Quantum computing at ORNL…and beyond

Presented at the

NP-QI Workshop, ANL

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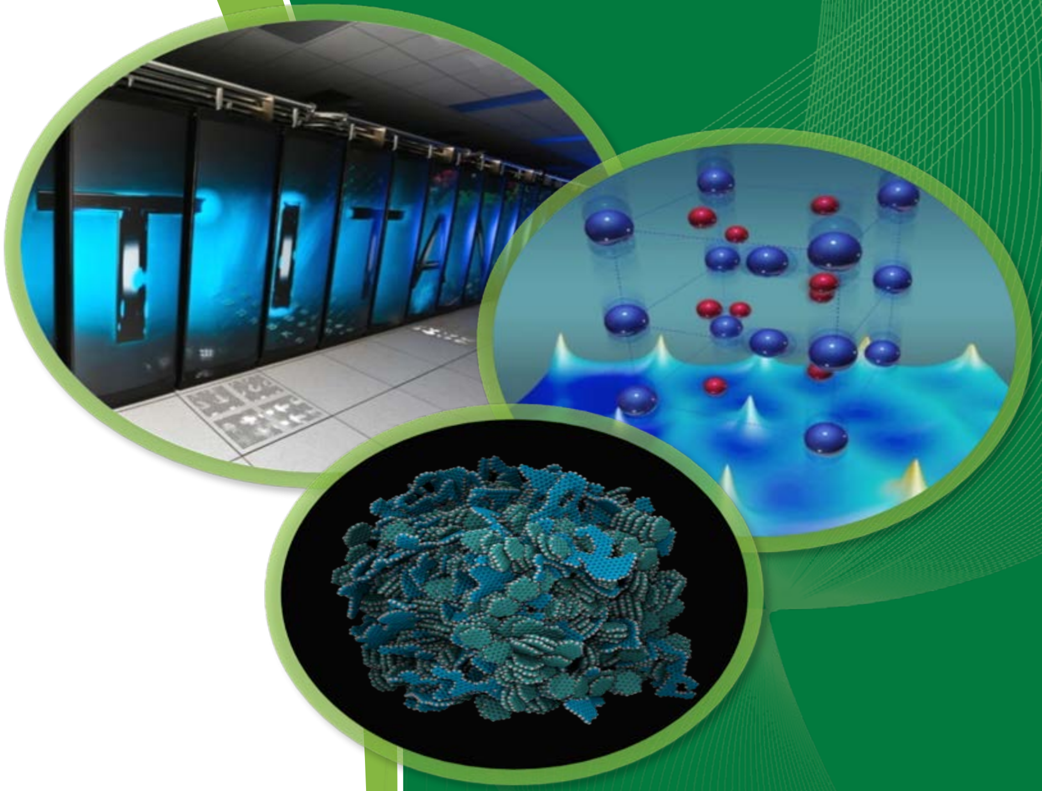
Director, Physics Division

Chicago
March 28, 2018



ORNL is managed by UT-Battelle
for the US Department of Energy

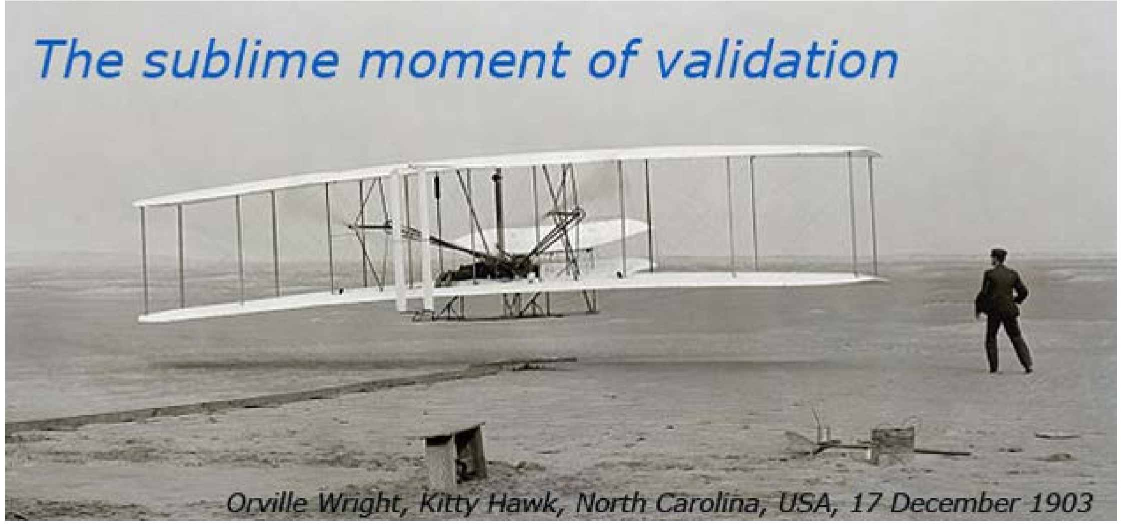
OAK RIDGE
National Laboratory

Outline

- Why do we compute?
- Trends in Classical and quantum computing
- ORNL efforts in QC and Quantum Materials
- Application to the Deuteron

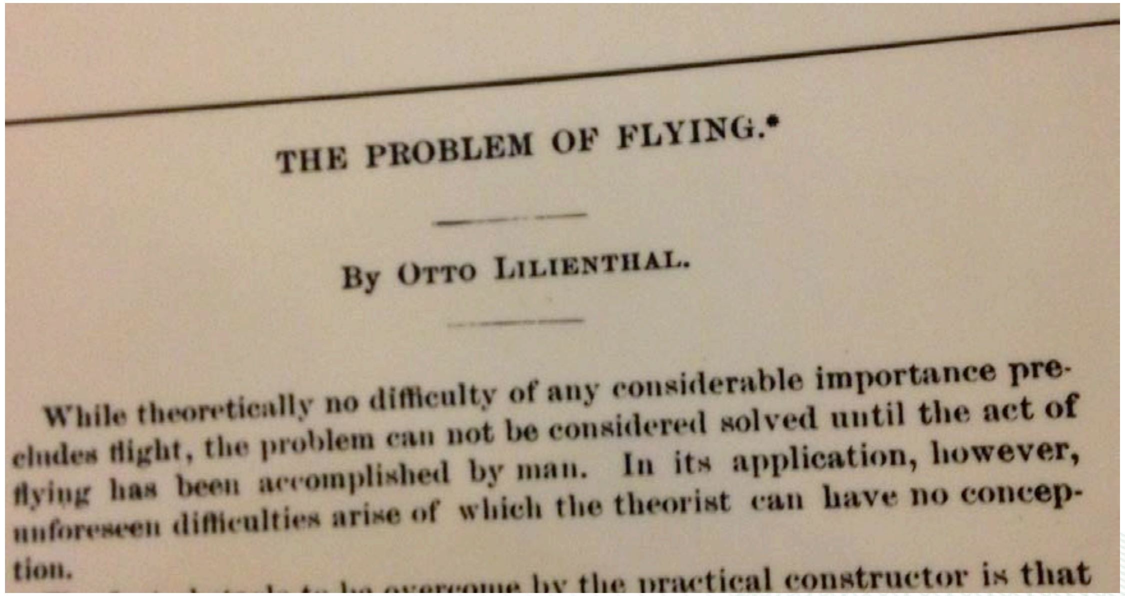
Why, how and purpose of computing

- Why
  - Very few instances of analytical, closed form, real life solutions exist.
  - Nonlinearity and emergent behavior exist everywhere
- How
  - We employ methods of Validation and Verification (V&V)
    - Doing the problem right (numerically sound approaches)
    - Doing the right problem (physically sound approaches)
- Purpose
  - We compare theory (as codified in equations) to experiment
  - We discover new phenomena
  - We predict the outcomes of experiments to test theory
  - We quantify our uncertainties (UQ)
- We ‘always’ apply liberal amounts of physics intuition



The sublime moment of validation

Orville Wright, Kitty Hawk, North Carolina, USA, 17 December 1903



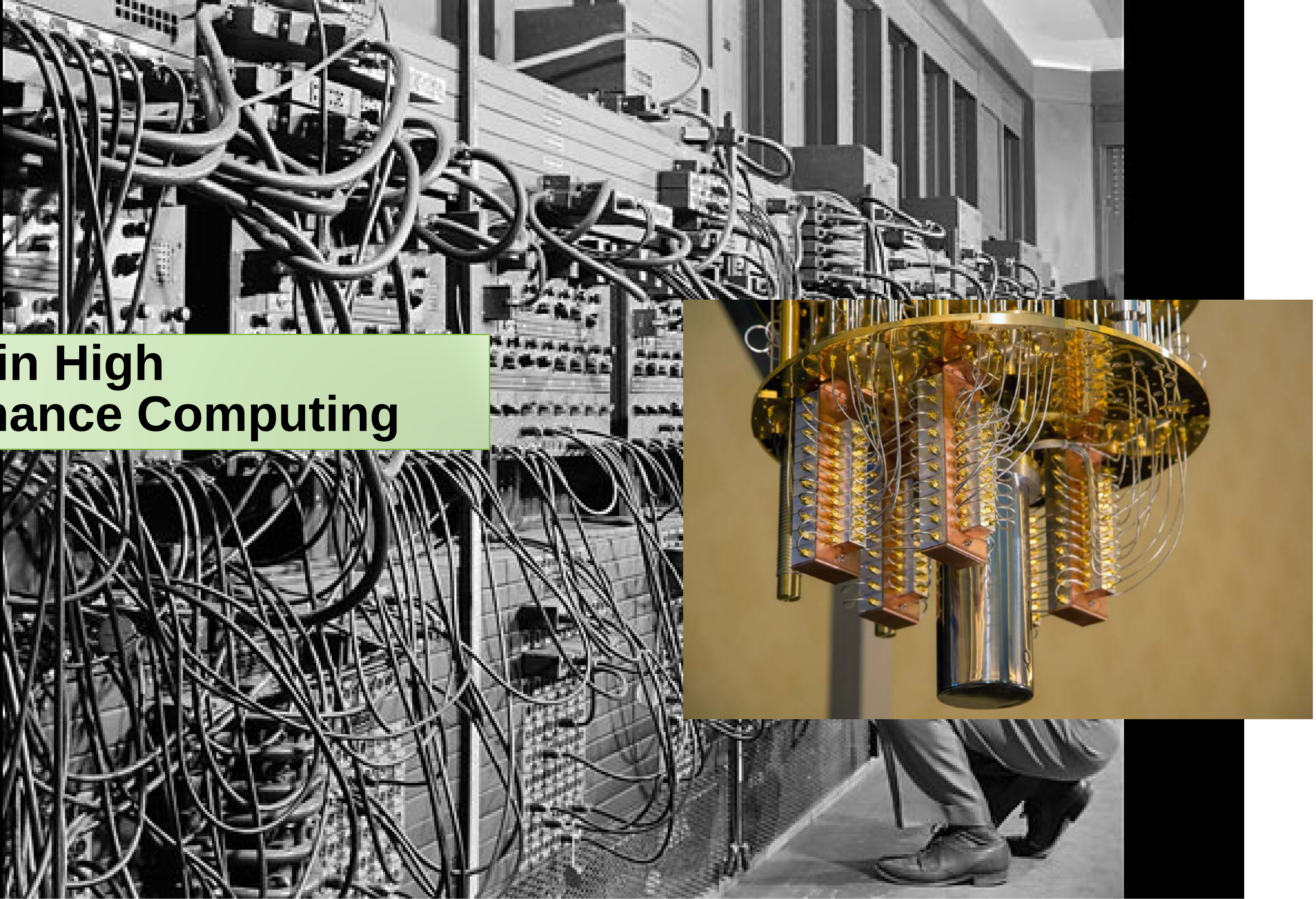
THE PROBLEM OF FLYING.*

By Otto Lilienthal.

