QuCQC 2021 workshop - talk details

All times are in CET, please see the [conference timetable](#) for other timezones.

Monday, February 22

<u>Frank Wilhelm-Mauch</u> *(1545 CET)*: *Simulating quantum matter on controlled artificial quantum systems*

This talk serves multiple purposes. On the one hand, it aims at pulling together some basic notions of NISQ quantum computing for participants with various backgrounds and aims at establishing joint vocabulary. On the other hand, it promotes the idea that an early quantum computer should be used efficiently by optimal and error-aware methods, and will highlights how the heuristic nature of variational algorithms is in particular well suited for that approach.

<u>Alan Aspuru-Guzik</u> *(1600 CET)*: *Keynote overview: 'Open problems in chemistry'*

<u>Nathan Wiebe</u> *(1740 CET)*: *Keynote overview: 'Fault-tolerant quantum computing'*

<u>James Whitfield</u> *(1820 CET)*: *Keynote overview: 'Quantum-classical interfaces and hybrid quantum computing'*

I will begin with a review and reminder of what is typically meant by "hybrid quantum computing." We will then narrow our attention to the variational quantum methods that have received much attention in the computational chemistry community. The goal is to survey quantum-classical optimizations techniques relevant to near-term quantum chemistry including dynamical evolutions, excited states characterization, and parameter reduction schemes. Obstructions and opportunities for hybrid schemes will also be discussed. Some of the existing programmatic quantum-classical interfaces are listed to give immediate next steps for getting started with hybrid quantum computing.

<u>Nicholas Rubin</u> *(2000 CET)*: *Electronic structure on today's devices*

<u>William Huggins</u> *(2100 CET, repeated 1500 CET Tuesday)*: *Discussion session: 'Near-term quantum computing'*

Ivan Kassal *(2330 CET)*: *Analog quantum simulation of chemical dynamics*

Ultrafast chemical reactions are difficult to simulate because they involve entangled, many-body wavefunctions whose computational complexity grows rapidly with molecular size. In photochemistry, the breakdown of the Born-Oppenheimer approximation further complicates the problem by entangling nuclear and electronic degrees of freedom. Here, we show that analog quantum simulators can efficiently simulate molecular dynamics using commonly available bosonic modes to represent molecular vibrations. Our approach can be implemented in any device with a qudit controllably coupled to bosonic oscillators and with quantum hardware resources that scale linearly with molecular size, and with more than a ten-fold resource savings compared to digital quantum simulation algorithms. Advantages of our approach include a time resolution orders of magnitude better than ultrafast spectroscopy, the ability to simulate large molecules with limited hardware using a Suzuki-Trotter expansion, and the ability to implement realistic system-bath interactions with only one additional interaction per mode. Our approach can be implemented with current technology; e.g., the conical intersection in pyrazine can be simulated using a single trapped ion. Therefore, we expect our method will enable classically intractable chemical dynamics simulations in the near term.

Reference: R.J. MacDonell, C.E. Dickerson, C.J.T. Birch, A. Kumar, C.L. Edmunds, M.J. Biercuk, C. Hempel, I. Kassal, arXiv:2012.01852

Keisuki Fujii *(0000 Jan 23 CET)*: *NISQ-aware methodologies for variational quantum algorithms*

NISQ devices have various limitations for practical applications, such as the number of qubits and the problem of statistical errors in estimating the expectation value. In this talk, I will introduce several algorithms and methodologies aimed at solving these problems. First, I will introduce deep VQE [1], a divide-and-conquer method for handling larger problems on small quantum computers. Second, I present a method for efficiently benchmarking lower bounds on performance in the regime of large number of qubits such as 48 qubits [2]. Third, I will introduce a variational quantum algorithm based on classical optimization by making use of classically simulatable quantum circuits and its application to quantum machine learning [3].

[1] K. Fujii et al., "Deep Variational Quantum Eigensolver: a divide-and-conquer method for solving a larger problem with smaller size quantum computers." arXiv:2007.10917.
[2] K. Mitarai et al,. "Quadratic Clifford expansion for efficient benchmarking and initialization of variational quantum algorithms." arXiv:2011.09927.
[3] K. Osaki et al., "Classically Optimized Variational Quantum Eignensolver for Topological Orderd Systems", AQIS 2020
https://www.uts.edu.au/sites/default/files/2020-11/Osaki__Classically_Optimized_Variational_Quantum_Eignensolver_for_Topological_Orderd_Systems.pdf.

