

# Advances in Numerical Optimal Transportation

Jean-David Benamou (INRIA),  
Yann Brenier (Ecole Polytechnique),  
Adam Oberman (McGill U.)

Feb 15 – Feb 20, 2015

## 1 Introduction

*Optimal Transportation* (OT) is a mathematical research topic which began two centuries ago the French mathematician Monge's work on "des remblais et déblais" in 1781. This engineering problem consists in minimizing the transport cost between two given mass densities. In the 40's, Kantorovitch solved the dual problem and interpreted it as an economic equilibrium. The *Monge-Kantorovitch* problem became a specific research topic in optimization and Kantorovitch obtained the 1975 Nobel prize in economics for his contributions to resource allocation problems. Following the seminal discoveries of Brenier in the 90's, Optimal Transportation has received renewed attention from mathematical analysts, resulting in the Fields Medal awarded in 2010 to C. Villani, who gave important contributions to Optimal Transportation, arrived at a culminating moment for this theory. *Optimal Transportation* is today a mature area of mathematical analysis. Numerical methods and applications are comparatively underdeveloped. The workshop was dedicated to recent results and methods pertaining to modelization and numerical simulations using Optimal Transportation tools and concepts.

## 2 Numerical approaches to Optimal Transportation

The Augmented Lagrangian method applied to the CFD Optimal Transportation [31] and its variants has been for a long time the main tool in numerical optimal transportation. It was used in particular for warping and registration in image processing. Three other numerical approaches have recently been explored :

**Solving the Monge-Kantorovich linear program :** Cuturi [8, 9, 10, 11, 4] presented the idea of regularizing optimal transport problems with an entropic penalty to enforce desirable properties for optimal couplings, such as balanced flows between equally expensive routes and overall smoothness. Only recently was it shown that such a regularization can provide an extremely efficient computational framework to approximate optimal transport using the toolbox of (strict) convex optimization. This presentation was followed by Peyré's with various applications of this family of numerical method to JKO gradient flows [20], and Wasserstein barycenters [4] in particular. For applications in neuroscience see [15] [14].

Ruan Yuanlong also presented a **multiscale linear programming solver** for optimal transportation (without Entropic regularisation).

**Laguerre Cells for Semi-Discrete Optimal Transportation :** Levy [17] presented a 3D implementation of quadratic OT between a density and a sum of Dirac masses. The modern implementation relies on the efficient computation of Laguerre Cells and the Newton or Quasi Newton minimisation of a convex objective function. Merigot proposed a hierarchical algorithm that improves the speed of convergence, together with an implementation in 2D [32]. The numerical algorithm has been tested on several datasets, with up to hundred thousands tetrahedra and one million Dirac masses.

**Finite difference Monge Ampère solvers and discretization of the cone of convex function :** Mirebeau reviewed the different approaches to discretize optimisation of functionals under convexity constraint [35]. This was illustrated on the Principal Agent problem in 3D. He then explained how it can be used to solve the Monge-Ampère equation [34] [33]. This is the only monotone FD scheme for Optimal Transportation after [40, 41].

### 3 Extensions

**Optimal Transportation on graphs :** Qinglan Xia [42] also presented his numerical simulations approach of the ramified optimal transportation.

**Multi-Marginal Optimal Transport :** Multi-Marginal optimal transportation is a new concept extending Optimal Transportation when data consists in more than 2 densities. Pass [19] gave a general overview of the multi-marginal optimal transport problem and outlined several applications.

### 4 JKO gradient flows and fluids, new modelisation and numerical simulations

Minimizing the Wasserstein distance between a source measure and a target measure can be regarded as an infinite dimensional two point boundary problem. The mapping between the two densities also generates, by interpolation, a geodesic in the Wasserstein distance between the two measures (regarded as points).

A different extension is to consider a gradient flow in the Wasserstein metric, in other words, to evolve the density in order to minimize some functional. Computing the steepest descent direction with respect to the Wasserstein distance defines a semi discrete Wasserstein gradient flow, also known as a *JKO gradient flow* [30]. It is now well-known, that in the limit, several diffusion and aggregation equations of second and fourth order can be interpreted as gradient flows of an entropy in the  $L^2$ -Wasserstein metric. The theory is well developed [3] and continues to expand, see for instance new convergence results in [22]. An significant part of the workshop was devoted to new theoretical and numerical results in this field.