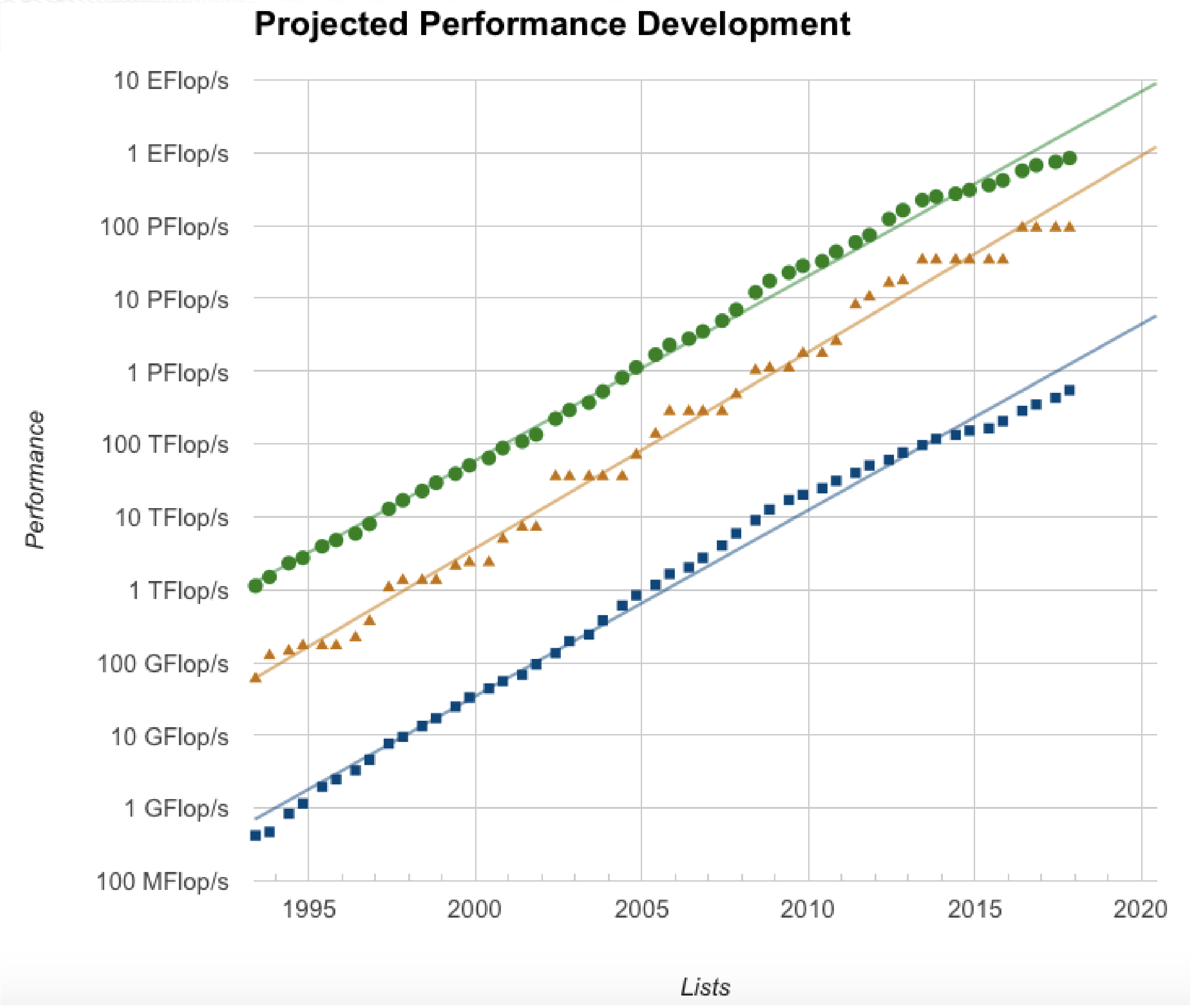
While theoretically no difficulty of any considerable importance precludes flight, the problem can not be considered solved until the act of flying has been accomplished by man. In its application, however, unforeseen difficulties arise of which the theorist can have no conception.

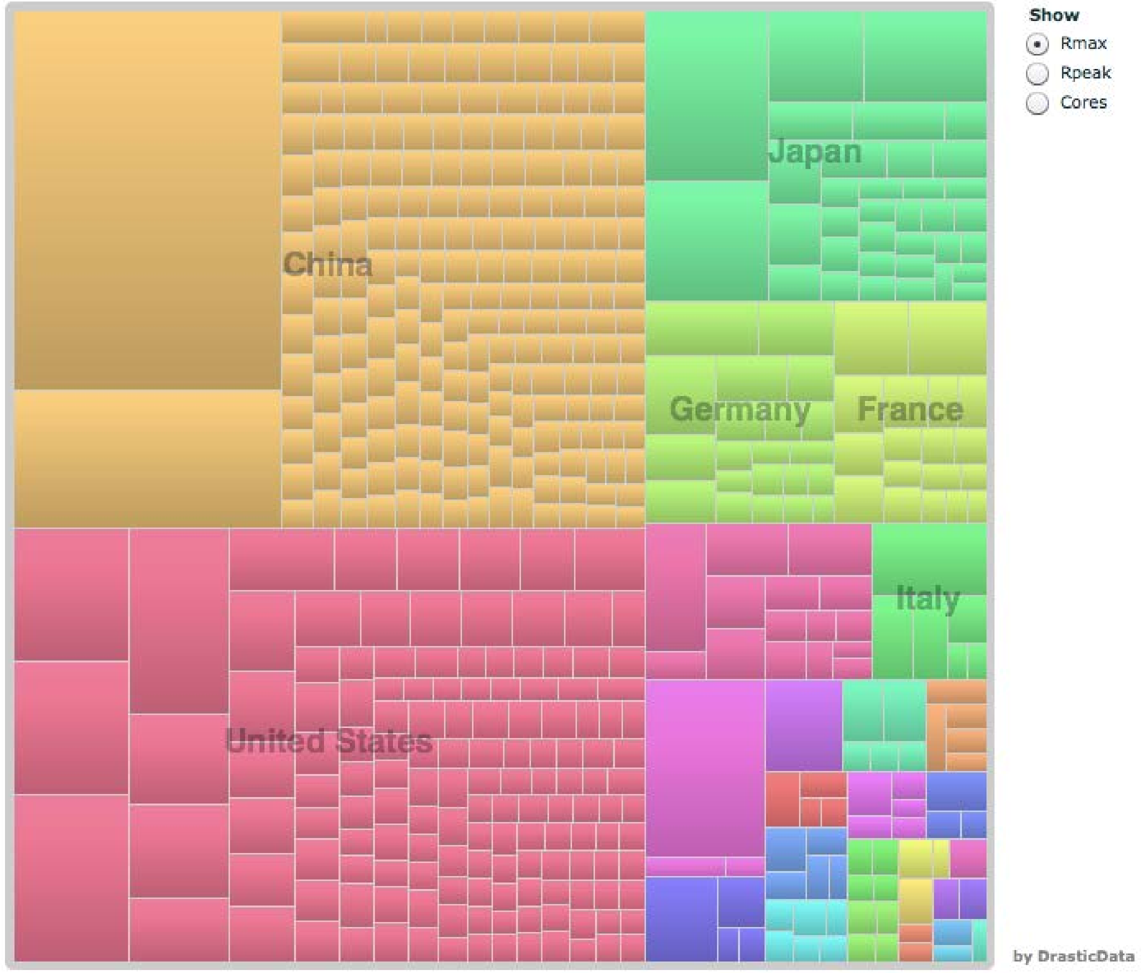
overcome by the practical constructor is that

Trends in High Performance Computing

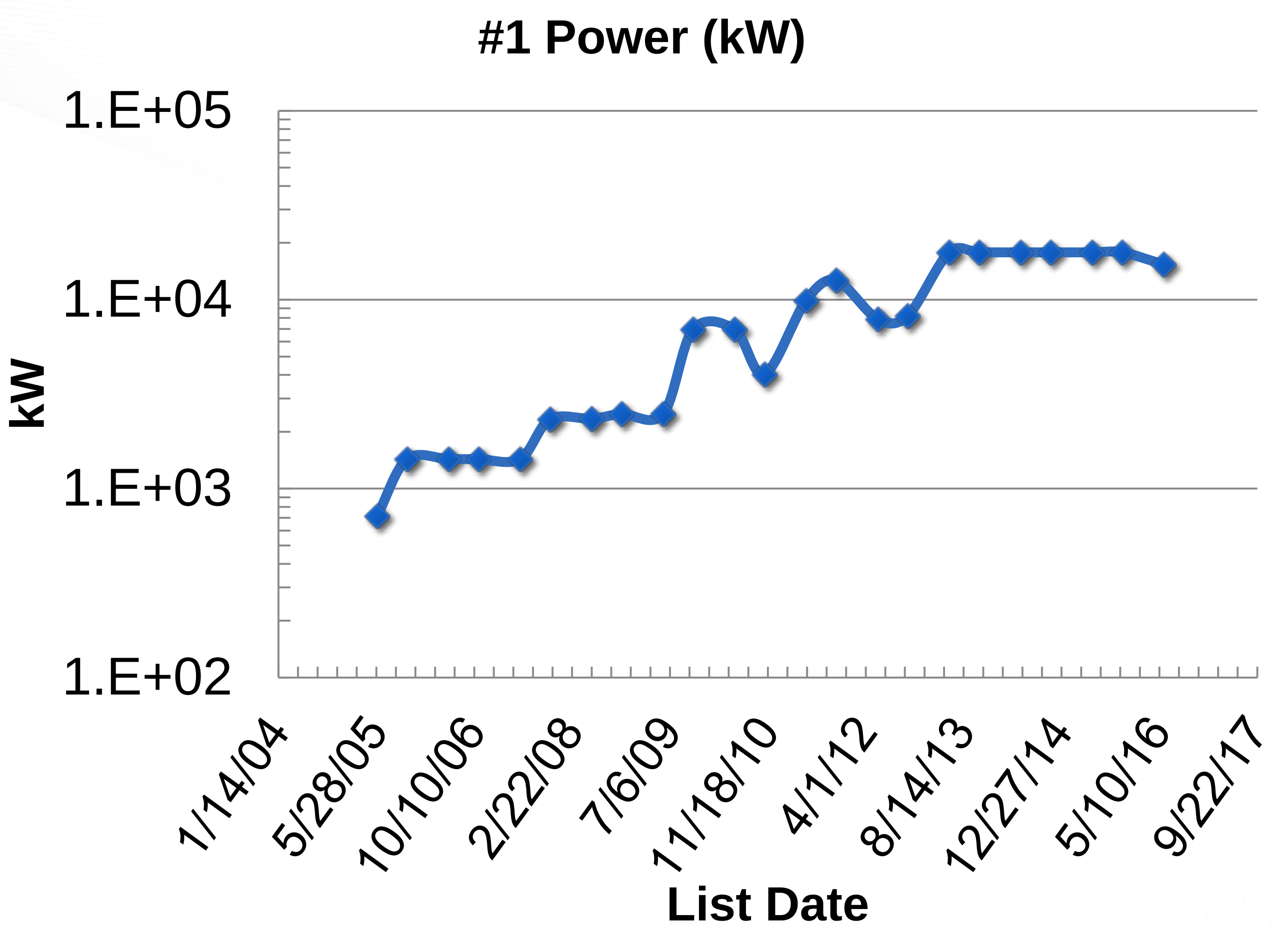


Development with time (top500.org)





A big issue: power



Incremental cost of running RHIC: $550k/week

Incremental cost of running Titan: $140k/week

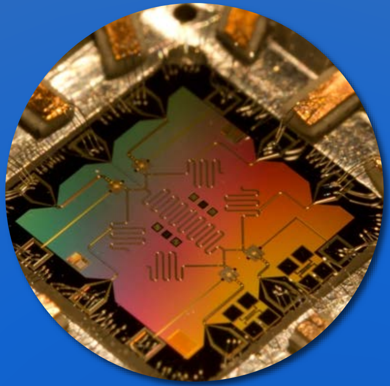
Incremental cost of running Sunway: $258k/week

(assume $0.1/kW-h)

