

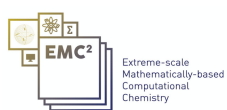
INTERNATIONAL JOINT WORKSHOP

MOANSI – ERC EMC² – CNRS IRP M4AS

Book of abstracts

16–18 November 2026

Laboratoire Jacques-Louis Lions, Sorbonne Université, Paris



<https://moansi2026.pages.math.cnrs.fr>

Contents

Monday, November 16 (afternoon)	3
Caroline Lasser — 13:30–14:15	3
Yoann Le Hénaff — 14:15–14:35	3
Marianne Curely — 14:35–14:55	3
Quentin Chauleur — 14:55–15:15	4
Asbjorn Baekgaard Lauritsen — 15:45–16:05	4
Jakob Oldenburg — 16:05–16:25	4
Théo Duez — 16:25–16:45	5
Louis Garrigue — 17:00–17:20	5
Thiago Carvalho Corso — 17:20–17:40	6
Chih-Chun Wang — 17:40–18:00	6
Markus Penz — 18:00–18:20	6
Tuesday, November 17 (morning)	7
Alice Allen — 09:00–09:45	7
Noe Blassel — 09:45–10:05	7
Lune Maillard — 10:05–10:25	7
Nour Alkhatib — 10:25–10:45	8
Laurent Vidal — 11:15–11:35	9
Mathias Oster — 11:35–11:55	9
Brice Kammegne — 11:55–12:15	10
Tuesday, November 17 (afternoon)	11
Michele Nottoli — 14:15–14:35	11
Laura Grazioli — 14:35–14:55	11
Lucien Dupuy — 14:55–15:15	12
Jonas Beck — 15:45–16:05	12
Alicia Negre — 16:05–16:25	13
Zhuoyao Zeng — 16:25–16:45	13
Solal Perrin-Roussel — 17:15–17:35	14
Etienne Obermeyer — 17:35–17:55	14
Maximilian Penka — 17:55–18:15	15
Wednesday, November 18 (morning)	16
David Gontier — 09:00–09:45	16
Virginie Ehrlicher — 09:45–10:05	16

Pierre Amenoagbadji — 10:05–10:25	17
Alfred Kirsch — 10:25–10:45	17
Bruno Ploumhans — 11:15–11:35	17
Ioanna-Maria Lygatsika — 11:35–11:55	18
Jonas Püschel — 11:55–12:15	18
Antoine Levitt — 12:15–12:35	18

Monday, November 16 (afternoon)

PLENARY TALK

Title to be announced

Caroline Lasser

13:30–14:15

School of Computation, Information and Technology, TU Munich

Abstract to be announced.

Numerical Bogoliubov approximation of bosonic quantum systems

Yoann Le Hénaff

14:15–14:35

Université de Tübingen

In this talk we will discuss an algorithm for the numerical simulation of the time-dependent bosonic Schrödinger equation with N particles in the case of a two-body interaction potential, based on the Bogoliubov approximation. This approximation holds in the limit $N \rightarrow \infty$, which is what we want to be able to simulate numerically.

By taking naturally into account the symmetries of the system, the Bogoliubov ansatz allows us to obtain a method whose computational complexity is independent of the number of particles. The essential idea consists in representing numerically the condensate function and a small number of interaction functions that are outside the condensate.

The approximate time evolution of all functions is given by the Dirac-Frenkel time-dependent variational principle. The interaction functions are low-rank approximated and a BUG integrator is used so that the method is robust to small singular values arising from the low-rank approximation. A tensorization property of the interaction functions, given by the Bogoliubov approximation, also allows us to compute the time evolution of only one of them and to deduce the time evolution of all others. Overall, the numerical scheme we obtain has a computational complexity independent of N .

Propagation of wave packets close to conical intersections

Marianne Cureau

14:35–14:55

Université d'Angers

In this presentation, we study the propagation of wave packets close to conical intersections for a system of two Schrödinger equations exhibiting a conical crossing of codimension two. We focus on the dynamics that occur when the wave packets pass through an area close to the crossing and our main results provide an explicit formula for the outgoing wave packet in terms of the incoming one, with a complete description of its phase and of the classical trajectories it follows, including a drift.

