WORKSHOP:
Optimal Transport meets Density Functional Theory

University of Jyäskylä

OT-DFT, 31st May - 2nd June 2017

Multi-marginal optimal transport

Brendan Pass
University of Alberta, Canada

I will discuss recent progress on multi-marginal optimal transport. I will try to provide some insight into the delicate dependence of the uniqueness and structure of solutions on the cost function, a phenomenon which is largely absent in the classical, two marginal problem. Examples of costs for which the solution is always unique and of Monge type will be contrasted with those (including the Coulomb cost from DFT) which do not exhibit this behavior.

Density functional theory and many-marginals optimal transport with Coulomb and Riesz costs

Codina Cotar
University College London, United Kingdom

Multi-marginal optimal transport with Coulomb cost arises as a dilute limit of density functional theory, which is a widely used electronic structure model. The number N of marginals corresponds to the number of particles. I will discuss the question whether "Kantorovich minimizers" must be "Monge minimizers" (yes for $N = 2$, open for $N > 2$, no for $N =$ infinity), and derive the surprising phenomenon that the extreme correlations of the minimizers turn into independence in the large N limit. Time permitting, I will also discuss open problems on the next order term and work in progress on the topic.

The talk is based on joint works, among others, with Gero Friesecke (TUM), Claudia Klueppelberg (TUM), Brendan Pass (Alberta) which appeared in CPAM (2013) and Calc.Var.PDE (2014), and on joint work in progress with Mircea Petrache on the next order term.

Properties of the Zero-Point Oscillation wavefunction in the strong-coupling limit of DFT

Derk Kooi
Vrije Universiteit Amsterdam

The zero-point oscillations around the degenerate SCE minimum represent the next-to-leading order contribution to the interaction energy in the strong-coupling limit of DFT [1]. We explicitly construct the corresponding wavefunction for a number of examples and study its properties. The examples are one-dimensional two-particle systems and include: Lorentzian and uniform density with renormalized Coulomb interaction and a Gaussian density with a repulsive harmonic interaction.

[1] M. Seidl, P. Gori-Giorgi, and A. Savin. Phys. Rev. A, 75:042511, 2007.

Locality of Electronic Structure Models

Faizan Nazar
Université Paris-Dauphine CEREMADE, France

I will give an overview of locality results for electronic structure models and discuss their applications in materials simulations. These include the construction of QM/MM coupling methods and linear scaling algorithms.

Optimal Sampling Patterns via Mass Transportation Theory

Giuseppe Buttazzo
Università di Pisa, Italy

In digital control systems, the state is sampled at given sampling instants and the control is kept constant between two consecutive instant. The choice of sampling instants is crucial in order to perform an optimal control and to govern efficiently the system. By optimal sampling problem we mean the selection of sampling instants and control inputs, such that a given function of the state and input is minimized. We consider a linear quadratic control problem and we discuss several sampling methods. Using the optimal mass transport theory we propose a new quantization-based sampling strategy that is capable of achieving the optimal cost in several situations.

Effect of statistics in the strongly correlated electron limit of DFT

Juri Grossi
Vrije Universiteit Amsterdam

We try to understand and implement the effects of the fermionic statistics in the first order correction of the strictly correlated electrons limit (SCE) [1] in DFT which, in the present form, does not distinguish between different spin states [2], taken into account in the KS kinetic energy but not in the XC SCE functional. Spin effects arise from the overlapping of the wavefunctions of the electrons due to zero point oscillations when the kinetic energy is not completely suppressed. This is crucial in order to capture the physics and chemistry of strongly correlated systems, which is determined by the subtle interplay between correlation and effects related to the spin state. We compare our calculations with the numerical results obtained through the constrained search method [3] for 2 electrons in 1D in a Lorentzian density for the expansion of the adiabatic connection at large λ.

[1] M. Seidl, P. Gori-Giorgi, and A. Savin. Phys. Rev. A, 75:042511, 2007.
[2] P. Gori-Giorgi, G. Vignale, and M. Seidl. J. Chem. Theory Comput., 5:743, 2009.
[3] P. Mori-Sanchez A. Cohen. arXiv:1506.02230.

Numerical Methods for Multi-Marginal Optimal Transportation

Luca Nenna
Université Paris-Dauphine & INRIA-Paris, France

In this talk we aim at giving a general numerical framework to approximate solutions to optimal transport (OT) problems. The general idea is to introduce an entropic regularization of the initial problems. The regularized problem corresponds to the minimization of a relative entropy with respect a given reference measure. Indeed, this is equivalent to find the projection of the joint coupling with respect the Kullback-Leibler divergence. This allows us to make use the Bregman/Dykstra' s algorithm and solve several variational problems related to OT. We are especially interested in solving multi-marginal optimal transport problems (MMOT) arising in Quantum Physics (e.g. Density Functional Theory). In this cases we show that the entropic regularization plays a more important role than a simple numerical stabilization.

Approximation of wave functions by transport plans and applications

Luigi De Pascale
Università di Firenze, Italy

The probability measure $|\psi|^2 dX$ associated to the square of a wave function ψ is a N-marginal transport plan for the single electron density ρ. As a transport plan $|\psi|^2 dX$ can be approximated in several way by sequences of transport plans.

The next question if whether or not to the approximation of $|\psi|^2 dX$ by a sequence of transport plans corresponds an approximation of ψ by a sequence of wave functions with specific properties. The fermionic conditions and the spin variable, for example, plays a crucial role in the study of this last question.

I will discuss an application to the semiclassical limit of the Hohenberg-Kohn energy and, if time permits, to a family of questions concerning the operator which associate ρ to ψ. (Joint work with Ugo Bindini).

