

Error Mitigation of Hamiltonian Simulations from an Analog-based Compiler (SimuQ)

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Abstract—Quantum computing has emerged as a revolutionary paradigm with the potential to solve computationally intractable problems. However, the practical realization of quantum algorithms faces significant challenges due to noise and errors inherent in quantum systems. Hamiltonian simulations serve as a cornerstone in quantum computing, providing insights into quantum dynamics and enabling the study of quantum algorithms. This paper studies error mitigation in analog-based Hamiltonian simulations as they have native support for generating Hamiltonians as opposed to digital-based simulations, which results in shorter pulse schedules to simulate the Hamiltonians. We further aim to enhance the accuracy and reliability of these simulations through error mitigation techniques.

This research explores several error mitigation techniques tailored for analog-based Hamiltonian simulations. Among them, Zero-Noise Extrapolation (ZNE) mitigates errors by extrapolating simulation results to the ideal noise-free scenario. Building upon ZNE, Folding-Free ZNE (FFZNE) introduces novel use of the infinite error point to address the challenges posed by folding techniques. Additionally, Reliability-Based ZNE (RBZNE) leverages a mix of both techniques, utilizing the folding method and the infinite error point.

Through empirical studies and rigorous analysis, this paper evaluates the efficacy and limitations of these error mitigation techniques in analog-based Hamiltonian simulations on both noise simulator and real quantum hardware. The experimental results shed light on the comparative performance of ZNE, FFZNE, and RBZNE, understanding their strengths and weaknesses in mitigating errors across different quantum systems and noise conditions. By providing the understanding of these techniques, this research contributes to the advancement of error mitigation strategies in quantum computing, paving the way for more reliable and accurate quantum simulations.

Index Terms—Hamiltonian Simulation, Quantum Error Mitigation

I. INTRODUCTION

Quantum simulation [12], inspired by Richard Feynman’s vision, has emerged as a promising avenue in modern physics, aiming to simulate quantum systems using other quantum systems [11]. While classical computers struggle with the complexities of quantum simulation [10], [25], quantum computers offer a natural fit for this task.

One significant application lies in simulating the time evolution of quantum systems, offering insights into phenomena previously inaccessible. This capability has profound implications across various domains, including machine learning,

where Quantum Hamiltonian Descent [18] outperforms classical counterparts like Gradient Descent. Also it has applications in Quantum Walks [5], which is used in understanding network dynamics and graph-based machine learning. Moreover, quantum Hamiltonian simulations play a vital role in elucidating molecular properties [8], [15]–[17], facilitating advancements in drug discovery, materials science, and catalysis. Additionally, they offer a deeper understanding of magnetic materials at the quantum level [14], propelling the development of transformative technologies like spintronics and quantum computing. These diverse applications underscore the profound impact of Hamiltonian simulations in pushing the boundaries of scientific discovery.

The quest for quantum simulation has led researchers to explore digital quantum simulators, utilizing gates to evolve the Hamiltonian of the system. However, recent experimental insights [25] have underscored the advantages of Hamiltonian-oriented Analog Quantum simulation, particularly within the realm of Noisy Intermediate-Scale Quantum (NISQ) machines. Unlike their digital counterparts, analog quantum simulators offer a more direct pathway to emulate the intricate dynamics of quantum systems. This paradigm shift has prompted the development of SimuQ [25], an analog-based compiler designed to simulate Hamiltonian systems on quantum computers. We leverage the SimuQ compiler for simulating Ising Model Hamiltonians in this paper.

While analog simulations exhibit promise in reducing noise encountered within quantum systems when probing a Hamiltonian [25], imperfections persist when implementing these simulations on real hardware, as evidenced by experiments conducted in this research. In light of these challenges, our research endeavors to explore error mitigation techniques commonly employed in digital quantum circuits [13], [24] to ascertain their efficacy in enhancing the accuracy of simulations on analog-based devices.