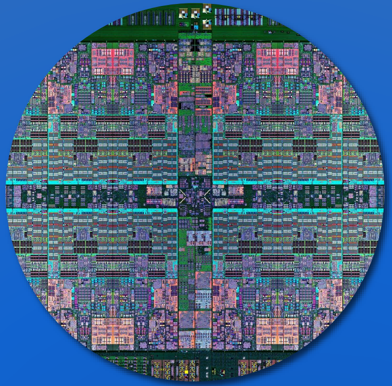
June 2005 Tflop/kW = 0.191
Nov. 2017 Tflop/kW = 6.05

32x technology improvement

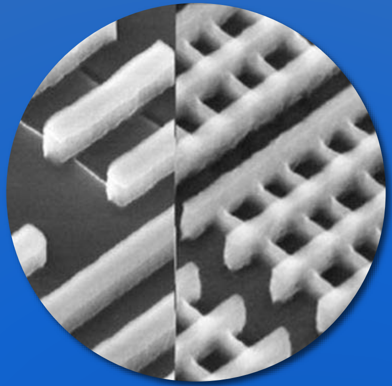
Beyond exascale landscape



Quantum, Neuromorphic



Squeeze out everything one can from CMOS



Beyond CMOS

Materials Science; Device Physics; Software

Quantum computing in context

In the sciences

1980s– 1990s

A curious idea; first quantum algorithms

2000s

Proof-of-principle demonstrations
Initial QC hardware

Error correction and control theory

2010s

Focus on practicality and improving quality and control

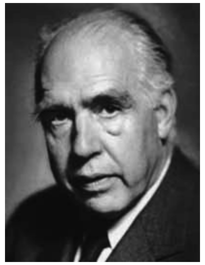
Circuit synthesis

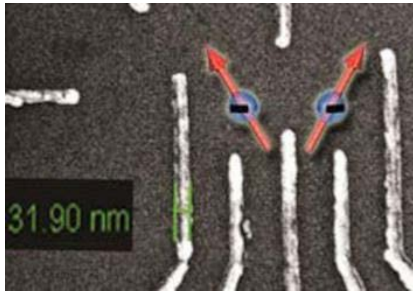
Current status

Qubit fragility presents tremendous challenges

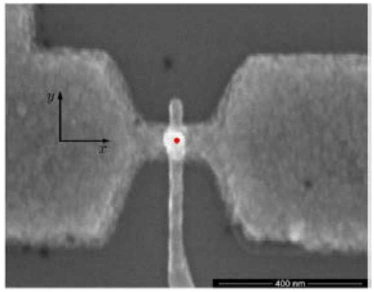
Attempt to broaden suite of applications

> *If quantum mechanics hasn't profoundly shocked you, you haven't understood it yet.*
> – Niels Bohr

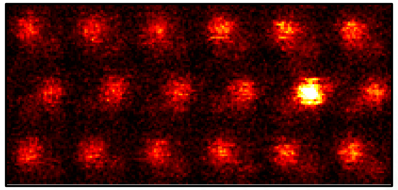




Si Ge qubits
Julich

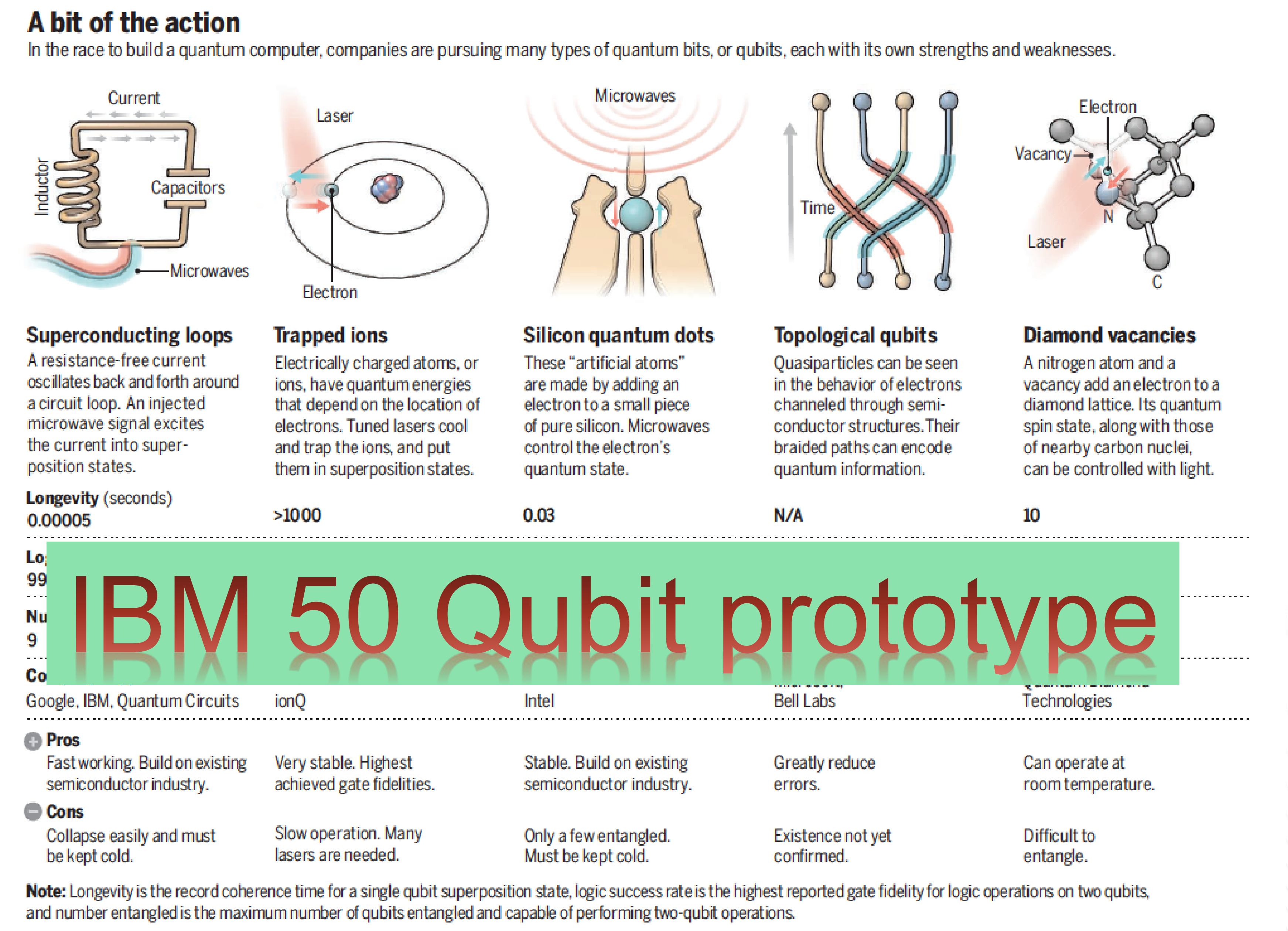


Phosphorous donor
Sydney



Scientific motivator: "…potential ability to realize full control of large-scale quantum coherent systems…"
BES: Challenges at the frontiers of matter and energy, 2015
Quantum Pathfinder and Quantum Algorithms funding awarded by ASCR (FY17)
BES: Quantum Information Science Round Tables (October, 2017)
HEP funding in FY18 PBR, NP interest – INT and this workshop

Science 354, 1091 (2016) – 2 December



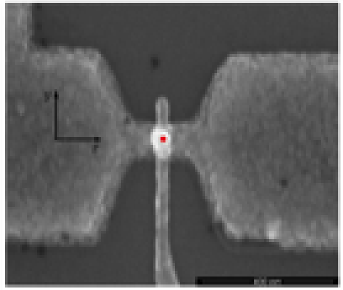
A bit of the action

In the race to build a quantum computer, companies are pursuing many types of quantum bits, or qubits, each with its own strengths and weaknesses.

	Superconducting loops	**Trapped ions**	**Silicon quantum dots**	**Topological qubits**	**Diamond vacancies**
	A resistance-free current oscillates back and forth around a circuit loop. An injected microwave signal excites the current into superposition states.	Electrically charged atoms, or ions, have quantum energies that depend on the location of electrons. Tuned lasers cool and trap the ions, and put them in superposition states.	These "artificial atoms" are made by adding an electron to a small piece of pure silicon. Microwaves control the electron's quantum state.	Quasiparticles can be seen in the behavior of electrons channeled through semiconductor structures. Their braided paths can encode quantum information.	A nitrogen atom and a vacancy add an electron to a diamond lattice. Its quantum spin state, along with those of nearby carbon nuclei, can be controlled with light.
Longevity (seconds)	0.00005	>1000	0.03	N/A	10
Lo	99				
Nu	9				
Co	Google, IBM, Quantum Circuits	ionQ	Intel	Bell Labs	Technologies
Pros	Fast working. Build on existing semiconductor industry.	Very stable. Highest achieved gate fidelities.	Stable. Build on existing semiconductor industry.	Greatly reduce errors.	Can operate at room temperature.
Cons	Collapse easily and must be kept cold.	Slow operation. Many lasers are needed.	Only a few entangled. Must be kept cold.	Existence not yet confirmed.	Difficult to entangle.

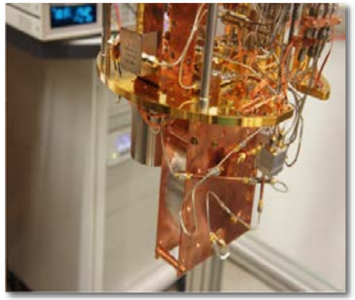
Note: Longevity is the record coherence time for a single qubit superposition state, logic success rate is the highest reported gate fidelity for logic operations on two qubits, and number entangled is the maximum number of qubits entangled and capable of performing two-qubit operations.

IBM 50 Qubit prototype



characterize

HREM, APT, SPM
Multiscale modeling



Classical quantum interface

From mK to 300K

Program Qubits

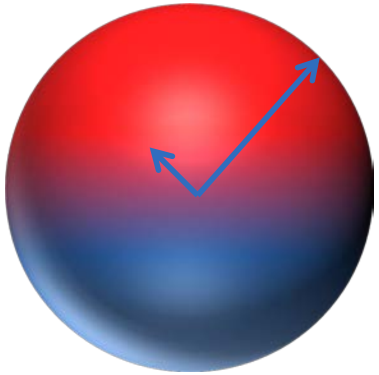
QIS and other groups

Quantum computing and its algorithms

● 1 = on

● 0 = off

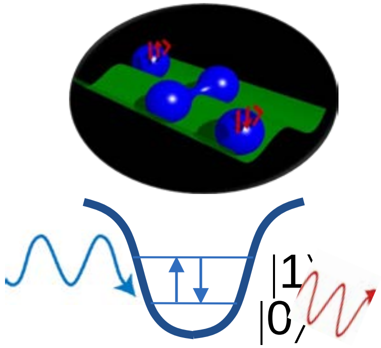
Classical:
Definite state



$$|\Psi\rangle = a|0\rangle + b|1\rangle$$

$$|a|^2 + |b|^2 = 1$$

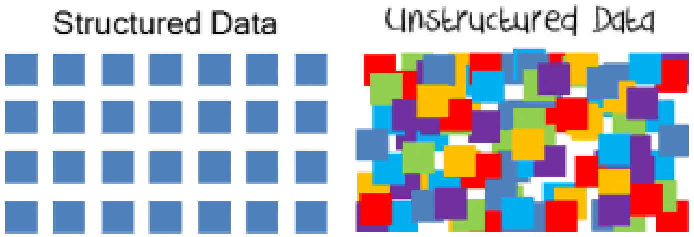
Quantum: State superposition



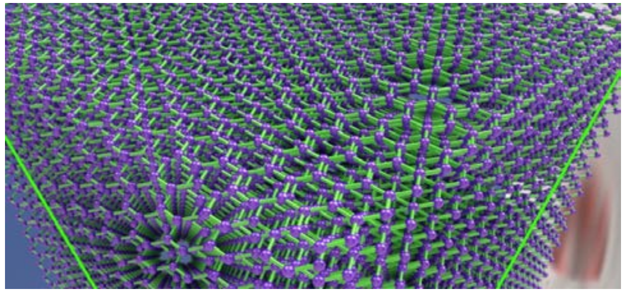
Must prepare
and probe with external fields

