BIRS Workshop-Report: Shape Analysis, Stochastic Mechanics and Optimal Transport

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2 Overview of the Field

The mathematical and computational analysis of shape and shape changes has, over the last few years, been at the center of focused research efforts, driven by a wide range of applications, from biological imaging to fluid dynamics. Problems in areas as diverse as shape optimisation, functional data analysis and computer graphics can all be formulated in terms of shape analysis.

Mathematically, shape analysis combines ideas from infinite-dimensional Riemannian geometry, geometric mechanics, fluid dynamics and, recently, also sub-Riemannian geometry and stochastic analysis. This interplay of different areas continues the historically very fruitful exchange of ideas between geometry, mechanics and applications.

In many instances, shape spaces can be endowed with the structure of an infinite-dimensional Riemannian manifold. Examples include the shape space of curves or surfaces in Euclidean space, the space of densities as well as more general spaces of mappings. The diffeomorphism group in particular plays a central role in the field of shape analysis and medical imaging.

The main objective of the workshop was to bridge the gap between shape analysis, stochastic geometric mechanics and applied optimal transport communities and to advance research that crosses the boundaries of the three fields in addition to communicating important challenges in shape analysis to researchers in stochastic geometric mechanics and optimal transport.

2.1 Shape analysis and medical imaging

The space of images is acted upon by the diffeomorphism group and, in the spirit of Grenander's pattern theory [1], differences between images can be encoded by diffeomorphisms. In this way medical images can be investigated with the help of Riemannian metrics on the diffeomorphism group. One of the major applications of Grenander's pattern theory is in computational anatomy [2], a field that uses modern imaging techniques, such as magnetic resonance, computed tomography and positron emission tomography, to perform a precise computational study of functional and anatomical morphology. Currently, the extension of statistical tools such as kernel PCA and regression, that are well understood in the linear setting, to finite and infinite-dimensional Riemannian shape manifolds is of great interest to the medical imaging and computer vision communities. This in addition provide links with geometric statistics [3], statistical analysis of data taking values in geometric spaces.

2.2 Stochastic geometric mechanics

Shapes observed in nature exhibit variations that are often best described stochastically. Thus there is a need, arising from applications, for stochastic shape models, that would enable statistical analysis of shape populations and describe stochastic nonlinear shape variations in a geometrically intrinsic way. The diffeomorphism group, which describes shape variations through its action on shape space [4], allows us to transfer developments happening in the new and growing field of stochastic geometric mechanics to problems in stochastic shape analysis.

Recent work has shown that the Euler-Poincaré equation on the diffeomorphism group has a stochastic analog [5], derived from a stochastic variational principle, that yields natural stochastic models of shape evolution. The diffeomorphism group can be equipped with a Lie group structure giving rise to Brownian type flows that are mapped from the Lie algebra to the group. Lagrangian Navier-Stokes flows [6] also constitute an alternative approach to stochastic flows. In very recent work, it has been shown how such flows can induce stochastic shape evolutions [7] but very little is known about their properties, such as existence, invariant distributions or ergodicity. Stochastic geometric mechanics is still a new field, and the similarity between stochastic flows on finite-dimensional Lie groups and stochastic flows on shape spaces induced by the diffeomorphism group enables developments in both fields to be transferred between them. For example, Riemannian stochastic models in shape analysis are used to construct stochastic models in geometric mechanics, whose definition relies on the affine connection. The workshop had as an objective to introduce in the shape community models from stochastic geometric mechanics, and to link ideas from shape analysis back to geometric mechanics.

2.3 Optimal transport

Independently, optimal transport has seen significant development as an area of pure mathematics. One can consider optimal transport as a special case of Riemannian shape analysis, with shapes being probability densities. Improved numerical methods, such as Monge-Ampère type solvers and entropic regularization schemes, have recently expanded the applications of optimal transport to include computer vision, biomedical imaging, machine learning and statistics. Compared to optimisation problems encountered in shape analysis, those in optimal transport often stand out by being convex, thus simplifying and speeding up computations. Nevertheless, embedding optimal transport into the more general framework of shape analysis allows one to consider possible extensions of optimal transport; for example the recently developed unbalanced optimal transport was partly inspired by ideas in shape analysis.

