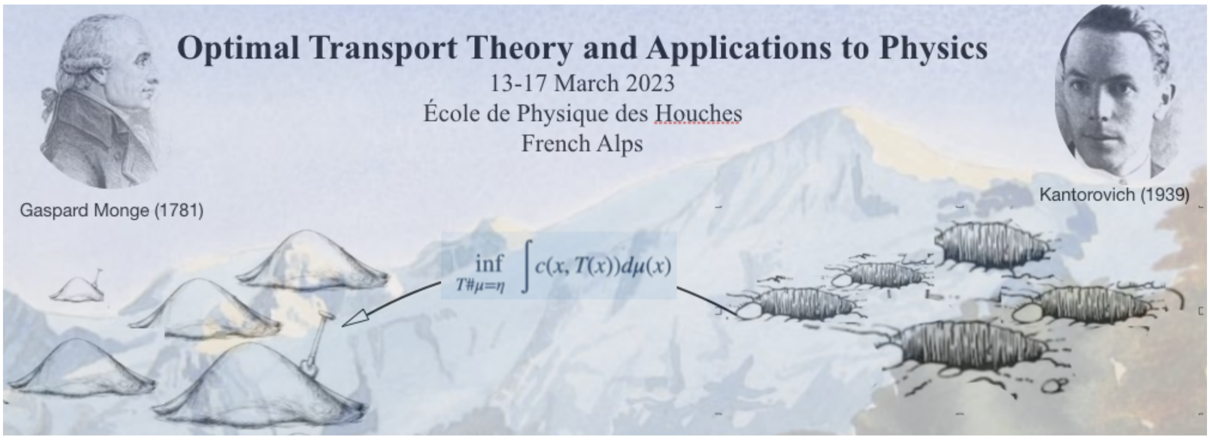
OPTIMAL TRANSPORT THEORY AND APPLICATIONS TO PHYSICS
École de physique des Houches, 13-17 march 2023



PLANNING

BREAKFAST: 7h45-8h30

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DINNER (19h30)</td><td>DINNER</td><td>SPECIAL DINNER</td><td>“SAVOYARD” DINNER</td><td>DINNER</td></tr>
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TITLE AND ABSTRACTS

Aymeric Baradat
Title: Monge-Ampère gravitation as a Γ-limit of good rate functions

Monge-Ampère gravitation is a modification of the classical Newtonian gravitation where the linear Poisson equation is replaced by the nonlinear Monge-Ampère equation. In this presentation, I will explain how to derive a model where a finite number of particles interact according to Monge-Ampère gravitation, starting from the basic model of indistinguishable Brownian particles. I will proceed in two steps. First, I will study a large deviation problem related to this model at fixed positive diffusivity, and then I will show that this problem converges when the diffusivity tends to zero. The limiting problem corresponds to minimizing a singular Lagrangian encoding Monge-Ampère gravitation. In addition, its singularities lead to sticky collisions in dimension 1. This is a joint work with Y. Brenier and L. Ambrosio.

David Bourne
Title: Optimal transport problems in microstructure modelling

In this talk I will describe how semi-discrete optimal transport theory arises naturally in materials science. The microstructure of foams and metals are often modelled as generalised Voronoi diagrams (Laguerre diagrams or anisotropic power diagrams). The challenge is to generate realistic geometric models with prescribed statistical properties, such as the distribution of cell volumes and shapes. These geometric models are then used as RVEs (Representative Volume Elements) for computational homogenisation. I will describe how geometric modelling of polycrystalline microstructures gives rise to some interesting problems in numerical semi-discrete optimal transport and optimal quantization. This is joint work with researchers from Tata Steel Research & Development, Heriot-Watt University, University of Glasgow, and Ghent University.

Ana Bela Cruzeiro
Title: On a pathwise stochastic control problem

We consider a pathwise stochastic optimal control problem and derive the associated (not necessarily adapted) Hamilton-Jacobi-Bellman stochastic partial differential equation. The value process is the unique solution of this equation, in the viscosity sense. This is joint work with Neeraj Bhauryal and Carlos Oliveira.

Maria Colombo
Title: Neural Networks, the interpretation as Wasserstein gradient flows.

Mike Cullen
Title: Application of optimal transport to the semi-geostrophic equations with variable rotation.

