

Lena Funcke



with Karl Jansen, Stefan Kühn, Tobias Hartung, et al.

Lattice 2022 Conference, Bonn, 8 August 2022

Computational costs of lattice field theory

Computational challenges of lattice field theory

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Supercomputer usage for different fields (INCITE 2019)



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Computational costs of lattice field theory

Supercomputer usage for different fields (INCITE 2019) \rightarrow Lattice QCD: $\sim 40\%$ Figure credit: Jack Wells, Kate Clark Biophysics Astrophysics Combustion Turbulence Plasma Physics LQCD Materials/Chemistry Al-Materials Weather/Climate Nuclear Physics Seismology Subsurface Flow

Computational challenges of lattice field theory

Critical slowing down, large autocorrelation times, ... \rightarrow Machine learning (*Algorithms* 8/10 Aug.)

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Figure credit:

BNL/RHIC



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Seismology

Nuclear Physics

Turbulence
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Figure credit: BNL/RHIC, CfA



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→ Quantum computing (Algorithms 9/10/11 Aug.)



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Example: finite baryon chemical potential

Reweighting procedure

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Partition function $Z = \int DUD\overline{\psi} D\psi e^{-S} = \int DUe^{-S_g} \det M$

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Figure credit: BNL/RHIC Example: phase quenched theory $\langle O \rangle = \frac{\int DUe^{-S_g} |\det M| e^{i\phi}O}{\int DUe^{-S_g} |\det M| e^{i\phi}} = \frac{\langle e^{i\phi}O \rangle_{pq}}{\langle e^{i\phi} \rangle_{pq}}$

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Highly oscillatory integrands

Near-cancellation of positive & negative contributions



Figure credit: BNL/RHIC, de Forcrand



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Near-cancellation of positive & negative contributions Sample number grows *exponentially* with volume V



Classical approaches to tackle the sign problem

Why is(n't) classical computing enough?

Classical approaches to tackle the sign problem

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Tensor networks

Describe quantum state $|\psi\rangle$ by network of small tensors

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Deep learning for path integral contour deformations¹ ...

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Simulate chemical potential, θ -term, real-time dynamics²



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Dalluis et al. (2

No efficient parametrization of highly entangled states

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Bañuls et al. (2013) Challenges

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No efficient parametrization of highly entangled states

In real-time evolution, tensor size can grow exponentially

Example: 1+1D Bose-Hubbard model

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Hamiltonian

$$\mathcal{H} = \sum_{j} -J\left(\hat{a}_{j}^{\dagger}\hat{a}_{j+1} + h.c.\right) + \frac{U}{2}\hat{n}_{j}(\hat{n}_{j} - 1)$$



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Real-time simulation¹

Analog quantum simulator: ultracold atoms

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Experimental results

"the controlled [quantum] dynamics runs for longer times than present classical algorithms can keep track of" ¹

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Practical quantum advantage in quantum simulation²

Here we overview the state of the art and future perspectives for quantum simulation, arguing that a first practical quantum advantage already exists in the case of specialized applications of analogue devices

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Quantum hardware

Quantum algorithms

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Achievements

Quantum advantage: outperformed classical computers¹



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cryptography, optimization problems, ...



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new technology \rightarrow need fundamentally new algorithms competition \rightarrow classical algorithms quickly advance



Example: "quantum advantage" (2019)

Example: "classical advantage" (2021)

Example: "quantum advantage" (2019)

Quantum supremacy using a programmable superconducting processor

The promise of quantum computers is that certain computational tasks might be executed exponentially faster on a quantum processor than on a classical processor¹. A fundamental challenge is to build a high-fidelity processor capable of running quantum algorithms in an exponentially large computational space. Here we report the use of a processor with programmable superconducting qubits²⁻⁷ to create quantum states on 53 qubits, corresponding to a computational state-space of dimension 2⁵³ (about 10¹⁶). Measurements from repeated experiments sample the resulting probability distribution, which we verify using classical simulations. Our Sycamore processor takes about 200 seconds to sample one instance of a quantum circuit a million times—our benchmarks currently indicate that the equivalent task for a state-of-the-art classical supercomputer would take approximately 10,000 years. This dramatic increase in speed compared to all known classical algorithms is an experimental realization of quantum supremacy⁸⁻¹⁴ for this specific computational task, heralding a much-anticipated computing paradigm.

