# Quantum Computing Overview

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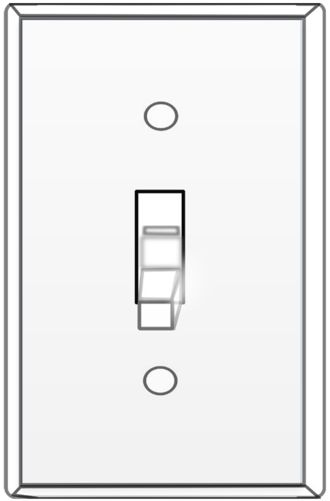
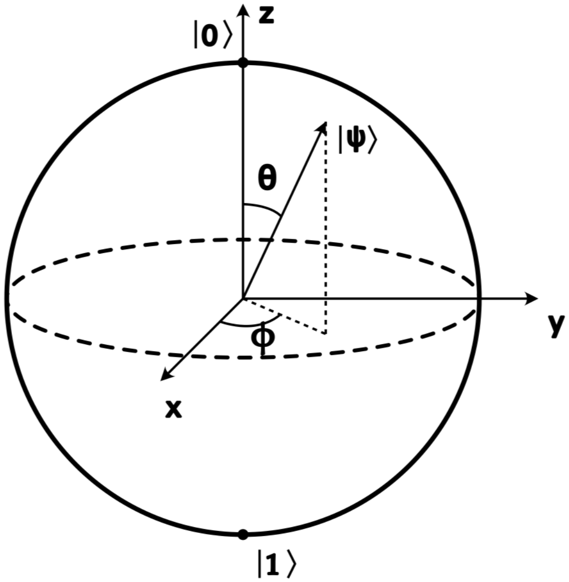
# What is quantum computation: Qubits



Either On (1) or Off (0)



