

Title: Classical simulation of noisy quantum circuits via locally entanglement-optimal unravelings

Speakers: Hakop Pashayan

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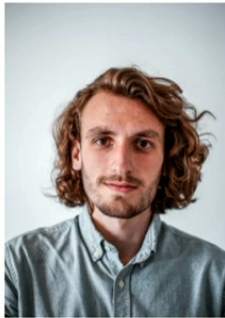
Abstract:

We present a tensor-network-based classical algorithm (equipped with guarantees) for simulating n -qubit quantum circuits with arbitrary single-qubit noise. Our algorithm represents the state of a noisy quantum system by a particular ensemble of matrix product states from which we stochastically sample a pure quantum state. Each single qubit noise process acting on a pure state is then represented by the ensemble of states that achieve the minimal average entanglement (the entanglement of formation) between the noisy qubit and the rest of the system. This approach provides a connection between the entanglement of formation and the accuracy of the simulation algorithm. For a given maximum bond dimension χ and circuit, our algorithm comes with an upper bound on the simulation error (in total variation distance), runs in $\text{poly}(n, \chi)$ -time and improves upon related prior work (1) in scope: by extending from the three commonly considered noise models to general single qubit noise (2) in performance: by employing a state-dependent locally-entanglement-optimal unraveling and (3) in conceptual contribution: by showing that the fixed unraveling used in prior work becomes equivalent to our choice of unraveling in the special case of depolarizing and dephasing noise acting on a maximally entangled state. This is joint work with Simon Cichy, Paul K. Faehrmann, Lennart Bittel and Jens Eisert.



Classical simulation of noisy quantum circuits via locally entanglement-optimal unravelings

Simon Cichy, Paul Fährmann, Lennart Bittel, Jens Eisert, Hakop Pashayan



Motivation

How does the presence of noise diminish the power of quantum computation?

Noise can decay entanglement.

Tradeoffs: noise level vs run-time & noise type vs run-time

Tool : Guage Freedom that Witnesses Entanglement UB.

Outline

1. Prelims:

- Unravelings
- Noise
- Entanglement
- Matrix Product States (MPS)

2. Simulation Task:

3. Algorithm & Performance

4. Outlook

Preliminaries: Unravelings

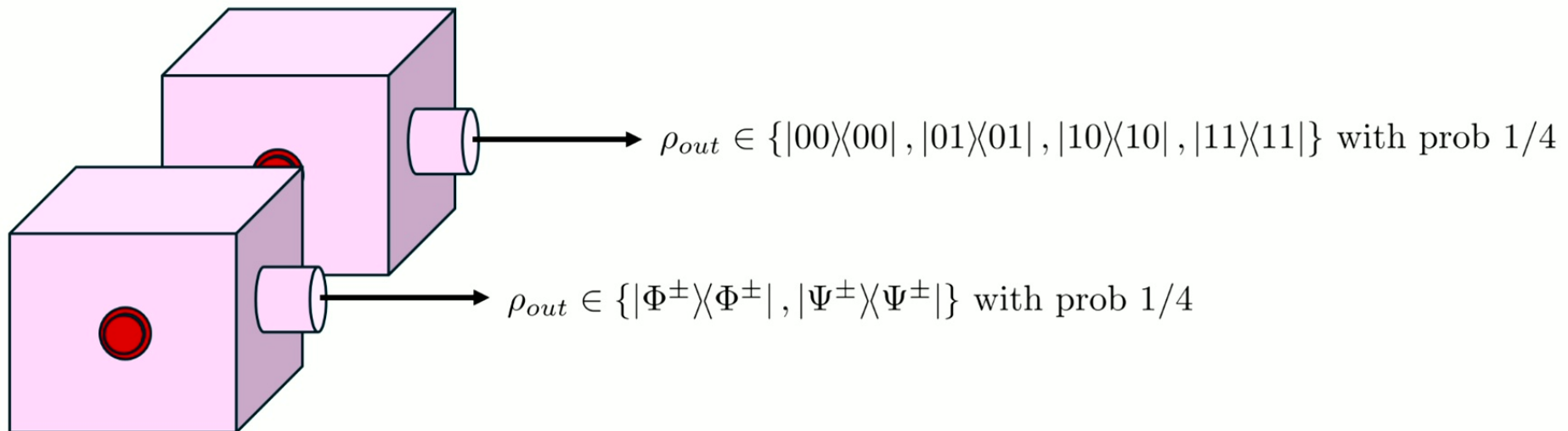
$$\begin{aligned}\rho &= \frac{1}{4}I \\ &= \frac{1}{4}[|00\rangle\langle 00| + |01\rangle\langle 01| + |10\rangle\langle 10| + |11\rangle\langle 11|] \\ &= \frac{1}{4}[|\Phi^+\rangle\langle\Phi^+| + |\Phi^-\rangle\langle\Phi^-| + |\Psi^+\rangle\langle\Psi^+| + |\Psi^-\rangle\langle\Psi^-|]\end{aligned}$$

$$|\Phi^+\rangle = \frac{|00\rangle + |11\rangle}{\sqrt{2}}$$

$$|\Phi^-\rangle = \frac{|00\rangle - |11\rangle}{\sqrt{2}}$$

$$|\Psi^+\rangle = \frac{|01\rangle + |10\rangle}{\sqrt{2}}$$

$$|\Psi^-\rangle = \frac{|01\rangle - |10\rangle}{\sqrt{2}}$$



Preliminaries: Unravelings

$$\rho = \Phi \Lambda \Phi^\dagger \quad \Lambda \in \mathbb{C}^{r \times r}, \text{ diagonal} \quad \& \quad \Phi \in \mathbb{C}^{d \times r} \equiv [|\phi_1\rangle \dots |\phi_r\rangle]$$

$$= [|\phi_1\rangle \quad |\phi_2\rangle \quad |\phi_3\rangle \quad \dots \quad |\phi_r\rangle] \times \begin{bmatrix} \lambda_1 & 0 & 0 & \dots & 0 \\ 0 & \lambda_2 & 0 & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \dots & \lambda_r \end{bmatrix} \times \begin{bmatrix} \langle \phi_1 | \\ \langle \phi_2 | \\ \langle \phi_3 | \\ \vdots \\ \langle \phi_r | \end{bmatrix}$$

$$= [\sqrt{\lambda_1} |\phi_1\rangle \quad \dots \quad \sqrt{\lambda_r} |\phi_r\rangle] \times U U^\dagger \times \begin{bmatrix} \sqrt{\lambda_1} \langle \phi_1 | \\ \vdots \\ \sqrt{\lambda_r} \langle \phi_r | \end{bmatrix}$$

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$$= \underbrace{|\tilde{\phi}_1\rangle}_{\sqrt{\lambda_1}|\phi_1\rangle} \quad \dots \quad \underbrace{|\tilde{\phi}_r\rangle}_{\sqrt{\lambda_r}|\phi_r\rangle} \times UU^\dagger \times \begin{bmatrix} \sqrt{\lambda_1} \langle \phi_1| \\ \vdots \\ \sqrt{\lambda_r} \langle \phi_r| \end{bmatrix} = \sum_i |\tilde{\phi}_i\rangle \langle \tilde{\phi}_i| = \sum_i \lambda_i |\phi_i\rangle \langle \phi_i|$$

$$= \underbrace{|\tilde{\psi}_1\rangle}_{\sum_i \sqrt{\lambda_i} u_{i1} |\phi_i\rangle} \quad \dots \quad \underbrace{|\tilde{\psi}_k\rangle}_{\sum_i \sqrt{\lambda_i} u_{ik} |\phi_i\rangle} \times \begin{bmatrix} \sum_j \sqrt{\lambda_j} u_{j1}^* \langle \phi_j| \\ \vdots \\ \sum_j \sqrt{\lambda_j} u_{jr}^* \langle \phi_j| \end{bmatrix} = \sum_i |\tilde{\psi}_i\rangle \langle \tilde{\psi}_i| = \sum_i \omega_i |\psi_i\rangle \langle \psi_i|$$