Weak solutions of the semi-geostrophic equations have been successfully used to describe important phenomena in meteorology. Rigorous results proving the existence of such solutions have been obtained with constant rotation. However, these equations are only an accurate approximation to the complete atmospheric equations on large scales, where the Earth's geometry is important and so the variable effects of rotation have to be included. The only rigorous results for the existence of semi-geostrophic solutions in this case are results for classical solutions. These results depend on a convexity condition, which has only been proved to be maintained for a short time. The optimal transport method should give weak solutions which maintain convexity for long times. However, there are significant obstacles to its use with variable rotation. These will be described and possible solutions suggested.

Hugo Lavenant
Title: A probabilistic view on unbalanced optimal transport

Optimal transport asks the question: what is the optimal way to transport a distribution of mass from one configuration to another. One of its variant, regularized optimal transport, is closely connect to large deviation principle and entropy minimization with respect to the law of the Brownian motion (a.k.a. the Schrödinger problem), a problem coming from physics consideration. In short: regularized optimal transport has a neat and fruitful probabilistic interpretation. I will explain what happens when we replace Brownian motion by branching Brownian motion (that is, when particles may also split or die at random instants): the optimal transport counterpart becomes regularized unbalanced optimal transport, enabling to match distributions of unequal mass.

Cédric Deffayet (Cancelled)
Title:

Job Feldbrugge
Title:

The cosmic web is the largest geometric structure in our universe, consisting of an intricate network of empty voids bounded by thin walls, elongated filaments, and dense clusters. Given the array of upcoming cosmological redshift surveys, new analytic tools are needed to study the formation of the various structures, quantify the geometry and topology, and isolate the elements of the cosmic web. New techniques might, for example, help to understand the link between the properties of galaxies and their placement in the large-scale structure. In this talk, I will present my recent developments in the study of the caustic skeleton of the cosmic web. By tracing the phase-space structure of the dark matter sheet, I identify the relevant caustics and illustrate their role in the cosmic web. I quantify the topology of the phase-space structure using persistent homology. Finally, I will present a non-linear extension of constrained Gaussian random field theory. When combined with caustic skeleton theory, this extension allows us to create a specialized set of initial conditions dissecting the elements of the cosmic web. These initial conditions will help cosmologists to systematically study the properties and interplay of the elements of the cosmic web, and their influence on the embedded galaxies.

Gero Friesecke
Title: Numerical methods for high-dimensional multi-marginal OT problems as arising in DFT

Multi-marginal OT problems arise naturally in application fields such as electronic structure, fluid dynamics, and data science, but pose a huge challenge for computation. This is because the number N of marginals corresponds, respectively, to the number of particles, timesteps, and datasets, hence one is interested in large N, but the number of unknowns after discretization scales exponentially in N. I will survey some promising recent avenues for tackling the curse of dimension in these problems, with particular focus on the multi-marginal Coulomb problem relevant to electronic structure.

Thomas Gallouët

Title: Lagrangian scheme for fluids mechanics based on Semi discrete Optimal Transport

In this talk we will explain how based on Brenier's ideas, it is possible to construct particle methods for a large class of fluids mechanics problems such that Wasserstein gradient flows of an internal Energy or Euler flows/Hamiltonian flows for the same energy. This class contains incompressible Euler equations, compressible (barotropic) fluids, fluid-structure interactions,...

In order to build these scheme the internal energy is replaced by its Moreau-Yosida regularization in the L2 sense, which can be efficiently computed as a semi-discrete optimal transport problem. Using a modulated energy argument which exploits the convexity of the problem in Eulerian variables, one can prove quantitative convergence estimates towards smooth solutions of the considered system of PDE.

Jun Kitagawa

Title: An embedding of sliced optimal transport metrics

The sliced and max Wasserstein metrics were originally developed to ease the computational burden of optimal transport by exploiting the explicit nature of 1D transport. However, there has not been a very in-depth systematic study of the geometric structure that these metrics induce on the space of probability measures with finite p-th moment. In this talk, I will first discuss some of this finer structure, and in particular point out that these metrics have some rather undesirable properties. In the second half of the talk, I will introduce a larger family of metric spaces into which these sliced and max metrics can be embedded, which in some senses seem to have more natural geometric properties. This talk is based on joint work with Asuka Takatsu.

