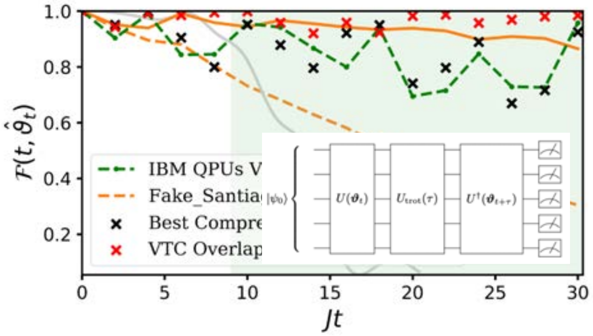
IOWA STATE UNIVERSITY
Department of Physics and Astronomy

Quantum algorithms for many-body dynamics simulations on noisy intermediate-scale quantum computers

Peter P. Orth (Iowa State University & Ames Laboratory)

Quantum Focus Semester Workshop, Saarland University, Dec 6, 2022



References:

- B. McDonough *et al.*, arXiv:2210.08611 (2022).
- I.-C. Chen *et al.*, Phys. Rev. Res. 4, 043027 (2022)
- N. F. Berthusen *et al.*, Phys. Rev. Res. 4, 023097 (2022)
- Y.-X. Yao *et al.*, Phys. Rev. X Quantum 2, 030307 (2021)

SQMS SUPERCONDUCTING QUANTUM MATERIALS & SYSTEMS CENTER

Collaborators

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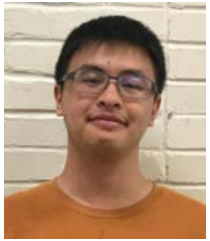
B. McDonough



I.-C. Chen

T. Iadecola

Y.-X. Yao

Quantum dynamics simulations

$$|\Psi(t)\rangle = \sum_n c_n e^{-iE_n t}|n\rangle$$

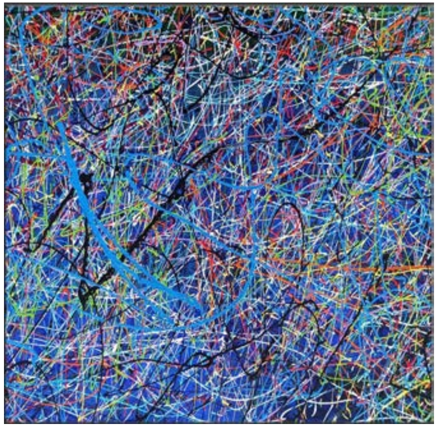
Initial state

Energy eigenstate of many-body H

$$|\Psi(0)\rangle = \sum_n c_n |n\rangle$$

Dynamics

$$|\Psi(t)\rangle = \sum_n c_n e^{-iE_n t}|n\rangle$$

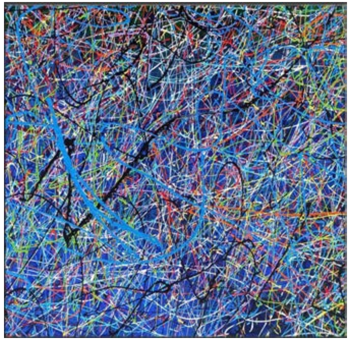


Dynamics of an observable O

$$\langle \mathcal{O}(t)\rangle = \sum_{n,m} c_n c_m^* e^{i(E_m - E_n)t}\langle m|\mathcal{O}|n\rangle$$

- Quantum dynamics simulations appear in many areas of physics and chemistry
- Classically hard due to rapid growth of entanglement in nonequilibrium for generic H
  - Reason: contains highly excited states ➢ Volume-law entanglement entropy.
  - Need many parameters to classically represent the quantum state
- Quantum simulators and computers can naturally time-evolve a quantum state

Entanglement growth makes classical simulations hard

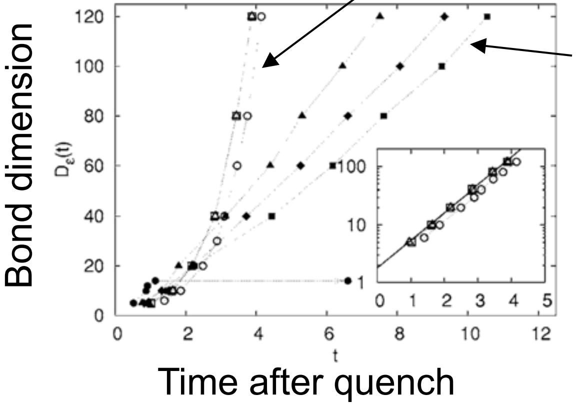


> Time-evolved state $|\Psi(t)\rangle = \sum_n c_n e^{-iE_n t}|n\rangle$ is strongly entangled

> Contains highly excited states of H ➢ Volume-law entanglement entropy

Minimal dimension of matrix product operators (MPO) grows exponentially in time for nonintegrable models (mixed-field Ising model)

Prosen, Znidaric (2007)

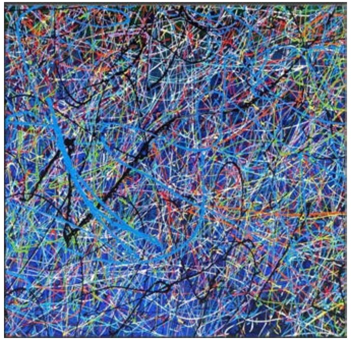


Growth is polynomially for integrable models (transverse-field Ising model)

$$H(h^x,h^z) = \sum_{j=0}^{n-2} \sigma^x_j \sigma^x_{j+1} + \sum_{j=0}^{n-1} (h^x \sigma^x_j + h^z \sigma^z_j)$$

FIG. 3. $D_\epsilon(t)$ for local initial operators. We consider three cases $O(0)=\sigma^{x,y,z}_{n/2}$ (empty circles, squares, and triangles), for nonintegrable evolution H_C, and four cases, $O(0)=\sigma^{x,y}_{n/2}$ (full squares, diamonds), $\sigma^z_{n/2-1}\sigma^y_{n/2}$ (full triangles) with infinite index, and $O(0)=\sigma^z_{n/2-1}\sigma^z_{n/2}$ (full circles) with index 2, for integrable evolution H_R.

Entanglement growth makes classical simulations hard



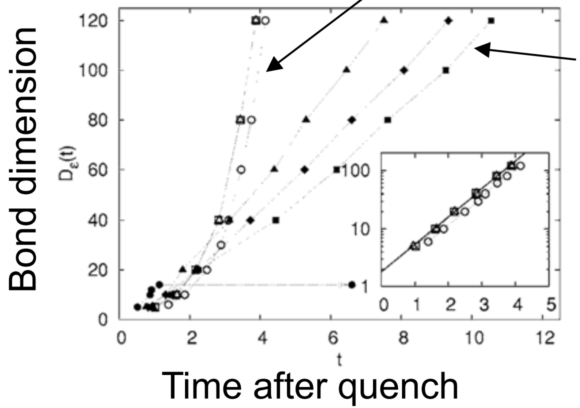
- Time-evolved state $|\Psi(t)\rangle = \sum_n c_n e^{-iE_n t}|n\rangle$ is strongly entangled
- Contains highly excited states of H ➢ Volume-law entanglement entropy

Entanglement entropy $S_A = -\mathrm{Tr}[\rho_A \ln \rho_A]$

Reduced density matrix $\rho_A = \mathrm{Tr}_B \rho$

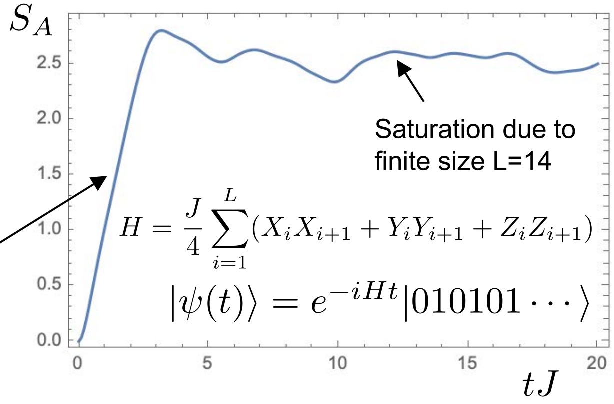
Minimal dimension of matrix product operators (MPO) grows exponentially in time for nonintegrable models

Prosen, Znidaric (2007)



Growth is polynomially for integrable models

Quench dynamics in Heisenberg model

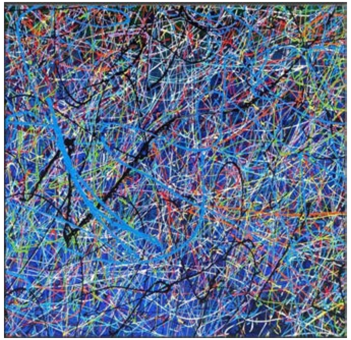


$$H = \frac{J}{4}\sum_{i=1}^{L}(X_i X_{i+1} + Y_i Y_{i+1} + Z_i Z_{i+1})$$

$$|\psi(t)\rangle = e^{-iHt}|010101\cdots\rangle$$

Entanglement entropy grows ballistically $\propto t$ after global quench

Entanglement growth makes classical simulations hard

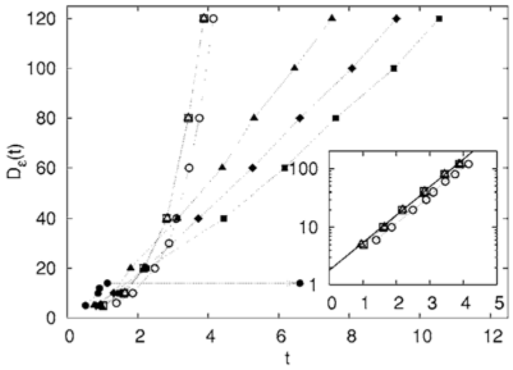


- Time-evolved state $|\Psi(t)\rangle = \sum_n c_n e^{-iE_n t}|n\rangle$ is strongly entangled
- Contains highly excited states of H ➢ Volume-law entanglement entropy

Entanglement = complexity of classical calculation

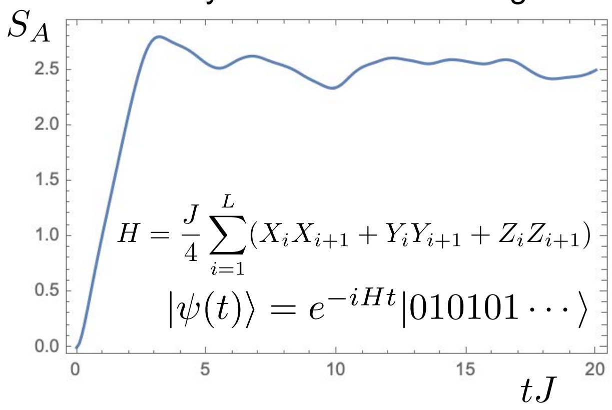
Exponential growth of classical resources like the bond dimension in tensor networks.
Exact diagonalization is limited by memory.

