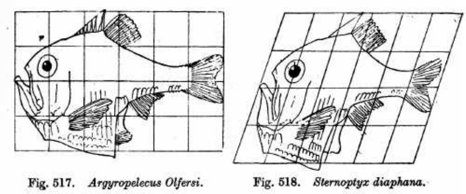
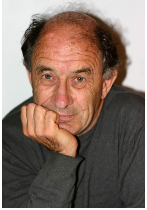
What is computational anatomy?

Origin in evolutionary biology by **Sir D'Arcy Thompson** (1860–1948)





Modern mathematical foundation: **topological hydrodynamics**



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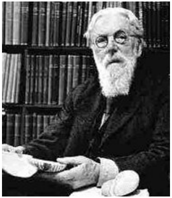

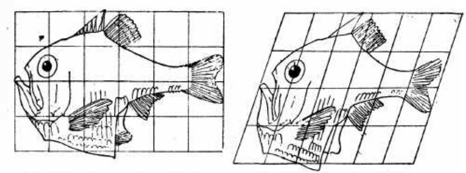

Fig. 517. *Argyropelecus Olfersi.* Fig. 518. *Sternoptyx diaphana.*

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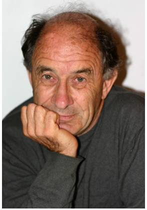


Vladimir Arnold (1937–2010)

What is topological hydrodynamics?

Recall Euler's equations for a rigid body:

$$\mathcal{I}\dot{\boldsymbol{\omega}} = \boldsymbol{\omega} \times \mathcal{I}\boldsymbol{\omega}$$

where

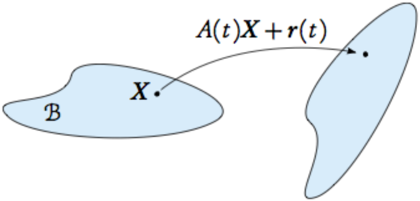
- $\boldsymbol{\omega} = (\omega_x, \omega_y, \omega_z)$ is the angular velocity vector
- $\mathcal{I} = \begin{bmatrix} a_{xx} & a_{xy} & a_{xz} \\ a_{xy} & a_{yy} & a_{yz} \\ a_{xz} & a_{yz} & a_{zz} \end{bmatrix}$ is the inertia tensor

Basic idea of topological hydrodynamics (Arnold, 1966)

Can the rigid body equations be generalized?
What geometric structures are present?

Arnold's approach:

- Configuration of object described by transformation acting on it
- Set of admissible transformations form a Lie group G
- Motion takes place on the group: $\gamma(t) \in G$

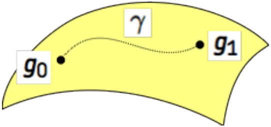


Basic idea of topological hydrodynamics, cont.

- Dynamics on *tangent bundle* TG, where G a Lie group

Connection between geometry and mechanics:

Mechanics	**Geometry**
Kinetic energy $L(g, \dot{g})$	Riemannian metric $\langle\langle \dot{g}, \dot{g} \rangle\rangle_g$
Euler–Lagrange equation	Geodesic equation
Symmetry $L(G \cdot (g, \dot{g})) = L(g, \dot{g})$	Left invariant metric



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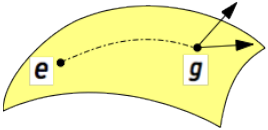
- Left invariant metric $\Leftrightarrow$ inner product on $\mathfrak{g} = T_e G$



$$\langle\langle u, v \rangle\rangle_g = \left\langle \mathcal{A} g^{-1} \cdot u, g^{-1} \cdot v \right\rangle$$

$$\mathcal{A} : \mathfrak{g} \to \mathfrak{g}^* \quad \text{(inertia operator)}$$

Basic idea of topological hydrodynamics, cont.

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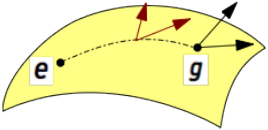

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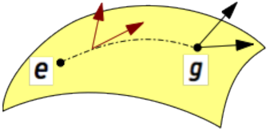

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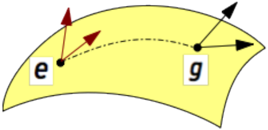

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Basic idea of topological hydrodynamics, cont.

Left invariance $\Rightarrow$ symmetry group G $\Rightarrow$ reduced phase space $TG/G \simeq \mathfrak{g}$

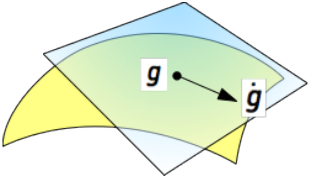
Euler-Lagrange equation

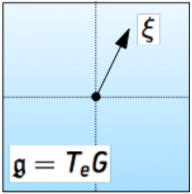
$$\frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial L}{\partial \dot{g}} = \frac{\partial L}{\partial g}$$

$\Longrightarrow$

Euler–Arnold equation

$$\mathcal{A}\dot{\xi} = \mathrm{ad}^*_{\xi}(\mathcal{A}\xi), \quad \xi \in \mathfrak{g}$$





First two examples

	Rigid body	Ideal incompressible fluid
$G, \mathfrak{g}$	$SO(3), \mathfrak{so}(3) \simeq \mathbf{R}^3$	$SDiff(M), \mathfrak{X}_\mu(M)$
L	$\int_{\mathcal{B}} \rho(\boldsymbol{x}) \lvert \dot{A}\boldsymbol{x} \rvert^2 \mathrm{d}V$	$\int_M \lvert \dot{\varphi}(\boldsymbol{x}) \rvert^2 \mathrm{d}\mu$
E-A eq.	$\mathcal{I}\dot{\boldsymbol{\omega}} = \boldsymbol{\omega} \times \mathcal{I}\boldsymbol{\omega}$	$\dot{u} + u^\top \nabla u = -\nabla p, \operatorname{div} u = 0$