Through empirical studies and rigorous analysis, this paper evaluates the efficacy and limitations of the following error mitigation techniques in analog-based Hamiltonian simulations: Zero-Noise Extrapolation (ZNE) [13], Folding-free ZNE [24], and reliability-based ZNE. Our findings include: (1) FFZNE being more effective error mitigation technique than

ZNE and RBZNE on the noise simulator with noise profiles. (2) In contrast, ZNE and RBZNE outperform FFZNE on the real backends. The achieved improvement in the fidelities of the Hamiltonian simulations on average is by 16.11% on the noise simulator and 4.80% on the real backends.

The remainder of this paper is organized as follows. Section II provides a background on the Hamiltonian of a system, Ising Hamiltonian models, Hamiltonian Simulations, and the SimuQ compiler which generates the analog circuits for our experiments. Section III discusses the implementation of the error mitigation strategies and explains how the fidelity is calculated to assess the accuracy of the simulations. Section IV discusses the findings from our experiments. Section V concludes the paper and discusses the future directions.

II. BACKGROUND

A. Ising Models

Ising Hamiltonian models [23] serve as fundamental frameworks for understanding the behavior of complex systems in various fields, including statistical mechanics [3], condensed matter physics [2], and computational biology [9], [21]. Originating from the study of magnetic materials, Ising models describe the interaction between spins (quantum or classical) arranged on a lattice. The Hamiltonian of an Ising model typically consists of terms representing the interaction between neighboring spins and an external magnetic field,

In this research paper, these are the target Hamiltonian systems which we are aiming to simulate on quantum computers. More specifically, we are utilizing Ising Chain models of site sizes from 4 to 10. The hamiltonian of an Ising chain is represented by:

$$\hat{H} = \sum_{1 \leq j < k \leq n} J_{jk} Z_j Z_k + \sum_{j=1}^n h_j X_j \quad (1)$$

where $J_{jk}, h_j \in \mathbb{R}$.

B. Hamiltonian Simulation

The evolution of a quantum system, starting from a quantum state represented by a high-dimensional complex vector $|j(0)\rangle$, obeys the Schrödinger equation [1], [4], [25]:

$$\frac{d}{dt} |j(t)\rangle = -iH(t)|j(t)\rangle \quad (2)$$

Hamiltonian simulation describes the dynamics of quantum systems by utilizing the Schrödinger equation, which governs the evolution of quantum states over time. In essence, the Hamiltonian operator encapsulates the total energy of the system and dictates how it changes with time [1]. By solving the Schrödinger equation, one can predict the time evolution of quantum states under the influence of a given Hamiltonian operator.

The output of a Hamiltonian simulation typically includes the evolution of quantum states over time, providing insights into how the system's properties change as it undergoes dynamic processes. This output can manifest as wavefunctions,

density matrices, or expectation values of observables, depending on the specific simulation method employed. For instance, in simulating chemical reactions, the output might reveal the probabilities of different reaction pathways or the final state of the system after a specified duration. In this study, we focus on the final state of a quantum system after a specified time interval as the output of the quantum simulation.

Moreover, Hamiltonian simulations can help us understand key physical phenomena such as quantum phase transitions, entanglement dynamics, and energy transfer mechanisms. By studying the time evolution of quantum systems through Hamiltonian simulation, researchers can gain deeper insights into the behavior of complex systems that are otherwise challenging to analyze using classical computational methods.

C. SimuQ Analog Compiler

SimuQ [25] is the first framework for quantum Hamiltonian simulation that supports Hamiltonian programming and pulse-level compilation [7] to heterogeneous analog quantum simulators. We need to specify the target quantum system with Hamiltonian Modeling Language (HML), and the Hamiltonian-level programmability of analog quantum simulators is specified through a new abstraction called the abstract analog instruction set (AAIS) and programmed in AAIS Specification Language by hardware providers. Through a solver-based compilation, SimuQ generates executable pulse schedules for real devices to simulate the evolution of desired quantum systems. SimuQ uses the Lie-Trotter formula, which is a first order product formula for the trotterization step [19] which also introduces approximation errors in the simulation. In this paper, we are not focusing on mitigating this approximation error, but only on the environmental error that is caused by executing the simulations on NISQ era quantum computers.