Opportunity for quantum computing



Prosen, Znidaric (2007)

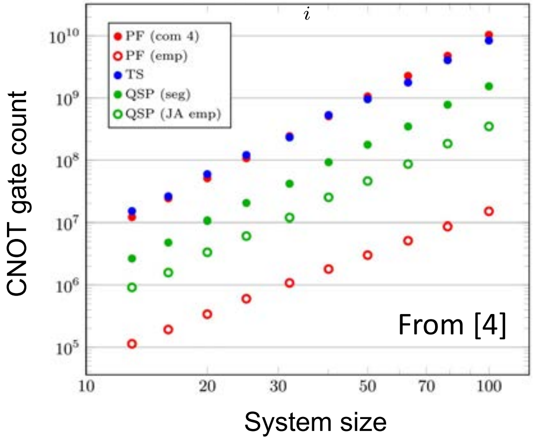
Quench dynamics in Heisenberg model



Overview of quantum algorithms for dynamics simulations

$$H = J\sum_i (Z_i Z_{i+1} + h_i Z_i)$$

- Lie-Suzuki-Trotter Product formulas (PF)
  - Simple yet limited to early times for current hardware noise
  - Trotter circuit depth scales as $\mathcal{O}(t^{1+1/k})$ ➢ fixed t_{max}
- Algorithms with best asymptotic scaling have significant overhead
  - Linear combination of unitaries (TS) [1], quantum walk methods [2], quantum signal processing (QSP) [3]
- Hybrid quantum-classical variational methods [5, 6]
  - Work with fixed gate depth ☞ ideally tailored for NISQ hardware
  - Trading gate depth for doing many QPU measurements



Variational Dynamics Simulations

$$|\Psi[\boldsymbol{\theta}]\rangle = \prod_{\mu=0}^{N_{\boldsymbol{\theta}}-1} e^{-i\theta_\mu \hat{A}_\mu} |\Psi_0\rangle$$

⇕ E.g. MacLachlan principle [5, 6]

$$\sum_\nu M_{\mu\nu}\dot{\theta}_\nu = V_\mu.$$

[1] Berry et al. (2015); [2] Childs (2004); [3] Low, Chuang (2017); [4] Childs et al., PNAS (2018);
[5] Li, Benjamin, Endo, Yuan (2019); Y. Yao, PPO, T. Iadecola *et al.* (2021).

Simulation methods presented in this talk

- First-order Trotter product formula
  - Benchmark of postquench dynamics in 1D spin model
  - Testing different error mitigation methods
- Variational Trotter Compression algorithm
  - Combines Trotter with variational compression step to simulate to long times
  - Simulation beyond coherence device time, but scaling requires difficult classical optimization
- Variational quantum dynamics of 1D spin models based on MacLachlan principle
  - Classical propagation of variational parameters using EOM that is determined on QC

Demonstration on IBM hardware

Chen, Burdick, Yao, PPO, Iadcola, PRR (2022); McDonough, ..., PPO, arXiv (2022); Berthusen, Trevisan, Iadecola, PPO, PRR 2022; Yao, ..., PPO, PRXQ (2021).

Trotter dynamics simulations of postquench dynamics in mixed-field Ising model

I-Chi Chen, Benjamin Burdick, Yongxin Yao, PPO, Thomas Iadecola
Error-Mitigated Simulation of Quantum Many-Body Scars on Quantum Computers with Pulse-Level Control
Phys. Rev. Res. **4**, 043027 (2022).

Trotter product formula approach

- Decompose Hamiltonian into sum of terms that include commuting operators
- Example for mixed-field quantum Ising model

$$H = H_{ZZ} + H_Z + H_X = V\sum_{i=1}^{L-1} Z_i Z_{i+1} - 2V\sum_{i=2}^{L-1} Z_i - V(Z_1 + Z_L) + \Omega\sum_{i=1}^{L} X_i.$$

Time evolution operator in 1st order Trotter approximation

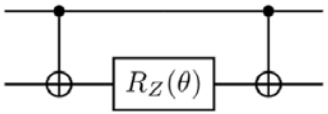
$$U(\Delta t) \approx e^{-iH_{ZZ}\Delta t} e^{-iH_Z\Delta t} e^{-iH_X\Delta t}.$$

$$R_X(\theta_i^X) = e^{-i\theta_i^X X_i/2}$$

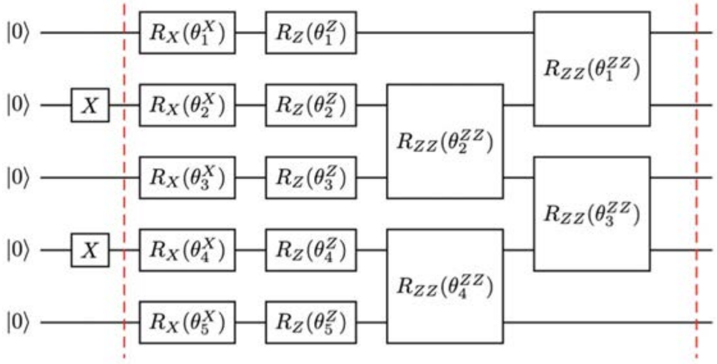
$$R_Z(\theta_i^Z) = e^{-i\theta_i^Z Z_i/2}$$

$$R_{ZZ}(\theta_i^{ZZ}) = e^{-i\theta_i^{ZZ} Z_i Z_{i+1}/2}$$

Standard decomposition of RZZ into CNOT and RZ



One step of Trotter circuit in L=5 system, starting in Neel state.



NISQ Trotter simulations of mixed field Ising model

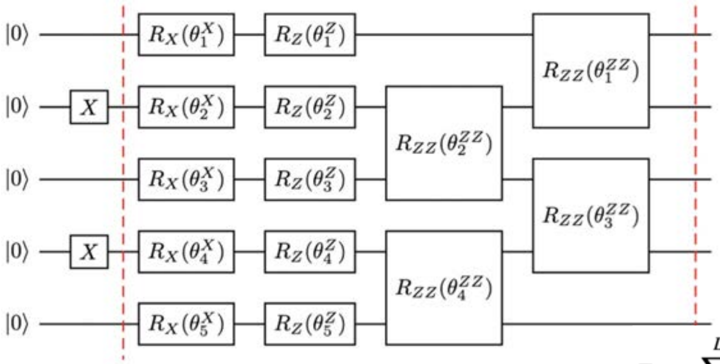
- Benchmark Trotter simulations of mixed-field Ising model on current NISQ hardware

$$H = H_{ZZ} + H_Z + H_X = V\sum_{i=1}^{L-1} Z_i Z_{i+1} - 2V\sum_{i=2}^{L-1} Z_i - V(Z_1 + Z_L) + \Omega \sum_{i=1}^{L} X_i.$$

Displays many-body coherent dynamics for $V \gg \Omega$

Bernien, Lukin (2017)

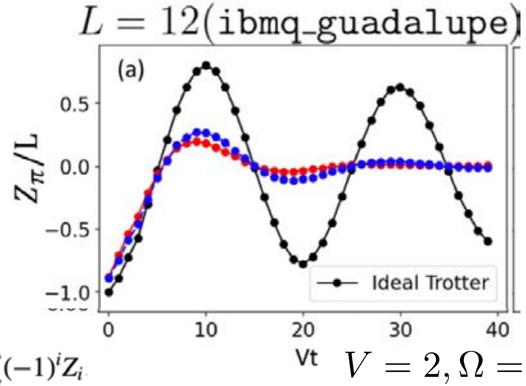
- Naïve Trotter simulation limited to short times due to finite coherence time on device



One step of Trotter circuit in L=5 system, starting from Neel state.

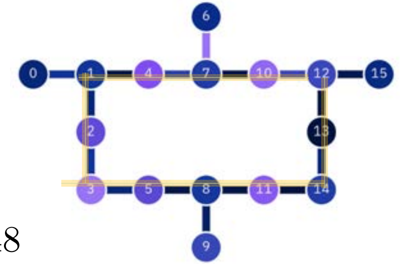
Chen et al, PRR (2022)

$$Z_\pi = \sum_{i=1}^{L} (-1)^i Z_i$$



$V = 2, \Omega = 0.48$

Trotter simulation on QPU ibmq_guadelupe
12 qubits, periodic boundary conditions

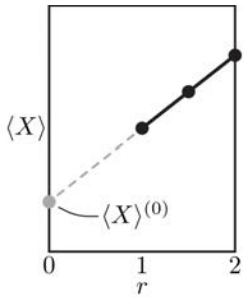


Use pulse level control and error mitigation to extend simulation time

Pulse level control and quantum error mitigation

- Pulse level control allows to make optimal use of finite coherence time on device
  - Direct implementation of R_{zz} gate via cross-resonance pulse ➢ cuts program in half
- Quantum error mitigation further extends final time of simulation
  - Readout error mitigation (tensor product assumption): $C_{\text{ideal}} = M^{-1} C_{\text{noisy}}$. $M = \begin{bmatrix} 1-\epsilon_1 & \eta_1 \\ \epsilon_1 & 1-\eta_1 \end{bmatrix} \otimes \cdots$
  - Zero-noise extrapolation (ZNE) after increasing noise via gate folding $G \mapsto GG^{\intercal}G$.
  - Pauli twirling: transforming noise to Pauli error channel
  - Dynamical decoupling: apply $X(\pi)$ and $X(-\pi)$ during qubit idle time
  - Symmetry-based postselection: physically motivated

ZNE



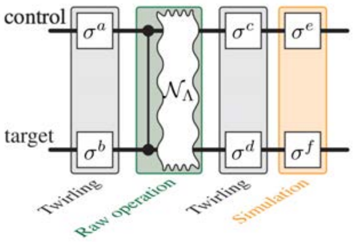
Kraus form of generic error channel $\mathcal{N}_\Lambda \rho = \sum_h E_h \rho E_h^\dagger$