Derk Kooi

Title: Bosonic and Fermionic Sinkhorn Algorithms for Multi-Marginal Optimal Transport with particle statistics

There exists a deep connection between ``diagonal approximations" to universal energy functionals in reduced density (matrix) functional theories and the field of Multi-Marginal Optimal Transport (MMOT). Similarly there is a deep connection between those ``diagonal approximations" at finite temperature and entropically regularized MMOT. However, particle statistics (whether bosonic or fermionic) results in some slight subtleties. As an example, we introduce One-body Reduced Density Matrix Functional Theory (1-RDMFT) in the canonical ensemble and then proceed to approximate the interacting ensemble by a non-interacting ensemble that maximizes the entropy, independently of temperature. Even though there is no ``cost", only entropic regularization, the problem is rendered non-trivial due to particle statistics. Bosonic and Fermionic Sinkhorn algorithms are derived and used to invert the relationship between the Natural Orbital Occupation Numbers (NOONs) and the effective orbital energies of the non-interacting ensemble. Both the Bosonic and Fermionic Sinkhorn algorithms are shown to perform well in reproducing the NOONs of simulated distributions and the ground-state NOONs of several molecules. It is shown that we can see the effect of particle statistics as an effective cost as well.

Christian Léonard
Title: A glance at entropic optimal transport

This short overview of the Schrödinger problem, a.k.a. entropic optimal transport, is intended to spread the word to physicists. It is tightly connected to Jean-Claude Zambrini's talk. We shall have a look at entropic interpolations and also sketch an optimal transport interpretation of thermal diffusion and basic quantum mechanics (non-relativistic without spin). Most of these not so new results were proved by a slowly (but surely) growing community of mathematicians.

Mathieu Lewin
Title: Optimal transport in quantum chemistry and statistical mechanics

In this lecture we will review how the multimarginal optimal transport problem naturally occurs in statistical mechanics and is used in quantum chemistry to describe strictly correlated electrons. We will also mention some recent mathematical results in this direction.

Amos Maritan
Title: Optimal River Networks

The most successful river basin model is based on a variational principle that minimizes energy dissipation. This leads to optimal river networks with universal scaling properties indistinguishable from real river basins.

Daniel Matthes
Title: A two-component variant of the famous result on equilibration in scalar Fokker-Planck equations

One of the most striking by-now-classical results on Wasserstein gradient flows is the one about exponential equilibration in nonlinear Fokker-Planck equations: if the nonlinearity satisfies McCann's condition, and the potential is lambda-uniformly convex, then any solution tends to the steady state at exponential rate lambda. The proof a la Felix Otto is a remarkable application of uniform displacement convexity.

Until now — despite lots of efforts — no result of comparable generality and simplicity has been derived for a system of two such Fokker-Planck equations that are coupled by means of cross diffusion. In this talk, we indicate the main difficulty, which is the total break-down of the displacement convexity as soon as coupling is introduced, no matter how tame. Our main result is that for sufficiently weak coupling, equilibration still happens exponentially fast, with a rate lambda, reduced by the coupling strength. The proof is based on the lambda-uniform displacement convexity of the decoupled system, and treats the non-convexity as perturbation. The latter requires the use of non-standard nonlinear functional inequalities.

This is joint work with Lisa Beck (Augsburg) and Martina Zizza (SISSA).

Ludovic Métivier et Jean-Marie Mirebeau
Title: Optimal transport distances for seismic imaging: how to deal with signed data? The Kantorovich-Rubinstein norm and the graph space approach

Modern seismic imaging methods are based on the interpretation of the "full waveform": from a mathematical standpoints it means solving a PDE-constrained minimization problem where the PDE describes the propagation of seismic waves in the subsurface. One of the main difficulty in the practical application of these strategies to field data is the non-convexity of the underlying minimization problem. This makes the success of such applications strongly dependent to an accurate initial guess of the solution and/or the availability of low frequency data. Recently, we have investigated how we can reformulate this PDE-constrained minimization problem using optimal transport distances instead of the conventional least-squares distance to mitigate the non-convexity. This idea is supported by the convexity of the optimal transport distances with respect to translation and dilation and the fact that, at first-order, perturbations of the wave velocity result in such translation and dilation on the seismic data. The main difficulty is that seismic data are oscillatory, therefore they can not be interpreted straightforwardly as measures, which is required by the optimal transport theory. In these two presentations, we will review different strategies we have proposed to extend and apply optimal transport distances to seismic data. The first is based on the dual formulation of 1-Wasserstein distance, which is linked to the so-called Kantorovich-Rubinstein norm. The second is based on a graph space lift: the discrete graph of each seismic records is compared using the 2-Wasserstein distance. More recently, taking advantage of the multi-component nature of the seismic data, we have proposed to use a lift of the data into a space of positive matrices, where we can apply a generalization of the Kantorovich-Rubinstein approach, which can be interpreted as a Beckmann's minimal flow problem. This last approach will be developed in the second of these two presentations.

Klas Modin
Title: On the gradient flow structure of the continuous Toda and incompressible porous medium flows.

