Computing Topological Field Theories

Lecture 3: Tensor Networks & Quantum Computing for Lattice Field Theories

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Tensor Networks and Quantum Computing

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Overview: computing topological field theories

Numerical computations

Lecture 1: Monte Carlo method High-precision lattice computations Computational issues

Lecture 2: Machine learning Efficient sampling, thermodynamic observables...

Lecture 3: Tensor networks & quantum computing Topological θ-terms, chemical potentials... **Theoretical models**

Standard Model "Real world" Quarks, gluons, Higgs...

1+1D ϕ^4 **theory** Higgs toy model Symmetry breaking...

1+1D Schwinger model QCD toy model θ-term, confinement... Experiments

Observables Spectrum, free energy, entropy, pressure...

LHC, cosmology, ... Heavy-ion collisions, Early-universe physics...



(Image credit: ALICE Collaboration / CERN)

Reminder: MCMC is hungry & challenging

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Computational costs of lattice field theory

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

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Computational challenges of lattice field theory

No direct computation of thermodynamic observables, … → Machine learning (lecture yesterday)



Baryon density

Reminder: MCMC is hungry & challenging

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Computational costs of lattice field theory



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Computational challenges of lattice field theory

No direct computation of thermodynamic observables, ... \rightarrow Machine learning (lecture yesterday) Baryon chemical potential, θ -term, real-time evolution, ...





Reminder: MCMC is hungry & challenging

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Computational costs of lattice field theory



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Computational challenges of lattice field theory

No direct computation of thermodynamic observables, ... \rightarrow Machine learning (lecture yesterday) Baryon chemical potential, θ -term, real-time evolution, ... \rightarrow Tensor networks

→ Quantum computing (lecture today)



Baryon density

Reminder: Why is the sign problem exponentially hard?

Example: finite baryon chemical potential

Computing observables

$$\langle O \rangle = \frac{1}{Z} \int DUD\bar{\psi} D\psi e^{-S_E}O = \frac{1}{Z} \int DUe^{-S_g} \det M O$$

MCMC sampling

Interpretation of $e^{-S_g} \det M$ as *real* probability weight **Sign problem**

For $\mu \neq 0$, *complex* det *M*: $[\det M(\mu)]^* = [\det M(-\mu^*)]$



- \rightarrow no probability weight
- \rightarrow no MCMC sampling



Reweighting procedure

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

Highly oscillatory integrands

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



 $\int dx \exp(-x^2 + i\lambda x) \to \int dx \exp(-x^2) \cos(\lambda x)$

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Do we really need quantum computing?

Classical approaches to tackle the sign problem

Tensor networks

Describe quantum state $|\psi\rangle$ by network of small tensors E.g. $|\psi\rangle = \sum c_{i_1,\dots,i_N} |i_1\rangle \otimes \dots |i_N\rangle = \sum A_1^{i_1} \dots A_N^{i_N} |i_1\rangle \otimes \dots |i_N\rangle$ Variational algorithm: minimize energy $E(\vec{\alpha}) = \langle \psi | \mathcal{H} | \psi \rangle$





Bañuls et al. (2013)

Why is(n't) classical computing enough?

Prospects

Simulate chemical potential, θ -term, real-time dynamics² Mostly focus on 1+1D, first simulations in 2+1D & 3+1D³



Other approaches

Deep learning for path integral contour deformations,¹...

No efficient parametrization of highly entangled states

In real-time evolution, tensor size can grow *exponentially*

¹ Wynen et al. (2020), ..., ² Bañuls et al. (2017), Byrnes et al. (2002), Pichler et al. (2016), ..., ³ Kuramashi et al. (2018), Felser et al. (2020), Akiyama et al. (2019), Magnifico et al. (2021), ...

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Do we really need quantum computing?

Example: 1+1D Bose-Hubbard model

Hamiltonian

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



Real-time simulation¹

- Analog quantum simulator: ultracold atoms
- Classical benchmark: tensor networks (MPS)

Experimental results

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

Why is(n't) classical computing enough?

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



¹ Trotzky et al. (2012), ² Daley et al. (2022)

Quantum computing: where do we stand?

