Novel Computing Approaches to Quantum Chemistry

Telluride Science Research Center
08/10/2015 - 08/14/2015

1 General Information

1.1 Meeting Description

Quantum chemistry has evolved from its beginnings at the turn of the century aided by continuous computational developments from early computer technology in the 1940s, into a huge field in its own right. It is now applied to nearly all fields of scientific interests, such as medicine, pharmaceuticals, engineering, biology, and materials science. Now it is again on the verge of several frontiers due to new developments in computer science both on the software and hardware side. The purpose of the *Novel computing approaches to quantum chemistry* workshop will be to examine and push further several of these innovative approaches by inviting experts in the various new and emerging subfields of quantum chemistry.

To achieve the goal of examining new ways of understanding and using computers in quantum chemistry, we hope to combine leading methodology developers with experts from the fields of quantum information theory, quantum computational simulations and machine learning. This will give an appropriately wide breadth of expertise to be explored within the five day time span of the proposed workshop. To facilitate the exchange of ideas, we will arrange discussions between the talks.

1.2 Meeting Venue

The workshop will be held in Telluride Elementary School, 447 West Columbia Ave Telluride CO 81435.

1.3 List of Participants

Babbush, Ryan (Google)
Cao, Yudong (Purdue University)
Kivlichan, Ian (Harvard University)
Kovyrshin, Arseny (ETH Zürich)
Love, Peter (Tufts University)
Romero Fontalvo, Jhonathan (Harvard University)
Sugisaki, Kenji (Osaka City University)
Szilvási, Tibor (Wigner Research Center, Budapest)
Tranter, Andrew (Imperial College London & UCL)
Whitfield, James (University of Vienna)
Wiebe, Nathan (Microsoft Research)
Zimborás, Zoltán (University College London)

2 Conference Schedule

Monday

10:00-10:30: Opening (J. Whitfield and Z. Zimborás)
10:30-12:00: Plenary talk
Nathan Wiebe:*Practical methods for simulating quantum chemistry on quantum computers*
12:00-12:30: Discussion
12:30-14:00: Lunch break
14:00-15:00: **Jhonathan Romero Fontalvo**: *Quantum Computing Molecular Energies using the Variational Quantum Eigensolver*
15:00-15:30: Discussion

Tuesday

10:00-11:30: Plenary talk
Ryan Babbush: *Exponentially more precise quantum simulation of chemistry*
11:30-12:00: Discussion
12:00-14:00: Lunch break
14:00-15:00: **Ian Kivlichan**: *Exponentially more precise simulation of chemistry using the sparsity of the CI matrix*
15:00-15:30: Discussion
15:30-16:30: **Andrew Tranter**: *Optimal Trotter orderings for Jordan-Wigner and Bravyi-Kitaev Hamiltonians*

Wednesday

10:00-11:30: Plenary talk
Peter Love: *State preparation - out from under the rug*
11:30-12:00: Discussion
12:00-14:00: Lunch break
14:00-15:00: **Arseny Kovyrshin**: *Tensor Network Parameterizations for Strong-Correlation Problems*
15:00-15:30: Discussion
15:30-16:30: **Kenji Sugisaki**: *Molecular electron spin based quantum computations*

Thursday

10:00-11:30: Plenary talk
Zoltán Zimborás: *The computational complexity of self-consistent field problems*
11:30-12:00: Discussion
12:00-14:00: Lunch break
14:00-15:00: **Yudong Cao**: *Perturbative reductions for quantum many-body systems*
15:00-15:30: Discussion
15:30-16:30: **James Whitfield**: *New ideas in computational chemistry*

Friday

10:00- : Discussions on future plans, ideas, papers

3 Abstracts

Nathan Wiebe
(Microsoft Research)

Practical methods for simulating quantum chemistry on a quantum computer

Quantum simulation is widely regarded as the most promising application of quantum computing, allowing efficient simulation of quantum systems that are not believed to be efficiently simulated using known classical methods. Among such proposals quantum chemistry simulation holds special promise because of the commercial and scientific importance of modeling chemical systems. While quantum simulation has long been known to lead to exponential speedups for such simulations, the overheads of the methods that were originally proposed were sufficiently large that such simulations would take millions of years to run on a quantum computer. I will present recent work from Microsoft research that slashes these costs leading to simulations that could conceivable be executed within minutes to hours. This shows that quantum computers allow for practical simulations of quantum chemistry.

