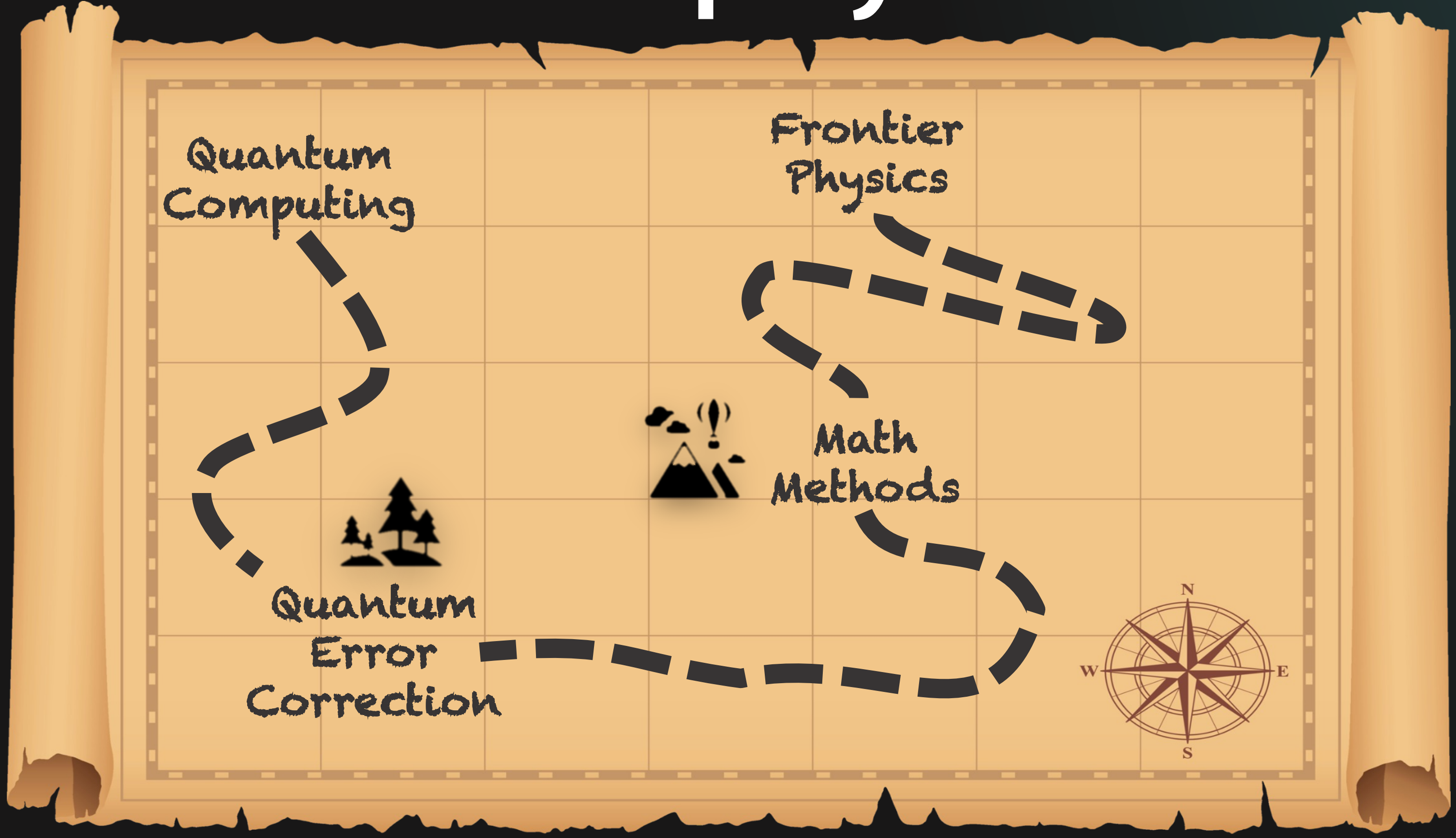
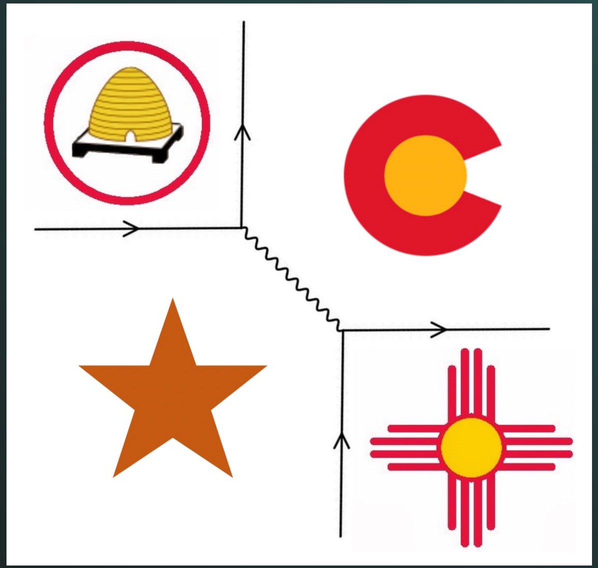
SAND2022-14236C

Quantum computing as a wayfinder for frontier physics





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October 14, 2022

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Breaking “unbreakable” cryptography

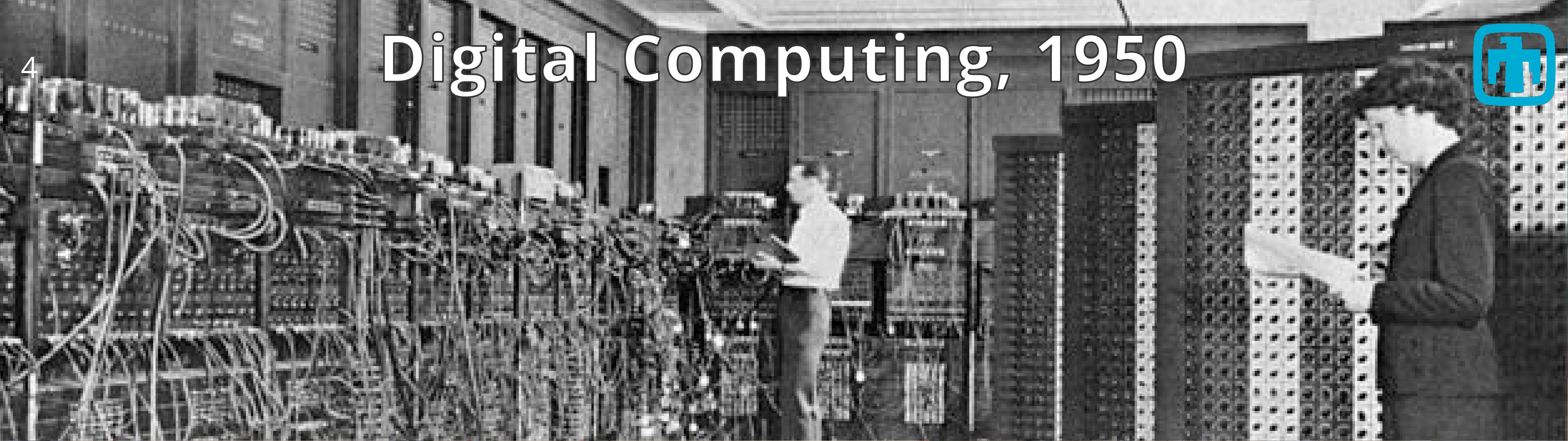
Quantum Computing
- Decoherence
- Data types
- Compiling

Frontier Physics
- Materials science
- Chemistry
- Nuclear physics

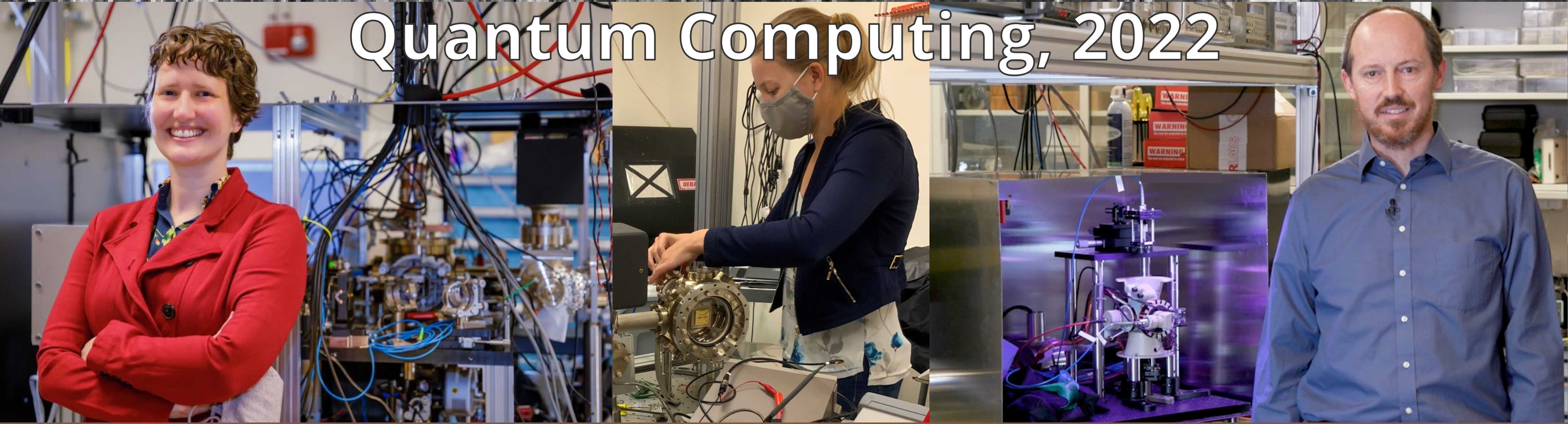
Math Methods
- Linear algebra
- PDEs
- Machine learning

Quantum Error Correction
- Codes
- Extrapolation
- Decoupling

Digital Computing, 1950



Quantum Computing, 2022



What else could you do with a quantum computer?

CYBER

- Cybersecurity
- Machine Learning
- Search
- Software verification

DEFENSE

- Armor design
- Inertial guidance
- Radar, imaging
- Autonomy, C&C

ENERGY

- Mineral & oil exploration
- Oil well optimization
- Energy distribution
- Battery & solar cell design

FINANCE

- Portfolio optimization
- Asset pricing
- Risk analysis & trading strategies
- Fraud detection & market simulation

PHARMA

- Drug discovery
- Catalyst & enzyme design
- Bioinformatics, genomics
- Patient diagnostics, improved MRI

MANUFACTURING

- Materials: OLEDs, composites
- Logistics: Planning and scheduling
- Automotive: Autonomous driving
- Semiconductors: Chip layout & fab

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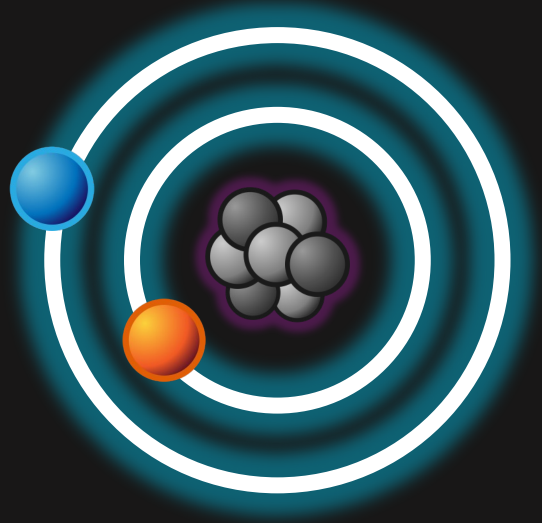
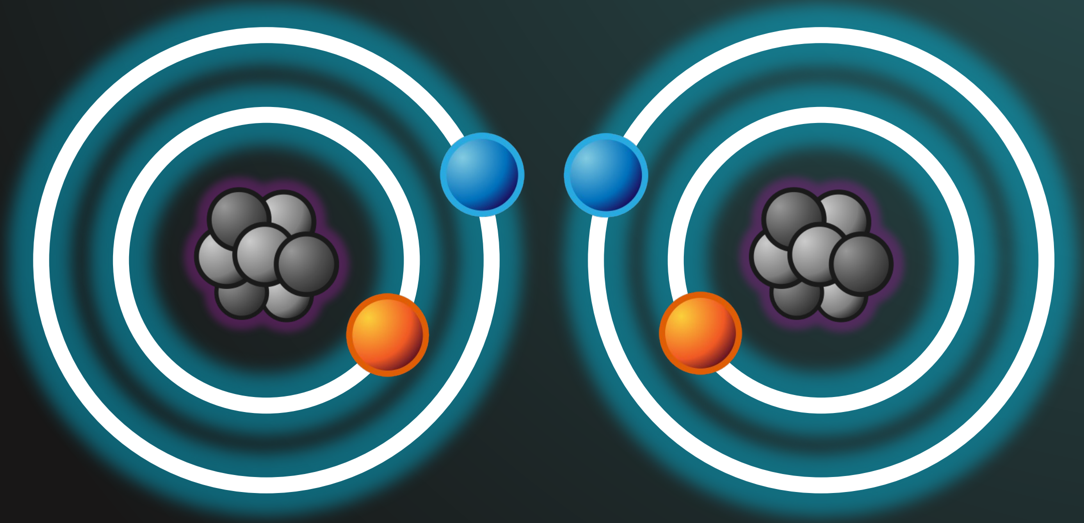
Step 1: Learn basics of quantum computing

Superposition



$\sqrt{}$NOT

Entanglement



$\sqrt{}$SWAP

Step 2: Access a quantum computer

Industry

- Maximum size & speed
- Difficult to study how it works

IBM Q

rigetti

IONQ

aws

Amazon Braket

QUANTINUUM

Open Quantum Testbeds

- Versatile, configurable, flexible
- Not optimized for performance

QSCOUT

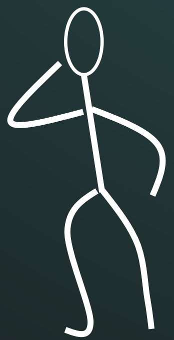
AQT

Sandia National Laboratories

BERKELEY LAB

Build your own

- Total control
- Costly and difficult

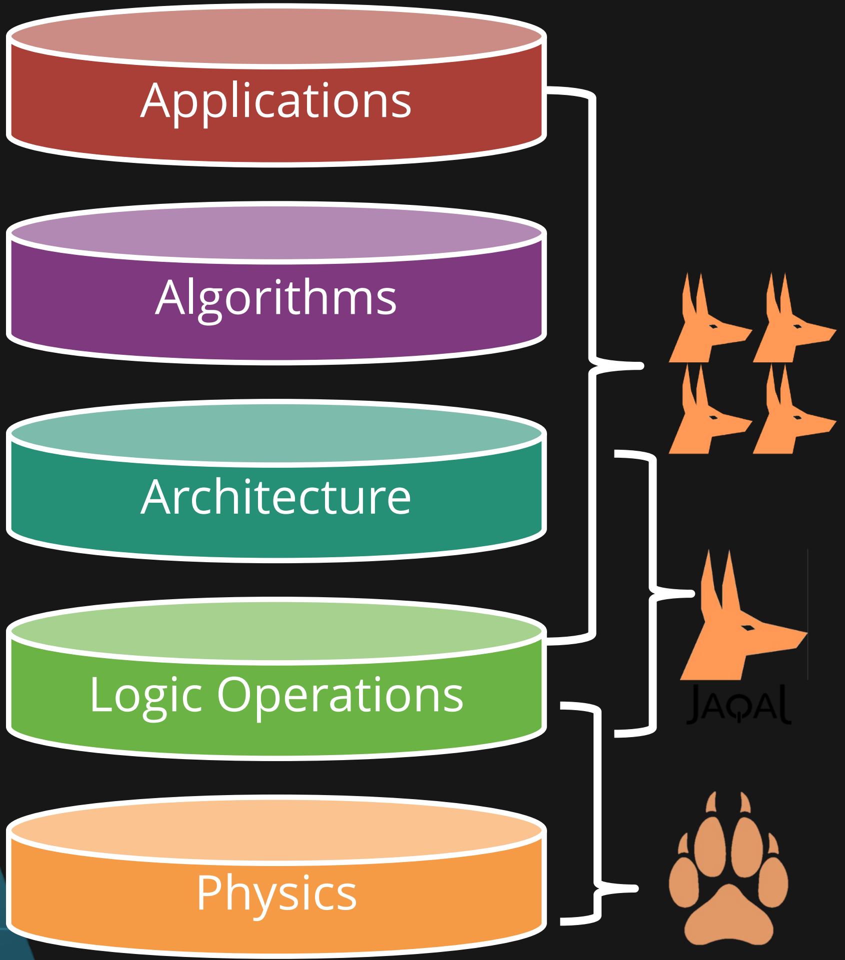


Low-level control →

← Ease of access

Sat., Oct. 15, 9:06 am: J04.00003 QSCOUT: A Transparent Quantum Computing Testbed

Step 2b: Learn quantum programming



JaqalPaq
(Meta-programming with python)

+pyGSTi
Ion Sim

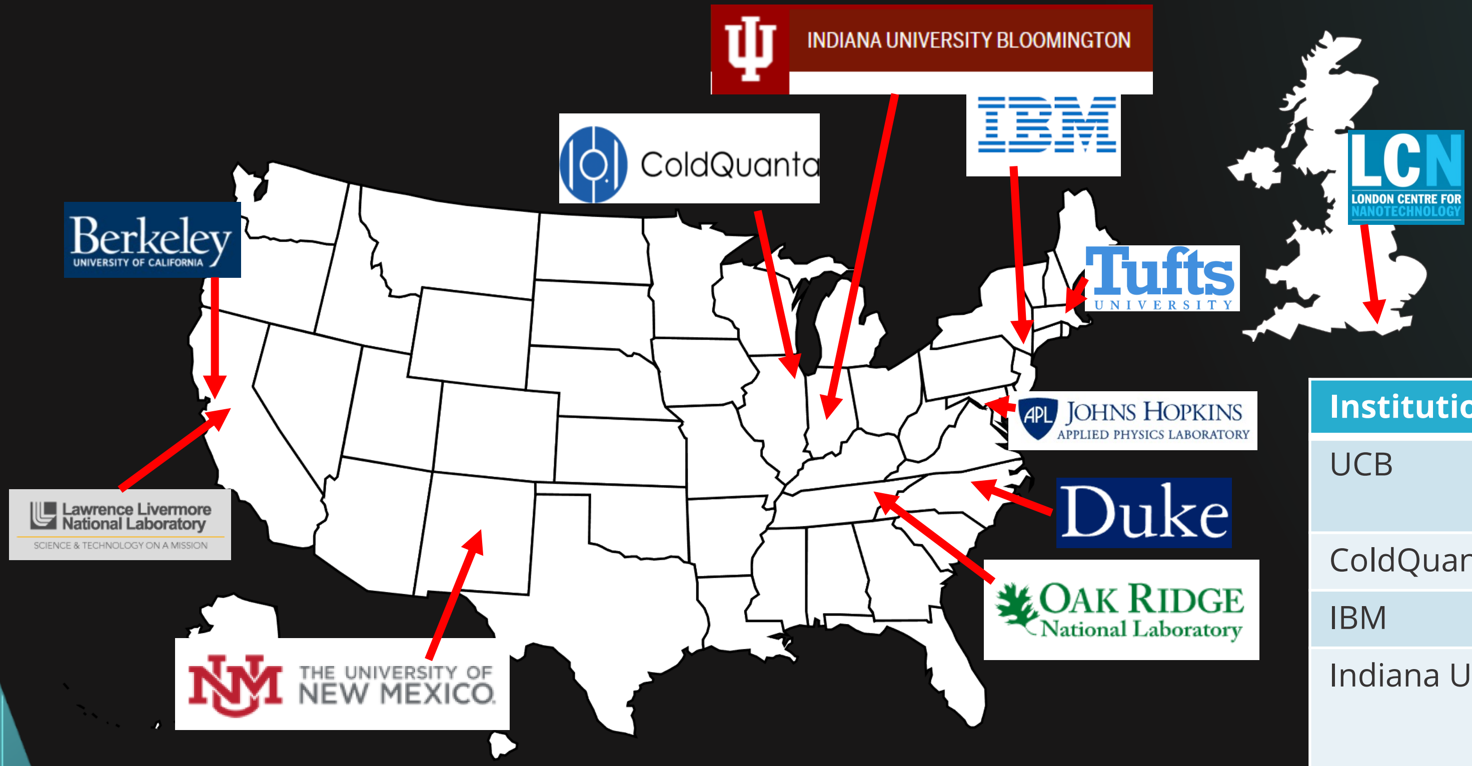
Jaqal
(Just Another Quantum Assembly Language)

JaqalPaw
Pulse-level control

gitlab.com/jaqal

```
from qscout.std.v1 usepulses *

register q[8]

let pi4    0.78539816339
let mpi2 -1.57079632679

macro Hadamard target {
  Sy target
  Px target
}

macro CNOT control target {
  Sy control
  MS control target 0 pi4
  < Rx control mpi2 | Rx target mpi2 >
  Sy control
}

prepare_all
Hadamard q[1]
CNOT q[2] q[1]
measure_all
```

Step 3: Explore the quantum computing frontier



Interested in becoming a user? See qscout.sandia.gov for details.

Institution	Project
UCB	Assessing the Performance of the Randomized Analog Verification protocol for gate-based devices
ColdQuanta	Native gate optimizations and performance benchmarking
IBM	Quantum volume benchmarking
Indiana U.	Simulating quantum chemical nuclear dynamics problems. Simulating the quantum dynamics of proton-coupled electron transport problems in quantum chemistry.
JHU	Characterization and optimal control of time-correlated amplitude control noise
LBNL	Using control pulse engineering to improve the effective fidelity of ion trap quantum computers
LCN	Simulating quantum evolution of infinite systems using tensor networks
ORNL	Connecting low level characterization metrics to higher level algorithmic performance with a tractably small simulation
UNM	Digital simulation of non-stoquastic Hamiltonians

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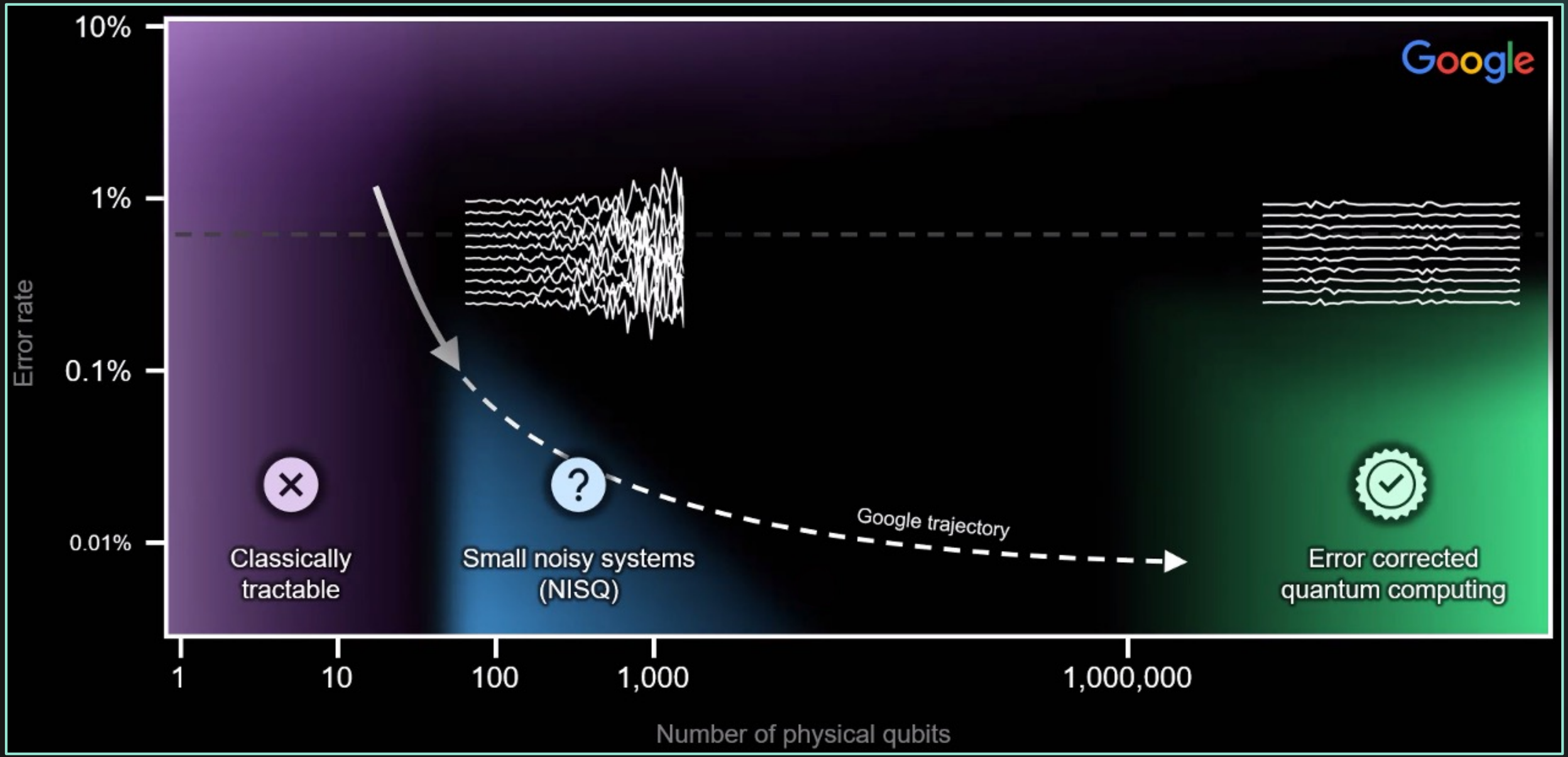
What's the principal challenge?

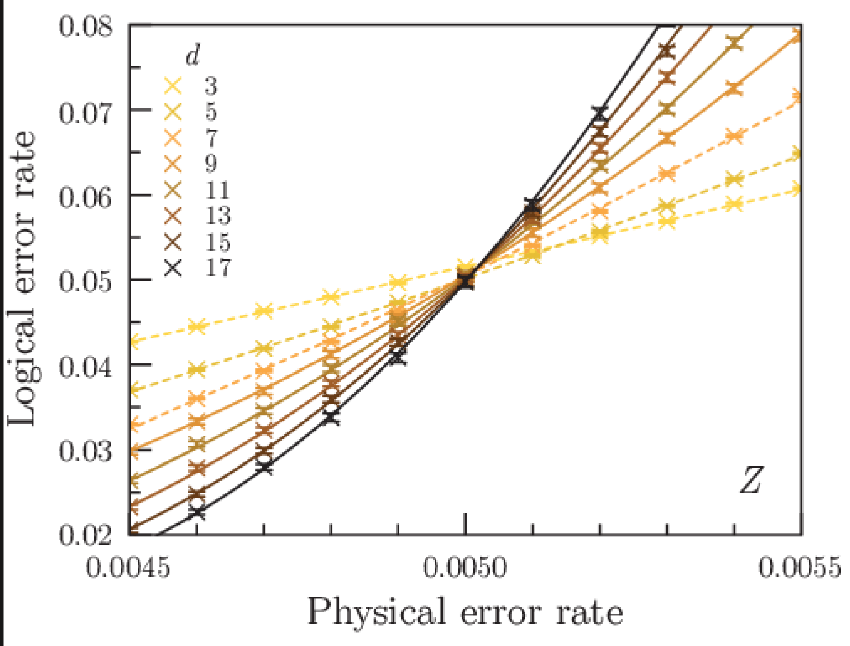
- **Decoherence:** With great power comes great fragility.
    - Today: Noisy Intermediate Scale Quantum (NISQ) Computers



Fri., Oct. 14, 3:06 pm: E02.00003 Demonstration of Mølmer–Sørensen Gates Robust to 10 kHz Trap Frequency Error

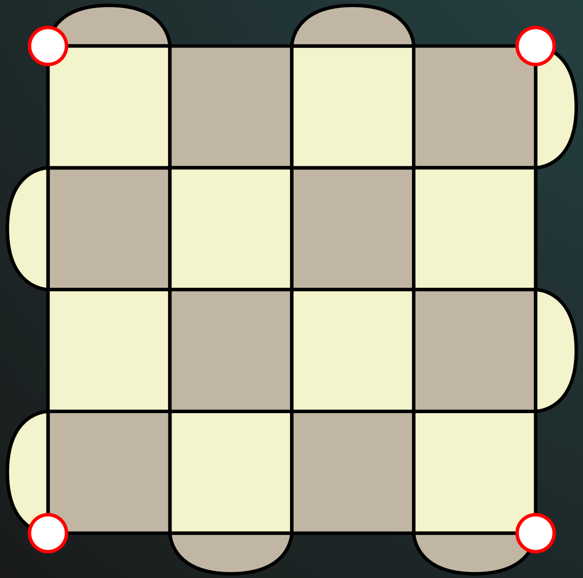
The miracle of fault-tolerant quantum computing

Threshold behavior



[Stephens, PRA 89, 022321 (2013)]

Surface code patch



- Qubits = vertices
- Checks = Pauli ops on faces
- Logical Majorana fermions = "twist" defects on corners*
- Logical qubit = patch

Eventually, we will trade quality for quantity!

*[Landahl, Morrison, arXiv:2110.10280]

How far do we need to go?

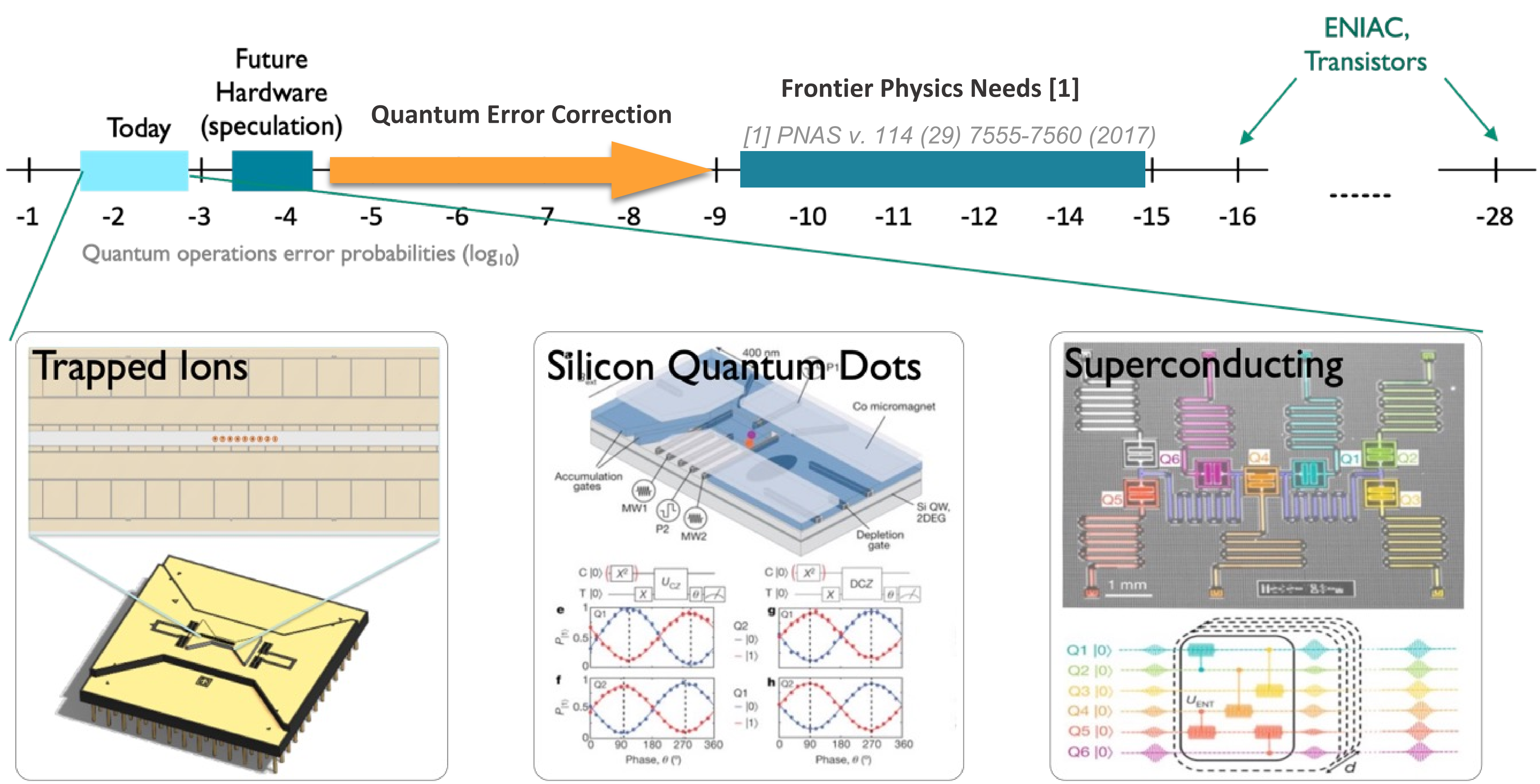


Image: SNL, [1] IonQ (https://ionq.co)

Nature v. 555, pages 633–637 (2018)