21=7*3

Shor's
algorithm



Grover's algorithm (or inversion)

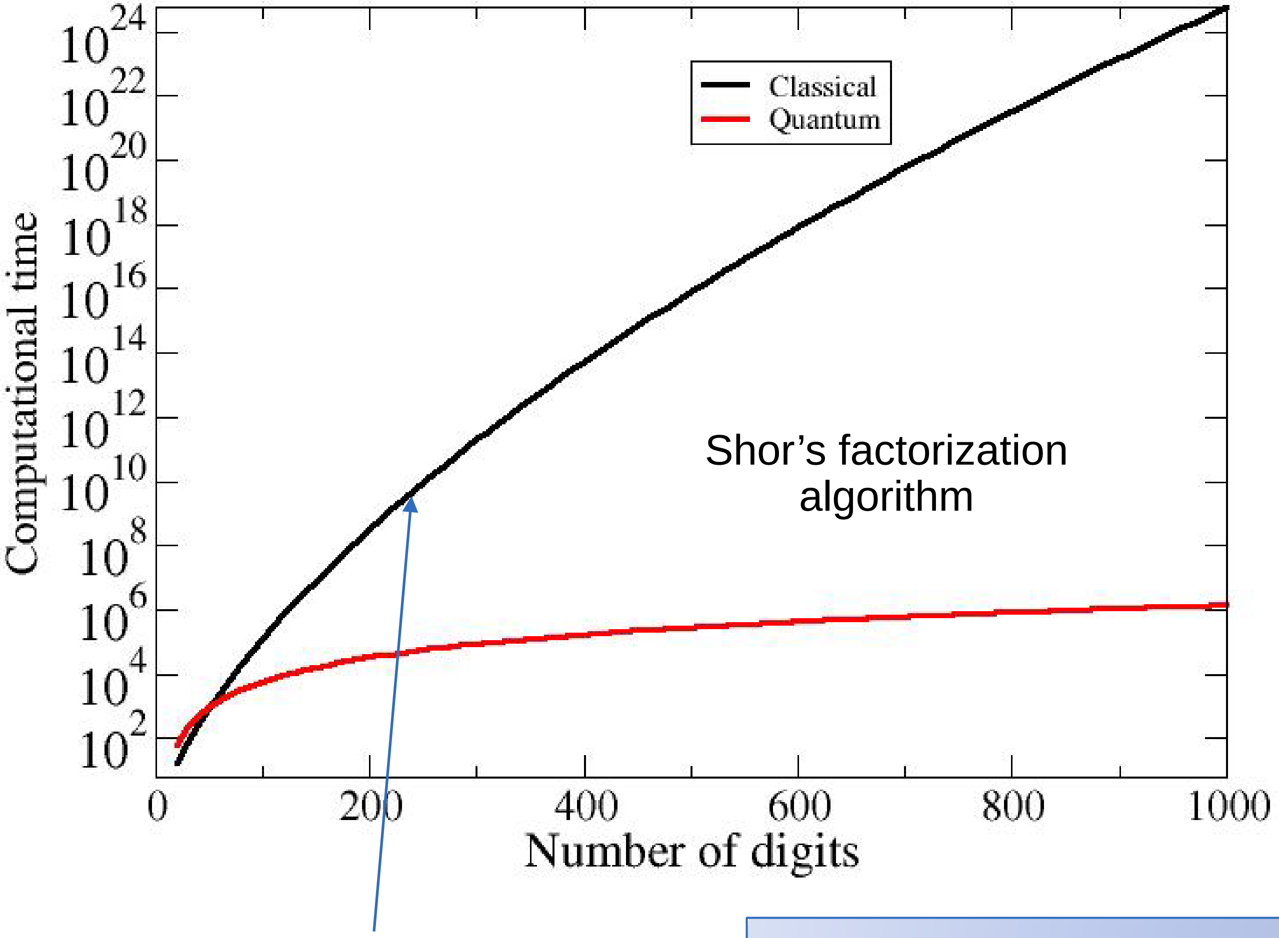


Quantum many-body
simulation: Feynman, Lloyd

~15 algorithms exist; others can be expected as QC develops

Quantum computing could crack some really tough problems!

The promise of quantum computing:
Scaling of some of the most difficult algorithms



Shor's factorization algorithm

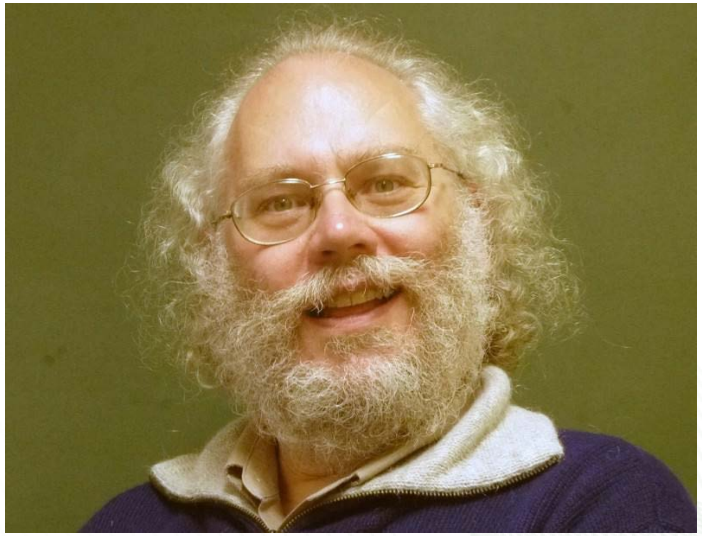
Today AES-256

Quantum

O((log N)^2(log log N)(log log log N))

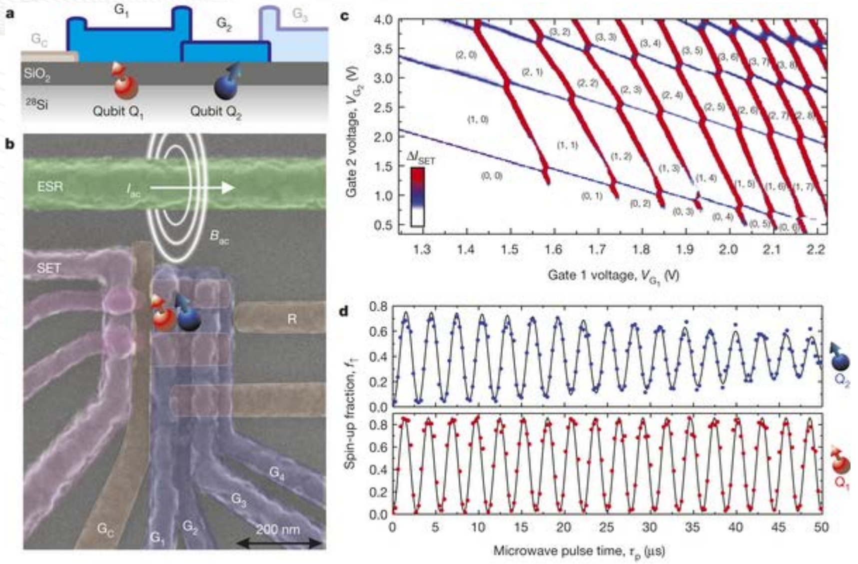
Classical

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



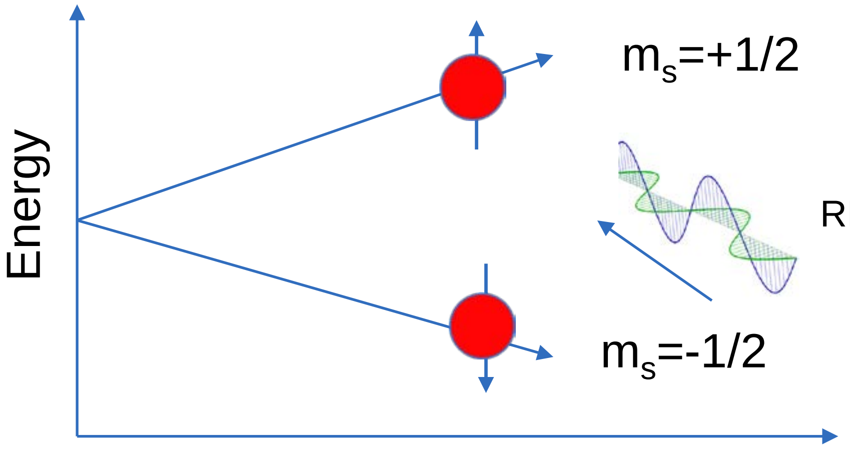
http://math.nist.gov/quantum/zoo/

How to make a qubit



Veldhorst et al., Nature 526, 410 (2015)

B-field splits the orbital into its projections



Energy

m_s=+1/2 $U=\frac{1}{2}g\mu_B B$

RF induced transition

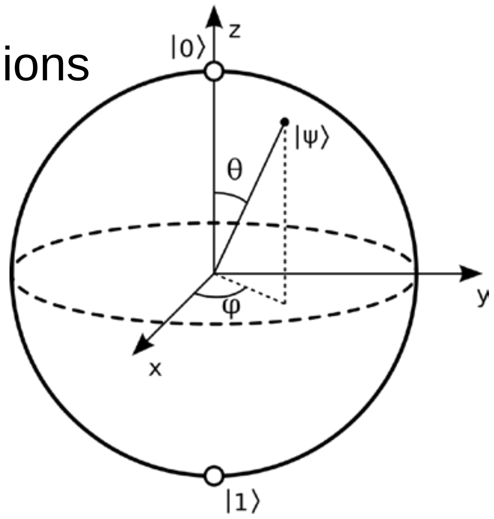
m_s=-1/2 $U=-\frac{1}{2}g\mu_B B$

B_0=0 B_0>0 Magnetic field

Electrons are spin ½ fermions

$$|\Psi> = a|\tfrac{1}{2}>+b|-\tfrac{1}{2}>$$

$|a|^2+|b|^2=1$



Order of magnitude estimates…

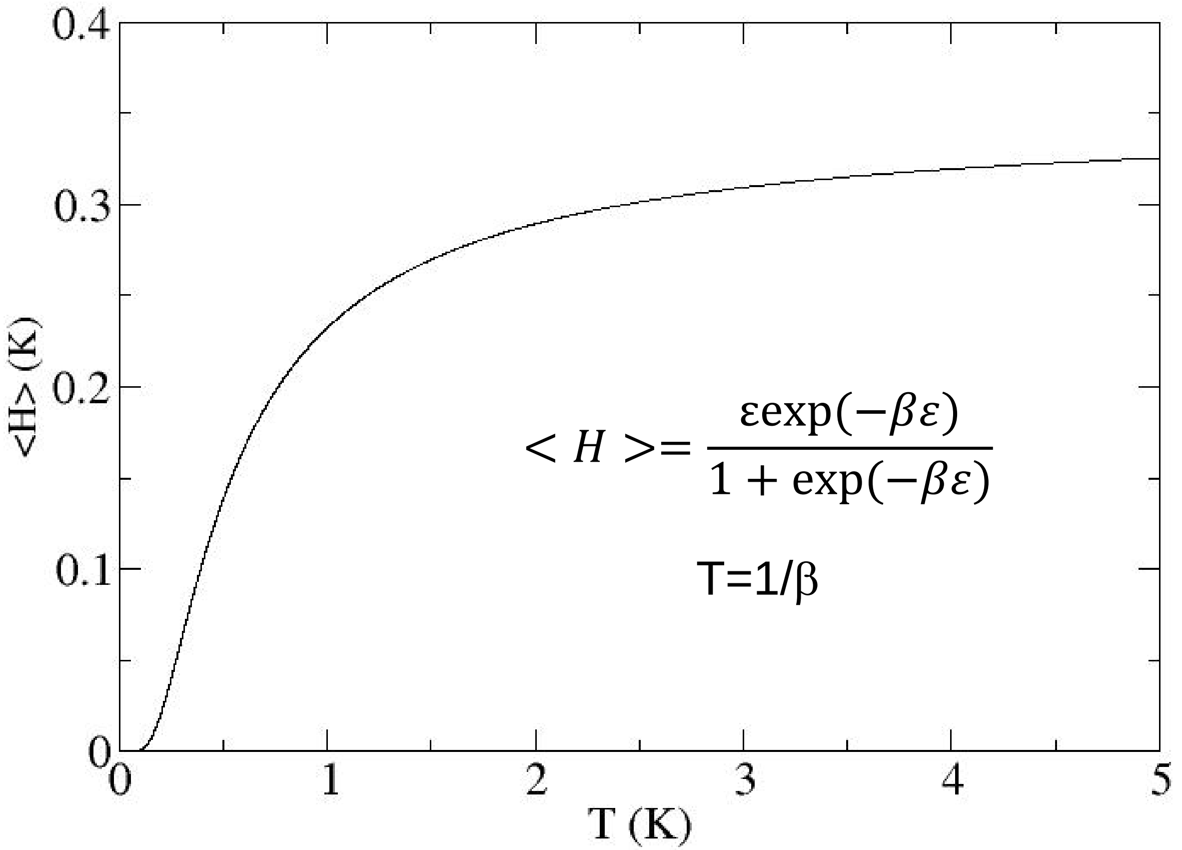
- Landau g factor ~1
- μ_B=5.8x10^{-5} eV/Tesla
- B=1 Tesla
- ε=0.7 K
- 1 K = 20 GHz