Tuesday, February 23

Sam McArdle *(1600 CET)*: *Learning from physics experiments, with quantum computers: Applications in muon spectroscopy*

Computational physics is an important tool for analysing, verifying, and - at times - replacing physical experiments. Nevertheless, simulating quantum systems and analysing quantum data has so far resisted an efficient classical treatment in full generality. In this talk, I discuss a new target for quantum simulation algorithms; analysing the data arising from muon spectroscopy experiments. These experiments can be used to probe the quantum interactions present in both condensed matter, and molecular systems. However, fully analysing their results can require classical computational resources scaling exponentially with the simulated system size, which can limit our understanding of the studied system. I show that this task may be a natural fit for the coming generations of quantum computers, as the algorithm developed appears to exhibit good noise resilience.

Kristan Temme *(1700 CET)*:

Claudia Filippi *(1815 CET)*: *Recent developments in (real-space) quantum Monte Carlo*

Wibe de Jong *(2000 CET, repeated 1500 CET Wednesday)*: *Discussion session: 'Open problems in chemistry'*

In this talk I will tee up some of the questions we will be discussing in the 'Open problems in Chemistry' session, with the hope of provoking some thought, maybe a bit of controversy that will lead to a lively discussion session.

Steven White *(2200 CET)*: *Improved Hamiltonians for Quantum Chemistry*

The performance of both classical and quantum simulation approaches for molecules are highly dependent on the size and structure of the Hamiltonian. Gaussian basis sets constitute the standard formulation, but they are highly optimized for the size of the Hilbert space, but not for the complexity of the Hamiltonian, with the number of two-electron terms scaling as N^4. We have been developing different representations, based on a new type of basis function called a gausslet, which are derived from wavelets. The Hamiltonians we have developed have only N^2 interaction terms, at the cost of somewhat higher N. These Hamiltonians can also be used as intermediate representations allowing further compression. The high locality of these basis sets

mean that they better obey area laws, allowing for better tensor network simulations. I will summarize the current status of this work, where we have had substantial success simulating hydrogen chains.

Joonho Lee *(2230 CET)*: *Challenges in quantum chemistry beyond the electronic ground state*

One of the main target applications for near-term and fault-tolerant quantum computers is the computation of the ground state of electronic Hamiltonians. However, recently, there has been increasing interest in simulating the ground state of coupled electron-phonon systems and electronic systems at finite temperatures in quantum chemistry. This talk will present examples of these problems with numerical results using auxiliary-field quantum Monte Carlo (AFQMC). We will first present a new AFQMC algorithm for simulating electron-phonon problems will be discussed with the Hubbard-Holstein model as an example. Next, we will discuss accurate AFQMC results on the uniform electron gas in the warm dense regimes. In each problem, the regimes for which currently no accurate scalable classical methods exist will be mentioned.

Wednesday, February 24

Libor Veis *(1600 CET)*: *DMRG-based methods for large-scale applications in strongly correlated quantum chemistry*

In the past decade, the quantum chemical version of the density matrix renormalization group method (QC-DMRG) [1, 2] has established itself as a method of choice for accurate calculations of strongly correlated molecular systems requiring large active spaces. In this talk, I will introduce MOLMPS [3], the new scalable C++ DMRG implementation, which we have recently developed in order to push the envelope of QC-DMRG calculations. The MOLMPS parallel scheme is based on the in-house MPI global memory library, combines operator and symmetry sector parallelisms, and exploits data locality at maximum. I will present the performance tests with the largest calculation of nitrogenase FeMo cofactor cluster with the active space comprising 113 electrons in 76 orbitals and bond dimension equal to 6000, where we achieved scaling up to approximately 2000 CPU cores. The DMRG method is very successful in recovering the strong (static) electron correlation, however, in order to treat the real-life problems with chemical accuracy, one needs some post-DMRG method for capturing the missing dynamical electron correlation. I will discuss two such approaches, which we have recently introduced and tested in connection with DMRG, namely the tailored coupled clusters [4] and the adiabatic connection [5]. I will demonstrate their performance on the examples of Fe(II)-porphyrine molecule and polyacenes series. Last but not least, I would like to sketch how the matrix product state (MPS) wave function produced by the DMRG algorithm may potentially help as an initial guess of hybrid quantum-classical algorithms [6].

[1] S. R. White, Phys. Rev. Lett. 69, 2863 (1992).
[2] G. Chan, S. Sharma, Annu. Rev. Phys. Chem. 62, 465 (2011).

[3] J. Brabec, J. Brandejs, Ö. Legeza, K. Kowalski, S. Xanteas, L. Veis, J. Comp. Chem. 1-11 (2020), DOI: 10.1002/jcc.26476.

[4] L. Veis, A. Antalík, J. Brabec, F. Neese, Ö. Legeza, J. Pittner, J. Phys. Chem. Lett. 7, 4072 (2016).

[5] K. Pernal, Phys. Rev. Lett. 120, 013001 (2018).