Nature v. 549, pages 242–246 (2017)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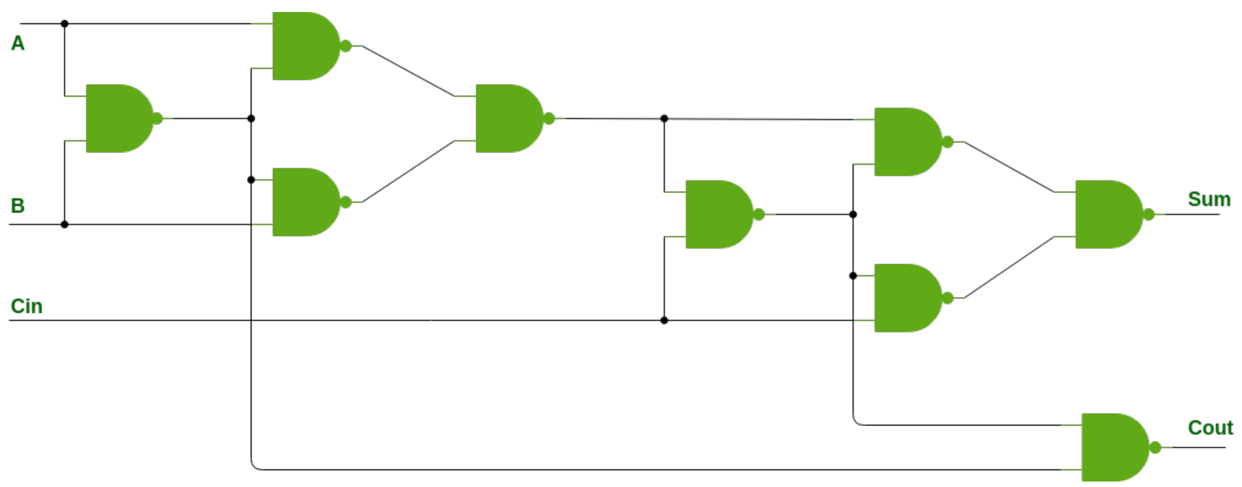
Math methods on a fault-tolerant QC

How do you add two numbers on a quantum computer?

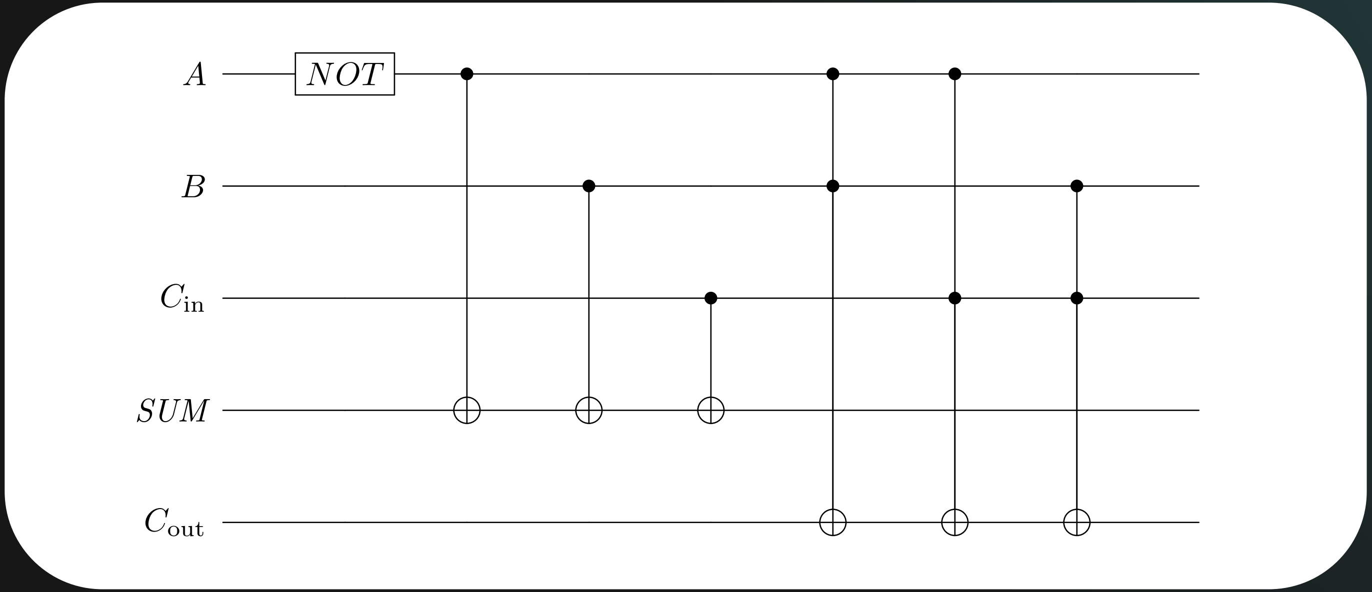


[www.geeksforgeeks.org/full-adder-in-digital-logic]

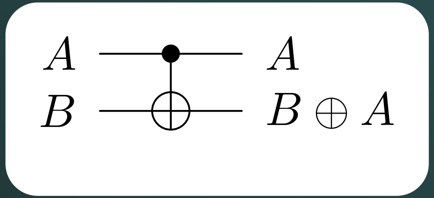
- **Problem 1:** NAND uses irreversible logic.
- **Problem 2:** FANOUT makes copies.
- **Solution:** Convert to reversible logic without FANOUTs.

Math methods on a fault-tolerant QC

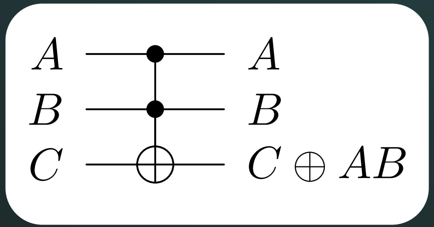
Reversible full adder



CNOT



Toffoli (CCNOT)



- Completely classical circuit: ***No quantum speedup!***
- Speedups still available for superposition inputs…
  - ”Are the sums of these million pairs of numbers all even?”

Advanced problem on a quantum computer

Input
↓
Pre-processing
↓
Q. State Preparation
↓
Q. Alg. Primitive
↓
Q. Measurement
↓
Post-processing
↓
Output

Example: Solving $Ax = b$ on a quantum computer

Conjugate gradient

$$\mathcal{O}(Ns\sqrt{\kappa}\log(1/\varepsilon))$$

Quantum HHL Algorithm [1]

$$\mathcal{O}(\log(N)s^2\kappa \text{ polylog}(1/\varepsilon))$$

Three big caveats

- Only returns *x* as a quantum state: $|x\rangle = A^{-1}|b\rangle$
  - Can compute expectation values though: $\langle M\rangle = \langle x|M|x\rangle$
- κ might scale like *O*(*N*).
- Doesn't account for complexity in preparing $|b\rangle$.

