Numerical method for solving EPDiff equation in Computational Anatomy

Felipe Arrate, Laurent Younes, and J.T. Ratnanather

Johns Hopkins University

Introduction

Computational anatomy (CA) introduces the idea of anatomical structures being transformed by geodesic deformations on groups of diffeomorphisms. Among these geometric structures, landmarks and image outlines in CA become singular solutions of the geodesic Euler-Poincaré equation on the diffeomorphisms, or EPDiff.

The obtained setting in CA shares several similarities with the mechanics of perfect fluids (divergence-free), both involving a right-invariant stationary principle, with an action in the fluid dynamics case and a cost function in the CA case.

As emphasized by Arnold (1966), the underlying relation is that many fundamental properties of Lie groups in rigid body mechanics, which can be proved in the finite-dimensional case, can be formally extended to the infinite-dimensional functional setting for the study of high dimensional shapes via diffeomorphisms. This point of view will relate the geodesic deformation of shapes with the conservation of momentum law in Lagrangian coordinates.

In the following, EPDiff is analyzed as an expression of the evolution of the generalized momentum of diffeomorphic flow of least energy/cost, in Eulerian and Lagrangian coordinates. In particular, the momentum map for singular solutions of the EPDiff will yield their a canonical Hamiltonian formulation, which in turn will provide a complete parametrization of the landmarks by their canonical positions and initial momenta.

Recently numerical methods for EPDiff based on geometric integration have been proposed (McLachlan & Marsland, 2006; Cotter and Holm 2006). In particular Cotter's approach allows a considerably speed up of the main calculation. In this study, the implementation an alternative of Cotter's approach in 2 and 3 dimensions will be presented.

Mathematical Model

The anatomic orbit of an image template is made into a metric space with the definition of a distance between elements, by constructing curves through the space of diffeomorphisms connecting them. The length of the curve becomes the basis for the construction, the metric distance corresponding to the geodesic shortest length curves.

$$Cost(v) = \int_0^1 \|v_t\|_V^2 \, dt \qquad (1)$$

Following Trouvé (1995), the construction of the cost function is based on the design of the Lie algebra V, which in turns it is used to generate the elements of the group of diffeomorphisms $\varphi_t^v \in \mathcal{G}_\mathcal{V}$. Our space of action will be an open bounded set $\Omega \subset \mathbb{R}^d$.

1. Take the Hilbert space $H = L^2(\Omega, \mathbb{R}^d)$. Select a symmetric and strongly monotone operator $L \in H^*$, $L : u \mapsto Lu$, whose domain (D_L) is a subspace of H. This operator induces an inner product on D_L, called the energetic inner product

$$\langle u\,,\, v \rangle_{D_L} := \langle Lu\,,\, v \rangle_H \qquad (2)$$

2. D_L is not complete for $\|\cdot\|_{D_L}$, but it can be completed following *Friedrich's extension Theorem* (Zeidler, 1995), to form a Hilbert subspace $V \subset H$, and extending the operator L to $L_E : V \to V^*$, restricted to any $u \in V$ such that $L_E u \in H^*$. Therefore, the following definition can be expressed

$$\langle u\,,\, v \rangle_V = \langle Lu\,,\, v \rangle_H = (L_E u \mid v)$$

3. Assume in addition that V can be embedded into $C^p(\Omega)$, $p \geq 1$. This condition makes V **p-admissible**. $\mathcal{X}_V^2(\Omega) \subset L^2(\Omega, \mathbb{R}^d)$ is defined to be the set of time-dependent vector fields, v_t, $(t \in [0,1])$ such that for each t, v_t is in V, and

$$\|v_t\|_{\mathcal{X}_V^2} := \int_0^1 \|v_t\|_V^2 \, dt < \infty$$

4. It has been proven that if $v_t \in \mathcal{X}_V^2(\Omega)$, the flow $\partial\varphi_t^v/\partial t = v \circ \varphi_t^v$ with initial conditions $\varphi_0(x) = x, x \in \Omega$, can be integrated over $[0,1]$. This construction makes φ_1 a diffeomorphism of Ω, denoted φ_1^v and a member of the group of diffeomorphisms $\mathcal{G}_\mathcal{V}$.
5. Since the flow φ_t^v is an extremal of the cost function (1), its first variation is taken equal to 0

$$\delta \int_0^1 \|v_t\|_V^2 \, dt = 0$$

yielding (Miller et al.)

$$\boxed{\frac{dLv_t}{dt} + ad_{v_t}^* Lv_t = 0} \qquad (3)$$

The dual adjoint operator ad_v^* is defined as

$$ad_v w = [v, w] \qquad (ad_v^* f \mid w) = (f \mid ad_v w)$$

6. This equation is another way of expressing the principle of conservation of momentum, that in Lagrangian coordinates is

$$m_t = Ad_{\varphi_{t0}}^* m_0, \qquad m_0, m_t \in V* \qquad (4)$$

or as $v_t = Ad_{\varphi_{t0}}^* v_0$. $\left(Ad_\varphi^* f \mid w\right) = \left(f \,\middle|\, Ad_\varphi w\right)$ and $Ad_\varphi w = D_{\varphi^{-1}}\varphi \cdot v \circ \varphi^{-1}$.