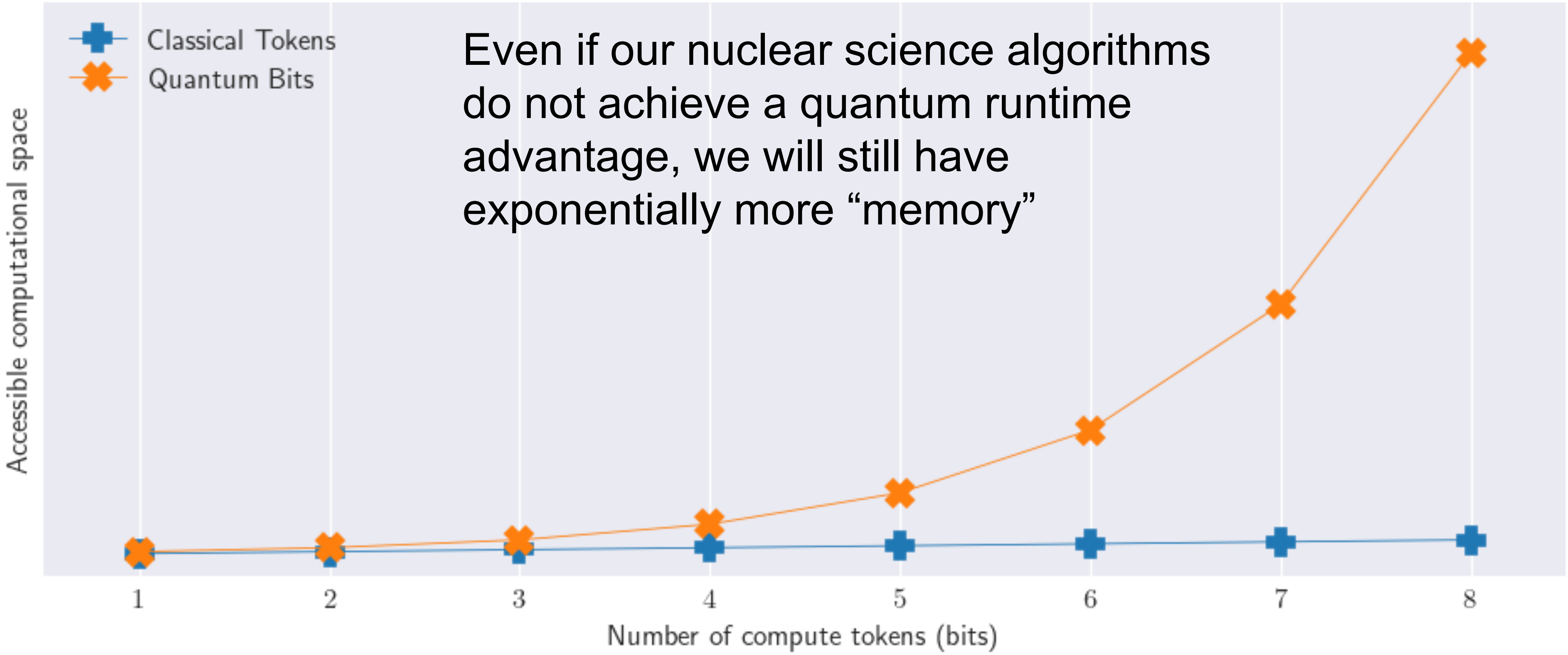

$$|\psi\rangle = \cos\frac{\theta}{2}|0\rangle + e^{i\phi}\sin\frac{\theta}{2}|1\rangle$$

# What is quantum computation: Gates

- $X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, Y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, Z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$
- $H = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}, S = \begin{pmatrix} 1 & 0 \\ 0 & i \end{pmatrix}, T = \begin{pmatrix} 1 & 0 \\ 0 & e^{\frac{i\pi}{4}} \end{pmatrix}$
- $CNOT = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix} = |0\rangle\langle 0| \otimes I_2 + |1\rangle\langle 1| \otimes X_2$

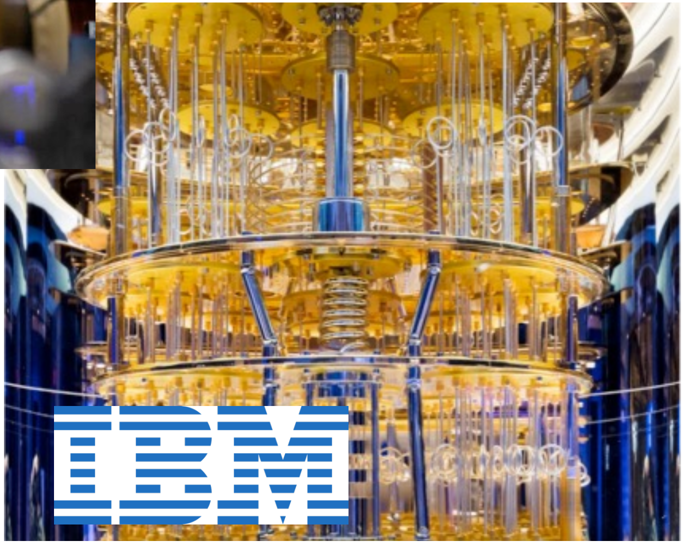
Operations on a quantum computer are unitary, i.e., fully reversible.

# What is quantum computation: Entanglement




Even if our nuclear science algorithms do not achieve a quantum runtime advantage, we will still have exponentially more “memory”

# ORNL OLCF Quantum Computing User Program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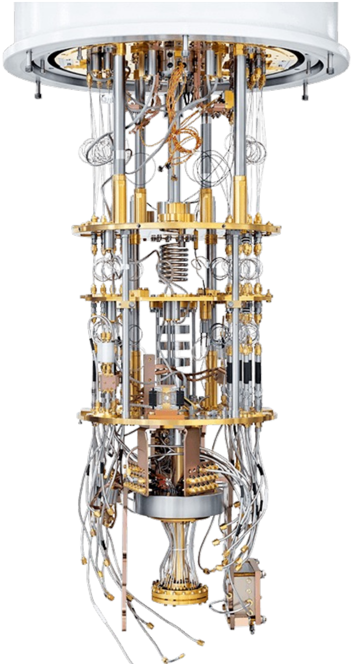
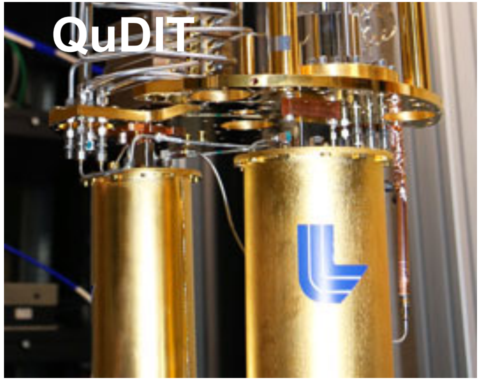
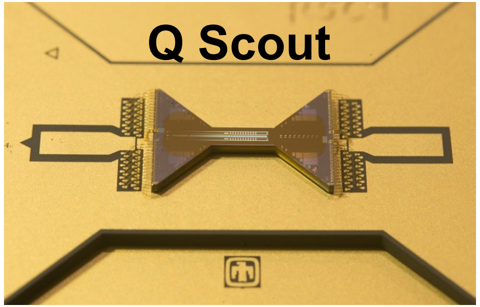


