SAND2022-14473C

Richardson extrapolation for small diatomic molecules on the QSCOUT device

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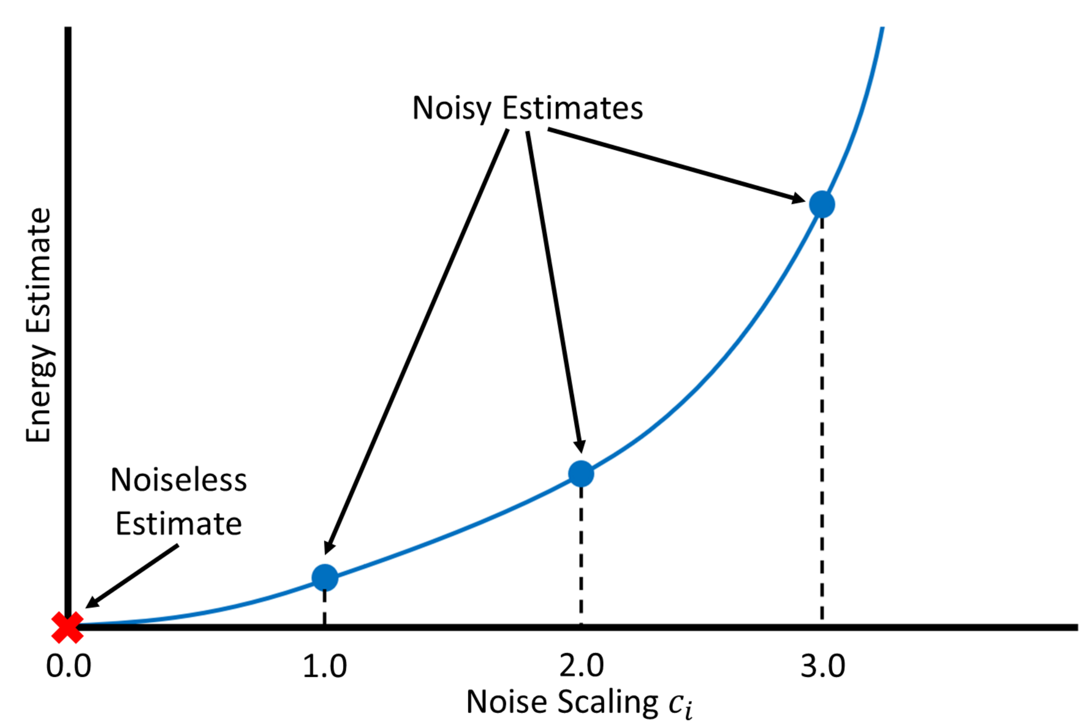
1. Richardson Extrapolation

Noisy Intermediate Scale Quantum (NISQ) devices are hindered by large error rates, particularly for multi-qubit gates. Richardson Extrapolation can improve device accuracy given more samples. We studied its effect on estimates of the ground state energy of small diatomic molecules. We simulated extrapolation using our noise model IonSim, which emulates the variation in experimental control parameters. Experiments were carried out on the Quantum Scientific Computing Open User Testbed (QSCOUT) device **[1, 2].**

We Taylor expand the noisy expectation value around a noiseless estimate to order n. If the unmitigated circuit has an error rate $\lambda = 1.0$, then n noisy measurements with noise scaled by $c_i\lambda > 1.0$ are fit to a polynomial of order $n-1$. The mitigated energy estimate corresponds to $\lambda = 0$ on this curve, with reduced error $\mathcal{O}(\lambda^{n+1})$.

