QI 12: Quantum Computing and Algorithms

Time: Thursday 15:00–18:15 Location: H8

QI 12.1 Thu 15:00 H8

Partitioning methods for solving optimization problems on NISQ-devices — •Federico Dominguez[1], Kaonan Campos Micadei[1], Christian Ertler[1], and Wolfgang Lechner[1,2] — [1]Parity QC Germany GmbH, Munich, Germany — [2]Institute for Theoretical Physics, LFUI, and Parity QC GmbH, Innsbruck, Austria

Partitioning methods are hybrid quantum-classical algorithms aimed at overcoming the memory limitations of current quantum devices. These methods decompose large problems into smaller pieces suitable for running on small quantum devices. The partial solutions to the problem are recombined using classical algorithms that can deal with both the error from the partition approximation and the intrinsic errors of the NISQ devices.

In this work, we solve optimization problems by developing partitioning methods based on the Parity encoding [1,2] and we benchmark the results using simulated quantum annealing. The Parity transformation is capable of encoding all-to-all graphs, hypergraphs, and side conditions of optimization problems using only local qubit interactions and allowing for a high gate parallelizability and hence scalability [3,4]. The resulting locality property is especially suited for the partitioning approach. The performance of our method shows that large optimization problems can be efficiently run on small quantum devices. [1] Lechner, W. et al. (2015). Science advances,1(9), e1500838. [2] Ender, K. et al. (2021).arXiv preprint arXiv:2105.06233. [3] Lechner, W. (2020). IEEE Transactions on Quantum Engineering,1, 1-6. [4] Drieb-Schön, M. et al. (2021). arXiv preprint arXiv:2105.06235.

QI 12.2 Thu 15:15 H8

Calculation of Correlated Electronic States on Noisy Intermediate Scale Quantum Computers — •Jannis Ehrlich[1], Daniel Urban[1], and Christian Elsässer[1,2] — [1]Fraunhofer-Institut für Werkstoffmechanik IWM, Freiburg, Germany — [2]Freiburger Materialforschungszentrum, Universität Freiburg, Germany

The numerical description of correlated electrons on conventional computers is limited to small system sizes. For the exact diagonalization approach, for example, all configurations in the many-particle space have to be considered, and their number grows exponentially with the number of one-particle states. This limitation can be overcome by simulating the correlated electrons with one of the artificial quantum systems that recently became available through the advance in quantum computing technologies. On such systems, each one-particle state can be represented by one qubit, which can be entangled with each other to generate superpositions. Thus, a linear scaling in the number of qubits is sufficient to cover the full many-particle space. Here, we describe strongly correlated systems within the dynamical mean-field theory (DMFT) and investigate its possible realization on a quantum computer. As a proof of concept, we study the simplified version of two-site DMFT both, by using simulators and an IBMQ quantum computer. We show that a solution of this model can be obtained using the quantum-classical variational quantum eigensolver (VQE). As the quality of the results is limited by the noise level of current quantum computers (NISQ type), we further investigate how different error mitigation strategies can improve the results.

QI 12.3 Thu 15:30 H8

Optimal gradient estimation for variational quantum algorithms — •Lennart Bittel, Jens Watty, and Martin Kliesch — Heinrich Heine Universität, Düsseldorf

Variational quantum algorithms (VQAs) are a leading approach for achieving a practically relevant near-term quantum advantage. A bottleneck of this approach is the estimation of derivatives of a given energy functional w.r.t. the parameters of the underlying variational quantum circuit. The parameter shift rule and its extensions allow for such and estimation without systematic errors. However, due to the measurement shot noise, they can have a large statistical error. As a consequence, many measurement rounds are required, which result in non-optimal VQA run-times.

In this work, we reduce this measurement overhead by using a Bayesian estimation framework. For this, we use prior knowledge about the circuit to then determine optimal measurement settings that minimize the expected statistical and systematic errors simultaneously. With accurate priors, this approach can significantly outperform traditional methods. We test our estimation algorithm numerically for a common quantum approximate optimization algorithm (QAOA). For a desired estimation accuracy we can reduce the number of measurements by an order of magnitude compared to traditional estimation methods. This also leads to significantly improved convergence times for the gradient descent algorithm.

