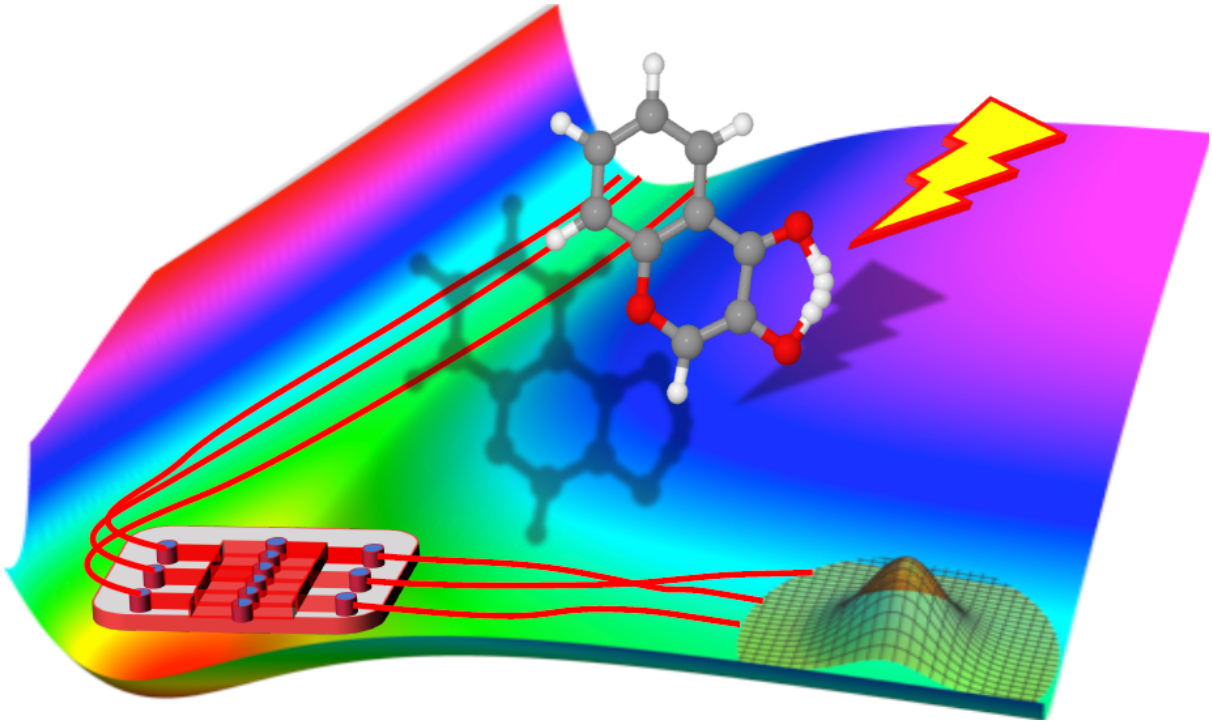
MLQC4Dyn - Week 3

Abstracts



Simulating open quantum systems with quantum computers

Michael Marthaler
HQS Quantum Simulations

From electron transport to light-matter interaction, considering quantum mechanical systems including their environment can often be off substantial interest or even strictly necessary. When trying to solve problem involving open quantum system on conventional computers it is necessary to solve the master equation for the density matrix instead of the Schrödinger equation for the wave function. This squares the already exponentially large state of a quantum mechanical problem and makes it therefore even more challenging. Solving quantum mechanical problems is one of the most obvious use cases for quantum computers. But it is interesting to note that the current generation of NISQ computers are intrinsically open quantum systems. In this presentation we will discuss in how far it is possible to map interesting open quantum system to NISQ devices and include the fact that qubits are open quantum systems themselves as part of the mapping. Additionally we discuss relatively common problems in ab-initio simulation which can in fact be mapped onto an open quantum system.