Computing discrete ground states of rotating Bose-Einstein condensates

Quentin Chauleur

14:55–15:15

INRIA, Univ. Lille

In this presentation, I will show how space discretization affects the convergence of the normalized gradient flow to compute the Gross-Pitaevskii energy minimizers with rotation. In the non-symmetric case, I will present the key steps to prove local convergence to the ground state manifold under a quasi-coercivity condition of the Hessian of the energy and under a fundamental spectral gap assumption. Numerical simulations and perspectives on the symmetric case will also complete the discussion. This talk is based on a joint work with Guillaume Dujardin and Robin Roussel.

Well-posedness of geometric time-dependent Kohn–Sham theory

Asbjorn Baekgaard Lauritsen

15:45–16:05

CNRS & CEREMADE, Université Paris-Dauphine, PSL

Standard time-dependent density-functional theory is based on the construction of the universal functional potential, which is the potential reproducing an externally given one-particle density. We recently proposed a different model, based on geometric concepts, called geometric TDDFT, where a given density is reproduced instead using a purely imaginary potential, or equivalently a nonlocal hermitian operator. Establishing the existence of either the universal functional potential or the corresponding imaginary geometric function are delicate mathematical questions in the theory of nonlinear PDE's. In this talk, I will explain the solution to the geometric problem in the class of analytic-in-space densities for non-interacting systems and explain how this leads to the well-posedness of geometric time-dependent Kohn–Sham theory.

Joint work with Mathieu Lewin and Jakob Oldenburg.

The inverse problem of time-dependent density functional theory on the torus

Jakob Oldenburg

16:05–16:25

CNRS & Université Paris Dauphine

We prove that for any given time-dependent one-particle density, there exists a unique external potential for which the solution to the many-body Schrödinger equation has this prescribed density. This implies in particular that one can exactly reproduce the time-dependent density of an interacting system using non-interacting electrons, which is at the heart of time-dependent density functional theory. Our result covers the Coulomb interaction for particles on the torus.

Joint work with Asbjørn Bækgaard Lauritsen and Mathieu Lewin.

V-Representability Beyond Singular Times in TDDFT: The Hubbard Dimer Case

Théo Duez

16:25–16:45

CNRS, CERMICS

The v-representability problem is a long-standing question in density functional theory: can the density of an interacting system of electrons be reproduced by non-interacting ones under a suitable effective potential? It is what makes the Kohn–Sham construction legitimate. In the time-dependent setting, where an entire density trajectory must be reproduced at all times, it is largely open.

In finite dimension the effective potential is determined at each time by a linear system, obtained by differentiating the density constraint in time, and local existence follows as long as that system is invertible. The difficulty is that it may degenerate at isolated singular times, where the usual inversion formulas break down and it is unclear whether the auxiliary dynamics can be continued. For the two-site problem, the explicit form of the potential and the existence of a boundary where the inversion fails are known [1], but not whether one can cross it.

In this talk I consider the Hubbard dimer in the singlet sector, a finite-dimensional model simple enough for the mechanism to be analysed explicitly, and for two formulations of the theory: the traditional variational principle, and a geometric principle introduced recently in [2], where the same question arises and is likewise open. We show that singular times obstruct neither of them. The price of crossing one is paid in uniqueness rather than in existence, and the two principles pay very differently: one binary choice per crossing in the variational case, an entire circle of admissible continuations in the geometric one.

- [1] M. Ruggenthaler, M. Penz, R. van Leeuwen, "Existence, uniqueness, and construction of the density-potential mapping in time-dependent density-functional theory", *J. Phys.: Condens. Matter* 27 (2015) 203202.
- [2] É. Cancès, T. Duez, J. van Gog, A. B. Lauritsen, M. Lewin, J. Toulouse, "Geometric theory of constrained Schrödinger dynamics with application to time-dependent density-functional theory on a finite lattice", *Phys. Rev. A* 113 (2026) 062210.

High density limit of the Kohn-Sham inverse potential

Louis Garrigue

17:00–17:20

Laboratoire AGM - UMR 8088, CNRS - CY Cergy Paris Université

Consider a target density having integral one and multiply it by the number of particles N . We study the inverse Kohn-Sham potential of this scaled density, in the limit where N goes to infinity. We prove that the corresponding inverse potential converges to the inverse potential of the Thomas-Fermi theory, which is analytically known. We numerically study the rate of convergence.