$E_h = \sum_{a=0}^{3} \sum_{b=0}^{3} \alpha_{h;a,b} \sigma_c^a \sigma_t^b$

Pauli twirling

$\bar{\mathcal{N}}_\Lambda = F_\Lambda[\mathbb{1}] + \sum_{(a,b)\neq(0,0)} \epsilon_{a,b}[\sigma_c^a \sigma_t^b]$,

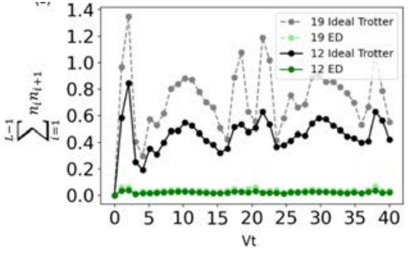
Error twirling



Pauli twirling converts noise to stochastic form ➢ justification for ZNE

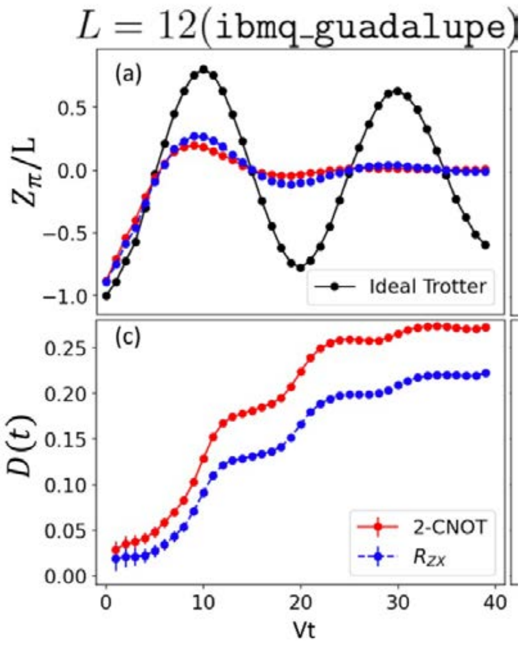
Wallmann; Li, Benjamin (2017)

Postselection into physically relevant part of Hilbert space



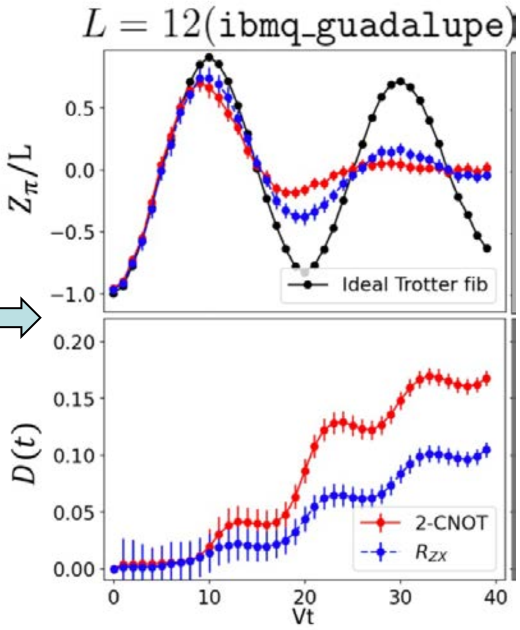
Quantum error mitigation toolbox mitiq

Extending simulation time using pulse control and error mitigation

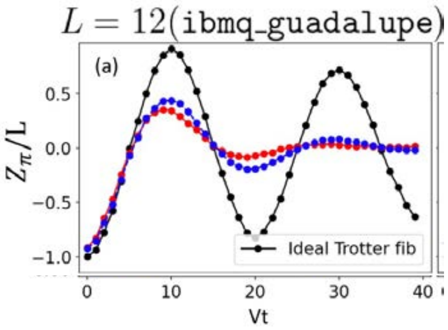


Pulse control

QEM



Postselection only



Pulse and zero-noise extrapolation (ZNE) are effective strategies to reduce errors.
But: ZNE is heuristic and cannot extend simulation time beyond coherence time of device.

Automated quantum error mitigation based on probabilistic error reduction

Benjamin McDonough, Andrea Mari, Nathan Shammah, Nathaniel T. Stemen, Misty Wahl, William J. Zeng, PPO
Automated quantum error mitigation based on probabilistic error reduction
arXiv:2210.08611 (2022)
Presented at SC22 and accepted at IEEE Proceedings

https://github.com/benmcdonough20/AutomatedPERTools

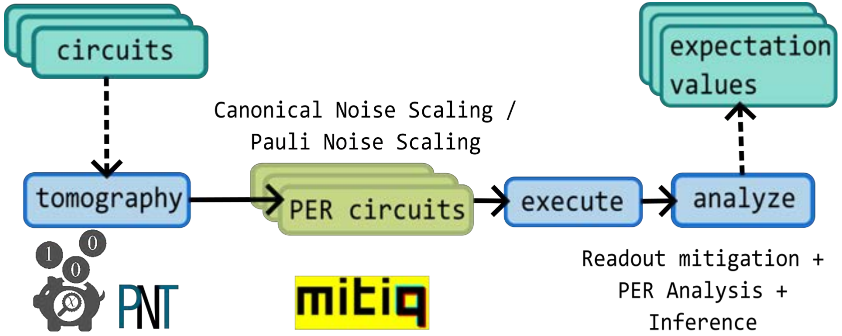
Automated quantum error mitigation

- Need for automated and noise aware quantum error mitigation methods
- Probabilistic error cancellation (PEC) is a systematic ways to remove quantum errors in observables
- Probabilistic error reduction (PER) combined with virtual ZNE
  - Noise can be scaled predictably above or below hardware level
  - Zero-noise limit does not need to be evaluated directly

Software framework for automated QEM

Input: *list of circuits and observables*

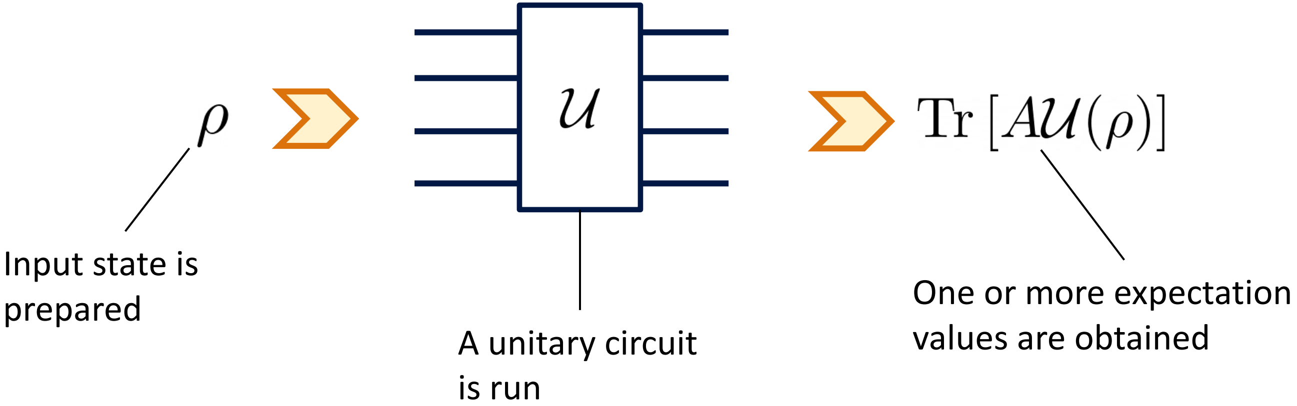
Output: *error-mitigated expectation values*



Probabilistic Error Cancellation

Applicable to algorithms in which the figure of merit is an expectation value averaged over many shots of a unitary circuit

ideal circuit:

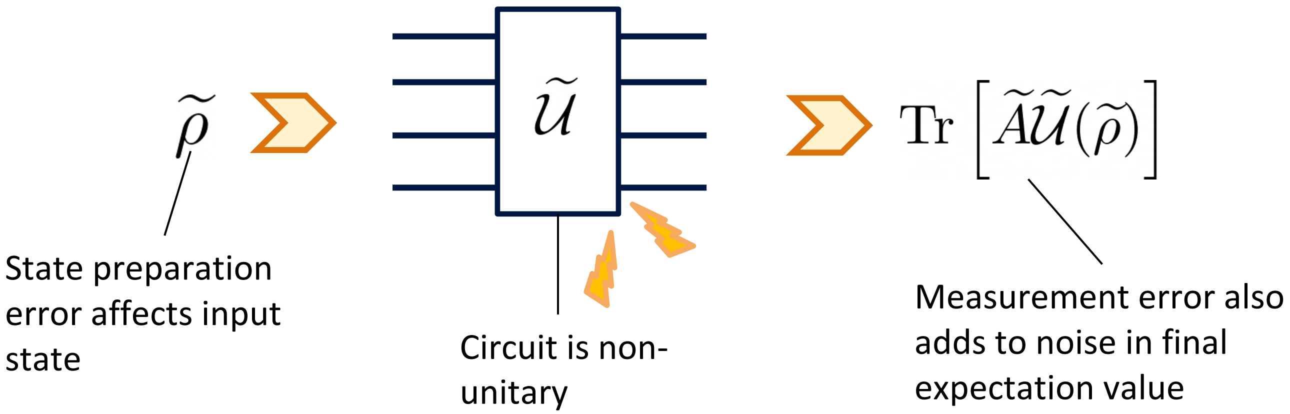


[1] Temme, Kristan, Sergey Bravyi, and Jay M. Gambetta. "[2] Endo, Suguru, Simon C. Benjamin, and Ying Li. "Practical quantum error mitigation for near-future applications." *Physical Review X* 8, no. 3 (2018): 031027.
Error mitigation for short-depth quantum circuits." Physical review letters 119, no. 18 (2017): 180509.
[3] Cai, Zhenyu, Ryan Babbush, Simon C. Benjamin, Suguru Endo, William J. Huggins, Ying Li, Jarrod R. McClean, and Thomas E. O'Brien. "Quantum error mitigation." arXiv preprint arXiv:2210.00921 (2022).