In turn, stochastic variants of optimal transport such as the Schrödinger problem of minimizing the relative entropy with respect to a Wiener process does not, at the moment, have a counterpart in stochastic shape analysis or stochastic geometric mechanics. An important outcome of entropic regularization of optimal transport is the development of algorithms that allow for fast computations of entropically regularized transport maps. For many problems in shape analysis, for example the computation of geodesics on the diffeomorphism group, computational time is still prohibitive for large scale applications. Ideas from optimal transport could prove useful in developing new numerical methods for these problems.

3 Presentation Highlights

We here discuss the topics presented in the range of excellent talks at the workshop. These highlights start with optimal transport and related topics followed by geometry of diffeomorphisms and hydrodynamics, stochastic geometric mechanics and stochastic shape analysis, and finally mathematical foundations of shape and image analysis.

3.1 Applied optimal transport and related topics

Talks concerned with optimal transport started with Ana-Bela Cruzeiro who presented an extension of the Schrödinger problem to Lie group valued processes. The infinite dimensional case and its connection with fluid dynamics ([8]), currently an open research area, was also touched upon. In particular it is not known how to obtain more regularity for the weak generalized flows associated to the Navier-Stokes equations through optimal transport methods and how to approach compressible Navier-Stokes equations.

On the space of probability densities, Christian Léonard presented a reformulation and a generalization of the so-called entropic interpolation of Wasserstein geodesics in terms of Newton equations on the space of densities ([9]). He was able to present a general contraction inequality for the Schrödinger problem on a Riemannian manifold with Ricci lower bound.

Other talks in optimal transport were centered on extensions of optimal transport and applications. Based on [10], semi-discrete numerical solutions of unbalanced optimal transport were presented by Bernhard Schmitzer and interesting connections and applications in fluid dynamic for the generalized Camassa-Holm equations were presented by Andrea Natale as in [11]. Unbalanced optimal transport appears to have applications not only in quantization but more surprisingly in crystallization.

Tryphon Georgiou presented a numerical approximation to optimal transport using Gaussian approximations, and also presented extensions of optimal transport to vector valued and matrix valued optimal mass transport. Based on a matrix continuity equation, the Linblad equation known in quantum theory was obtained as a gradient flow of the Von Neuman entropy which is a non-commutative counterpart of the pioneering result of Jordan-Kinderlehrer-Otto. An open question of interest in this field consists in providing a unified framework to all these generalizations of optimal transport to cone valued measures.

Tom Needham introduced the Gromov-Monge quasimetric, which is a notion of distance between arbitrary compact metric measure spaces that blends the Monge formulation of optimal transport with the Gromov-Hausdorff construction. He discussed applications to metric trees, which appear in shape analysis and data visualization. Alice Le Brigant spoke on optimal quantization on Riemannian manifolds, which is the problem of finding the best (with respect to Wasserstein distance) finite discrete approximation to a given probability distribution. She presented a new online algorithm as well as an application to summarizing air traffic complexity in which she compared summaries using discrete optimal transport.

Carola Schönlieb has shown the use of the Wasserstein distance in unsupervised learning of regularizers in inverse imaging problems such as tomography, the Wasserstein distance being here approximated via the dual formulation on the space of 1-Lipschitz functions. Another use of optimal transport was proposed by Jean Feydy in shape matching where a similarity divergence [12] was built upon entropic regularization. Importantly, numerical advances on the computation of these metrics for a large number of data were shown.