Preliminaries: Unravelings

$$\rho = \Phi \Lambda \Phi^\dagger \quad \Lambda \in \mathbb{C}^{r \times r}, \text{ diagonal} \quad \& \quad \Phi \in \mathbb{C}^{d \times r} \equiv [|\phi_1\rangle \dots |\phi_r\rangle]$$

$$= [|\phi_1\rangle \quad |\phi_2\rangle \quad |\phi_3\rangle \quad \dots \quad |\phi_r\rangle] \times \begin{bmatrix} \lambda_1 & 0 & 0 & \dots & 0 \\ 0 & \lambda_2 & 0 & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \dots & \lambda_r \end{bmatrix} \times \begin{bmatrix} \langle \phi_1 | \\ \langle \phi_2 | \\ \langle \phi_3 | \\ \vdots \\ \langle \phi_r | \end{bmatrix}$$

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$$\| |\psi_i\rangle \|_2 = 1$$

$$\omega_i \geq 0$$

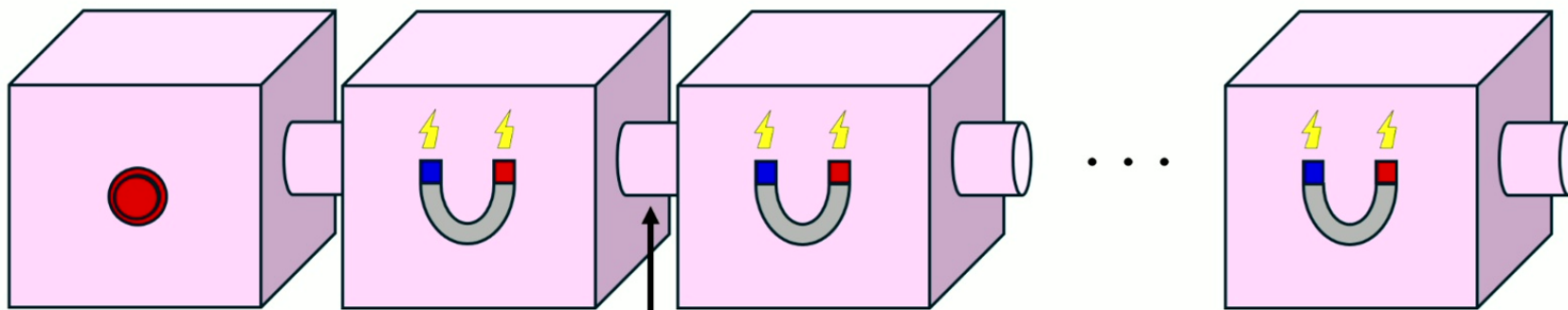
$$\sum_i \omega_i = 1$$

Preliminaries: Unravelings

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product state

maximally entangled



Want: Pure State

Want: Low Entanglement States

Preliminaries: Noise

CPTP maps specified by Kraus operators $\{K_i\}_i$ where $\sum_i K_i K_i^\dagger = I$

$$\rho \mapsto \mathcal{N}(\rho) = \sum_i K_i \rho K_i^\dagger$$

Noise	$\mathcal{N}(\rho)$	Kraus Representation
Depolarizing	$(1 - \frac{3p}{4}) \rho + \frac{p}{4}(X\rho X + Y\rho Y + Z\rho Z)$	$\left\{ \sqrt{1 - \frac{3p}{4}} I, \frac{\sqrt{p}}{2} X, \frac{\sqrt{p}}{2} Y, \frac{\sqrt{p}}{2} Z \right\}$
Dephasing	$(1 - \frac{p}{2}) \rho + \frac{p}{2} Z\rho Z$	$\left\{ \sqrt{1 - \frac{p}{2}} I, \sqrt{\frac{p}{2}} Z \right\}$
Amplitude Damping	$\begin{pmatrix} 1 & 0 \\ 0 & \sqrt{1-\gamma} \end{pmatrix} \rho \begin{pmatrix} 1 & 0 \\ 0 & \sqrt{1-\gamma} \end{pmatrix} + \begin{pmatrix} 0 & \sqrt{\gamma} \\ 0 & 0 \end{pmatrix} \rho \begin{pmatrix} 0 & 0 \\ \sqrt{\gamma} & 0 \end{pmatrix}$	$\left\{ \begin{pmatrix} 1 & 0 \\ 0 & \sqrt{1-\gamma} \end{pmatrix}, \begin{pmatrix} 0 & \sqrt{\gamma} \\ 0 & 0 \end{pmatrix} \right\}$

Preliminaries: Entanglement Measures

von Neumann entanglement entropy:

$$E(|\psi\rangle_{A:B}) = -\text{Tr}(\rho_A \log \rho_A) \quad \text{where} \quad \rho_A = \text{Tr}_B(|\psi\rangle\langle\psi|)$$

Ensemble-averaged entanglement entropy:

Defined on any decomp $\sum_i p_i |\phi_i\rangle\langle\phi_i| = \rho$

$$E_{\text{av}}(\{p_i, |\phi_i\rangle\}) = \sum_i p_i E(|\phi_i\rangle_{A:B})$$

Entanglement of formation:

Infimum of E_{av} over all decompositions of ρ

Computing the EoF:

Even deciding separability is NP-hard [Gharibian 2010]

Gradient decent works without guarantees

Fast, method for 2-qubits [Wootters 1998]

Optimal unraveling

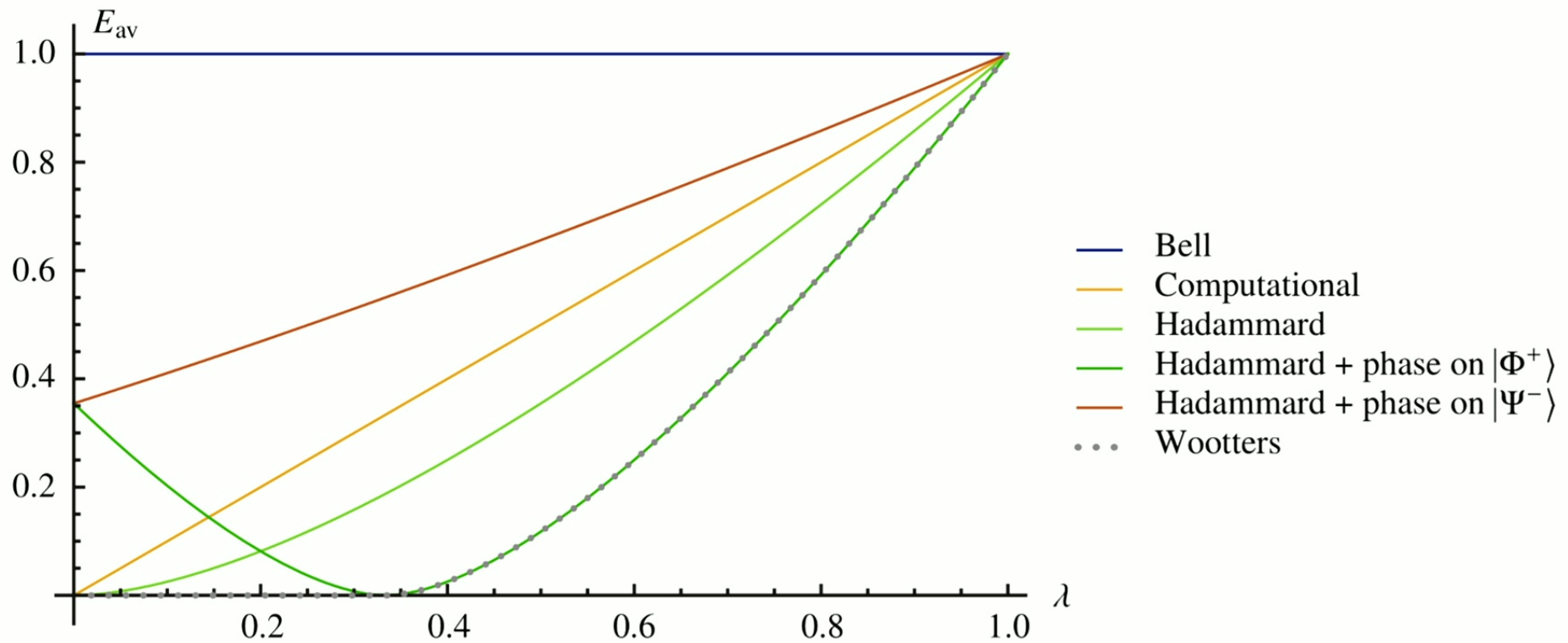
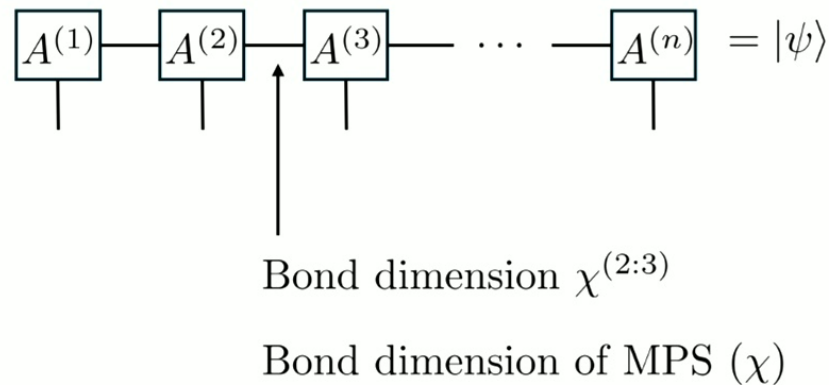


FIG. 8. Ensemble-averaged entanglement entropy for some unravelings of the Werner state.

Preliminaries: Matrix Product States (MPS)

Algebraic form: $|\psi\rangle = \sum_x c_x |x\rangle$ where $c_x = A_{x_1}^{(1)} \times \dots \times A_{x_n}^{(n)}$

Graphical form:



Preliminaries: Matrix Product States (MPS)

Efficient contractions:

$$A^{(1)} - B^{(2)} - B^{(3)} - \dots - A^{(n)} = U |\psi\rangle$$

Thm (Schmidt decomposition): For any bi-partate $|\psi\rangle_{LR}$, there are orthonormal states $\{|L_i\rangle\}$ on L and $\{|R_i\rangle\}$ on R s.t.

$$|\psi\rangle_{LR} = \sum_i \lambda_i |L_i\rangle |R_i\rangle,$$

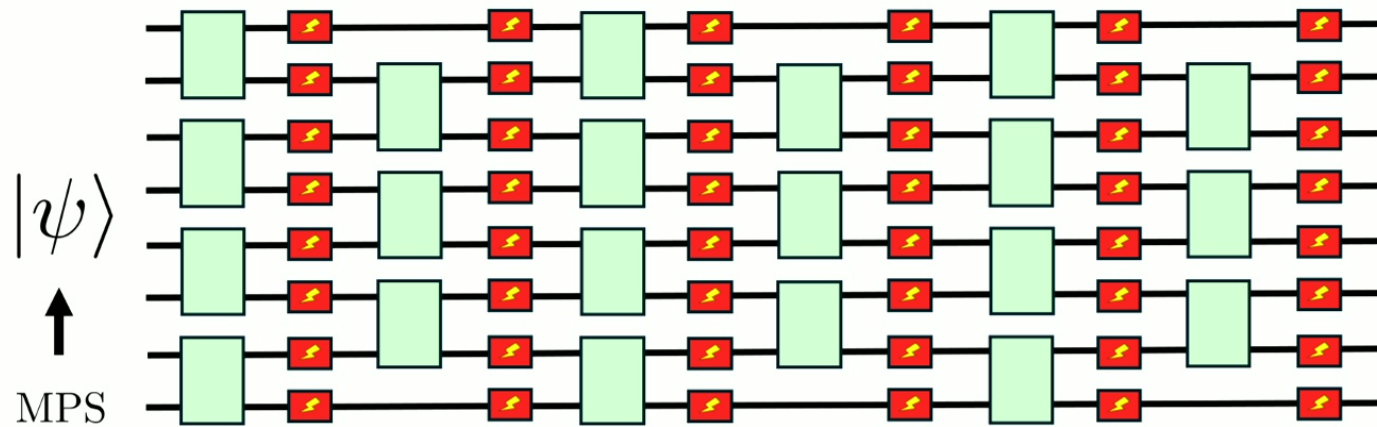
where $\lambda_i \geq 0$ and $\sum_i \lambda_i^2 = 1$.

Efficient Schmidt decomp:

$$B^{(1)} - B^{(2)} - \overset{i}{\diamond} - B^{(3)} - \dots - B^{(n)} = \sum_i \lambda_i |L_i\rangle |R_i\rangle$$

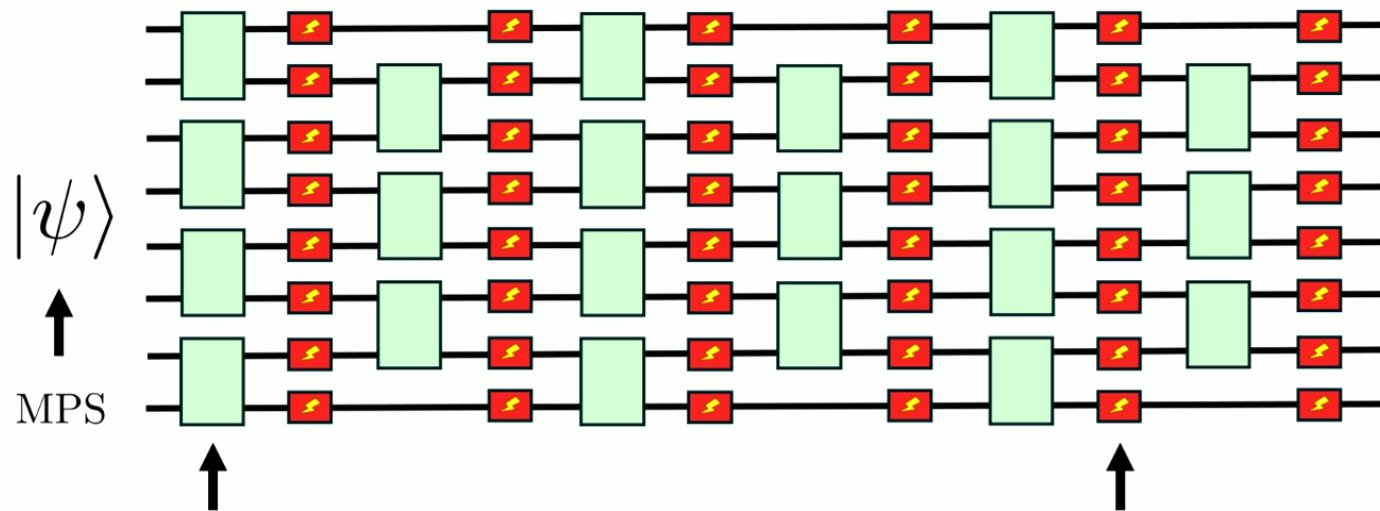
Simulation Tasks:

\mathcal{D} (Noisy Quantum Circuit Description)



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\mathcal{D} (Noisy Quantum Circuit Description)