Probabilistic Error Cancellation

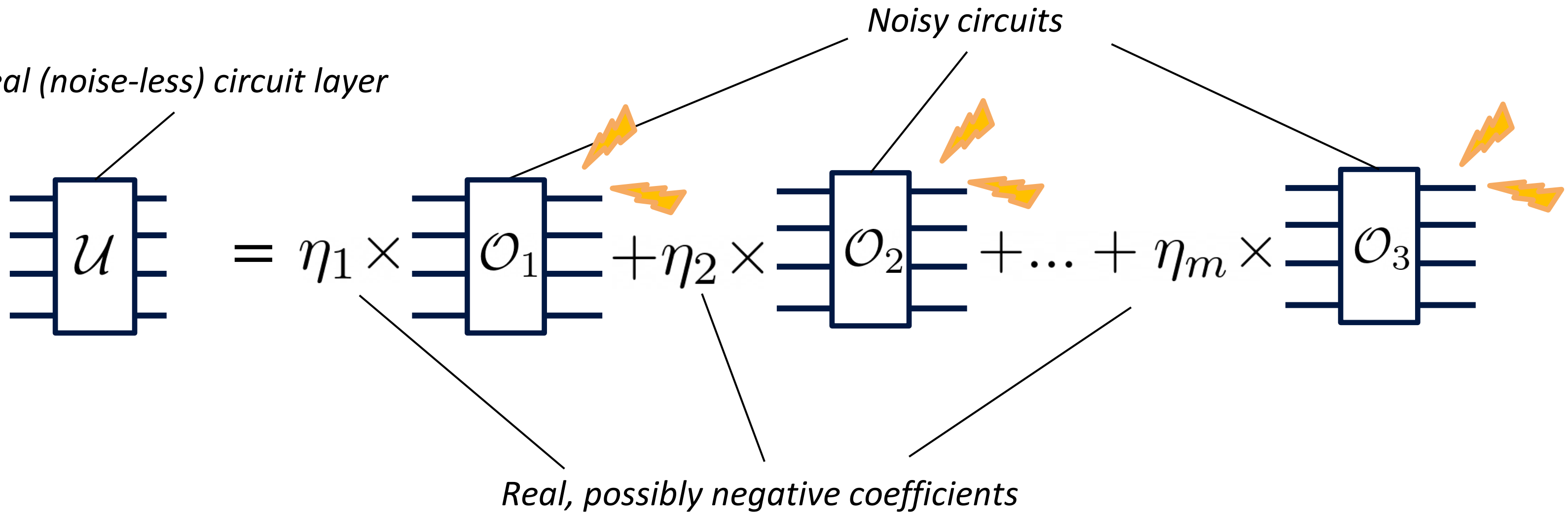
Noise introduces bias into the estimator of this expectation value.

noisy circuit:



Probabilistic Error Cancellation

After characterizing the noisy operations $\{\mathcal{O}_\alpha\}$, the ideal circuit is decomposed into $\mathcal{U}(\rho) = \sum_\alpha \eta_\alpha \mathcal{O}_\alpha(\rho)$ where the η_α are real.



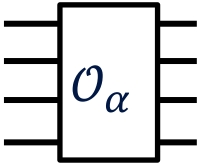
The linearity of the expectation value allows the ideal value to be written as $\langle A \rangle_{ideal} = \sum_\alpha \eta_\alpha \langle A \rangle_\alpha$

Probabilistic Error Cancellation

Number of terms grows exponentially with circuit depth…

The linear combination can be converted into a quasi-probability distribution (QPD) and sampled.

Sample



with probability $\frac{|\eta_\alpha|}{\gamma}$

Scale expectation value by $\gamma \, \mathrm{sgn}(\eta_\alpha)$, where $\gamma = \sum_\alpha |\eta_\alpha|$

The sign problem:

- Since η can be negative, $\gamma > 1$. The magnitude of γ is generally determined by the noise strength
- γ determines the variance of the estimator, related to the strength of noise on the hardware
- If γ_i is the overhead of a single layer, then the total overhead is $\gamma = \prod_i \gamma_i \sim \gamma_i^n$

PEC with Mitiq

$$\widetilde{RX}\left(\frac{\pi}{2}\right) =$$

```
[[ 0.504+0.j   , -0.015-0.488j, -0.015+0.488j,  0.493+0.j   ],
 [-0.014-0.489j,  0.502-0.03j ,  0.489+0.003j,  0.021+0.487j],
 [-0.014+0.489j,  0.489-0.003j,  0.502+0.03j ,  0.021-0.487j],
 [ 0.496+0.j   ,  0.015+0.488j,  0.015-0.488j,  0.507+0.j   ]]
```

Mitiq: *an open-source toolkit for implementing error mitigation techniques [1].*

Constrained optimization algorithm for finding QPD representation with least overhead:

```
mitiq.pec.representations.optimal.find_optimal_representation
```

- Set of superoperators with maximum span is constructed using sequences of noisy gates.

$$\tilde{G}_1, \tilde{G}_2 \rightarrow \tilde{G}_1\tilde{G}_1\tilde{G}_1, \tilde{G}_1\tilde{G}_1\tilde{G}_2, \dots, \tilde{G}_2\tilde{G}_2\tilde{G}_1, \tilde{G}_2\tilde{G}_2\tilde{G}_2$$

Set of noisy operations (e.g. obtained using gate set tomography on QPU) → mitiq → QPD representation of the ideal gate

$$\rightarrow \quad RX_{PEC}\left(\frac{\pi}{2}\right) = \begin{bmatrix} 0.4999900 + 0.0000000j & 0.0000099 + -0.4999900j & 0.0000099 + 0.4999900j & 0.4999900 + 0.0000000j \\ 0.0000100 + -0.5000059j & 0.4999900 + -0.0000092j & 0.4999900 + 0.0000090j & 0.0000100 + 0.4999941j \\ 0.0000100 + 0.5000059j & 0.4999900 + -0.0000090j & 0.4999900 + 0.0000092j & 0.0000100 + -0.4999941j \\ 0.5000100 + -0.0000000j & -0.0000099 + 0.4999900j & -0.0000099 + -0.4999900j & 0.5000100 + -0.0000000j \end{bmatrix}$$

[1] LaRose, R., A. Mari, N. Shammah, P. Karalekas, and W. Zeng. "Mitiq: A software package for error mitigation on near-term quantum computers." (2020).

Canonical Noise Scaling

PER Representation:

$$\mathcal{U}(\rho) = \sum_\alpha \eta_\alpha \mathcal{O}_\alpha(\rho) = \gamma^+\Phi^+(\rho) - \gamma^-\Phi^-(\rho)\,,$$

- Positive volume, overhead: $\Phi^+ = \sum_{\eta_\alpha>0} \frac{|\eta_\alpha|}{\gamma^+}\mathcal{O}_\alpha(\rho)$
- Negative volume, overhead: $\Phi^- = \sum_{\eta_\alpha<0} \frac{|\eta_\alpha|}{\gamma^-}\mathcal{O}_\alpha(\rho)$

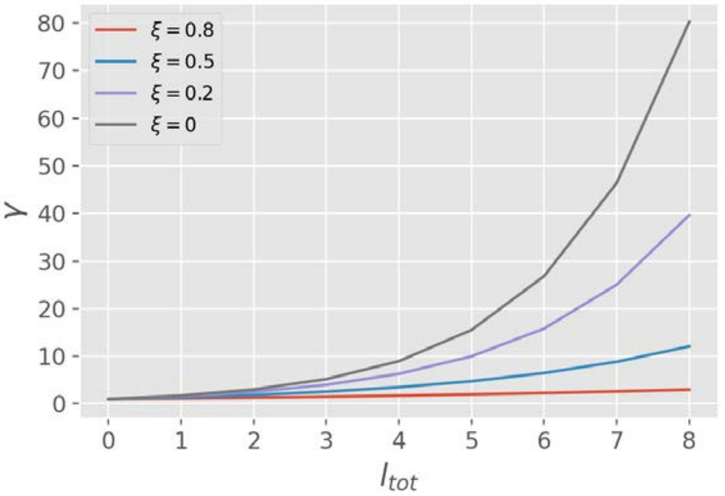
Canonical noise scaling [1]:

$$\mathcal{U}^{(\xi)}(\rho) = (\gamma^+ - \xi\gamma^-)\Phi^+(\rho) - (1-\xi)\gamma^-\Phi^-(\rho)$$

Controlling ξ interpolates between

- $\mathcal{U}^{(0)}(\rho) = \mathcal{U}(\rho)$
- $\mathcal{U}^{(1)}(\rho) = \tilde{\mathcal{U}}(\rho)$

Overhead is reduced to $\gamma^{(\xi)} = \gamma - \xi(\gamma - 1)$ for $\xi \in [0,1]$



The overhead interpolates between the hardware noise value $\gamma^{(1)} = 1$ and the noiseless value $\gamma^{(0)} = \gamma$.

Number of circuits for fixed precision $\propto \gamma^2$

- At $\xi = 0, \gamma = 1.73$. At depth $8, \gamma \approx 80$
- At $\xi = 0.5, \gamma = 1.37$. At depth $8, \gamma \approx 12$
- By combining estimates at $\xi = .5$, $\xi = 1$, and $\xi = 2$, the total number of circuits $\approx 14/\delta^2$

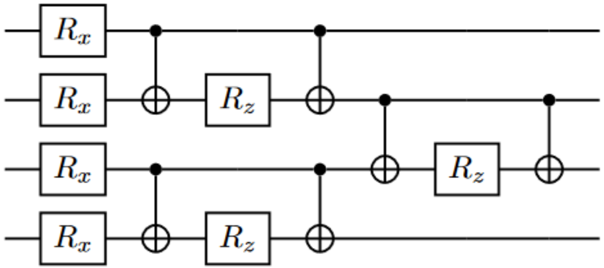
[1] Mari, Andrea, Nathan Shammah, and William J. Zeng. "Extending quantum probabilistic error cancellation by noise scaling." *Physical Review A* 104, no. 5 (2021): 052607.