Types of decoherence

T_1 – relaxation time

T_2^* – 'dephasing' time

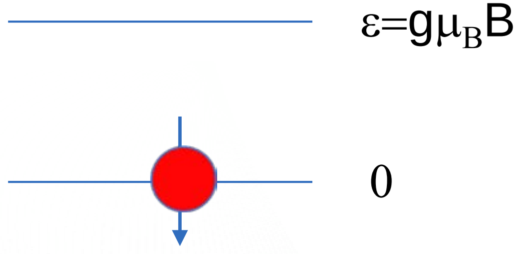
Thermal effects



$$< H >= \frac{\varepsilon \exp(-\beta\varepsilon)}{1+\exp(-\beta\varepsilon)}$$

$T=1/\beta$

Landau g factor ~1
$\mu_B = 5.8\times10^{-5}$ eV/Tesla
B=1 Tesla
$\varepsilon = 0.7$ K
1 K = 20 Ghz



Implies very low temperature operation (mK)

Quantum Computing at ORNL

ORNL Quantum computing materials and interfaces strategy

Opportunity

- Integrate core competencies in materials, modeling, and isotopes to establish a broad R&D effort in quantum computing
- Create S&T base to drive computing beyond exascale and into quantum computing

ORNL assets

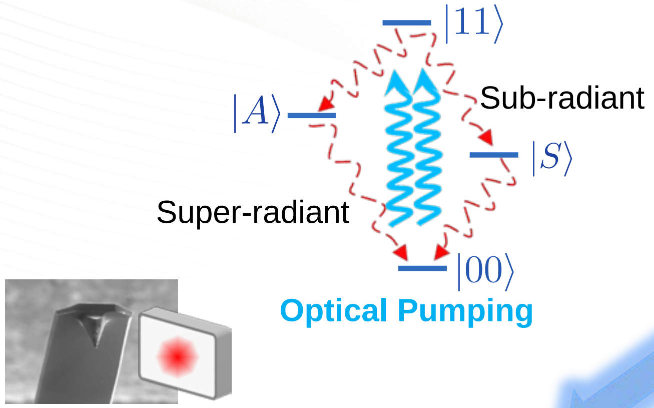
- Expertise in quantum information science and quantum computing
- Unique resources for materials characterization
- Strengths in first principles theory, modeling, and simulation for quantum materials
- National User Facilities: CNMS, OLCF, SNS

Strategy

- Develop tools necessary to characterize and design high-fidelity physical qubits
- Explore methods to interface qubits to traditional computers
- Develop a multi-qubit research test bed
- Research methods to program multi-qubit systems
- Foster multiagency ties to secure long-term funding

Outcome
Cross-cutting R&D portfolio establishing ORNL as a national leader in quantum computing

The Quantum Information Science Group supports research and development in a variety of quantum technologies



QUANTUM
INFORMATION SCIENCE
OAK RIDGE NATIONAL LABORATORY

Quantum Sensing

- Compressive Quantum Imaging
- Quantum Plasmonic Sensors
- Ultra-sensitive MEMS Displacement
- Standoff Spectroscopy
- Opto-mechanical Force Microscopy

Quantum Computing

- Circuit Model Simulations
- Analog Digital Quantum Simulations
- Physical Qubits Modeling
- Quantum Characterization, Verification and Validation

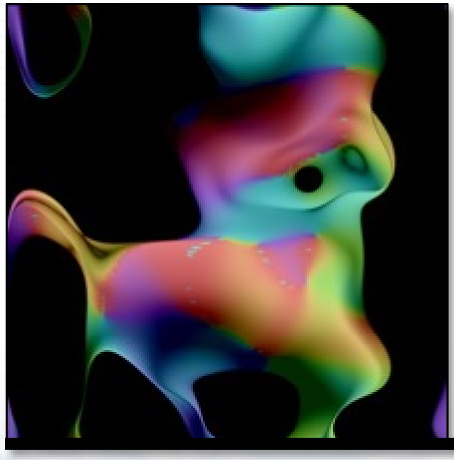
Quantum Communication

- Quantum Networks
- Quantum Key Distribution
- Quantum Secret Sharing
- Quantum Random Number Generators

More information:
https://www.ornl.gov/division/csed/quantum-information
Contact: gricew@ornl.gov

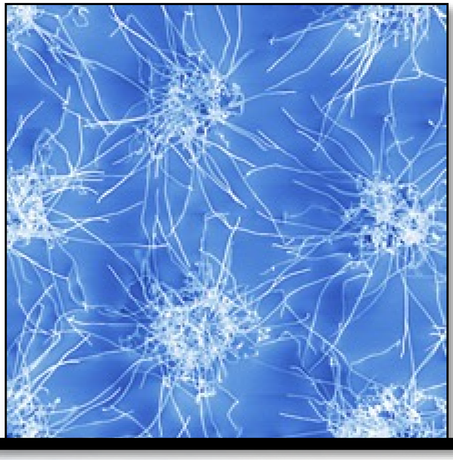
Center for Nanophase Materials Sciences provides capabilities for qubit research

Synthesis



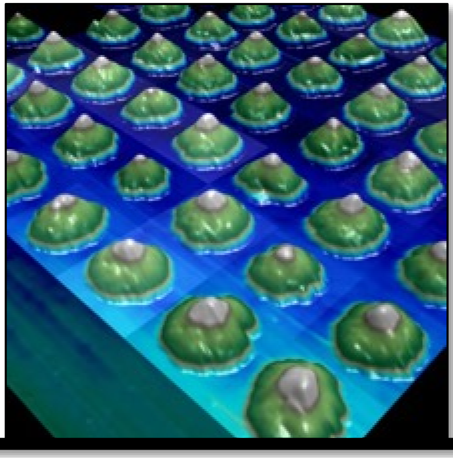
2D, precision synthesis, selective deuteration

Nanofabrication



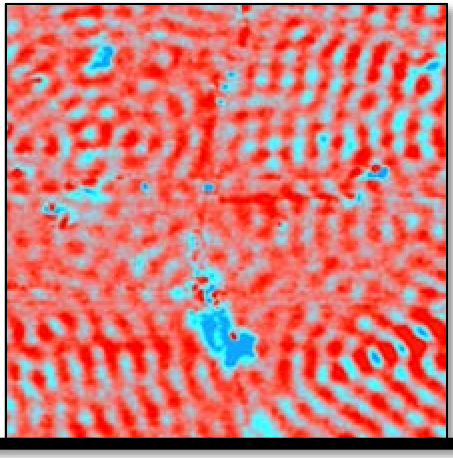
Direct-write, microfluidics, cleanroom

Advanced microscopy



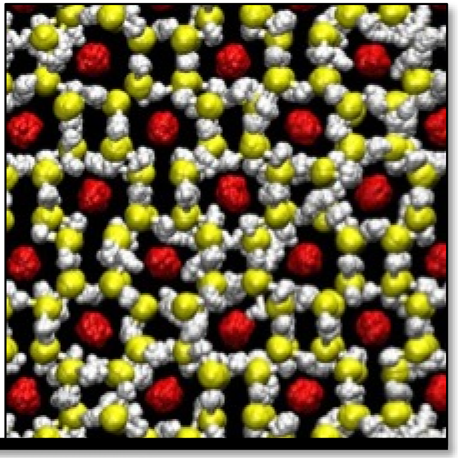
AFM (a CNMS specialty), STM, aberration-corrected TEM/STEM, atom probe tomography

Functional characterization



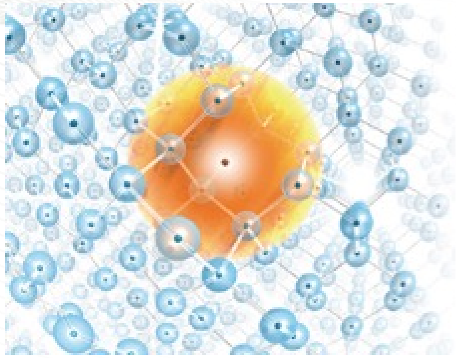
Laser spectroscopy, transport, magnetism, electromechanics

Theory and modeling



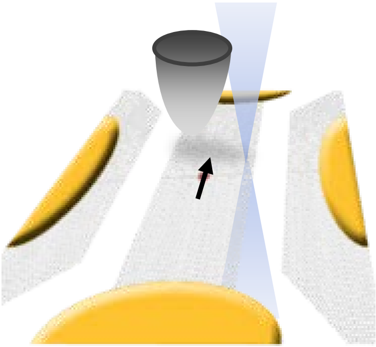
Nanomaterials Theory Institute; gateway to leadership-class high-performance computing

Current Quantum Computing LDRD initiative (FY16-18)

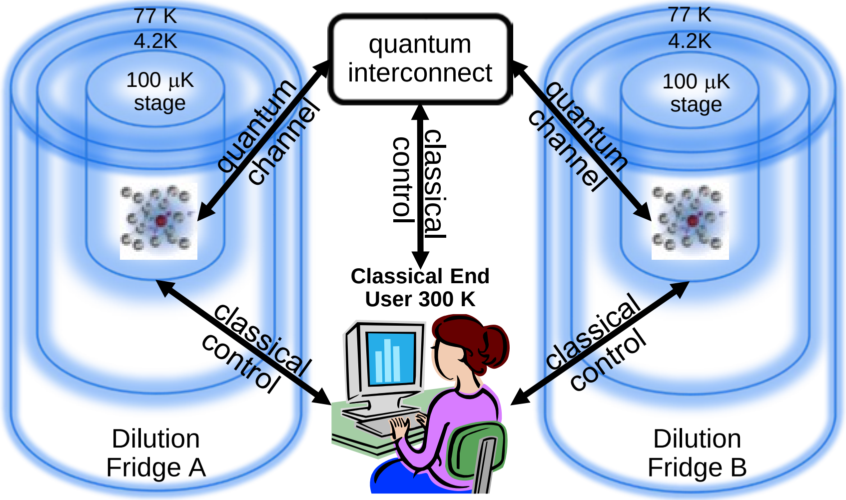


P donor in Si
(Humble, Lupini)

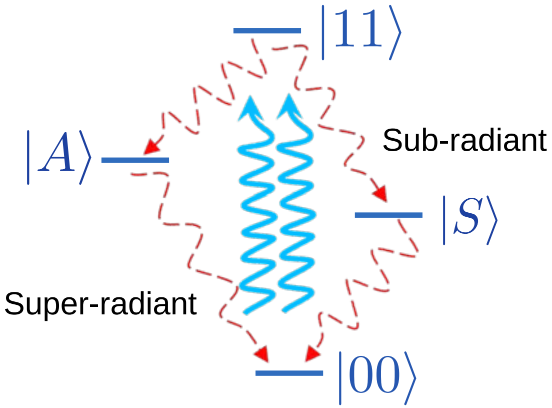
Qubit operations
Heat dissipation
(Peters)