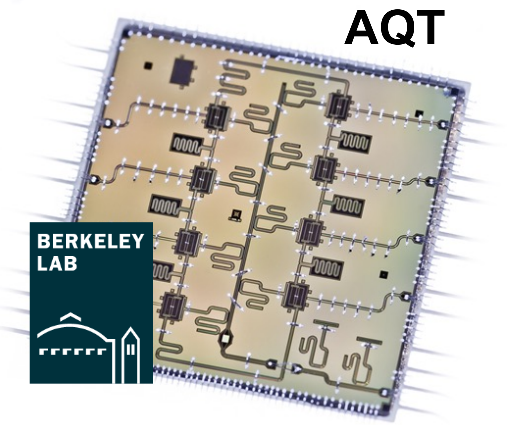
# DOE Quantum Testbed Programs

DOE has several quantum computing testbeds that enable low level engagement with the quantum hardware and experts.

Our community has limited engagement with these resources



# Challenges in quantum computing

Quantum computers are unitary (reversable) computers

$$|\Psi_{\mathrm{f}}\rangle = \boldsymbol{U}|\Psi_{\mathrm{i}}\rangle \rightarrow |\Psi_{\mathrm{i}}\rangle = \boldsymbol{U}^{\dagger}\,|\Psi_{\mathrm{f}}\rangle$$

Most of our established methods are built on some sort of projection:

$|\Psi\rangle = e^{\boldsymbol{T}}|\Phi\rangle$ (similarity transformations)

$|\Psi_{\mathrm{n}}\rangle \propto H|\Psi_{\mathrm{n-1}}\rangle - \frac{\alpha_n}{\beta_n}\left|\Psi_{\mathrm{n-1}}\right\rangle - \beta_j|\Psi_{\mathrm{n-2}}\rangle$ (Lanczos iterations)

$|\Phi\rangle \propto \lim_{n\rightarrow\infty} e^{-\tau\,\boldsymbol{H}}|\Phi_{\mathrm{ref}}\rangle$ (QMC projection)

# Challenges in quantum computing

Quantum computers are unitary (reversable) computers

$$|\Psi_{\mathrm{f}}\rangle = \boldsymbol{U}|\Psi_{\mathrm{i}}\rangle \rightarrow |\Psi_{\mathrm{i}}\rangle = \boldsymbol{U}^{\dagger}\,|\Psi_{\mathrm{f}}\rangle$$

And we only have access to final state probabilities

$$P(0101\ldots) = \left|\langle 0101\ldots|\Psi_f\rangle\right|^2$$

We need to express our simulations in a unitary form whose output can be extracted from a semi-positive definite distribution.

# Opportunities in quantum computing

Real time dynamics is naturally expressed on quantum hardware

$$|\Psi(t_f)\rangle = \mathcal{T} e^{-i \int_{t_i}^{t_f} \boldsymbol{H}(t) dt} |\Psi(t_i)\rangle$$

- Nuclear Scattering and Reactions
  - Fission
  - Fusion
- Nonperturbative leptonic probes

Dynamics is very hard classically!

**How do we get our initial state for the dynamics?**

# Two broad classes of problems need to be solved for dynamics

$$\langle \Psi_f(t_f) | \boldsymbol{O} | \Psi_i(t_i) \rangle$$

# Two broad classes of problems need to be solved for dynamics

$$\langle 0|\boldsymbol{U}_f^{\dagger}\boldsymbol{U}^{\dagger}(\Delta t_f)\boldsymbol{O}\boldsymbol{U}(\Delta t_i)\boldsymbol{U}_i|0\rangle$$

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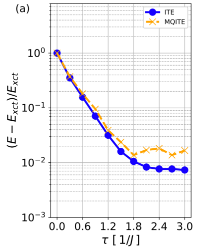
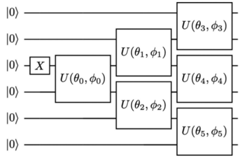
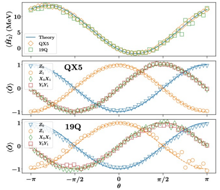
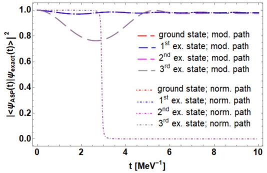
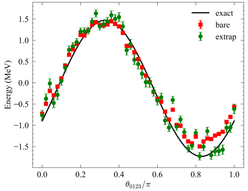
$$\langle 0|\boldsymbol{U}_f^\dagger \boldsymbol{U}^\dagger(\Delta t_f)\,\boldsymbol{O}\,\boldsymbol{U}(\Delta t_i)\boldsymbol{U}_i|0\rangle$$