Check left invariance for rigid body: $R \in SO(3), (A, \dot{A}) \in T\,SO(3)$

$$L(RA, R\dot{A}) = \int_{\mathcal{B}} \rho(\boldsymbol{x}) \lvert R\dot{A}\boldsymbol{x} \rvert^2 \mathrm{d}V = \int_{\mathcal{B}} \rho(\boldsymbol{x}) \lvert \dot{A}\boldsymbol{x} \rvert^2 \mathrm{d}V = L(A, \dot{A})$$

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Other examples of Euler–Arnold equations

Group	Metric	Equation
$SO(3) \ltimes \mathbf{R}^3$	quadratic forms	Kirchhoff's body in a fluid
$SO(n)$	Manakov's metrics	n–dimensional top
$\mathit{Diff}(S^1)$	L_2	Inviscid Burgers' equation
Virasoro	L_2	KdV equation
$\mathit{Diff}(S^1)$	H^1	Camassa–Holm equation
$\mathit{Diff}(S^1)/S^1$	$\dot{H}^1$	Hunter–Saxton equation
$\mathit{SDiff}(M)$	H^1	Averaged Euler fluid
$\mathit{SDiff}(M) \ltimes \mathfrak{X}_\mu(M)$	$L_2 + L_2$	Magnetohydrodynamics
$C^\infty(S^1, SO(3))$	H^{-1}	Heisenberg magnetic chain
$\mathit{Diff}(M)$	H^s	EPDiff equation

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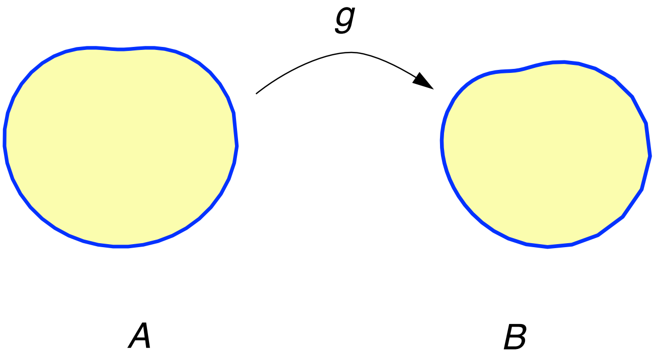
Back to computational anatomy: abstract formulation

- G Lie group acting on **shape space** S
- d right-invariant Riemannian distance on G
- $\bar{d}$ metric distance on S

Problem: given **source** $A \in S$ and **target** $B \in S$, find minimizer

$$\min_{g \in G} \left(\sigma d^2(e, g) + \bar{d}^2(g \cdot A, B) \right), \qquad \sigma > 0$$



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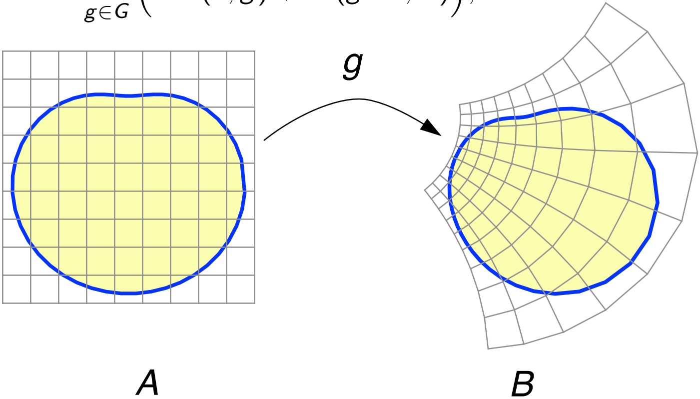
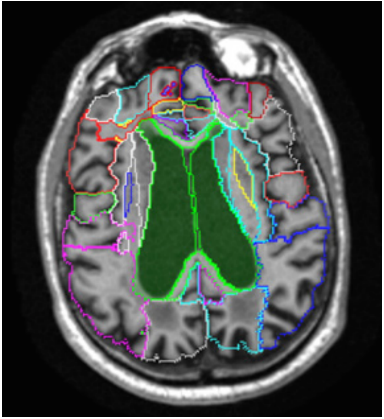


Typical application of CA: medical image registration

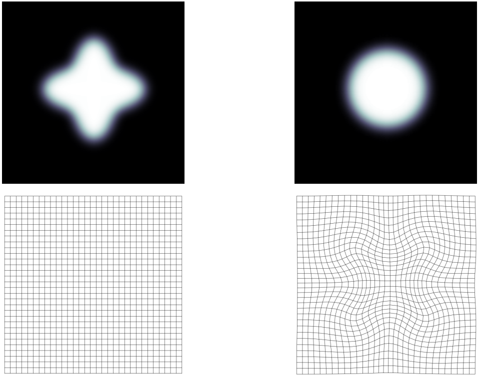


Outline of talk

1. What is computational anatomy?
2. Diffeomorphic density matching
   - Optimal mass transport
   - Optimal information transport
3. Examples

Density transport problem

μ_0 (source) μ_1 (target)



$$M \ni x \longmapsto \varphi(x) \in M$$

Basic problem: find map $\varphi\colon M \to M$ such that

$$\varphi_* \mu_0 = \mu_1$$

First complication: φ is not unique

Regularized problem formulation

- Manifold M (domain)
- $Dens(M)$, smooth, strictly positive probability densities
- $Diff(M)$, diffeomorphisms
- Distance $d(\cdot,\cdot)$ on $Diff(M)$

Exact density matching (optimal transport)

Given $\mu_0, \mu_1 \in Dens(M)$, find $\varphi \in Diff(M)$ minimizing

$$d(id, \varphi)$$

under **constraint** $\varphi_* \mu_0 = \mu_1$

Inexact density matching (computational anatomy)

Given $\mu_0, \mu_1 \in Dens(M)$, find $\varphi \in Diff(M)$ minimizing

$$E(\varphi) = \sigma d^2(id, \varphi) + \bar{d}^2(\varphi_* \mu_0, \mu_1), \quad \sigma > 0$$

