Quantum computing for nuclear physics Part I: Introduction to Quantum Computation

REYES Nuclear Mentoring Program Aug 9, 2022

James Mulligan University of California, Berkeley



Also see talk by D. Grabowska





The strong nuclear force — interactions of quarks and gluons



QCD interactions comprise $\approx 99\%$ of the visible mass in the universe!

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Quantum chromodynamics





Can we solve the "equations of motion" given that we know the Lagrangian?





Perturbative QCD

For $\alpha_s \ll 1$, compute scattering amplitudes with Feynman diagrams



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Solving the equations of motion



For low-density systems, compute static quantities with lattice regularization



- Hadron spectra
- Deconfinement transition
- Chiral symmetry restoration



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Perturbative QCD

For $\alpha_s \ll 1$, compute scattering amplitudes with Feynman diagrams



...but no strong coupling!

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Solving the equations of motion



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While we know the Lagrangian...we still often don't know how to solve it

What is the landscape of QCD matter?



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What are the dynamics that confine quarks and gluons into hadrons?



Opportunity to study a strongly-interacting, many-body quantum field theory











I. What is a quantum computer?

2. What are potential uses of quantum computing?

3. What are the challenges to achieve quantum advantage?

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Outline











I. What is a quantum computer?



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Given a scientific problem, there are two main questions we want to know:

Given infinite time and memory, can a computer eventually solve the problem?

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Computability

Can a computer find an answer in a reasonable amount of time?









Given a scientific problem, there are two main questions we want to know:

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Example: The Halting Problem



Given an arbitrary computer program, is there an algorithm that can tell us whether the program will finish running? No!

Given infinite time, classical computers can solve the same problems as quantum computers

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Computability

Can a computer find an answer in a reasonable amount of time?



But quantum computers can solve more problems efficiently









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P: Polynomial-time solution on classical computer



a_{11}	a_{12}		a_{1n}		b_{11}	b_{12}		b_{1p}		c_{11}	c_{12}		c_{1p}
a_{21}	a_{22}	• • •	a_{2n}		b_{21}	b_{22}	• • •	b_{2p}		c_{21}	c_{22}	• • •	c_{2p}
:	÷	·	:	×	:	÷	·	:	=	:	÷	·	:
a_{m1}	a_{m2}		a_{mn}		b_{n1}	b_{n2}		b_{np}		c_{m1}	c_{m2}		c_{mp}

Classical computer: Time = $\mathcal{O}(N^{2.373})$





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P: Polynomial-time solution on classical computer

NP: Polynomial-time verification on classical computer

Example: Traveling salesman problem



What is the shortest route between N cities? Classical computer: Time = $\mathcal{O}(\sim 2^N)$

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- P: Polynomial-time solution on classical computer
- NP: Polynomial-time verification on classical computer
- **BQP:** Polynomial-time solution on quantum computer









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- P: Polynomial-time solution on classical computer
- NP: Polynomial-time verification on classical computer
- **BQP:** Polynomial-time solution on quantum computer



QC can solve some classically hard problems









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2019

Article

Quantum supremacy using a programmable superconducting processor Google

Martinis et al., Nature (2019)



53-qubit superconducting circuit device

Algorithm: sampling of random circuits



times faster than best classical *F*_{xEB} *supercomputers* See also: Pan et al., PRL (2021)

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Quantum advantage

2020-2021

Cite as: H.-S. Zhong et al., Science

Quantum computational advantage using photons

Han-Sen Zhong^{1,2*}, Hui Wang^{1,2*}, Yu-Hao Deng^{1,2*}, Ming-Cheng Chen^{1,2*}, Li-Chao Peng^{1,2}, Yi-Han Luo^{1,2}, Jian Qin^{1,2}, Dian Wu^{1,2}, Xing Ding^{1,2}, Yi Hu^{1,2}, Peng Hu³, Xiao-Yan Yang³, Wei-Jun Zhang³, Hao Li³, Yuxuan Li⁴, Xiao Jiang^{1,2}, Lin Gan⁴, Guangwen Yang⁴, Lixing You³, Zhen Wang³, Li Li^{1,2}, Nai-Le Liu^{1,2}, Chao-Yang Lu^{1,2}, Jian-Wei Pan^{1,2}⁺

Pan et al., Science (2020)



Photonic device — special-purpose

Algorithm: boson sampling

Claim: $\mathcal{O}(10^{14})$ times faster than best classical supercomputers







Article

Not so fast!

Ordinary computers can beat Google's quantum computer after all

Superfast algorithm put crimp in 2019 claim that Google's machine had achieved "quantum supremacy"

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https://www<mark>.science.org</mark>/content/article/ordinary-computers-can-beat-google-s-quantum-computer-after-all

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Photonic device — special-purpose

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The building block of computation

Classical bit: 0 or 1

A classical bit can only be in one of two states

Quantum bit (qubit): $|\psi\rangle = a_0 |0\rangle$

A quantum mechanical wave function that is a *superposition* of 0 and 1

When we measure the state $|\psi\rangle$, we obtain either: \Box State $|0\rangle$, with a probability $|a_0|^2$ \Box State $|1\rangle$, with a probability $|a_1|^2$

A quantum bit can be in an infinite number of states, but when we measure it it can only be in one of two states

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$$\rangle + a_1 | 1 \rangle = \begin{pmatrix} a_0 \\ a_1 \end{pmatrix}$$

 $|0\rangle$ $\frac{|0\rangle - |1\rangle}{\sqrt{2}} \psi$ $\frac{|0\rangle - i|1\rangle}{\sqrt{2}}$ $|0\rangle + i |1\rangle$ $\frac{|0\rangle + |1\rangle}{\sqrt{2}}$ $|1\rangle$





We represent a quantum state of multiple qubits using a **tensor product**:

$|a\rangle =$ Two qubits:

where $|00\rangle = |0\rangle \otimes |0\rangle$ denotes the tensor product

N qubits: $a\rangle$

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Multiple qubits

- Quantum computations start to get interesting when we have multiple qubits

$$= a_0 |00\rangle + a_1 |01\rangle + a_2 |10\rangle + a_3 |11\rangle = \begin{pmatrix} a_0 \\ a_1 \\ a_2 \\ a_3 \end{pmatrix}$$

$$= a_0 | 0...0 \rangle + \ldots + a_K | 1...1 \rangle = \begin{pmatrix} a_0 \\ \vdots \\ a_K \end{pmatrix}$$





We represent a quantum state of multiple qubits using a **tensor product**:

Example:

 $|01\rangle =$

 $|\psi_{ab}\rangle$ =

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Multiple qubits

- Quantum computations start to get interesting when we have multiple qubits

$$= |0\rangle \otimes |1\rangle = \begin{pmatrix} 1\\0 \end{pmatrix} \otimes \begin{pmatrix} 0\\1 \end{pmatrix} = \begin{pmatrix} 1 \times 0\\1 \times 1\\0 \times 0\\0 \times 1 \end{pmatrix} = \begin{pmatrix} 0\\1\\0\\0 \end{pmatrix}$$

$$= |a\rangle \otimes |b\rangle = \begin{pmatrix} a_0 \\ a_1 \end{pmatrix} \otimes \begin{pmatrix} b_0 \\ b_1 \end{pmatrix} = \begin{pmatrix} a_0 b_0 \\ a_0 b_1 \\ a_1 b_0 \\ a_1 b_1 \end{pmatrix}$$



Where does quantum advantage come from?

$$|\psi\rangle = \sum_{i=1}^{2^N} a_i |\psi_i\rangle$$
 For N qubits

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pits, there are 2^N amplitudes

e.g. $|\psi\rangle = a_1 |000\rangle + a_2 |001\rangle + a_3 |010\rangle + a_4 |011\rangle + a_5 |100\rangle + a_6 |101\rangle + a_7 |110\rangle + a_8 |111\rangle$





Where does quantum advantage come from?

$$|\psi\rangle = \sum_{i=1}^{2^N} a_i |\psi_i\rangle$$
 For N qubits

A quantum operation (gate) modifies all of these 2^N amplitudes simultaneously!

$$|a\rangle = \sum_{i=1}^{2^{N}} a_{i} |\psi_{i}\rangle \rightarrow |b\rangle = \sum_{i=1}^{2^{N}} b_{i} |\psi_{i}\rangle$$

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$$|a\rangle = \sum_{i=1}^{2^{N}} a_{i} |\psi_{i}\rangle \rightarrow |b\rangle = \sum_{i=1}^{2^{N}} b_{i} |\psi_{i}\rangle$$

This is the major challenge: How can we take advantage of the exponential efficiency of quantum operations when we only access one randomly sampled state at a time?

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e.g. $|\psi\rangle = a_1 |000\rangle + a_2 |001\rangle + a_3 |010\rangle + a_4 |011\rangle + a_5 |100\rangle + a_6 |101\rangle + a_7 |110\rangle + a_8 |111\rangle$

However: we cannot access the quantum amplitudes $\{a_i\}$ directly!







Digital quantum computers

Universal





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Quantum computing

Analog quantum computers

Application-specific



In this program we will focus on digital, universal quantum computers







Quantum states: column vectors

Quantum logic gates: unitary matrice

Single-qubit gates:



Multi-qubit gates: Any quantum gate can be composed from CNOT and single-qubit gates

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um Gates

$$a
angle = a_0 |0
angle + a_1 |1
angle = \begin{pmatrix} a_0 \\ a_1 \end{pmatrix}$$

es $U^{\dagger}U = I$
NOT
 $A |0
angle + \alpha |1
angle$
 $X \equiv \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$
 $X \equiv \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$
 $X \equiv \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$
 $H \equiv \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}$

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NOT









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Example: CNOT Gate

controlled-NOT

 $|A\rangle$ • $|A\rangle$ How do we construct the matrix



NOT











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Example: CNOT Gate

controlled-NOT

 $|A\rangle$ How do we construct the matrix representation of the gate A



The i^{th} column determines how the i^{th} basis state transforms: NOT $|00\rangle \rightarrow |00\rangle$

FANIN













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controlled-NOT

 $|A\rangle$ How do we construct the matrix representation of the gate A



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Example: CNOT Gate

controlled-NOT

 $|A\rangle$ How do we construct the matrix representation of the gate A



The i^{th} column determines how the i^{th} basis state transforms: NOT $|10\rangle \rightarrow |11\rangle$

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Example: CNOT Gate

controlled-NOT

 $|A\rangle$ How do we construct the matrix representation of the gate A



The i^{th} column determines how the i^{th} basis state transforms: NOT $|11\rangle \rightarrow |10\rangle$

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Example: SWAP circuit



 $SWAP(|a\rangle \otimes |b\rangle) = CNOT_{0,1} \times CNOT_{1,0} \times CNOT_{1,0}$

 $= \bigcap \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix} \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ F_{A} Q_{IN} 0 & 1 \\ 0 & 1 & 0 \end{bmatrix}$ FAN UT

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$$IAX A HART A H$$









2. What are potential uses of quantum computing?

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Simulation of quantum field theory







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Shor's factoring algorithm

Task: Find prime factors of an integer



Exponential speedup compared to classical algorithms

 $\mathcal{O}((\log N)^2...)$ vs. $\mathcal{O}(e^{1.9(\log N)^{1/3}...})$



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Quantum algorithms

Grover's search algorithm

Task: Find marked entry in an unordered list

Grover diffusion operator



Repeat $\approx \frac{\pi}{4}\sqrt{N}$ times

Polynomial speedup compared to classical algorithms

$$\mathcal{O}\left(\sqrt{(N)}\right)$$
 vs. $\mathcal{O}(N)$

And more...









Task: Given the Hamiltonian of a quantum mechanical system, simulate its dynamical evolution Quantum chemistry, material design, nuclear dynamics, …

That is, solve the time-dependent Schrödinger equation: $H|\psi(t)\rangle = i\hbar\frac{d}{dt}|\psi(t)\rangle$

The solution is just a unitary evolution! $|\psi(t)\rangle = U_H |\psi(0)\rangle$ whe

computer: 2^N amplitudes! \Box Cannot simulate more than $\mathcal{O}(10 - 100)$ particles

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Quantum simulation

Feynman `81 Lloyd `96



re
$$U_H = e^{-iHt/\hbar}$$

It is exponentially expensive to simulate an N-body quantum system on a classical





A quantum computer can naturally simulate a quantum system

(I) Initial state preparation

$$0...0\rangle \rightarrow |\psi(0)\rangle$$

(2) Time evolution

$$|\psi(0)\rangle - U_H(t)$$

Need efficient encoding of U_H into quantum gates, e.g. local interactions

(3) Measurement

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Quantum simulation

Feynman `81 Lloyd `96













3. What are the challenges to achieve quantum advantage?

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DiVincenzo Criteria

A quantum computer must satisfy the following:

- Scalable physical system with well-defined qubits Ability to initialize qubits Ability to measure qubits Universal set of quantum gates Qubit decoherence times much longer than gate latency

A variety of different physical systems are being explored, each with strengths

- Superconducting circuits
- Trapped ions
- Rydberg atoms

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- Photonics
- Topological materials
- . . .







