MOANSI Annual Meeting 2025

Book of Abstracts

Munich, November 20th and 21st

Contents

Titles and Abstracts

Reducing Errors in Traditional and Machine-Learned Density Functional Calculations

20 Nov
11:00am

Stefan Vučkovic
Université de Fribourg

Density Functional Theory (DFT) is the most widely used electronic structure method, yet significant challenges of standard Kohn–Sham DFT remain for several classes of systems. Large DFT errors often arise from self-interaction and static correlation, and, more recently, unexpectedly poor performance in charged systems has been observed [3]. In this talk, I will discuss our group's recent strategies for reducing these errors, focusing on two directions:

1. improvements in traditional DFT for charged systems, and
2. machine-learning developments targeting self-interaction–prone systems and bond breaking.

On the Regularity of the discretized Coupled Cluster Amplitudes

20 Nov
11:45am

Jonas Beck
Universität Stuttgart

One of the most widely used and accurate methods for calculating ground-state energies of molecules within the Born–Oppenheimer approximation is the coupled cluster method. The accuracy comes at a high cost, as the coupled cluster method is computationally intensive. Moreover, this method must be applied over a large set of nuclear coordinates in order to obtain a reasonable potential energy surface. Understanding the regularity of the coupled cluster amplitudes with respect to the nuclear coordinates would therefore have multiple practical implications. High regularity would suggest that only a small number of nuclear geometries need to be calculated, and that subsequent application of interpolation methods could be used to obtain approximate solutions for all geometries. These solutions could either serve as a computationally inexpensive standalone approach or provide initial estimates for the actual coupled cluster calculations, potentially leading to significantly faster convergence.

In this talk, our theoretical work on the regularity of the coupled cluster amplitudes is presented, which is closely related to the regularity of the underlying SCF procedure itself. Furthermore, the results are illustrated with several practical examples. For certain molecules, the coupled cluster amplitudes are interpolated using a polynomial-like interpolation along Chebyshev nodes, and the corresponding error decay is demonstrated.

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20 Nov
12:10pm

A rigorous formulation of density functional theory for electrons in one dimension

Thiago Carvalho Corso

Universität Stuttgart

In this talk, I will present a completely rigorous formulation of Kohn-Sham density functional theory for spinless electrons living in one dimensional space. More precisely, we first present a complete characterization of the set of v-representable densities for a broad class of distributional potentials. In particular, this characterization shows that the v-representable set is independent of the interaction potential. Next, we present a Hohenberg-Kohn theorem that applies to the class of potentials considered here. Lastly, we establish the differentiability of the exchange-correlation functional and therefore the existence of a unique exchange-correlation potential. From these results, we conclude that the Kohn-Sham scheme is rigorously exact in this setting. Time permitting, we discuss some unexpected regularity properties of the exchange-correlation potential.

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20 Nov
14:00pm

A posteriori error estimates for LCAO basis

Mi-Song Dupuy

Sorbonne Université

TBA.

Geometric and topological potentials guiding protein self-assembly

20 Nov
14:25pm

Ivan Spirandelli
Universität Potsdam

The simulated assembly of molecular building blocks into functional complexes is central to computational biology and materials science. Protein-assembly simulations, driven by short-range nonpolar interactions, can in principle reach their biologically correct structures, but rugged energy landscapes often trap simulations in non-functional local minima.

We introduce a long-range topological potential, quantified by weighted total persistence, and combine it with the morphometric approach to solvation free energy. Across simulations of four different protein assemblies, this combination increases assembly success rates by as much as sixteen-fold relative to the morphometric model alone and enables successful assembly in cases that otherwise fail.

Unlike previous topology-based approaches, which have been primarily descriptive, our method uses topological measures as an active energetic bias. The method is independent of electrostatics or chemical specificity and depends only on atom geometry. While here presented for proteins, the geometry-only formulation in principle allows for the method's extension to other classes of self-assembling systems. Integrating topological descriptions into energy functions offers a general strategy for overcoming kinetic barriers in molecular simulations, with potential applications in drug design, materials development, and the study of complex self-assembly processes.