[6] N. P. Bauman, J. Chládek, L. Veis, J. Pittner, K. Kowalski, Variational Quantum Eigensolver for Approximate Diagonalization of Downfolded Hamiltonians using Generalized Unitary Coupled Cluster Ansatz, arXiv:2011.14715.

Ors Legeza *(1700 CET)*: *Tensor product approximation based methods for electronic structure calculations*

Tensor network states and specifically matrix-product states have proven to be a powerful tool for simulating ground and excited states of strongly correlated spin and fermionic models. In this contribution, we briefly overview tensor network states techniques, like density matrix renormalization group (DMRG) method, tree-tensor network (TTNS) and three-legged tree tensor network (3TNS) state methods [1,2,3]. These can be used for the treatment of high-dimensional optimization tasks used in many-body quantum physics with long range interactions, ab initio quantum chemistry, and nuclear structure theory. We will also discuss the controlled manipulation of entanglement, which is in fact the key ingredient of such methods, and which provides relevant information about correlations [4]. We will present recent developments on fermionic orbital optimization [5], long time evolution based on time dependent variational principle (TDVP) and mode optimization [6], externally corrected coupled cluster (DMRG-TCCSD) [7] and its extension towards the relativistic domain [8], and recent developments for extended periodic systems.

[1] Density matrix formulation for quantum renormalization groups,
S. R. White, Phys. Rev. Lett. 69, 2863 (1992).

[2] Tensor product methods and entanglement optimization for ab initio quantum chemistry,
Sz. Szalay, M. Pfeffer, V. Murg, G. Barcza, F. Verstraete, R. Schneider, Ö. Legeza,
INTERNATIONAL JOURNAL OF QUANTUM CHEMISTRY 115:(19) pp. 1342-1391. (2015)

[3] T3NS: three-legged tree tensor network states,
K. Gunst, F. Verstraete, S. Wouters, Ö. Legeza, D. Van Neck,
J. Chem. Theory Comput., 14, 4, 2026–2033 (2018)

[4] The correlation theory of the chemical bond,
Sz. Szalay, G. Barcza, T. Szilvási, L. Veis, Ö. Legeza,
Scientific Reports 7, Article number: 2237 (2017)

[5] Fermionic orbital optimisation in tensor network states,
C. Krumnow, L. Veis, Ö. Legeza, J. Eisert,

Phys. Rev. Lett. 117, 210402 (2016)

[6] Coupled cluster method with single and double excitations tailored by matrix product state wave functions,
L. Veis, A. Antalik, F. Neese, Ö. Legeza, J. Pittner,
Journal of Physical Chemistry Letters, 7 (20) 4072-4078 (2016)

[7] Towards overcoming the entanglement barrier when simulating long-time evolution,
C. Krumnow, J. Eisert, Ö. Legeza arXiv:1904.11999 (2019)

[8] Toward DMRG-tailored coupled cluster method in the 4c-relativistic domain,
J. Brandejs, J. Višňák, L. Veis, M. Maté, Ö. Legeza, and J. Pittner
J. Chem. Phys. 152, 174107 (2020)

Ryan Babbush *(1815 CET)*: *The Promise of First Quantized Quantum Simulations of Chemistry*

The majority of work on quantum computing for chemistry has thus far focused on simulating second quantized representations of the molecular Hamiltonian. However, this talk will make the case that first quantization has many preferable characteristics for large fault-tolerant quantum simulations, especially when it comes to bulk materials or surface chemistry. We will discuss the implications of combining first quantization with various different basis sets and review the existing literature of quantum algorithms leveraging such representations. We will take an especially close look at the algorithms of arXiv:1807.09802 and reveal the results of some unpublished work obtaining the constant factors associated with those algorithms.

Bela Bauer *(2000 CET, repeated 1500 CET Thursday)*: *Discussion session: 'Fault-tolerant quantum computing'*

Guang-Hao Low *(2200 CET)*:

Lin Lin *(2230 CET)*: *Quantum computation of Green's functions*

Green's functions play a central role in describing excited state electronic structures in quantum chemistry and materials science. At the heart of Green's function computation is the solution of a linear system of size $2^N \times 2^N$, where N is the number of spin-orbitals in the quantum system. We will discuss how to use quantum linear system solvers to compute Green's functions, and how to accelerate such computations using a new quantum primitive called the fast inversion, as well as preconditioning techniques.

