

Simulating Quantum Magnetism on Noisy Quantum Computers: An Analysis of Trotter-Suzuki and qDRIFT

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Introduction

Quantum computing is a new paradigm of computing that:

- Makes use of quantum mechanics to perform calculations on quantum bits (qubits).
- Can perform some algorithms for simulating quantum systems in much fewer operations than classical computers.
- If perfected, could be used to efficiently simulate chemical interactions for drug design and materials development.
- Is currently limited by noise from interactions between the qubits and the environment and performing operations.

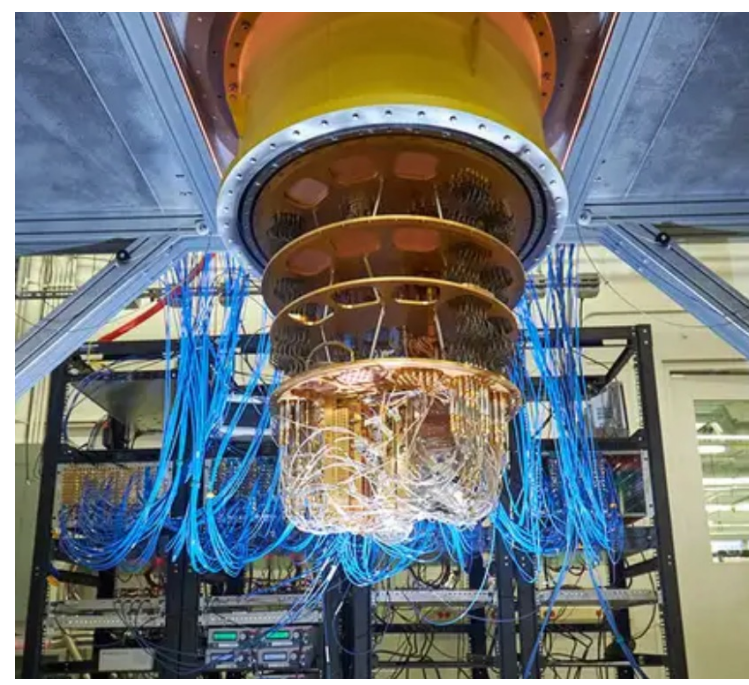


Image of a quantum computer



The qubit layout of the *ibmq_manila* device that we mainly utilized through out this project [3].

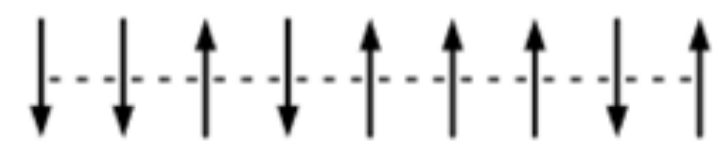
In this project, we investigate the performance of quantum algorithms for simulating magnetic materials on current quantum computing hardware. The key challenge with these systems is noise, which we tackle by examining a newly developed algorithm, qDRIFT [1,2].

Most of the tests were run on *ibmq_manila*, which is a cloud-accessible quantum computer developed by IBM with qubits connected linearly to one another [3].

Background

Ising Model of Ferromagnetism

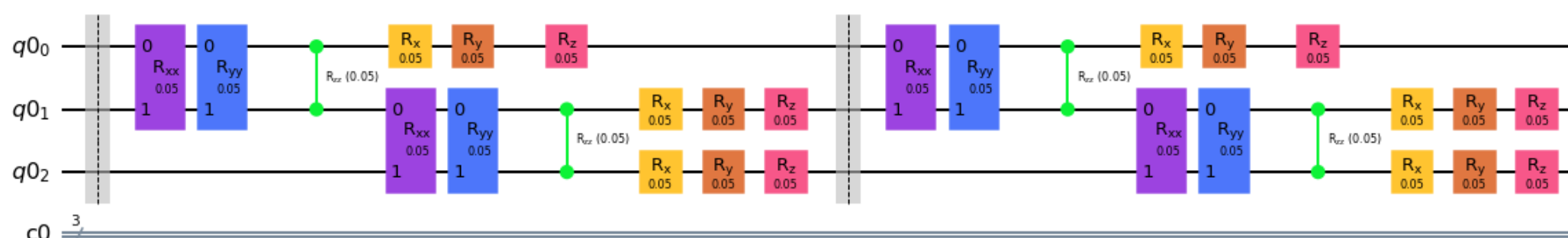
- Physical model for quantum magnetic materials.
- Each particle represents an atomic spin.
- Each spin tries to align with external magnetic fields and interacts with neighboring spins.
- The Ising chain is a one-dimensional version of the generalized model.