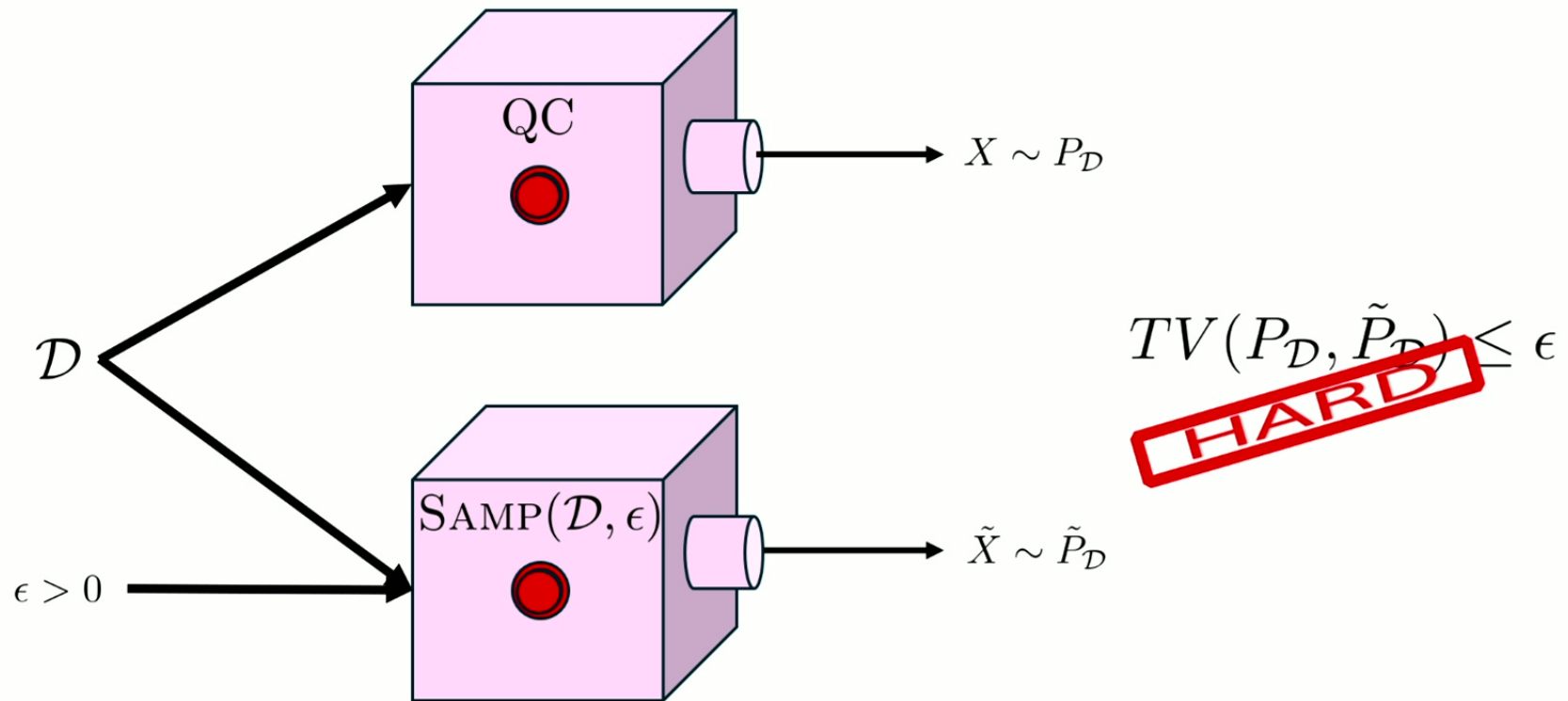
(Local) Unitaries: $\rho \mapsto U\rho U^\dagger$

1D architecture is the natural setting

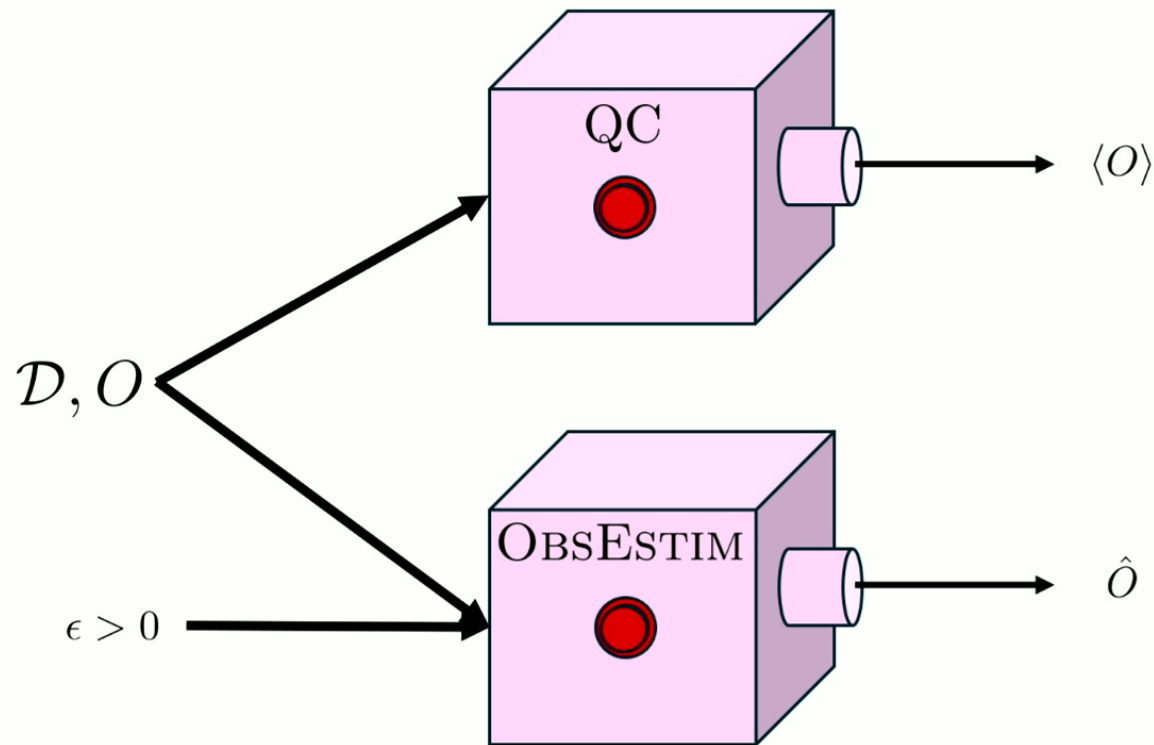
Single qubit noise channels \mathcal{N}

$$\mathcal{N}(\rho) = \sum_j K_j \rho K_j^\dagger$$

Simulation Tasks: $\text{SAMP}(\mathcal{D}, \epsilon)$



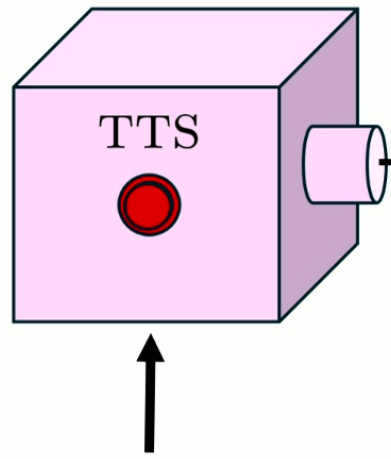
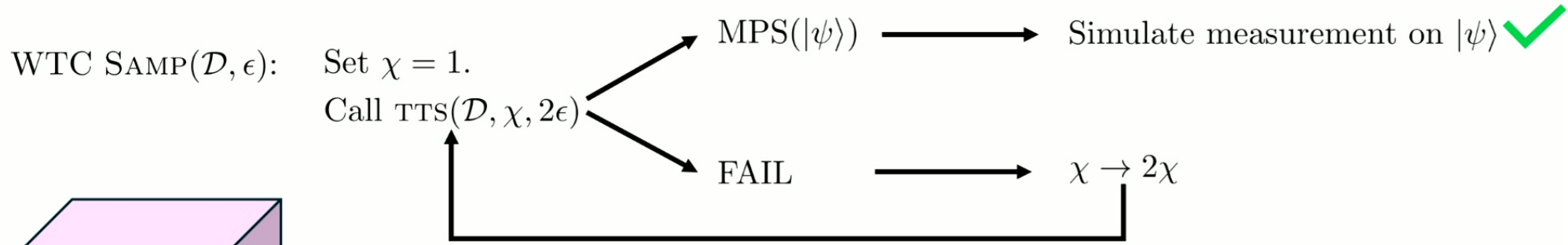
Simulation Tasks: $\text{OBS_ESTIM}(\mathcal{D}, O, \epsilon)$



$$\Pr \left(\left| \langle O \rangle - \hat{O} \right| \geq \epsilon \right) \leq \delta$$

HARD

Simulation Tasks: TTS to SAMP



MPS($|\psi_i\rangle$) with prob p_i

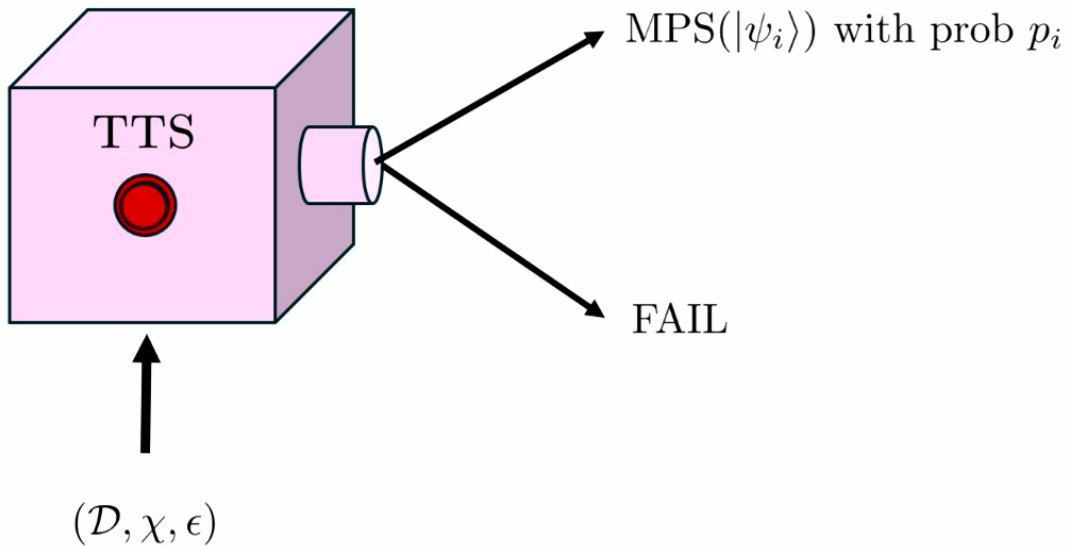
$|\psi_i\rangle$ is an MPS with BD $\leq \chi$

$$\left\| \rho_{\mathcal{D}} - \sum_i p_i \psi_i \right\|_{Tr} \leq \epsilon$$

\mathcal{D}
 $\chi \in \{1, 2, \dots\}$
 $\epsilon \geq 0$

If \exists 2ϵ -approx χ -BD MPS decomp. of $\rho_{\mathcal{D}}$, then one can solve SAMP(\mathcal{D}, ϵ) in $poly(\chi, n)$ time.

Algorithm



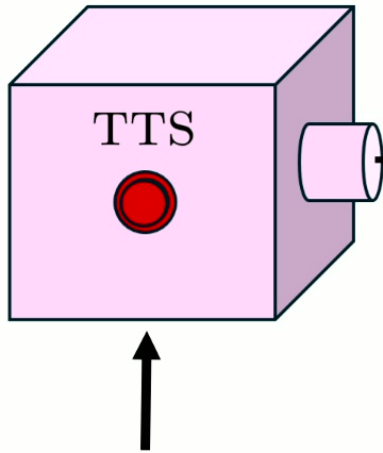
If $\exists \{p_i, |\psi_i\rangle\}_i$ s.t. $\text{BD}(|\psi_i\rangle) \leq \chi$ and

$$\left\| \rho_{\mathcal{D}} - \sum_i p_i \psi_i \right\|_{Tr} \leq \epsilon.$$

otherwise

Our algorithm will output “FAIL” on more inputs!

Algorithm

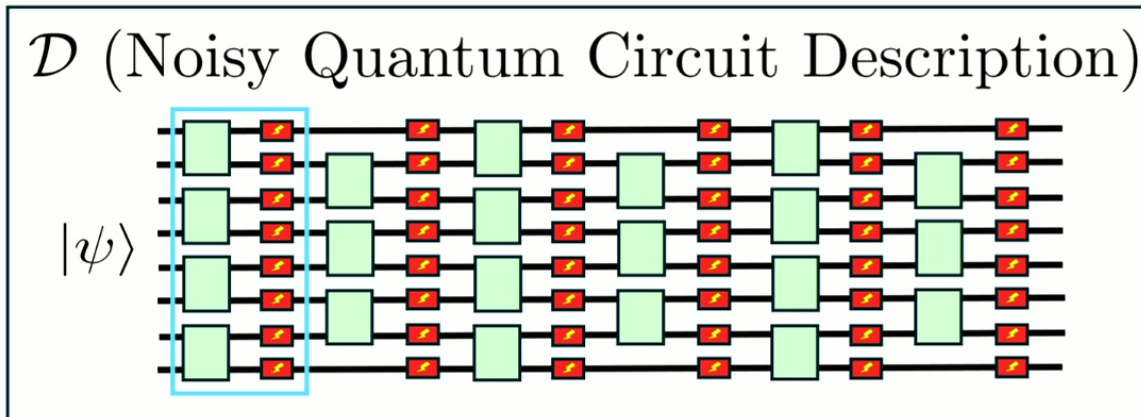


$(\mathcal{D}, \chi, \epsilon)$

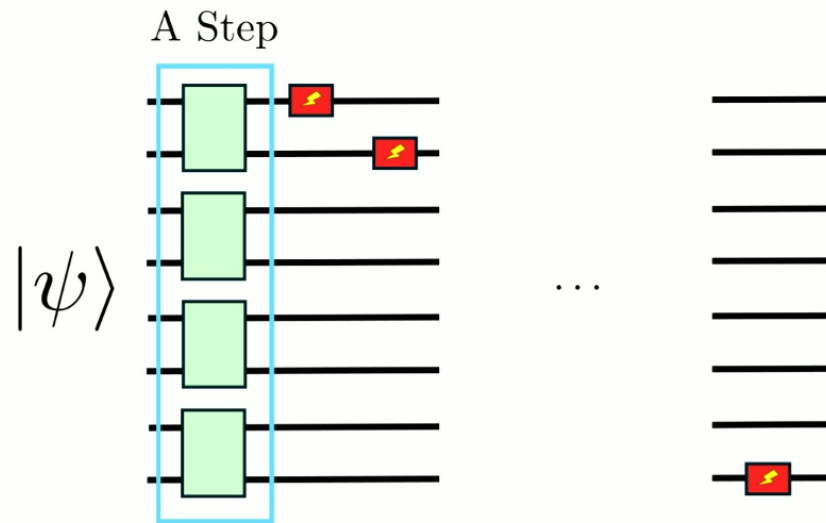
MPS($|\psi_i\rangle$) with prob p_i

$|\psi_i\rangle$ is an MPS with $\text{BD} \leq \chi$

$$\left\| \rho_{\mathcal{D}} - \sum_i p_i \psi_i \right\|_{Tr} \leq \epsilon(\mathcal{D}, \chi)$$

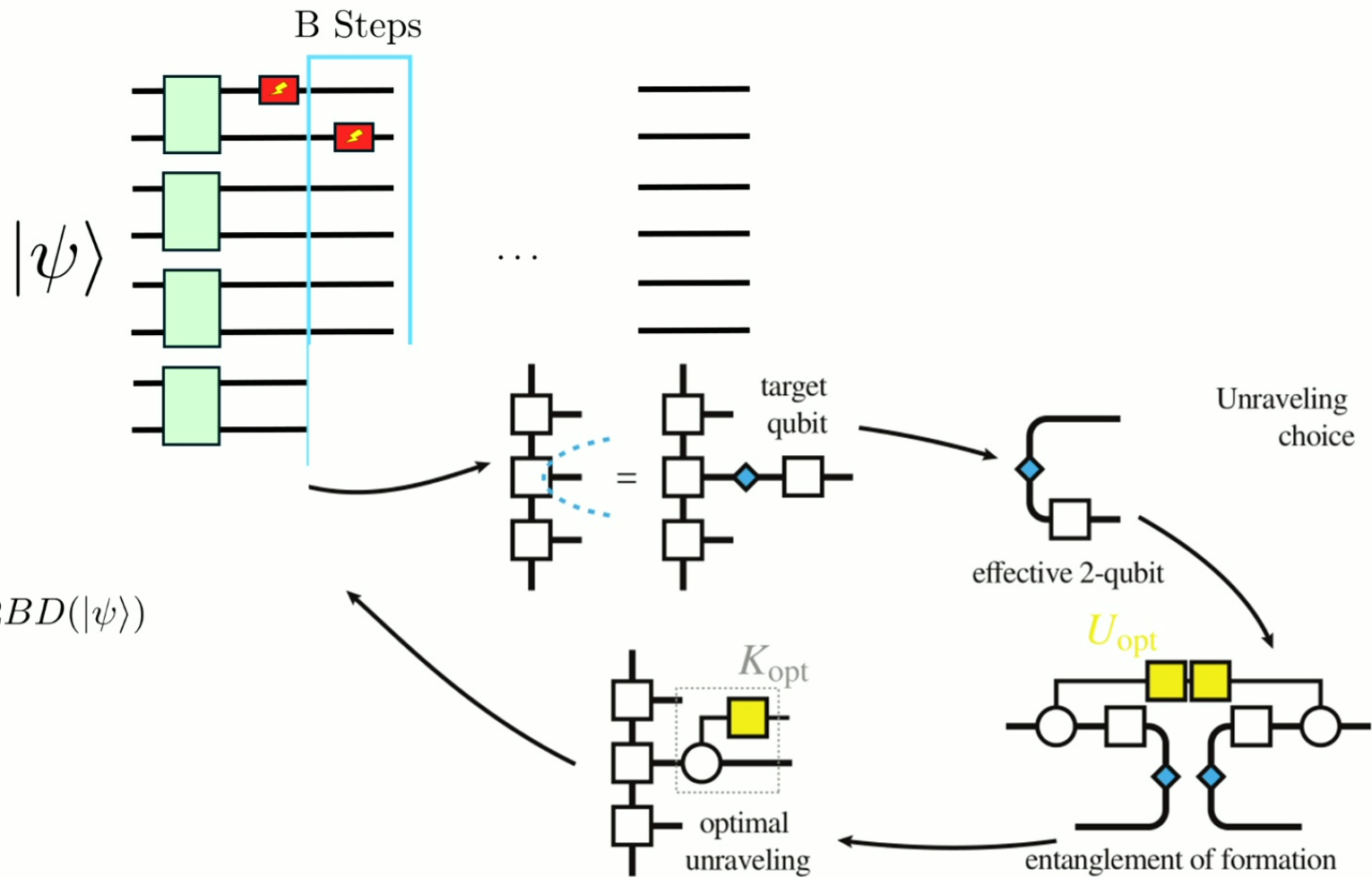


Algorithm

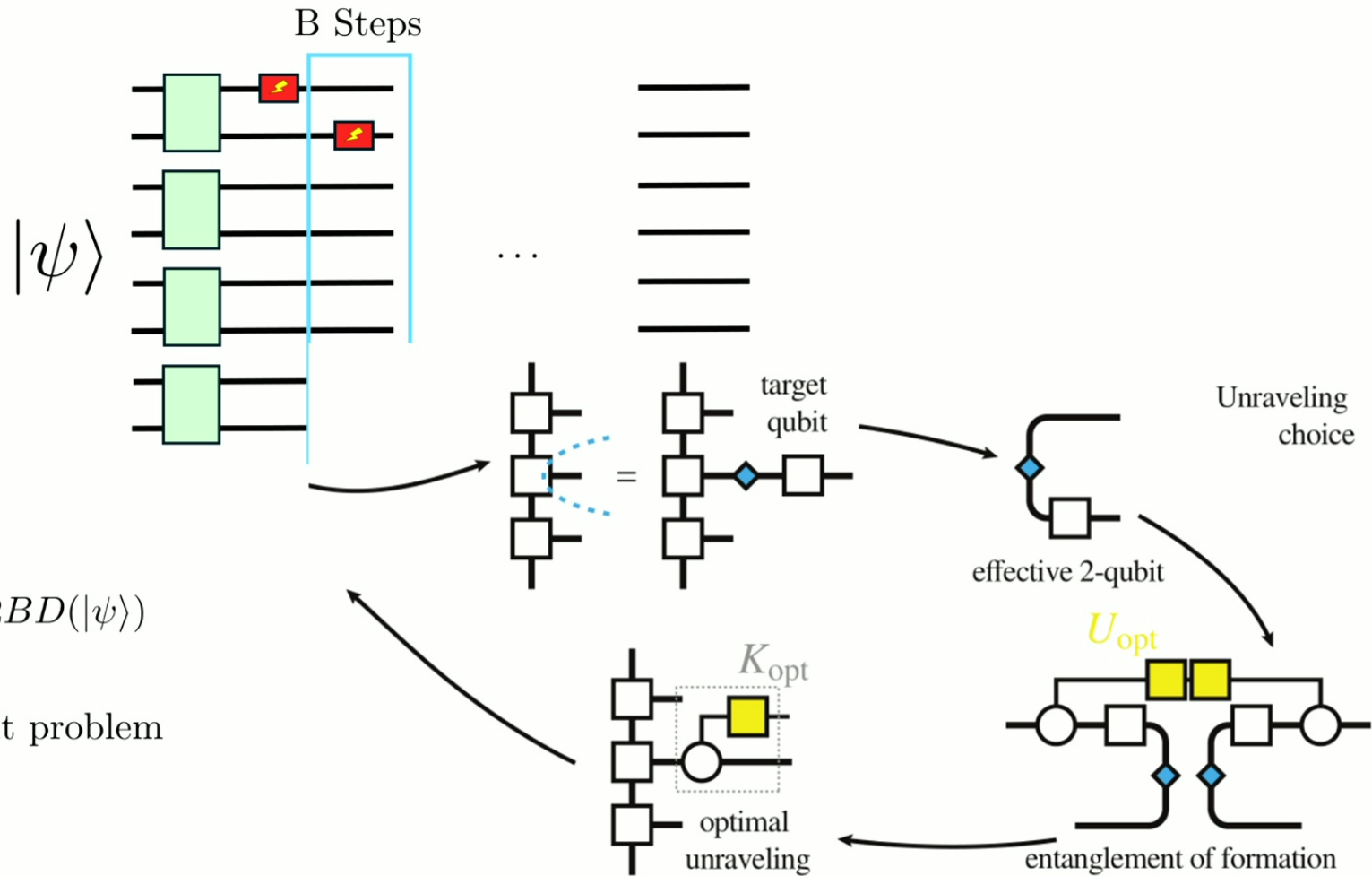


A Step: $BD(|\psi\rangle) \mapsto 2BD(|\psi\rangle)$

Algorithm



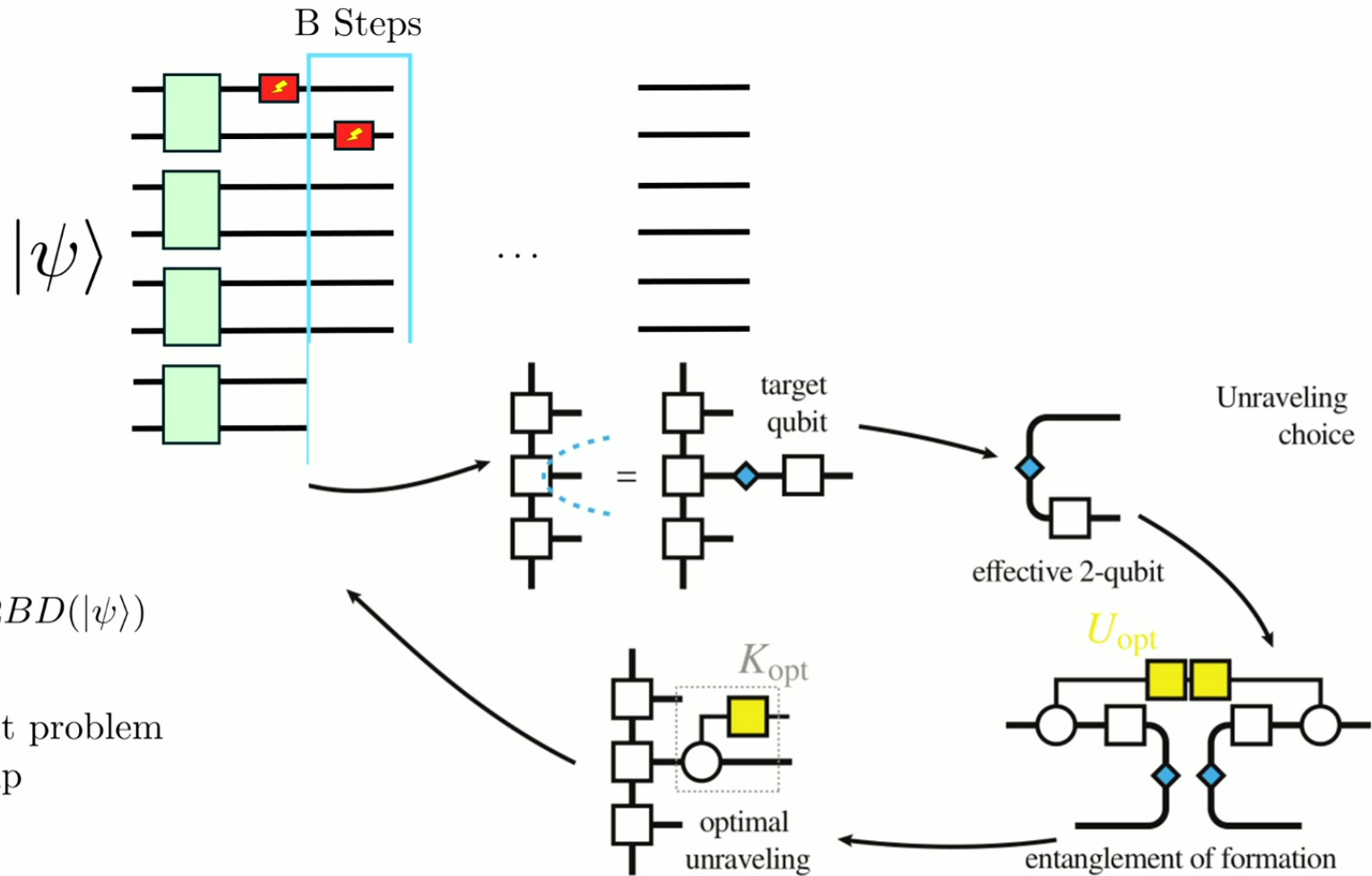
Algorithm



B Steps: $2BD(|\psi\rangle) \mapsto 2BD(|\psi\rangle)$

- (1) SVD
- (2) Transform to 2-qubit problem

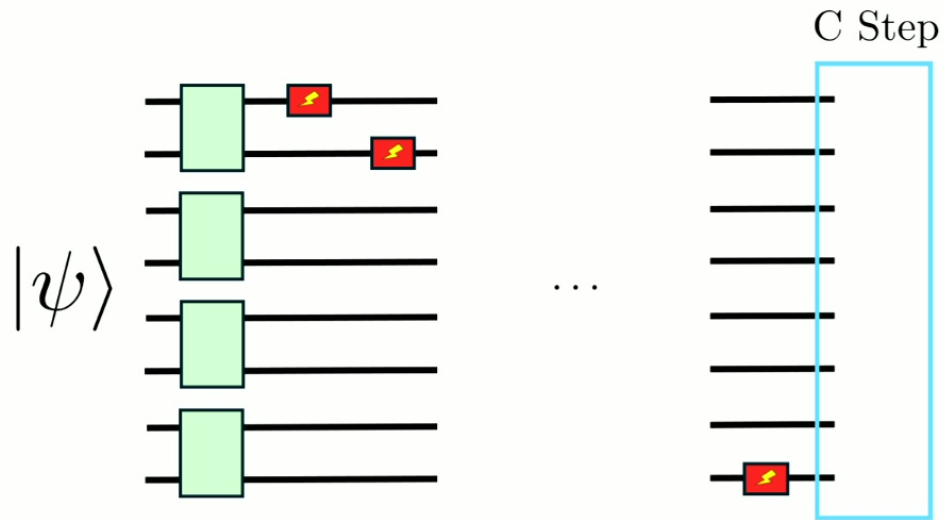