Example Circuit

1D Transverse-Field Ising Model

$$H = -J\sum_i Z_i Z_{i+1} + h\sum_i X_i$$

Trotter step



$$R_x = RX(2h\delta t)$$

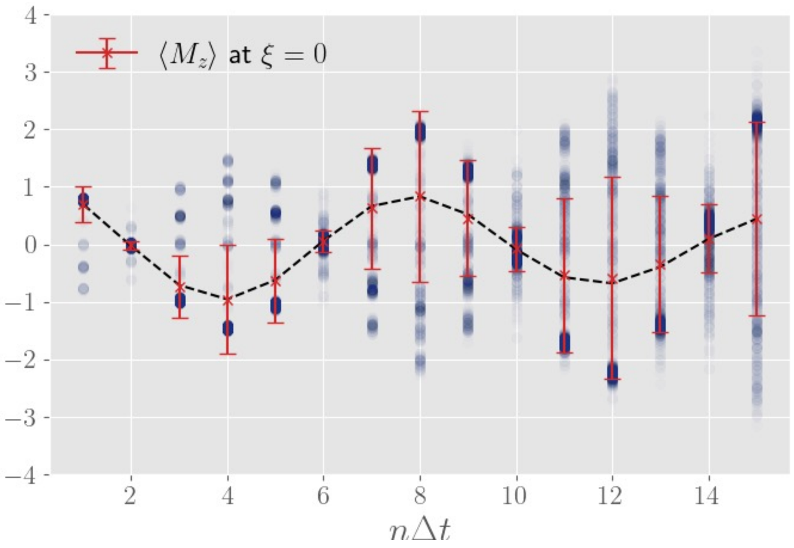
$$R_z = RZ(-2J\delta t)$$

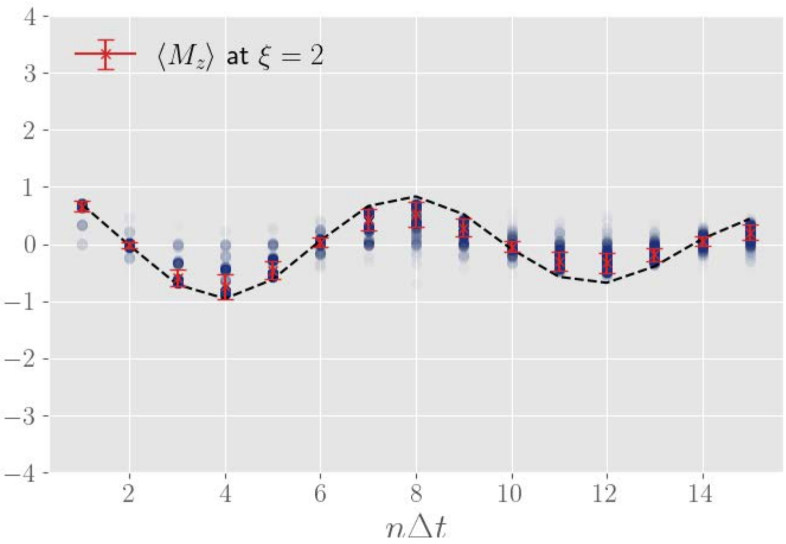
Quantity to measure

Global Z-Magnetization:

$$M_z = \frac{1}{N}\sum_i \langle Z_i \rangle$$

Visualization of PER





The tradeoff between bias and variance controlled by ξ

- Each blue dot represents 1024 shots of a single PER circuit
- Scaling down the noise incurs a higher variance
- This overhead is a symptom of the negativity of the distribution

Parameters

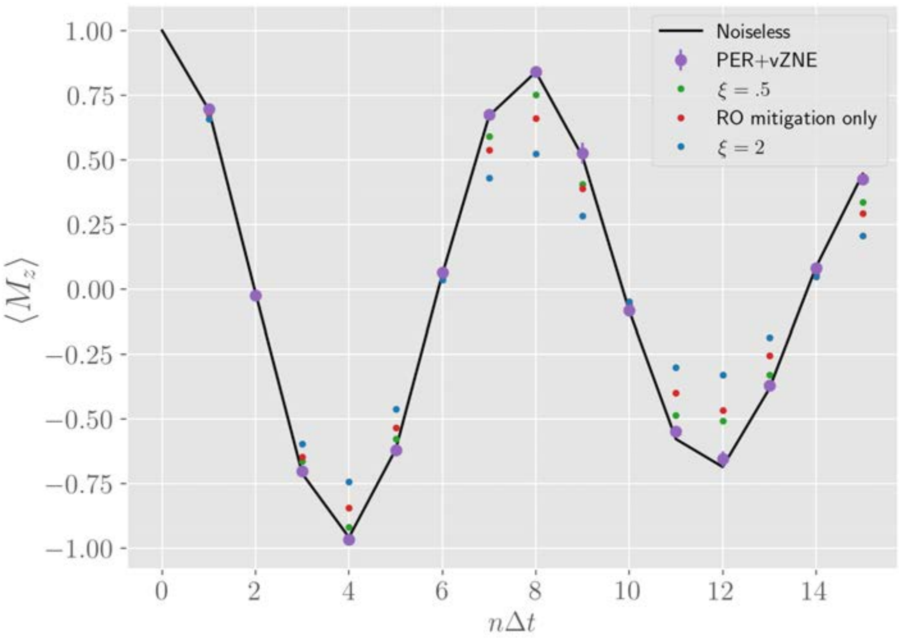
- 1000 PER samples
- 1024 shots per circuit
- Simulator: *FakeVigo*

Results

Simulation of PER carried out on Z-magnetization of TFIM on four qubits

- Red, blue, and green dots show how the estimator converges with ξ
- The purple dots show extrapolation using $\xi = 0.5, 1$, and 2
- Extrapolation shows good agreement with noiseless simulation

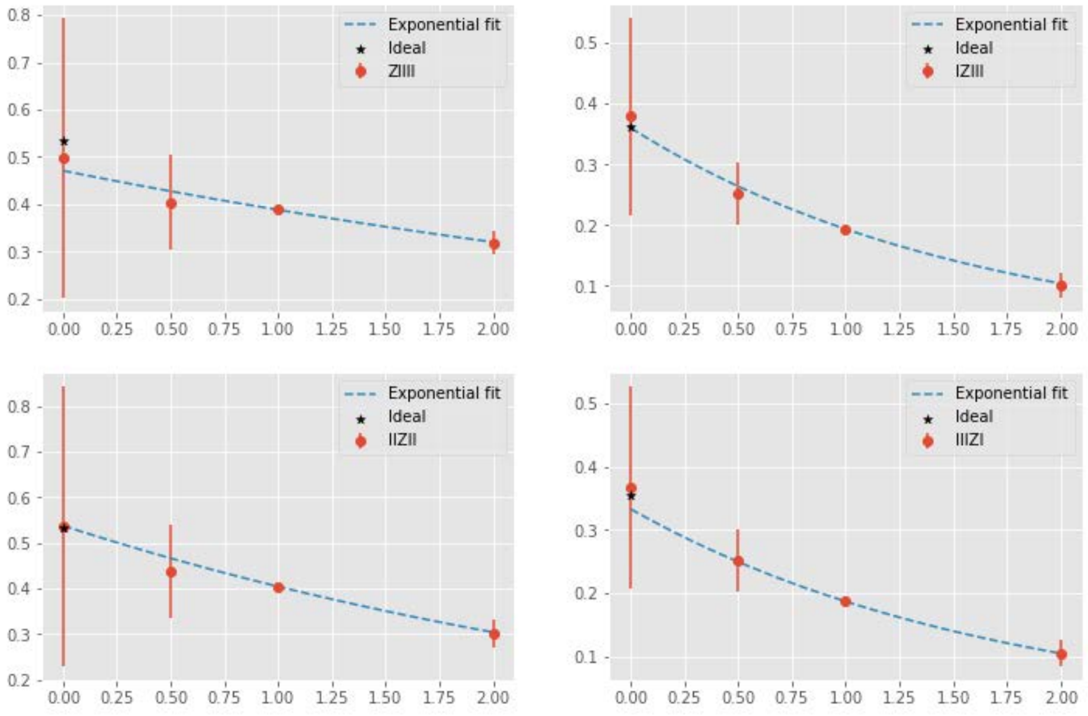
Parameters:
- 1000 PER samples
- 1024 shots
- $\Delta t = 0.2$
- $J = 0.15$
- $h = 1$



Results

Convergence of the individual estimators

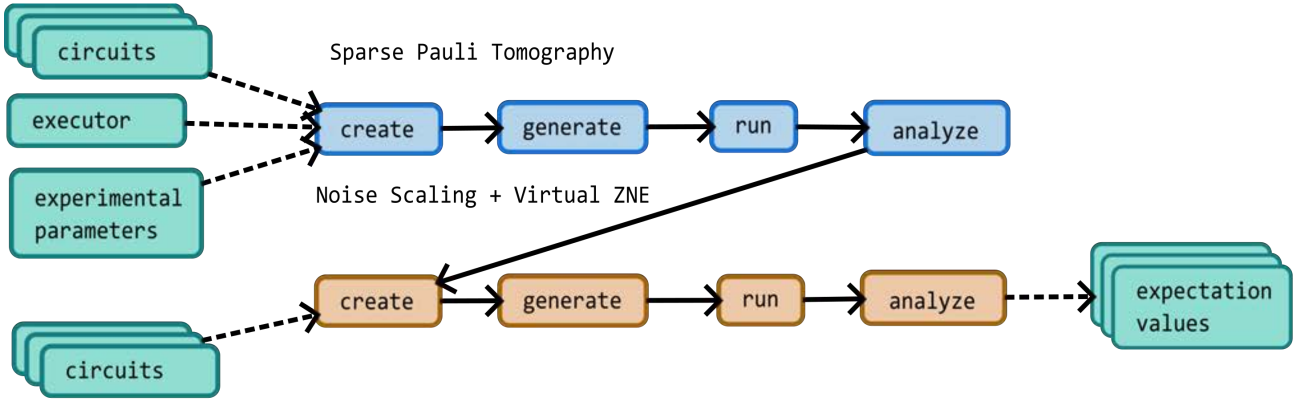
- The convergence is exhibited by each expectation value $\langle Z_n \rangle$
- The extrapolation shown uses only the values $\xi \in \{.5,1,2\}$.
- Extrapolation using an exponential fit can yield results with accuracy similar to PEC without evaluating the expectation at $\xi = 0$.



Pauli Noise Tomography

- We implement a previously described procedure to characterize a Pauli-noise channel under Pauli twirling [1],[2].
- We extend this procedure to carry out PER, and we develop software to automate this process.

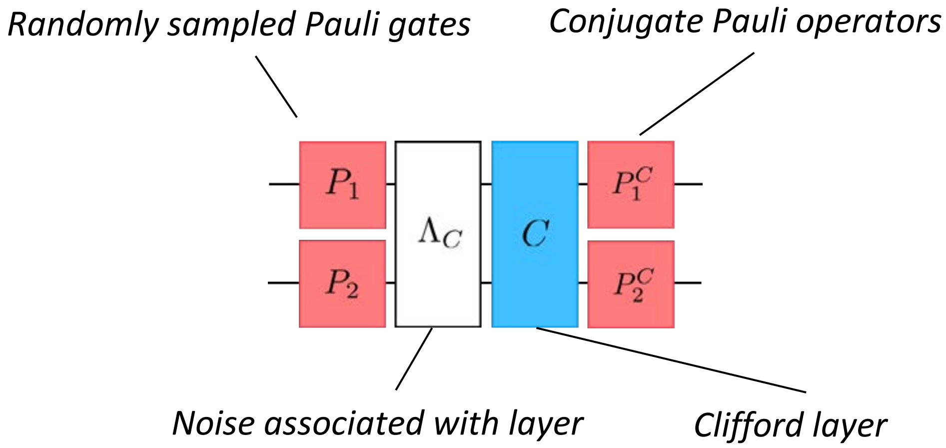
custom toolchain



[1] Berg, Ewout van den, Zlatko K. Minev, Abhinav Kandala, and Kristan Temme. "Probabilistic error cancellation with sparse Pauli-Lindblad models on noisy quantum processors." arXiv preprint arXiv:2201.09866 (2022).
[2] Flammia, Steven T., and Joel J. Wallman. "Efficient estimation of Pauli channels." ACM Transactions on Quantum Computing 1, no. 1 (2020): 1-32.

