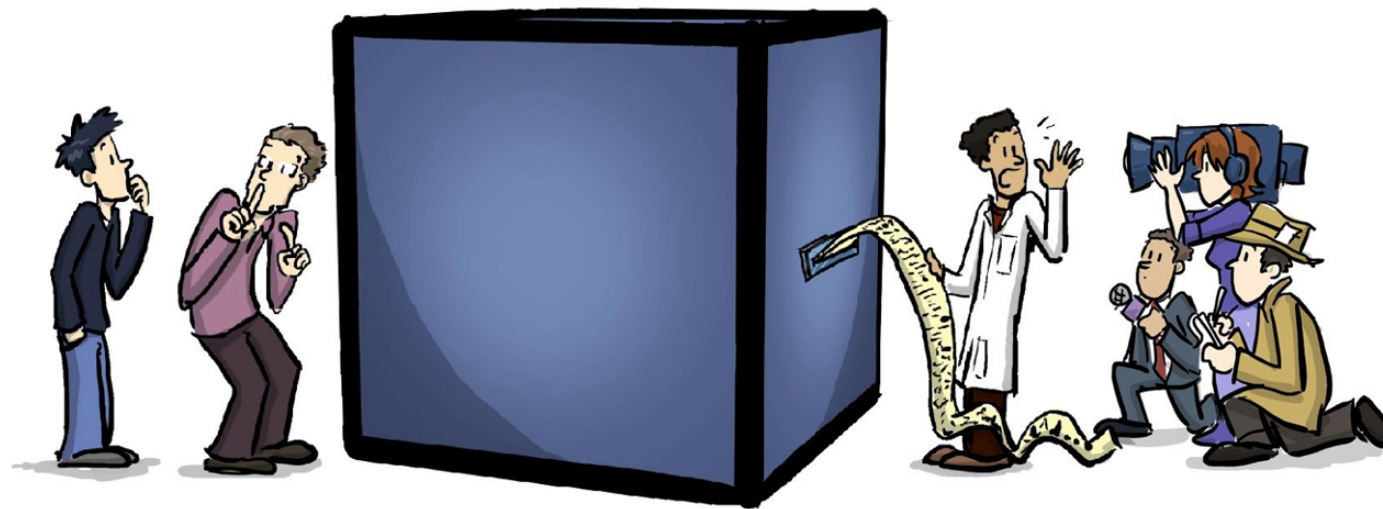


An Invitation to the intersection of Quantum Computing & Programming Languages

Tutorial at POPL 2021

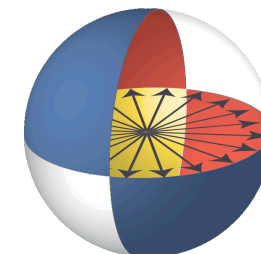
A Quantum COMPUTER



Xiaodi Wu
QuICS & UMD



UNIVERSITY OF
MARYLAND



JOINT CENTER FOR
QUANTUM INFORMATION
AND COMPUTER SCIENCE

About this Tutorial:

Goal: An Invitation due to limited time

Cover Some Basic Quantum Computing & PL

Provide References / Pointers for further study

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Format: Tutorial divided into 3 parts:

(1) Introduction to Quantum Computing and Potential Roles of Programming Languages **(25 min + 5 Q & A)**

(2) A Mini-Course of Quantum Hoare Logic on Quantum While Language **(30 min + 5 Q & A)**

(3) Discussion on existing and potential Programming Language research opportunities **(20 min + 5 Q & A)**

About the Speaker:

Wu: assistant professor at UMD working on quantum computing from CS perspective in general.

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Teaching in Q. Computing

Past Courses

This is a collection of courses that I have taught in the past for your references. Please be cautious as thes

University of Maryland, College Park (2017 - present)

- Complexity Theory (CMSC 652): graduate-level theory core course
 - Fall 2017
- Introduction to Quantum Computing (CMSC/PHYS 457): undergraduate-level introduction to quantum computing
 - Spring 2018, Spring 2020, Spring 2021
- Introduction to Quantum Information Processing (CMSC 657): graduate-level introduction to quantum information processing
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-

Mini-Library on Quantum Information and Computation

This page is meant to be a collection of representative and available references for the study and research of the **theoretical** aspects of quantum computing as possible and will be regularly maintained. Send me an email if you have any good suggestion.

Expository Writings and Lecture Notes by myself

- **Tutorial at POPL 2021:** An Invitation to the Intersection of Quantum Computing and Programming Languages
 - (Part I) A brief introduction to quantum computing and potential roles of programming languages
 - (Part II) A mini-course on the verification of quantum while languages based on quantum Hoare logic
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 - Quantum Algorithms for Linear Equation Systems
 - Quantum Algorithms for Semidefinite Programs

Scientific Reports from Relevant Research Communities

- National Academies of Sciences, Engineering, and Medicine. 2019. [Quantum Computing: Progress and Prospects](#). Washington, DC: National Academies Press.
- National Academies of Sciences, Engineering, and Medicine. 2020. [Manipulating Quantum Systems: An Assessment of the State of the Field](#). Washington, DC: National Academies Press.
- Quantum Frontiers Report on community input to the Nation's Strategy for Quantum Information Science, October, 2019.
- Next Steps in Quantum Computing: Computer Science's Role: Computing Community Consortium Workshop Report
- More Reports at [Quantum|Gov](#).

General Study: Courses, Lecture Notes & Textbooks

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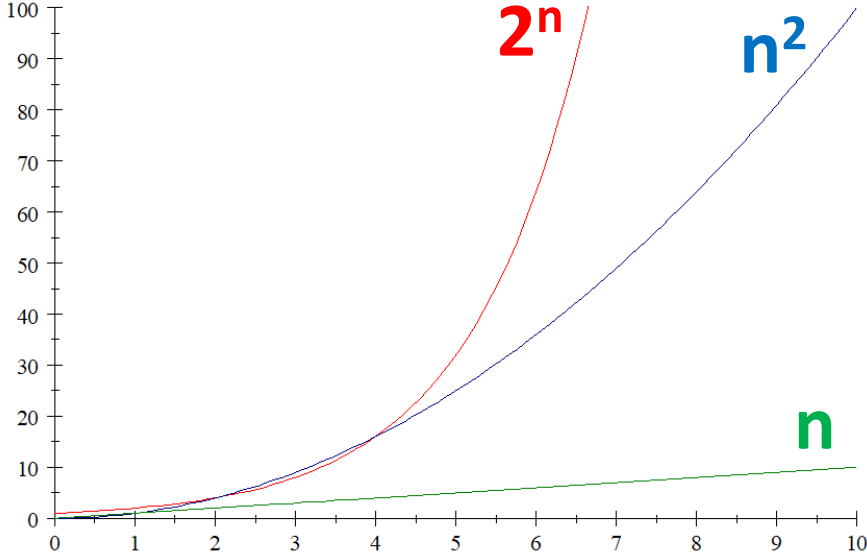
Reference: tutorial slides and some references are available at https://www.cs.umd.edu/~xwu/mini_lib.html



What Quantum Computing is NOT

Credit: Scott Aaronson

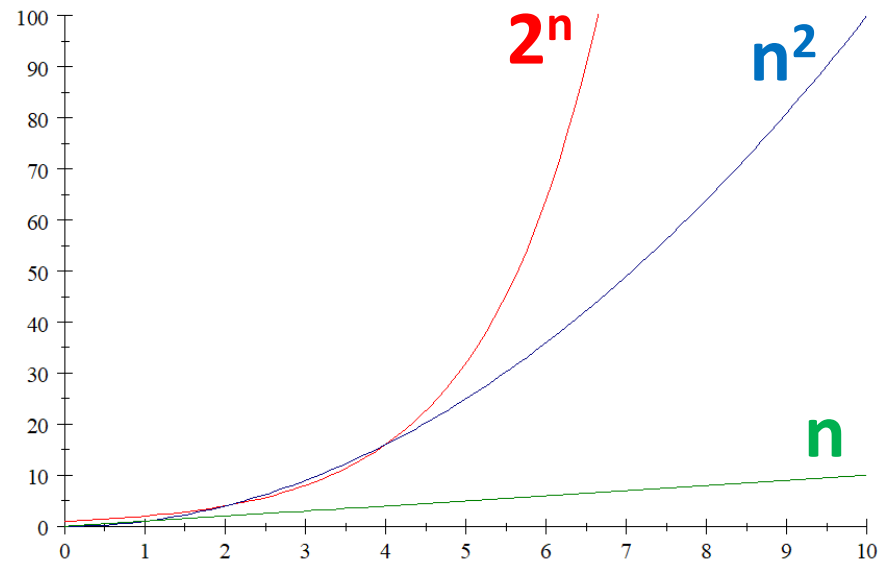
It Isn't Just Today's Computers But
Smaller or Faster



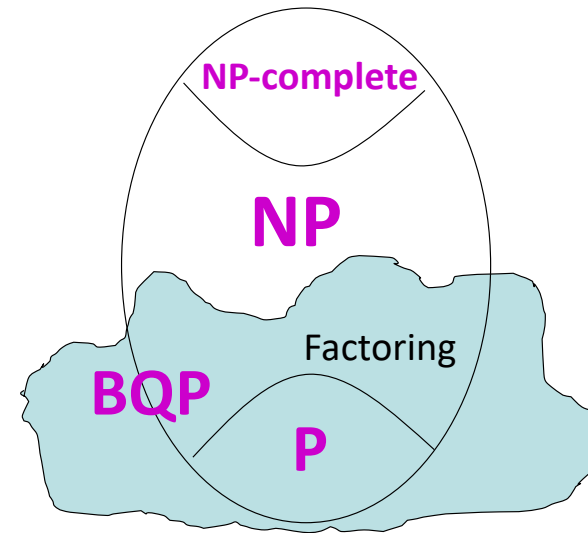
What Quantum Computing is **NOT**

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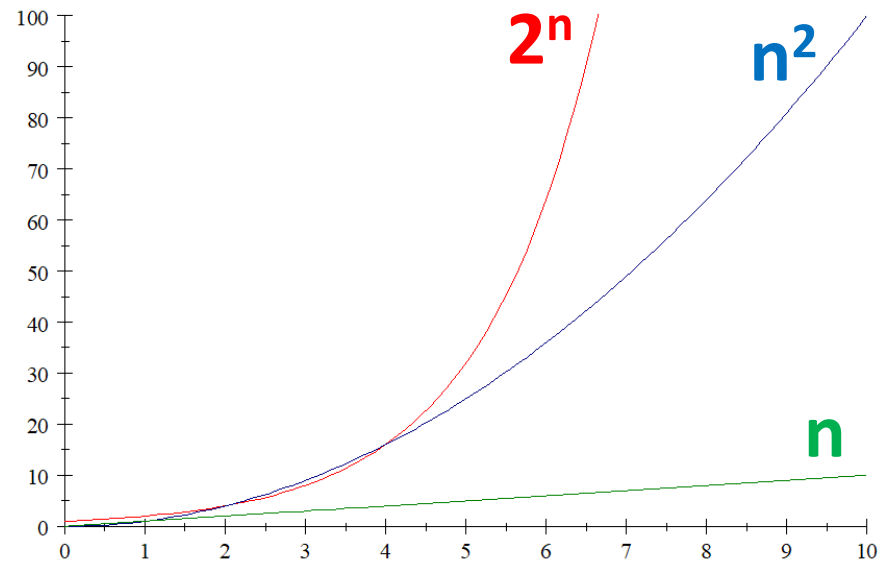
It Isn't A Magic Bullet That Solves
All Problems Instantly



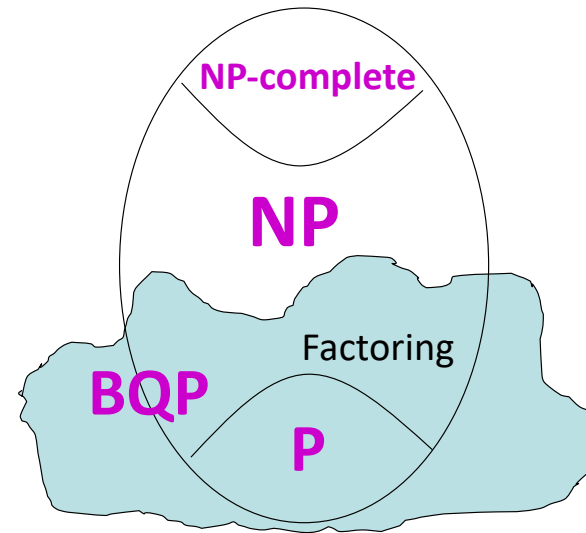
What Quantum Computing is **NOT**

Credit: Scott Aaronson

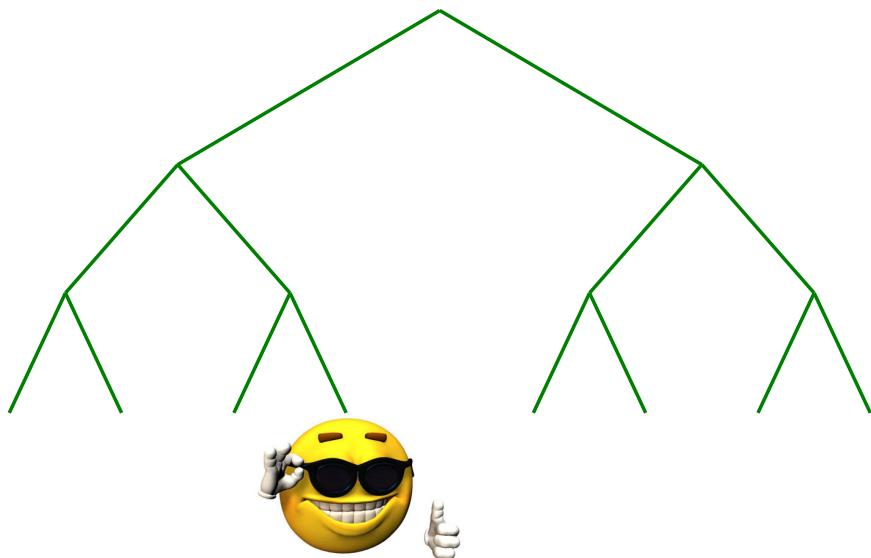
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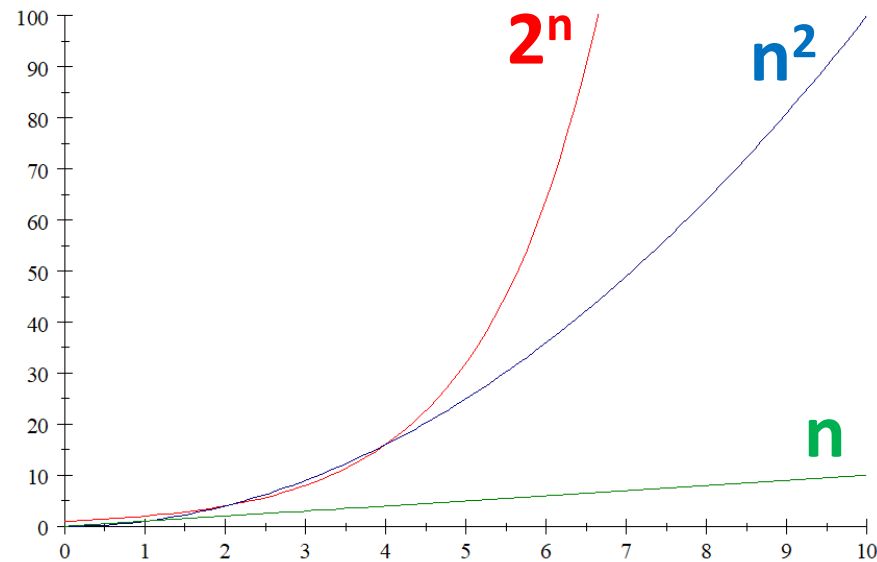
It Isn't A Simple Matter of Trying
All Possible Answers In Parallel



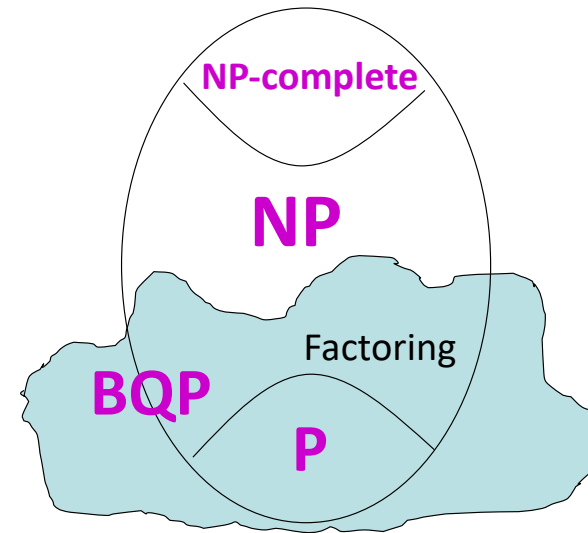
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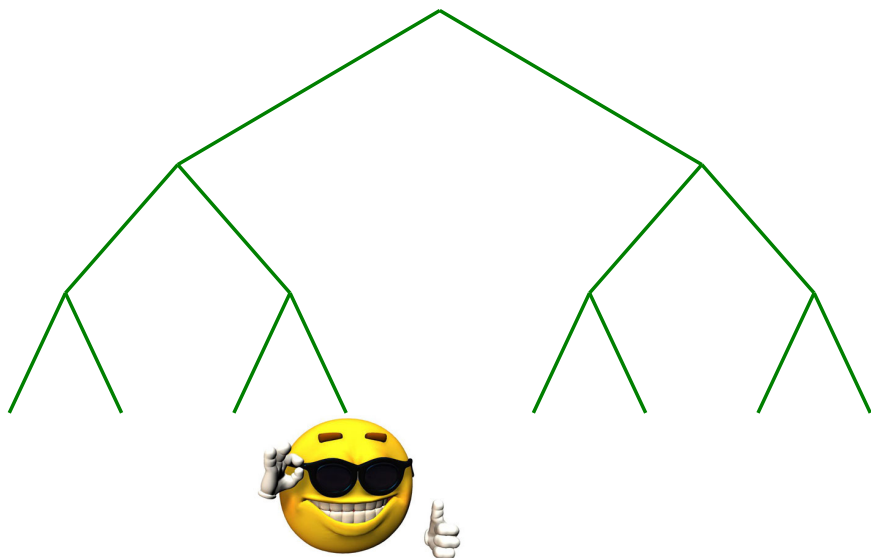
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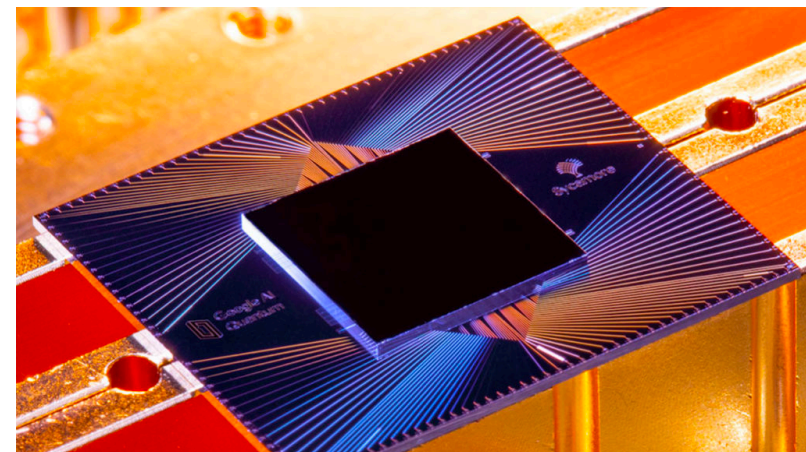
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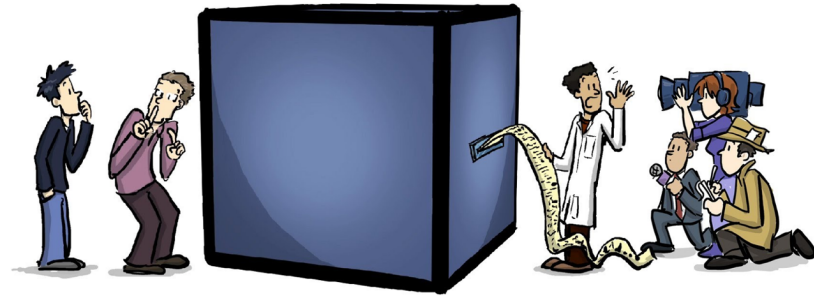


But Nor Is It Science Fiction



Roadmap in 2010s

A Quantum COMPUTER



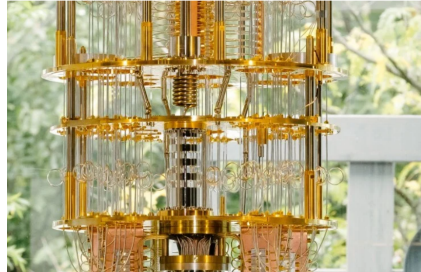
(2012)



Ion-Trap (UMD)

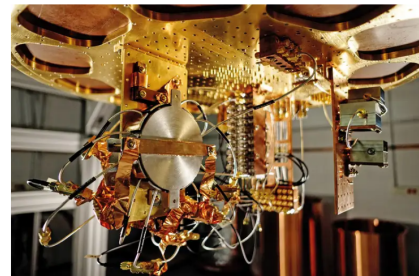
IBM will soon launch a 53-qubit quantum computer

Frederic Lardinois @frederic / 8:00 am EDT • September 18, 2019



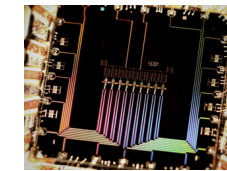
Google has reached quantum supremacy – here's what it should do next

TECHNOLOGY | ANALYSIS | 26 September 2019
By Chelsea Whyte

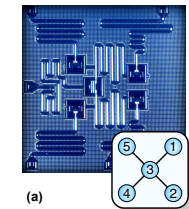


(2019)

Super-conducting

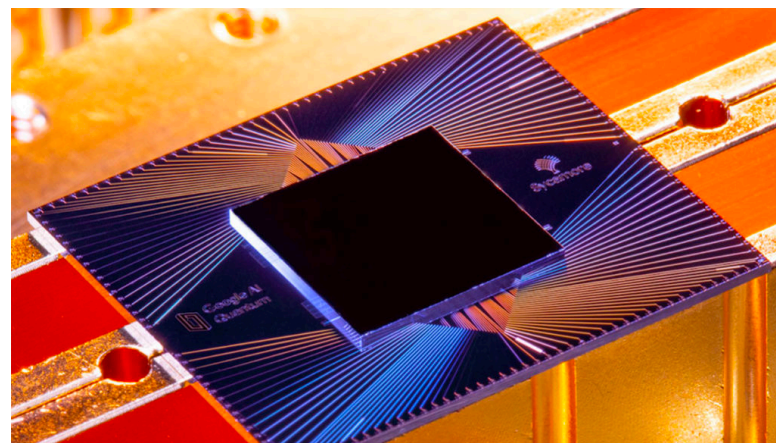
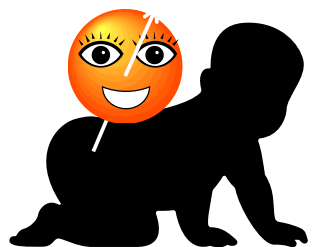


Google



(a) IBM

(2017)

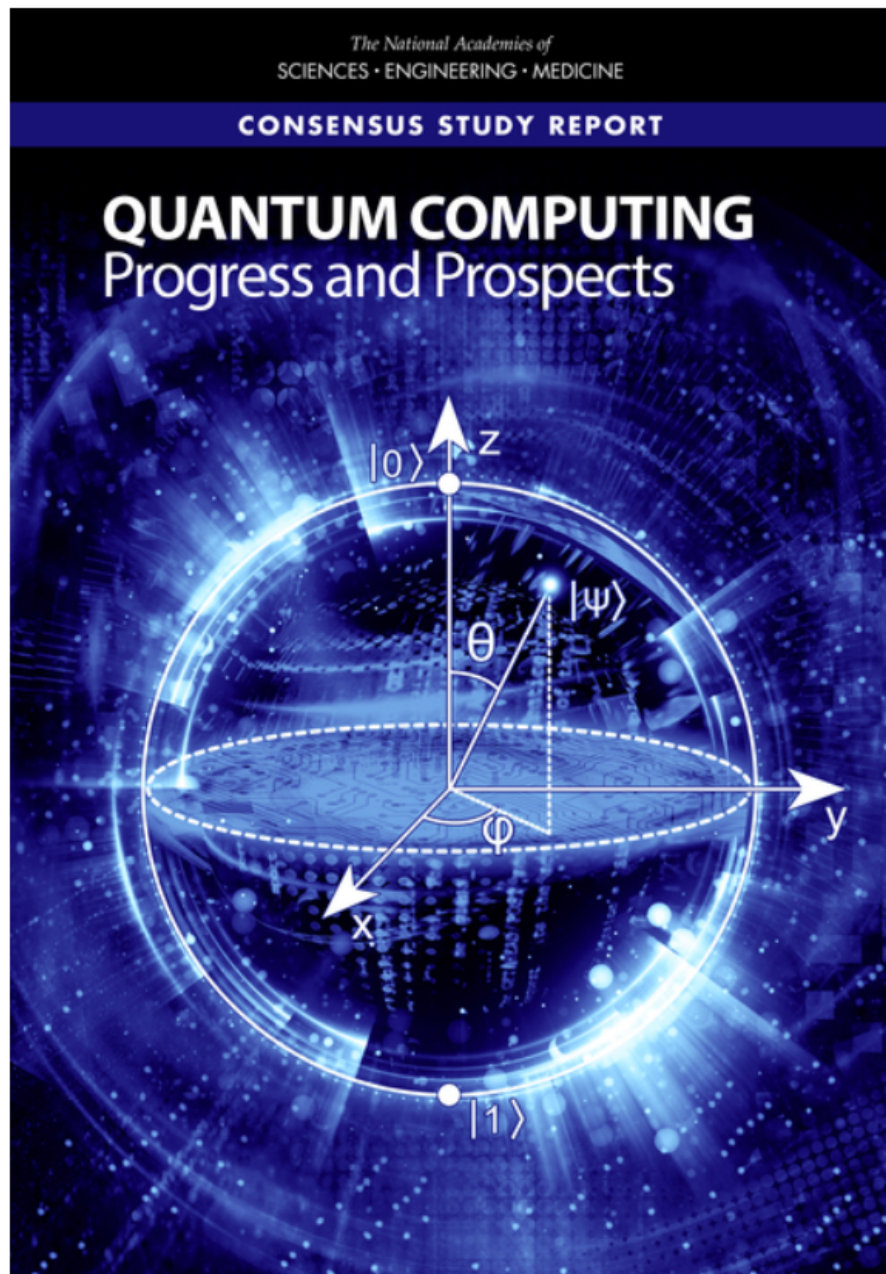


Google Supremacy: RCS (2019)



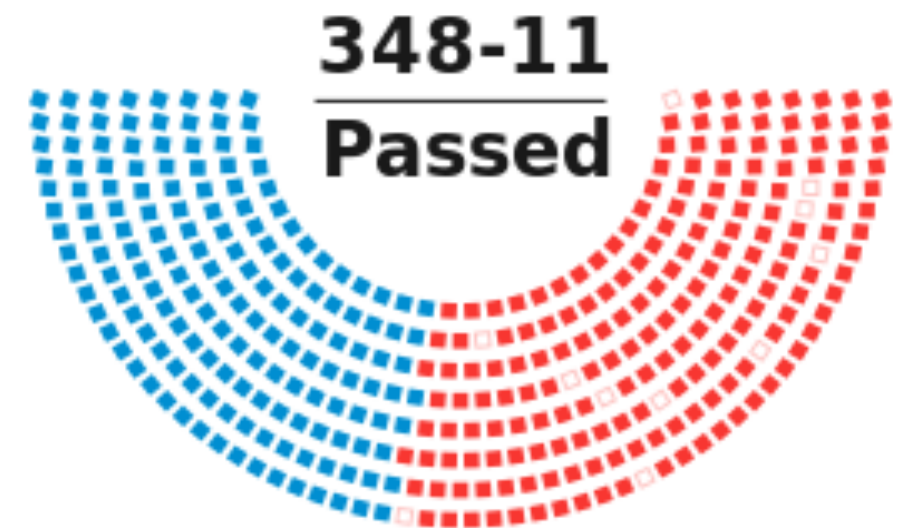
USTC: Boson Sampling (2020)

Surge of Interests from Gov, Academia, & Industry



MARK A. HOROWITZ,
Stanford University, *Chair*
ALÁN ASPURU-GUZIK,
University of Toronto
DAVID D. AWSCHALOM,
University of Chicago
BOB BLAKLEY,
Citigroup
DAN BONEH,
Stanford University
SUSAN N. COPPERSMITH,
University of Wisconsin, Madison
JUNGSANG KIM,
Duke University
JOHN M. MARTINIS,
Google, Inc.
MARGARET MARTONOSI,
Princeton University
MICHELE MOSCA,
University of Waterloo
WILLIAM D. OLIVER,
Massachusetts Institute of Technology
KRYSTA SVORE,
Microsoft Research
UMESH V. VAZIRANI,
University of California, Berkeley

H. R. 6227
National Quantum Initiative Act



House Vote #442 -- 12/19/18

Gov: US (NSF, DOE + National Labs, DoD, NIST), China, Europe,

Industry: Google, IBM, Microsoft, Amazon, Alibaba, Tencent, Baidu,

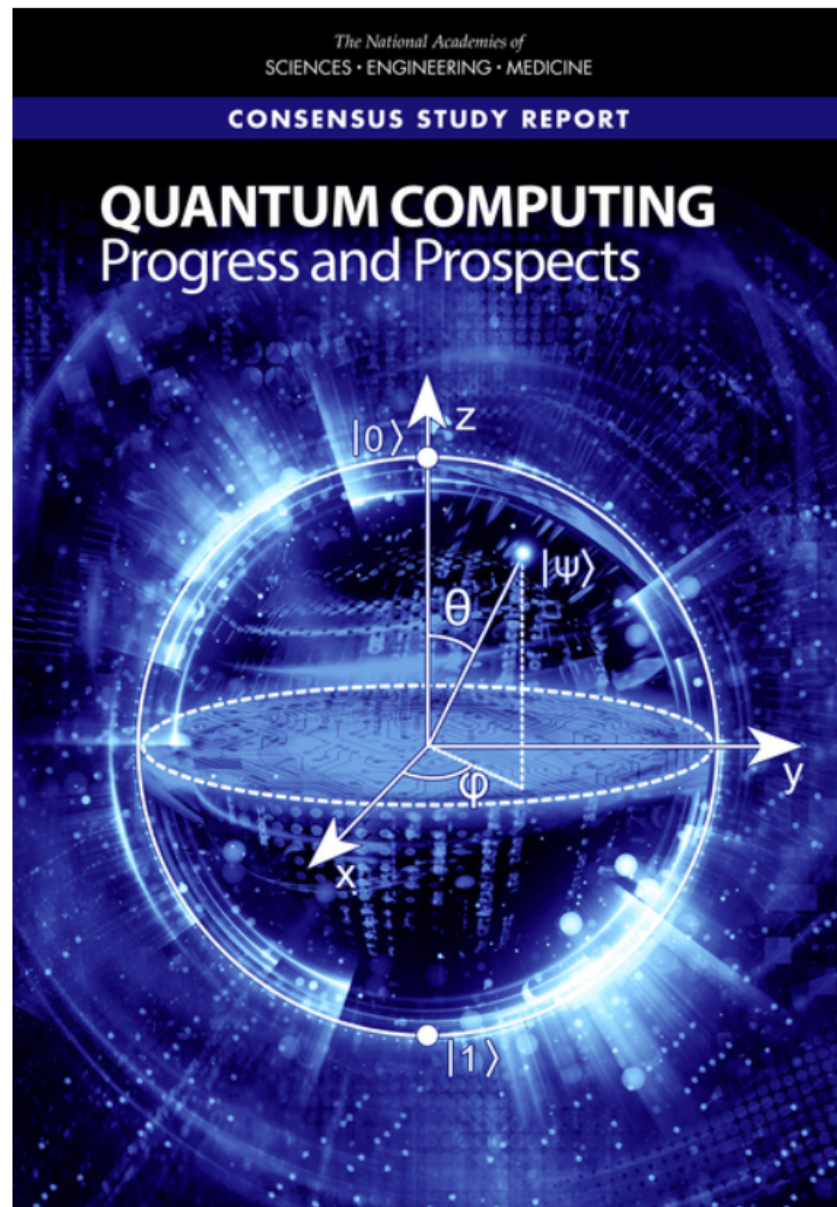
Academia: #faculty in quantum computing ++

US GOV Policy & Efforts:

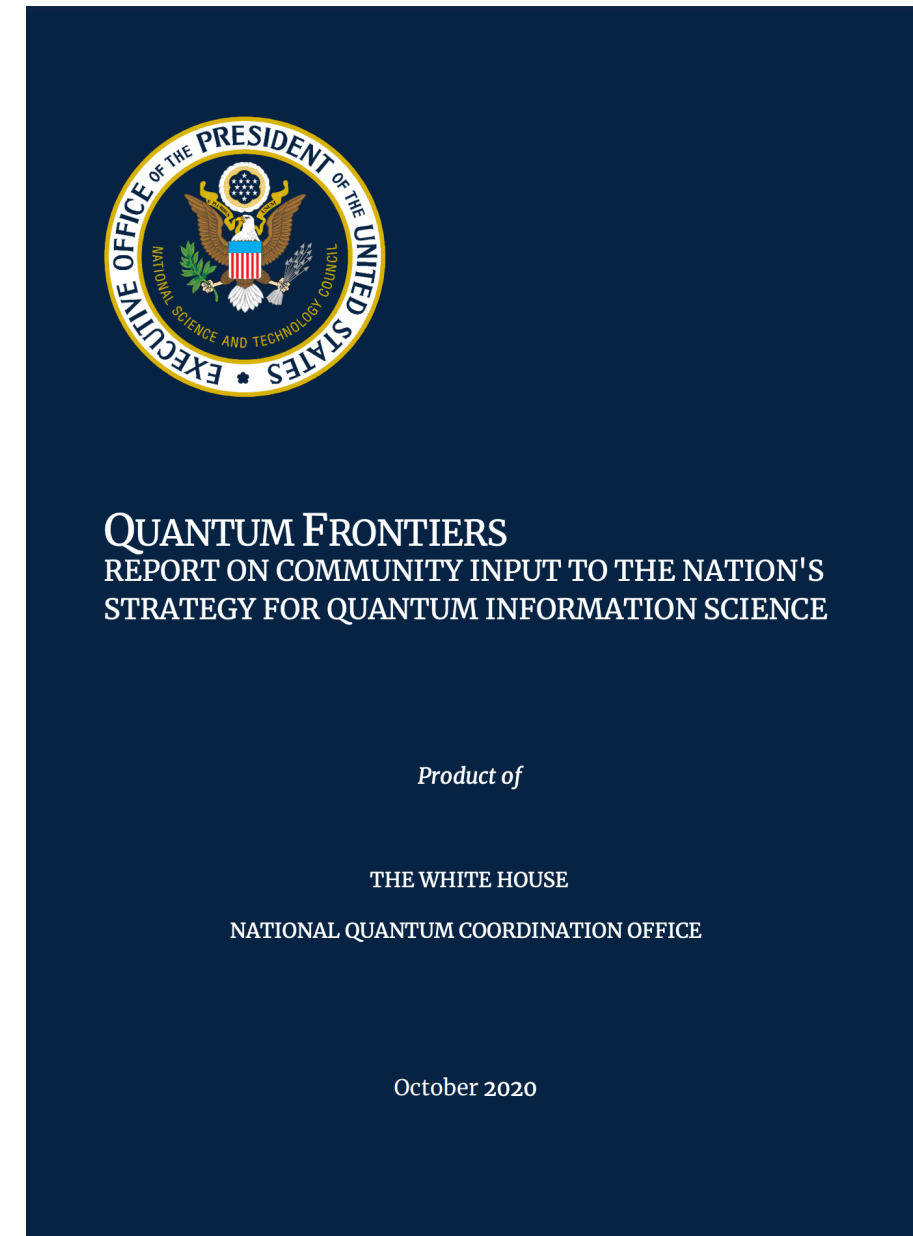


<quantum|gov>

Scientific Reports from relevant research communities



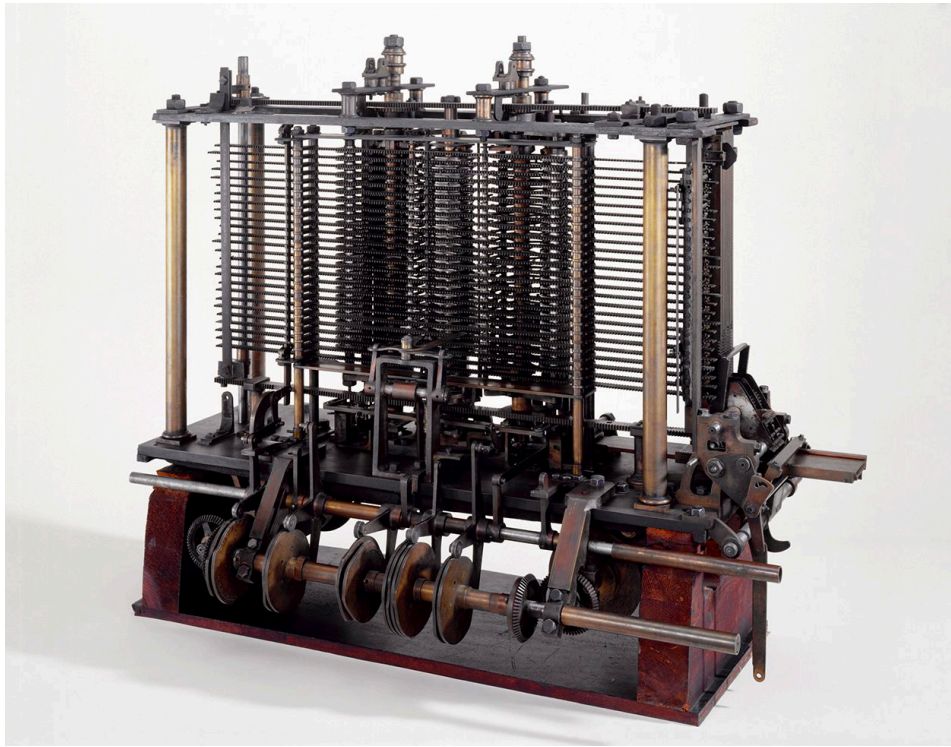
Next Steps in Quantum Computing: Computer Science's Role



Reference: links are available at [https://www.cs.umd.edu/~xwu/mini lib.html](https://www.cs.umd.edu/~xwu/mini_lib.html)



What is Quantum Computing?



A Mechanical Computer

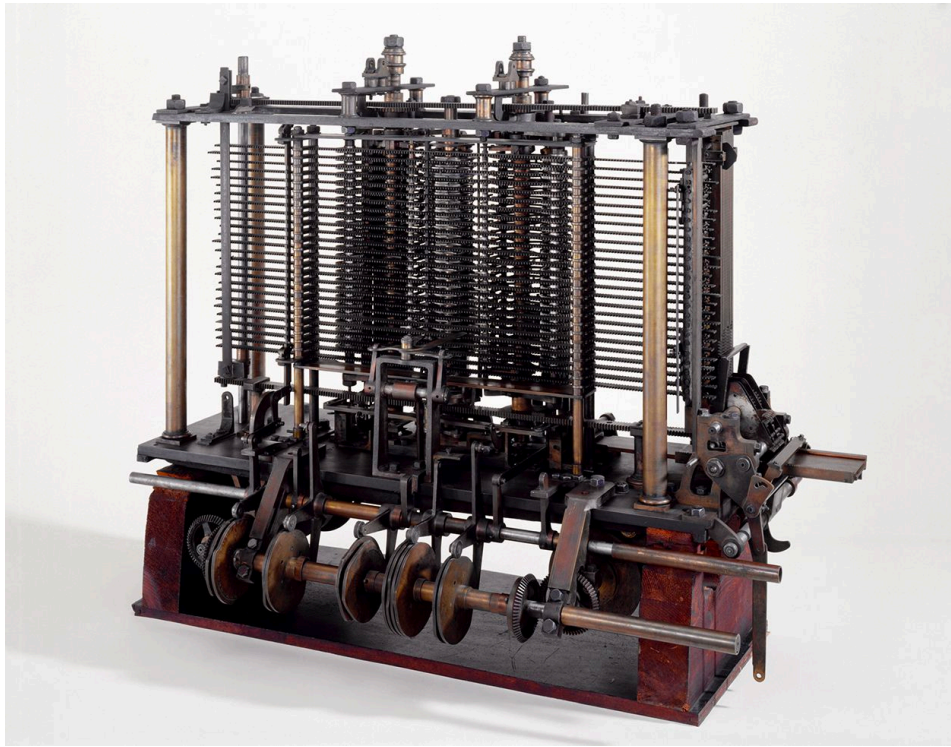
An **Operation** O — — — \rightarrow A **Physical Evolution** P

Computation:

Evolution of the Machine: P_1, P_2, P_3, \dots

The accumulative evolution carries some computation!

What is Quantum Computing?



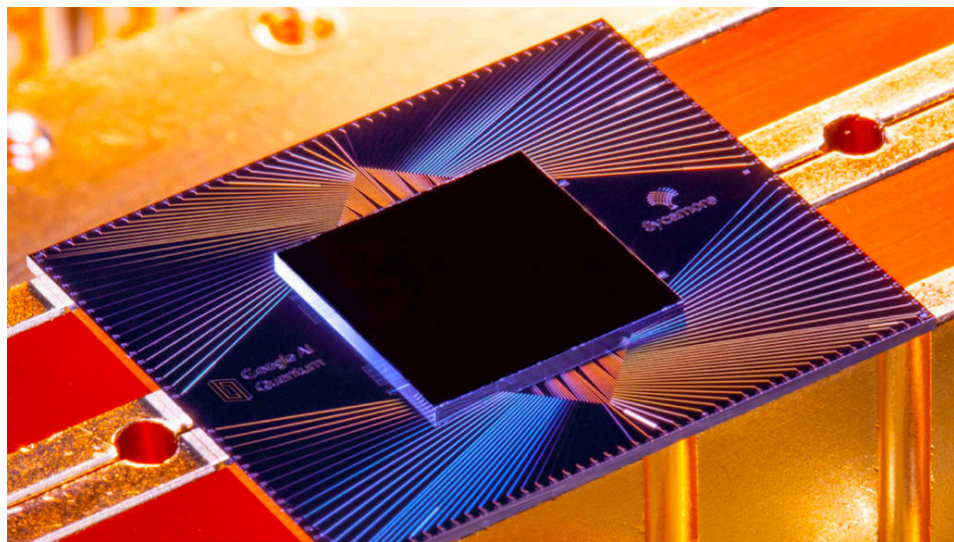
A Mechanical Computer

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The accumulative evolution carries some computation!



A Quantum Computer

An **Operation** O \rightarrow A **Quantum** Physical Evolution Q

Computation:

Evolution of the Machine: Q_1, Q_2, Q_3, \dots

The accumulative evolution carries some computation!

What is Quantum Computing **good** at?

Assume a *unit* operation requires a *unit* time on respective machines.

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Computation can be
carried out by P_1, P_2, \dots, P_T

Classical Computing (T)

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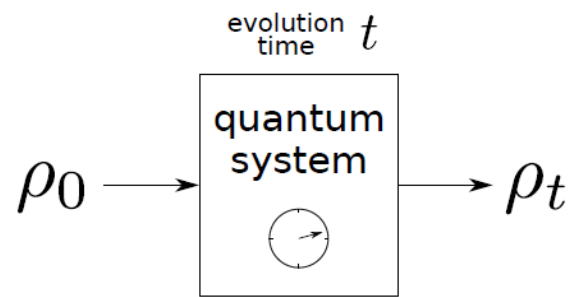
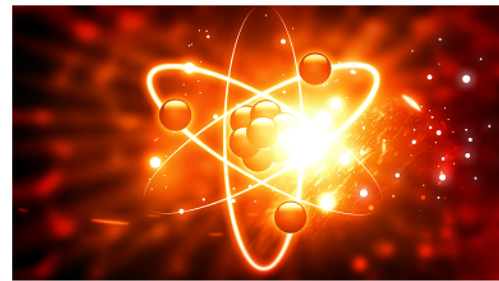
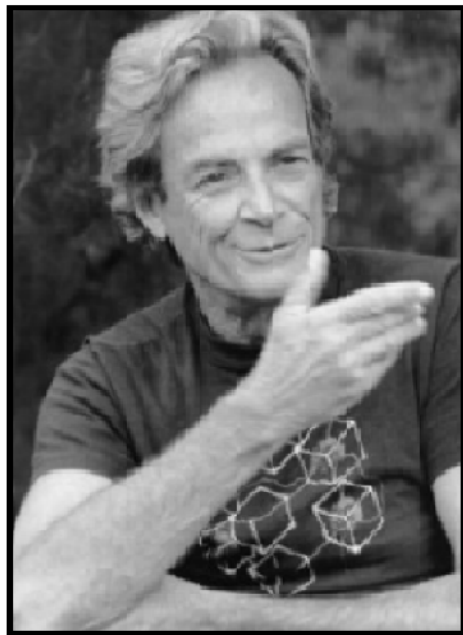
Classical Computing (T)



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Quantum Computing (T)

Quantum Simulation



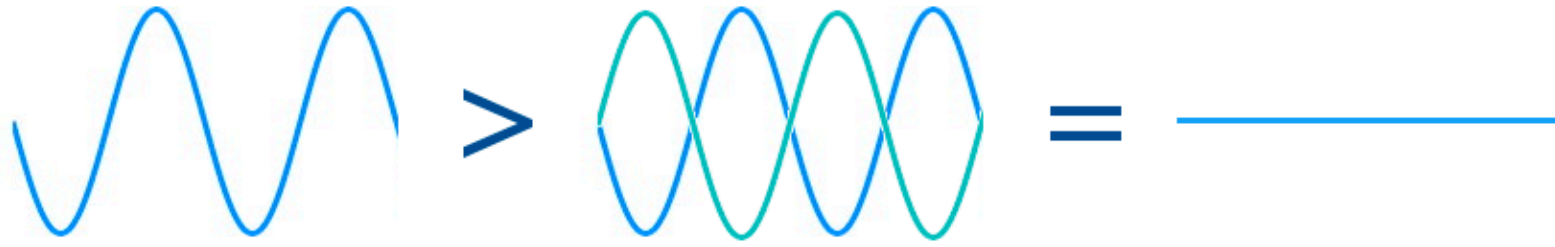
Nature isn't classical, and if you want to make a simulation of Nature, you'd better make it quantum mechanical, and by golly it's a wonderful problem, because it doesn't look so easy.

Richard Feynman, 1982

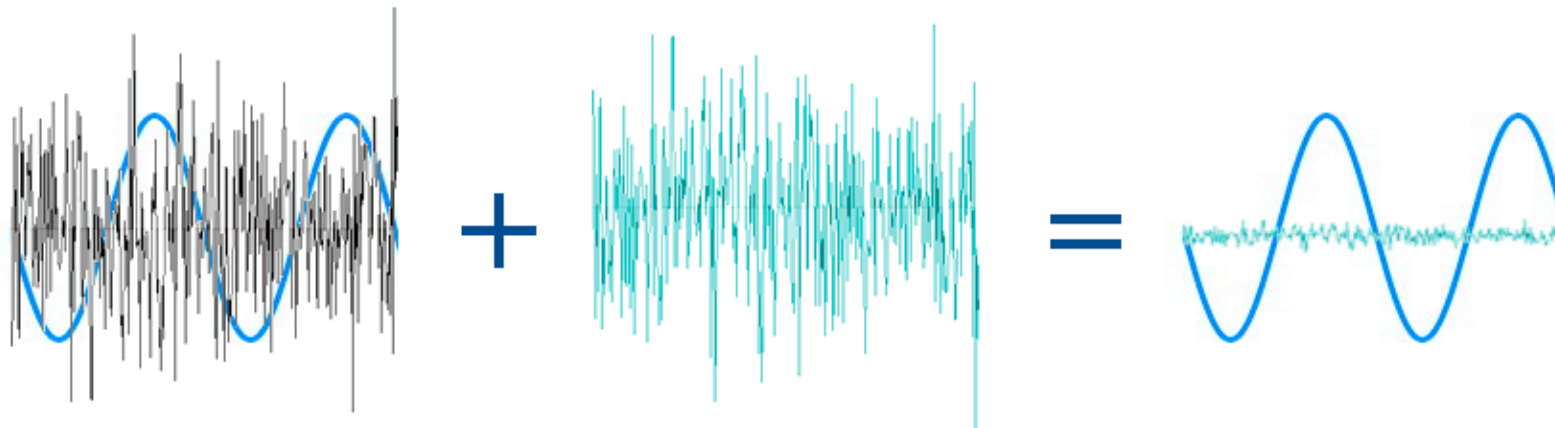
Simulating quantum systems is critical for the scientific discovery for natural science include physics, chemistry, biology, material science, and so on. And nowadays, it consumes a significant amount of our HPC computing power.

Make Interference Work:

Waves of equal amplitude and opposite phase cancel out



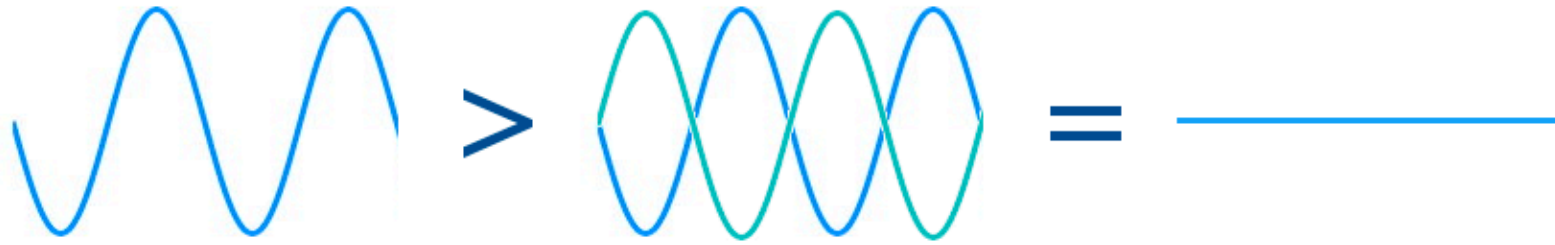
Recording and inverting noise leaves you with your desired signal



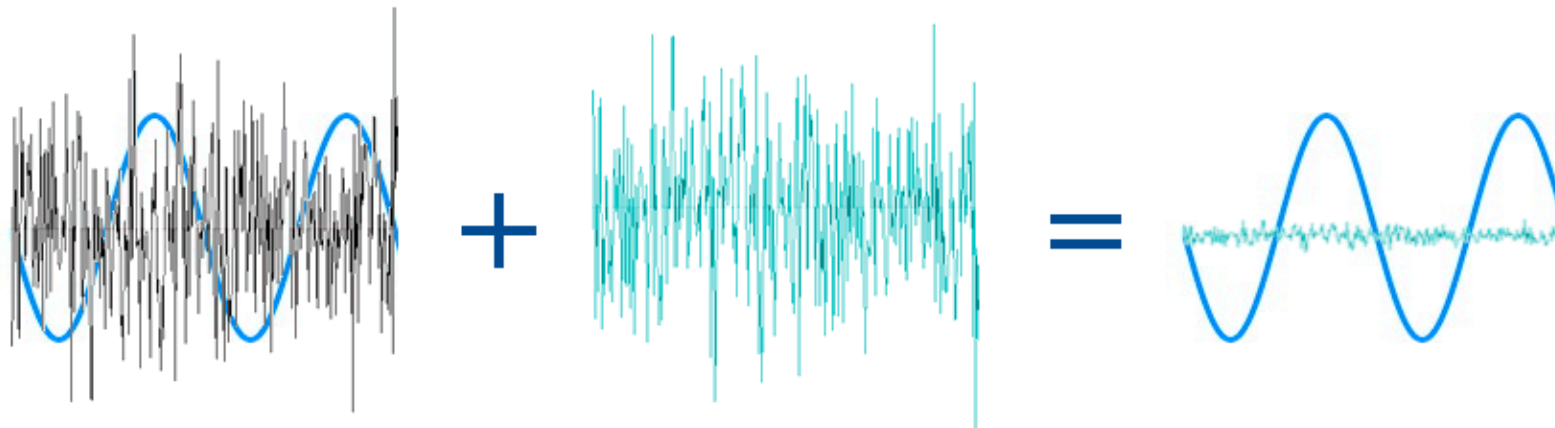
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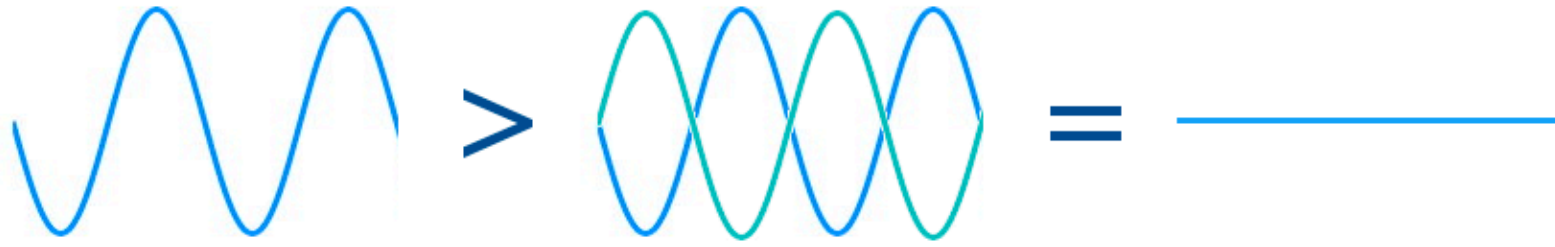
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Make Interference Work for Computation:

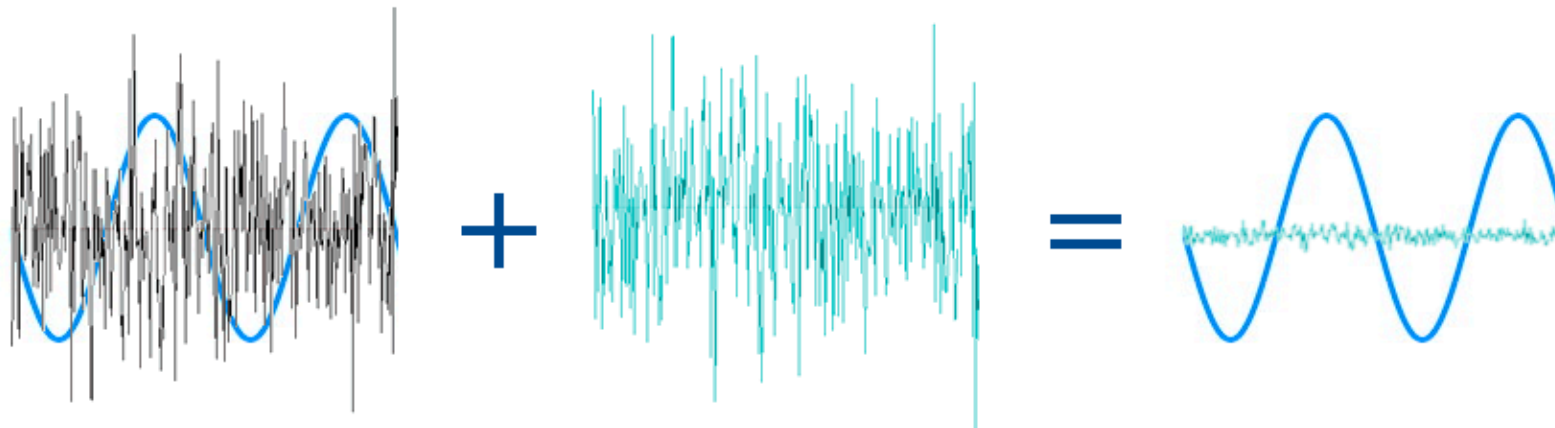
Quantum Computation: Get computational paths leading to *incorrect* answers to **interfere destructively** and cancel each other out.

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Quantum vs Randomized:

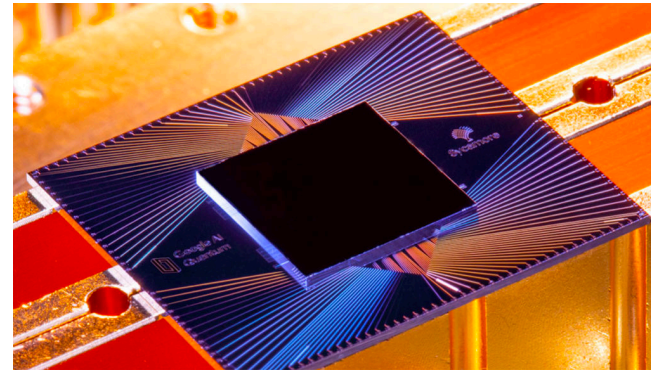
Randomized Computation: Probabilities of computational paths leading to *incorrect* answers only **add up**, never cancel out.

A Rough Timeline of Quantum Applications

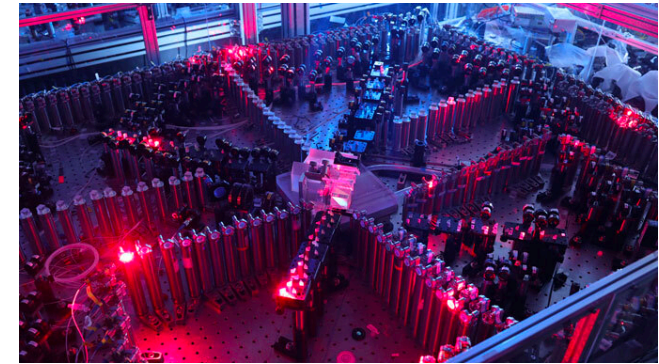
NOW: Quantum Supremacy

Computational tasks, *not necessarily useful*, which is feasible to implement w/ current q. machines, but hard to simulate by classical computation.

A **Milestone** Toward Useful Quantum Computation



Google: Random Circuit Sampling



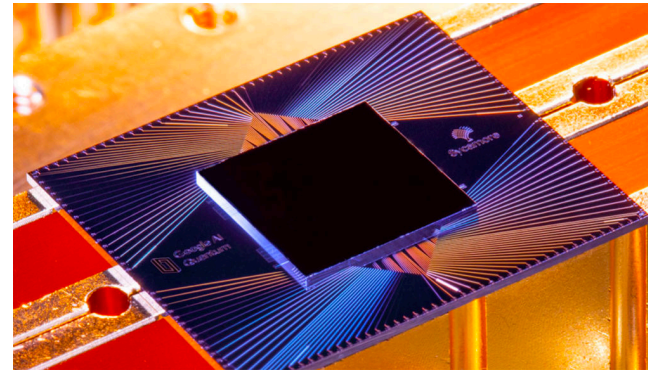
USTC: Boson Sampling

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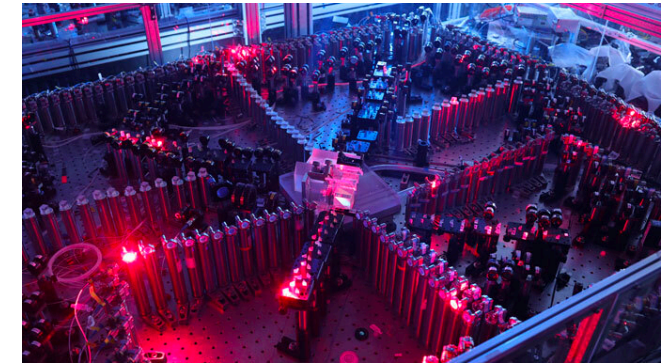
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USTC: Boson Sampling

NISQ: Noise Intermediate-Scale Quantum machines ~ near future

50 ~ 200, ~ 1000 controllable but noisy qubits, no fault-tolerant qubits

Or special-purpose quantum machines, like analog quantum simulators

Quantum Simulation

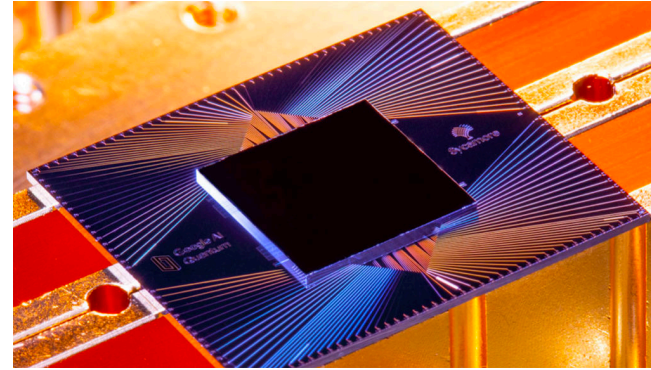
Variational Q. Methods

A Rough Timeline of Quantum Applications

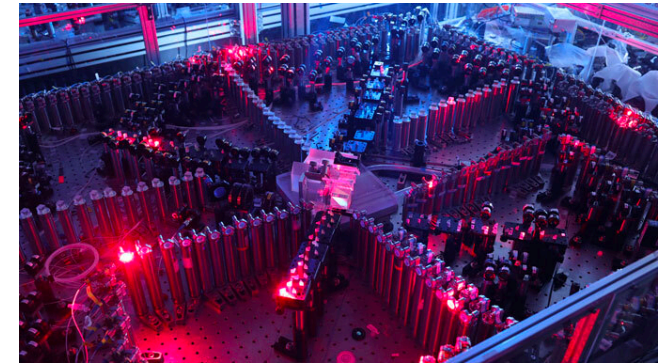
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Other quantum applications not in the computation domain: *quantum sensing, quantum communication*

Quantum Simulation

Variational Q. Methods

The **Role** of Programming Languages

Like the role of PL played for any other computing models, many *similar first-principle questions* can be asked in the context of quantum computing as well!

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But of course, quantum computing model demonstrates some *fundamental differences and unique needs*, which requires **new** techniques to deal with.

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How to Program Q. Applications, Debug, and Verify Correctness?

How to Develop Software for Q. Computing, e.g., compiler, system?

How to Design and Implement Architecture for Quantum Computing?

How to Handle Quantum Security Issues in Design&Implementation?

How to Scale and Automate the Design of Quantum Hardware ?

How to Program Q. Applications, Debug, and Verify Correctness?

The natural question with MOST investigation, but still a huge gap!

How to **Program Q.** Applications, **Debug**, and **Verify Correctness**?

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THEORY: quantum lambda-calculus, functional quantum PL, q. while language semantics in various pictures, q. Hoare logic and verification, ...

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LANGUAGES: **Quipper** (embedded in Haskell), **Scaffold** (based on LLVM), **Q#** (based on F#, MSR),
QWIRE/SQIR (embedded in Coq), **SILQ**, ... <- **academia**
python-lib **Qiskit** (IBM), **Cirq** (Google), **Forrest** (Rigetti), **Braket** (AWS), <- **industry**

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Gap: (1) **too-low-level-abstraction**: very hard to write **complex** programs

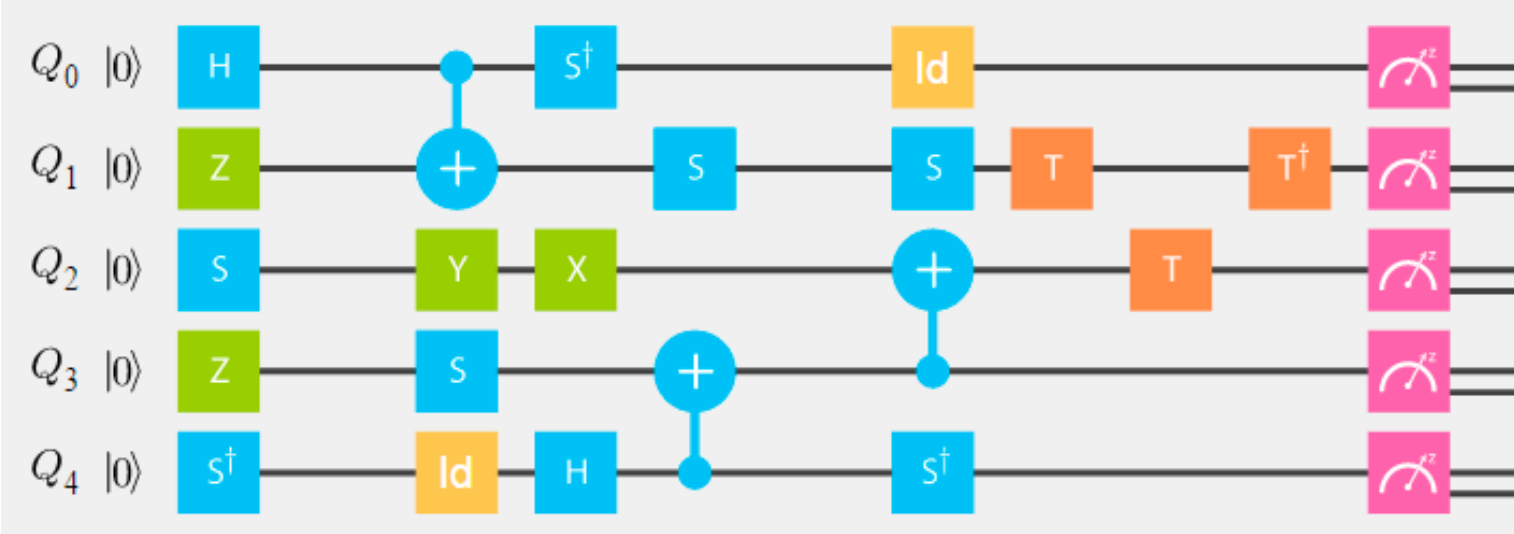
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LANGUAGES: **Quipper** (embedded in Haskell), **Scaffold** (based on LLVM), **Q#** (based on F#, MSR), **QWIRE/SQIR** (embedded in Coq), **SILQ**, ... **<- academia**
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Gap: (1) **too-low-level-abstraction:** very hard to write **complex** programs
(2) **lack of scalable verification:** very hard to write **correct** programs



Verifying the circuit by observation
.... not scalable ...

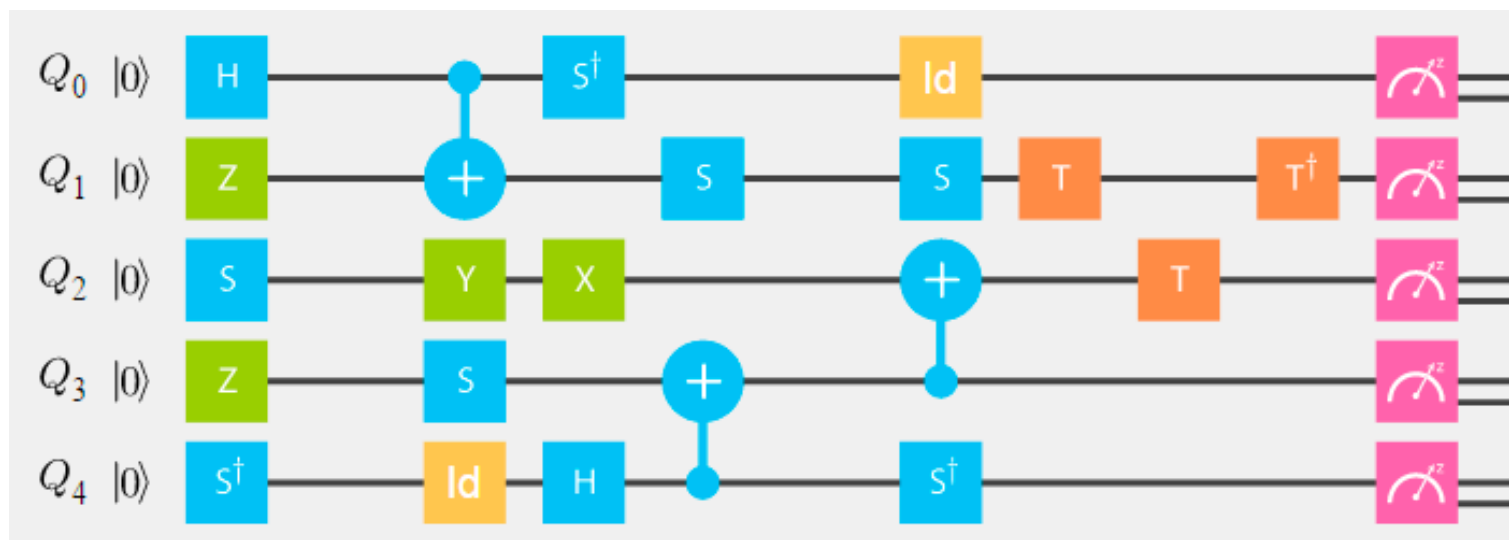
How to Program Q. Applications, Debug, and Verify Correctness?