ADAPTive Variational Quantum Algorithms for Gibbs State Preparation

Ada Warren
Virginia Tech

The preparation of Gibbs states is a centrally important task in quantum computation, with applications in quantum simulation, quantum optimization, and quantum machine learning. Inspired by the successes of the variational quantum eigensolver in the preparation of molecular ground states, a number of previous approaches to Gibbs state preparation have been variational in nature. As with other variational algorithms, however, the *a priori* selection of a variational ansatz is either too restrictive or can lead to unnecessarily long circuits. Additionally, many algorithms for preparing Gibbs states rely on quantum subroutines which are difficult to implement on near-term hardware, such as estimation of the Gibbs free energy. In this talk, we address this by (i) introducing an objective function that, unlike the free energy, is easily measured and (ii) using dynamically generated ansatze which are more compact and problem-tailored. This allows for arbitrarily accurate Gibbs state preparation using low-depth circuits. To verify the effectiveness of our approach, we numerically demonstrate that our algorithm can prepare high-fidelity Gibbs states across a broad range of temperatures and for a variety of Hamiltonians.

Using molecular symmetries to perform quantum simulations on current quantum hardware

David Muñoz Ramo

Cambridge Quantum Ltd.

The simulation of complex chemical systems on quantum computers is one of the main applications expected to yield quantum advantage in the near term. However, the current generation of quantum hardware is difficult to use for molecular simulations due to the high levels of noise during device operation. Improvements on hardware promise to make these simulations possible, either by improvements in fidelities and coherence time, or by making quantum error correction possible. In parallel, research in algorithms to combat noise is actively being developed.

In this talk, I'll present work performed by my team on the simulation of a variety of molecular and solid state systems on different quantum hardware architectures. Examples include protein-ligand interactions, different phases of iron metal and the chemistry of atmospheric reactions. I will highlight the impact of noise on the results we obtained, and the need to mitigate it. For this purpose, I will introduce two strategies. First, I will describe a novel noise mitigation technique, called Partition Measurement Symmetry Verification (PMSV), which exploits the symmetries present in molecular systems to reduce noise in NISQ experiments. Second, I will discuss strategies to reduce circuit depth in the state preparation step of the algorithms we use for our simulations, based again on analysis of symmetries present in the systems being simulated. I will show how these techniques greatly help in improving results from hardware experiments and pushes us closer to making quantum computers useful for the simulation of chemical systems.

QUANTUM COMPUTING EMULATION

Quantum computation is a new, emerging, disruptive technology capable of boosting computational performance in selected areas of science and technology. Not being a universal HPC technology, we are facing the challenging issue of identifying its area of applicability.

In this context, quantum emulation on classical computers is a relevant approach. On one side, deep understanding of quantum algorithms requires getting the hands under the hood to manipulate them. On the other side, real tests of new computational protocols on quantum platforms are limited by the decoherence limit, which prevents the execution of deep, powerful algorithms. However, in a hybrid quantum-classical computational platform, they can be executed by an emulator operating on the classical side. These lectures will provide examples on these issues.

Inspired by these observations, a quantum emulator library was developed to serve both as a pedagogical and research tool, for exploring quantum circuits and implementing computational protocols. The need for cooperation in hybrid simulations imposed strong requirements of computational performance. The software package is in fact composed of four different, fully portable C++ libraries:

- PQubits (Parallel Qubits) Shared memory, multithreaded library
- CQubits (Cuda Qubits) Shared memory with Cuda GPU support
- DQbits (Distributed Qubits) Distributed memory, MPI library
- CDQbits (MPI + Cuda qubits) Distributed memory, cuda aware MPI

MPI and Cuda subtleties are mostly hidden to client codes, and programming interfaces are largely universal. There are in addition architectural choices that significantly boost performance. First, the support of multiqubit gates (only one and two qubit gates are needed, but we support up to five qubit gates). Secondly, a gate fusion optimization that allows us to replace complex multiqubit circuits by a single multiqubit gate. In some quantum chemistry codes, cuda plus gate fusion provide a 50x speedup with respect to a single CPU without gate fusion.