Graphene Qubit
(Jesse)



Quantum/Classical Interfaces (Lougovski)

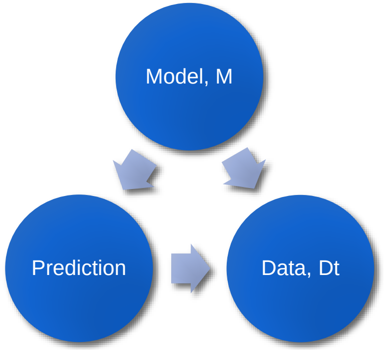


Optical Pumping

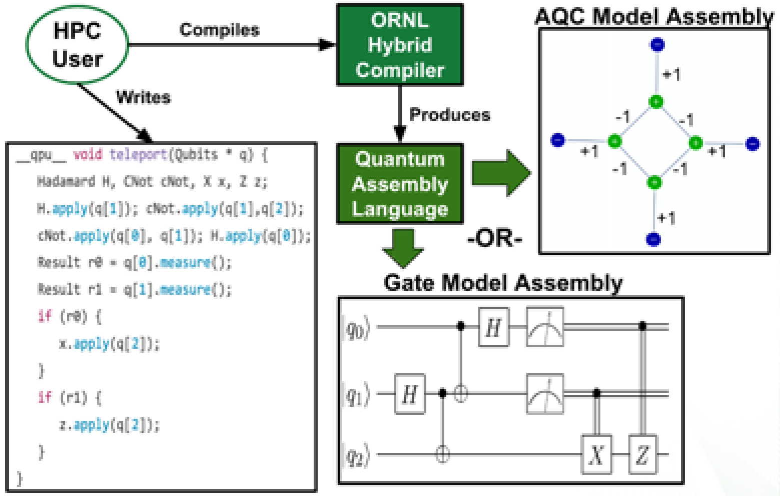
$$|S\rangle = |01\rangle + |10\rangle$$

$$|A\rangle = |01\rangle - |10\rangle$$

Dissipative QC (Evans)



Qubit fidelity modeling
(Bennink)

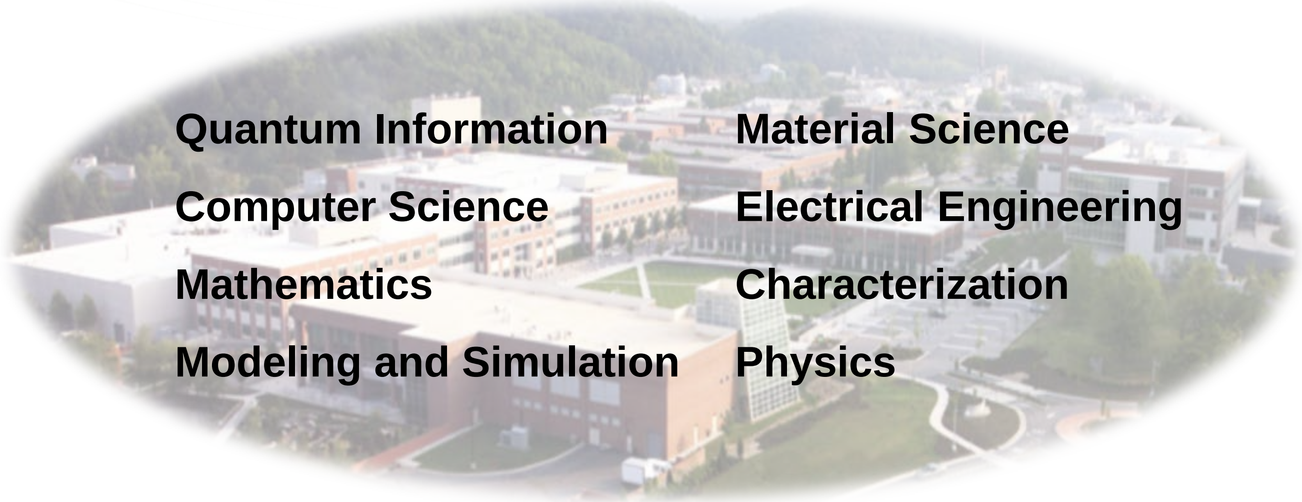


```
__qpu__ void teleport(Qubits * q) {
   Hadamard H, CNot cNot, X x, Z z;
   H.apply(q[1]); cNot.apply(q[1],q[2]);
   cNot.apply(q[0], q[1]); H.apply(q[0]);
   Result r0 = q[0].measure();
   Result r1 = q[1].measure();
   if (r0) {
      x.apply(q[2]);
   }
   if (r1) {
      z.apply(q[2]);
   }
}
```

Qubit Compiler
(McCaskey)

The Quantum Computing Institute provides lab-wide integration of our unique capabilities and partnerships

- **ORNL interaction point for resources in quantum computing**
  - *Our mission is to foster collaborations and partnerships in developing quantum computing for scientific applications of next generation computing systems*
- **The QCI leverages expertise across ORNL:**



Quantum Information	**Material Science**
Computer Science	**Electrical Engineering**
Mathematics	**Characterization**
Modeling and Simulation	**Physics**

- **Focused Research, Community Outreach, Partnerships, User Support, Facilities**
- **40+ staff and associates working on collaborative research**

More information available at quantum.ornl.gov

Our partnership network leverages expertise from academia, industry, and government

IBM

Georgia Tech

University of Virginia

The University of Tennessee UT

VirginiaTech

APL
Johns Hopkins
Applied Physics Laboratory

MIT Lincoln Laboratory

Georgia Tech Research Institute

University of Toronto

Illinois
University of Illinois at Urbana-Champaign

Purdue University

Sandia National Laboratories

NASA

ARL

Texas
The University of Texas at Austin

Vanderbilt University

University of Nebraska Lincoln

D-Wave

GE Global Research

Qubitekk

Pacific Northwest National Laboratory
Proudly Operated by Battelle Since 1965

Naval Air Systems Command

The University of Oklahoma

Lockheed Martin

جامعة خليفة
Khalifa University

Raytheon
BBN Technologies

WKU

SIU
Southern Illinois University
Carbondale

QxBranch

IDQ

Florida State University
1851

Schola Genevensis 1559

Applied Communication Sciences

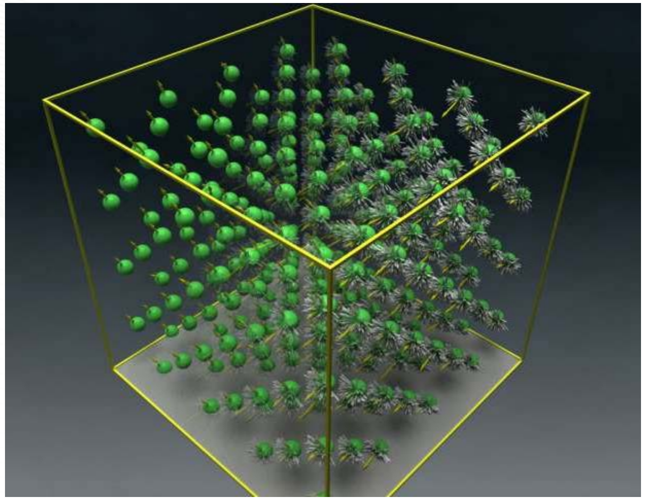
NC State University

Universidad del País Vasco
Euskal Herriko Unibertsitatea

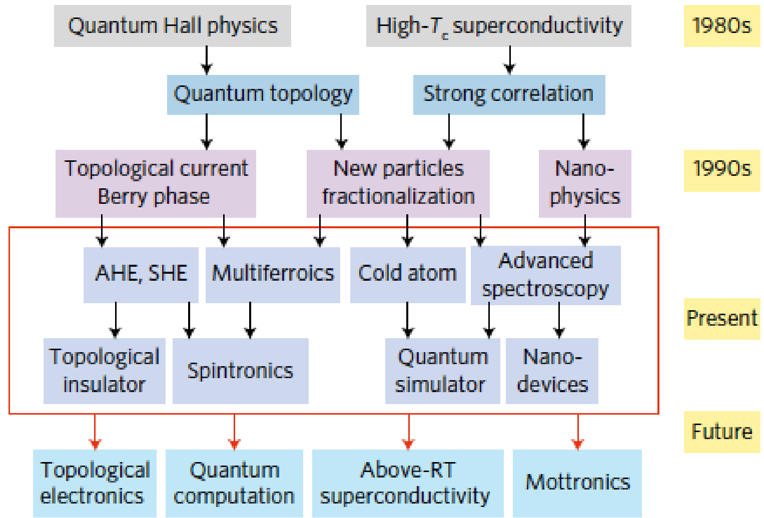
Current activities and near-term opportunities in QC

- At ORNL
  - FY16 – FY18 Quantum Computing Materials and Interfaces LDRD focused on the testbed concept; QCI,…
  - ASCR (funded): Pathfinder Testbed (Pooser, PI)
  - ASCR (funded): Quantum Algorithms (Loubovski, PI)
- Nationally
  - BES Round Table Reports on QIS
    - Possible funding opportunity to follow (through Linda Horton)
  - NP White Paper on QC
    - Significant FY18 or FY19 funding for enriched materials production for QC (PBR)
  - HEP workshops on QC and QIS
    - Quantum sensing is the main focus
    - RFPs are on the street
  - Congressional (House S&T Committee) discussing a ‘national quantum initiative’

Quantum Materials



Yang et al., *Nature* **542**, 75 (2017)



Quantum Hall physics

High-T_c superconductivity

1980s

Quantum topology

Strong correlation

Topological current Berry phase

New particles fractionalization

Nano-physics

1990s

AHE, SHE

Multiferroics

Cold atom

Advanced spectroscopy

Present

Topological insulator

Spintronics

Quantum simulator

Nano-devices

Future

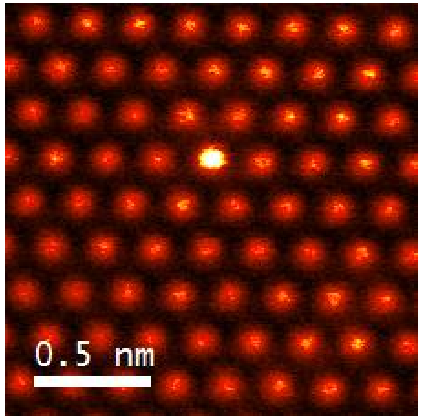
Topological electronics

Quantum computation

Above-RT superconductivity

Mottronics

Nat. Phys. **13**, 1056 (2017)



Lupini LDRD

The Science

- Strongly correlated electron systems and emergent behavior
- Requires a strong theoretical basis
- Requires advanced characterization techniques
- Neutrons provide an excellent probe of magnetic properties
- Light sources yield structural info

Why it is important

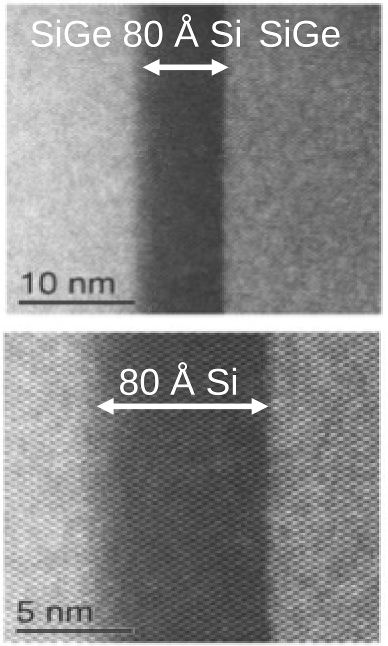
- Miniaturization of electronics toward <7 nm structures requires quantum mechanics
- Strong connection to quantum information and quantum computing
- Used in sensors, high-density memory…

ORNL Strategy

- Pursue both basic and applied R&D
- Identify expertise gaps and utilize LDRD to fill them
- Capitalize on current strengths in neutron scattering from these materials and computation of their properties