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Closing the "Quantum Supremacy" Gap: Achieving Real-Time Simulation of a Random Quantum Circuit Using a New Sunway Supercomputer

We develop a high-performance tensor-based simulator for random quantum circuits(RQCs) on the new Sunway supercomputer. Our major innovations include: (1) a near-optimal slicing scheme, and a path-optimization strategy that considers both complexity and compute density; (2) a threelevel parallelization scheme that scales to about 42 million cores; (3) a fused permutation and multiplication design that improves the compute efficiency for a wide range of tensor contraction scenarios; and (4) a mixed-precision scheme to further improve the performance. Our simulator effectively expands the scope of simulatable RQCs to include the 10×10 (qubits) \times (1+40+1)(depth) circuit, with a sustained performance of 1.2 Eflops (single-precision), or 4.4 Eflops (mixed-precision)as a new milestone for classical simulation of quantum circuits; and reduces the simulation sampling time of Google Sycamore to 304 seconds, from the previously claimed 10,000 years.

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53- and 54-Qubit Sycamore Circuits with Single

Note: classical runtime improved from 2.5 days (2019) to 304 seconds (2021)

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→ Quantum-classical race: algorithms and hardware quickly advance

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→ For exponentially hard problems:
small quantum step ↔ giant classical leap

Example: "classical advantage" (2021)

Closing the "Quantum Supremacy" Gap: Achieving Real-Time Simulation of a Random Quantum Circuit Using a New Sunway Supercomputer

We develop a high-performance tensor-based simulator for random quantum circuits(RQCs) on the new Sunway supercomputer. Our major innovations include: (1) a near-optimal slicing scheme, and a path-optimization strategy that considers both complexity and compute density; (2) a threelevel parallelization scheme that scales to about 42 million cores; (3) a fused permutation and multiplication design that improves the compute efficiency for a wide range of tensor contraction scenarios; and (4) a mixed-precision scheme to further improve the performance. Our simulator effectively expands the scope of simulatable RQCs to include the 10×10 (qubits) \times (1+40+1)(depth) circuit, with a sustained performance of 1.2 Eflops (single-precision), or 4.4 Eflops (mixed-precision)as a new milestone for classical simulation of quantum circuits; and reduces the simulation sampling time of Google Sycamore to 304 seconds, from the previously claimed 10,000 years.

53- and 54-Qubit Sycamore Circuits with Single

Note: classical runtime improved from 2.5 days (2019) to 304 seconds (2021)

The Path to Go...

A Rough Sketch...

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State of the Art

IBM: 27 physical qubits (2019) \rightarrow 65 (2020) \rightarrow 127 (2021)



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IBM: 433 (2022) → 1121 (2023) → 4158 (2025) → ...



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Arute et al. (2019) Carlow (2018)



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Far Future

Need $\mathcal{O}(10^7 - 10^8)$ logical qubits for lattice volume of 96³



Number of logical qubits

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Far Future

Need $O(10^7 - 10^8)$ logical qubits for lattice volume of 96³

 \rightarrow Analogy: lattice QCD from 1980s to 2020s?



Noisy quantum circuit

Error mitigation versus error correction

Noisy quantum circuit

Error mitigation versus error correction



Noisy quantum circuit



Error mitigation versus error correction

Noisy quantum circuit



Error mitigation versus error correction

Problem

Quantum noise: affecting qubits, gates, measurement

Noisy quantum circuit



Error mitigation versus error correction

Problem

Quantum noise: affecting qubits, gates, measurement Near-term solution Error mitigation: reduce noise on NISQ devices

Noisy quantum circuit



Error mitigation versus error correction

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Quantum noise: affecting qubits, gates, measurement Near-term solution Error mitigation: reduce noise on NISQ devices Long-term solution Error correction (EC): fault-tolerant quantum computation

Noisy quantum circuit



Error mitigation versus error correction

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Quantum noise: affecting qubits, gates, measurement **Near-term solution** Error mitigation: reduce noise on NISQ devices **Long-term solution** Error correction (EC): fault-tolerant quantum computation E.g. bit-flip code,¹ Shor code,² toric code,³ GKP code,⁴ ...