Andrea Natale
Title: Gradient flows of interacting Voronoi cells and their continuous limits

Voronoi diagrams are a popular approach to describe neighborhood relations within particle systems and therefore to model their interaction and dynamics. In this talk we consider a class of models where a weighted Voronoi diagram evolves in time following the gradient flow of an energy depending on the cell areas. We describe the link of such models with semidiscrete optimal transport, and study their convergence towards nonlinear diffusion PDEs of porous-medium type. Finally, we will show how similar ideas can be used to construct particle discretizations of fluid models with multiple advected quantities, such as the thermal shallow water equations.

Adi Nusser
Title: Reconstruction of the late large scale structure: from Wiener to ML

Using a modified Wiener estimation, will present results of the analysis of redshift surveys and peculiar velocity measurements with a special emphasis on error estimation. Will also discuss the estimation using ML and its relation to Wiener filtering.

Henry Orland
Title: Statistical Physics of Optimal Transport at Finite Temperature

We show how optimal transport (OT) can be studied at finite temperature, using the formalism of statistical physics. The method applies to balanced and unbalanced transport, and reduces to standard OT at zero temperature. The saddle-point approximation provides simple algorithms to implement the finite temperature OT. Examples of these methods are presented for some image recognition and bioinformatics applications.

Felix Otto
Title:

Beatrice Pelloni
Title: Semi-discrete optimal transport: application to geophysical fluids

Mario Putti
Title: Gradient flow for L^1 optimal transport and its extensions to ramified transport

We present a numerical approach for the approximation of the L^1 optimal transport density μ^*, here intended as the unique L^∞ solution of the Monge-Kantorovich equations. Our numerical approximation scheme relies upon the combination of a FEM-inspired variational approximation of an appropriate discrete energy functional and its minimization via gradient flow. The energy functional is formed by the sum of two terms, one identifiable with the Dirichlet energy of the Monge-Kantorovich elliptic PDE and the other with the total transport mass, i.e., the integral of the transport density.
We first prove convergence of the unique minimizer of the discrete energy functional towards the L^1 optimal transport density as the sequence of FEM spaces is refined. Then we derive a gradient flow minimization of the discrete transport energy based on the variational implicit Euler scheme. We show that the proposed scheme converges towards the asymptotic solution exponentially in time. This allows the use of an increasing time-step sequence in combination with Newton iteration for the efficient solution of the nonlinear equations at each time step. The overall scheme is shown to converge superlinearly towards the approximate L^1 transport density.
We will present several applications of the proposed approach related to the calculation of Wasserstein distances and to the approximation of the cut locus of a three-dimensional embedded surface.

The discrete energy functional can be shown to be equivalent to Beckman problem. As a consequence, a simple modification of the functional and the ensuing gradient flow leads to a model seemingly capable of describing both congested and ramified optimal transport. In the latter case the functional is non convex and multiple local minima appear. However, experimental results show that meaningful numerical approximations that resemble solutions of ramified transport problems are obtained.

This approach has been applied to the simulation of real-world problems, ranging from multi-commodity routing on graphs (e.g., dynamics of passengers in the London underground) to hydrological applications (formation of river basins and deltas) and, more recently, to the dynamical growth of plant roots.

Simon Rezchikov
Title:

Filippo Santambrogio
Title: The role of OT in some physical problems

I will review some well-known physical evolution problems which can be interpreted in terms of optimal transport and/or of its several variants. These problems will include

- evolution PDEs, such as diffusion equations which can be seen as gradient flows for the W_2 distance ; in this case, and in particular for the Fokker-Planck equation, I will insist on the difference between the interpretation in terms of OT and the interpretation as the law of a Brownian process
- other evolution PDEs, such as the semi-geostrophic equation, where gradients of convex functions, and their regularity, and hence quadratic OT, allow to study the equation in dual variables. Yet another evolution equation, the incompressible Euler system, which has a variational interpretation due to Arnold and then relaxed by Brenier which is reminiscent of OT, and where OT can appear as a brick to approximate the solution
- the static and dynamic formulation of the problem of the reconstruction of the early universe, which lets an OT appear if using the Zeldovich approximation, but also a variant of the Benamou-Brenier problem in the non-approximated case

Bernhard Schmitzer
Title: A review of Numerical OT

In the first part we will introduce the Monge formulation of optimal transport, its subsequent relaxation to the Kantorovich problem, duality of the latter, and finally demonstrate their relation via Brenier's theorem. The second part will focus on the structure of the quadratic Wasserstein distance, shortest paths, the celebrated Benamou--Brenier formula, and the implied weak Riemannian structure. The third part introduces entropic regularization, the updated dual problem, Sinkhorn's algorithm, and statistical implications. Finally, if time allows we will briefly touch on multi-marginal transport and the Wasserstein barycenter problem.