Representation of Ising Chain

First Order Trotter-Suzuki (FOTS) Algorithm for Quantum Simulation

- Deterministic approximation of the time-evolution operator in terms of the Trotter-Suzuki Decomposition.
- Splits the simulation into many small, equal time steps [2].
- Total gate count, and therefore error from noise, scales with the number of terms of the Hamiltonian. For example, chemical systems can have millions of Hamiltonian terms [1].

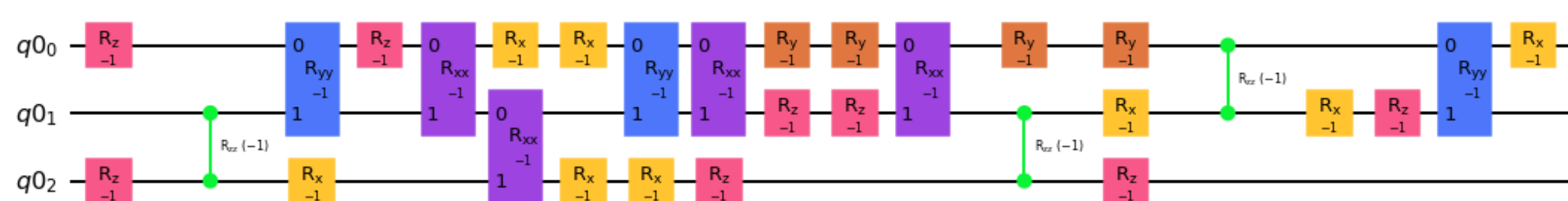


Two layers of a FOTS circuit with 30 color-coded gates.

Dotted lines are circuit barriers representing the beginning of a new time step

qDRIFT Algorithm for Quantum Simulation

- Weighs operations based on their importance to the simulation [1].
- Randomly selects operations based on their weights [1].
- Total gate count scales with the sum of coefficients of Hamiltonian [1,2], promising drastic improvements compared to FOTS.



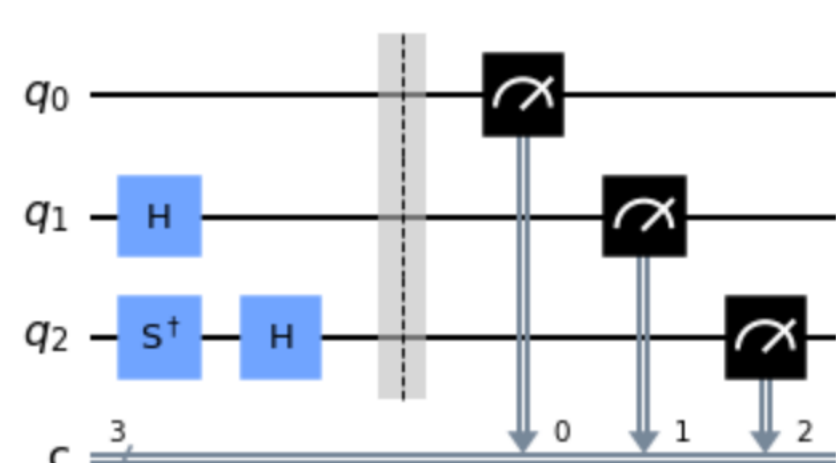
An example of a qDRIFT circuit with 30 color-coded quantum gates