QI 12.4 Thu 15:45 H8

Synthesis of and compilation with time-optimal multi-qubit gates — •Pascal Bassler[1], Matthias Zipper[1], Christopher Cedzich[1], Patrick Huber[2], Michael Johanning[2], Markus Heinrich[1], and Martin Kliesch[1] — [1]Heinrich Heine University Düsseldorf, Germany — [2]University of Siegen, Germany

We develop a method to synthesize a class of entangling multi-qubit gates for a quantum computing platform with fixed Ising-type interaction with all-to-all connectivity. The only requirement on the flexibility of the interaction is that it can be switched on and off for individual qubits. Our method yields a time-optimal implementation of the multi-qubit gates. We numerically demonstrate that the total multi-qubit gate time scales approximately linear in the number of qubits. Using this gate synthesis as a subroutine, we provide compilation strategies for important use cases: (i) we show that any Clifford circuit on n qubits can be implemented using at most n multi-qubit gates without requiring ancilla qubits, (ii) we decompose the quantum Fourier transform in a similar fashion, (iii) we compile a simulation of molecular dynamics into native gates, and (iv) we propose a method for the compilation of diagonal unitaries with time-optimal multi-qubit gates, as a step towards general unitaries. As motivation, we provide a detailed discussion on a microwave controlled ion trap architecture with magnetic gradient induced coupling (MAGIC) for the generation of the Ising-type interactions.

QI 12.5 Thu 16:00 H8

Estimating molecular forces and other energy gradients efficiently on a quantum computer — •Michael Streif[2], Thomas O'Brien[1], Nicholas C. Rubin[1], Raffaele Santagati[2], Yuan Su[1], William J. Huggins[1], Joshua J. Goings[1], Nikolaj Moll[2], Elica Kyoseva[2], Matthias Degroote[2], Christofer S. Tautermann[3], Joonho Lee[1,4], Dominic W. Berry[5], Nathan Wiebe[6,7], and Ryan Babbush[1] — [1]Google Research, USA — [2]Quantum Lab, Boehringer Ingelheim, Germany — [3]Boehringer Ingelheim Pharma GmbH & Co KG, Germany — [4]Department of Chemistry, Columbia University, USA — [5]Department of Physics and Astronomy, Macquarie University, Australia — [6]Department of Computer Science, University of Toronto, Canada — [7]Pacific Northwest National Laboratory, USA

The calculation of energy derivatives underpins many fundamental properties for molecular systems, such as dipole moments or molecular forces. Nevertheless, most methods for quantum chemistry on quantum computers have focused on electronic structure calculations, even though energy derivatives are fundamental for many practical applications. Here, I will introduce quantum algorithms for the calculation of energy derivatives on noisy intermediate scale (NISQ) and fault tolerant (FTQC) quantum computers, with substantially reduced cost compared to previous methods. Our results suggest that the calculation of molecular forces has a similar cost to estimating energies. However, since molecular dynamics (MD) simulations typically require millions of force calculations, current known methods for MD on quantum computers are impractical and new approaches need to be found.

QI 12.6 Thu 16:15 H8

Towards the Simulation of Large Scale Protein-Ligand Interactions on NISQ-era Quantum Computers — •Nikolaj Moll[1], Fionn D. Malone[2], Robert M. Parrish[2], Alicia R. Welden[2], Thomas Fox[3], Matthias Degroote[1], Elica Kyoseva[1], Raffaele Santagati[1], and Michael Streif[1] — [1]Quantum Lab, Boehringer Ingelheim, 55218 Ingelheim, Germany — [2]QC Ware Corporation, Palo Alto, CA, 94301, USA — [3]Medicinal Chemistry, Boehringer Ingelheim Pharma GmbH & Co. KG, 88397 Biberach, Germany