7. Assuming $\{e_1, \ldots, e_d\}$ as an orthonormal basis of $\mathbb{R}^d$, for $y \in \Omega$, we have

$$Ad_\varphi^T v(y) = \sum_{i=1}^d \left(m \mid Ad_\varphi K(\cdot, y) e_i\right) e_i$$

8. Using the fact that $d\varphi_t^v/dt = v(t, \varphi_t^v)$, and combining the conservation of momentum (4) with this last equation, we obtain

$$\boxed{\frac{d\varphi_t^v(y)}{dt} = \sum_{i=1}^d \left(m_0 \,\middle|\, (D\varphi_t)^{-1} K^i(\varphi_t^v(\cdot), \varphi_t^v(y))\right) e_i}$$

9. After the derivation of the last equation w.r.t. t, the evolution of $D\varphi_t^v$ becomes

$$\frac{d}{dt} D\varphi_t^v(y).\beta = \sum_{i=1}^d \left(m_0 \,\middle|\, (D\varphi_t)^{-1} D_2 K^i(\varphi_t^v(\cdot), \varphi_t^v(y)) D\varphi_t^v(y).\beta\right) e_i$$

Defining $M_t := (D\varphi_t^v)^{-1}$, we obtain $dM/dt = -M\frac{d}{dt}(D\varphi_t^v)M$. So

$$\boxed{\frac{dM_t(y)}{dt}.\beta = -\sum_{i=1}^d \left(m_0 \middle| M_t(\cdot) D_2 K^{(i)}(\varphi(\cdot), \varphi(y)).\beta\right) M_t(y) e_i}$$

Landmark Evolution

Take two collections of points: $X_{ii=1,N}$ and $Y_{ii=1,N}$ in Ω. Find the deformation path with minimal cost, under the constraint that it carries X_i points to Y_i points. In this setting, one suitable definition for the momentum: $m_0 = \sum_{k=1}^N (a_k \otimes \delta_{x_k}) \in V^*$. Defining $b_k(t) := M_t(x_k)^T a_k$, the system of ODE equations reduces to:

$$\frac{d\varphi_t^v(y)}{dt} = \sum_{i=1}^d \sum_{k=1}^N b_k(t)^T K^i(\varphi_t^v(x_k), \varphi_t^v(y)) e_i$$

$$\frac{dM_t(y)}{dt} = -\sum_{i=1}^d \sum_{k=1}^N b_k(t)^T D_2 K^{(i)}(\varphi(x_k), \varphi(y)) M_t(y) e_i$$

Selecting a Gaussian Kernel $K(x,y) = \gamma(x-y) I_d$, with $\gamma(x-y) = e^{\|x-y\|^2/\sigma^2}$ and solving for $y = x_k$, we obtain an ODE Hamiltonian system of equations in terms of the landmark points x_k,

$$\frac{d\varphi_t^v(x_i)}{dt} = \sum_{k=1}^N b_k(t)^T \gamma(\varphi_t^v(x_k) - \varphi_t^v(x_i)) \qquad (5)$$

$$\frac{dM_t(x_i)}{dt} = -M_t(x_i) \sum_{k=1}^N b_k(t) \nabla\gamma_k(\varphi_t^v(x_k) - \varphi_t^v(x_i))$$

Conservation of Energy The first variation of the energy (1) vanishes along the extremal path described by the last set of equations. Following a mechanical point of view, this implies that the Hamiltonian energy is conserved. Combining equation (5) with $d\varphi_t^v/dt = v(t, \varphi_t^v)$ and with the definition of the momenta, we obtain for the energy in the system:

$$\begin{aligned}
\langle Lv_t\,,\, v_t \rangle &= \sum_{kl}^N \left(b_k(t) \otimes \delta_{\varphi_t^v(x_k)} \mid v_t(\cdot)\right) \\
&= \sum_{k=1}^N \sum_{l=1}^N \left(b_k(t) \otimes \delta_{\varphi_t^v(x_k)} \,\middle|\, K(\cdot, \varphi_t^v(x_l)) M_t(x_l)^T a_l\right) \\
&= \sum_{k=1}^N b_k(t)^T \sum_{l=1}^N K(\varphi_t^v(x_k), \varphi_t^v(x_l)) M_t(x_l) a_l \\
&= \sum_{k=1}^N b_k(t)^T \frac{d\varphi_t^v(x_k)}{dt}
\end{aligned}$$

Results

The double sum in each equation can be implemented as a convolution using FFT transforms. The process involves a dual interpolation of the discrete vector field $b_k(t)$ into a grid that covers the whole evolution space, proceeded by the filtering of this grid with the Gaussian Kernel and its derivative. The following figures show the evolution of several 2 and 3 dimensional set of landmarks.