On the numerical side of optimal transport, Jean-David Benamou presented the extension of the Sinkhorn algorithm to a multi-marginal setting as in [13] for the simulation of the generalized incompressible Euler equation which was introduced by Brenier in the 90s. The Sinkhorn algorithm is known to converge linearly with respect to a Hilbert norm in the case of standard optimal transport with two marginals. Although the multimarginal scheme proposed by Jean-David Benamou is variational and provably convergent, it is an open question to prove the linear convergence with respect to a modified Hilbert norm.

Related to these generalized incompressible Euler equations, Andrea Natale presented, as in [11], a generalized Camassa-Holm equation based on the unbalanced optimal transport problem, which is related to Bernhard Schmitzer's talk. He has introduced a convex relaxation of the Camassa-Holm equation à la Brenier. The main open question is the tightness of this relaxation in dimension greater or equal to 2. Andrea Natale showed that in a particular case this relaxation was tight and his construction was similar to the one proposed by Cy Maor in his vanishing distance result on the diffeomorphism group.

These optimal transport talks have shown that generalizations of optimal transport are a very active topic of research in connections with fluid dynamic, quantum theory and practical applications. In all these talks, the entropic interpolation stands out and was a central tool for practical use and extensions, and also motivated theoretical developments.

3.2 Geometry of the diffeomorphism group and mathematical hydrodynamics

The first series of talks on infinite dimensional Riemannian geometry concerned the geometry of the diffeomorphism group in the particular context of mathematical hydrodynamics. Boris Khesin focused in his talk on the geometry of the Madelung transform, which is known to relate Schrödinger-type equations in quantum mechanics and the Euler equations for barotropic-type fluids. He presented a recent result by himself, K. Modin and G. Misiolek [14] in which they showed that the Madelung transform is a Kähler map (i.e. a symplectomorphism and an isometry) between the space of wave functions and the cotangent bundle to the density space equipped with the Fubini-Study metric and the Fisher-Rao information metric, respectively.

Gerard Misiolek's lecture centered around Arnold's geometric picture [15] for the incompressible Euler equations as geodesic equation on the group of diffeomorphisms of the fluid domain equipped with a L^2-metric given by fluid's kinetic energy. Misiolek gave a detailed overview of the study of the exponential map of this metric and described several recent results concerning its properties. These investigations of the geometric properties of the L^2-metric on the group of volume preserving diffeomorphisms date back to the seminal paper by Ebin and Marsden [16], in which they proved local well-posedness and uniqueness of the solutions to the corresponding geodesic initial value problem. These techniques have been later extended to the class of *right invariant* Sobolev metrics on the full diffeomorphism group. This observation lead to geometric interpretations of many prominent equations of mathematical hydrodynamics, including for example the Camassa-Holm [17, 18] or KdV-equation [19]. In his talk Stephen Preston discussed how many of these one-dimensional Euler-Arnold equations can be recast in the form of a central-force problem

$$\Gamma_{tt}(t,x) = -F(t,x)\Gamma(t,x),$$

where Γ is a vector in $\mathbb{R}^2$ and F is a nonlocal function possibly depending on Γ and Γ_t. Angular momentum of this system is precisely the conserved momentum for the Euler-Arnold equation. In the solar model, breakdown comes from a particle hitting the origin in finite time, which is only possible with zero angular momentum. In his talk Preston discussed some conjectures and numerical evidence for the generalization of this picture to other equations such as the μ-Camassa-Holm equation or the DeGregorio equation. Klas Modin presented a recent result with Martin Bauer [20] in which they prove extensions of the Ebin and Marsden result to higher order Sobolev metrics on diffeomorphism groups that are only invariant with respect to volumorphisms. This study reveals many pitfalls in going from fully right invariant to semi-invariant Sobolev metrics; the regularity requirements, for example, are higher. Nevertheless the key results, such as no loss or gain in regularity along geodesics, can be adopted.