Dominic Berry *(2300 CET)*:

Thursday, January 25

<u>Matthias Troyer</u> *(1700 CET)*:

<u>Jens Eisert</u> *(1815 CET)*: *Making quantum computation for quantum chemistry more useful*

Recent years have witnessed an increased excitement about the possibility of using near-term quantum computers to tackle practically relevant problems in quantum chemistry, and hence realizing a "practical quantum advantage" beyond purely conceptual problems. In this talk, we will have a look at two new developments in this direction. On the one hand, we will see how randomness may help in compiling circuits for the Hamiltonian simulation of interacting quantum problems in quantum chemistry. Specifically, we will have a look at a new scheme for quantum simulation that unites the advantages of randomized compiling and higher-order linear-combination-of-unitaries algorithms [1]. On the other hand, we will stress the importance of classical control in variational hybrid quantum algorithms as they are relevant for applications in quantum chemistry [2,1]. (If time allows, I will sketch some recent progress on certifiable conceptual quantum advantages [3] and on quantum advantages in learning tasks [4].)

[1] In preparation (2021).
[2] Quantum 4, 314 (2020).
[3] Phys. Rev. Lett. 125, 250501 (2020).
[4] arXiv:2007.14451 (2020).

<u>Jarrod McClean</u> *(2000 CET repeated 1400 CET Friday)*: *Discussion session: 'Quantum-classical interfaces and hybrid quantum computing'*

<u>Sophia Economou</u> *(2100 CET)*: *Problem-tailored ansatze for efficient variational quantum eigensolvers*

The performance of variational quantum eigensolvers (VQEs) critically depends on the form of the variational ansatz. A good ansatz translates to relatively shallow circuits and involves a low number of classical optimization parameters. These features can be achieved more easily if the ansatz knows something about the problem that is simulated. In this talk, I will present our techniques for problem-tailored ansatze, including symmetry-preserving circuits [1], ADAPT-VQE [2,3], and ctrl-VQE [4]. Our simulations show that these techniques can outperform competing ansatze in terms of circuit depth and accuracy.

[1] B. T. Gard, L. Zhu, G. S. Barron, N. J. Mayhall, S. E. Economou, and E. Barnes, npj Quantum Inf. 6, 10 (2020)

[2] H. R. Grimsley, S. E. Economou, E. Barnes, N. J. Mayhall, Nature communications 10, 1-9 (2019)

[3] H. L. Tang, E. Barnes, H. R. Grimsley, N. J. Mayhall, and S. E. Economou, arXiv:1911.10205

[4] O. R. Meitei, B. T. Gard, G. S. Barron, D. P. Pappas, S. E. Economou, E. Barnes, and N. J. Mayhall, arXiv:2008.04302

Friday, January 26

<u>Saad Yalouz</u> *(1530 CET)*: *A state-averaged quantum algorithm for an equal footing description of ground and excited states on a near term quantum computer*

In quantum computing, solving the electronic structure problem from quantum chemistry is considered as the ``killer application'' for near term quantum computers. Recently, many efforts have been devoted to the development of quantum algorithms capable of solving this problem on the current ``Noisy Intermediate-Scale Quantum'' computers. In this context, the hybrid quantum/classical ``Variational-Quantum-Eigensolver'' (VQE) algorithm is considered as one of the best methods due to its low requirement of quantum resources. While VQE has been proficiently applied to find electronic eigenstates/energies of various small molecules, using this approach on more complex systems is still a genuine challenge especially when peculiar spectral features such as degeneracies are present. Motivated by this issue, our work focuses on the following idea: using a VQE algorithm to accurately describe conical intersections (singular points of degeneracy between electronic states). In nature, conical intersections are crucial and play a keyrole in many prominent reactions. For instance, in the process of vision, the retinal molecule is known to undergo a photoisomerisation mediated by a non-radiative relaxation through a conical intersection. In such a situation, characterizing the phenomenon requires to precisely describe the shape of the conical intersection, with both qualitative and quantitative high-level treatments. This makes it a difficult target to current quantum algorithms, such as VQE. To solve this problem on a near term quantum computer, we introduce an algorithm called ``State-Averaged Orbital-Optimized VQE'' designed to treat on an equal footing degenerate states. We apply this method on the formaldimine molecule (a minimal model for retinal featuring a similar conical intersection) and we show that the latter is able to qualitatively and quantitatively reproduce the molecule's conical intersection.

<u>Sabre Kais</u> *(1600 CET)*: *Quantum Algorithms for Evolving Open Quantum Dynamics on Quantum Computing Devices*

In this talk I will discuss a general quantum algorithm to evolve open quantum dynamics on quantum computing devices. The Kraus operators governing the time evolution can be converted into unitary matrices with minimal dilation guaranteed by the Sz.-Nagy theorem. This allows the evolution of the initial state through unitary quantum gates, while using significantly less resources than required by the conventional Stinespring dilation. Then, I will present

results of the algorithm on a simple amplitude damping channel and simulating the dynamics of the Fenna-Matthews-Olson (FMO) complex. The proposed algorithm does not require particular models of dynamics or decomposition of the quantum channel, and thus can be easily generalized to other open quantum dynamical models.

Ivano Tavernelli *(1700 CET)*:

Garnet Chan *(1815 CET)*: