IOWA STATE UNIVERSITY

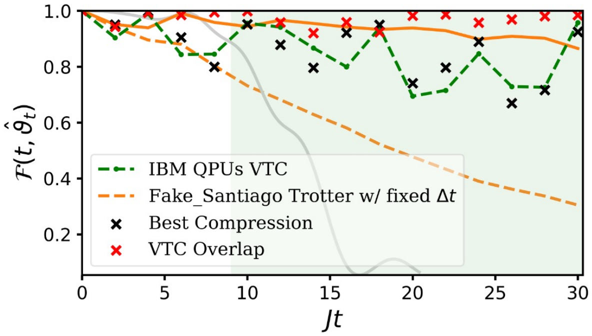
Department of Physics and Astronomy

Variational Trotter compression algorithm for quantum dynamics simulations on noisy intermediate-scale quantum computers

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

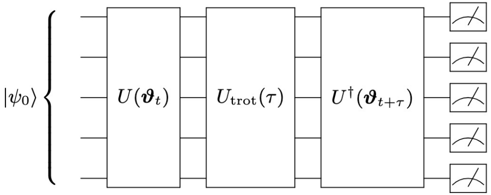
Collaboration with Noah F. Berthusen, Thaís V. Trevisan, and Thomas Iadecola (Iowa State University & Ames Lab)

APS March Meeting, Chicago, March 15, 2022



Reference:

- N. F. Berthusen, T.V. Trevisan, T. Iadecola, PPO, arXiv:2112.12654



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Quantum dynamics simulations

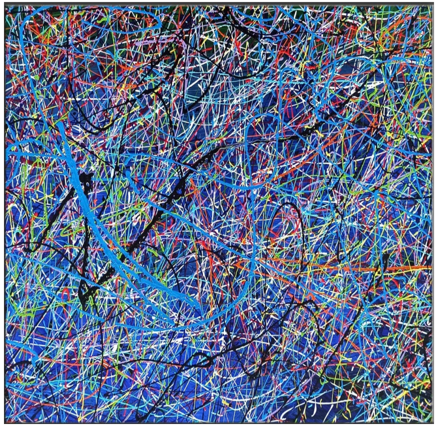
Initial state

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

Energy eigenstate of many-body H

Dynamics

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



Dynamics of an observable *O*

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

- Classically hard due to rapid growth of entanglement in nonequilibrium for generic H
- Reason: contains highly excited states ➢ Volume-law entanglement entropy

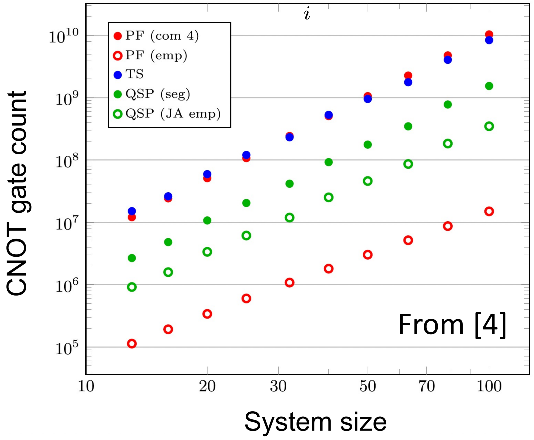
Entanglement = complexity of classical calculation

Exponential growth of classical resources like the bond dimension in tensor networks →

Opportunity for quantum computing

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).

Overview of quantum algorithms for dynamics simulations

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In this talk:
Combine simplicity of Trotter product with a variational approach to simulate for long times.

Demonstrate full algorithm on IBM hardware [6].

[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); [6] Berthusen, Trevisan, Iadecola, PPO (2021).

Variational Trotter Compression (VTC) algorithm

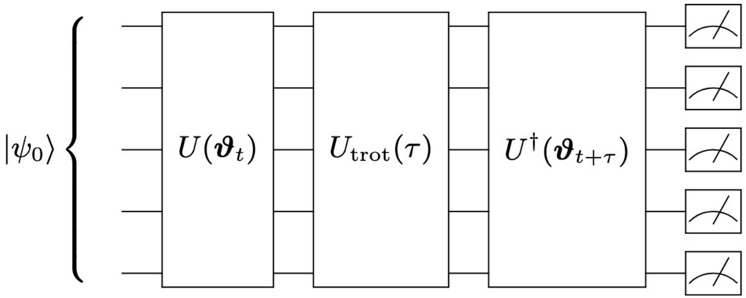
Key idea of VTC algorithm [1, 2]:

- First, propagate state using Trotter: $|\psi(\boldsymbol{\vartheta}_t)\rangle \Longrightarrow U_{\mathrm{trot}}(\tau)\,|\psi(\boldsymbol{\vartheta}_t)\rangle$
- Then, update variational parameters $\vartheta_t \to \vartheta_{t+\tau}$ 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 $H_0 = \frac{J}{4}\sum_{i=1}^{M}(X_i X_{i+1} + Y_i Y_{i+1} + Z_i Z_{i+1})$

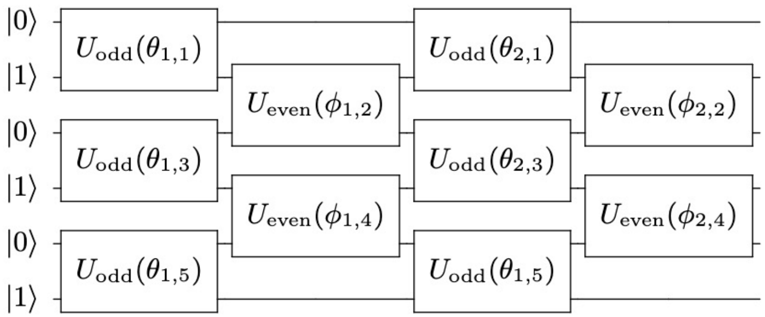
> Start from classical Néel state and time-evolve with H_0: $|\psi(t)\rangle = e^{-iH_0 t}|010101\cdots\rangle$

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

$$U_{\text{odd}}(\boldsymbol{\theta}_l) = \prod_{j \text{ odd}} e^{-i\,\theta_{l,j}\,(X_j X_{j+1} + Y_j Y_{j+1} + Z_j Z_{j+1})}$$

$$U_{\text{even}}(\boldsymbol{\phi}_l) = \prod_{j \text{ even}} e^{-i\,\phi_{l,j}\,(X_j X_{j+1} + Y_j Y_{j+1} + Z_j Z_{j+1})}$$

Brickwall form of quantum circuit



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

Required layer numbers versus time

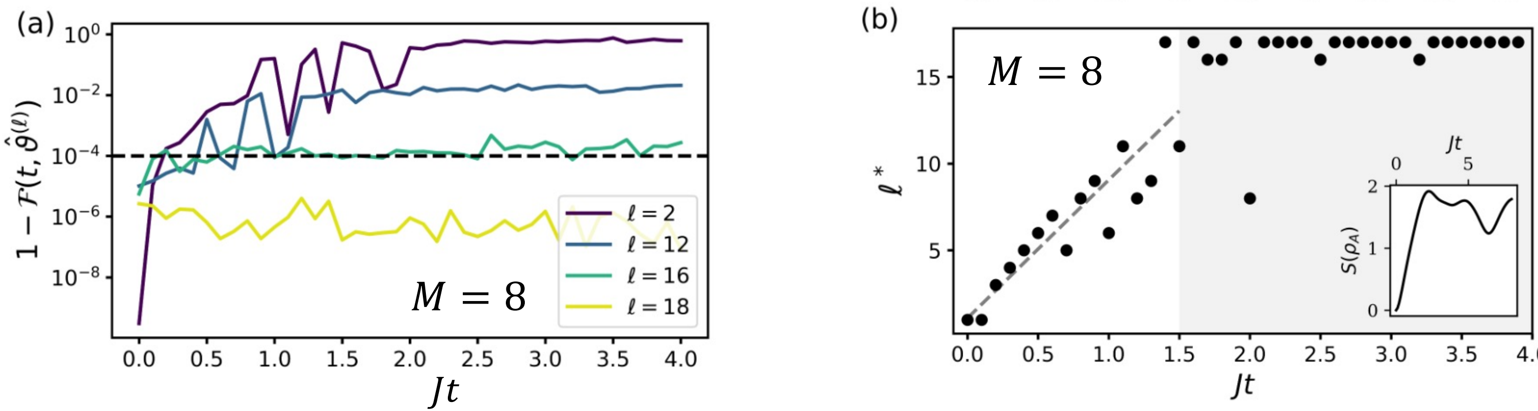
- Start from classical Néel state and time-evolve with H_0: $|\psi(t)\rangle = e^{-iH_0 t}|010101\cdots\rangle$
- Determine depth of layered ansatz ℓ to accurately describe $|\psi(t)\rangle$