[1] Harrow, Hassidim, Lloyd, PRL 103, 150502 (2009)]

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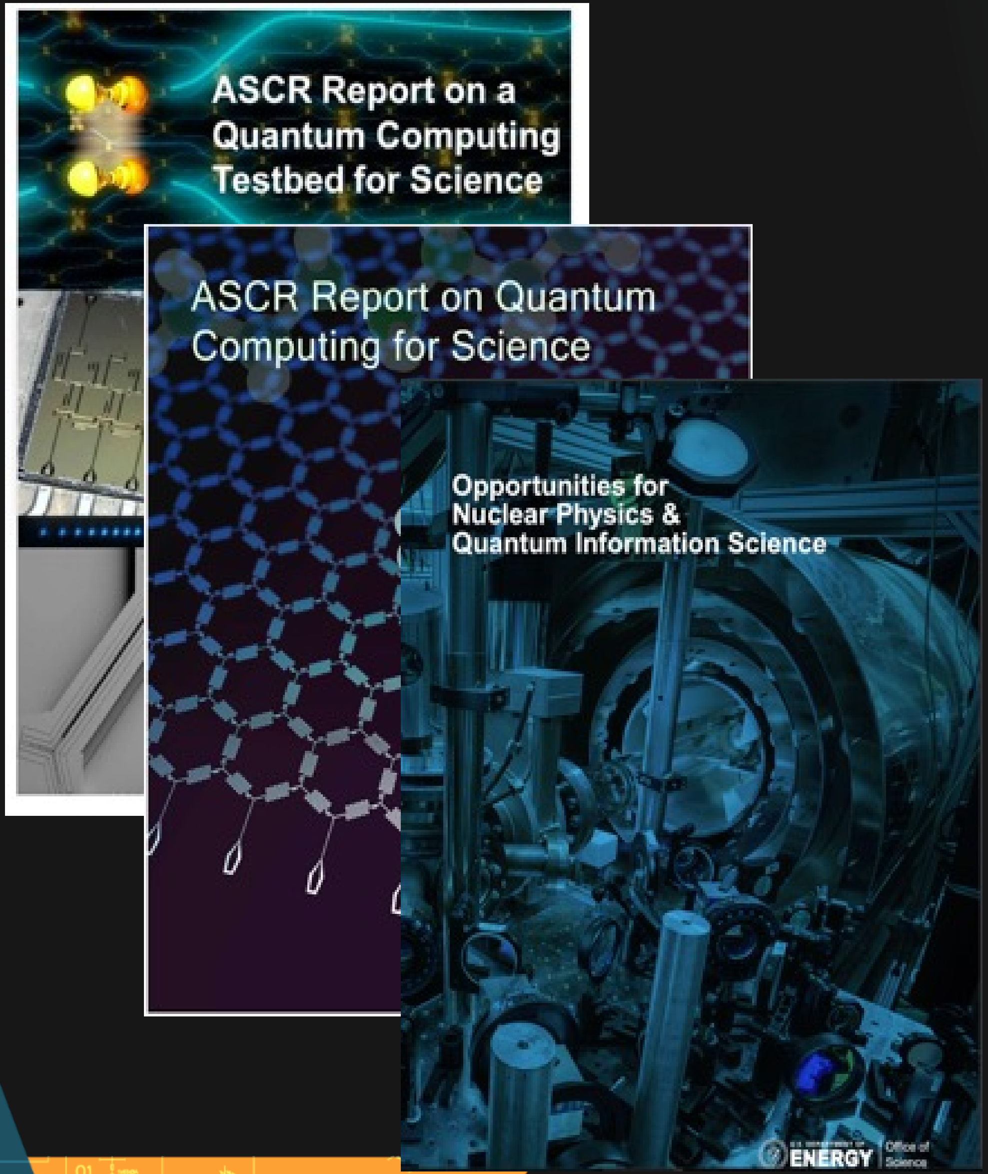
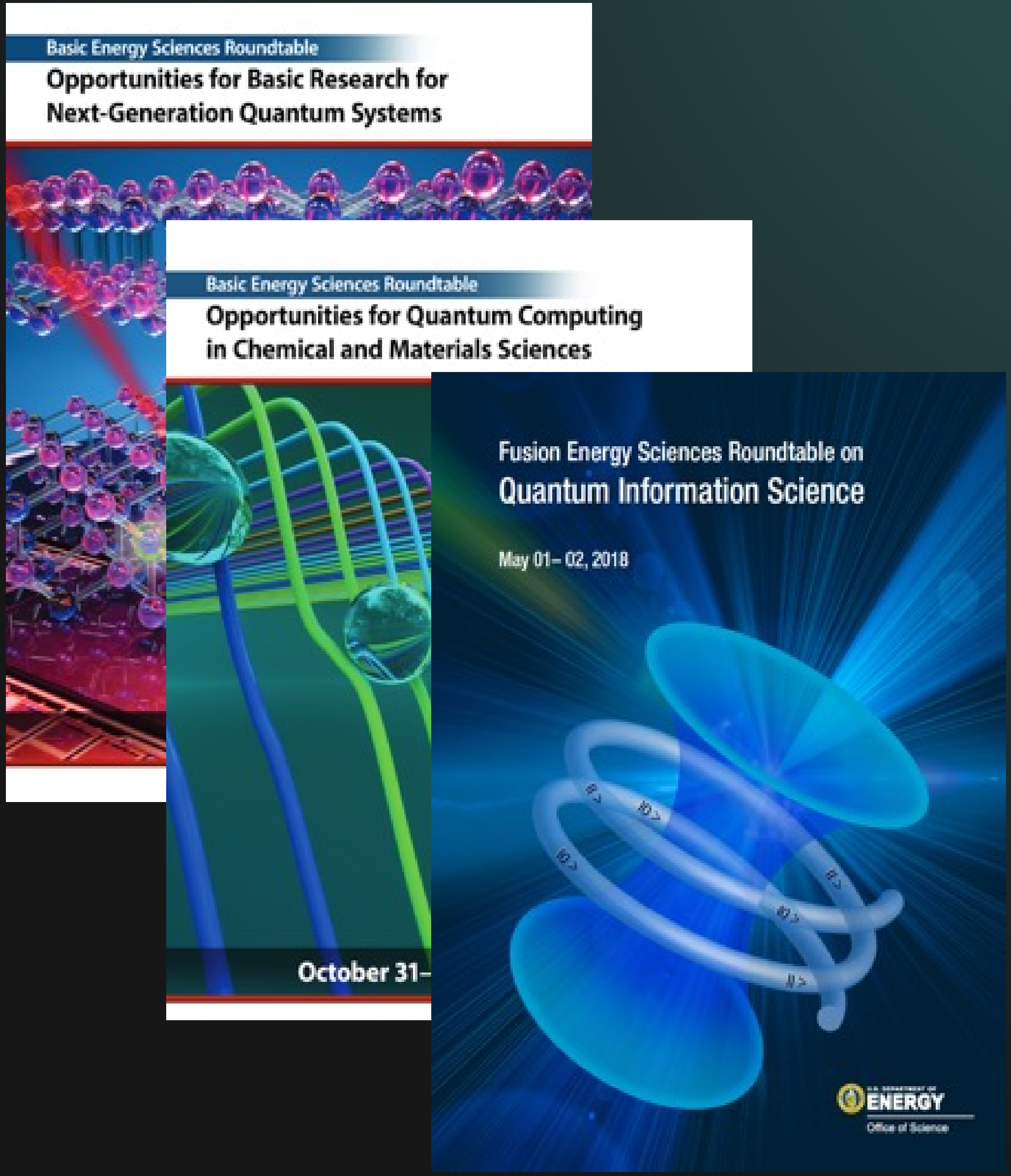
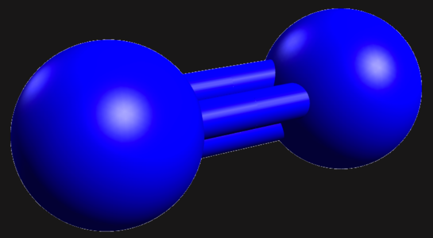
Frontier Physics on a quantum computer