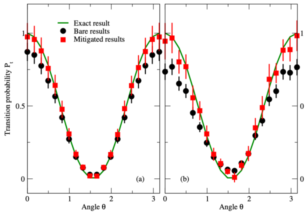


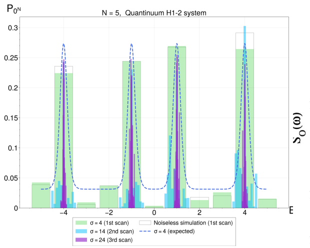



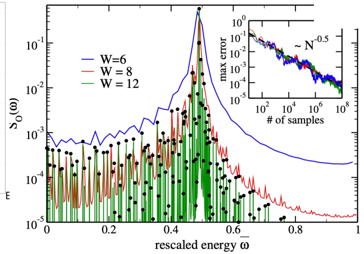



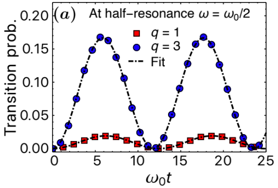



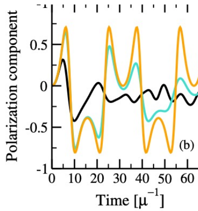



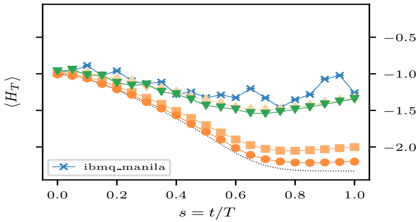



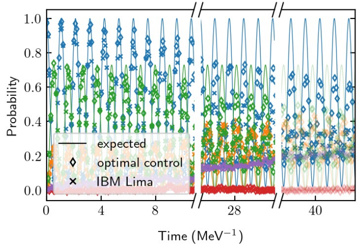

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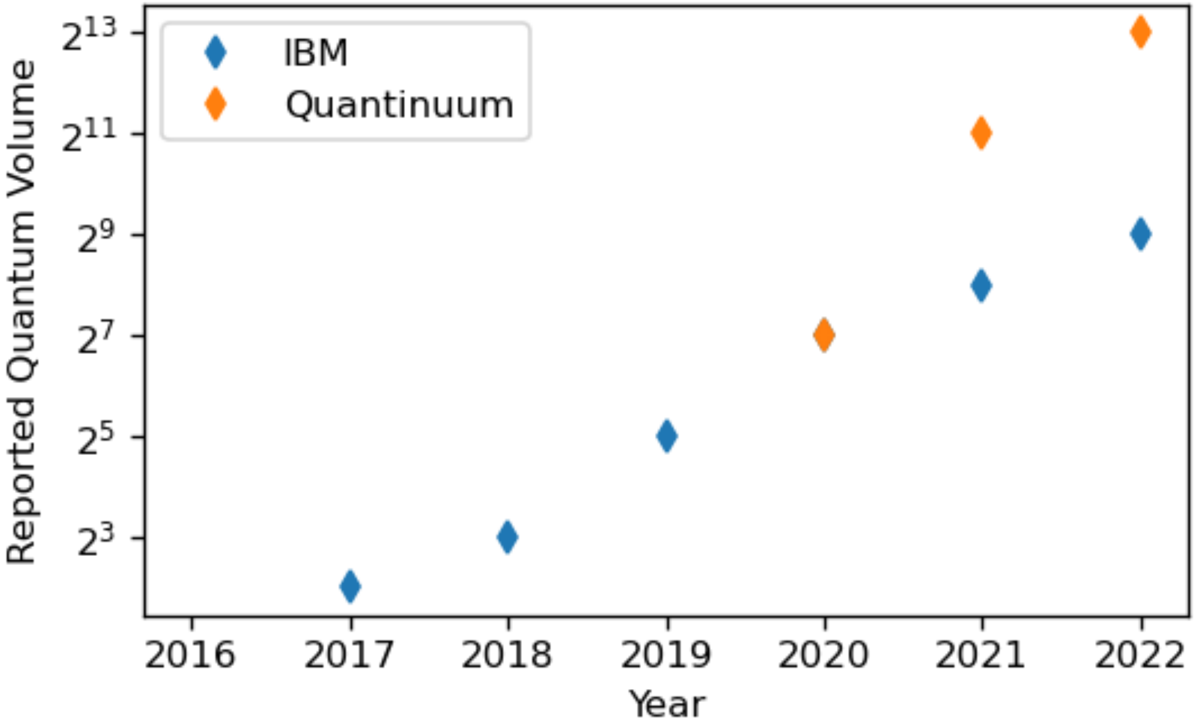
PRL 127, 040505