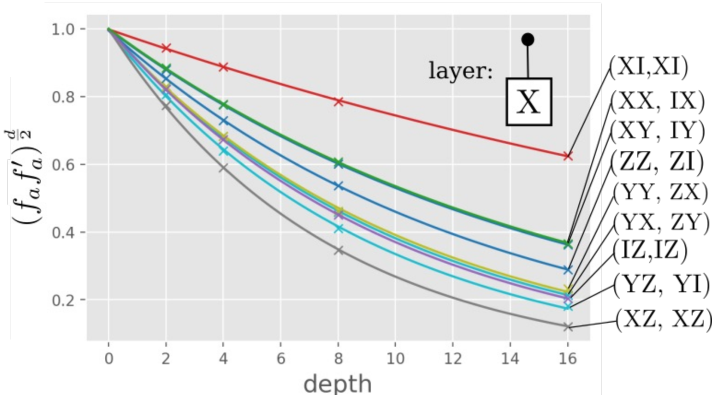
Pauli Twirling

- Pauli operator P_a is an eigenvector of twirled noise channel with eigenvector f_a [2]



- Even number of repetitions of noisy Clifford layer
- Noise associated with dressed Clifford layers is learned

- Self-adjoint Clifford layers result in fidelity pairs $\sqrt{f_a f_a'}$ [1]



Simulated with random Pauli noise + amplitude damping noise

[1] Berg, Ewout van den, Zlatko K. Minev, Abhinav Kandala, and Kristan Temme. "Probabilistic error cancellation with sparse Pauli-Lindblad models on noisy quantum processors." arXiv preprint arXiv:2201.09866 (2022).
[2] Flammia, Steven T., and Joel J. Wallman. "Efficient estimation of Pauli channels." ACM Transactions on Quantum Computing 1, no. 1 (2020): 1-32.

Sparse Pauli-Lindblad Model

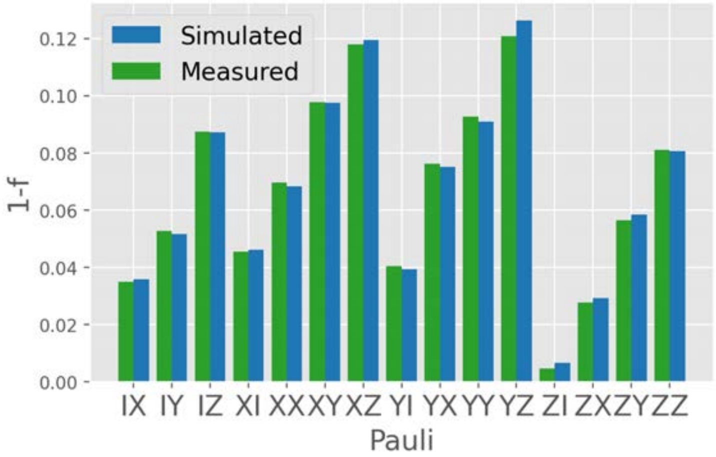
- Even repetitions of noisy Clifford layer result in exponential decays giving fidelity products:

$$\frac{1}{d}Tr\big(P_a\Lambda(P_a)\big) = (f_a f_a')^{\frac{d}{2}}$$

- Several direct fidelity measurements can lift the degeneracy for pairs where $f_a \neq f_a'$ [1]

Simulation of learning procedure

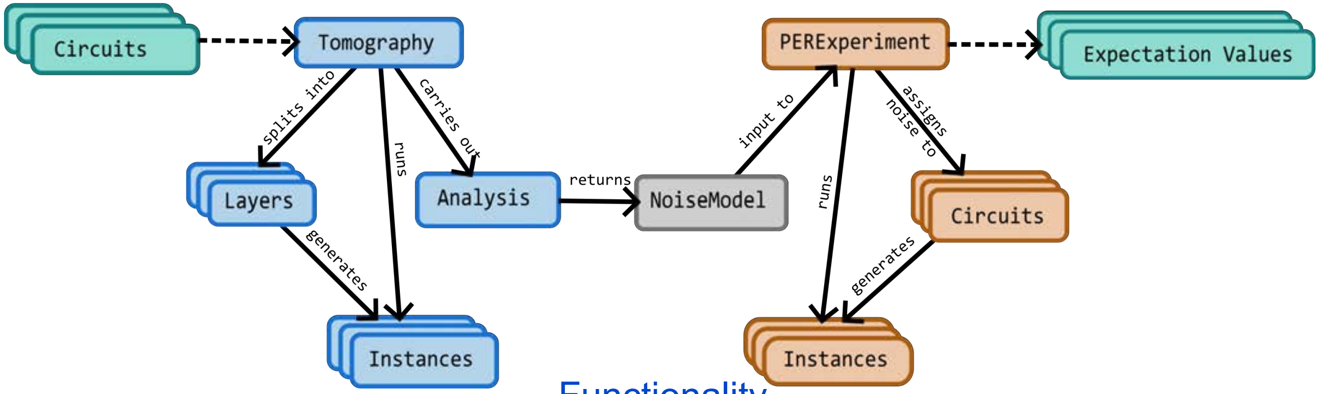
- random Pauli noise and amplitude damping channel.
- software automatically generates benchmark circuits based on input circuit
- data is automatically processed to obtain model estimate.



[1] Berg, Ewout van den, Zlatko K. Minev, Abhinav Kandala, and Kristan Temme. "Probabilistic error cancellation with sparse Pauli-Lindblad models on noisy quantum processors." arXiv preprint arXiv:2201.09866 (2022).

Software Package

Design



Functionality

Automates tomography and scaling process

- Breaks user-defined circuit into layers
- Generates & runs tomography circuits (skip some of these)
- Runs vZNE and extracts expectation values

Built on a multi-platform wrapper

- Processor
- Circuit
- Instruction
- Pauli

https://github.com/benmcdonough20/AutomatedPERTools

Adaptive variational quantum dynamics simulations

Yong-Xin Yao, Niladri Gomes, Feng Zhang, Thomas Iadecola, Cai-Zhuang Wang, Kai-Ming Ho, PPO
Adaptive Variational Quantum Dynamics Simulations
Phys. Rev. X Quantum **2**, 030307 (2021)

Time-dependent variational quantum algorithms

Variational form of quantum state

$$|\Psi[\boldsymbol{\theta}]\rangle = \prod_{\mu=0}^{N_{\boldsymbol{\theta}}-1} e^{-i\theta_\mu \hat{A}_\mu} |\Psi_0\rangle$$

Variational parameters evolve in time

Von Neumann equation

$$\frac{d\rho}{dt} = \mathcal{L}(\rho) = -i[\mathcal{H}, \rho]$$

$$L^2 \equiv \left\| \sum_\mu \frac{\partial \rho[\boldsymbol{\theta}]}{\partial \theta_\mu} \dot{\theta}_\mu - \mathcal{L}[\rho] \right\|^2 = \sum_{\mu\nu} M_{\mu\nu} \dot{\theta}_\mu \dot{\theta}_\nu - 2 \sum_\mu V_\mu \dot{\theta}_\mu + \mathrm{Tr}[\mathcal{L}[\rho]^2].$$

MacLachlan distance b/w exact and variational time evolution

[1] Li, Benjamin, Endo, Yuan (2019).

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MacLachlan distance b/w exact and variational time evolution

Minimize L^2

M measures state change under parameter change

$$M_{\mu\nu} \equiv \mathrm{Tr}\left[\frac{\partial \rho[\boldsymbol{\theta}]}{\partial \theta_\mu} \frac{\partial \rho[\boldsymbol{\theta}]}{\partial \theta_\nu}\right]$$

$$V_\mu \equiv \mathrm{Tr}\left[\frac{\partial \rho[\boldsymbol{\theta}]}{\partial \theta_\mu} \mathcal{L}[\rho]\right]$$

V depends on Hamiltonian

EOM for variational parameters

$$\sum_\nu M_{\mu\nu} \dot{\theta}_\nu = V_\mu.$$

Matrix $M_{\mu\nu}$ and vector V_μ measured on QPU

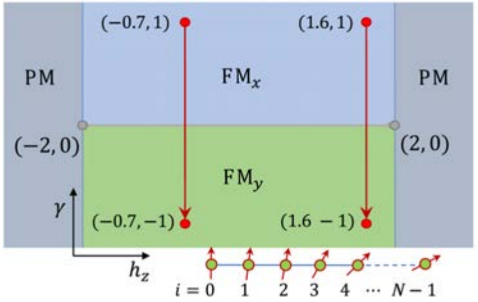
Scaling to large system sizes challenging as $N_{meas} \propto N_\theta^2$ and N_θ can grow exponentially with system size for nonintegrable models
☞ Opportunity at early times and for integrable models

[1] Li, Benjamin, Endo, Yuan (2019).

Application: continuous quench in spin chain

> Linear quench of anisotropic XY chain in transverse magnetic field

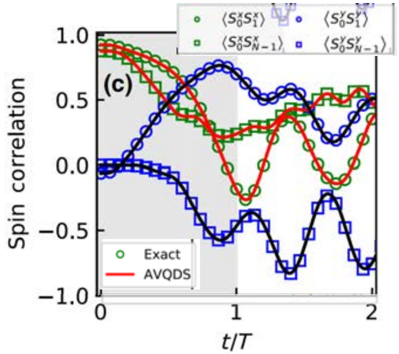
$$\hat{\mathcal{H}} = -J \sum_{i=0}^{N-2} \left[(1+\gamma)\hat{X}_i\hat{X}_{i+1} + (1-\gamma)\hat{Y}_i\hat{Y}_{i+1} \right] + h_z \sum_{i=0}^{N-1} \hat{Z}_i \quad \text{with} \quad \gamma(t) = 1 - \frac{2t}{T}$$

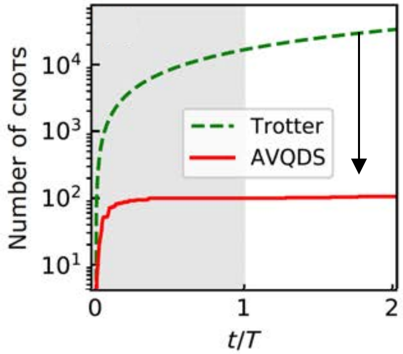


> Follows exact solution during and after quench, shown for $N = 8$

> **Circuit depth saturates at 100 CNOTs** << **Trotter circuit depth 10^4 CNOTs**

> Simulate system with gate depth independent of time t ➢ can simulate to arbitrary times!