Ravi Sheth
Title: Optimal Transport and the Cosmic Web

It has been known for some time that Optimal transport provides an elegant framework for reconstructing the initial field which gave rise to the cosmic web we see today. I will review recent progress in this methodology for standardizing the rod that is used for calibrating the expansion history of the universe, especially when one only observes a biased subset of the elements which make up the cosmic web. I will point to some open problems in this approach, as well as discuss potential new directions.

François-Xavier Vialard

Title: On the Gromov-Wasserstein problem, existence of Monge maps and Unbalanced Gromov-Wasserstein

This talk has two parts. First we present a possible extension of the Gromov-Wasserstein problem to the setting of metric measures spaces, whose total mass is not necessarily equal to 1. We propose a true distance and a lower bound which is more friendly for computations. Second, we study the existence of Monge maps as optimizer of the standard Gromov-Wasserstein problem for two different costs in euclidean spaces. The first cost for which we show existence of Monge maps is the scalar product, the second cost is the quadratic cost between the squared distances for which we show the structure of a bi-map. We present numerical evidence that the last result is sharp.

Philipp Windischhofer

Title: Calibrating stochastic simulations with optimal transport

Stochastic simulators are an indispensable tool in many branches of science. Often based on first principles, they deliver a series of samples whose distribution implicitly defines a probability measure to describe the phenomena of interest. However, the fidelity of these simulators is not always sufficient for all scientific purposes, necessitating the construction of ad-hoc corrections to “calibrate” the simulation and ensure that its output is a faithful representation of reality. In this talk, I will show how methods from transportation theory can be leveraged to construct such corrections in a systematic way. Building on recent advances in machine learning, I will explain how minimal modifications to the individual samples produced by the simulator can be computed such that the resulting distribution becomes properly calibrated. The need for calibrated stochastic simulators is particularly pronounced in particle physics, and I will use examples from this field to illustrate the method and its benefits.

Jean-Claude Zambrini

Title: Quantum Mechanics via Schrödinger's problem, Mass Transportation (and back).

After a brief summary of (Von Neumann's) Quantum Mechanics in Hilbert space, we shall mention some of its mathematical and conceptual difficulties.They motivated Schrödinger, in 1931-32, to overcome basic ones by an unusual variational problem in classical statistical physics.We shall summarize the (geometric) stochastic dynamical theory founded on his solution.It justifies Schrödinger's initial hunch that his quantum analogy was more than an accidental one.

REGISTERED PARTICIPANTS

Baradat	Aymeric
Benamou	Jean-David
Boldrini	Pierre
Bourne	David
Brenier	Yann
Brizzi	Camilla
Colombo	Maria
Cruzeiro	Ana Bela
Cullen	Mike
Deffayet	Cédric
Egan	Charlie
Eichinger	Katharina
FACCA	ENRICO
Feldbrugge	Job
Feydy	Jean
Friesecke	Gero
Gallouët	Anatole
Gallouët	Thomas
Hamprecht	Fred
Khosravi	Nima
Kitagawa	Jun
Kooi	Derk
Koren	Zvi
Lavenant	Hugo
Lavier	Theo
Lelotte	Rodrigue
Léonard	Christian
Levy	Bruno
Lewin	Mathieu
Li	Baojiu
Luca	Nenna
Makinen	Timothy Lucas
Malamut	Hugo
Maritan	Amos
Matarrese	Sabino
Matthes	Daniel
Mérigot	Quentin
Métivier	Ludovic

Mirebeau	Jean-Marie
Modin	Klas
Mohayaee	mohayaee
Müller	Bastian
Natale	Andrea
Nikakhtar	Farnik
Nikjoo	Mehraveh
Nusser	Adi
Orland	Henri
Otto	Felix
Padmanabhan	Nikhil
Pearce	Mason
Pelloni	Beatrice
Putti	Mario
Ravve	Igor
Rezchikov	Semon
Ried	Tobias
Santambrogio	Filippo
Schmitzer	Bernhard
Sheth	Ravi
Sylvestre	Maxime
Tan	Justin
Tertois	Anne-Laure
Thibert	Boris
Todeschi	Gabriele
van de Weygaert	Rien
Vialard	François-Xavier
von Hausegger	Sebastian
Windischhofer	Philipp
Zambrini	Jean-Claude
Zhong	Adrianne