Partnerships: Interfacial optimization for improved qubit devices

Understand electrostatically gated quantum dot structures in SiGe/Si/SiGe heterostructures

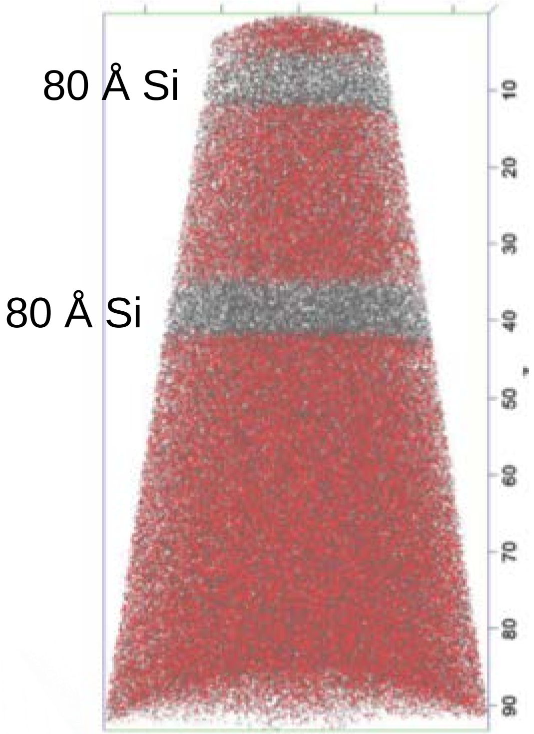


Z-contrast STEM images of 80 Å Si well reveal an atomically “sharp” Si/SiGe interface and a “10 Å diffuse” Si/SiGe interface

Collaboration to investigate SiGe/Si/SiGe interfacial structures and chemistries at the sub-Å level

Partner grows SiGe/Si/SiGe via chemical vapor deposition (CVD) and molecular beam epitaxy (MBE) under various deposition conditions

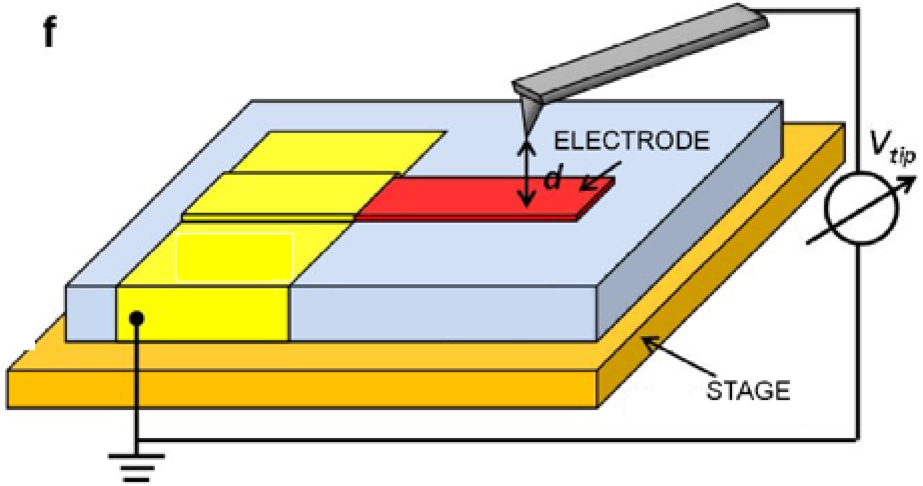
ORNL optimizes CVD and MBE processing variables and reliably produces high-fidelity interfaces through application of expertise in aberration-corrected Z-contrast STEM imaging, electron energy loss spectroscopy, and atom probe tomography to provide the single-atom-level understanding of defects, interfacial steps/terraces, chemistry, composition, and structural thermal stability



Atom probe tomography map of a double-Si-well heterostructure (Si: grey; Ge: red)

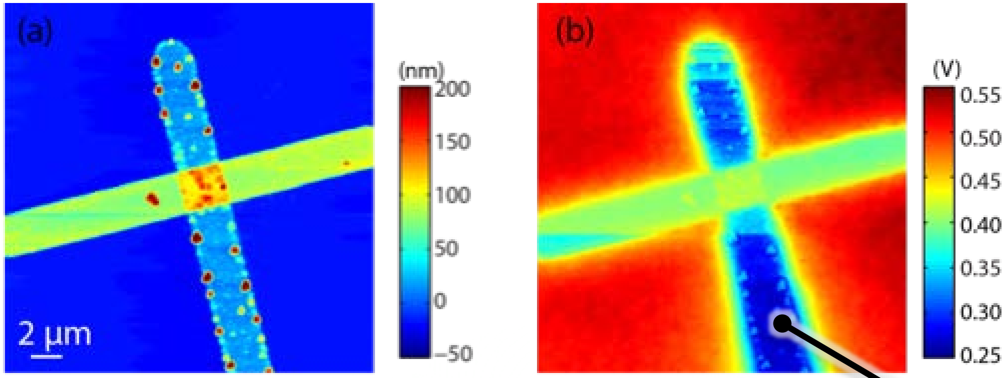
Kelvin probe force microscopy with MIT Lincoln Laboratory

Understanding anomalous heating of ion-trap qubits using Kelvin probe force microscopy (KPFM) and X-ray photoelectron spectroscopy



Kelvin probe AFM: DC/AC biased probe detects electrostatic forces on a sample surface, mapping work function on a surface with nanometer precision

Understanding surface contamination of superconducting qubits: Standard AFM and KPFM imaging on model Au/Si sample

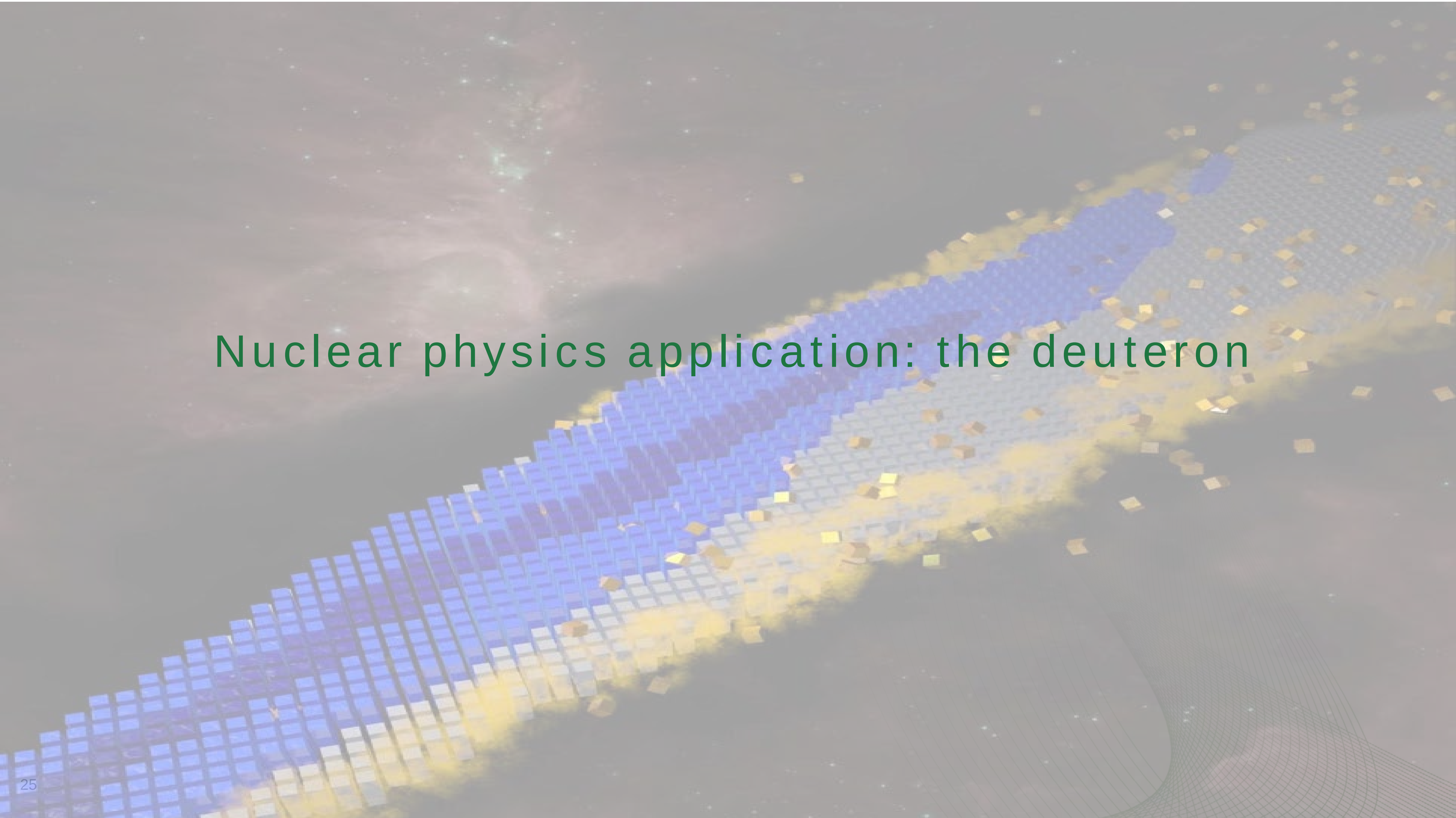


Topography

CPD

Small blue dots: Distortions in work function map may be due to localized distortions in the electric field caused by residual contaminants (both distortions and contaminants may be detectible using this technique)

L. Collins et al., "Multifrequency spectrum analysis using fully digital G-mode-Kelvin probe force microscopy," ***Nanotechnol.*** In press



Nuclear physics application: the deuteron

Game plan (“simplest deuteron”)

1. Hamiltonian from pionless EFT at leading order; fit to deuteron binding energy; constructed in harmonic-oscillator basis of $^3S_1$ partial wave [à la Binder et al. (2016); Bansal et al. (2017)]; cutoff at about 150 MeV.

$$H_N = \sum_{n,n'=0}^{N-1} \langle n'|(T+V)|n\rangle a_{n'}^\dagger a_n$$

$$\langle n'|V|n\rangle = V_0 \delta_n^0 \delta_n^{n'}$$

$$V_0 = -5.68658111 \text{ MeV}$$

2. Map single-particle states |n⟩ onto qubits using |0⟩ = |↑⟩ and |1⟩ = |↓⟩. This is an analog of the Jordan-Wigner transform.

$$a_p^\dagger \leftrightarrow \sigma_-^{(p)} \equiv \frac{1}{2}(X_p - iY_p) \qquad a_p \leftrightarrow \sigma_+^{(p)} \equiv \frac{1}{2}(X_p + iY_p)$$

3. Solve H_1, H_2 (and H_3) and extrapolate to infinite space using harmonic oscillator variant of Lüscher’s formula [More, Furnstahl, Papenbrock (2013)]

$$E_N = -\frac{\hbar^2 k^2}{2m}\left(1 - 2\frac{\gamma^2}{k} e^{-2kL} - 4\frac{\gamma^4 L}{k} e^{-4kL}\right) + \frac{\hbar^2 k \gamma^2}{m}\left(1 - \frac{\gamma^2}{k} - \frac{\gamma^4}{4k^2} + 2 w_2 k \gamma^4\right) e^{-4kL}$$