Methods

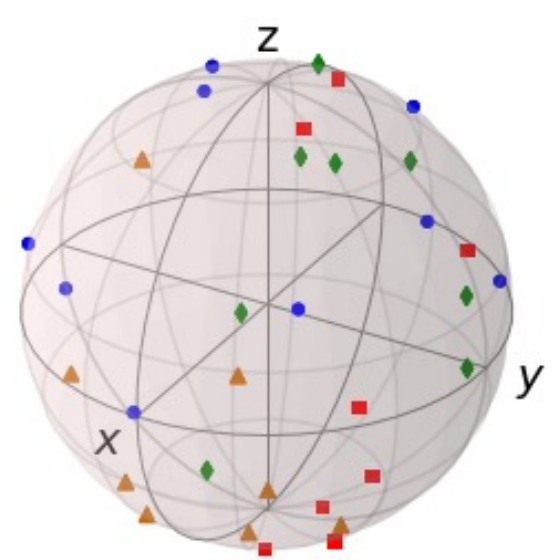
We analyzed both quantum algorithms for simulating the Ising chain with a set Hamiltonian under several scenarios:

- 1) specific initial state and measurement observable,
- 2) randomized initial state and specific measurement observable,
- 3) randomized initial state and observable.

Circuits for the qDRIFT and FOTS protocols were created using Python libraries Qiskit and Qutip [4].



Circuit which measures qubits 0, 1, and 2 using the Z, X, and Y observables respectively



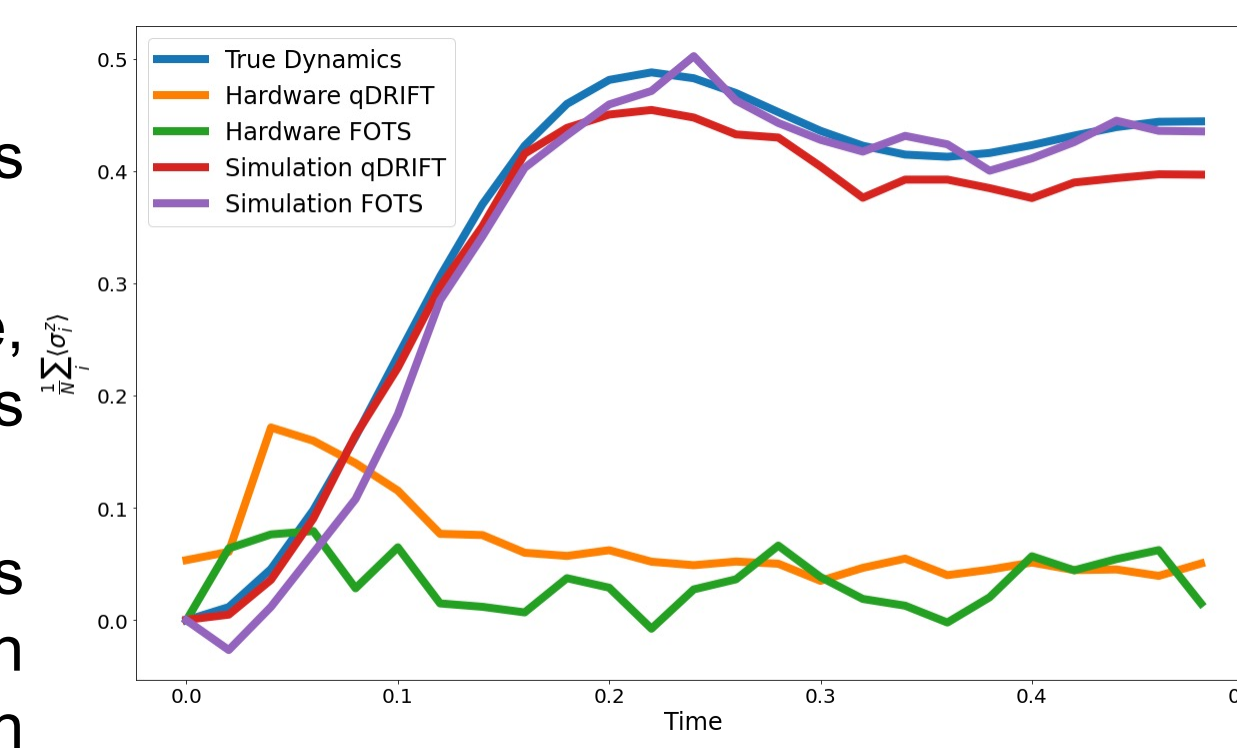
Bloch sphere with 30 Haar random initial states