Y. Yao, .., PPO, PRX Quantum (2021)

Variational Trotter Compression algorithm

Noah F. Berthusen, Thaís V. Trevisan, Thomas Iadecola, PPO
Quantum dynamics simulations beyond the coherence time on noisy intermediate-scale quantum hardware by variational Trotter compression
Phys. Rev. Res. **4**, 023097 (2022).

Trotter simulations of quantum dynamics of Heisenberg model

- Decompose Hamiltonian into sum of terms that include commuting operators $H = H_{\text{even}} + H_{\text{odd}}$

$$H_{\text{even}} = \frac{J}{4} \sum_{i \,\text{even}} (X_i X_{i+1} + Y_i Y_{i+1} + Z_i Z_{i+1}) \quad \text{and} \quad H_{\text{odd}} = \frac{J}{4} \sum_{i \,\text{odd}} (X_i X_{i+1} + Y_i Y_{i+1} + Z_i Z_{i+1})$$

- Trotter product formula expansion (first order)

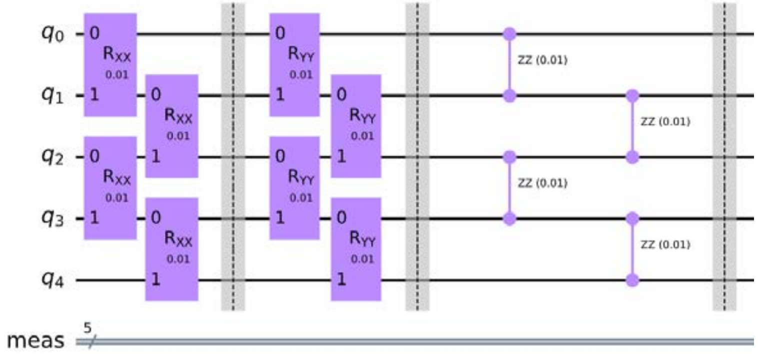
$$\left[e^{-i(H_{\text{even}}+H_{\text{odd}})\frac{t}{N}}\right]^N = \prod_{\alpha=1}^{N} \left[e^{-iH_{\text{even}}\frac{t}{N}} e^{-iH_{\text{odd}}\frac{t}{N}} + \mathcal{O}(t^2/N^2)\right]$$

Trotter step size

$\tau = t/N$

Must be chosen small ➢ deep circuits

Can be easily implemented as product of two-qubit unitaries



Single Trotter step circuit

While product formulas are straightforward to implement, they result in **deep circuits for long and precise simulations**

Lloyd (1996); Trotter, Suzuki; Childs, Wiebe

Variational Trotter Compression (VTC) algorithm

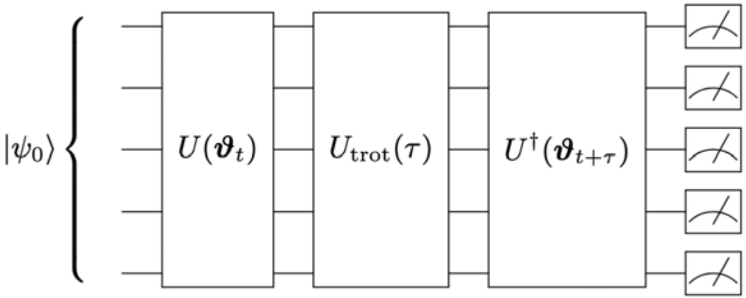
Key idea of VTC algorithm [1, 2]:

- First, propagate state using Trotter: $|\psi(\boldsymbol{\vartheta}_t)\rangle \Longrightarrow U_{\mathrm{trot}}(\tau)\,|\psi(\boldsymbol{\vartheta}_t)\rangle$
- Then, update variational parameters $\vartheta_t \rightarrow \vartheta_{t+\tau}$ by optimizing fidelity cost function

Fidelity cost function $\mathcal{C} = |\,\langle\psi_0|U^\dagger(\boldsymbol{\vartheta}_{t+\tau})U_{\mathrm{trot}}(\tau)U(\boldsymbol{\vartheta}_t)|\psi_0\rangle\,|^2$

Our variational state: $$|\psi(\boldsymbol{\vartheta})\rangle = U(\boldsymbol{\vartheta})\,|\psi_0\rangle = \prod_{l=1}^{\ell}\prod_{i=1}^{N} e^{-i\vartheta_{l,i}A_i}\,|\psi_0\rangle$$

ℓ = number of layers
N = number of parameters per layer
A_i= Hermitian operator (e.g. Pauli matrix)



Return probability to initial state is maximal for optimal parameters $\vartheta_{t+\tau}$

Measure cost function on QPU [3]

[1] Lin, Green, Smith, Pollmann (2020); [2] Barison, Carleo (2021), [3] Berthusen, Trevisan, Iadecola, PPO (2021).

Application to Heisenberg model: choice of ansatz

1D AF Heisenberg model $H_0 = \frac{J}{4}\sum_{i=1}^{M}(X_iX_{i+1} + Y_iY_{i+1} + Z_iZ_{i+1})$

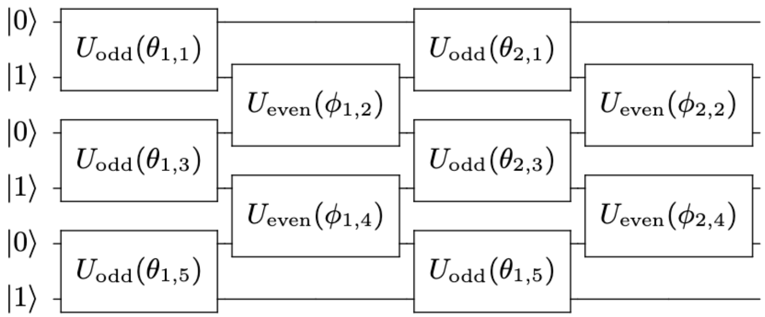
> Start from classical Néel state and time-evolve with H_0: $|\psi(t)\rangle = e^{-iH_0t}|010101\cdots\rangle$

$$|\psi(\boldsymbol{\vartheta}^{(\ell)})\rangle = \prod_{l=1}^{\ell} U_{\text{even}}(\boldsymbol{\phi}_l)\, U_{\text{odd}}(\boldsymbol{\theta}_l)\, |\psi_0\rangle$$

$$U_{\text{odd}}(\boldsymbol{\theta}_l) = \prod_{j \text{ odd}} e^{-i\,\theta_{l,j}\,(X_jX_{j+1}+Y_jY_{j+1}+Z_jZ_{j+1})}$$

$$U_{\text{even}}(\boldsymbol{\phi}_l) = \prod_{j \text{ even}} e^{-i\,\phi_{l,j}\,(X_jX_{j+1}+Y_jY_{j+1}+Z_jZ_{j+1})}$$

Brickwall form of quantum circuit



> Determine depth of layered ansatz $\ell \equiv \ell^*$ to accurately describe $|\psi(t)\rangle$

Required layer numbers versus time

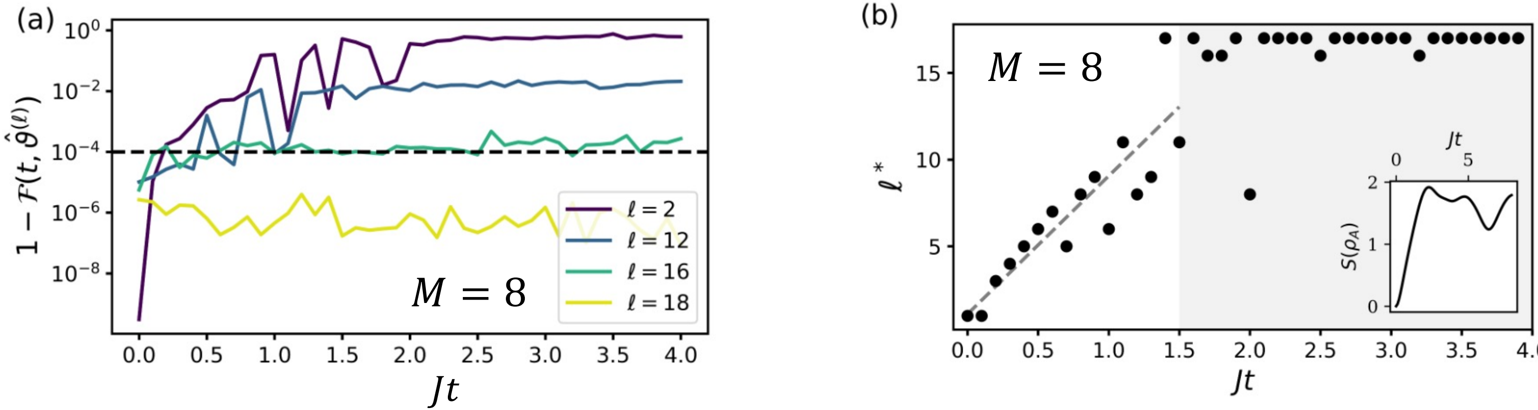
- Start from classical Néel state and time-evolve with H_0: $|\psi(t)\rangle = e^{-iH_0 t}|010101\cdots\rangle$
- Determine depth of layered ansatz ℓ to accurately describe $|\psi(t)\rangle$

Variational form

$$|\psi(\boldsymbol{\vartheta}^{(\ell)})\rangle = \prod_{l=1}^{\ell} U_{\text{even}}(\boldsymbol{\phi}_l)\, U_{\text{odd}}(\boldsymbol{\theta}_l)\, |\psi_0\rangle$$