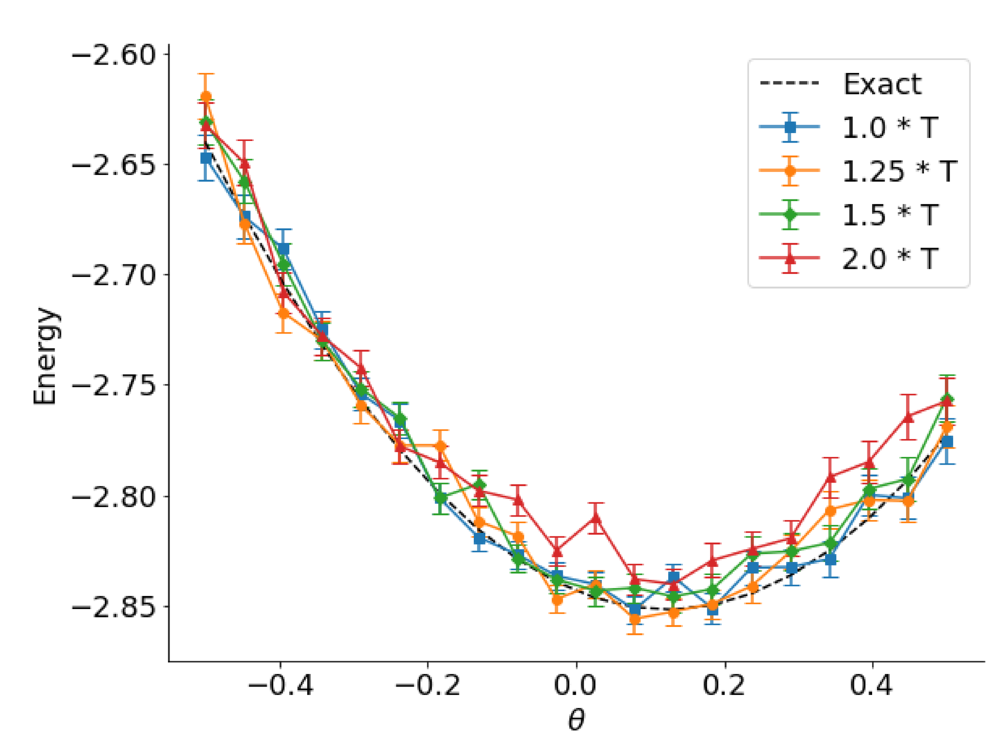
Figure 1 – Schematic of Richardson Extrapolation. Noisy estimates are extrapolated using a polynomial of order n.



2. Time Stretching Methods

We increase the error in our circuits by stretching the duration of our control pulses **[3, 4]**. Simulations varied the duration by $c_i = \{1.0, 1.25, 1.5, 2.0\}$ using 2000 samples per measurement.

Figure 2 – Simulation results of time-stretch extrapolation. Increasing gate duration has little effect. It is difficult to differentiate the noisy energy estimates.



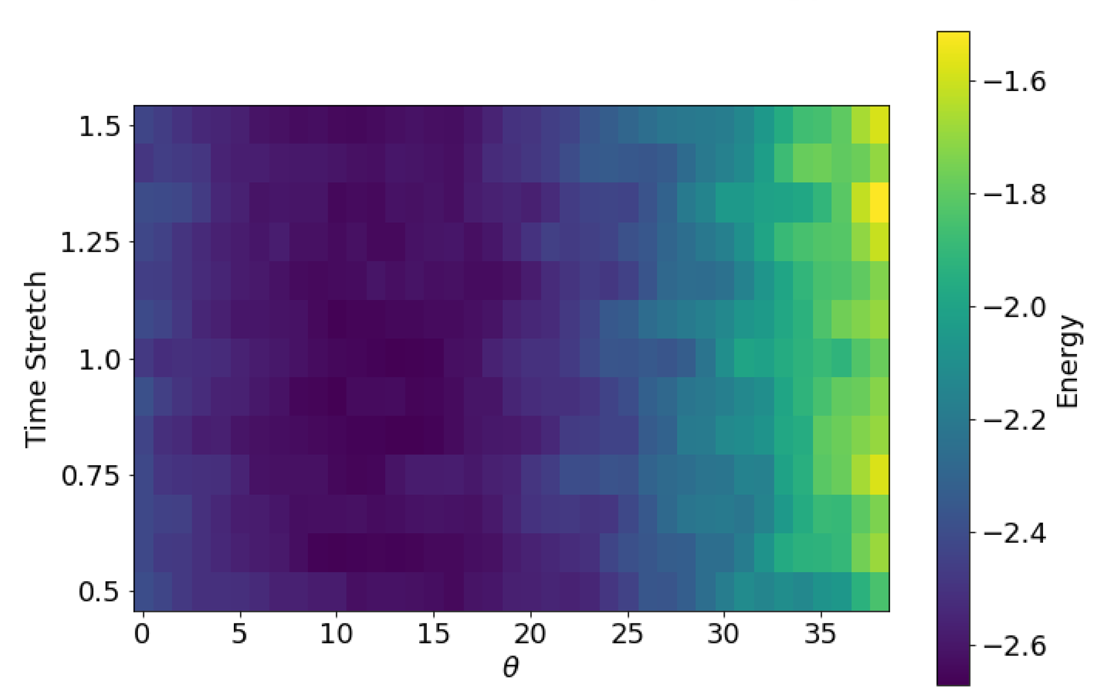
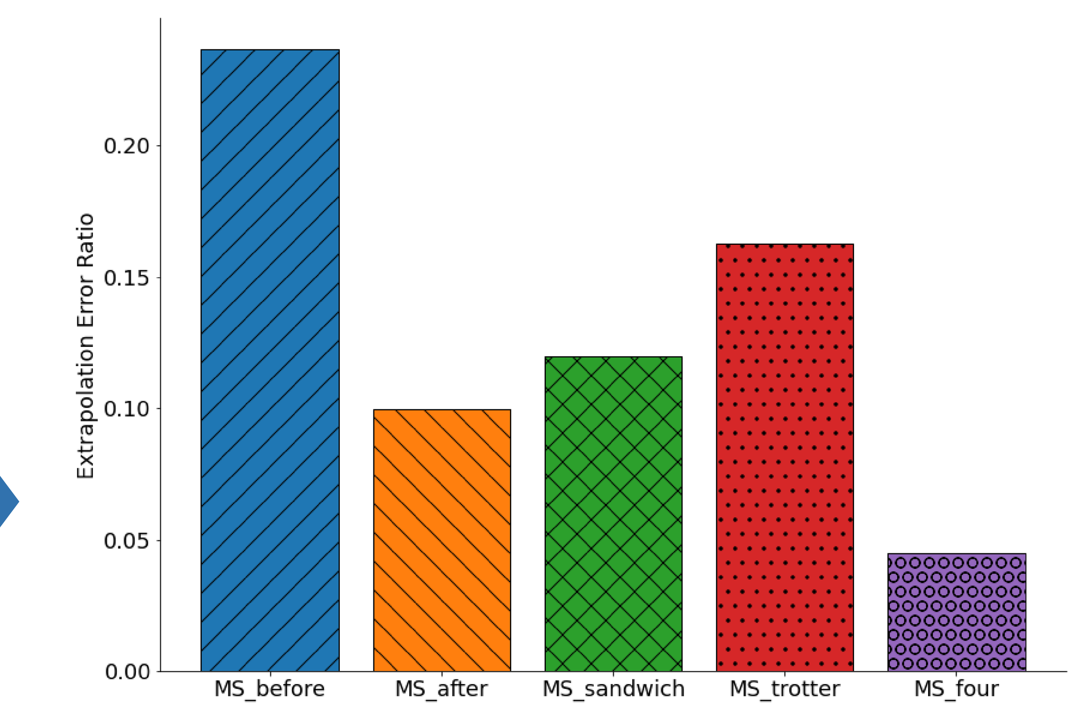