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$$d(id, \varphi)$$

under **constraint** $\varphi_* \mu_0 = \mu_1 \quad \mu_0 = I_0 \mu \quad \Rightarrow \quad \varphi \cdot I_0 = |D\varphi^{-1}| I_0 \circ \varphi^{-1}$

Inexact density matching (computational anatomy)

Given $\mu_0, \mu_1 \in Dens(M)$, find $\varphi \in Diff(M)$ minimizing

$$E(\varphi) = \sigma d^2(id, \varphi) + \bar{d}^2(\varphi_* \mu_0, \mu_1), \quad \sigma > 0$$

Optimal Mass Transport (OMT)

Exact density matching with

- $M = \Omega \subset \mathbf{R}^n$
- $d^2(id, \varphi) = \int_\Omega |x - \varphi(x)|^2 \mu_0$
- **Wasserstein distance**: metric distance on $Dens(M)$

$$\bar{d}_W(\mu_0, \mu_1) := \inf_{\varphi_* \mu_0 = \mu_1} d(id, \varphi)$$

Existence and uniqueness by Brenier 1991:

- Based on **polar factorization** of maps

$$\varphi = \nabla f \circ \psi \quad \text{where} \quad \psi_* \mu_0 = \mu_0 \quad \text{and} \quad f \text{ convex}$$

Solution fulfils **Monge–Ampere equation**

$$|\nabla^2 f| = \frac{I_1}{I_0 \circ \nabla f}$$

Riemannian geometry of OMT (Otto calculus)

Formal geometric description by Otto 2001:

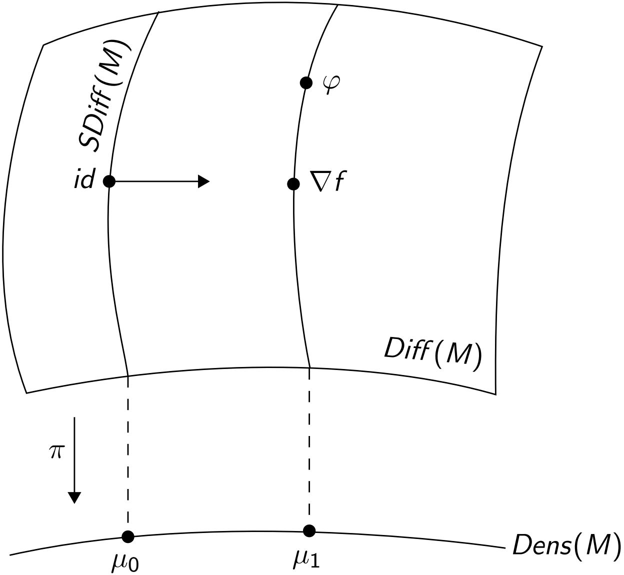
- $\mathit{Diff}(M)$ **infinite-dimensional** Riemannian manifold with metric

$$G_\varphi(U,V) = \int_M g(U,V)\mu, \quad U,V \in C^\infty(M,TM)$$

- G is **right-invariant** w.r.t. $\mathit{SDiff}(M) = \{\psi \in \mathit{Diff}(M); \psi_*\mu = \mu\}$

$$G_{\varphi\circ\psi}(U\circ\psi, V\circ\psi) = G_\varphi(U,V)$$

- Consequence: G induces Riemannian metric $\bar{G}$ on quotient $\mathit{Diff}(M)/\mathit{SDiff}(M)$
- **Moser's lemma** (1965): $\mathit{Diff}(M)/\mathit{SDiff}(M) \simeq \mathit{Dens}(M)$ by $\pi\colon \varphi \mapsto \varphi_*\mu$
- Magic: distance of $\bar{G}$ is **Wasserstein distance**
- Otto's "flagship": heat equation is gradient flow of entropy w.r.t. $\bar{G}$



SDiff(M)
φ
id
∇f
Diff(M)
π
Dens(M)
μ0
μ1

Fisher–Rao metric on $Dens(M)$

Canonical metric on $Dens(M)$, important in **information geometry**

Fisher–Rao metric

$$\bar{G}^F_\mu(\alpha,\beta) = \int_M \frac{\alpha}{\mu}\frac{\beta}{\mu}\mu$$

Properties

1. Unique right-invariant metric on $Dens(M)$

$$\bar{G}^F_{\varphi^*\mu}(\varphi^*\alpha,\varphi^*\beta) = \bar{G}^F_\mu(\alpha,\beta), \quad \forall\,\varphi \in Diff(M)$$

2. **Geodesics are explicit** $\Rightarrow$ distance function is explicit

Idea: use Fisher–Rao distance instead of Wasserstein
Question: Riemannian metric on $Diff(M)$ descending to Fisher–Rao?

Geometry of the Hunter–Saxton equation

$$u_{txx} + 2u_x u_{xx} + u u_{xxx} = 0, \quad u\colon [0,1] \times S^1 \to \mathbf{R}$$

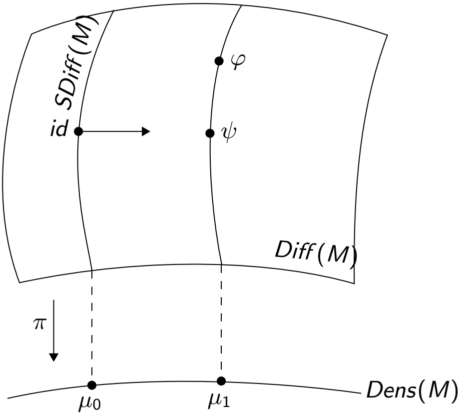
- Model for rotors in liquid crystal [Hunter and Saxton, 1991]
- Geodesic eq. on $S^1 \backslash \mathit{Diff}(S^1) = \{(\varphi + \mathbf{R})\, \mathit{mod}\, 2\pi \mid \varphi \in \mathit{Diff}(S^1)\}$ [Khesin and Misiolek, 2003]
- Astonishing geometry! [Lenells, 2007]