Most quantum computing research for quantum chemistry applications has focused on the calculation of ground state energies, while in the pharmaceutical industry, one is often more interested in gaining insight into the interaction of drugs and proteins. The interaction energy to-

gether with entropic contributions allows the determination of the efficacy of a potential drug. Here we explore the use of symmetry-adapted perturbation theory (SAPT) as a simple means to compute interaction energies between two molecular systems with a hybrid method combing NISQ-era quantum and classical computers. From the one- and two-particle reduced density matrices of the monomer wavefunctions obtained by the variational quantum eigensolver (VQE), we compute SAPT contributions to the interaction energy. At first order, this energy yields the electrostatic and exchange contributions for non-covalently bound systems. Ideal statevector simulations show that the SAPT(VQE) interaction energy components display orders of magnitude lower absolute errors than the corresponding VQE total energies which sub kcal/mol accuracy in the SAPT interaction energies.

15 min. break

QI 12.7 Thu 16:45 H8

Resilience of quantum approximate optimization against correlated errors — Joris Kattemölle and •Guido Burkard — Universität Konstanz, Konstanz, Deutschland

The Quantum Approximate Optimization Algorithm (QAOA) has the potential of providing a quantum advantage in large-scale optimization problems, as well as in finding the ground state of spin glasses. This algorithm is especially suited for Noisy Intermediate Scale Quantum (NISQ) devices because of its noise resilience. So far, this noise resilience has only been studied under the assumption of uncorrelated noise. However, in recent years, it has become increasingly clear that the noise impacting NISQ devices is significantly correlated. In this work, we introduce a model for both spatially and temporally (non-Markovian) correlated errors that allows for the independent variation of the marginalized local error probability and the correlation strength. Using this model, we study the effects of noise correlations on QAOA by full density matrix simulation. We find evidence that the performance of QAOA improves as the strength of noise correlations is increased at fixed marginalised local error probability. This shows that, as opposed to algorithms for fully error-corrected quantum computers, noise correlations need not be detrimental for NISQ algorithms such as QAOA, and may actually improve the performance thereof.

QI 12.8 Thu 17:00 H8

Exploiting symmetry in variational quantum machine learning — Johannes Jakob Meyer[1], Marian Mularski[1,2], Elies Gil-Fuster[1,3], •Antonio Anna Mele[1], Francesco Arzani[1], Alissa Wilms[1,2], and Jens Eisert[1,3,4] — [1]Dahlem Center for Complex Quantum Systems, Freie Universität Berlin, 14195 Berlin, Germany — [2]Porsche Digital GmbH, 71636 Ludwigsburg, Germany — [3]Fraunhofer Heinrich Hertz Institute, 10587 Berlin, Germany — [4]Helmholtz-Zentrum Berlin für Materialien und Energie, 14109 Berlin, Germany

Variational quantum machine learning is an extensively studied NISQ application. The success of variational quantum learning models crucially depends on finding a suitable parametrization of the model that encodes an inductive bias relevant to the learning task. However, little is known about guiding principles for constructing suitable parametrizations. We explore when and how symmetries of the learning problem can be exploited to construct quantum learning models with outcomes invariant under the symmetry of the learning task. Using tools from representation theory, we show how a standard gateset can be transformed into an equivariant one that respects the symmetries of the problem through a process of symmetrization. We benchmark the proposed methods on two toy problems that feature a non-trivial symmetry and observe a substantial increase in generalization performance. As our tools can also be applied in a straightforward way to other variational problems with symmetric structure, we show how equivariant gatesets can be used in variational quantum eigensolvers.

QI 12.9 Thu 17:15 H8

Preparation of Hardware-Efficient Graph States on IBM QX — •Sebastian Brandhofer[1], Jelena Mackeprang[2], Daniel Bhatti[2], Ilia Polian[1], and Stefanie Barz[2] — [1]Institute of Computer Architecture and Computer Engineering & IQST, University of Stuttgart, Germany — [2]Institute for Functional Matter and Quantum Technologies & IQST, University of Stuttgart, Germany

Near-term quantum computers are characterized by heterogeneous errors that occur at a high rate, a short decoherence time, and a limited number of qubits. Preparing a quantum state on these near-term quantum computers must be performed with these limitations in mind. Especially, when preparing highly entangled multi-qubit quantum states one would like to reach quantum state fidelities as high as possible. For this, the quantum state preparation algorithm needs to be adapted to the specific quantum hardware and the respective limitations. In this work, a method is proposed for determining the optimal preparation algorithm of a specific class of graph states. The proposed method is based on one of the winning submissions to the 2020 IBM Quantum's Open Science Prize - Graph State Challenge.