Joint work with Thiago Carvalho Corso

A maximal Hohenberg-Kohn theorem via potential theory

Thiago Carvalho Corso

17:20–17:40

University of Stuttgart

In this talk, we present a characterization of regular single-particle densities in the continuum setting via tools from classical potential theory. As an application, we show that the Hohenberg-Kohn theorem holds within the class of Laplace form-bounded distributions if and only if the ground state density is quasi-everywhere positive. Moreover we show that this condition is always satisfied for non-interacting systems, thereby establishing the uniqueness of the Kohn-Sham potential.

Physical Significance of Generalized Pauli Constraints

Chih-Chun Wang

17:40–18:00

LMU

A mathematical breakthrough two decades ago by Klyachko revealed that, for pure states, fermionic exchange symmetry constrains natural occupation numbers beyond the Pauli exclusion principle. The physical significance of these generalized Pauli constraints (GPCs) has remained a subject of debate, with their near saturation (quasipinning) in few-electron ground states providing suggestive evidence. Here we establish their physical significance via reduced density matrix functional theory (RDMFT), an exact reformulation of the many-body ground-state problem. We derive a square-root boundary law for the pure-state universal functional, with an explicit expression for its prefactor. The resulting divergence of the functional's gradient translates fermionic exchange symmetry into a repulsive kinematic force in the one-particle picture. This force precludes exact pinning and is missed by common functional approximations. We further prove that the family of ensemble functionals obtained by varying the pair interaction determines the pure-state domain and hence the GPCs. Ensemble relaxation therefore does not eliminate these constraints: it shifts them from the geometry of the domain into the structure of the functionals themselves.

Unified Framework for Functional Theories of Quantum Systems

Markus Penz

18:00–18:20

LMU Munich

This talk presents a unified framework for density-functional theory and its variants for quantum systems on finite-dimensional Hilbert spaces. These theories reduce the complexity inherent in the many-body quantum problem by describing ground states through reduced variables. One can identify a minimal mathematical structure (called the scope of a functional theory) that yields all ingredients of a functional theory: It is possible to define universal functionals, establish their convexity and differentiability properties, address representability questions, and prove a Hohenberg-Kohn-type uniqueness result. An emphasis is placed on functional theories with Lie-algebra observables and examples of possible realizations are given.

Tuesday, November 17 (morning)

PLENARY TALK

Title to be announced

Alice Allen

09:00–09:45

Max Planck Institute for Polymer Research

Abstract to be announced.

Quantitative decorrelation estimates beyond the low-temperature regime

Noe Blassel

09:45–10:05

EPFL

The estimation of decorrelation times, which governs how fast a molecular system converges to a metastable equilibrium, is an important practical question for accelerated molecular dynamics (AMD) algorithms. Despite this, the only quantitative results available are in the low-temperature setting, which excludes most biological systems. Therefore, AMD simulations of biological systems rely on suboptimal heuristics and a posteriori validation.

In this presentation, we will introduce a recent approach to obtain quantitative estimates under milder physical conditions than previously considered. We will describe a framework to analyse the transient behavior of Markov processes conditioned on non-absorption, and present non-asymptotic estimates we obtained for finite-state space jump processes. The approach, based on the backward numerical analysis of coarse-grained semigroups, is expected to generalize beyond this simple setting. We will finally discuss some implications of these results for the construction of principled quasi-stationary diagnostics in AMD algorithms.

Importance sampling for Adaptive Multilevel Splitting

Lune Maillard

10:05–10:25

CERMICS, ENPC, Institut Polytechnique de Paris, CNRS

Computing the probability of rare events is a challenging task. Indeed, in that case, performing direct molecular dynamics simulations is often computationally prohibitive. Hence, we use the Adaptive Multilevel Splitting (AMS) algorithm. However, AMS struggles to converge when the initial momentum distribution corresponds to low values of the committor (i.e. the probability to observe the rare event): this results in a high variance. Therefore, we introduce an importance sampling method on the initial momenta, which allows to reduce the variance of the probability estimator. The method is first tested on a 1D double well potential before being applied to a 2D potential and a real-life example: the alanine dipeptide.