Figure 3 – Experimental results of time-stretch extrapolation. We increased the duration of only our two qubit Mølmer–Sørensen gates by $c_i = \{0.5 \ldots 1.5\}$. The time-stretched energy curves are too close together to differentiate in the presence of sampling noise.

3. Gate-Based Simulation

Another noise scaling method is to discretely insert gates **[5, 6, 7]**. This targets control errors in our circuit, rather than the minimal decoherence our qubits experience. We tested five different methods: inserting the identity $MS\,MS^{-1}$ into our circuit *before and/or after* our parameterized gate, *trotterizing* our gate $(\sqrt[n]{MS})^n$ and inserting the identity *4x* $(MS(\frac{\pi}{2}))^4$.

Figure 4 – Simulation error comparison with and without extrapolation. Four noisy energy curves were estimated for twenty parameters between $[-1.0, 1.0]$. The noisy estimates measured at the minimum parameter for the bare circuit $c_i = 1.0$ were extrapolated. All methods show improvement. We used 2000 samples per measurement.



4. Gate-Based Experiment

Extrapolation experiments on the hardware show mixed results. We tested the effects of the above noise scaling methods except for gate trotterization, varying the order n of our extrapolation. These results are uncertain with our limited sampling budget as shown in **Figure 6**.

Figure 5 – Experimental error comparison with and without extrapolation. Methods are the same as in simulation results. Extrapolated estimates were compared with order $n = 2, 3, 4$. Some methods show improvement over no extrapolation, some do not.