QI 12.10 Thu 17:30 H8

A single T-gate makes distribution learning hard — Marcel Hinsche[1], Marios Ioannou[1], •Alexander Nietner[1], Jonas Haferkamp[1], Yihui Quek[1], Dominik Hangleiter[2], Jean-Pierre Seifert[3], Jens Eisert[1,4,5], and Ryan Sweke[1] — [1]FU Berlin, 14195 Berlin, Germany — [2]University of Maryland, MD 20742, USA — [3]TU Berlin, 10587 Berlin, Germany — [4]Helmholtz-Zentrum Berlin, 14109 Berlin, Germany — [5]Fraunhofer Heinrich Hertz Institute, 10587 Berlin, Germany

The task of probabilistic modelling is at the core of many practical applications. As such, the efficient learnability of natural classes of probability distributions is a question of both fundamental and practical interest. The output distributions of local quantum circuits is a particularly interesting class of distributions, of key importance both to quantum advantage proposals and a variety of quantum machine learning algorithms. In this work, we provide an extensive characterization of the learnability of the output distributions of local quantum circuits. We prove that the density modelling problem can be solved efficiently in case of Clifford circuits, while adding a single T gate renders the task computationally hard. Evidently, the simulability of this class does not imply its learnability. Next we show that the generative modelling task is hard for depth $n^{\Omega(1)}$ universal local quantum circuits for both, classical and quantum algorithms. Finally we obtain a similar hardness result already for depth $\omega(\log(n))$ local Clifford circuits when restricting to practically relevant learning algorithms, such hybrid-quantum classical algorithms.

QI 12.11 Thu 17:45 H8

Avoiding barren plateaus via transferability of smooth solutions in Hamiltonian Variational Ansatz — Antonio Anna Mele[1,2], Glen Bigan Mbeng[3], Giuseppe Ernesto Santoro[2], Mario Collura[2], and •Pietro Torta[2] — [1]Dahlem Center for Complex Quantum Systems, Freie Universität Berlin, 14195 Berlin, Germany — [2]SISSA, Via Bonomea 265, I-34136 Trieste, Italy — [3]Universität Innsbruck, Technikerstraße 21 a, A-6020 Innsbruck, Austria

A large ongoing research effort focuses on Variational Quantum Algorithms (VQAs), representing leading candidates to achieve computational speed-ups on current quantum devices. The scalability of VQAs to a large number of qubits, beyond the simulation capabilities of classical computers, is still debated. Two major hurdles are the proliferation of low-quality variational local minima, and the exponential vanishing of gradients in the cost function landscape, a phenomenon referred to as barren plateaus. Here we show that, by employing iterative search schemes one can effectively prepare the ground state of paradigmatic quantum many-body models, circumventing also the barren plateau phenomenon. This is accomplished by leveraging the transferability to larger system sizes of iterative solutions, displaying an intrinsic smoothness of the variational parameters, a result that does not extend to other solutions found via random-start local optimization. Our scheme could be directly tested on near-term quantum devices, running a refinement optimization in a favorable local landscape with non-vanishing gradients.

QI 12.12 Thu 18:00 H8

Hay from the haystack: explicit examples of exponential quantum circuit complexity — •Yifan Jia and Michael M. Wolf — Department of Mathematics, Technische Universität München, Germany

The vast majority of quantum states and unitaries have circuit complexity exponential in the number of qubits. In a similar vein, most of them also have exponential minimum description length, which makes it difficult to pinpoint examples of exponential complexity. In this work, we construct examples of constant description length but exponential circuit complexity. We provide infinite families such that each element requires an exponential number of two-qubit gates to be generated exactly from a product and where the same is true for the approximate generation of the vast majority of elements in the family.

The results are based on sets of large transcendence degree and discussed for tensor networks, diagonal unitaries and maximally coherent states.