Quantum Computing User Forum

Agenda

April 21-24, 2020

Hosted by the

Oak Ridge Leadership Computing Facility

at

Oak Ridge National Laboratory

Quantum Computing User Forum

The Quantum Computing User Forum brings together users to discuss common practices in the development of applications, software, and simulations for quantum computing devices and systems. Hosted by the Oak Ridge Leadership Computing Facility at Oak Ridge National Laboratory, the four-day virtual meeting scheduled April 21-24, 2020 includes invited presentations from leading researchers in the field of quantum computer science. Keynote presentations by Dr. Eleanor Rieffel from NASA Ames Research Center and Dr. Sergey Bravyi from IBM open the event organized in four topical sessions:

- Applications of Quantum Computing
- Software for Quantum Computing
- Numerical Simulation of Quantum Computing
- Error Mitigation for Quantum Computing

Agenda

- All times presented in the agenda reference Eastern Daylight Time (UTC-4).
- Sessions will adhere strictly to the scheduled timetable.

Presentations

- The user forum will use a moderated online videoconferencing platform.
- Videoconferencing details are sent by email to registered attendees and should not be shared due to limits on videoconferencing capacity.
- Attendees may submit questions for a speaker through the videoconferencing chat.
- Session chairs will address questions as time permits.
- Speaker presentations will be recorded for online distribution after the user forum closes.

Tuesday, April 21, 2020

Time	Speaker	Topic
11:00	Travis Humble Oak Ridge National Laboratory	*Opening Remarks*
		Keynote Presentation
11:05	Eleanor Rieffel NASA Ames Research Center	*Utilizing NISQ Devices for Evaluating Quantum Algorithms* With the advent of quantum supremacy, we have an unprecedented opportunity to explore quantum algorithms in new ways. The emergence of general-purpose quantum processors opens up empirical exploration of quantum algorithms far beyond what has been possible to date. Challenging computational problems arising in the practical world are often tackled by heuristic algorithms. While heuristic algorithms work well in practice, by definition they have not been analytically proven to be the best approach or to outperform the best previous approach. Instead, heuristic algorithms are empirically tested on benchmark and real-world problems. With the empirical evaluation NISQ hardware enables, we expect a broadening of established applications of quantum computing. What to run and how best to utilize these still limited quantum devices to gain insight into quantum algorithms remain open research questions. We discuss opportunities and challenges for using NISQ devices to evaluate quantum algorithms, including in elucidating quantum mechanisms and their uses for quantum computational purposes, in the design of novel or refined quantum algorithms, in compilation, error-mitigation, and robust algorithms design, and in techniques for evaluating quantum algorithms empirically.
11:45	Chair: Pavel Lougovski Oak Ridge National Laboratory	*Session: Applications of Quantum Computing*
11:50	Bert de Jong Lawrence Berkeley National Laboratory	*Advancing Physical Sciences on Near-Term Quantum Computers* In recent years significant advances have been made to deliver quantum computing as a platform enabling scientific discovery. I will discuss some of the advances made by the QAT4Chem Quantum Algorithms Team, the Accelerated Research in Quantum Computing Team AIDE-QC, and the high-energy physics QuantiSED effort led out of Lawrence Berkeley National Laboratory. These programs involve quantum algorithm developers, mathematicians, and computer scientists with a mission to deliver algorithmic, computational, and mathematical advances to enable scientific discovery on quantum computers.

Tuesday, April 21, 2020 (continued)

Time	Speaker	Topic
12:10	Alexander McCaskey Oak Ridge National Laboratory	*Quantum Chemistry as a Benchmark for Near-term Quantum Computers* We present a quantum chemistry benchmark for noisy intermediate-scale quantum computers that leverages the variational quantum eigensolver, active-space reduction, a reduced unitary coupled cluster ansatz, and reduced density purification as error mitigation. We demonstrate this benchmark using 4 of the available qubits on the 20-qubit IBM Tokyo and 16-qubit Rigetti Aspen processors via the simulation of alkali metal hydrides (NaH, KH, RbH), with accuracy of the computed ground state energy serving as the primary benchmark metric. We also show how to reduce the noise in post processing with specific error mitigation techniques. For specific benchmark settings and a selected range of problems, our results show that the accuracy metric can reach chemical accuracy when computing over the cloud on certain quantum computers.
12:30	Break	
12:40	Andrew Sornborger Los Alamos National Laboratory	*Variational Fast Forwarding for Quantum Simulation Beyond the Coherence Time* Trotterization-based, iterative approaches to quantum simulation are restricted to simulation times less than the coherence time of the quantum computer, which limits their utility in the near term. Here, we present a hybrid quantum-classical algorithm, called Variational Fast Forwarding (VFF), for decreasing the quantum circuit depth of quantum simulations. VFF seeks an approximate diagonalization of a short-time simulation to enable longer-time simulations using a constant number of gates. Our error analysis provides two results: (1) the simulation error of VFF scales at worst linearly in the fast-forwarded simulation time, and (2) our cost function's operational meaning as an upper bound on average-case simulation error provides a natural termination condition for VFF. We implement VFF for the Hubbard, Ising, and Heisenberg models on a simulator. Finally, we implement VFF on Rigetti's quantum computer to show simulation beyond the coherence time.
13:00	Andy Li Fermi National Accelerator Laboratory	*Quantum Computing for Neutrino-nucleus Scattering with NISQ Devices* Neutrino-nucleus cross-section uncertainties are expected to be a dominant systematic in future accelerator neutrino experiments. In this talk, I will present an analysis of the required resources and expected scaling for scattering cross-section calculations on quantum computers with a simple neutrino-nucleus model. A small-scale experiment consisting of the variational state preparation and the relevant time evolution is also demonstrated using the IBM Quantum Experience as a first step to implement the cross-section calculations.