While these previous talks focused mainly on properties of the geodesic spray (geodesic initial value problem resp.), the lecture of Cy Maor studied a different geometric question that arises in this context: properties of the geodesic distance induced by right invariant metrics on diffeomorphism groups and in particular the question whether it is positive between distinct diffeomorphisms or not. In this talk he presented a recent preprint by him with Robert Jerrard [21] which shows that the geodesic distance on the diffeomorphism group of an n-dimensional manifold, induced by the $W^{s,p}$ norm, does not vanish if and only if $s \geq 1$ or $sp > n$. The first condition detects changes of volume, while the second one detects transport of arbitrary small sets. In particular he discussed how the failure of these two conditions enables the construction of arbitrarily short paths between distinct diffeomorphisms. This work extends previous results on vanishing geodesic distance by Michor, Mumford and others [22, 23, 24, 25].

3.3 Stochastics in geometric mechanics and shape analysis

The talks on stochastics in geometric mechanics and shape analysis concerned symmetry reduction for two different stochastic models, the stochastic variational principle in Lie groups by Arnaudon, Chen, and Cruzeiro [6] and the variational model by Holm [5], together with particle samplers for Feynman-Kac measures on path spaces.

Ana-Bela Cruzeiro's presented the variational principle and Euler-Poincaré reduction of [6]. The setting is a left- or right-invariant metric on a general Lie group. Noise is introduced in Stratonovich form through a set of vector fields on the Lie algebra, and the resulting stochastic perturbations are transported by the push-forward of left-translation to the group. From this, a stochastic action functional is derived. Critical points of this functional are then shown to be amenable to Euler-Poincaré reduction in a setting resembling the deterministic case (see e.g. [26]). In particular, the motion can be described by

$$\frac{d}{dt}u(t) = \mathrm{ad}^*_{\tilde{u}(t)}u(t) + K(u(t))$$

with

$$\tilde{u}(t) = u(t) - \frac{1}{2}\sum_i \Delta_{H_i} H_i$$

and subsequently reconstructed to the group. In the reconstruction equation, a coupling term appears that comes from the Itô to Stratonovich conversion terms.

Alexis Arnaudon discussed the stochastic model of [5] in the context of shape analysis. Stochastic perturbations are here introduced by perturbing the Hamiltonian that before perturbation comes from a right-invariant metric on e.g. the diffeomorphism group. This leads to a different variational principle, again with Euler-Poincaré reduction for critical paths, however in a different form than considered by Cruzeiro et al.. In coadjoint form, the reduced dynamics are governed by

$$d\mu(t) + \mathrm{ad}^*_{dX}\mu(t) = 0$$

with

$$dX = udt - \sum_i \partial_\mu \Phi_i(\mu) \circ dW^i_t \quad \mu = \frac{\partial l(u)}{u}$$

where Φ_i constitute a basis for the noise and l is a reduced lagrangian. Arnaudon showed how the stochastic dynamics through the action of the diffeomorphism group descend to shape spaces, e.g. the landmark shape space. Here, Arnaudon related the model to Langevin dynamics in different forms, particularly the stochastic model of [27], and he introduced a dissipation term on the Hamilton equations as a general link between the two stochastic landmark equations.

Marc Arnaudon discussed continuous time Feynman-Kac measures on path spaces. There equations are central in applied probability, PDE theory, and quantum physics. Arnaudon presented a new duality formula between normalized Feynman-Kac distributions and their mean field particle interactions. This allows rerversible particle Gibbs-Glauber samplers for continuous time Feynman-Kac integration on path spaces. Arnaudon in addition discussed new estimates for propagation of chaos for continuous time genealogical tree based particle models, allowing sharp quantitative estimates of the convergence rate of particle Gibbs-Glauber samples.