Molecular Principles to Data Science, investigating Metal–Organic Frameworks for Atmospheric Water Harvesting

Nour Alkhatib

10:25–10:45

NYUAD

Freshwater scarcity is a pressing global challenge, and atmospheric water harvesting (AWH) using porous materials offers a sustainable route for water production in arid environments. Many of the efforts have been in discovering new materials for AWH; a major challenge remains in the physical understanding of this process. This work investigates how metal–organic frameworks (MOFs) capture and release water, establishing molecular principles that connect the application of these materials with physical principles. For that, computer simulations validated by experimental adsorption trends are used to uncover mechanisms of AWH. We studied MOF-303, which emerges as a benchmark material due to its sharp adsorption step at low humidity and mild regeneration. We elucidate how water molecules anchor at pyrazole sites, creating local interactions that nucleate water clustering and result in a cooperative transition leading to overall adsorption. This heterogeneous nucleation of water at the pores was later compared with bulk water under the same conditions. We found that, unlike bulk water, a hydrogen-bond network stabilizes in small aggregates inside the MOF, resulting in favorable release afterwards. Comparative studies of aluminum-based frameworks, including MOF-333 and MOF-LA2-1, highlight how subtle changes in linker chemistry and pore geometry shift adsorption profiles. MOF-303, with compact hydrophilic cavities, supports early nucleation and rapid network growth, whereas MOF-333, with fewer polar groups, delays percolation and produces a gradual uptake. MOF-LA2-1 achieves higher capacity due to larger pores but exhibits delayed connectivity because adsorption sites are less symmetrically accessible. These results demonstrate how the spatial distribution of adsorption sites governs both the uptake onset and the isotherm steepness. Scaling up, large-scale simulations, and machine learning have been performed across 2,600 MOFs. Our analysis of a diverse set of MOF structures reveals that uptake capacity is not dictated solely by topological factors such as surface area or pore volume. Instead, framework chemistry, such as charge distribution, metal electronegativity, and functional group polarity, plays the dominant role. Frameworks that balance hydrophilic sites consistently achieve high performance under dry conditions. Our study bridges physical insight with data science and provides transferable design rules to establish a roadmap for the rational design of next-generation MOFs optimized for sustainable water harvesting.

Confidence-Aware Graph Diffusion for Molecular Structure Elucidation

Laurent Vidal

11:15–11:35

DAVID, Université Versailles Saint-Quentin, Paris-Saclay

Inferring a molecule’s structure from spectroscopic measurements, such as NMR and IR, is a challenging inverse problem, with applications in drug and materials design. Classical approaches generate candidate structures, predict their spectra using quantum chemistry calculations, and compare them with the measurements, but are too costly for high-throughput use. Generative deep-learning methods — using chemical language models or diffusion models — offer a faster alternative by learning a distribution of molecular structures conditioned on measured spectra. Recent generative models, however, provide limited information about the reliability of their predictions. To tackle this issue, we present a proof-of-concept diffusion-based approach that estimates confidence through efficient repeated sampling. We introduce a fast, training-free sampling procedure based on closed-form transitions between arbitrary diffusion times. It reduces model evaluations by a factor of 50 on our benchmark while preserving generation quality, resulting in a $56\times$ reduction in sampling time. This makes repeated sampling for a given spectrum practical, allowing us to estimate confidence from the resulting empirical distribution, both for complete structures and individual molecular regions. These confidence scores enable candidate ranking and abstention when the spectroscopic evidence is insufficient. With a small model and almost no hyperparameter tuning, our approach achieves comparable or higher confidence-ranked accuracy while using substantially fewer network evaluations than the reference methods in our benchmark. These results suggest that efficient repeated sampling provides a simple basis for confidence-aware molecular structure elucidation.

Neural Networks in DFT: new findings

Mathias Oster

11:35–11:55

RWTH Aachen

We are presenting some new theoretical results in learning universal functionals and energies. We will especially focus on restricted and compactly observed Moreau-Yosida regularisation. Furthermore, we will present a numerical comparison of learning functionals vs. energy.

Numerical tensor methods for three-particle systems with arbitrary angular momentum and parity

Brice Kammegne

11:55–12:15

University of Sussex, UK

Accurate solutions of the Schrödinger equation for all-particle few-body systems remain a central challenge in theoretical chemistry and molecular physics. The main obstacle is the so-called curse of dimensionality, which makes fully correlated, non-Born–Oppenheimer treatments prohibitively expensive with conventional methods. In this talk, I will present numerical tensor methods developed and implemented for solving the all-particle Schrödinger equation for three-body Coulomb systems — the simplest quantum systems exhibiting electron correlation and coupled nuclear-electronic motion — where the equation is recast in tensor format and solved using low-rank decompositions, dramatically reducing computational cost without sacrificing precision.