Tuesday, April 21, 2020 (continued)

Time	Speaker	Topic
13:20	Kaiwen Gui University of Chicago	*Term Grouping and Travelling Salesperson for Digital Quantum Simulation* In the digital simulation of quantum dynamics, the corresponding quantum circuits have large numbers of quantum gates and Trotter errors. We first propose a term ordering technique that improves the Trotter fidelity compared with previously proposed optimization by reordering Pauli terms and partitioning them into commuting families. Secondly, we describe a gate cancellation technique that reduces the high gate counts by formulating the gate cancellation problem as a traveling salesperson problem.
13:40	Mike McGuigan Brookhaven National Laboratory	*Discrete Gauge Theories on Quantum Computers* In this talk we introduce lattice gauge theories based on discrete groups that can be realized on quantum computers and can be used as a simplified version of lattice QCD. We discuss how to do the Hamiltonian mapping for the system, calculate the ground state energy, impose gauge invariance and calculate thermal observables for the system. Finally, we will discuss scaling studies for the performance of these systems on IBM quantum hardware.
14:00	Session Adjourns	

Wednesday, April 22, 2020

Time	Speaker	Topic
11:00	Chair: Alex McCaskey Oak Ridge National Laboratory	*Session: Software for Quantum Computing*
11:05	Moin Quereshi Georgia Tech	*Reducing Errors in Quantum Computation via Program Transformation* In this talk, I will discuss some of our recent proposals that aims to improve the reliability of NISQ computers by developing software techniques to mitigate the hardware errors. Our first proposal exploits the variability in the error rates of qubits to steer more operations towards qubits with lower error rates and avoid qubits that are error-prone. Our second proposal looks at executing different versions of the programs each crafted to cause diverse mistakes so that the machine becomes less vulnerable to correlated errors. Our third proposal looks at exploiting the state-dependent bias in measurement errors (state 1 is more error prone than state 0) and dynamically flips the state of the qubit to perform the measurement in the stronger state.
11:35	Vlad Gheorghiu softwareQ Inc.	*staq – A Full Stack Quantum Processing Toolkit* I will describe 'staq', a full-stack quantum processing toolkit written in standard C++. 'staq' is a quantum compiler toolkit, comprising of tools that range from quantum optimizers and translators to physical mappers for quantum devices with restricted connectives. The design of 'staq' is inspired from the UNIX philosophy of "less is more", i.e. 'staq' achieves complex functionality via combining (piping) small tools, each of which performs a single task using the most advanced current state-of-the-art methods."
11:55	Alexandru Paler Johannes Kepler University Linz	*The Toolset for Quantum Resource Estimation* Reliable resource estimation of quantum algorithms is a critical component of the development cycle of viable quantum applications for quantum computers of all sizes. Determining critical resource bottlenecks in algorithms, especially when resource intensive error correction protocols are required, is crucial to reduce the cost of implementing viable algorithms on actual quantum hardware. This talk presents the components of a "Swiss army knife" for estimating the number of physical qubits and the execution time of arbitrary quantum algorithms.