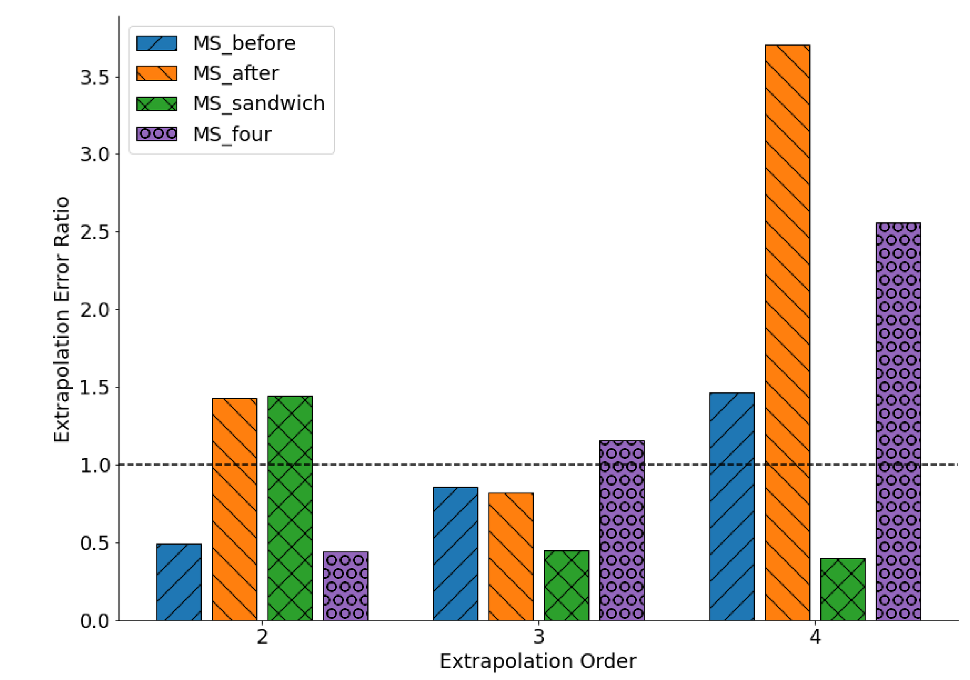
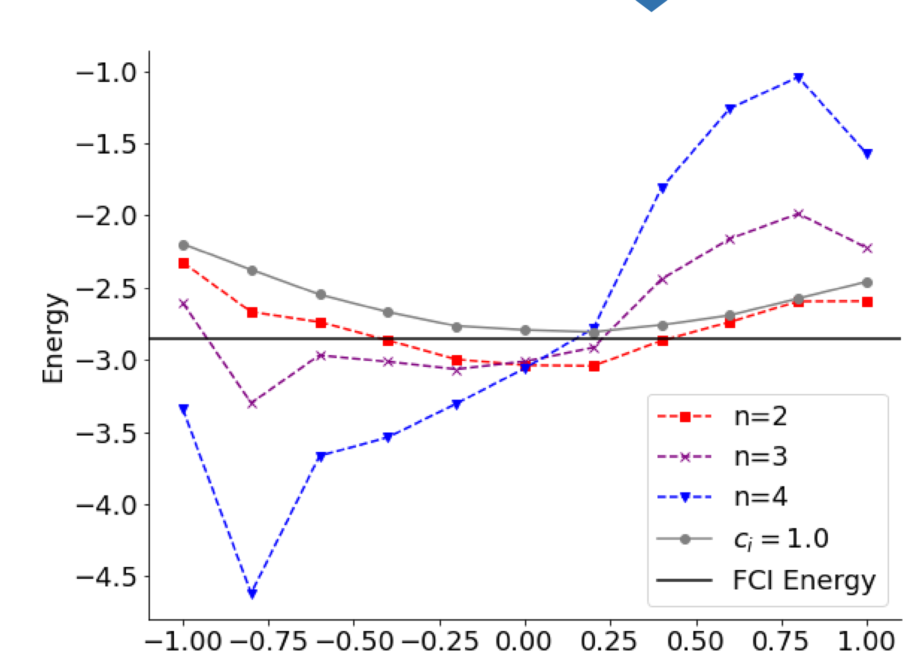


Figure 6 – Experimental results for inserting identity $MS\,MS^{-1}$ before and after our parameterized gate (MS_sandwich). The extrapolated energy curves for $n = 2, 3, 4$ estimates are wildly inaccurate for most parameter values. Errors happen to be improved for the minimum parameter of the base circuit.



5. Conclusions

Richardson Extrapolation can work for a trapped-ion device in the right circumstances. We find time-stretching gates does not increase the circuit noise enough for extrapolation, as our qubits do not experience much decoherence.

Discrete gate-based methods increase the noise better. However, they require many samples per measurement and are susceptible to coherent errors. Such errors are not conducive to extrapolation.

Further data with more samples is needed, and the addition of other error mitigation techniques such as Randomized Compiling **[8]** may improve results.

This project was funded by the U.S. Department of Energy, Office of Science, Office of Advanced Scientific Computing Research Quantum Testbed Program. *Sandia National Laboratories is a multimission laboratory managed and operated by National Technology & Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525*

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