Jhonathan Romero Fontalvo
(Harvard University)

Quantum Computing Molecular Energies using the Variational Quantum Eigensolver with a Unitary Coupled Cluster Ansatz

The recently proposed variational quantum eigensolver (VQE) algorithm [1] stands as an alternative procedure for state preparation and quantum simulation that requires shorter coherent times as compared with other quantum algorithms, constituting one of the most promising applications for near-term quantum computers. The VQE scheme involves the preparation of a quantum state based on a chosen ansatz whose parameters are optimized by minimizing the energy for a given problem Hamiltonian. In this contribution we present a practical guide for implementing VQE on a quantum computer, focusing on solving the electronic structure problem with a Unitary Coupled Cluster (UCC) ansatz [2]. We present a description of the construction of the circuits for preparing a UCC wavefunction on a quantum computer along with a discussion of the energy measurement and parameter optimization steps. A new scheme for reducing the computational cost

of UCC based on an active space approximation is also proposed. We complement our discussion with numerical simulations performed with EXACTA, a new software for assisting the implementation of quantum algorithms for quantum chemistry developed by the Aspuru-Guzik group. Finally, we present an experimental realization of the VQE algorithm with a UCC ansatz for molecular hydrogen using an ion trap quantum computer [3].

[1] Peruzzo, Alberto, et al. *A variational eigenvalue solver on a photonic quantum processor.* Nature communications 5 (2014).

[2] Taube, Andrew G., and Rodney J. Bartlett. *New perspectives on unitary coupledcluster theory.* International Journal of Quantum Chemistry 106.15 (2006): 3393-3401.

[3] Lanyon, B. P., et al. *Universal digital quantum simulation with trapped ions.* Science 334.6052 (2011): 57-61.

Ryan Babbush
(Google)

Exponentially more precise quantum simulation of chemistry

In this talk we review recent advances in Hamiltonian simulation based on truncating the Taylor series (arXiv:1412.4687) and the application of those techniques to the quantum simulation of chemistry (arXiv:1506.01020). These quantum simulations scale logarithmically with the inverse of the desired precision, an exponential improvement over Trotterization. We will discuss two algorithms which both rely on a second quantized encoding of the wavefunction in which the state of an N spin-orbital system is encoded in $O(N)$ qubits. Up to polylogarithmic factors, our first algorithm has gate complexity $O(N^8 t)$. Our second algorithm involves on-the-fly computation of molecular integrals, in a way that is exponentially more precise than classical sampling methods, by using the truncated Taylor series simulation technique. This algorithm has the lowest asymptotic gate complexity of any approach to the quantum simulation of chemistry in the literature, $O(N^5 t)$ up to polylogarithmic factors.

Ian Kivlichan
(Harvard University)

Exponentially more precise simulation of chemistry using the sparsity of the CI matrix

I will introduce a new algorithm for quantum simulation of chemistry using the sparse structure of the configuration-interaction (CI) matrix. This algorithm scales exponentially better in terms of precision than methods based on the Trotter-Suzuki decomposition, logarithmically rather than polynomially in the inverse precision (arXiv:1506.01029). Similar to work using a second-quantized encoding of the wave function (arXiv:1506.01020), this algorithm computes the necessary molecular integrals on-the-fly. Up to poly-logarithmic factors, with n the number of electrons and N the number of spin-orbitals, we encode the wave function in O(n) qubits, and the gate count of the algorithm scales as $O(n^5N^3t)$ or $O(nN^5t)$ depending on how we choose to decompose the CI matrix. I will additionally present a thorough and intuitive analysis of how the truncated Taylor series techniques (arXiv:1412.4687) we apply work.

Andrew Tranter
(Imperial College & University College London)

Optimal Trotter orderings for Jordan-Wigner and Bravyi-Kitaev Hamiltonians

In this talk we discuss ordering strategies in the Trotterization of quantum chemical Hamiltonians. Using molecular Hydrogen as a simple test case, we consider the characteristics of what an optimised ordering would look like. We examine this using random Hamiltonians and small chemical test cases. We finally consider the implications of such an ordering for both Jordan-Wigner and Bravyi-Kitaev transformed Hamiltonians.

Peter Love
(Tufts University)

State preparation - out from under the rug

In this talk we discuss ordering strategies in the Trotterization of quantum chemical Hamiltonians. Using molecular Hydrogen as a simple test case, we consider the characteristics of what an optimised ordering would look like. We examine this using random Hamiltonians and small chemical test cases. We finally consider the implications of such an ordering for both Jordan-Wigner and Bravyi-Kitaev transformed Hamiltonians.

Arseny Kovyrshin
(ETH Zürich)

Tensor Network Parameterizations for Strong-Correlation Problems

Wave functions represented by the matrix product states (MPS) [1,2] ansatz proved to be very useful in tackling systems with a complicated electronic structure. However, for systems with multidimensional entanglement MPS may suffer from convergence problems. The MPS ansatz, being a special case of the tensor network states ansatz, features an artificial one-dimensional ordering of tensors which can be inappropriate in cases with multidimensional entanglement. A solution to this problem are tensor network states of which tree tensor network states are currently intensely investigated [3,4,5]. Our complete graph tensor network state (CGTNS) ansatz [6,7] describes one- and multi-dimensional entanglement on equal footing. Thus, it is a suitable ansatz for a general tensor network which is able to adapt to the system under study and yields energy estimates with controlled accuracy. Here, we analyze the applicability of CGTNS [8] for chemical systems representing difficult electron-correlation scenarios.