PRC 100, 034610
PRA 101, 062307
PRD 105, 083020
arXiv:2105.08910

# Useful quantum compute is not that far off in the horizon!




All example shown yesterday and today are small systems using only a few qubits (2-8)

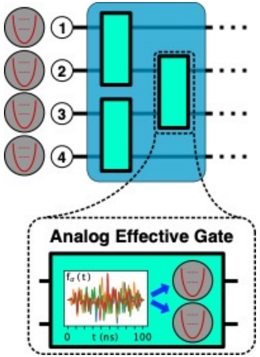
Accessible Quantum platforms are growing at a rapid pace!

# Opportunities for the next decade

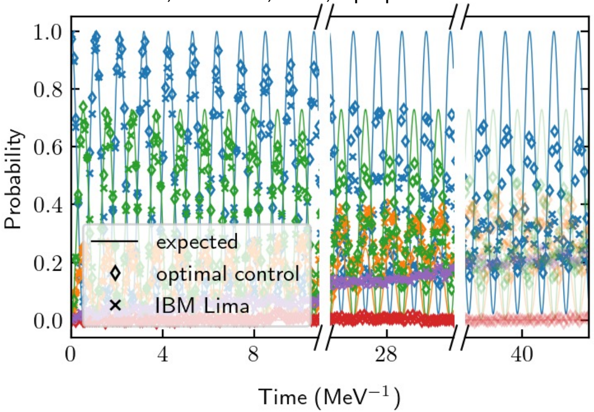
- We will likely see the possibility of the first “useful” simulations on quantum planforms within the next 10 years.
  - Large scale (100s to 1000s qubits) simulations on noisy, but mitigatable, platforms.
  - Insight into our many-body approximations more than leading edge nuclear physics predictions.
- We have only started to explore how to express our theories on quantum hardware
  - Most of our current algorithms and demonstrations reflect us adapting our classical methods to quantum devices instead of directly exploiting the nature of the quantum devices.
  - Real-time dynamics come naturally on quantum hardware, offering an opportunity to a deeper and more precise simulations of nuclear reactions.
- Better engagement with the DOE Quantum Testbed program
  - Unique opportunity for collaborations with hardware experts.  Low level access to quantum hard can yield insight not possible with commercial platforms.

# ~~Physics~~ Problem Informed Quantum Computing

- “White-box” platforms can enable hybrid digital-analog computing.
- Opens a pathway to dynamical real-time simulations of nuclei.
- Replace blocks of our quantum algorithm with analog inputs that enact custom gates tune to the simulation at hand.




Holland, et. al. ,Phys. Rev. A 101, 062307 (2020)
X. Wu, K. Wendt, et. al, inprep

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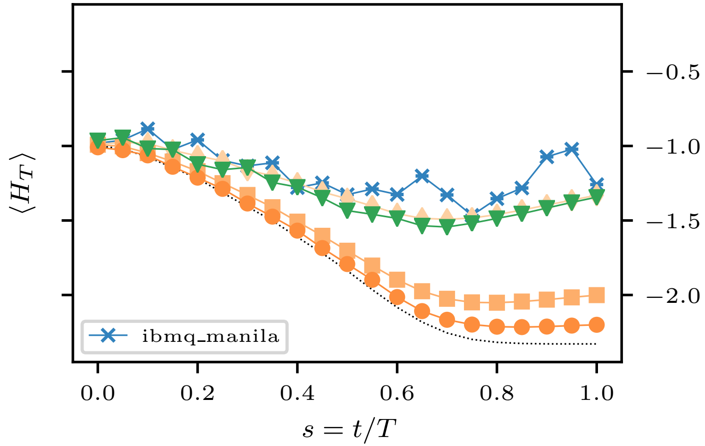

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