Variational wave function

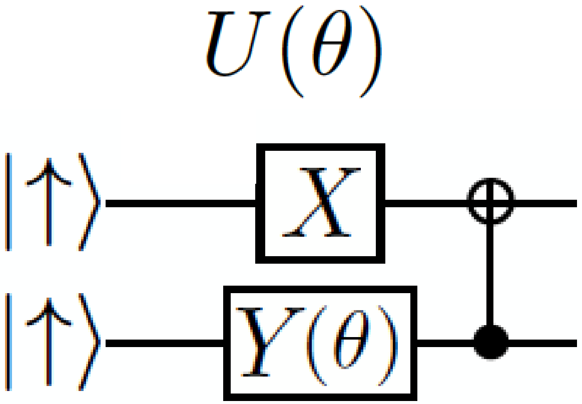
Wave functions on two qubits

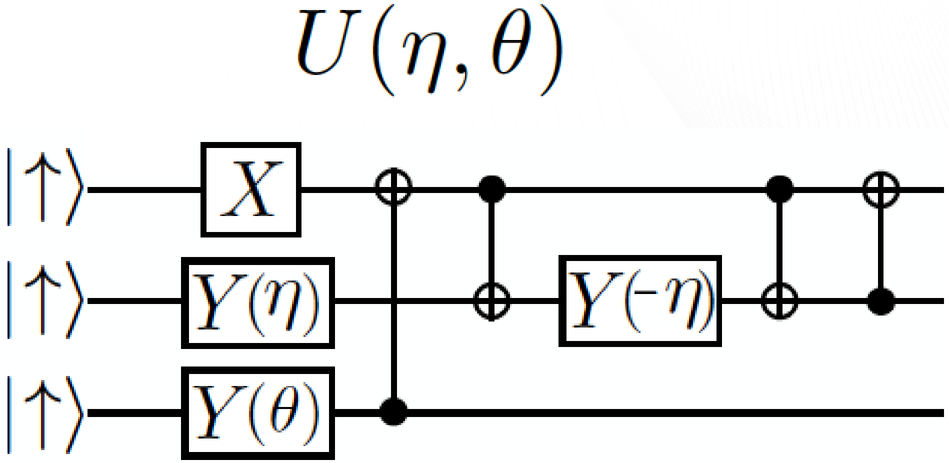
$$U(\theta)|\downarrow\uparrow\rangle \qquad U(\theta) \equiv e^{\theta\left(a_0^\dagger a_1 - a_1^\dagger a_0\right)} = e^{i\frac{\theta}{2}(X_0Y_1 - X_1Y_0)}$$

Wave functions on three qubits

$$U(\eta,\theta)|\downarrow\uparrow\uparrow\rangle \qquad U(\eta,\theta) \equiv e^{\eta\left(a_0^\dagger a_1 - a_1^\dagger a_0\right)+\theta\left(a_0^\dagger a_2 - a_2^\dagger a_0\right)}$$

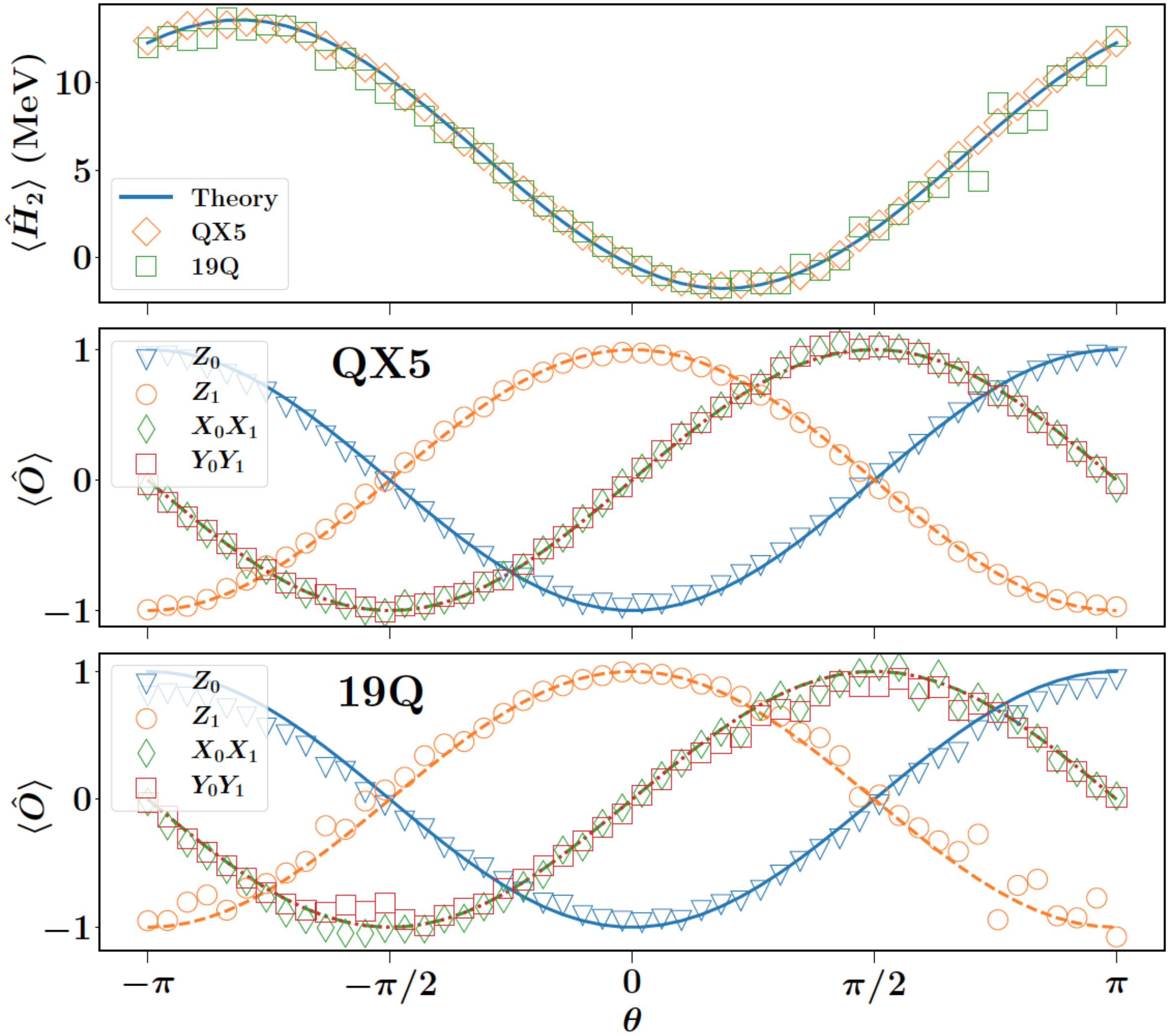
Minimize number of two-qubit CNOT operations to mitigate low two-qubit fidelities (construct a “low-depth circuit”)





Hamiltonian expectation value on two qubits

$$H_2 = 5.906709I + 0.218291Z_0 - 6.125Z_1 - 2.143304\,(X_0X_1 + Y_0Y_1)$$

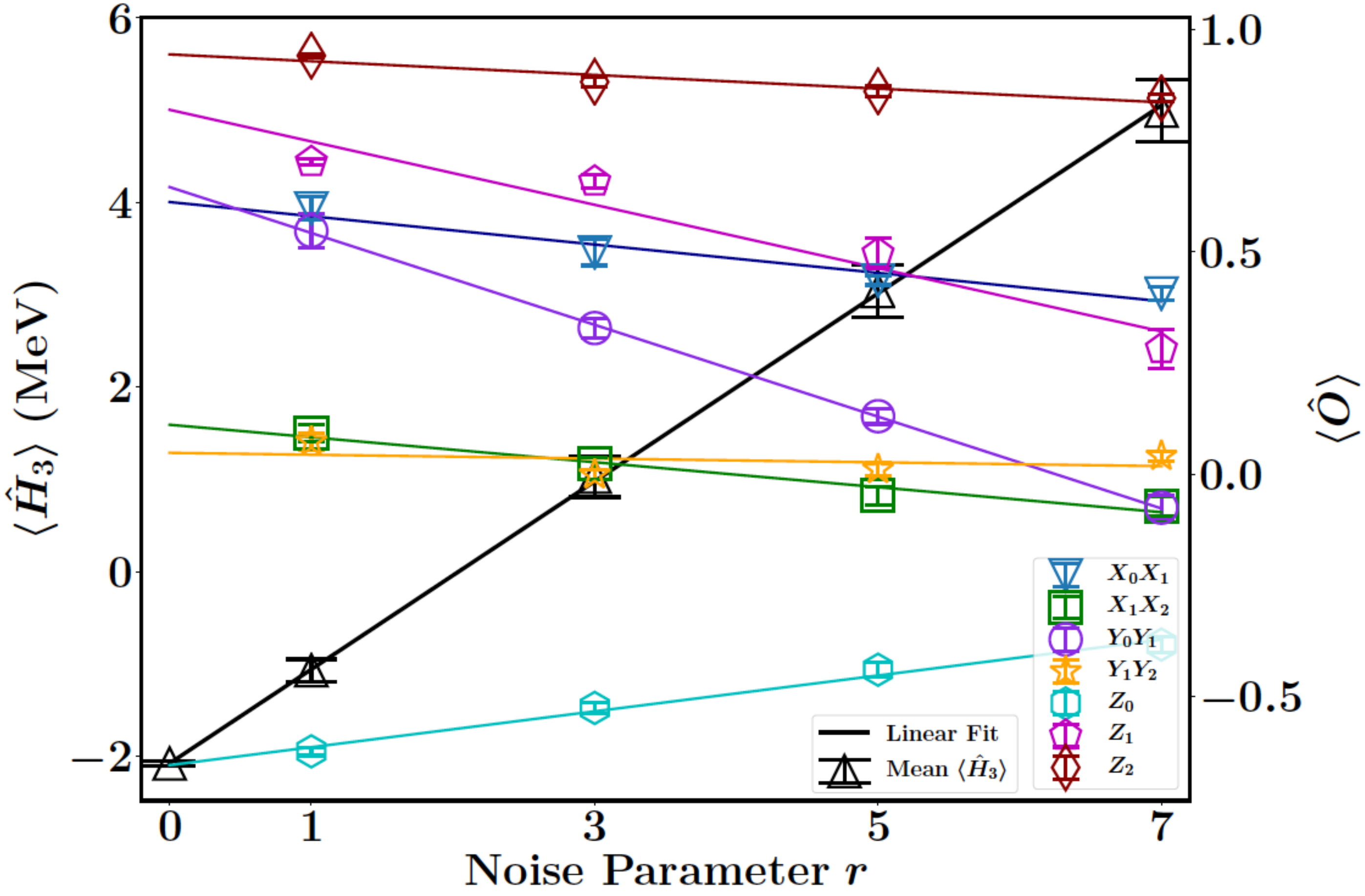


Quantum-classical hybrid algorithm VQE [Peruzzo et al. 2014; McClean et al 2016]:

Expectation values on QPU.
Minimization on CPU.

Three qubits

$$H_3 = H_2 + 9.625(I - Z_2) - 3.913119\,(X_1X_2 + Y_1Y_2)$$



Three qubits have more noise. Insert *r* pairs of CNOT (unity operators) to extrapolate to *r*=0. [See, e.g., Ying Li & S. C. Benjamin 2017]

Final results

Deuteron ground-state energies from a quantum computer compared to the exact result, E_∞=-2.22 MeV.

E from exact diagonalization				
N	E_N	$\mathcal{O}(e^{-2kL})$	$\mathcal{O}(kLe^{-4kL})$	$\mathcal{O}(e^{-4kL})$
2	-1.749	-2.39	-2.19	
3	-2.046	-2.33	-2.20	-2.21
E from quantum computing				
N	E_N	$\mathcal{O}(e^{-2kL})$	$\mathcal{O}(kLe^{-4kL})$	$\mathcal{O}(e^{-4kL})$
2	$-1.74(3)$	$-2.38(4)$	$-2.18(3)$	
3	$-2.08(3)$	$-2.35(2)$	$-2.21(3)$	$-2.28(3)$

$$E_N = -\frac{\hbar^2 k^2}{2m}\left(1 - 2\frac{\gamma^2}{k}e^{-2kL} - 4\frac{\gamma^4 L}{k}e^{-4kL}\right) + \frac{\hbar^2 k\gamma^2}{m}\left(1 - \frac{\gamma^2}{k} - \frac{\gamma^4}{4k^2} + 2w_2 k\gamma^4\right)e^{-4kL}$$

[Dumitrescu, McCaskey, Hagen, Jansen, Morris, Papenbrock, Pooser, Dean, Lougovski, arXiv:1801.03897]

Discussion