3.4 Mathematical Foundations of Shape and Image Analysis

Several of the talks on Shape and Image analysis concerned new developments for the LDDMM-framework [28]. The first in this direction was by L. Younes, who presented recent work on equivolumic layers estimation in the cortex. B. Gris described a constrained version of LDDMM and showed how this approach can help to understand the variability within a population of shapes. A crucial ingredient for deformation based approaches such as LDDMM is the construction of efficient data attachment terms. Towards this aim, N. Charon presented several deformation models on spaces of oriented varifolds, which embeds many previously considered geometric structures like curves, surfaces but also orientation distribution fields. In particular he discussed compressing/quantizing oriented varifold representations in order to numerically accelerate diffeomorphic registration procedures. D. Kuang presented a completely different method for nonlinear image registration using unsupervised neural networks. This led to some discussion about the relative merits of, on one hand, data driven methods such as Kuang's, and on the other hand, variational and geometric methods such as LDDMM.

A central concept in LDDMM is the momentum vector field; in a related theoretical talk, T. Ratiu introduced a new generalization of the momentum map concept: a group-valued momentum map, inspired by the Poisson Lie setting.

A second theme in this part of the workshop consisted in the study of intrinsically defined metrics on spaces of geometric objects, such as curves or surfaces. E. Klassen presented a new Riemannian metric on the space of vector valued one-forms, that has potential applications for the shape analysis of surfaces. The proposed metric is a direct generalization of the elastic metric associated to the SRV framework [29], that has been proven successful for the analysis of unparametrized curves. Related to this talk was the presentation of P. Harms, who showed that (fractional) Laplacians depend real analytically on the underlying Riemannian metric in suitable Sobolev topologies. As an application he presented local well-posedness of geodesic equations for (fractional) Sobolev metrics on the space of mappings. While these two talks focused mainly on the existence and form of geodesic curves, M. Rumpf studied the existence and construction of spline curves in the context of Riemannian shape spaces. In his talk he introduced a variational time discretization for the spline energy, that leads to a constrained optimization problem over discrete paths on the manifold. Existence of continuous and discrete spline curves is established using the direct method in the calculus of variations and the convergence of discrete spline paths to a continuous spline curve follows from the Γ-convergence of the discrete to the continuous spline energy.

4 Outcomes of the Meeting

This meeting provided an excellent occasion to open discussions and develop connections between several related fields: Applied optimal transport, methods involving diffeomorphic matching, the so-called large deformation by diffeomorphisms, and stochastic geometric mechanics. Different applications context have shown fundamental differences as well as similarities. In addition, the link between these fields and fluid flows was discussed several times in the talks.

A central discussion topic at conference was the question of finite explosion time of Brownian motion on landmark spaces. We consider the LDDMM landmark manifold [30] with metric inherited from a right-invariant metric on the diffeomorphism group. This Riemannian manifold has a global representation as an open subset of Euclidean space. It is thus not compact, which raises the question of finite time blowup of Riemannian Brownian motion. Several recent works use the landmark Brownian motion in applied settings [31, 32] which underlines the interest in the existence question. Furthermore, understanding the structure in the Brownian case may shed light on similar questions for stochastic shape models such as discussed in the talks in this workshop. We made significant progress on this question by finding sharper conditions for finite time collision of the landmarks. Current ongoing work evolves around evaluating these conditions to either prove or disprove finite time explosion.

In informal discussion about applications to medical image registration, tips and tricks were shared, and a divergence of opinion appeared about the likelihood of large practical improvements over the current state of the art, given that the practical registration problem isn't entirely well-posed.

In addition several new projects and discussions have been initiated during the workshop, including: Cy Maor and Philipp Harms on the physics of stress and strain in shape analysis; Martin Bauer, Nicolas Charon, Philipp Harms and Martin Rumpf discussed a new collaboration to obtain a numerical framework for shape analysis of surfaces with respect to higher order Sobolev metrics; Tryphon Georgiou and Tanya Schmah discussed the restriction of the Wasserstein metric to the space of Gaussian mixtures. Martin Bauer, Klas Modin and Cristina Stoica discussed and started a new project related to the existence of 'peakon' singular-suported solutions for non-Newtonian fluids.

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