Isometric mapping to convex subset of $L^2(S^1)$–sphere

$$\varphi \mapsto \sqrt{\varphi_x}$$

Generalization to higher dimensions [Khesin, Lenells, Misiolek, Preston, 2013]

- Fisher–Rao induces metric on $SDiff(M)\backslash Diff(M)$



New Riemannian metric on $\mathit{Diff}(M)$ (information metric)

$$G^I_{id}(u,v) = \int_M \operatorname{tr}(\mathcal{L}_u g (\mathcal{L}_v g)^\top)\mu + \sum_{i=1}^{k} \langle \xi_k, u\rangle \langle \xi_k, v\rangle$$

Lemma (M. 2014)

G^I descends to Fisher–Rao under projection

$$\pi\colon\ \mathit{Diff}(M) \to \mathit{Dens}(M), \quad \varphi \mapsto \varphi^*\mu$$

Corollary

Horizontal geodesics *on $\mathit{Diff}(M)$ by lifting equations*

$$\Delta f(t) = \frac{\dot\mu(t)}{\mu(t)} \circ \varphi(t)^{-1}$$

$$v = \operatorname{grad} f(t)$$

$$\dot\varphi(t) = v(t)\circ\varphi(t)$$

Optimal Information Transport (OIT)

- $\bar{d}_F$ the Fisher–Rao distance function
- d_I the distance function of G^I

OIT problem (exact density matching)

Given $\mu_0, \mu_1 \in Dens^{s-1}(M)$, find $\varphi \in Diff^s(M)$ minimizing

$$d_I(id, \varphi)$$

under constraint $\varphi_* \mu_0 = \mu_1$

Theorem (M. 2015)

Every $\phi \in Diff^s(M)$ has a unique decomposition $\varphi = \psi \circ \exp_{G^I}(\nabla f)$ with $\psi \in SDiff^s(M)$ and $f \in H^{s+1}(M)$

Corollary

OIT problem has unique solution of the form $\exp_{G^I}(\nabla f)$

Fast numerical method using information transport

Algorithm 1 (Bauer, Joshi, and M., 2015)

1. Use explicit $[0,1] \ni t \mapsto \mu(t) \in Dens(M)$ (Fisher–Rao geodesic)
2. At each time $t_k = k/N$
   - Lift $\dot\mu(t_k)$ to vector field $v(t_k) = \operatorname{grad} f(t_k)$ (solve Poisson problem)
   - Use Lie–Trotter formula to advance horizontal geodesic $\varphi(t_{k+1}) = \exp(v(t_k)) \circ \varphi(t_k)$

Algorithm 2 (Bauer, Joshi, and M., 2015)

1. Fisher–Rao gradient flow on $Dens(M) \times Dens(M)$
2. At each time t_k
   - Lift $\dot\mu(t_k)$ to vector field $v(t_k) = \operatorname{grad} f(t_k)$ (solve Poisson problem)
   - Use Lie–Trotter formula to advance horizontal geodesic $\varphi(t_{k+1}) = \exp(v(t_k)) \circ \varphi(t_k)$

Applications

1. **Medical image registration**
2. Texture mapping in computer graphics
3. Image morphing techniques
4. Random sampling
5. Mesh adaptivity in numerical PDE

Outline of talk

Example: random sampling from non-uniform distribution

- Let $M = \mathbb{T}^2$
- Non-uniform distribution, for example

$$\mu_1 = (1 - 0.8\cos(x)\cos(2y))dx \wedge dy$$

Problem formulation

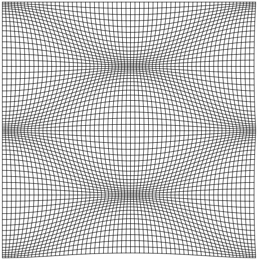
Draw N random samples from distribution μ_1

Approach

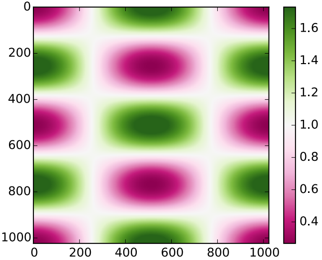
- Use OIT to match μ with μ_1, i.e., $\varphi \in \mathit{Diff}(M)$ s.t. $\varphi_* \mu = \mu_1$
- Draw N uniform samples (x_i, y_i) on $\mathbb{T}$
- Non-uniform samples given by $(\tilde{x}_i, \tilde{y}_i) = \varphi(x_i, y_i)$