Wednesday, April 22, 2020 (continued)

Time	Speaker	Topic
12:15	Jonathan Baker University of Chicago	*Multivalued and Mixed Radix Quantum Computing* Typical quantum computation is performed using two level systems or qubits. However, in many current technologies this simplification is unnecessary. Similar to higher radix classical computation, multivalued quantum computation typically confers limited advantage, for example constant depth and gate count improvements. An alternative, mixed-radix, strategy is to take advantage of higher dimensional states temporarily which can reduce total resource requirements substantially. In this talk I will introduce the basics of multivalued quantum computation and examine a few examples of mixed radix quantum techniques, like the Generalized Toffoli and arithmetic circuits.
12:35	Thien Nguyen Oak Ridge National Laboratory	*Scalable Pulse-level Software Infrastructure for the XACC Framework* XACC is a system-level software infrastructure for heterogeneous quantum-classical computing incorporating compilers, simulation or remote execution runtimes, and high-level quantum programming concepts in a service-oriented fashion. In this talk, we will present recent extensions of the XACC framework to enable pulse-level quantum programming and simulation in a multi-layered and hardware-agnostic approach. This includes quantum hardware modeling, pulse-level intermediate representation, and a pulse backend simulator.
12:55	Session Adjourns	

Thursday, April 23, 2020

Time	Speaker	Topic
11:00	Travis Humble Oak Ridge National Laboratory	*Introductions*
		Keynote Presentation
11:05	Sergey Bravyi IBM	*Classical Algorithms for Quantum Mean Values* Variational quantum algorithms such as VQE employ variational states generated by parameterized quantum circuits to minimize the expected value of a Hamiltonian encoding the problem of interest. Whether or not VQE can outperform classical computers in some tasks is an actively debated question. Our work contributes to this debate by isolating the quantum part of VQE - computing expected values of multi-qubit observables and studying its hardness for classical computers as a function of the circuit depth and qubit connectivity. Finally, I will discuss classical algorithms for the Forrelation Problem and highlight its connection to variational quantum optimization algorithms. Based on arXiv:1909.11485.
11:45	Chair: Yuri Alexeev Argonne National Laboratory	*Session: Numerical Simulation of Quantum Computing*
11:50	Dmitry Liakh Oak Ridge National Laboratory	*Leveraging Tensor Networks for an Efficient Classical Simulation of Quantum Circuits with the ExaTN Library* Tensor network machinery provides a natural and often efficient representation of quantum many-body states, in particular the multi-qubit states in quantum computing. We discuss different flavors of tensor network theory as applied to the classical HPC simulation of quantum circuits. We consider both the exact tensor contraction of arbitrary quantum circuits as well as approximate (fixed-fidelity) simulations where a tensor network delivers a compressed representation of the multi-qubit wave-function. We also demonstrate the utility of our ExaTN library for HPC processing of arbitrary tensor networks in both cases.

Thursday, April 23, 2020 (continued)

Time	Speaker	Topic
12:10	Benjamin Villalonga University of Illinois at Urbana-Champaign and Google	*Simulating Large Shallow Quantum Circuits using qFlex* Quantum computers are entering the Noisy Intermediate-Scale Quantum (NISQ) era, with devices of about 50-100 qubits with high enough gate fidelities to run for depths that challenge and even surpass what classical simulation techniques can achieve on the largest supercomputers. At this time, classical simulators play a versatile role: they aid in benchmarking the performance of quantum computers, they are a useful tool in quantum algorithm exploration, and they help map out the boundary of what is classically achievable, hence giving insight on where NISQ applications might show an advantage. In this talk I will present qFlex, an open source simulator of large shallow quantum circuits. I will demonstrate the simulation of random quantum circuits on different qubit layouts, including shallow circuits on square lattices of up to 121 qubits.
12:30		Break
12:40	Matthew Otten Argonne National Laboratory	*Simulating Quantum Devices with QuaC* As quantum devices progress in scale and quality, understanding the effects of noise sources beyond single qubit Pauli errors, such as leakage errors in superconducting qubits, becomes critical. I will discuss the QuaC simulator, a high-performance Lindblad master equation solver designed to simulate the underlying physics, including noise processes, of various quantum devices.
13:00	Martin Suchara Argonne National Laboratory	*Running Large Quantum Circuits on Small Quantum Computers* In this talk I will describe a technique that splits large quantum circuits into smaller fragments, evaluates these fragments, and recombines the fragment outputs to reconstruct the original circuit outputs. I will demonstrate the technique on Quantum Approximate Optimization Algorithm circuits and present results obtained on IBM Poughkeepsie, a 20-qubit processor. I will also systematically analyze the effects of noise on the fidelity of the outputs.