As a proof of concept, two strategies are first presented for S states. The first uses a Chebyshev–Lagrange approach on a bounded domain, achieving nano-Hartree accuracy, but suffers from quadrature errors and a dense eigenvalue problem. The second overcomes these limitations by employing a triple-orthogonal Laguerre basis on $[0, \infty)^3$, reaching pico-Hartree accuracy, eliminating quadrature errors, and keeping the Hamiltonian sparse. Building on this foundation, the framework is extended to states with non-zero angular momentum: the angular motion is separated exactly from the radial motion, with correct permutational symmetry enforced for both natural and unnatural parity, and the formalism is generalised to arbitrary angular momentum L , providing a unified framework valid for any angular momentum and parity. Throughout, low-rank decompositions reduce CPU time by several orders of magnitude compared to full-tensor calculations, while pico-Hartree accuracy is maintained across a wide range of atomic, molecular, and exotic systems.

Tuesday, November 17 (afternoon)

An extrapolation strategy for high performance Born-Oppenheimer molecular dynamics with DFT

Michele Nottoli

14:15–14:35

University of Stuttgart

Born-Oppenheimer molecular dynamics (BOMD) simulations are a powerful computational tool for the study of molecules and materials. Since calculations are repeated on geometries that are relatively close, it is possible to reuse the electronic density matrices at previous BOMD time steps to provide an accurate guess for the upcoming calculation at the current BOMD step. In recent works, a strategy which uses molecular descriptors and that takes into account the structure of the Grassmann manifold has been applied to provide accurate guesses for DFT in both BOMD[1,2] and geometry optimizations[3]. While this strategy provided very good results, it cannot be directly applied to high performance methods like those implemented in CP2K due to a computational cost higher than the DFT calculation itself.

In this contribution, we overcome the problem by reformulating the strategy in simpler terms, by keeping the descriptor based approach but working directly in the ambient space and not on the manifold[4]. The reformulation avoids both cubically scaling operations and the storage of square matrices, and it is more accurate than the existing state-of-the-art alternatives in CP2K.

- [1] Polack, Dusson, Stamm, Lipparini J. Chem. Theory Comput. (2021) 17 (11): 6965–6973.
- [2] Pes, Polack, Mazzeo, Dusson, Stamm, Lipparini J. Phys. Chem. Lett. (2023) 14 (43): 9720–9726.
- [3] Askarpour, Nottoli, Stamm, J. Chem. Theory Comput. (2025) 21 (4): 1643–1651.
- [4] Wilhelm et al. arXiv:2607.22916

A unified geometrical framework for computing molecular excitation energies

Laura Grazioli

14:35–14:55

CERMICS and CNRS, ENPC

In the many-body Schrödinger theory, electronic excitation energies admit two mathematically equivalent characterisations. On the one hand, excited states arise as higher-energy solutions of the many-body Schrödinger equation and therefore as critical points of the corresponding energy functional; under suitable regularity assumptions, they are saddle points whose Morse indices equal the excitation levels. On the other hand, excitation energies appear as the normal modes of the linearised dynamics around the ground state through linear response theory.

In approximate theories, the two routes to excitation energies do not coincide, making their comparison interesting both from the mathematical and chemical point of view. In this work, we make a step forward by providing a unified geometrical framework, through the investigation of the inherent manifold structures. For the critical point approach, we develop saddle-point search algorithms on the manifold of admissible wave functions. These algorithms target critical points of prescribed Morse index while respecting the intrinsic geometry of the underlying variational manifold, an essential ingredient for the stable computation of inherently unstable saddle points. In parallel, we provide a systematic geometrical derivation of linear response theory for

variational wave-function models by exploiting the Kähler structure of the corresponding manifolds. Our derivations reduce to well-known linear response equations in quantum chemistry, which may necessitate ad hoc technicalities for different levels of theory.

We apply the general framework to the variational quantum chemical methods Complete active Space Self-Consistent Field (CASSCF) theory and Density Matrix Renormalisation Group (DMRG) theory. We conduct computational studies on some molecular systems and provide chemical interpretations of the obtained results.