III. METHODS

A. Error Mitigation Schemes

In this paper, we explore the following error mitigation strategies:

1. Zero-Noise Extrapolation (ZNE): This method [13] introduces errors into the system through circuit folding. Specifically, we concentrate on the global folding of the gates. By incrementally varying the noise factor in the steps of 2 (i.e., $U^\dagger U$), starting from a noise factor of 1, we conduct simulations for different circuits. Subsequently, we extrapolate the results to the zero noise case.

2. Folding-free Zero-Noise Extrapolation (FFZNE): Unlike ZNE, this approach [24] does not use circuit folding. It operates on the assumption that under infinite depolarization noise conditions, the state probability distribution would be maximally mixed, with each state having an equal probability of occurrence. Utilizing this assumption, we can extrapolate to the ideal state distribution using only two points. To represent the infinite error case on graphs, the x-axis can be adjusted to denote circuit reliability, where a reliability of 0 signifies the infinite error scenario. Determining the reliability of the

circuit is essential to fix the x-axis for the graph, with the y-axis representing the state probability of occurrence.

To calculate the circuit reliability, we use Estimated Success Probability (ESP) [22] defined as follows:

$$\text{Circuit Reliability} = \prod_i (1 - E_i)^{N_i} \quad (3)$$

where,

I : Number of different types of instructions

E_i : Error rate of the instruction type i

N_i : Number of times the instruction type i was applied.

To compute the circuit reliability, we need the error rates of different types of instructions (or gates) and their counts in the circuit. Let us examine one sample circuit that SimuQ generates. In this case, we have considered the scenario where $N = 4$, $T = 1$ (N: number of qubits and T: Time duration of the simulation), and the backend system for which it is compiled is `ibmq_brisbane`.

TABLE I
INSTRUCTION TYPES AND THEIR COUNTS USED IN SIMUQ GENERATED
CIRCUIT OF $N = 4$ AND $T = 1$

Instruction Name	Counts
rz	61
sx	18
rxz	18
rx	10
measure	4

We can readily obtain the error rates of the instructions `sx` and `rz` from the backend properties. However, the instructions `rxz` and `rx` are custom instructions compiled specifically for each backend. Hence, for each backend, we must acquire the error rates of these `rxz` and `rx` gates. To obtain these error rates, we conduct the Interleaved Randomized Benchmarking (InterleavedRB) experiments.

Interleaved Randomized Benchmarking (RB) [6], [7], [20] serves as a reliable technique for estimating the average error-rate associated with a specific quantum gate. In an interleaved RB experiment, two sequences are generated: one containing random Cliffords as per the standard RB protocol, and the other incorporating the interleaved gate under examination. These sequences are executed on a quantum backend, following which the probabilities of returning to the ground state are computed. Subsequently, the experiment fits two exponentially decaying curves to the obtained data, facilitating the estimation of the error associated with the interleaved gate.

3. Reliability-based Zero-Noise Extrapolation (RBZNE): This method combines elements of both ZNE and FFZNE. It involves global folding to introduce errors into the system while also leveraging the maximally mixed state assumption used in FFZNE. Similar to FFZNE, RBZNE necessitates circuit reliability values for setting the x-axis. The process for calculating circuit reliability is the same as for FFZNE.

There is a scalability challenge to use these extrapolation techniques to refine the output states, as the state has 2^N

coefficients, where N is the number of qubits. To address this, a *top-k* approach is adopted for error mitigation of state probabilities. This involves finding top k state probabilities (or coefficients) and exclusively performing extrapolation for just these *top-k* values. This way, the post-processing overhead is constrained to a constant factor [24]. For consistency, in all the experiments, a top-k factor of 10 is maintained. In other words, we perform error mitigation for the 10 highest state coefficients.