Coarse-grained simulation of protein self-assembly

20 Nov
14:50pm

Lukas Mayrhofer
Technische Universität Munich

We study how large protein systems self-assemble, focusing on how the tobacco mosaic virus coat protein forms a helical shell. The size and timescales of these systems make all-atom molecular dynamics simulations impractical. Each protein is fixed in a single conformation, and we use a coarse-grained energy model capturing van der Waals, electrostatic, and hydrophobic interactions. The rigidity assumption requires careful tuning of the approximation for each interaction type. Our simulations employ overdamped Langevin dynamics to drive the assembly process. A key finding is that high interaction specificity, which is essential for robust self-assembly, emerges only through the collective interplay of the interactions we model.

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20 Nov
15:15pm

Neural Network Acceleration of Iterative Methods for nonlinear Schrödinger eigenvalue problems

Jonas Püschel

Universität Augsburg

We present a novel approach to accelerate iterative methods to solve nonlinear Schrödinger eigenvalue problems using neural networks. Nonlinear eigenvector problems are fundamental in quantum mechanics and other fields, yet conventional solvers often suffer from slow convergence in extreme parameter regimes, as exemplified by the rotating Bose-Einstein condensate (BEC) problem. Our method uses a neural network to predict and refine solution trajectories, leveraging knowledge from previous simulations to improve convergence speed and accuracy. Numerical experiments demonstrate significant speed-up over classical solvers, highlighting both the strengths and limitations of the approach.

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20 Nov
16:15pm

Homogeneous Sobolev spaces in Maxwell's equation and density-functional theory

Markus Penz

Ludwig-Maximilians-Universität München

A Hilbert-space setting for density-functional theory is suggested that integrates Maxwell's equations into the geometry of the spaces. This does not only allow for a very elegant formulation but also leads to automatic regularization of the theory, completely avoiding the usual representability problems.

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20 Nov
16:40pm

Local convergence of Riemannian optimization methods for rotating multicomponent BECs

Martin Hermann

Universität Augsburg

We investigate Riemannian optimization methods for ground states of rotating multicomponent Bose-Einstein condensates. The local convergence properties are determined by an eigenvalue problem that reflects both the interaction between the components as well as the complex-valued nature of the rotating gas and therefore poses a new challenge beyond previously established results.

Efficient generation of group-equivariant and permutation-invariant polynomials

20 Nov
17:05pm

Liwei Zhang
RWTH Aachen

Group-equivariant and permutation-invariant polynomials serve as commonly employed descriptors for physical properties in machine learning (ML), such as interatomic potentials, Hamiltonian operators, and density matrices in Kohn-Sham density functional theory (DFT). In this talk, we will introduce an efficient method for constructing such polynomials using the Lie algebra of the group. Furthermore, we will explore the approximation properties and dimensionality of the corresponding function space for several typical groups, thereby demonstrating the significance of incorporating symmetry into machine learning models.

Projection-based Coarse Graining for Underdamped Langevin Dynamics

20 Nov
17:30pm

Vahid Nateghi
Max Planck Institute for Dynamics of Complex Technical Systems

Coarse-graining has gained significant attention in recent decades, driven by an increasing interest in understanding the slow dynamics of molecules. This work presents a projection-based coarse-graining method for general underdamped Langevin dynamics. Following Mori-Zwanzig projection formalism, we derive a closed-form expression for the effective dynamics. Leveraging the well-established Koopman generator Extended Dynamic Mode Decomposition (gEDMD) method, we evaluate the slowest timescales of the system. Using a two-dimensional model system, we demonstrate that the proposed method accurately captures the thermodynamic and kinetic properties of the full-space model.

A Numerical Study of the Landau Hamiltonian

20 Nov
17:55pm

Rafael Antonio Lainez Reyes
Universität Stuttgart

Despite its simplicity the Landau Hamiltonian display some interesting, unexpected behavior. In this talk we explore the Landau Hamiltonian subject to a periodic potential. We will first recall Bloch theory for this system, and then exploit its consequences in order to perform numerical simulation on said system.

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21 Nov
09:00am

Alchemical Perturbations Characterizing Chemical Space: Intepretability, Intrinsic Dimension and Sampling

Guido Falk van Rudorff
Universität Kassel

Alchemical Perturbations Characterizing Chemical Space: Intepretability, Intrinsic Dimension and Sampling

Understanding molecular properties across regions in chemical space requires methods that go beyond traditional one-by-one evaluations of individual systems. With "quantum alchemy", a perturbative approach, many diverse properties such as energies, orbital eigenvalues, electron densities, photoelectron circular dichroism parameters, protonation energies and more can be predicted for millions of related systems with a simple closed form expression. At heart, a Taylor or Padé approximant is built from the first low-order response functions of the property w.r.t. changes in the nuclear charges and geometry. End-to-end, this is typically five orders of magnitude cheaper than quantum chemistry methods of comparable accuracy.