Beyond-Born-Oppenheimer One-Electron Equations through the Exactly-Factorized Molecular Kohn-Sham Density Functional Theory

Lucien Dupuy

14:55–15:15

Institut de Chimie de Strasbourg, Université de Strasbourg

Density Functional Theory (DFT) shaped the field of computational chemistry around itself. It owes this impact to its cheap one-electron working equation that can be made to reproduce ground-state many-electrons properties through the use of a universal functional of the electronic density. While this functional is unknown, its known approximations are surprisingly accurate, and can be refined depending on the specific application. However the description of excited states, typically done through DFT’s time-dependent extension (TDDFT), is comparatively less reliable. A case where TDDFT fails to be even qualitatively faithful is around degeneracies of the ground and first-excited states, whose description is crucial for studying dynamics and properties of molecules excited by light. This failure comes from the Born-Oppenheimer framework over which DFT and TDDFT are built, with electronic states unaffected by dynamical correlation with nuclei, the latter being reduced to static point-charges. In this contribution, I will present a beyond-Born-Oppenheimer DFT using electronic and nuclear densities as its basic variables. In addition to the general framework of molecular DFT, I will discuss the modeling of its functional as well as deriving and solving its one-electron beyond-BO equations.

Coupled Cluster Amplitude Extrapolation in Geometry Optimization

Jonas Beck

15:45–16:05

University of Stuttgart

In the Born-Oppenheimer picture, finding the ground state of a molecule practically boils down to minimizing the electronic energy with respect to the nuclear coordinates. For medium-sized molecules, the coupled cluster method offers a highly accurate and systematically improvable approach. At each geometry in the gradient descent along the potential energy surface, both the coupled cluster equations for the energy and the subsequent Lambda equations for the gradient are solved using a quasi-Newton method. The main computational cost in this procedure stems from the steep time scaling associated with evaluating the residuals in each iteration.

In this work, we present an extrapolation ansatz for the coupled cluster and Lambda amplitudes that leverages calculations from previous steps to construct an initial guess for the quasi-Newton solver at each new geometry, significantly accelerating convergence. The ansatz incorporates a necessary amplitude transformation to mitigate discontinuities associated with orbital energy crossings at the Hartree–Fock level of theory, all while remaining computationally and memory efficient.

A quadratic Grassmann manifold optimization problem arising from quantum embedding methods

Alicia Negre

16:05–16:25

CERMICS, Ecole des ponts et chaussées - Institut Polytechnique de Paris, Inria

Density Matrix Embedding Theory (DMET) is a quantum embedding method designed to study large and strongly correlated quantum systems through a domain-decomposition strategy. In DMET, the central object is the one-particle reduced density matrix (1-RDM) of the global quantum system. The method proceeds by first fragmenting the system into smaller subsystems. These subproblems are then solved iteratively by embedding each subsystem in a bath (the "high-level" stage), while the results are integrated through a self-consistent procedure (the "low-level" stage).

In the conventional DMET formulation, the global 1-RDM is constrained to be a projector. This constraint severely restricts the class of admissible solutions and thus reduces accuracy, particularly in strongly correlated regimes. The present work investigates how to overcome this limitation by extending the set of admissible 1-RDMs to include mixed states across all key stages of the method, highlighting the subproblems arising with this extension. In particular, it proposes an alternative approach for constructing the bath spaces using a Riemannian optimization framework, enabling a more expressive high-level solution. The goal is to enhance the accuracy and flexibility of DMET within a broader framework while remaining consistent with its underlying philosophy.

Model Order Reduction for Parametric Dissipative Quantum Systems

Zhuoyao Zeng

16:25–16:45

University of Stuttgart

We consider the approximation of trace-one elements in the kernels of parameter-dependent Lindblad operators acting on the space of Hermitian matrices. Since the dimension of the ambient matrix space grows exponentially with system size, direct solution throughout the parameter domain rapidly becomes prohibitive. We develop a residual-driven reduced basis framework for this problem. Building on the reduced eigenvalue approach previously proposed for Lindbladian steady states, we introduce a trace-constrained residual formulation and derive concrete offline–online algorithms with corresponding residual-driven greedy selection rules.

For problems with a unique steady state, we derive residual-based state-error estimates and prove that both indicators are equivalent to the squared projection error. For real-analytic parameter dependence, we establish generalized-exponential width decay and greedy convergence.

Numerical experiments for boundary-driven Fermi–Hubbard and dissipative XYZ chains corroborate the theoretical analysis and demonstrate the effectiveness of the reduced models. Among the methods considered, the results suggest that the trace-constrained greedy method, AffGreedy, provides the most favorable overall balance of accuracy and computational cost.