Subsequently, the top-k extrapolated values are normalized to adhere to the additive principle of probabilities, wherein the total probability equals 1.

B. Evaluating Simulation Results

As the output of the simulations in this study is the state probabilities of the quantum system after a time interval T , we use the following two ways to evaluate the simulation accuracy or the noise impact.

Hellinger Fidelity: This metric quantifies the similarity between two probability distributions. It is calculated using the Hellinger distance, a measure of the difference between probability distributions. A higher Hellinger fidelity indicates a closer resemblance between the simulated and target probability distributions. The range of the hellinger fidelity lies from 0 to 1.

$$F_H(\mathbf{p}; \mathbf{q}) = \sqrt{\sum_i p_i q_i} \quad (4)$$

where \mathbf{p} and \mathbf{q} are probability distributions.

Total Variation Distance: This metric measures the discrepancy between two probability distributions by calculating the total difference between corresponding probabilities. A lower total variation distance suggests a more accurate simulation, with smaller deviations between the simulated and target probability distributions. Again, the range for Total Variation distance lies between 0 to 1.

$$\text{TV}(\mathbf{p}; \mathbf{q}) = \frac{1}{2} \sum_i |p_i - q_i| \quad (5)$$

where \mathbf{p} and \mathbf{q} are probability distributions.

IV. RESULTS

A. Evidence of Noise in Simulations

Fig. 1 displays a color-coded matrix of Total Variation Distance for each of the simulations, indicating the closeness of the state probability distributions between an ideal simulation (free from environmental noise and approximation errors by Trotterization) and a noise-free simulator. In this matrix, dark purple hues represent an accurate simulation as they have low TV values as seen in the legend.

For instance, in the case of $N = 4$ and $T = 0.1$, the TV value is 0.0043, indicating a highly accurate simulation. Observing the trend, simulations with higher T values tend to diverge from the ideal scenario, particularly notable in the column representing $T = 2.0$. Additionally, as the N value

increases, there's a gradual decrease in the fidelity, although not as pronounced as the variations observed with increasing the T values.