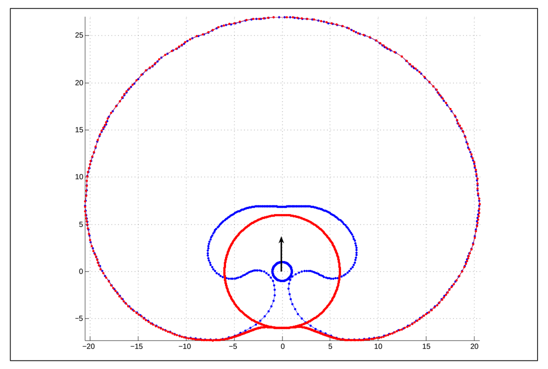

Fig 1. 2D Evolution, 1000 points, speed factor: 15

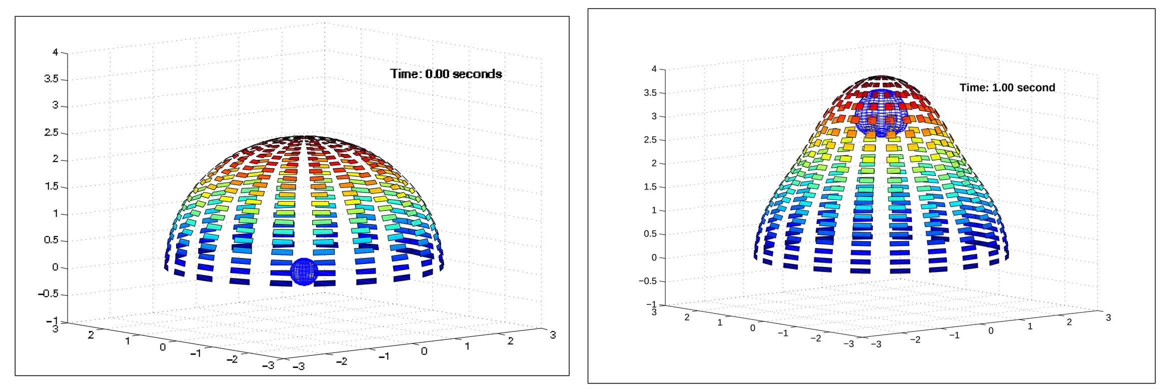

Fig 2. 3D Evolution, 1000 points, speed factor 10

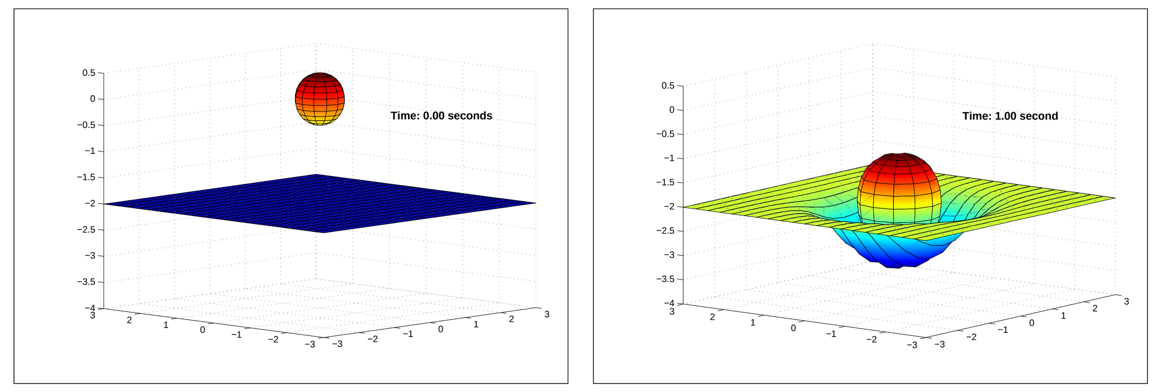

Fig 3. 3D Evolution, 1000 points, speed factor 10

References

- Arnold, V.I., (1966). *Mathematical Methods of Classical Mechanics*, Springer, New York.
- Hairer, E., Lubich, C., Wanner, G., (2002). *Geometric Numerical Integration. Structure-Preserving Algorithms for Ordinary Differential Equations*. Springer-Verlag Berlin, Heidelberg.
- Holm, D.D., Ratnanather JT, Trouv A, Younes L., (2004). *Soliton dynamics in computational anatomy*. NeuroImage, vol 23, S170-S178
- Holm, D.D., (2005). *Geometry, Symmetry and Mechanics*. Notes for the course M4A34, Imperial College London.
- Cotter, C., and Holm, D.D., (2006). *Discrete momentum maps for EPDiff*. http://arxiv.org/abs/math/0602296v1
- Marsden, J., Ratiu, T., (2001). *Manifolds, Tensor Analysis and Applications*. Springer, New York.
- McLachlan, R.I. and Marsland, SR. (2006). *The Kelvin-Helmholtz instability of momentum sheets in the Euler equations for planar diffeomorphisms*. SIAM Journal on Applied Dynamical Systems, 5, 726-758.
- Miller, M, Trouv A, Younes L. (2006). *Geodesic Shooting for Computational Anatomy*. J Math Imaging, vol 24, p209-228

Supported by NSF (DMS-0456253) and NIH (R01-MH064838, P41-RR15241, RO1-MH60883, P20-MH071616, P01-AG003991, P01-AG026276).