Kohn-Sham models for encapsulated 2D moiré materials

Solal Perrin-Roussel

17:15–17:35

ENS de Lyon

We study Kohn-Sham Density Functional Theory (DFT) models describing the electronic structure of two-dimensional materials placed in a three-dimensional environment, encapsulated between two parallel conducting electrodes. In this geometry, the Dirichlet boundary conditions at the electrodes screen the Coulomb interaction, which becomes effectively short-ranged, of Yukawa type. We prove that some nonlinear Kohn-Sham DFT models are well-posed in this setting, both for periodic materials (such as graphene) and for quasi-periodic materials (such as twisted bilayer graphene and other moiré materials for generic incommensurate twist angles).

Quantum optimal transport and interpolations in quantum chemistry

Etienne Obermeyer

17:35–17:55

Université Marie et Louis Pasteur

Quantum optimal transport is a theory that adapts classical optimal transport to a framework where measures are replaced by density matrices, that is self-adjoint, positive, trace-one operators. These matrices arise naturally in quantum mechanics. Quantum optimal transport has drawn attention in recent years, with different formulations, most of which adapting Kantorovich problem from classical optimal transport.

In this talk, I will present a numerical method to compute the quantum optimal transport distance proposed by Carlen and Maas [2] in 2020. This distance is a Riemannian distance on the manifold of density matrices, based on the B enamou–Brenier formulation [5] and mimicking the Otto formulation of dynamical optimal transport [1].

I will present a numerical method to compute this distance, based on a sequential quadratic programming (SQP) method, following Chen and al. [3], with an extra interior-point strategy to tackle the problem of semidefinite matrices, inspired by a similar work on vanishing densities in the classical setting [4]. This method allows us to compute distances and geodesics for large matrices. We then study qualitatively the geodesics through the integral kernel of the matrices. We study the convergence with respect to the discretization in a Fourier basis.

I will then present examples of quantum chemistry density matrices. These matrices characterize some important properties of the wavefunction solution to the Schr odinger equation. These matrices have low rank, and these examples can only be treated with a careful numerical method. We will compare the Carlen–Maas geodesics with the solutions with varying nuclei positions, with the aim of giving approximations of solutions in quantum chemistry.

- [1] Felix Otto. The geometry of dissipative evolution equations: the porous medium equation (2001).
- [2] Eric A. Carlen and Jan Maas. Non-commutative calculus, optimal transport and functional inequalities in dissipative quantum systems. *Journal of Statistical Physics* 178.2 (2020): 319-378.
- [3] Yongxin Chen et al. An efficient algorithm for matrix-valued and vector-valued optimal mass transport. *Journal of Scientific Computing* 77.1 (2018): 79-100.
- [4] Andrea Natale and Gabriele Todeschi. Computation of optimal transport with finite volumes. *ESAIM: Mathematical Modelling and Numerical Analysis* 55.5 (2021): 1847-1871.
- [5] Jean-David Benamou and Yann Brenier. A computational fluid mechanics solution to the Monge-Kantorovich mass transfer problem. *Numerische Mathematik* 84.3 (2000): 375-393.

Model Order Reduction using Wasserstein Barycenter

Maximilian Penka

17:55–18:15

Laboratoire de mathématiques de Besançon

Abstract to be announced.

Wednesday, November 18 (morning)

PLENARY TALK

Optimization of Dirac's eigenvalue

David Gontier

09:00–09:45

CERMICS, École nationale des ponts et chaussées

I will talk about the Keller inequality, which concerns the optimization of the first eigenvalue of an operator depending on an external potential, under some L^p constraints on this potential. I will provide a novel technique which allows to tackle the problem both for all kinds of operators, including Schrödinger and Dirac, and which provides interesting numerical schemes for this optimization problem.

This is joint work with Hanne Van Den Bosch, Jean Dolbeault, and Fabio Pizzichillo.