Example: random sampling from non-uniform distribution

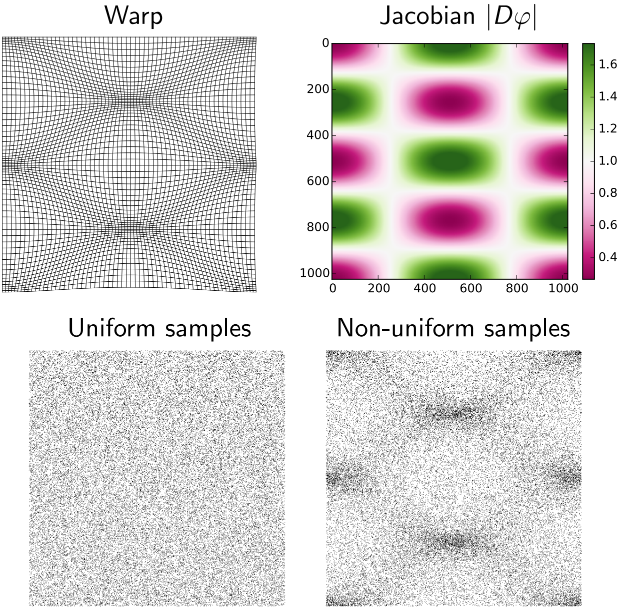
Warp



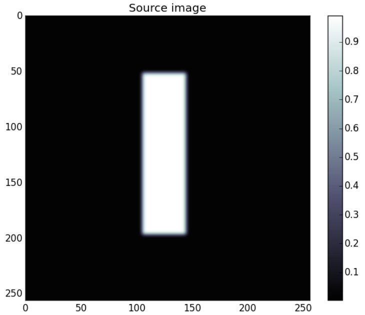
Jacobian $|D\varphi|$

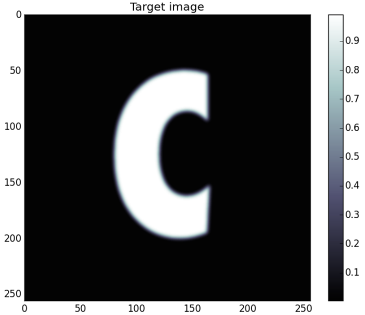


Example: random sampling from non-uniform distribution



Example: I to C





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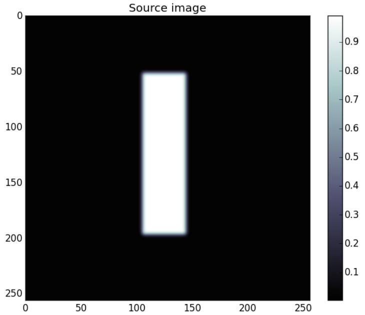
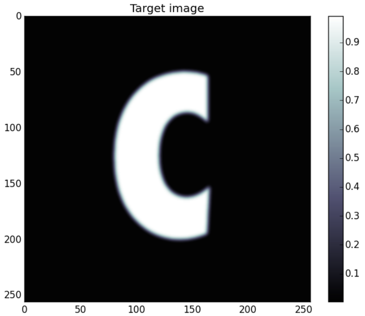
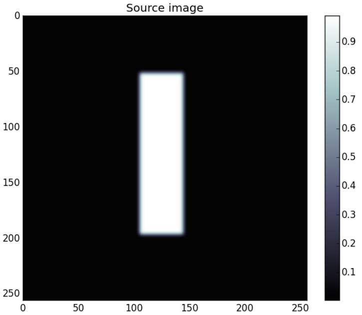
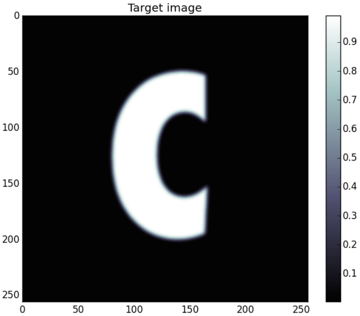




Example: I to C





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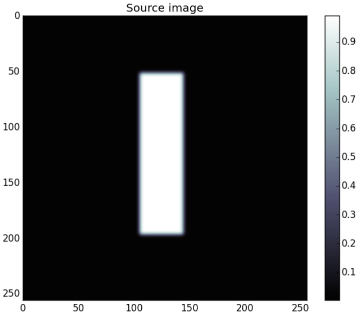

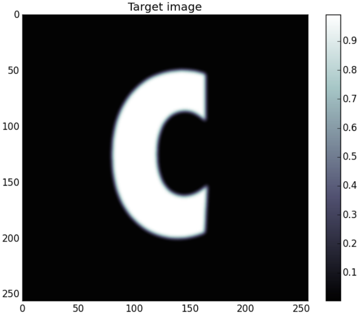

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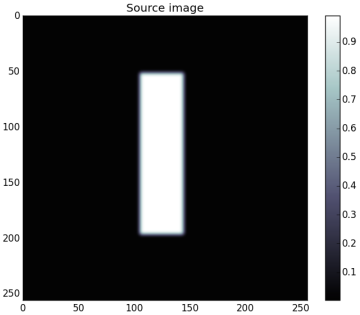

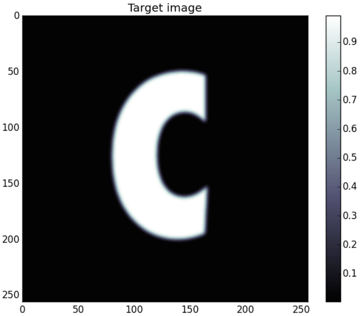

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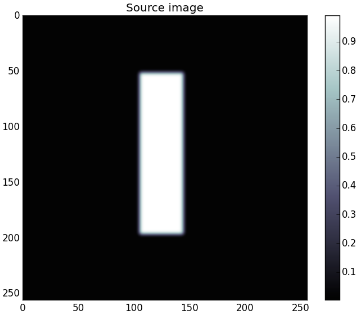

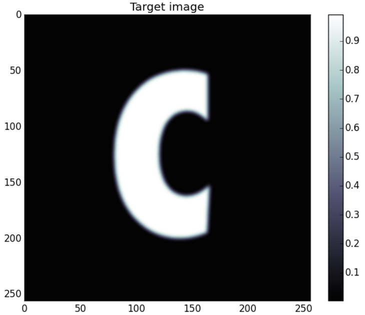

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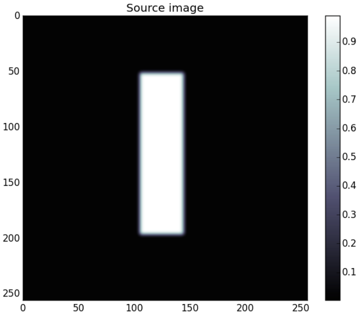

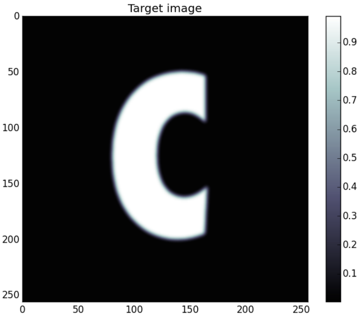

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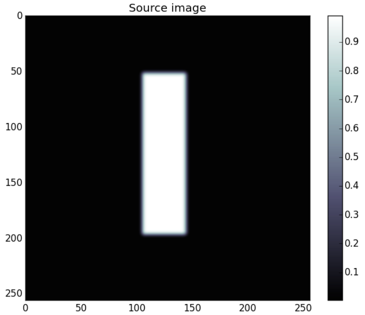