Lieb-Oxford inequality and the uniform electron gas

Mathieu Lewin
CNRS & Université Paris-Dauphine, France

In this talk I will recall the Lieb-Oxford inequality which plays an important role in DFT, and is linked to multi-marginal optimal transport. I will also discuss its relation with the uniform electron gas, a system of infinitely many electrons placed everywhere in space such as to build a constant density.

Merging SCE functional into the Green's function theory

Mehdi Farzanehpour
Vrije Universiteit Amsterdam

We propose a description of equilibrium and nonequilibrium systems through a hybrid model which combines exchange-correlation potentials from the strictly correlated limit of the density functional theory with self-energies of many-body perturbation theory. The hybrid construction is designed in a way that avoids double counting thorough separating the interaction into short-range and long-range. This allows us to treat the low and high correlation regions separately and thus better model the strongly correlated systems.

Large-N asymptotics for symmetric optimal transport with N marginals

Mircea Petrache
Max-Planck Institute Bonn, Germany

In this talk, I consider the Symmetric Optimal Transport problem with N equal marginals, with cost given by a $2-$particles interaction-type potential. I will discuss the recent developments regarding the asymptotics for large N for minimizers of such Optimal Transport problems. Several open questions and possible research directions are naturally appearing as a consequence of this discussion.

Strictly correlated electrons (SCE) in density functional theory (DFT)

Michael Seidl
University of Regensburg and Vrije Universiteit Amsterdam

In the strong-interaction limit of DFT, we are facing a hypothetic situation where the Coulomb repulsion between the electrons (of an atom, a molecule, etc.), multiplied with a factor $\lambda \geq 0$, becomes infinitely strong ($\lambda \to \infty$). The resulting strongly correlated (quantum mechanical) wave function is described by the concept of strictly correlated electrons (SCE). This situation is opposite to the familiar concept of a Slater determinant (SD) which describes non-interacting electrons ($\lambda = 0$) that are moving (independently of each other) in single-particle orbitals. The true wave function of a real-universe electron system ($\lambda = 1$) may be viewed as an intermediate stage between the extreme limiting situations described by a SD or by SCE, respectively.

I shall illustrate the SCE concept in detail for the simplest case of systems with $N = 2$ electrons in a spherically symmetric density $\rho(r)$, such as the He atom. Generalizations to $N = 3$ or more electrons and to symmetries less than spherical will also be discussed. In particular, we shall see that this SCE limit of quantum mechanical DFT, from the mathematics point of view, is a multimarginal optimal transportation (OT) problem. The SCE co-motion functions $\mathbf{f}_i(\mathbf{r})$ correspond to the optimizing transport maps $T_i(x)$.

Insight into the decomposition of the XC potential in the physical and in the strong-coupling limit cases

Sara Giarrusso
Vrije Universiteit Amsterdam

The theory of conditional probability amplitudes first developed by Hunter [1] offers an excellent tool for deriving an exact differential equation for the square root of the density and has proven very fruitful inasmuch as it allows an insightful decomposition of the XC potential into its kinetic, response, and XC hole contributions [2,3,4].

By adopting this formalism within a λ-dependent hamiltonian, we generalise the reduced one-electron form of the Schrödinger equation for any value of the interaction parameter. Focusing on the infinite coupling strength or strongly-correlated electrons (SCE) limit, we derive the corresponding form of the conditional amplitude. Our analysis shows from a different standpoint, the necessity of adding a kinetic correlation correction to the SCE energy, and to its functional derivative, in order to recover important informations like the ionization potential. A natural and consistent definition of the so-called response potential at the SCE level is also provided and we discuss preliminarily some of its peculiar features. A simple model for a dissociating alcaline hydride is used to compare its performances with the response potential at $\lambda = 1$ as in ref. [5].

Furthermore we introduce the concept of a response potential coupling-constant averaged (CCA) along the adiabatic connection, along with that of a CCA XC hole potential, which might be of help for the construction of approximate XC functionals, especially of a new generation of DFAs based on local quantities along the AC, and highlight the differences between these potentials and the 'traditional' ones, i.e. the kinetic, response, and XC hole potentials.

[1] G. Hunter. Int. J. Quant. Chem., 9:237–242, 1975.
[2] E. J. Baerends and O. V. Gritsenko. Phys. Rev. A, 54:1957–1972, Sep 1996.
[3] E. J. Baerends and O. V. Gritsenko. J. Phys. Chem. A, 101:5383–5403, July 1997.
[4] Oleg V. Gritsenko, Robert van Leeuwen, and Evert Jan Baerends. J. Chem. Phys., 104:8535, 1997.
[5] D. G Tempel, T. J Martínez, and N. T. Maitra. J. Chem. Theory Comput., 5:770–780, 2009.

Multimarginal optimal transport and structure of optimal plans: examples and counterexamples on SGS conjecture

Simone Di Marino
Scuola Normale Superiore Pisa, Italy

We will introduce the multimarginal optimal transport problem in its generality and discuss the structure of optimal plans in the 1d repulsive case, in which there exists a full characterization that shows SGS conjecture is true. Then we will move to the radial case, where only partial results are available, both on the positive and negative side for the SGS conjecture.

Continuity and estimates for multimarginal optimal transportation problems with singular costs

Thierry Champion
Université de Toulon, France

In this talk, we consider some repulsive multimarginal optimal transportation problems which include, as a particular case, the Coulomb cost. We will state a regularity property of the minimizers (optimal transportation plan) from which existence and some basic regularity of a maximizer for the dual problem follow. Applications to obtain some estimates of the cost and to the study of related continuity properties will also be ginven. Joint work with G. Buttazzo and L. De Pascale.