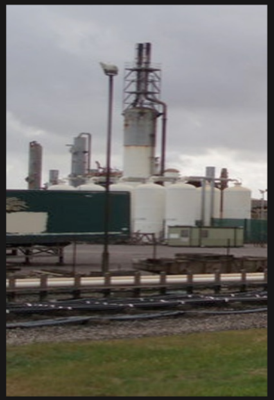




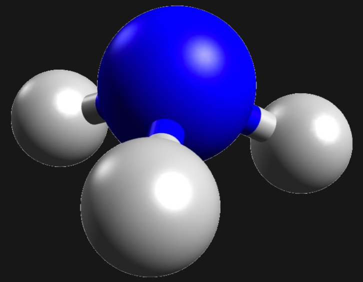
Energy-efficient fertilizer production

Nitrogen

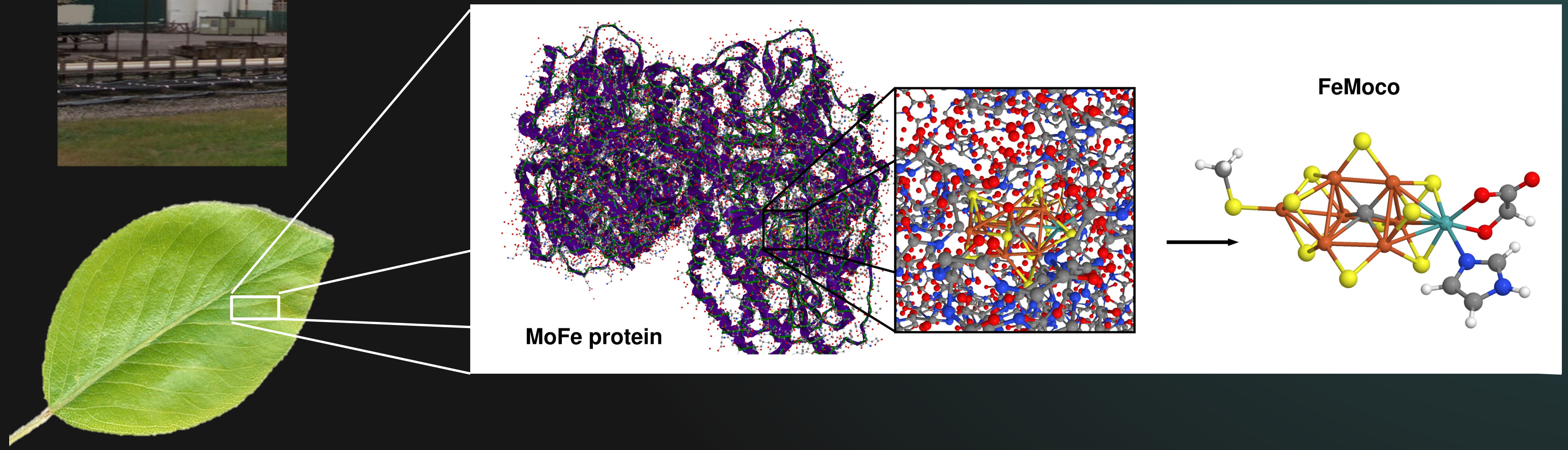




Ammonia



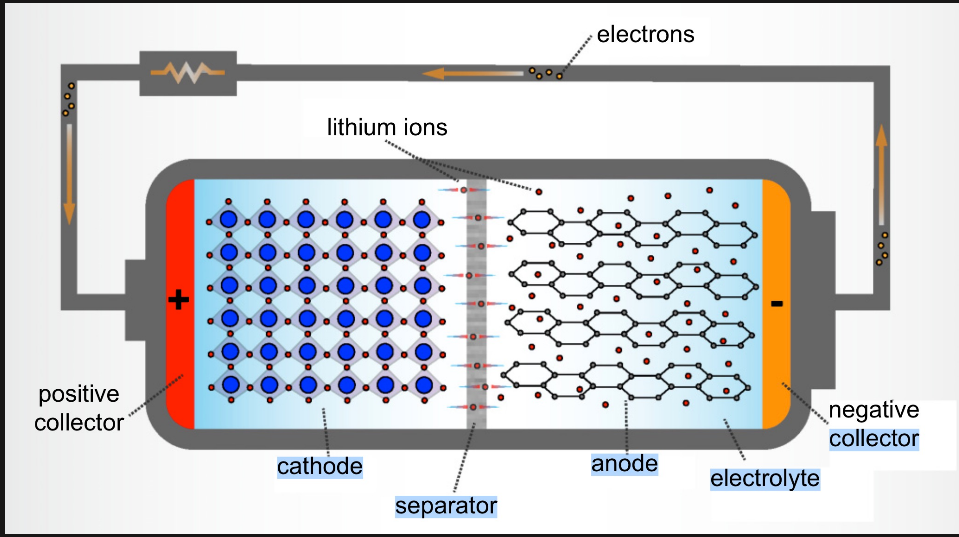
The Haber-Bosch process consumes 2% of the world's annual energy supply.



Q. Algorithm	Logical qubits	Toffoli gates
qDRIFT	328	1.8×10^{28}
Single factorization	3 628	1.2×10^{11}
Sparse	2 489	4.4×10^{10}
Double factorization	6 404	6.4×10^{10}
Tensor hypercontraction	2 196	3.2×10^{10}

Iimages: Andrew Baczewski/Sandia, Nathan Wiebe/Markus Reiher, MoFe, FeMoco
Wikipedia, Rabe!, "Pear Leaf;" Sharon Loxton "Haber Process."

Better batteries through quantum computing



[Delgado *et al.*, PRA 106, 032428 (2022)]

Goals

- Higher energy density
- Faster charging
- Longer lifetime
- Increased safety
- Lower cost

From ground state energy we can learn…

- Equilibrium cell voltage
- Ionic mobility
- Thermal stability
- Reaction rates

Material	Q. Algorithm	Logical qubits	T gates
Li_2FeSiO_4 cathode	1st quantized QPE	6 652	2.5×10^{13}
$LiPF_6$ electrolyte	2nd quantized QPE	84 721	6.7×10^{13}

The most important part of the physics frontier

UNM attendees at 2019 APS 4CS meeting

Quantum computers don't do physics. Humans do physics.

“Computers are useless.
They can only give you answers.”

--Pablo Picasso

Backup Slides