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Problem

Quantum noise: affecting qubits, gates, measurement **Near-term solution** Error mitigation: reduce noise on NISQ devices **Long-term solution** Error correction (EC): fault-tolerant quantum computation E.g. bit-flip code,¹ Shor code,² toric code,³ GKP code,⁴ ... **Quantum threshold theorem**

For EC, need extra qubits and noise below threshold⁵

¹ Peres (1985), ² Shor (1995), ³ Kitaev (1997), ⁴ Gottesmann et al. (2001), ... ⁵ Shor (1996), Knill et al. (1998), Kitaev (2003), Aharonov et al. (2008) 9

Noisy quantum circuit



Error mitigation versus error correction

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Quantum noise: affecting qubits, gates, measurement Near-term solution Error mitigation: reduce noise on NISQ devices Long-term solution Error correction (EC): fault-tolerant quantum computation E.g. bit-flip code,¹ Shor code,² toric code,³ GKP code,⁴ ... Quantum threshold theorem For EC, need extra qubits and noise below *threshold*⁵ E.g. surface code needs > 1000 extra qubits for p < 0.1%

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Error mitigation: how can we reduce the noise?

Example: measurement error mitigation

Operator rescaling method

Error mitigation: how can we reduce the noise?



Operator rescaling method

Error mitigation: how can we reduce the noise?



Operator rescaling method

Goal

mitigate bit-flip errors during readout: $0 \xrightarrow{p_0} 1 \text{ or } 1 \xrightarrow{p_1} 0$
Example: measurement error mitigation $|\psi(\vec{\alpha})\rangle = \begin{bmatrix} |0\rangle - U(\alpha_1) + U(\alpha_3) + U(\alpha_3$

Operator rescaling method

Goal

mitigate bit-flip errors during readout: $0 \xrightarrow{p_0} 1$ or $1 \xrightarrow{p_1} 0$ Method ¹

replace operators by noisy operators: $\langle \tilde{\psi} | \boldsymbol{O} | \tilde{\psi} \rangle \rightarrow \langle \psi | \tilde{\boldsymbol{O}} | \psi \rangle$

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Readout	Bit Flips	Probability	Noisy Operator
correct	$0 \rightarrow 0, 1 \rightarrow 1$	$(1-p_0)(1-p_1)$	$\tilde{\boldsymbol{\textit{0}}} = \boldsymbol{Z} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$

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for outcome 0	$0 \rightarrow 1, 1 \rightarrow 1$	$p_0(1-p_1)$	$\tilde{\boldsymbol{0}} = -\mathbb{I} = \begin{pmatrix} -1 & 0\\ 0 & -1 \end{pmatrix}$
for outcome 1	$0 \rightarrow 0, 1 \rightarrow 0$	$(1 - p_0)p_1$	$ ilde{oldsymbol{O}} = \mathbb{I} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$

Example: measurement error mitigation $U(\alpha_3)$ $|\psi(\vec{\alpha}) angle =$ $U(\alpha_2)$ $U(\alpha_4)$