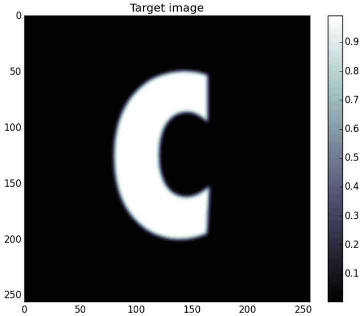

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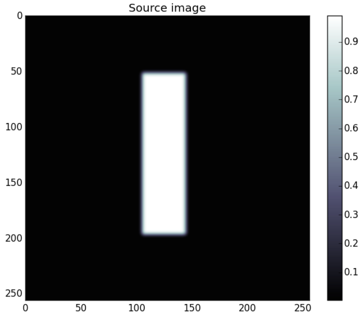

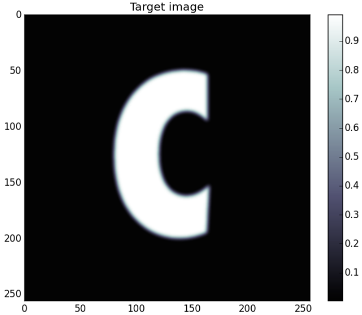

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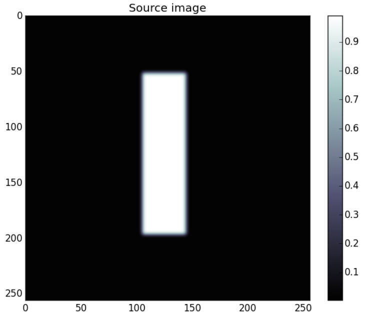

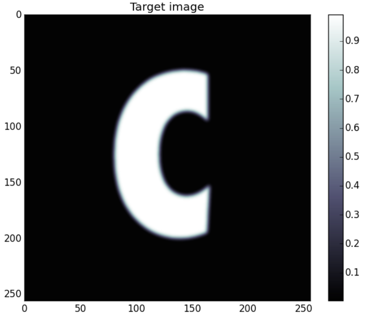

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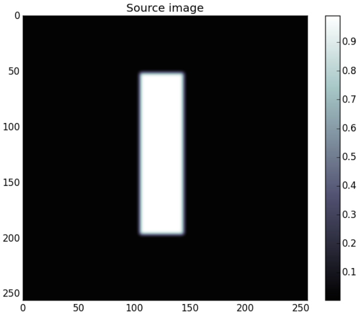

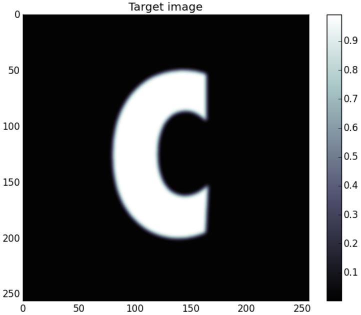

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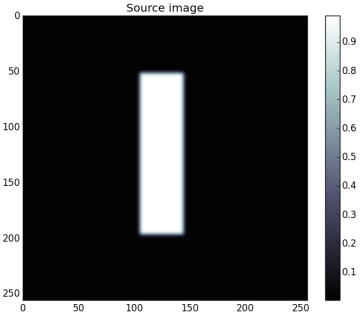
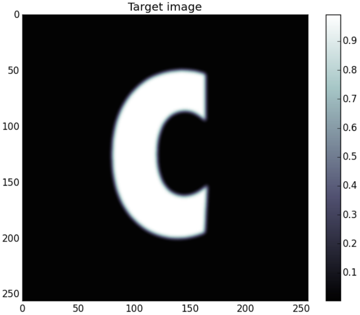
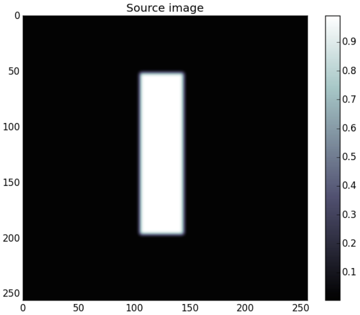
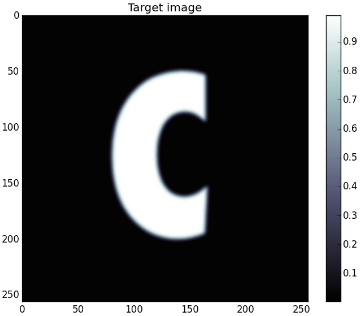


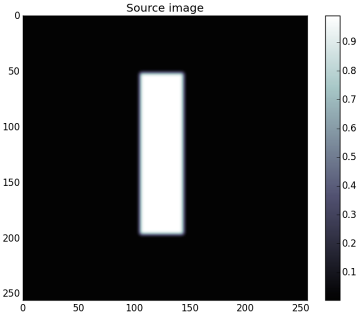


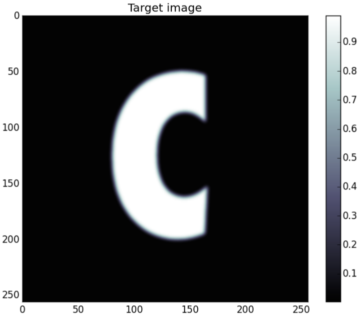
Example: I to C



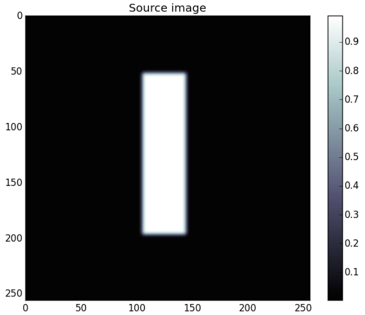


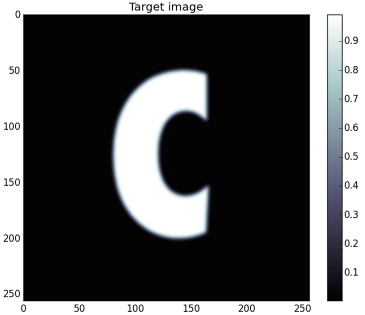
Example: I to C





Example: I to C





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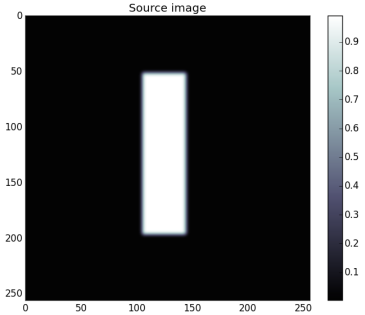