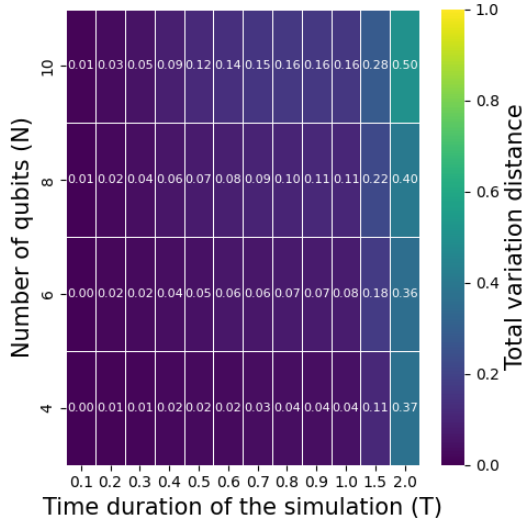


Fig. 1. TV values heatmap between ideal and noise-free case from simulators

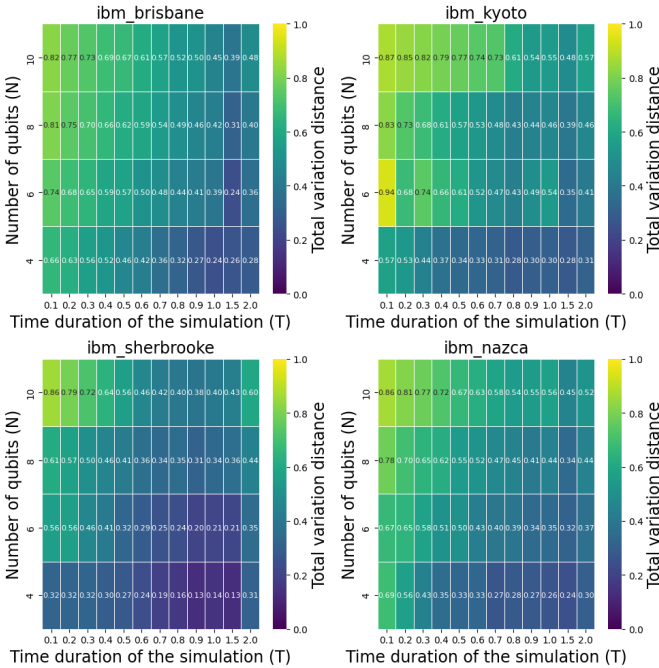


Fig. 2. TV values heatmap between ideal case and noisy case from real backend results

Fig. 2 depicts the TV value heatmaps for experiments which were conducted on four different real IBM quantum systems: *ibm_brisbane*, *ibm_kyoto*, *ibm_nazca*, and *ibm_sherbrooke*. The parameters N and T maintain the same range as in the simulator experiments. Here, we can observe discrepancies between the simulations, suggesting the significant effect of noise on conducting the simulations on the

real backends as there are very few regions with dark purple hues.

B. Experimentation on Simulator with Noise Profiles

For the below results, we have run the simulation circuits on a noise simulator loaded with noise profiles of the 4 IBM backends that were mentioned previously. The noise profiles for each system were created using the error rates of the custom gates generated by SimuQ, estimated using InterleavedRB experiments, and the error rates of the standard gates available in backend properties of each of the IBM systems considered.

1) *Trend line analysis*: Fig. 3 represents the line trend of TV values of the simulation results after performing error mitigation by ZNE, FFZNE and RBZNE methods, varying the parameters N and T on *ibm_nazca* noise simulator. Noise baseline represents the initial TV value when no error mitigation was performed. Noise free baseline represents the TV value for the noiseless simulation. All these TV values are computed w.r.t. the ideal case, which is free from noise and Trotterization approximation errors. Fig. 4 represents the percentage change of the TV values with reference to the initial noisy TV values where no error mitigation was performed. Any point above the baseline represents a positive improvement in the simulation accuracy.

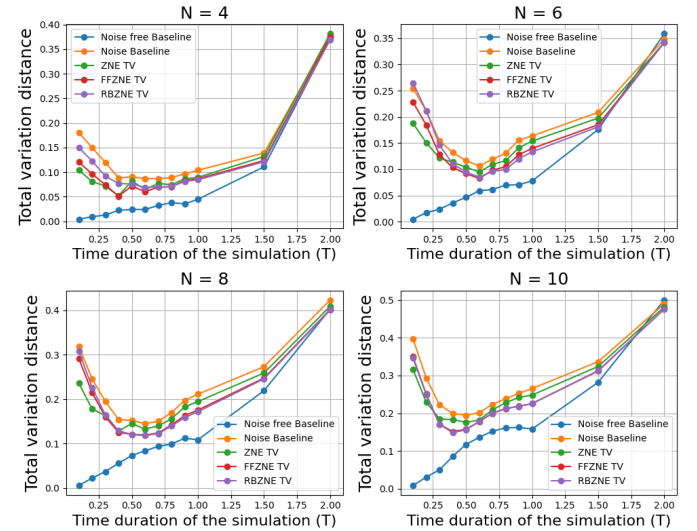


Fig. 3. Trend lines for TV values after each of the error mitigation techniques

From these figures, we can see that FFZNE performs on an average better than ZNE and RBZNE on the simulator with *ibm_nazca* noise profile. This can be attributed to the fact that FFZNE utilizes a linear extrapolation, which responds better to the simulator environment errors. ZNE performs better at the start of the simulation and the performance degrades with time evolution, whereas the RBZNE performance improves with time evolution.

2) *Aggregation analysis*: Figures 5 and 6 give a comprehensive idea about the performance of each of the methods on the simulator with noise profiles of different backends.