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incorrect for both outcomes	$0 \rightarrow 1, 1 \rightarrow 0$	$p_0 p_1$	$\tilde{\boldsymbol{O}} = -Z = \begin{pmatrix} -1 & 0\\ 0 & 1 \end{pmatrix}$	$ = (1 - p_0)(1 - p_1)\mathbf{Z} + p_0p_1(-\mathbf{Z}) + p_0(1 - p_1)(-\mathbf{I}) + (1 - p_0)p_1\mathbf{I} $
for outcome 0	$0 \rightarrow 1, 1 \rightarrow 1$	$p_0(1-p_1)$	$\tilde{\boldsymbol{\textit{0}}} = -\mathbb{I} = \begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix}$	
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incorrect for both outcomes	$0 \rightarrow 1, 1 \rightarrow 0$	p_0p_1	$\tilde{0} = -Z = \begin{pmatrix} -1 & 0\\ 0 & 1 \end{pmatrix}$	$= (1 - p_0)(1 - p_1)\mathbf{Z} + p_0p_1(-\mathbf{Z}) + p_0(1 - p_1)(-\mathbf{I}) + (1 - p_0)p_1\mathbf{I}$
for outcome 0	$0 \rightarrow 1, 1 \rightarrow 1$	$p_0(1-p_1)$	$\tilde{\boldsymbol{0}} = -\mathbb{I} = \begin{pmatrix} -1 & 0\\ 0 & -1 \end{pmatrix}$	Rescaled (zero-noise) operator:
for outcome 1	$0 \rightarrow 0, 1 \rightarrow 0$	$(1 - p_0)p_1$	$ ilde{oldsymbol{O}} = \mathbb{I} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$	$\int = \frac{1}{1 - p_0 - p_1} \tilde{O} - \frac{p_1 - p_0}{1 - p_0 - p_1} \mathbb{I}$

Example: measurement error mitigation

Example: gate error mitigation

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Operator rescaling method¹

Benchmark: Z and Z_1Z_2 operators on IBM-Q hardware



Carlow (2018)

¹ Kandala et al. (2017), Yeter-Aydeniz et al. (2019), LF et al. (2020)

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Benchmark: Z and Z_1Z_2 operators on IBM-Q hardware Result: measurement error reduced by factor 10





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Example: gate error mitigation

Other mitigation techniques

Zero-noise extrapolation,² randomized compiling,³ quasi-probability decomposition,⁴ ...

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Lattice field theory applications

Zero-noise extrapolation for lattice Schwinger model:



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Experimental results on "public" QC

Experimental results on "private" QC

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Experimental results on "private" QC

IBM-Q's superconducting qubits

Real-time evolution: Schwinger model,¹ SU(2),² SU(3),³ ...

1+1D SU(3) gauge theory, one plaquette³



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Real-time evolution: Schwinger model, 1 SU(2), 2 SU(3), 3 ...



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Experimental results on "private" QC

Trapped ions

Real-time evolution: Schwinger model, ⁵...



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Example: hybrid quantum-classical algorithms

Variational Quantum Eigensolver (VQE)¹

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Key concept

Classical computer: main computation

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Key concept	Goal
Classical computer: main computation	Find ground state and excited states of Hamiltonian ${\cal H}$
Quantum computer: classically hard/intractable part	
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Quantum computer: classically hard/intractable part	Variational approach
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	Classical computer	

Given $E(\vec{\alpha}_i)$, find optimized parameters $\vec{\alpha}_{i+1}$



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Variational Quantum Eigensolver (VQE)¹

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Find ground state and excited states of Hamiltonian \mathcal{H} **Variational approach** Minimize $E(\vec{\alpha}) = \langle \psi(\vec{\alpha}) | \mathcal{H} | \psi(\vec{\alpha}) \rangle$ w.r.t. parameters $\vec{\alpha}$ **Classical computer** Given $E(\vec{\alpha}_i)$, find optimized parameters $\vec{\alpha}_{i+1}$



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Variational Quantum Eigensolver (VQE)¹



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Quantum circuit design¹

Example: geometrical method²

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Quantum circuit design¹

Example: geometrical method²

Maximal expressivity

 $|\psi(\vec{\alpha})\rangle$ should reach all physical states in Hilbert space



Quantum circuit design¹

Maximal expressivity

 $|\psi(\vec{\alpha})\rangle$ should reach all physical states in Hilbert space

Minimality

 $|\psi(\vec{\alpha})\rangle$ should not contain any redundant parameters



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Quantum circuit design¹

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 $|\psi(\vec{\alpha})\rangle$ should not contain any redundant parameters

Symmetry

 $|\psi(\vec{\alpha})\rangle$ should include physical symmetries



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Example: geometrical method²

Manifolds

Circuit manifold *M*: states $|\psi(\vec{\alpha})\rangle$ reachable by circuit

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Example: geometrical method²

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State manifold S: states $|n(\vec{\alpha})\rangle$ of quantum device

Optimization

minimize: $\operatorname{codim}(M) = \dim(S) - \dim(M) \stackrel{!}{=} 0$

Quantum circuit design¹

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14
How to prepare the quantum state?