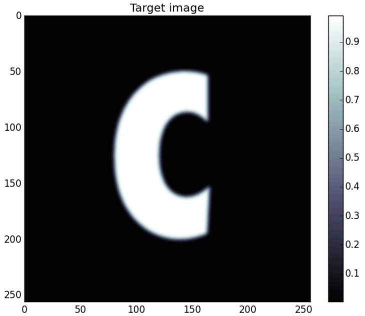

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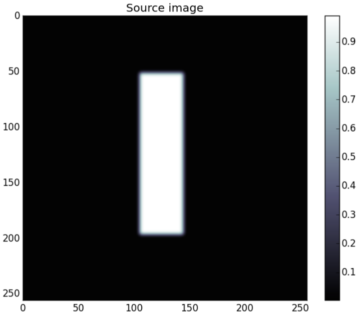
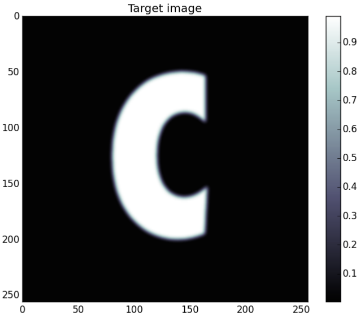
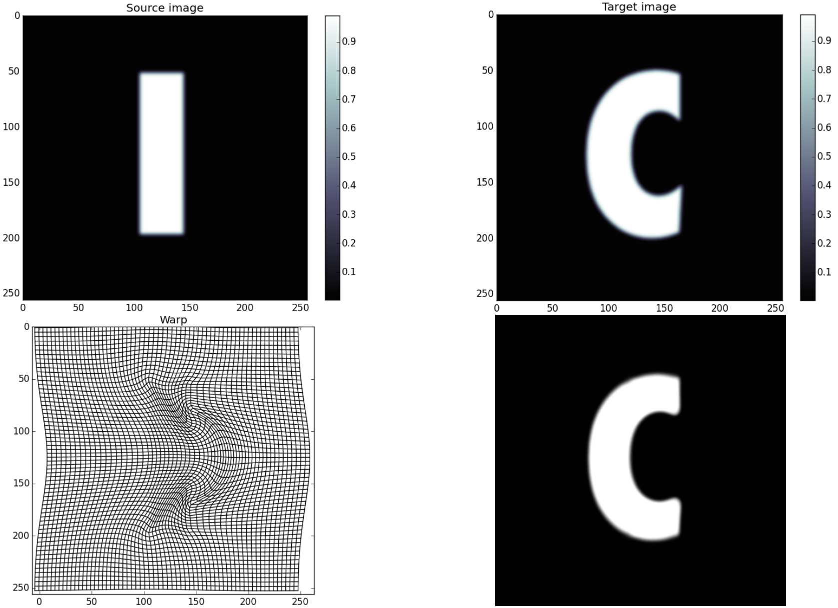




Example: I to C



Example: J to V

Example: J to V

Example: J to V

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Example: J to V

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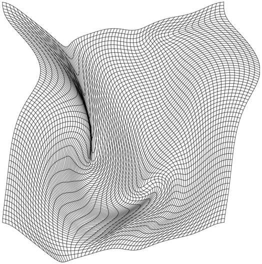
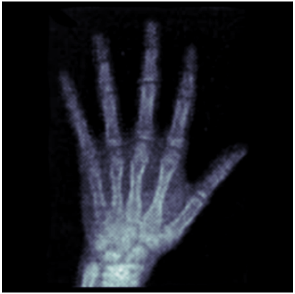


Example: hand x-ray registration



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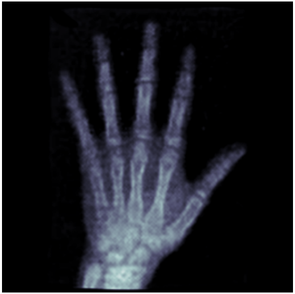

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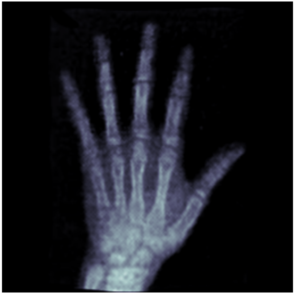

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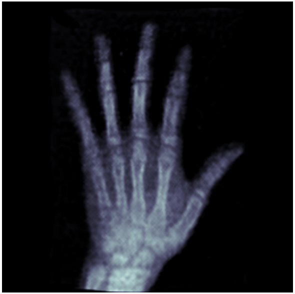

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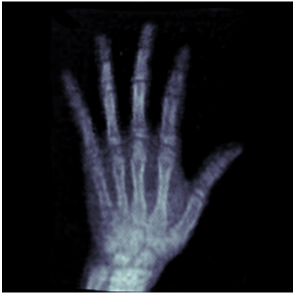

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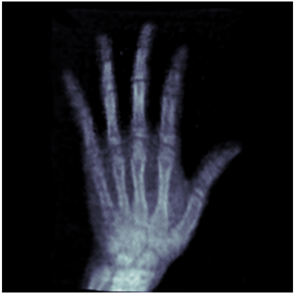