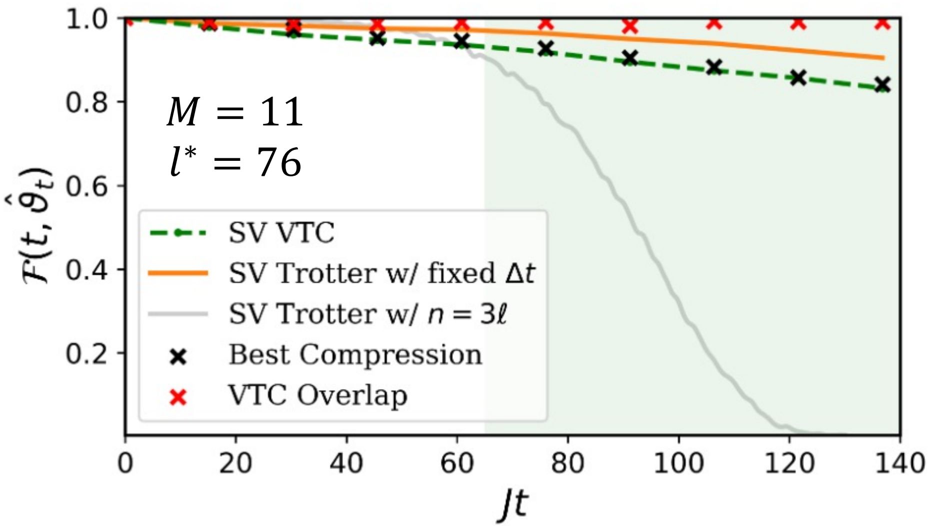
Overlap with exact state

$$1 - \mathcal{F}(t, \boldsymbol{\vartheta}^{(\ell)}) = 1 - |\langle\psi(\boldsymbol{\vartheta}^{(\ell)})|\psi(t)\rangle|^2$$



Required layer number ℓ to achieve $1 - \mathcal{F} < 10^{-4}$ grows **linearly with time** and then **saturates**.

VTC benchmark on statevector simulator



- VTC approximately follows Trotter with fixed small step size $\Delta t = \frac{0.2}{J}$
- Orange curve has depth $\mathrm{n} = 700$ at t_f
- Grey curve has depth $3\ell = 228$ at all t
- VTC cost function has fixed depth $3\ell = 228$
- Gradient based optimization using L-BFGS-B

Fidelity = Overlap with exact state $\mathcal{F}(t, \hat{\boldsymbol{\vartheta}}_t) = |\langle \psi(\hat{\boldsymbol{\vartheta}}_t) | \psi(t) \rangle|^2$

$$\text{Best Compression} \equiv |\langle \psi(t) | U_{\text{Trot}}(n = \ell) | \psi(\hat{\boldsymbol{\vartheta}}_{t-\tau}) \rangle|^2$$

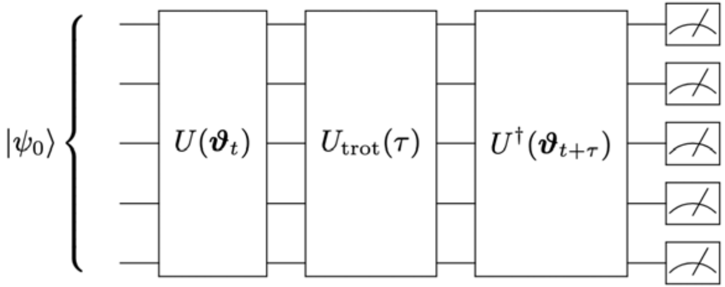
$$\text{VTC overlap} \equiv |\langle \psi(\hat{\boldsymbol{\vartheta}}_t) | U_{\text{Trot}} | \psi(\hat{\boldsymbol{\vartheta}}_{t-\tau}) \rangle|^2$$

VTC allows simulating to arbitrarily long times with high fidelity.

Parameters: $\ell = 76, n = 76$
$\tau = 15.2/J, \Delta t = 0.2/J$

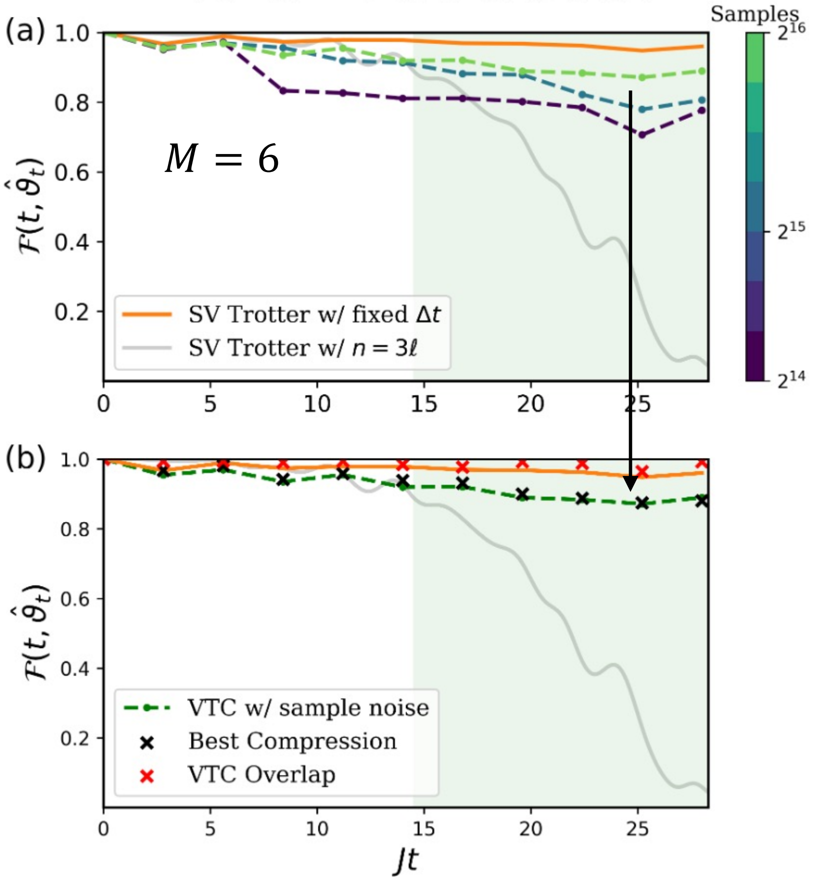
VTC on ideal circuit simulators

- Double-time contour cost function circuit
- Non-gradient-based optimizer: CMA-ES
- Larger shot numbers increase fidelity
- Single compression step takes few hours

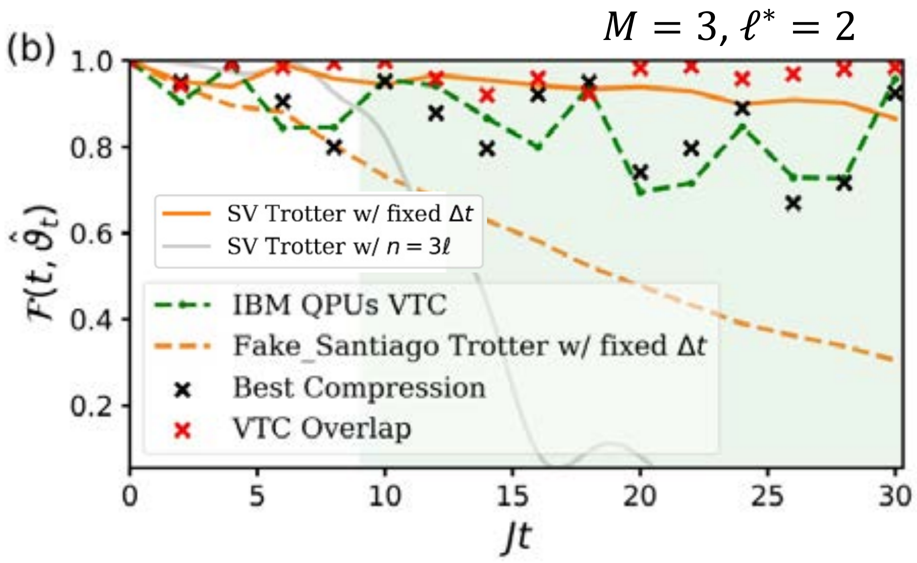


VTC is feasible for noisy cost function.

$$\mathcal{F}(t, \hat{\boldsymbol{\vartheta}}_t) = |\langle \psi(\hat{\boldsymbol{\vartheta}}_t)|\psi(t)\rangle|^2$$



VTC on IBM hardware

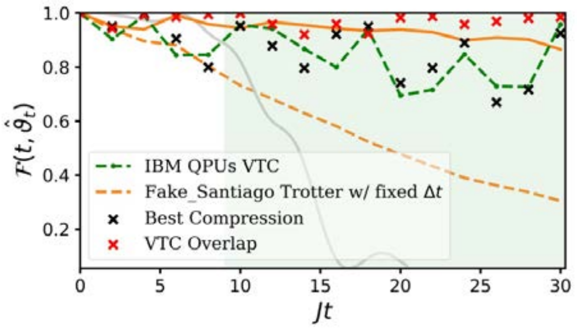


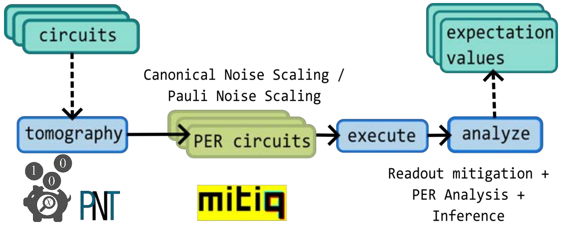
Explicit demonstration of dynamics simulations beyond QPU coherence time

- Cost function evaluation on IBM hardware `ibmq_santiago & ibmq_quito`
- Final fidelity = 0.96, where Trotter fidelity has decayed to < 0.4 already
- 15 compression steps
- Average fidelity $\langle F \rangle = 0.86$
- $\mathcal{M} = 5700$ measurement circuits in total
- Comparable number of measurements for MacLachlan simulations $\approx 10^4$

Summary

- Quantum dynamics simulations are one of the primary early applications of noisy quantum devices
- Hardware and software developments necessary to realize quantum advantage
- Trotter simulations have low overhead and can be improved using quantum error mitigation methods (ZNE, PEC/PER)
- Variational Trotter Compression (VTC) algorithm
  - Trotter propagation combined with variational compression
  - Effectively Trotter with fixed step size *and* fixed gate depth





Thank you for your attention!

References:
- B. McDonough *et al.*, arXiv:2210.08611 I.-C. Chen *et al.*, Phys. Rev. Res. (2022)
- N. F. Berthusen *et al.*, Phys. Rev. Res. (2022)
- Y.-X. Yao *et al.*, Phys. Rev. X Q (2021)