**JKO schemes Theory :** Santambrogio presented some new  $L^\infty$  estimates obtained in collaboration with J.-A. Carrillo. for the Keller-Segel model of chemotaxis, based on a JKO-like scheme, and on a fine analysis of the optimality conditions at every time step, combined with the use of the Monge-Ampère equation.

Carlier and Agueh [1] presented a new JKO approach to the analysis of kinetic models of granular materials.

**JKO schemes Numerical methods :** The JKO scheme is semi-discrete in time. These works (try to) address the space discretisation and the convergence of the resulting schemes.

Wolfram [6] presented a finite element methods for two optimal transportation problems, in particular a class of nonlinear convection-aggregation equations and the Monge-Ampere equation which discretize the associated JKO scheme. OT provides a Lagrangian change of variable into the non-linear PDE to be solved.

Osberger and Mathes [36] use the Lagrangian change of variable into the JKO scheme and perform the gradient flow descent on a galerkin approximation of the transport map. The mass densities can be viewed as weighted moving particles. They check convergence.

Pataccini also uses the Lagrangian approach but chooses to represent the densities as balls of various size along particles. Gamma convergence results are available. This is joint work with J. A. Carrillo, Y. Huang, P. Sternberg and G. Wolansky.

See also Peyré contribution in section 2.

## 5 Applications

**Fluids Dynamics :** Maury presented an optimal transportation framework to pressureless Euler equation with a maximal density constraint. This is a second order extension of the the macroscopic congested crowd motion models proposed in [37].

Cullen [29, 7] presented and discussed computations of singular solutions of the semi-geostrophic eady problem using solutions of the Euler problem. The Semi-Geostrophic problem is the asymptotic limit as the Rossby number tends to zero.

Méridot [18] presented a numerical method to solve Brenier Generalized Euler solutions in 2D which is an instance of Multi-Marginal optimal transportation.

**Seismology :** In seismic exploration a wave field is generated at the surface and reflections from the earths interior are recorded. The purpose is to find properties such as wave velocity and location of reflecting sub layers. This is done in an inverse process where the measurements are compared to a computed wave field with unknown coefficients in the wave equation. Engquist and Froese [13] propose to use the Wasserstein metric for this comparison. We will also remark on applications to registration in seismology.

**Non-Imaging optics :** Free-Forming or the automatic design of smooth refractors or reflectors can be modelled with Monge-Ampère type PDEs and optimal transportation.

Gutierrez [16] gave a complete mathematical overview of the refractor problem : design of interface surfaces between the two homogeneous materials, so the resulting lense refracts radiation in a prescribed manner.

The far-field reflector problem is also a well-known inverse problem arising in geometric optics. It consists in creating a mirror that reflects a given point light source to a prescribed target light at infinity. Thibert [12] presented how the combinatorics of this intersection can be efficiently computed using tools from computational geometry, thus providing an efficient algorithm for the far field reflector problem. This work is in common with Pedro Machado et Quentin Méridot. [12]

Thije Boonkamp [21] also addressed the reflector problem but using finite difference based discretisation of the reflector and in a far field regime.

**Image Processing :** Solomon [27, 28, 26, 25, 24, 23] reviewed several transportation techniques for Geometric Data Processing. Mainly based on accelerated LP solvers and entropic regularization.

Hongkai Zhao [39] uses a simplification of Wasserstein distance called Sliced-Wasserstein Distance to perform Multi-scale Non-Rigid Point Cloud Registration. He applies the Sliced-Wasserstein Distance density built with the Laplace-Beltrami Eigenmap Operator.

Saumier [38] presented a method based on Optimal Optimal Transport for Particle Image Velocimetry.

**Mesh Adaptation :** Budd [5] borrows idea from optimal transport to construct a moving mesh adapted to a transient solution. He uses a parabolic Monge-Ampère equation to compute an approximation of the optimal map at each time step. This is applied to the Semi-Geostrophic problem mentioned above.

## References

- [1] Martial Agueh, Guillaume Carlier, and Reinhard Illner. Remarks on a class of kinetic models of granular media: asymptotics and entropy bounds. *Kinetic and Related Models*, 8, 2015.