- We tested our results using a combination of classical numerical simulators, quantum circuit simulators, and quantum computing hardware.
- The qDRIFT algorithm involved averaging over many random circuit instances to improve accuracy of results.
- When comparing both methods, the number of gates was kept constant.

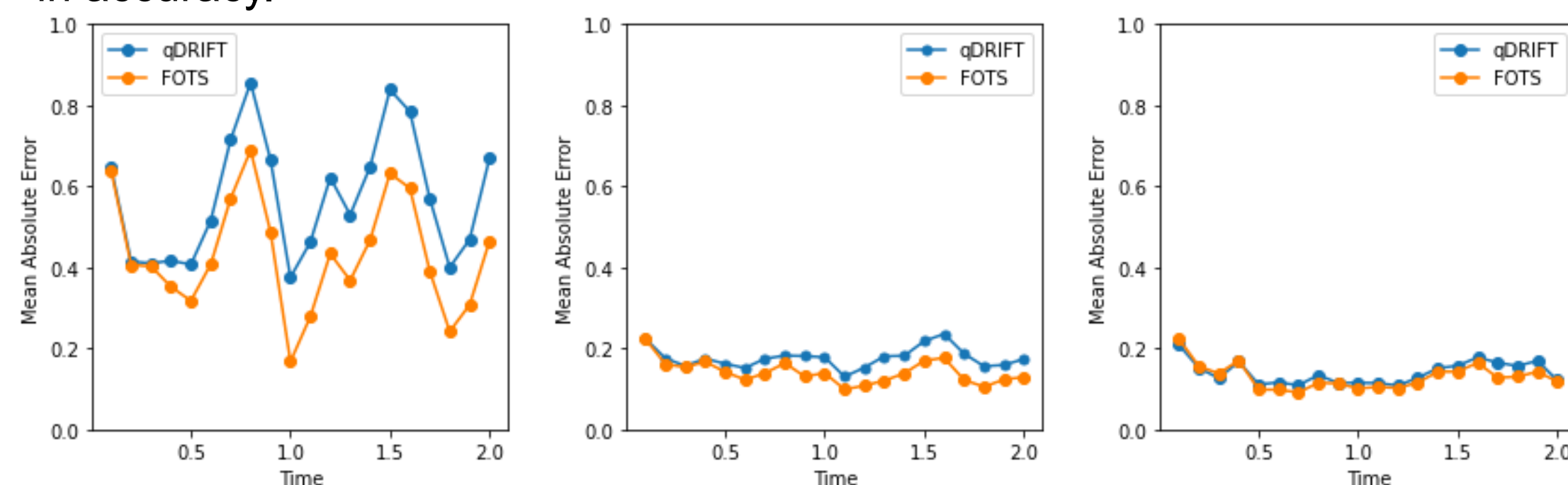
Results

Overall Summary:

- In simulation, both algorithms reproduce true dynamics.
- When implemented on hardware, the accuracy of both algorithms is severely limited by noise.
- In simulation, FOTS outperforms qDRIFT. However, tests on hardware showed that both methods to be more comparable in accuracy.



Dynamics of a 4-qubit quantum system



Hardware tests for set initial state and observable (left), randomized initial state and set observable (middle), and randomized initial state and observable (right)

Test Scenario 1: Specific initial state and observable:

- Neither algorithm was very accurate, with FOTS and qDRIFT having 0.431 and 0.571 mean error respectively.
- The error from qDRIFT was 32.5% higher than that of the FOTS approach.