Variational form

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

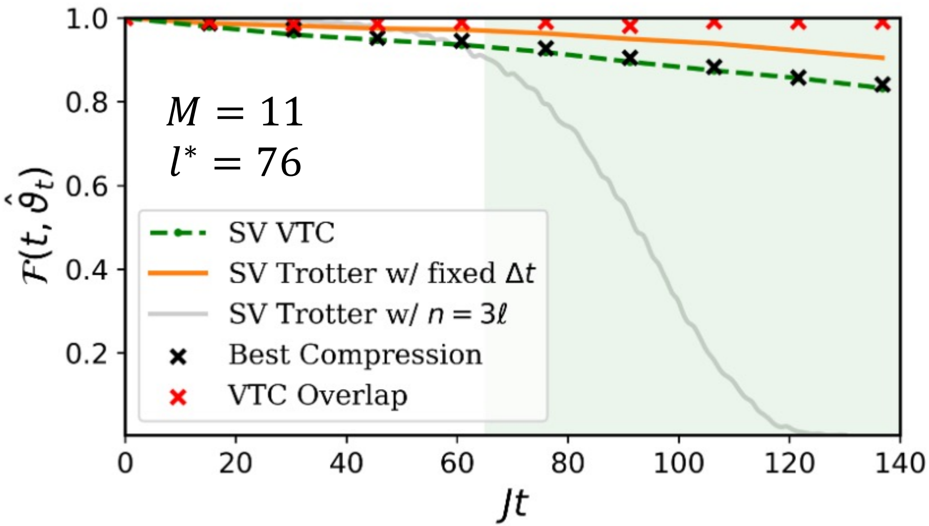
Overlap with exact state

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



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

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

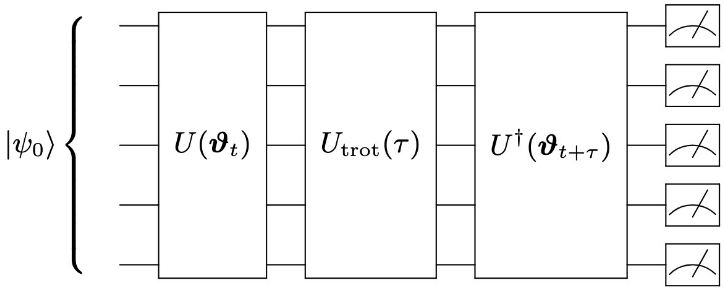
$$\text{VTC overlap} \equiv |\langle \psi(\hat{\boldsymbol{\vartheta}}_t) | U_{\mathrm{Trot}} | \psi(\hat{\boldsymbol{\vartheta}}_{t-\tau}) \rangle|^2$$

VTC allows simulating to arbitrarily long times with high fidelity.

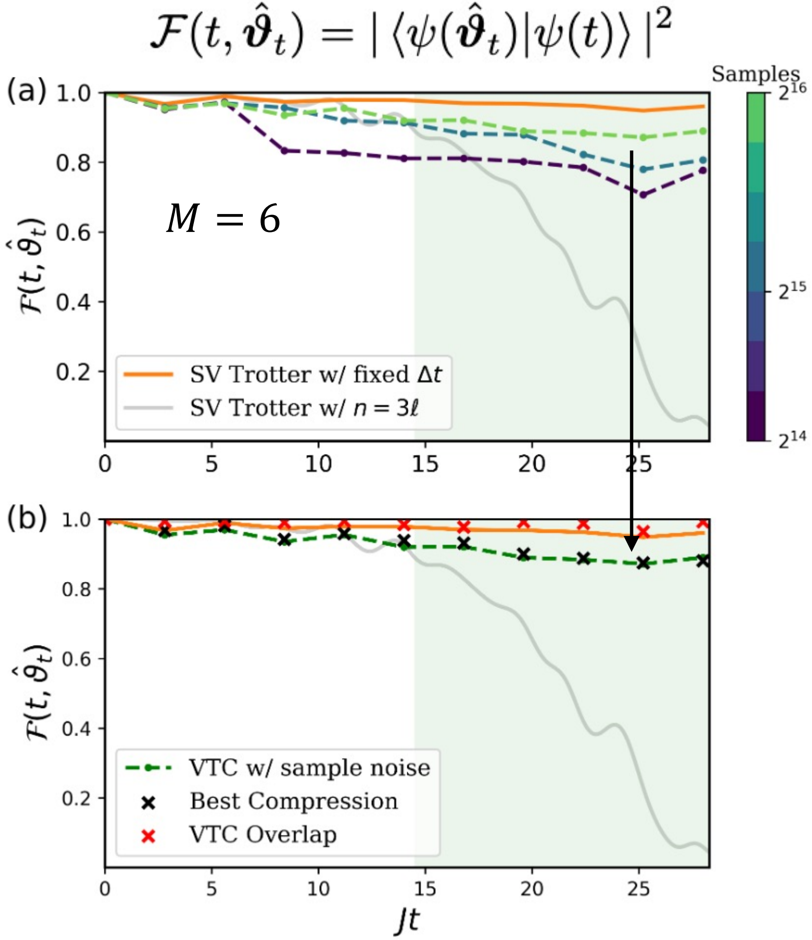
Parameters: $\ell = 76, n = 76$
$\tau = 15.2/J, \Delta t = 0.2/J$