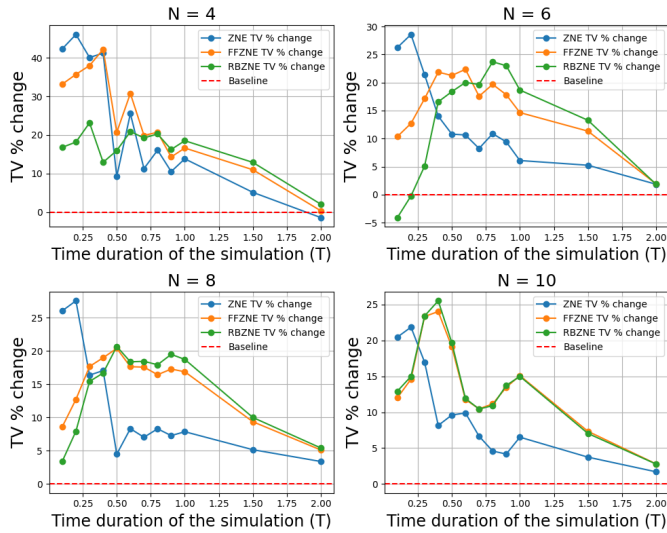


Fig. 4. Percentage change trend lines in TV values after the error mitigation techniques

These figures suggest a similar picture as suggested by the line plots in figures 3 and 4. Also, we can observe that the improvement in the fidelity of the simulation decreases with an increase in the number of qubits from figure 5. Except for *ibm_kyoto*, FFZNE outperforms ZNE and RBZNE. Also a maximum of 25.68% improvement in fidelity can be seen on *ibm_brisbane* for $N = 4$ case for the entire time evolution on an average.

Also, Fig. 6 gives the overall performance of the error mitigation techniques using the two metrics, Hellinger Fidelity and Total Variational Distance. We can observe that these techniques significantly improve the TV values than HF values. A maximum of 16.11% improvement can be observed for TV, whereas 2.23% can be observed for HF values. Also, a general trend of improvement in the fidelity is observed after performing any of the error mitigation technique. We can also observe the order of performance benefits from this figure, suggesting FFZNE having the maximum improvement on an average, followed by RBZNE and then ZNE.

C. Experimentation on Real IBM Backend Systems

For the below results, we have run the simulation circuits on the four real IBM backend systems mentioned previously.

1) *Trend analysis*: Figures 7 and 8 provide similar trends discussed in figures 3 and 4, with only difference being the experiments being conducted on real *ibm_nazca* hardware.

Upon examination of the graphs, it is evident that ZNE and RBZNE exhibit significant improvements compared to FFZNE. This disparity can be attributed to the use of a quadratic fit for extrapolating results in ZNE and RBZNE, whereas FFZNE employs a linear fit. This distinction is reflected in the volatility of the changing trend, with ZNE and RBZNE displaying greater fluctuations compared to the smoother progression observed with FFZNE. Another thing that we can observe is that there are more cases where there

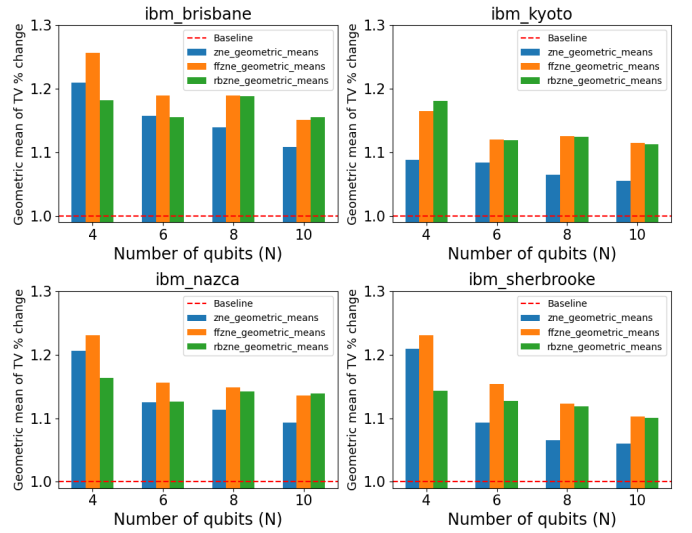


Fig. 5. Aggregated results of TV percentage change for different systems and N values using Geometric means