Algorithm



B Steps: $2BD(|\psi\rangle) \mapsto 2BD(|\psi\rangle)$

- (1) SVD
- (2) Transform to 2-qubit problem
- (3) Find optimal decomp

Algorithm



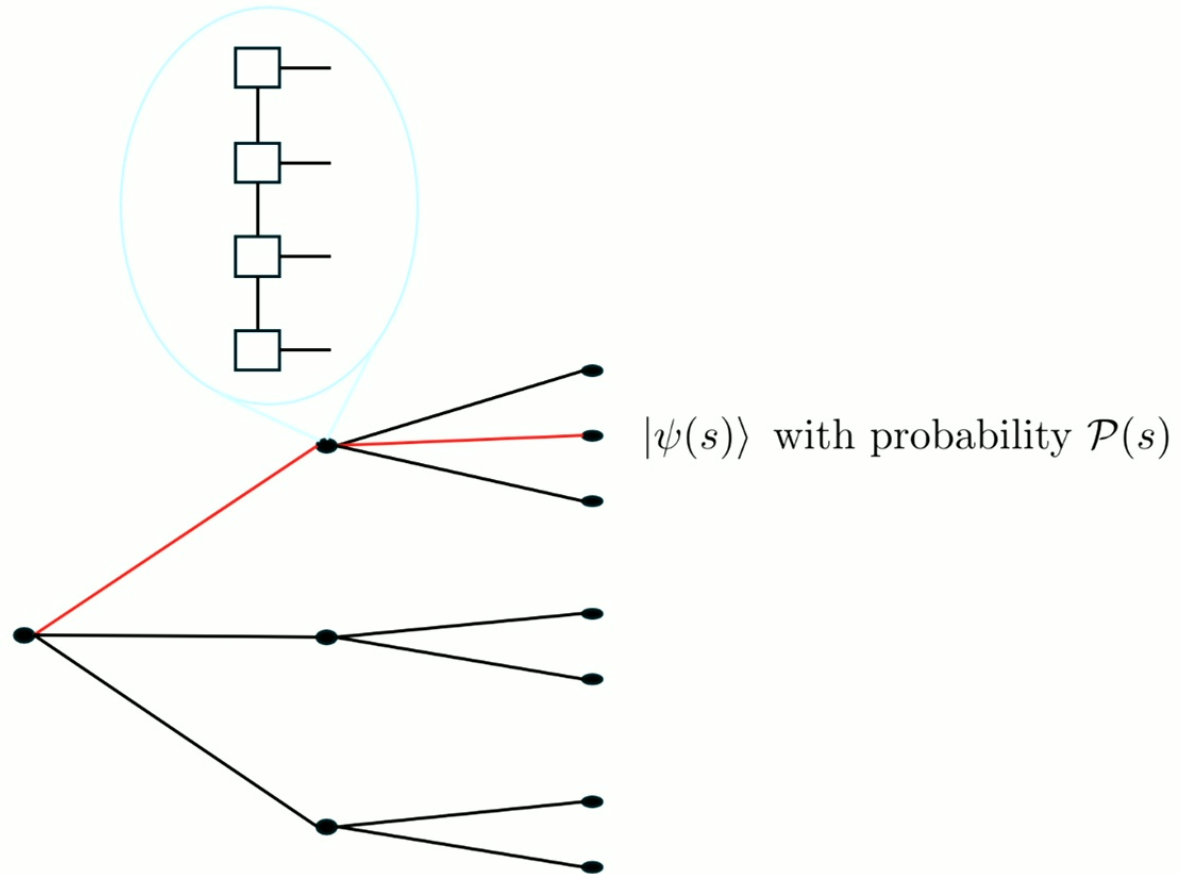
C Steps: $2BD(|\psi\rangle) \mapsto \chi$

Sweeps through MPS applying SVD at each bond.

If local BD $> \chi$ then truncate.