VTC on ideal circuit simulators

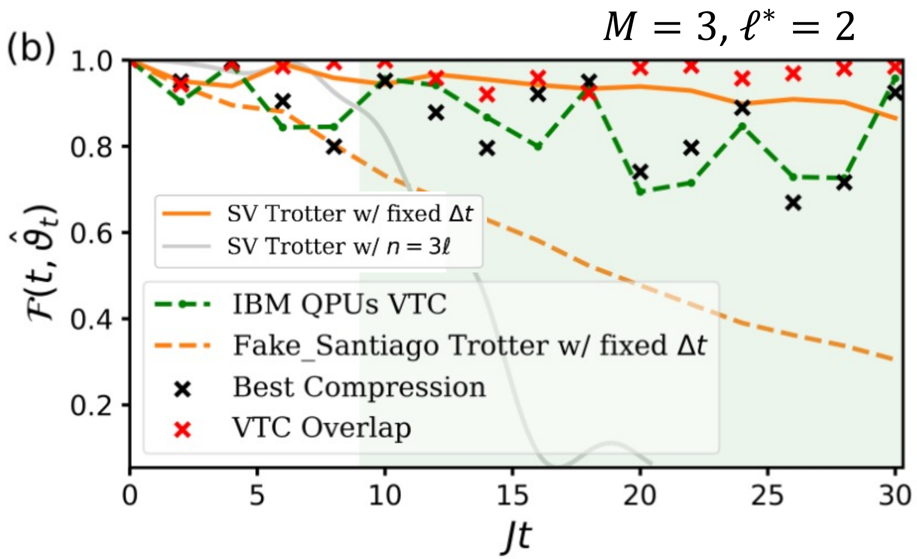
- Double-time contour cost function circuit
- Non-gradient-based optimizer: CMA-ES
- Larger shot numbers increase fidelity
- Single compression step takes few hours



VTC is feasible for noisy cost function.



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 $\approx 10^4$

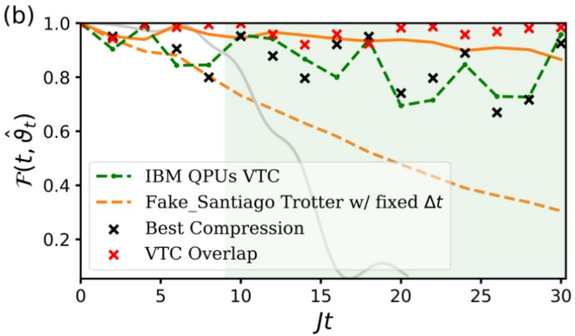
Summary

> Variational Trotter Compression (VTC) algorithm

> Trotter propagation combined with variational compression

> Can simulate out to arbitrary long times with high fidelity

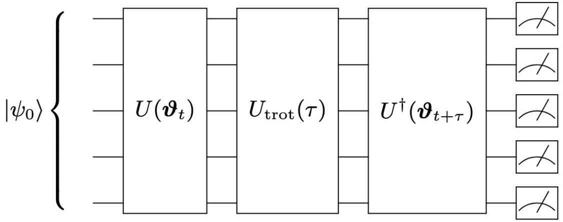
> Effectively Trotter with fixed step size *and* fixed gate depth



> Explicit demonstration of dynamics simulation beyond QPU coherence time

> Executed full algorithm using IBM hardware on $M = 3$ sites

> Simulation on $M = 11$ sites using statevector



> Main limitation is growth of number of variational parameters

> Exponential at long times, linear at short times (quantum advantage?)

Reference:

- N. Berthusen *et al.*, T.V. Trevisan, T. Iadecola, PPO, arXiv:2112.12654

Thank you for your attention!