Rapid advances in qubit coherence times and quantum gates

State-of-the-art: $\mathcal{O}(10 - 100)$ qubits, $\mathcal{O}(100)$ two-qubit operations

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Quantum devices



Noisy quantum devices

Few qubits

Current devices are limited to O(10) - O(100) qubits



Decoherence

Need more qubits to achieve quantum advantage

Need longer coherence times to increase the "gate depth" of circuits

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The quantum state of a qubit is stable only for a limited time

 $T_1: \text{decay time } |1\rangle \rightarrow |0\rangle$

 $T_2: \text{dephasing time} \\ |1\rangle \rightarrow \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$

Gate noise

Single- and two-qubit gate operations are imperfect





Need smaller gate noise to perform quantum error correction



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No cloning theorem

Can we copy arbitrary qubits, in order to provide redundancy?



Proof:



Quantum mechanics prevents us from using traditional error correction techniques

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Suppose
$$U_{\text{clone}} \left(|a\rangle \otimes |b\rangle \right) = |a\rangle \otimes |a\rangle$$

 $U_{\text{clone}} \left(|a'\rangle \otimes |b\rangle \right) = |a'\rangle \otimes |a'\rangle.$

Then taking inner product of both sides gives:

$$\langle a \, | \, a' \rangle = \langle a \, | \, a' \rangle^2$$

so $\langle a | a' \rangle = 0$ or 1 i.e. cannot copy arbitrary states.







Example: Bit flip code

 \Box Suppose a bit flip (X gate) occurs with probability p

Quantum error correction



Devitt, Munro, Nemoto (2013)







Example: Bit flip code

- \Box Suppose a bit flip (X gate) occurs with probability p
- \Box Encode our qubit $|\psi\rangle = a_0 |0\rangle + a_1 |1\rangle$ into three qubits: $|\psi_{\text{encoded}}\rangle = a_0 |000\rangle + a_1 |111\rangle$

Quantum error correction



Devitt, Munro, Nemoto (2013)







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- Introduce ancilla qubits to measure the parity of the three qubits

Quantum error correction



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- $\Box_{\psi} h troduce$ ancilla qubits to measure the parity of the three qubits

–	Error Location	Final State,
	No Error	$ \alpha 000 \rangle 00 \rangle$
	Qubit 1	$ \alpha 100\rangle 11\rangle$
	Qubit 2	$ \alpha 010 \rangle 10 \rangle$
	Qubit 3	$\mid \alpha \mid 001 \rangle \mid 01 \rangle$



Quantum error correction







There are a variety of error correction codes:

- □ Shor code
- □ Steane code
- Surface codes
- Ω...

correct errors faster than you introduce them

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Quantum error correction



- Quantum threshold theorem: If errors are below a certain threshold, then you can
 - Demonstrating "break-even" point is active goal of research







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2. What are potential uses of quantum computing?

3. What are the challenges to achieve quantum advantage?

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Outline











Basics:

- Introduction to qubits
- Unitary gates: <u>Nielsen+Chuang</u> Section 1.3

Introduction to complexity classes

Quantum computing overviews: https://arxiv.org/pdf/1905.07240.pdf https://arxiv.org/pdf/1801.00862.pdf

Quantum simulation: <u>https://arxiv.org/</u> pdf/1907.03505.pdf

Additional reading material Not required, but you may find them useful and interesting!

Qiskit tutorials from IBM Quantum Lab

Create an account: <u>https://quantum-computing.ibm.com/lab</u>

- Login and navigate to qiskit-tutorials/qiskit/circuits
- Complete the following two tutorials:

01_circuit_basics.ipynb

3_summary_of_quantum_operations.ipynb

- Navigate to qiskit-tutorials/qiskit/simulators
- Complete the following two tutorials:

2_device_noise_simulation.ipynb

3_building_moise_models.ipynb

- Navigate to giskit-tutorials/giskit-ibm-runtime
- Complete the following tutorial:

01_introduction_ibm_cloud_runtime.ipynb