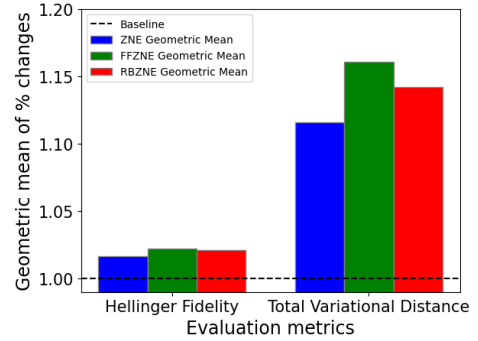


Fig. 6. Aggregated results of TV and HF percentage change using Geometric means

is a decrease in the fidelity after error mitigation, than for the simulator case which was discussed previously.

2) *Aggregation analysis*: Figures 9 and 10 represent similar information portrayed in Figures 5 and 6, with only difference being the experiments being conducted on real IBM backends.

Fig. 5 also suggests a similar trend where there is more improvement for lower values of N on an average, except for the case of *ibm_brisbane*. Fig. 9 gives a better view to analyze the performance on different systems with varying N, where only for *ibm_brisbane* we observe a decrease in the fidelities by any of the methods on an average. Fig. 10 gives an idea of the performance of each of the error mitigation techniques to improve the HF and TV values. We can observe that a difference from the simulator results that HF values are also improved on par with TV values on average.

V. CONCLUSIONS

In this paper, our exploration of error mitigation techniques for analog-based Hamiltonian simulations on quantum computers yields valuable insights. Through empirical analysis,

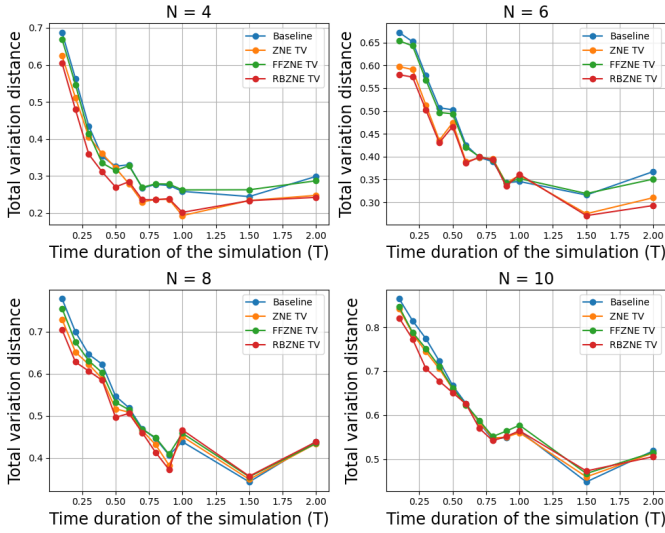


Fig. 7. Trend lines for TV values after the error mitigation techniques on the real `ibm_nazca` backend