Quantum hardware

Achievements

Quantum advantage: outperformed classical computers¹ Exponential speedup of *specific* classical computations

Challenges

O(100) digital / O(1000) analog qubits \rightarrow need more Noise \rightarrow need quantum error mitigation / correction



Arute et al. (2019)



Zhong et al. (2020)

¹Arute et al. (2019), Zhong et al. (2020, 2021), Yulin (2021), Zhu (2021), Madsen (2022). Applications

Quantum algorithms

Cryptography, optimization problems, ... Particle / nuclear / condensed matter physics, ...

Challenges

New technology \rightarrow need fundamentally new algorithms Competition \rightarrow classical algorithms quickly advance



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Quantum computing: where do we stand?

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.

→ Quantum-classical race: algorithms and hardware quickly advance → For exponentially hard problems: small quantum step \leftrightarrow 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 Precision Storage to Disk (8 bytes per amplitude)



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

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Quantum computing: where will we go?

The Path to Go...

A Rough Sketch...

State of the Art

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

Near Future

IBM: 433 (2022) \rightarrow 1121 (2023) \rightarrow 4158 (2025) \rightarrow ...

Google: 1,000,000 physical / 1000 logical qubits (2029)?



Far Future

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

Arute et al. (2019)

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



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11

How can we reduce the noise?

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 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. toric code needs > 1000 extra qubits for p < 0.1%

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)

Error mitigation: how can we reduce the noise?



¹ Single *Z* operator: Kandala et al. (2017), strings of *Z* operators: Yeter-Aydeniz et al. (2019), generalizations: LF, et al. (2020), (2021); Alexandrou, et al. (2021a), (2021b)

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Error mitigation: how can we reduce the noise?

Example: measurement error mitigation

Operator rescaling method¹

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



Example: gate error mitigation

Other mitigation techniques

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

Lattice field theory applications

Zero-noise extrapolation for lattice Schwinger model:



¹ Kandala et al. (2017), Yeter-Aydeniz et al. (2019), LF et al. (2020); ² Li et al. (2017), Wallman et al. (2016), ⁴ Temme et al. (2017), van den Berg (2020), ...

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14

Which field theories have already been simulated?



¹ Klco et al. (2018), de Jong et al. (2021), ² Klco et al. (2019), ³ Ciavarella et al. (2019a,b), ⁴ Atas et al. (2021), ⁵ Martinez et al. (2016), Nguyen et al. (2021), ⁶ Bloch et al. (2012), ⁷ Yang et al. (2020), Mil et al. (2020), ...

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How to simulate these field theories?

Example: hybrid quantum-classical algorithms

Key concept

Classical computer: main computation Quantum computer: classically hard/intractable part Advantages: already for small quantum hardware?



Variational Quantum Eigensolver (VQE)¹

Goal

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 $\vec{\alpha}_{i+1}$

Quantum device

Given $\vec{\alpha}_i$, prepare $|\psi(\vec{\alpha})\rangle$ and measure $E(\vec{\alpha}_i)$



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

Quantum device

Given $\vec{\alpha}_i$, prepare $|\psi(\vec{\alpha})\rangle$ and measure $E(\vec{\alpha}_i)$



How to prepare the quantum state?

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

Symmetry

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



Example: geometrical method²

Manifolds

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

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

Optimization

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

 $\det \begin{pmatrix} \operatorname{Re}|\partial_{\alpha_{1}}\psi\rangle & \cdots & \operatorname{Re}|\partial_{\alpha_{k}}\psi\rangle\\ \operatorname{Im}|\partial_{\alpha_{1}}\psi\rangle & \cdots & \operatorname{Im}|\partial_{\alpha_{k}}\psi\rangle \end{pmatrix} = 0 \text{ iff } \alpha_{k} \text{ redundant}$



¹ Martinez et al. (2016), Klco et al. (2018,2019), Ciavarella et al. (2019a,b), Schweizer et al. (2019), Yang et al. (2020), Mil et al. (2020), de Jong et al. (2021), Nguyen et al. (2021), Atas et al. (2021), ..., ² LF, Hartung, Jansen, Kühn, Stornati, *Quantum* (2021), *IEEE ICWS* (2021)

How to measure the energy on a quantum computer?