Cut-off Jastrow Factors and Spectral Barron Regularity of Coulombic Electronic Wave Functions

Virginie Ehrlacher

09:45–10:05

Ecole nationale des Ponts et Chaussées & INRIA

We study the spectral Barron regularity of Coulombic electronic eigenfunctions after extraction of a cut-off Jastrow factor. Let H be an N -electron Coulomb Hamiltonian with clamped nuclei, and let ψ be an eigenfunction associated with a discrete eigenvalue below the bottom of the essential spectrum of H . For the cut-off Jastrow factor of Fournais–Hoffmann–Ostenhof–Hoffmann–Ostenhof–Sørensen, we set φ the quotient of ψ with this factor. Whereas the original wave function ψ satisfies the sharp global threshold $\psi \in B_{\text{sp}}^s(\mathbb{R}^{3N})$ for $0 \leq s < 1$, we prove that the Jastrow quotient gains one full order: $\varphi \in B_{\text{sp}}^s(\mathbb{R}^{3N})$ for $0 \leq s < 2$. The endpoint $s = 2$ is shown to be natural through an explicit hydrogen-like eigenfunction. The many-body proof is a global Fourier-side resolvent argument. After conjugation by the cut-off Jastrow factor, the Coulomb singularities are converted into localized angular coefficient blocks with admissible Fourier-control measures. Low frequencies are controlled by the a priori H^1 -bound, while high frequencies are recovered by a Neumann fixed-point argument using the resolvent multiplier and annular estimates for the coefficient measures.

Continuum honeycomb Schrödinger operators with non-commensurate line defects

Pierre Amenoagbadji

10:05–10:25

LJLL, Sorbonne Université

In this work, we study wave propagation in two-dimensional honeycomb structures with a non-commensurate line defect or edge. Our model is a Schrödinger operator which interpolates, across the edge, between two distinct bulk (asymptotic) Hamiltonians with a common spectral gap about the Dirac point of an unperturbed honeycomb operator. We seek edge states, eigenstates that are bounded and oscillatory parallel to the edge, and decaying in the transverse direction. For non-commensurate edges, the rigorous definition of these states is nontrivial due to the lack of translation invariance along the edge. To address this, we exploit quasiperiodicity along the edge by expressing the Hamiltonian as the restriction of a 3D (degenerate elliptic) Hamiltonian describing a 3D medium with a 2D interface within which there is periodicity. Using perturbation theory, we construct edge states in this 3D setting and obtain by restriction 2D edge states which are quasiperiodic along the irrational edge. These edge states are seeded by eigenfunctions of an effective Dirac operator, which has an infinite block-diagonal structure due to the non-commensurate geometry. A consequence is that infinitely many edge state eigenpairs arise, whose energies are dense in the perturbed bulk spectral gap. The construction of the edge states requires an omnidirectional non-resonance (no-fold) condition on the dispersion functions of the unperturbed honeycomb Hamiltonian, as well as a Diophantine condition on the edge slope.

Title to be announced

Alfred Kirsch

10:25–10:45

Technische Universität München

Abstract to be announced.

Quantification of Discretization Error in Plane-Wave Density Functional Theory

Bruno Ploumhans

11:15–11:35

EPFL

I will present recent progress on estimating the plane-wave basis discretization error in density functional theory computations for materials.

Hardware-accelerated parallel eigensolvers for ab initio calculations of materials

Ioanna-Maria Lygatsika

11:35–11:55

Inria Paris

The computation of the electronic structure of materials from first principles in condensed matter physics requires solving the Kohn-Sham equations discretized on a plane-wave basis. This problem requires finding only a few eigenpairs of a large Hermitian matrix. We first present matrix-free eigensolvers for solving such problems. We focus on the spectrum slicing subspace iteration, an algorithm recently implemented in the open-source software package Abinit. We provide numerical results on the performance of the new eigensolver on hardware-accelerated architectures. This is joint work with Marc Torrent and Clémentine Barat.

Riemannian full multigrid methods for plane-wave density functional theory

Jonas Püschel

11:55–12:15

University of Augsburg

Riemannian multilevel optimization accelerates energy minimization under manifold constraints by exchanging first-order information across a hierarchy of discretizations, but it operates at a fixed finest level and depends on the initial guess supplied there. In the Euclidean setting, full multigrid (nested iteration) removes this dependence by solving on the coarsest level and prolonging each solution to initialize the next, reaching discretization accuracy in a small, level-independent number of cycles. We extend this idea to the manifold setting and introduce a Riemannian Full Multigrid method, building upon the Riemannian MGOPT and introducing a point-prolongation based coarse model and refinement strategy. We employ the method for plane-wave Kohn–Sham density functional theory, where the discretization hierarchy is a sequence of kinetic-energy cutoffs and observe significantly improved performance compared to single-level methods.

Title to be announced

Antoine Levitt

12:15–12:35

Université Paris Saclay

Abstract to be announced.