- [2] L. Ambrosio, N. Fusco, and D. Pallara. *Functions of Bounded Variation and Free Discontinuity Problems*. Oxford Mathematical Monographs. Oxford University Press Inc.: New York, 1st edition, 2000.
- [3] L. Ambrosio, N. Gigli, and G. Savaré. *Gradient Flows: in Metric Spaces and in the Space of Probability Measures*. Lectures in Mathematics ETH Zürich. Birkhäuser Verlag: Basel, 2nd edition, 2008.
- [4] J-D. Benamou, G. Carlier, M. Cuturi, L. Nenna, and G. Peyré. Iterative bregman projections for regularized transportation problems. *SIAM Journal on Scientific Computing*, to appear, 2015.
- [5] C.J. Budd and M.J.P. Cullen and E.J. Walsh Monge-Ampère based moving mesh methods for numerical weather prediction, with applications to the Eady Problem. , 2012.
- [6] J.A. Carrillo, H. Ranetbauer, and M.T. Wolfram. Numerical simulations of nonlinear convection-aggregation equations by evolving diffeomorphisms. preprint, 2015.
- [7] M. J. P. Cullen. A comparison of numerical solutions to the eady frontogenesis problem. *Quarterly Journal of the Royal Meteorological Society*, 134(637):2143–2155, 2008.
- [8] M. Cuturi, G. Peyré, and A. Rolet. A smoothed dual approach for variational wasserstein problems. Preprint 1503.02533, arXiv, 2015.
- [9] Marco Cuturi. Sinkhorn distances: Lightspeed computation of optimal transport. In *Advances in Neural Information Processing Systems 26*, pages 2292–2300, 2013.
- [10] Marco Cuturi and Arnaud Doucet. Fast computation of wasserstein barycenters. In *Proceedings of the 31st International Conference on Machine Learning (ICML 2014)*, *JMLR W&CP 32*, page pp. 685693, 2014.
- [11] Marco Cuturi, Gabriel Peyré, and Antoine Rolet. A smoothed dual approach for variational wasserstein problems. *arXiv preprint arXiv:1503.02533*, 2015.
- [12] Pedro Machado Manhães De Castro, Quentin Mérigot, and Boris Thibert. Intersection of paraboloids and application to minkowski-type problems. In *30th Annual Symposium on Computational Geometry, SOCG'14, Kyoto, Japan, June 08 - 11, 2014*, page 308, 2014.
- [13] Björn Engquist and Brittany D. Froese Application of the Wasserstein metric to seismic signals In *Communications in Mathematical Science*, 2014.
- [14] Alexandre Gramfort, Gabriel Peyré, and Marco Cuturi. Fast optimal transport averaging of neuroimaging data. In *Information Processing in Medical Imaging*, 2015.
- [15] A. Gramfort, G. Peyré, and M. Cuturi. Fast optimal transport averaging of neuroimaging data. In *Proc. IPMI'15*, 2015.
- [16] Cristian E. Gutiérrez and Qingbo Huang The near field refractor In *Annales de l'Institut Henri Poincaré (C) Non Linear Analysis*, 2014.
- [17] Bruno Levy A Numerical Algorithm for L2 semi-discrete optimal transport in 3D In *ESAIM M2AN (Mathematical Modeling and Numerical Analysis)* , 2015.
- [18] Quentin Mérigot and Jean-Marie Mirebeau. Minimal geodesics along volume-preserving maps, through semi-discrete optimal transport. 2015.
- [19] B. Pass. Multi-marginal optimal transport: theory and applications. To appear in *ESAIM: Math. Model. Numer. Anal.*
- [20] G. Peyré. Entropic wasserstein gradient flows. Preprint 1502.06216, arXiv, 2015.
- [21] CR Prins, Thijs Boonkkamp, WL IJzerman, and Teus TW Tukker. A least-squares method for optimal transport using the monge-ampère equation. 2014.