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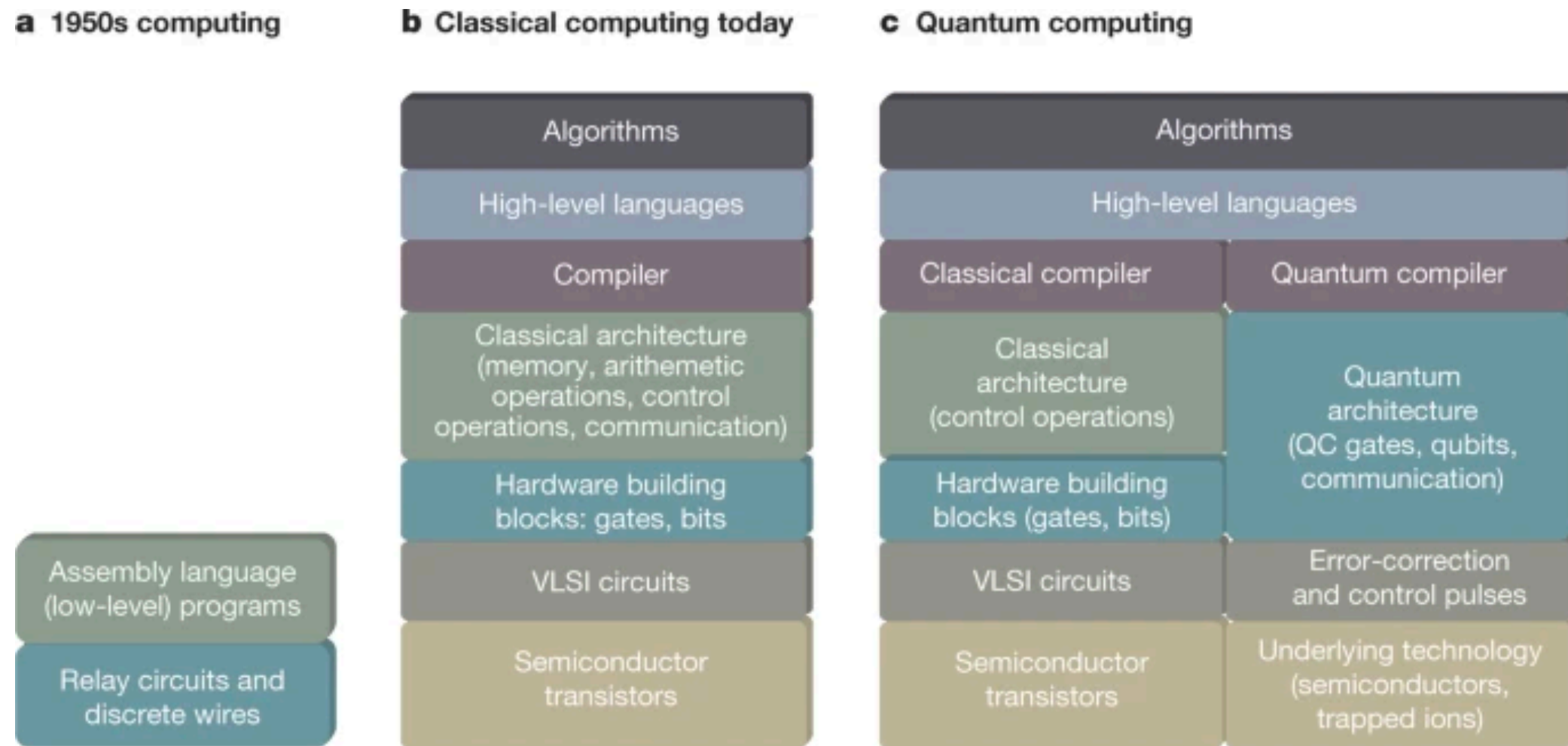
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Verifying the circuit
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(3) **lack of many desirable analyses, automation, & optimization**: a lot of burdens on the programmers

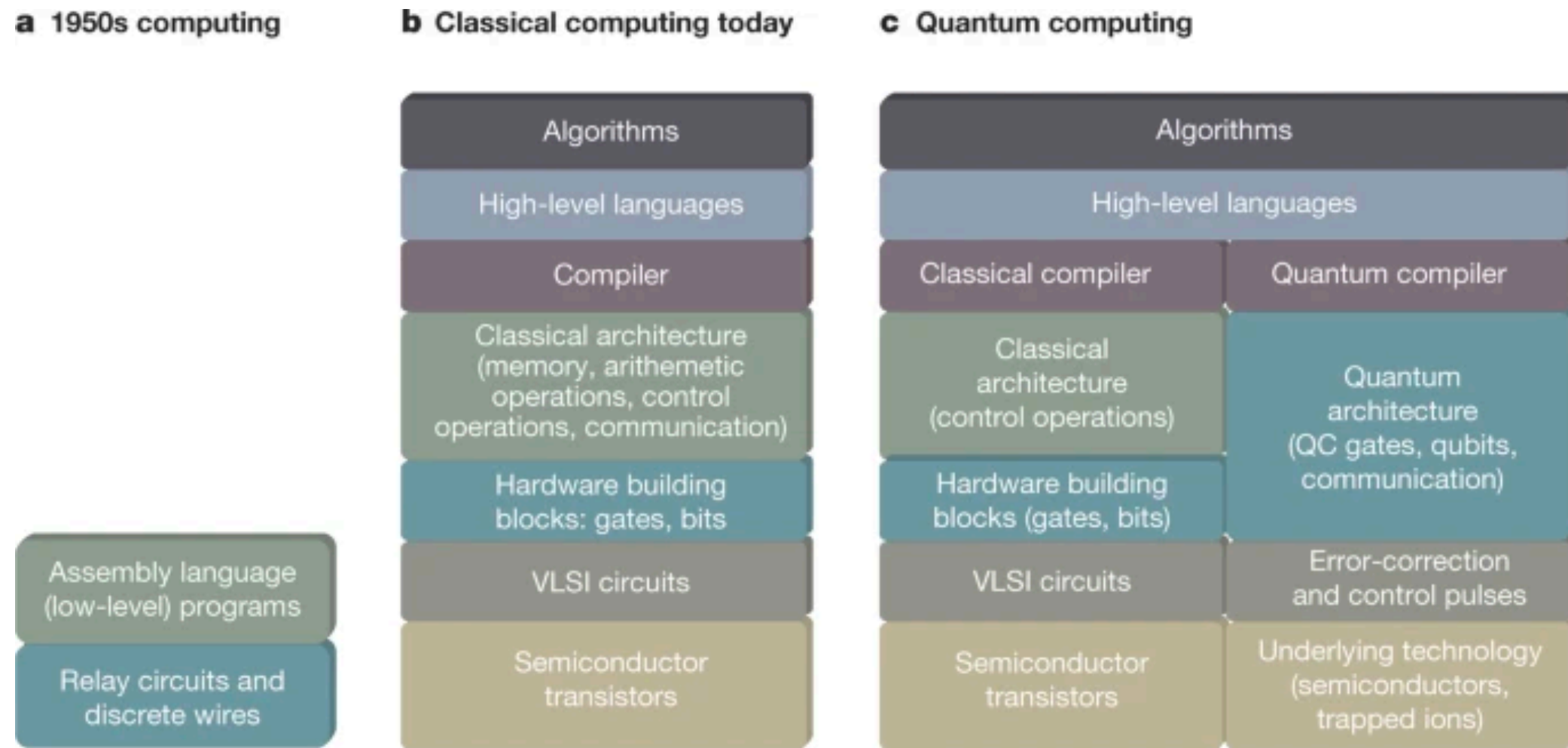
How to Develop **Software** for Q. Computing, e.g., **compiler, system?**



F. Chong, D. Franklin, M. Martonosi, Nature 549, 180

Large Design Space for System Software for Quantum Computers.

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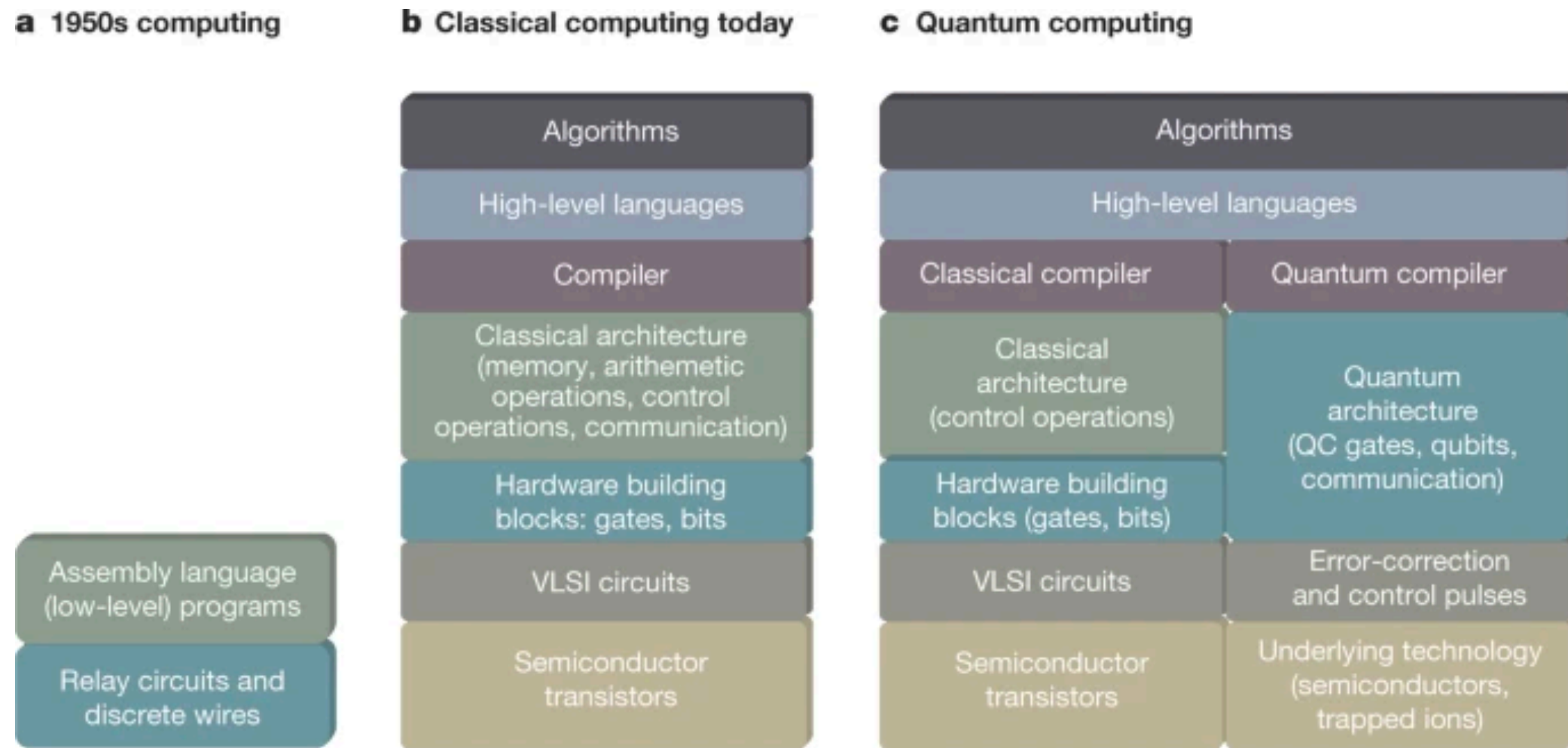
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High-Assurance Software Tool-chain both **desirable** and **challenging**.