Quantum circuit design¹

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14

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Infinite Hilbert space

Gauge invariance

Infinite Hilbert space

Gauge invariance

Problem

Continuous gauge theory requires ∞ -dim. Hilbert space

Infinite Hilbert space

Gauge invariance

Problem

- Continuous gauge theory requires ∞ -dim. Hilbert space
- **First approach**
- Integrate out gauge field: only possible in 1+1D

Infinite Hilbert space

Gauge invariance

Problem

- Continuous gauge theory requires ∞ -dim. Hilbert space
- **First approach**
- Integrate out gauge field: only possible in 1+1D
- Second approach
- Approximate gauge group:¹ e.g. $U(1) \rightarrow \mathbb{Z}_n$



Infinite Hilbert space

Gauge invariance

Problem

- Continuous gauge theory requires ∞-dim. Hilbert space
- **First approach**
- Integrate out gauge field: only possible in 1+1D
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Truncate irreps:² e.g. for $F_j |l\rangle = |l\rangle$, use finite |l| < L

Infinite Hilbert space

Gauge invariance

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The Path to Go...

A Rough Sketch...

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Present

Hardware: O(10 - 100) noisy qubits with error mitigation

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1.0

O NILSON LOOP

0.01 L

SU (2) $\beta = 3.0$ 2^4 4^4 6^4 8^4 10^4 LATTICE SIZE 4×1^4 6×6 Creutz (1980)



A Rough Sketch...

The Path to Go...

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Future

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The Way Forward...

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The Way Forward...

A Rough Sketch...

Quantum

new and quickly progressing \rightarrow high risk, high gain





The Way Forward...

A Rough Sketch...







Backup: details of Bose-Hubbard quantum simulation

Classical versus quantum simulation

Bose-Hubbard Hamiltonian

$$\mathcal{H} = \sum_{j} -J\left(\hat{a}_{j}^{\dagger}\hat{a}_{j+1} + h.c.\right) + \frac{U}{2}\hat{n}_{j}(\hat{n}_{j} - 1) + \frac{K}{2}\hat{n}_{j}j^{2}$$

Experimental goal¹

Simulate quantum *tunneling* from even to odd sites



Experimental setup

Quantum simulation: ultracold atoms in optical lattice Classical benchmark: tensor networks (MPS-based)

¹ Trotzky et al. (2012)

Why is(n't) classical computing enough?

Experimental results

Classical (line) vs. quantum (circles) simulation



this dynamical quantum simulator outperforms any continuous-time numerical simulation, for which the calculational effort increases with t. Simulation methods on classical computers, such as matrix-product state based t-DMRG used here, suffer from an extensive increase in entanglement entropy which limits the relaxation times accessible in the calculations^{24,25}.

Backup: analog versus digital quantum computers

Analog

Concept

- Use controllable quantum system to simulate the behavior of another quantum system
- Continuous time evolution
- Usually non-universal



Concept

Construct set of logical gates onto qubits

Digital

- Discrete time evolution
- Usually universal



Backup: how to measure the energy in VQE?