The following subjects will be developed, illustrated by examples and simulations codes available in the library (and executed on a laptop):

- Brief overview of the quantum computing landscape (20 to 30 minutes)
- Basic issues in quantum emulation: a high level overview of the emulation software (1 h 30')
- Discussion of the most important quantum algorithms with examples on linear algebra and optimization issues (2h ?)
- High level overview of large scale simulations (?):
  - Ground state of the H2 molecule, that exposes the speedup provided by gate fusion.
  - Itinerant ferromagnetism in the Hubbard model. This simulation develops computational protocols that explicitly shows the added value provided by the presence of an emulator in a quantum-classical hybrid context.
  - Probably, a simulation under development in computational finance.
- Conclusions.

Victor Alessandrini
Maison de la Simulation

Efficient quantum computation of molecular forces and other energy gradients

Matthias Degroote

Boehringer Ingelheim B.V.

While most work on the quantum simulation of chemistry has focused on computing energy surfaces, a similarly important application requiring subtly different algorithms is the computation of energy derivatives. Almost all molecular properties can be expressed an energy derivative, including molecular forces, which are essential for applications such as molecular dynamics simulations. We introduce new quantum algorithms for computing molecular energy derivatives with significantly lower complexity than prior methods. For noisy-intermediate scale quantum devices we demonstrate how low rank factorizations and other tomography schemes can be optimized for energy derivative calculations. We perform numerics revealing that our techniques reduce the number of circuit repetitions required by many orders of magnitude for even modest systems. In the context of fault-tolerant algorithms, we develop new methods of estimating energy derivatives with Heisenberg limited scaling incorporating state-of-the-art techniques for block encoding fermionic operators.

Quantum dynamics on quantum computers: where do we stand, where may we go?

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In this talk, we shall tentatively cover some aspects related to making use of the promised advantage of quantum computing in the context of quantum dynamics. A short review of the basic formalism will be provided first.

An evident valorisation concerns the on-the-fly production of highly-multiconfigurational quantum chemistry data (e.g., with SA-OO-VQE) to be further used in direct nonadiabatic quantum dynamics (e.g., DD-vMCG). This will be illustrated with a proof of concept, namely the photoisomerisation of formaldimine. Such developments strongly rely on the detailed material provided in the talks given by Saad Yalouz, Bruno Senjean, and Martin Beseda.

We shall also mention how the GUCCSD-based SA-OO-VQE Ansatz of an target ensemble of coupled electronic wavefunctions may provide a potential avenue for generating an ab initio diabatic representation for free when preventing the final diagonalisation step within the subspace of interest.

Finally, some open discussion will be provided in this context regarding the variational quantum description of the vibrational problem itself (eigensolver and propagator).

Green's functions algorithms on quantum computers for materials science

Ivan Rungger

National Physical Laboratory

Quantum embedding approaches for materials simulations, such as the dynamical mean-field theory (DMFT), provide corrections to first-principles calculations for strongly correlated electrons, which are poorly described at lower levels of theory. These embedding methods are computationally demanding on classical computers, and hence remain restricted to small systems, limiting the scope of their applicability. Quantum computers have the potential to overcome this limitation. In this talk we present different methods to obtain the Green's functions on quantum computers for materials science simulations, which are based either on the Lehman representation (arXiv:1910.04735, Nature Comp. Sci. 1. 410 (2021)), or on a continued fraction representation using the Krylov basis. We consider two methods to construct the Krylov states. The first is based on the Krylov variational quantum algorithm (KVQA, arXiv:2105.13298), while the second method uses the quantum subspace expansion for Green's functions (QSEG, arXiv:2205.00094).