[1] S. White, Phys. Rev. Lett., 69, 2863 (1992).
[2] S. Ostlund and S. Rommer, Phys. Rev. Lett., 75 3537 (1995).

[3] F. Verstraete, V. Murg, and J.I. Cirac, Adv. Phys., 57, 143 (2008).
[4] N. Nakatani and G. K.-L. Chan, J. Chem. Phys., 138 (2013) 134113. [5] V. Murg, F. Verstraete, R. Schneider, P. R. Nagy, and O. Legeza, J. Chem. Theory Comput. 11 (2015) 1027.
[6] K. H. Marti, B. Bauer, M. Reiher, M. Troyer, F. Verstraete, New J. Phys., 12, 103008 (2010).
[7] K. H. Marti and M. Reiher, Phys. Chem. Chem. Phys., 13, 6750 (2011).
[8] A. Kovyrshin and M. Reiher, in preparation.

Kenji Sugisaki
(Osaka City University)

Molecular electron spin based quantum computations

Implementation of molecular electron spin based quantum computers (MSQCs) is an emerging issue in the field of quantum computation and quantum information science. Since electron-electron (exchange and dipolar) and electron-nuclear (hyperfine) couplings are much stronger than nuclear spin-spin couplings, MSQC can afford to execute quantum operations faster than NMR-based QCs. In this talk we firstly present our recent progress on MSQC: (1) Design and synthesis of stable organic spin-triplet systems for quantum memory devices, and (2) Adiabatic quantum computations with electron/nuclear spin qubits. Secondly, our recent achievement in quantum chemical calculations on quantum computers will be discussed.

Zoltán Zimborás
(University College London)

On the computational complexity of self-consistent field problems

The self-consistent field method utilized for solving the Hartree-Fock (HF) problem and the closely related Kohn-Sham problem is typically thought of as one of the cheapest methods available to quantum chemists. This intuition has been developed from the numerous applications of the self-consistent field method to a large variety of molecular systems. However, as characterized by its worst-case behavior, the HF problem is NP-complete. In this talk, we map out boundaries of the NP-completeness by investigating restricted instances of HF. We construct two new NP-complete variants of the problem. The first is a set of Hamiltonians whose translationally invariant Hartree-Fock solutions are trivial, but whose broken symmetry solutions are NP-complete. Second, we demonstrate how to embed instances of spin glasses into translationally invariant Hartree-Fock instances and provide a numerical example. We have also extended this perspective with some initial investigation into random fermionic ensembles using exact diagonalization and Hartee-Fock. These findings [1] are the first steps towards understanding in which cases the self-consistent field method is computationally feasible and when it is not.

[1] J.D. Whitfield, Z. Zimborás, J. Chem. Phys. 141, 234103 (2014)

Yudong Cao
(Purdue University)

Perturbative reductions for quantum many-body systems

Perturbative reductions (or so-called gadgets) between various classes of Hamiltonians appear in many different contexts of quantum computation such as adiabatic quantum computing and quantum complexity theory. Realizing perturbative reductions with a physical scaling of parameters is therefore of great importance. A major shortcoming of the previously known constructions of perturbative gadgets is the polynomially large norm of interactions in the gadget Hamiltonian (which is unphysical), making them practically not very useful from the physics perspective. In this talk I will present gadget constructions that either has reduced degrees of polynomial interaction strength or requires arbitrarily weak interaction strength (at the cost of more ancilla qubits).

[1] Yudong Cao, Ryan Babbush, Jacob Biamonte, and Sabre Kais. *Hamiltonian Gadgets with Reduced Resource Requirements*. Physical Review A. Volume 91, Number 1: 012315. 2015. arXiv preprint 1311.2555.

[2] Yudong Cao, Daniel Nagaj. *Perturbative gadgets without strong interactions. Quantum Information and Computation*. Vol. 15, No. 13&14. 2015. 11971222. arXiv preprint 1408.5881.

James Whitfield
(University of Vienna)

New ideas in computational chemistry

Ideas from the theory of computation can be used to analyze, classify, and reexamine established approaches to electronic structure. Statistical approaches complement and suggest advances in computational complexity and allow new ways to systematically understand attributes of model chemistry including their convergence and error analysis. A first aim is to use theoretical computer science to achieve rigorous bounds on the spatial and temporal cost of model chemistries with an emphasis on classifying the interrelations between algorithms beginning with the foundations of density functional theory and its time-dependent formulation. Secondly, some directions in machine learning are suggested based on recent developments in quantum chemistry and quantum machine learnings.