Example: massless Schwinger model

Mapping the model to qubits

Original Hamiltonian

$$\mathcal{H} = -\frac{i}{2a} \sum_{n=0}^{N-2} \left(\phi_n^{\dagger} e^{i\theta_n} \phi_{n+1} - h.c. \right) + \frac{ag^2}{2} \sum_{n=0}^{N-2} F_n^2$$
with $\theta_n = -aqA_n^1$, $gF_n = E_n$, $[\theta_n, L_m] = i\delta_{nm}$, $\theta_n \in [0, 2\pi]$
Eliminate θ_n
 $\phi_n^{\dagger} e^{i\theta_n} \phi_{n+1} \rightarrow \phi_n^{\dagger} \phi_{n+1}$ from gauge transformation:
 $\phi_n \rightarrow (\prod_{k=0}^{n-1} e^{-i\theta_n}) \phi_n$ and $\phi_n^{\dagger} \rightarrow \phi_n^{\dagger} (\prod_{k=0}^{n-1} e^{i\theta_{n-k}})$
Eliminate F_n
 $F_n = \sum_{k=0}^n Q_k$ from solving Gauß law (for OBC):

$$F_n - F_{n-1} = Q_n \ \forall n$$
, where $Q_n = \phi_n^{\dagger} \phi_n - \frac{1}{2} [1 - (-1)^n]$

Dimensionless spin Hamiltonian¹ $\mathcal{H} = x \sum_{n=0}^{N-2} (\sigma_n^+ \sigma_{n+1}^- + \sigma_n^- \sigma_{n+1}^+) + \frac{1}{2} \sum_{n=0}^{N-2} \left\{ \sum_{k=0}^n [(-1)^k + \sigma_k^z] \right\}^2$ from mapping $\phi_n^\dagger \phi_{n+1} \to \sigma_n^+ \sigma_{n+1}^-$ and $\phi_n^\dagger \phi_n \to \frac{1}{2} (\sigma_n^z + \mathbb{I})$ Quantum computer Measurement of $\langle \psi | \boldsymbol{O} | \psi \rangle$ with $\boldsymbol{O} \in \{\mathbb{I}, \sigma^z\}^{\otimes N}$ $\mathcal{H} = \sum_k h_k U_k^* \boldsymbol{O}_k U_k$ with $U_k^* \boldsymbol{O}_k U_k \in \{\mathbb{I}, \sigma^x, \sigma^y, \sigma^z\}^{\otimes N}$



¹ Banks et al. (1976), Hamer et al. (1997)

Gokhale et al. (2020

Backup: quantum volume

Concept

Timeline

Motivation

Number of noisy qubits: no good performance measure

New performance measure

Measure capabilities and error rates of quantum device

IBM's definition

 $\log_2 V_Q = \arg \max_{n \le N} \{\min[n, d(n)]\}$

Example

Successfully run circuit of depth d = 8 on n = 8 qubits: quantum volume is $V_Q = 2^8 = 256 \rightarrow$ size of state space "Success"

Most likely outputs of the circuit are computed correctly 67% of the time with a 2σ confidence interval

Last three years

Early 2020: $V_Q = 32$ (IBM) for d = 5, n = 5Early 2021: $V_Q = 512$ (Honeywell) for d = 9, n = 9Early 2022: $V_Q = 4096$ (Quantinuum) for d = 12, n = 12



Chow, Gambetta (2020)

2017 2018 2019 2020 2021 2022 2023 2024 2025 2026 2027 2028 2029 2030

Backup: preparing for overcoming sign problems in 3+1D

Example: 3+1D compact U(1) theory with θ -term

Details: numerical ED results for single cube

Goal

Simulate phase transition at $\theta = \pi$ and large $g = \beta^{-1/2}$

Analytical results

Derivation of Hamiltonian lattice θ -term: $\theta Q = -\frac{ig^2\theta}{8\pi^2 a} \sum_{n,i,j,k,b} \varepsilon_{ijk} \operatorname{Tr} \left[E_{n,i}^b \lambda^b \left(U_{n,jk} - U_{n,jk}^\dagger \right) \right]$

Numerical results

Unlike in QCD, transition in U(1) might be not of first order

Near-future outlook

Larger-volume simulation with 3+1D tensor networks

Far-future outlook

First quantum simulation of 3+1D θ -term

Kan, LF, Kühn, Dellantonio, Zhang, Haase, Muschik, Jansen (2021a, 2021b)