Quantum embedding methods for simulations of materials on quantum computers

Giulia Galli
University of Chicago, and Argonne National Laboratory

Quantum computers hold promise to improve the efficiency of quantum simulations of materials and to enable the investigation of systems and properties more complex than tractable at present on classical architectures. We discuss computational frameworks to carry out electronic structure calculations of solids on noisy intermediate scale quantum computers [1] using embedding theories [2,3], and we give examples for a specific class of materials, i.e., spin defects in solids. These are promising systems to build future quantum technologies, e.g., computers, sensors and devices for quantum communications. Although quantum simulations on quantum architectures are in their infancy, some promising results for realistic systems appear to be within reach.

[1] Simulating the electronic structure of spin defects on quantum computers, Benchen Huang, Marco Govoni, and Giulia Galli, PRX Quantum 3, 010339 (2022).
[2] Green's function formulation of quantum defect embedding theory, Nan Sheng*, Christian Vorwerk*, Marco Govoni, and Giulia Galli (*equal contribution), J. Chem. Theory Comput. 18, 3512 (2022).
[3] Quantum Embedding Theories to Simulate Condensed Systems on Quantum Computers, Christian Vorwerk*, Nan Sheng*, Marco Govoni, Benchen Huang, and Giulia Galli (*equal contribution), Nature Comput. Sci. accepted (2022). arXiv:2105.04736.

Quantum algorithms for dynamics: from quantum simulations to quantum machine learning

Francesco Tacchino

IBM Research Zurich

In this talk, I will present recent progress in the field of quantum computing methods for quantum and molecular dynamics. In the first part, after briefly introducing the IBM Quantum hardware, software and applications roadmap, I will discuss quantum algorithmic methods for quantum dynamics, from digital quantum simulations of many body systems to applications in quantum chemistry, including grid-based calculations in first quantization, non-adiabatic evolution and molecular dynamics. In the second part, I will cover recently developed quantum approaches to force field generation, based on variational and quantum machine learning methods. In particular, I will discuss an application of quantum neural networks to this problem, highlighting challenges and opportunities of data-driven quantum solutions.

Variational Quantum Optimization Algorithms

Rick van Bijnen

Innsbruck University / IQOQI

Hybrid classical–quantum algorithms aim to variationally solve optimization problems using a feedback loop between a classical computer and a quantum co-processor, while benefiting from quantum resources. Originally designed for finding ground states of quantum many-body systems, the variational approach has recently also been successful in finding suitable states for quantum sensing. In this talk we discuss the noisy optimization algorithms running on the classical computer, the challenges of optimizing noisy quantum devices, and how we can use physical insights of the quantum platform combined with some machine learning to dramatically reduce the required number of measurements.

Algebraic techniques for dealing with difficult operators in quantum chemistry on a quantum computer

Artur Izmaylov

University of Toronto

Quantum chemistry problem is one of the attractive targets for demonstrating quantum advantage of quantum computing technology. Quantum computing algorithms for solving this problem require algebraic operations with the electronic Hamiltonian. Dealing with this Hamiltonian in the second quantized form can be facilitated by partitioning it into a sum of fragments diagonalizable using rotations from either small Lie groups or the Clifford group. These fragments are convenient for performing various algebraic manipulations required in circuit compiling and quantum measurement. In this talk, I will illustrate how the Hamiltonian partitioning can be used to improve performance of the Variational Quantum Eigensolver and Quantum Phase Estimation algorithms.

Quantum computing to describe properties of correlated many-body systems: from quantum chemistry to condensed matter physics

Saad Yalouz[1]

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Today, the development of quantum algorithms dedicated to the description of many-body systems is considered as one of the most promising applications for near term quantum computers. However, tackling such complex problems on emerging quantum devices requires caution, as experimental setups are still in their infancy and suffer from severe constraints (which will be gradually lifted in the coming years), thus prompting us to adapt our implementation accordingly. To this end, a great attention has been paid to the development of suitable methods, such as the well-known Variational Quantum Eigensolver (VQE), a hybrid classical-quantum algorithm. The VQE algorithm has been successfully applied to describe many simple problems. However, its application to more complex systems with strong many-body interactions remains a real challenge.