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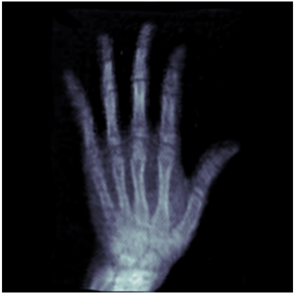

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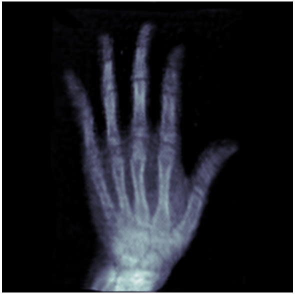

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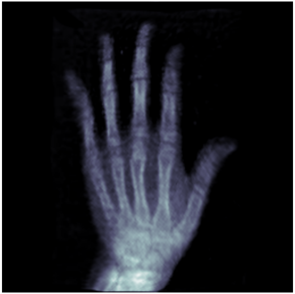

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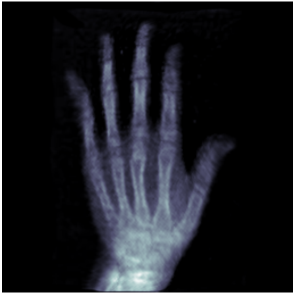

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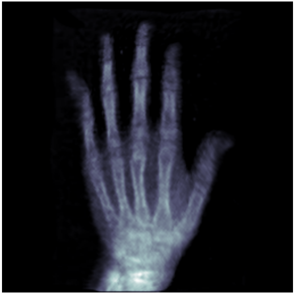

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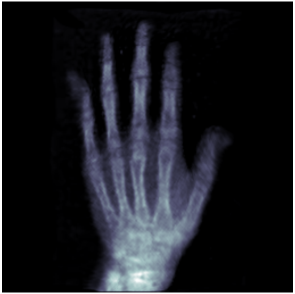

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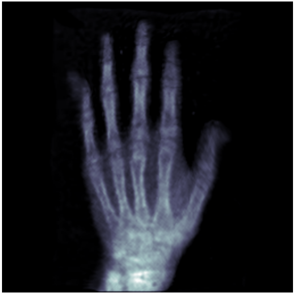
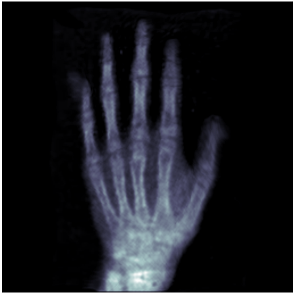


Example: hand x-ray registration



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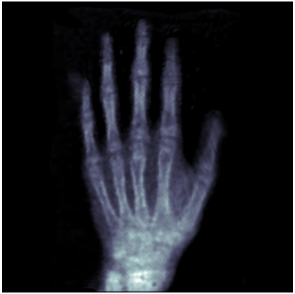
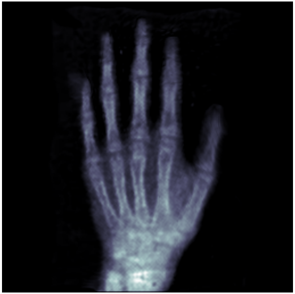


Example: hand x-ray registration



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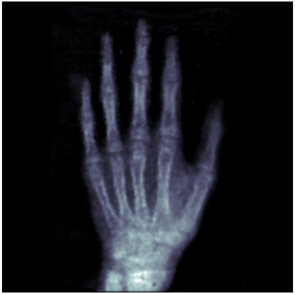

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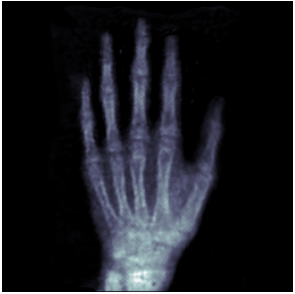

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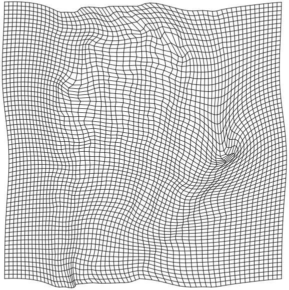
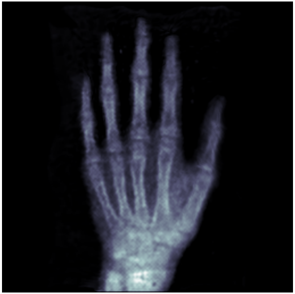
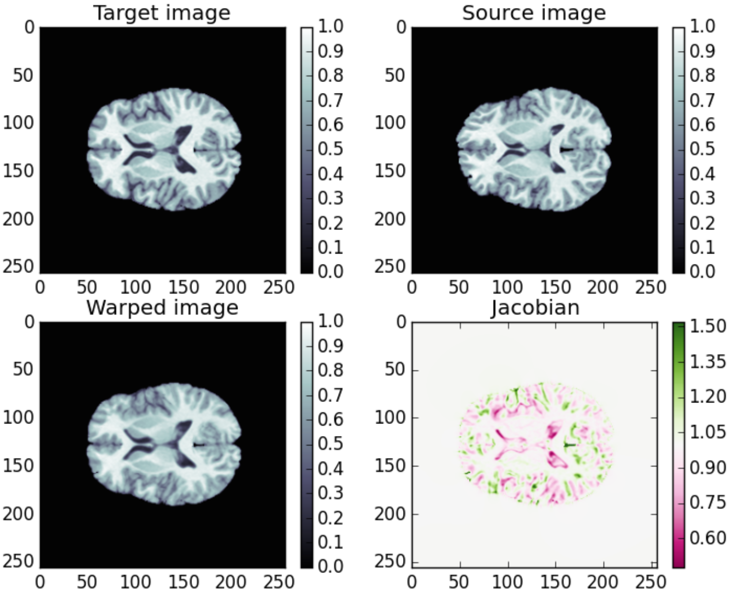




Example: brain MRI registration



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THANK YOU!