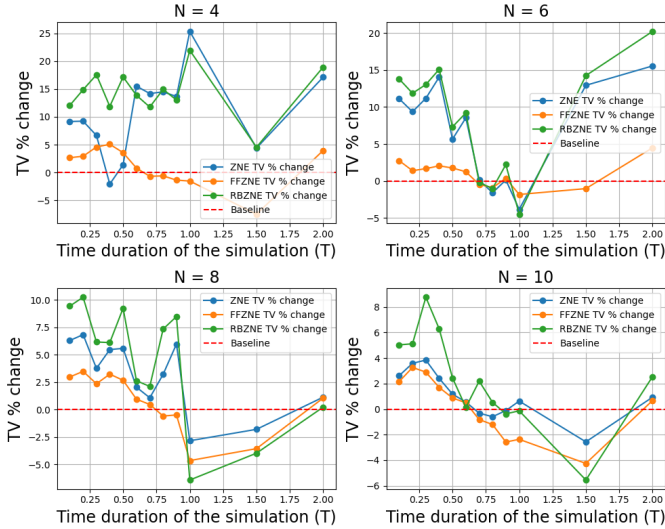


Fig. 8. Percentage change trend lines in TV values after the error mitigation techniques on the real `ibm_nazca` backend

we evaluated the effectiveness of three techniques: Zero-Noise Extrapolation (ZNE), Folding-Free ZNE (FFZNE), and Reliability-based ZNE (RBZNE). Our findings reveal that all three methods contribute to improving simulation accuracy by mitigating noise-induced errors in analog quantum systems. The choice of extrapolation technique, particularly quadratic fit utilized by ZNE and RBZNE, plays a pivotal role in their performance on the real hardware simulations, overshadowing the limited effectiveness of FFZNE’s linear fit, while the opposite was observed for noise simulator performance. Furthermore, experiments utilizing InterleavedRB provided critical insights into error rates of custom instructions and the validation of mitigation strategies by helping to create noise profiles to be used with simulators.

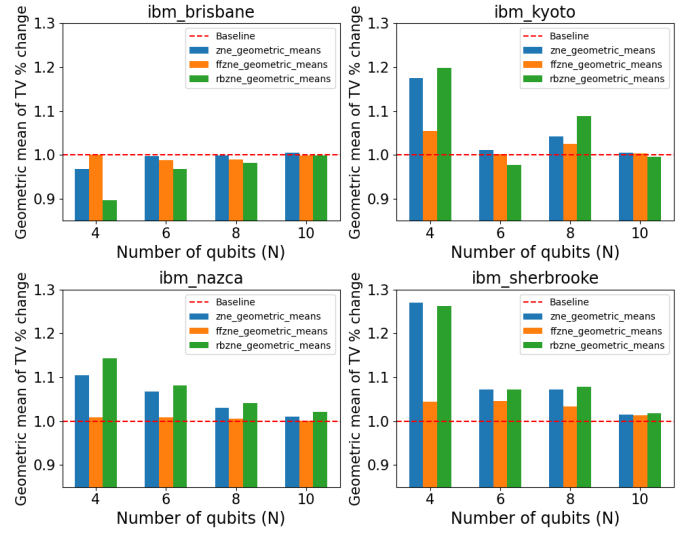


Fig. 9. Aggregated results of TV percentage change for different systems and N values using Geometric means on the real IBM backends

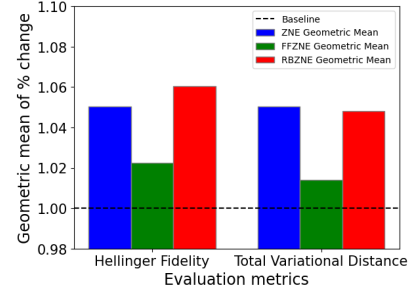


Fig. 10. Aggregated results of TV and HF percentage change using Geometric means on the real IBM backends

Looking forward, there are promising avenues for future research to expand upon these findings. Firstly, exploring error mitigation strategies across different Hamiltonian systems beyond the Ising model could offer insights into their adaptability and performance in diverse quantum computing applications, such as the Heisenberg model or Hubbard model. Secondly, extending the analysis to alternative backend systems beyond IBM, such as QuERA and IonQ, could help understand platform-specific nuances and inform optimization strategies tailored to specific hardware configurations. By pursuing these directions, we can further advance error mitigation in quantum computing, fostering the development of more robust and reliable simulations across a spectrum of applications and platforms.

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