In this talk, I will discuss recent work I have realized to cover the problem of strong many-body interactions on different types of systems in quantum chemistry and condensed matter physics. I will present several extensions of the VQE algorithm to describe photochemical [1, 2] systems, the so-called state-averaged orbital-optimization VQE (SA-OO-VQE), as well as the development of a circuit ansatz for photonics quantum computers to describe exotic transitions in the ground state of bosonic models [3].

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[1] S. Yalouz, B. Senjean, J. Günther, F. Buda, T. E. O'Brien, and L. Visscher, A state-averaged orbital-optimized hybrid quantum–classical algorithm for a democratic description of ground and excited states, Quantum Science and Technology **6**, 024004 (2021).

[2] S. Yalouz, E. Koridon, B. Senjean, B. Lasorne, F. Buda, and L. Visscher, Analytical nonadiabatic couplings and gradients within the state-averaged orbital-optimized variational quantum eigensolver, Journal of chemical theory and computation **18**, 776 (2022).

[3] S. Yalouz, B. Senjean, F. Miatto, and V. Dunjko, Encoding strongly-correlated many-boson wavefunctions on a photonic quantum computer: application to the attractive bose-hubbard model, Quantum **5**, 572 (2021).

Optimal quantum kernels for classification and regression problems

Roman Krems
University of British Columbia

I will describe our work that explores interplays of quantum physics and machine learning. The connection between quantum mechanics and machine learning is through kernels of reproducing kernel Hilbert spaces. I will describe an algorithm to construct kernels that yield Bayesian machine learning models capable of extrapolation in Hamiltonian parameter spaces. I will then show that this algorithm can be adapted for building optimal circuits of a gate-based quantum computer, yielding quantum kernels that outperform conventional classical kernels for small data machine learning tasks. If time permits, I will also show that support vector machines with a quantum kernel can be designed to have BQP-complete expressive power, i.e. quantum kernels can be designed to have quantum advantage for any classification problem that derives from a decision problem that cannot be classically solved in polynomial time.

Projective quantum algorithms for quantum chemistry

Francesco Evangelista

Emory University

Solving the electronic many-body Schrödinger equation for strongly correlated systems is a significant challenge in physics, materials science, and chemistry. Classical numerical simulations of these systems are limited by the exponential scaling of the many-body basis. Quantum computers can represent and manipulate quantum states efficiently and, therefore, could offer an alternative way to simulate many-body problems. Recent work has centered on quantum phase estimation (QPE) and the variational quantum eigensolver (VQE). These two techniques have been successfully applied to solve small molecular problems using quantum simulators and experiments on real hardware. Of these two approaches, VQE is seen as the most promising for near-term noisy quantum computers. In this talk, I will discuss several contributions from our group, including the Projective Quantum Eigensolver (PQE), a new quantum algorithm for trial-state optimization alternative to VQE. PQE is based on a projective formalism commonly used in quantum chemistry. If time permits, I will also discuss ways to leverage small quantum computers via hybrid quantum-classical schemes based on unitary transformations.

Towards Density Functional Theory on Quantum Computers

Bruno Senjean

CNRS Montpellier

Quantum computers have shown promises to solve problems that are currently intractable on classical computers. While quantum chemistry has been identified as one of the kil ler applications of quantum computers in the near term, the focus is on wavefunction theory that provides an exact solution to the quantum problem. However, the focus on th ese specific cases turns out to be extremely limited in terms of the size of affordable systems (even on quantum computers). Currently, computations on large systems rely m ainly on density functional theory, for which no quantum advantage has been envisioned so far. In this talk, we question this a priori by investigating the benefit of quant um computers to scale up not only many-body wavefunction methods, but also density functional theory, and consequently the whole range of application of quantum chemistry [1].