Moreover, the closed-form expression of quantum alchemy models can be analysed particularly well: it affords a way to make black-box predictors such as quantum chemistry calculations or machine learning models interpretable. This becomes possible through a unique decomposition of a global property into n-body k-order effects of individual atoms or functional groups. For energies, this decomposition unravels approximate symmetries which must hold true for all conceivable systems of certain structural properties, which can help machine learning models by reducing the dimensionality of the search space. Moreover, we show how perturbations allow to estimate the intrinsic dimensionality of a chemical space.

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21 Nov
09:45am

Accurate Ab-initio Neural-network Solutions to Large-Scale Electronic Structure Problems

Nicholas Gao
CUSP AI

Neural-network-based ansätze combined with variational Monte Carlo (NN-VMC) have seen tremendous success in solving the electronic Schrödinger equation for small molecules. While frequently offering the most accurate ground-state energies out-of-the-box, computational cost has so far prohibited the application to many or large systems. We tackle the computational scaling on two axes: 1) We present finite-ranged embeddings (FiRE). This novel neural network wave function reduces the complexity of NN-VMC by the number of electrons by restricting the range at which electrons interact. In practical calculations, this reduction in complexity yields a 10x speedup while consistently matching the most accurate reference data in relative energies, often outperforming CCSD(T). 2) We present an amortization scheme of NN-VMC. Instead of independently finding the ground

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Predicting Fractures in Disordered Material

21 Nov
10:10am

Maximilian Reihn
Universität Suttgart

TBA.

A mathematical analysis of the discretized IPT-DMFT equations

21 Nov
11:00am

Alfred Kirsch
Technische Universität München

Dynamical Mean-Field Theory (DMFT) stands as an insightful approximation in condensed matter physics. Using the Iterated Perturbation Theory (IPT) solver, it allows for instance to predict interaction-driven metal-to-insulator transition for the Hubbard model on several lattices. In this talk, I will provide a mathematical introduction to the IPT-DMFT formalism and present recent results on the discretization of these equations on the so-called Matsubara frequencies ([1], joint work with É. Cancès and S. Perrin-Roussel).

More precisely, I will discuss the existence and uniqueness of solution(s) to these equations, and demonstrate through numerical simulations that a given "causal" property is not preserved by this discretization scheme. If time permits, I will present an alternative discretization that preserves this "causal" property (based on results from a previous analysis of the continuous equations, see [2]).

Universal Approximation of the regularized Lieb functional by neural networks

21 Nov
11:25am

Mathias Oster
RWTH Aachen

We will provide existence results of neural networks with physical constraints approximating the Moreau-Yosida regularized Lieb functional for grand-canonical ensembles. We will furthermore provide a first error estimate of the approximated energy in terms of the regularization parameter.

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21 Nov
11:50am

Fluctuation relation beyond the Jarzynski equality and solvation models from a probabilistic view on the solute-solvent interaction energy

Christopher J. Stein
Technische Universität München

I will outline the derivation and initial application of a fluctuation relation that allows us to calculate free energy diIerences from general dynamics that do not need to be Liouvillian and are free from other constraints such as microscopic reversibility or (local) detailed balance. This framework is therefore more general than the Jarzynski equality, which we recover in the limit of Liouvillian dynamics. I will present both the derivation of this theory and an initial model application that highlights the advantage of our protocol. In the second part of the talk, I will outline how we intend to leverage the underlying probabilistic framework and a rigorous calculation of the moments of the system- environment interaction energy to define novel solvation models. These models enable us to focus the simulation eIort on a relatively small, explicit system while maintaining high accuracy for evaluating free energy diIerences through accurate coupling to the environment.

Bibliography

[1] E. Cancès, A. Kirsch, et al. A mathematical analysis of the discretized ipt-dmft equations. *arXiv preprint arXiv:2505.21287*, 2025.

[2] É. Cancès, A. Kirsch, and S. Perrin-Roussel. A mathematical analysis of ipt-dmft. *arXiv preprint arXiv:2406.03384*, 2024.

[3] C. J. Nickerson, K. R. Bryenton, A. J. Price, and E. R. Johnson. Comparison of density-functional theory dispersion corrections for the des15k database. *The Journal of Physical Chemistry A*, 127(41):8712–8722, 2023.