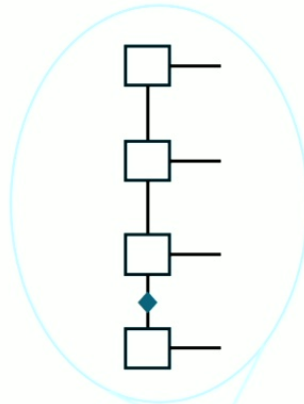
Store accumulated truncation error $\epsilon_{\text{layer}} = 4\sqrt{2} \sum_b \epsilon_b(\chi)$.

Performance Guarantee

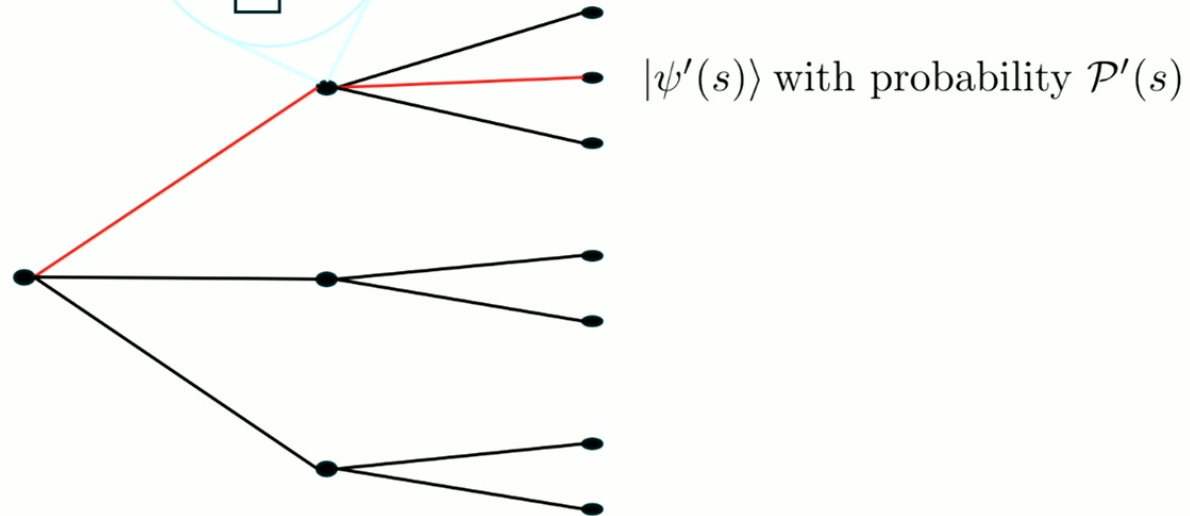


Performance Guarantee

$$\left\| \rho_{\mathcal{D}} - \sum_s \mathcal{P}'(s) \psi'(s) \right\|_{Tr} \leq \epsilon$$



$$\text{Result: } \epsilon_{tot} \leq \sum_s \epsilon(s) \mathcal{P}'(s)$$



Performance

		Our work
Simulation		Sampling
Run-time		$\text{poly}(\chi, n)$
Guarantee		A-postiori
Noise model		Any single qubit
Required assumptions		$\epsilon_{tot}^{UB}(\mathcal{D}, \chi)$ is small

Performance

	Pauli Path [Schuster 2024]	Our work
Simulation	Sampling	Sampling
Run-time	Quasi-polynomial	$\text{poly}(\chi, n)$
Guarantee	A-priori (avg. case)	A-posteriori
Noise model	Local depol.	Any single qubit
Required assumptions	Anti-concentration	$\epsilon_{tot}^{UB}(\mathcal{D}, \chi)$ is small

Performance

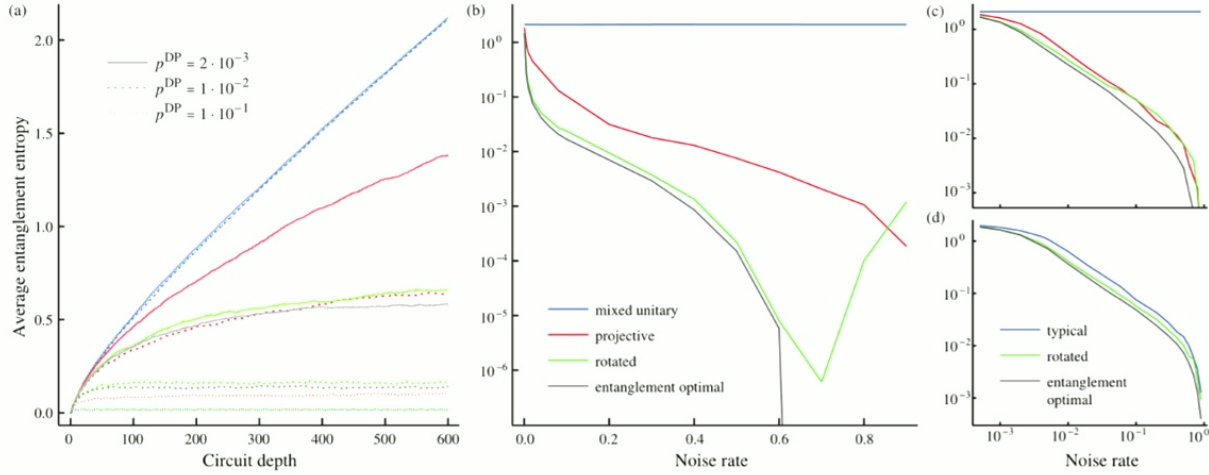


FIG. 4. Average entanglement entropy across the middle bond of the MPS in the numerical implementation of the trajectory unraveling algorithm to different random circuits with noise for different choices of unraveling. Each run results from one unraveled trajectory of a newly sampled circuit. For all settings, we computed the average entanglement after each layer. Panel (a) shows the growth of the entanglement with circuit depth for some noise rates of depolarizing noise on low-entangling random circuits. Panels (b) to (d) show the value of the entropy after the last layer (600) as a function of noise rates for (b) low-entangling random circuits with depolarizing noise (as in (a)), (c) dephasing noise and (d) low-entangling random circuits with local random rotations with amplitude damping noise. In these settings, the final value at depth 600 is representative of the relation between the different unravelings for all depths, like in panel (a).

Noise model	Typical	Projective	Rotated
Dephasing	$\sqrt{1 - \frac{p}{2}} \mathbb{1}, \sqrt{\frac{p}{2}} Z$	$\sqrt{1 - p} \mathbb{1}, \sqrt{p} 0\rangle\langle 0 , \sqrt{p} 1\rangle\langle 1 $	$U = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$
Depolarizing	$\sqrt{1 - \frac{3p}{4}} \mathbb{1}, \sqrt{\frac{p}{2}} X, \sqrt{\frac{p}{2}} Y, \sqrt{\frac{p}{2}} Z$	$\sqrt{1 - p} \mathbb{1}, \sqrt{\frac{p}{2}} 0\rangle\langle 0 , \sqrt{\frac{p}{2}} 0\rangle\langle 1 , \sqrt{\frac{p}{2}} 1\rangle\langle 0 , \sqrt{\frac{p}{2}} 1\rangle\langle 1 $	$U = \frac{1}{2} \begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & 1 & -1 & -1 \\ 1 & -1 & 1 & -1 \\ 1 & -1 & -1 & 1 \end{pmatrix}$
Amplitude damping	$\begin{pmatrix} 1 & 0 \\ 0 & \sqrt{1-\gamma} \end{pmatrix}, \begin{pmatrix} 0 & \sqrt{\gamma} \\ 0 & 0 \end{pmatrix}$	—	$U = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$

FIG. 5. Overview of some unravelings considered in the literature and implemented in the numerical simulations. The rotated unraveling is obtained by rotating the typical unraveling according to Eq. (5) using the specified unitary. More in Appendix A 5

Outlook

1. Minimizing entropy vs bond dimension
2. Globally optimal vs locally optimal
3. Noise reservoir and looking forward strategies
4. Multi-qubit optimization
5. A priori guarantees
6. Can noise reduce computational power through the decay of other computational resources?

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Thank You