Thursday, April 23, 2020 (continued)

Time	Speaker	Topic
13:20	Ryan Bennink Oak Ridge National Laboratory	*Quasiprobabilistic Representations of Quantum Mechanics for Insight and Simulation* Quantum mechanics can be formulated entirely in terms of probabilities in lieu of Hilbert space. Such a formulation more clearly elucidates some of the differences between quantum and classical mechanics. Interestingly, quantum states and processes can be understood in stochastic terms if one allows probabilities to be negative. Negative probability is a non-classical resource and total negativity of a state or process can be viewed as a measure of its quantumness. This perspective suggests new metrics for quantifying the power of noisy quantum computers and new approaches to simulating quantum phenomena as efficiently as possible on classical computers.
13:40	Edwin Pednault IBM	*Exploiting Memory Hierarchies in Quantum Circuit Simulation* Tensor representations, circuit partitioning, and tensor slicing operations provide basic tools for managing both memory footprints and distributed calculations in quantum circuit simulation. However, different ways of applying these tools can lead to dramatically different computational efficiencies that can vary over many orders of magnitude. To maximize efficiency, one must take into account the memory hierarchy of the compute cluster being utilized, the access times and storage capacities at each level, and the communication bandwidths between levels. On the Summit supercomputer, for example, a voluminous parallel file system occupies one end of the memory hierarchy, while the other end is occupied by the much smaller but significantly faster high-bandwidth memories and internal cache levels of the GPUs. This talk presents a circuit-partitioning and tensor-slicing strategy for minimizing data transfers that take place between levels in such hierarchies, which can thereby make it feasible to exploit secondary storage in quantum circuit simulation.
14:00	Session Adjourns	

Friday, April 24, 2020

Time	Speaker	Topic
11:00	Chair: Raphael Pooser Oak Ridge National Laboratory	*Session: Error Mitigation for Quantum Computing*
11:05	Ken Brown Duke University	*Hidden Inverses* The noise sources in quantum information processors fluctuate at different timescales allowing for a range of mitigation schemes from quantum control to quantum error correction. In this talk, we will consider relatively slow noise processes that vary from experiment to experiment but are relatively constant on the length scale of a circuit. These sorts of errors can often be handled by quantum control techniques like dynamic decoupling and composite pulses. In this talk, we will describe how to identify "hidden inverses" in a quantum circuit to reduce these errors. We will examine alternative gate compilation strategies, identification of inverses on subspaces, and approximate inverses.
11:35	Lukasz Cincio Los Alamos National Laboratory	*Machine Learning of Noise-resilient Quantum Circuits* In this work, we study how machine learning can be applied to formulate noise-aware circuit compilations that can be executed on near-term quantum hardware to produce reliable results. We will demonstrate that experimentally derived noise models can be used to go beyond naive circuit compilations for several example quantum algorithms. There are two inputs to our Noise-Aware Circuit Learning (NACL) method: a task, and a noisy gate alphabet. The task is defined by either a set of classical training data or a desired output quantum state or unitary. The output of NACL is a quantum gate sequence that optimally accomplishes the inputted task in the presence of the inputted noise model. Neither an ansatz nor the circuit depth of the gate sequence is an input to NACL. This is because NACL optimizes over the circuit structure and depth, which is in the spirit of task-oriented programming. We implement NACL for several different problems, such as computing state overlap, preparing multi-body entangled states, and implementing the quantum Fourier transform. In each case, we find that our overall figure-of-merit is significantly lower for NACL than for standard methods of circuit compilation.

Friday, April 24, 2020 (continued)

Time	Speaker	Topic
11:55	Yanzhu Chen Stony Brook University	*Detector Tomography on IBM 5-qubit Quantum Computers and Mitigation of Imperfect Measurement* We use quantum detector tomography to characterize the qubit readout in terms of measurement POVMs on IBM Quantum Computers IBM Q 5 Tenerife and IBM Q 5 Yorktown. Our results show noticeable deviation from the ideal projectors and signs of correlations in the detector behavior. We also discuss how the characterized detectors' POVM can be used to estimate the ideal detection distribution.
12:15	Sophia Economou Virginia Tech	*Efficient Ansatze for VQEs* A crucial aspect of VQE is the creation of a good variational ansatz, which allows for relatively shallow circuits and a low number of classical optimization parameters. In this talk, I will give an overview of VQEs for chemistry applications and present ADAPT-VQE, an algorithm which realizes efficient, problem-tailored ansatze on quantum computers.
12:35	Michael Geller University of Georgia	*Quantum Error Correction for SPAM* We discuss and experimentally demonstrate two new techniques for the mitigation of state preparation and measurement errors. The first is a scalable implementation of the well-known transition matrix technique. The second enables rigorous readout correction for a family of nonideal quantum measurement models.
12:55	Kathleen Hamilton Oak Ridge National Laboratory	*Scaling Up Error Mitigation for Data Driven Circuit Learning* The efficacy of data-driven circuit learning is reduced when training is done on noisy intermediate scale quantum (NISQ) devices. Incorporating matrix-based error mitigation methods can speed up gradient-based circuit training by reducing the number of spurious state counts. The construction of a full error kernel matrix can require an exponential number of circuit evaluations. In this talk we present several methods for reducing the computational overhead.
13:15	Session Adjourns	
13:15	Travis Humble Oak Ridge National Laboratory	Closing Remarks
13:20	Forum Adjourns	