- [22] S. Serfaty. Gamma-convergence of gradient flows on Hilbert and metric spaces and applications. *Discrete and Continuous Dynamical Systems*, 31(4):1427–1451, 2011.
- [23] J. Solomon, F. de Goes, G. Peyré, M. Cuturi, A. Butscher, A. Nguyen, T. Du, and L. Guibas. Convolutional wasserstein distances: Efficient optimal transportation on geometric domains. *ACM Transactions on Graphics (Proc. SIGGRAPH 2015)*, to appear, 2015.
- [24] Justin Solomon, Fernando de Goes, Gabriel Peyré, Marco Cuturi, Adrian Butscher, Andy Nguyen, Tao Du, and Leonidas Guibas. Convolutional wasserstein distances: Efficient optimal transportation on geometric domains. *ACM Trans. Graph.*, to appear (*Proc. SIGGRAPH 2015*), 2015.
- [25] Justin Solomon, Leonidas Guibas, and Adrian Butscher. Dirichlet energy for analysis and synthesis of soft maps. *Computer Graphics Forum*, 32(5):197–206, 2013.
- [26] Justin Solomon, Andy Nguyen, Adrian Butscher, Mirela Ben-Chen, and Leonidas Guibas. Soft maps between surfaces. *Comp. Graph. Forum*, 31(5):1617–1626, August 2012.
- [27] Justin Solomon, Raif Rustamov, Leonidas Guibas, and Adrian Butscher. Earth mover’s distances on discrete surfaces. *ACM Trans. Graph.*, 33(4):67:1–67:12, July 2014.
- [28] Justin Solomon, Raif Rustamov, Guibas Leonidas, and Adrian Butscher. Wasserstein propagation for semi-supervised learning. In *Proc. ICML*, pages 306–314, 2014.
- [29] AR Visram, CJ Cotter, and MJP Cullen. A framework for evaluating model error using asymptotic convergence in the eady model. *Quarterly Journal of the Royal Meteorological Society*, pages n/a–n/a, 2014.
- [30] Richard Jordan, David Kinderlehrer, and Felix Otto. The variational formulation of the Fokker-Planck equation. *SIAM J. Math. Anal.*, 29(1):1–17, 1998.
- [31] Jean-David Benamou and Yann Brenier. A computational fluid mechanics solution to the Monge-Kantorovich mass transfer problem. *Numer. Math.*, 84(3):375–393, 2000.
- [32] Q. Merigot, *A multiscale approach to optimal transport*, *Comp. Graph. Forum* **5** (2011), no. 30, 1583–1592.
- [33] Jean-Marie Mirebeau, *Discretization of the 3d monge-ampere operator, between wide stencils and power diagrams*, arXiv preprint arXiv:1503.00947 (2015).
- [34] Jean-David Benamou, Francis Collino, and Jean-Marie Mirebeau, *Monotone and consistent discretization of the monge-ampere operator*, arXiv preprint arXiv:1409.6694 (2014), to appear in *Math. of Comp.*
- [35] Jean-Marie Mirebeau. Adaptive, Anisotropic and Hierarchical Cones of Convex functions. *preprint*, 2014.
- [36] D. Matthes and H. Osberger. Convergence of a variational Lagrangian scheme for a nonlinear drift diffusion equation *ESAIM Math. Model. Numer. Anal.*, 2014.
- [37] Maury, B., Roudneff-Chupin, A., Santambrogio, F. A macroscopic crowd motion model of gradient flow type. *Mathematical Models and Methods in Applied Sciences* **20**(10), 1787–1821 (2010)
- [38] Saumier L.P. and Khouider B. and Agueh M. Optimal Transport For Particle Image Velocimetry *Commun. Math. Sci.* 2015.
- [39] R. Lai and H. K. Zhao. Multi-scale Non-Rigid Point Cloud Registration Using Robust Sliced-Wasserstein Distance via Laplace-Beltrami Eigenmap *preprint*
- [40] B. D. Froese and A. M. Oberman. Convergent filtered schemes for the Monge-Ampère partial differential equation. *SIAM J. Numer. Anal.*, 51(1):423–444, 2013.

- [41] J-D. Benamou, B. D. Froese, and A. Oberman. Numerical solution of the optimal transportation problem using the monge-ampère equation. *J. Comput. Physics*, 2014.
- [42] Qinglan Xia. Motivations, ideas, and applications of ramified optimal transportation. . To appear. *ESAIM: Mathematical Modelling and Numerical Analysis*, 2015.