Test Scenario 2: Randomized initial state and set observable:

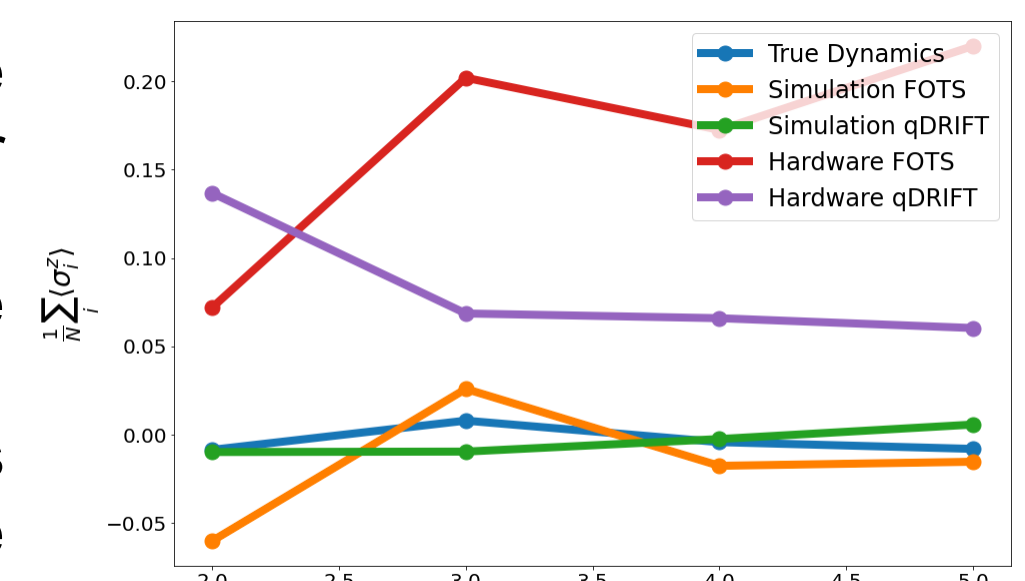
- In comparison to Test Scenario 1, the mean error for both methods drastically decreased (67.1% for FOTS and 69.0% qDRIFT).
- The mean error from qDRIFT is 24.8% higher than the algorithm.

Test Scenario 3: Randomization of both initial state and observables:

- Mean error dropped by a further 8.4% and 20.7% for FOTS and qDRIFT respectively, when compared to Test Scenario 2.
- Error in qDRIFT was very comparable to FOTS (only 8.0% higher).

We found some parameter regimes for the Ising model where qDRIFT outperforms FOTS on both hardware and simulation.

- These Hamiltonians had a single interaction term that was much larger than the other terms.
- In simulation, both algorithms reproduce the true dynamics.
- On hardware, accuracy of qDRIFT is better than FOTS and the difference between the two approaches increases with qubit count.



Dynamics of Ising chain with one dominant and several weaker interactions

Conclusions

In this work we have shown that noise plays an important role for simulation accuracy on current quantum computers. In summary,

- Both algorithms are more accurate for shorter simulation time.
- FOTS has less algorithmic error than qDRIFT for an equal number of gates.
- qDRIFT is less impacted by noise, but this is mostly when the algorithmic error is already high.
- Factoring in noise, qDRIFT and FOTS have similar accuracies.
- qDRIFT out-performs FOTS for some instances of the Heisenberg model featuring one dominant term and a few other small terms.

Future Work

The scale of systems tested in this project was limited by available quantum hardware. As larger quantum computers come online, it will enable the study of larger, more complex material models and larger molecules relevant to quantum chemistry with a wide variety of applications. These systems may exhibit more complex noise processes such as cross-talk, which will necessitate the design of noise-robust quantum algorithms.

Acknowledgments

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