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Advancing quantum computing as a platform for scientific discovery in chemical sciences

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The Quantum Algorithms Team led out of Lawrence Berkeley National Laboratory is an integrated team of quantum algorithm developers, mathematicians, and computer scientists with a mission to deliver algorithmic, computational and mathematical advances to enable scientific discovery in chemical sciences on quantum computers. Our focus is on quantum chemistry simulations, which are an early exemplar of quantum computing, demonstrating the potential of various types of quantum devices to aid in scientific discovery in the chemical sciences.

Our team has assessed the robustness of state preparation (https://arxiv.org/abs/1809.05523), devised new sparse techniques with lower gate depth (https://arxiv.org/abs/1810.02327), and have explored the use of tensor networks (https://arxiv.org/abs/1803.11537). Preparation of scientifically relevant states is a key challenge for chemical simulations. We have developed a protocol to discriminate between decoherence and information scrambling as a way to verify quantum circuits, which was experimentally validated on an ion trap (https://arxiv.org/abs/1807.09087). Our team is exploring a quantum autoencoder and its strongly reduced latent space for a quantum machine learning model. Gate depth of a quantum circuit plays a critical role in achieving results with high fidelity. The QAT team, in partnership with NASA, has demonstrated low depth circuits for k-local gates in QAOA and Trotterized fermionic Hamiltonians. We extended the open-source quantum simulation software framework ProjectQ with gate-level noise injection capabilities for error analysis, and used it to demonstrate that a rudimentary approach to mitigate errors in a CNOT gate operation can improve the gate fidelity. Additional efforts for error mitigation are ongoing. We have developed a large suite of stochastic classical optimizers, needed for variational quantum eigensolvers and qubit gate optimization. The optimizers have been packaged (github.com/scikit-quant) for integration in quantum computing software stacks. We are continuing to develop new and better stochastic optimizers.

Primary author: DE JONG, Wibe

Co-authors: Dr IANCU, Costin (LBNL); Dr METCALF, Mekena (LBNL); Dr URBANECK, Miroslav (LBNL); Dr LAVRIJSEN, Wim (LBNL)

Presenter: DE JONG, Wibe

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