[1] B. Senjean, S. Yalouz, M. Saubanère, arxiv:2204.01443

Quantum dynamics with state-averaged VQE in noisy environment

Martin Beseda

CNRS Montpellier

The talk will be mainly focused on the presentation of a new state-averaged orbital-optimized variational quantum eigensolver (SA-OO-VQE) in connection with Quantics, performing quantum dynamics simulations.

With the current technologies, there are many challenges still to be overcome for them to be generally useful in real-life applications. One of the most prominent ones is quantum noise, able to render results completely inaccurate if it is not compensated for. This is also the case for the nearby future, as noisy intermediate-scale quantum (NISQ) computers are not going to be, as their name already suggests, noise-resistant by themselves.

With that said, the talk will mainly address simulations focused on photoisomerization of formaldimine, going through a conical intersection, from “pure” statevector simulation to the real-computer runs, evaluate the significance of measurement error in the final simulation results and the possibility of its mitigation.

Alternatives to unitary coupled cluster Ansatz for variational quantum Eigensolver

Matthieu Saubanère

CNRS Montpellier

Variational Quantum Eigensolver (VQE) approaches allow to solve the Schrodinger equation associated to Quantum Chemistry/Condensed matter Physic problems on actual (Noisy) Quantum Computers. The VQE strategy consists in classically optimizing a unitary transformation that is applied on an initial state (generally the Hartree-Fock state) on the quantum device to obtain the ground state of the given Hamiltonian. A prominent way to build such VQE algorithm is based on the Unitary Coupled Cluster (UCC) Ansatz that provides a versatile template for the unitary transformation to be applied on the Hartree-Fock state. Such approaches have been shown to be realizable on real quantum computers and provide fair results in particular for weakly interacting systems. In this talk we explore the design of physically motivated alternatives to the UCC Ansatz applied to the strongly interacting limit rather than the Hartee-Fock limit.

Variational learning in the age of machine learning and quantum computing

Giuseppe Carleo

EPFL

The theoretical description of several complex quantum phenomena fundamentally relies on many-particle wave functions and our ability to represent and manipulate them. Variational methods in quantum mechanics aim at compact descriptions of many-body wave functions in terms of parameterised ansatz states, and are at present living exciting transformative developments informed by ideas developed in machine learning and quantum computing. In this presentation I will start by discussing variational representations of quantum states based on artificial neural networks [1] and their use in approximately solving the Schrödinger equation. I will further highlight the general representation properties of such states, the crucial role of physical symmetries, as well as the connection with other known representations based on tensor networks [2]. Finally, I will discuss hybrid classical-quantum variational approaches, such as the Quantum Natural Gradient [3], and the projected variational quantum dynamics (p-VQD) method [4].

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[1] Carleo and Troyer, Science 365, 602 (2017)

[2] Sharir, Shashua, and Carleo, arXiv:2103.10293 (2021)

[3] Stokes, Izaac, Killoran, and Carleo, Quantum 4, 269 (2020)

[4] Barison, Vicentini, and Carleo, Quantum 5, 512 (2021)

Quantifying quantum advantage through high-performance classical simulations: two examples

Thomas Ayral

Atos Quantum Lab

In this talk, I am going to discuss the proximity, or not, to quantum advantage with the help of two examples.

First, I will argue that one can simulate Google's random circuit experiment with a comparable fidelity and in a few hours using tensor-network techniques borrowed from many-body physics. I will also show that this task of reproducing finite-fidelity quantum computations with classical machines is even easier on "useful" circuits like circuits used for combinatorial optimization [1].

Second, I will show that that despite the fact that quantum advantage is yet to be reached, steady progress is being made in devising more and more accurate or fast quantum algorithms. I will illustrate this point in the field of quantum chemistry, with a comprehensive study of the performance of "adaptive" variational methods, thanks to two recently released quantum software packages, myQLM-fermion and openVQE [2].

[1] arXiv:2207.05612

[2] arXiv:2206.08798