Example: massless Schwinger model

Mapping the model to qubits

Original Hamiltonian

$$\mathcal{H} = -\frac{i}{2a} \sum_{n=0}^{N-2} \left(\psi_n^{\dagger} e^{i\theta_n} \psi_{n+1} - h. c. \right) + \frac{ag^2}{2} \sum_{n=0}^{N-2} F_n^2$$
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
 $\psi_n^{\dagger} e^{i\theta_n} \psi_{n+1} \rightarrow \psi_n^{\dagger} \psi_{n+1}$ from transformation:
 $\psi_n \rightarrow (\prod_{k=0}^{n-1} e^{-i\theta_n}) \psi_n$ and $\psi_n^{\dagger} \rightarrow \psi_n^{\dagger} (\prod_{k=0}^{n-1} e^{i\theta_{n-k}})$
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 $Q_n = \psi_n^{\dagger} \psi_n - \frac{1}{2} [1 - (-1)^n]$

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 $\psi_n^\dagger \psi_{n+1} \to \sigma_n^+ \sigma_{n+1}^-$ 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)

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How to deal with gauge fields?

Infinite Hilbert space

Continuous gauge theory requires ∞ -dim. Hilbert space

Integrate out gauge field: only possible in 1+1D

Truncate irreps:² e.g. for $F_i |l\rangle = |l\rangle$, use finite |l| < L

Approximate gauge group:¹ e.g. $U(1) \rightarrow \mathbb{Z}_n$

Gauge invariance

Problem

Gauge invariance requires imposing local constraints **First approach**

Penalize unphysical states,³ e.g. $\mathcal{H}_{\text{penalty}} = \lambda (\sum_{i=1}^{N} Q_i)^2$

Second approach

Analytically solve Gauß law at every site⁴

Third approach

Gauge-invariant formulation, e.g. loop-string-hadron⁵ Many more approaches...

¹Zohar et al. (2013), ..., ²Horn (1981), ..., ³Banerjee et al. (2012), ..., ⁴Klco et al. (2018), ..., ⁵Raychowdhury, Stryker (2020)

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Many more approaches...

Problem

First approach

Second approach

Third approach

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Outlook: how can we address the sign problem in 3+1D?

Example: U(1) lattice gauge theory with θ -term

Goal

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

Theoretical requirements

Derive $3+1D \theta$ -term in Hamiltonian formulation¹

Develop resource-efficient quantum algorithms for lattice gauge theories in 1+1D,² 2+1D,³ and finally 3+1D

First classical computations

Study phase transition with exact diagonalization¹

Future work

Larger volumes: tensor-network and *quantum* simulations

¹ Kan, LF, Kühn, Zhan, Haase, Muschik, Jansen, PRD (2021)
 ² Ferguson, ..., Jansen, PRL (2021), ..., and ongoing work
 ³ Haase, ..., Jansen, Muschik, Quantum (2021), Paulson, ..., Jansen, Zoller, Muschik, PRX Quantum (2021), Clemente, Crippa, Jansen (2022), ..., and ongoing work

$\langle \mathcal{H}_{\theta} \rangle (-8\pi^2 \beta / \theta V)$ = 0.750.80.60.4= 0.05= 0.00.2= 0.0050 opological charge -0.2-0.4-0.6-0.8-1 -0.6-0.4-0.20.20.40.60 $\theta/8\pi^2$

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First classical results for a single cube

Summary: where do we stand, where will we go?

The Path to Go...

Present

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

Algorithms: first QC implementations of 1+1D LGTs, first resource-efficient formulations of 2+1D LGTs

Future

Hardware: O(1000) error-corrected qubits by 2029?

Algorithms: improved Hamiltonians, resource-efficient formulations of 3+1D LGTs, ...

ATTICE SIZE

₩6×6

Creutz (1980)

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WILSON LOOP

0.01

SU (2)

B=3.0





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Summary: where do we stand, where will we go?



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