- standard software assurance techniques, e.g., black-box / unit test, expensive in q.
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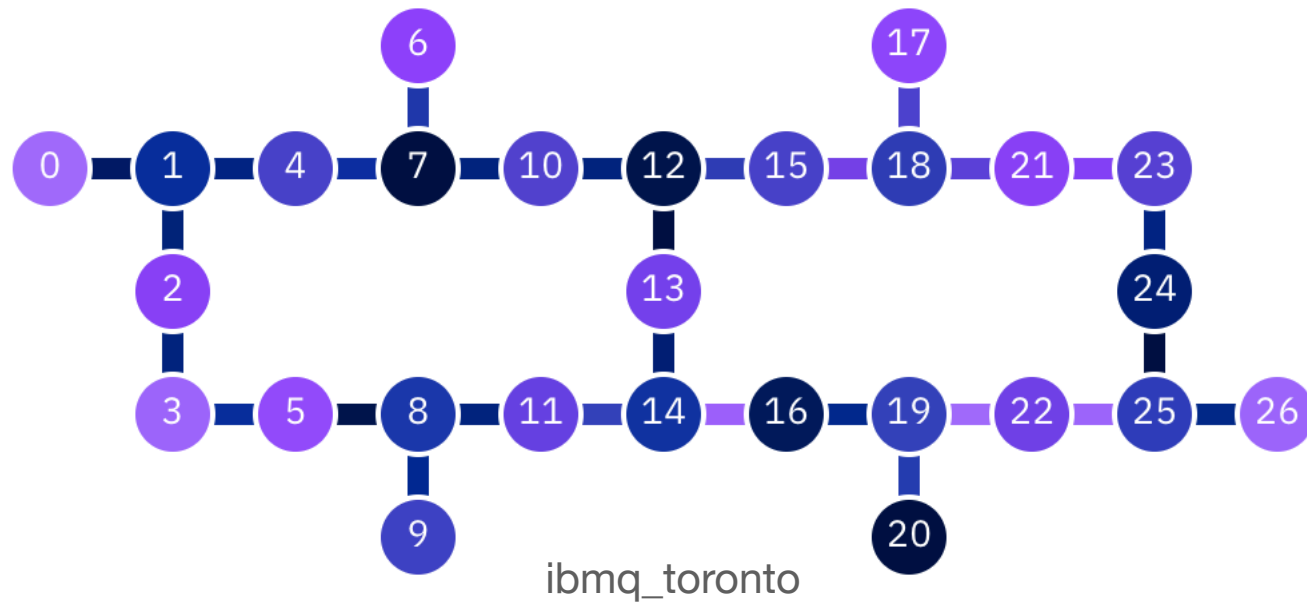
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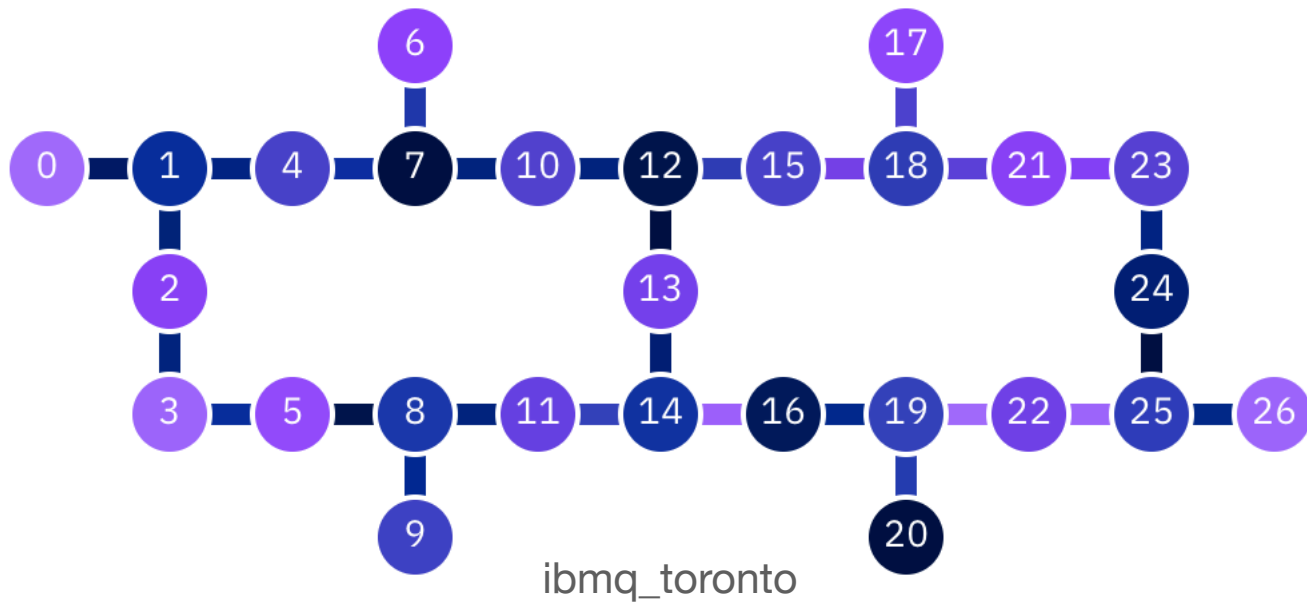
A possible **solution** : **fully certified software**, e.g., **VOQC (POPL 2021)**

How to Design and Implement **Architecture** for Quantum Computing?



Mapping, Error Mitigation, ...
approximate computing

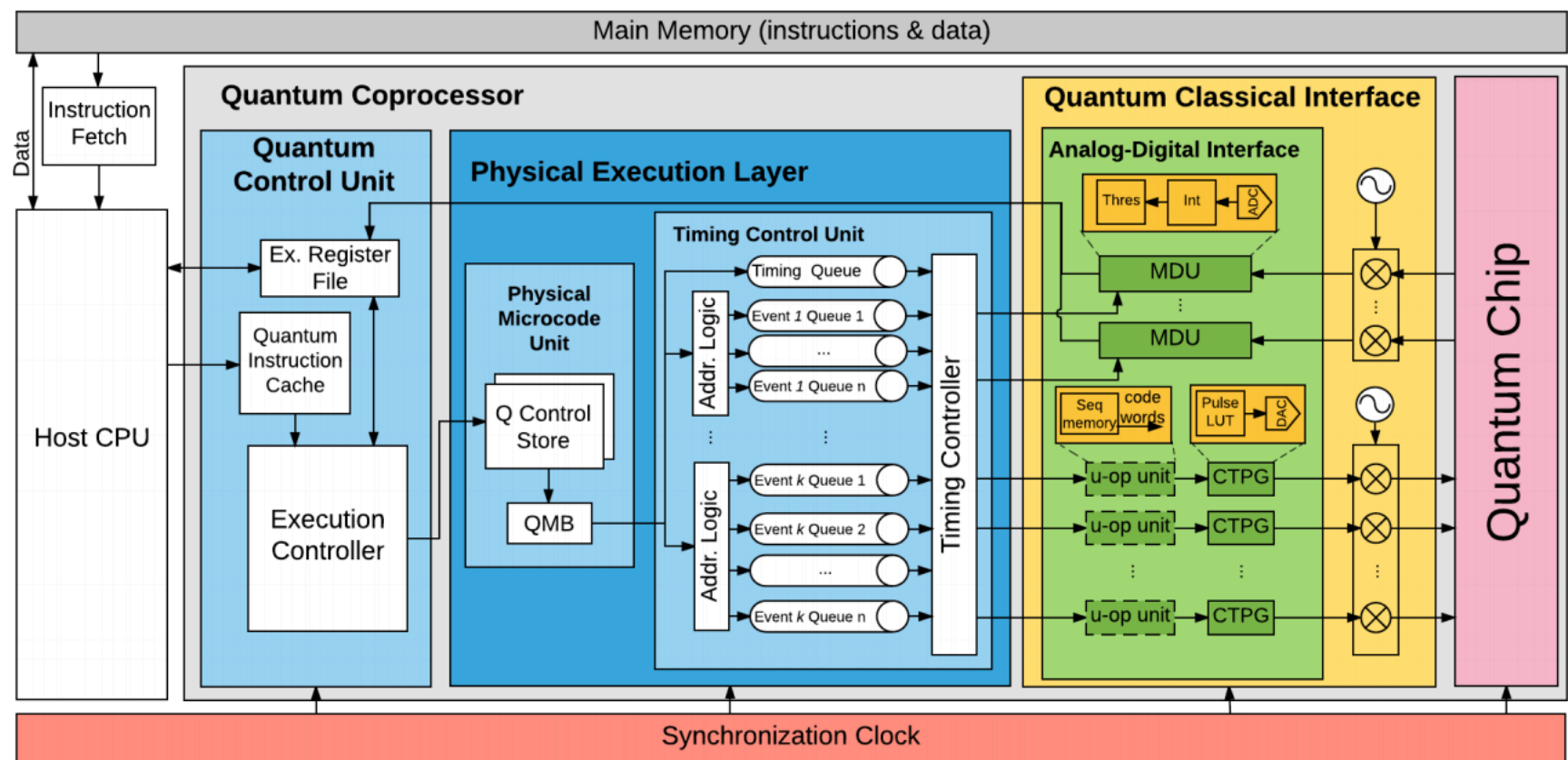
How to Design and Implement **Architecture** for Quantum Computing?



Mapping, Error Mitigation, ...
approximate computing

A lot of controlling operations need to be located close to quantum chips for small responsive time.

ISA + Fast Compilation



How to Handle Quantum **Security** Issues in Design and Implementation?

Verification of Quantum Cryptography:

Relational Quantum Hoare Logic (Unruh; Barthe et al.)



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Resource estimation of Complex Quantum Attack Programs

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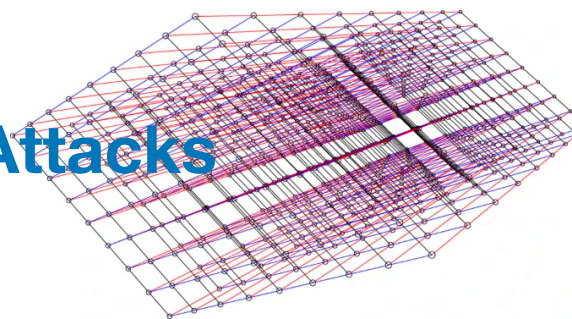


Quantum Cryptanalysis:

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Post-Quantum Cryptography:

Classical Cryptographic Systems Resilient to Quantum Attacks



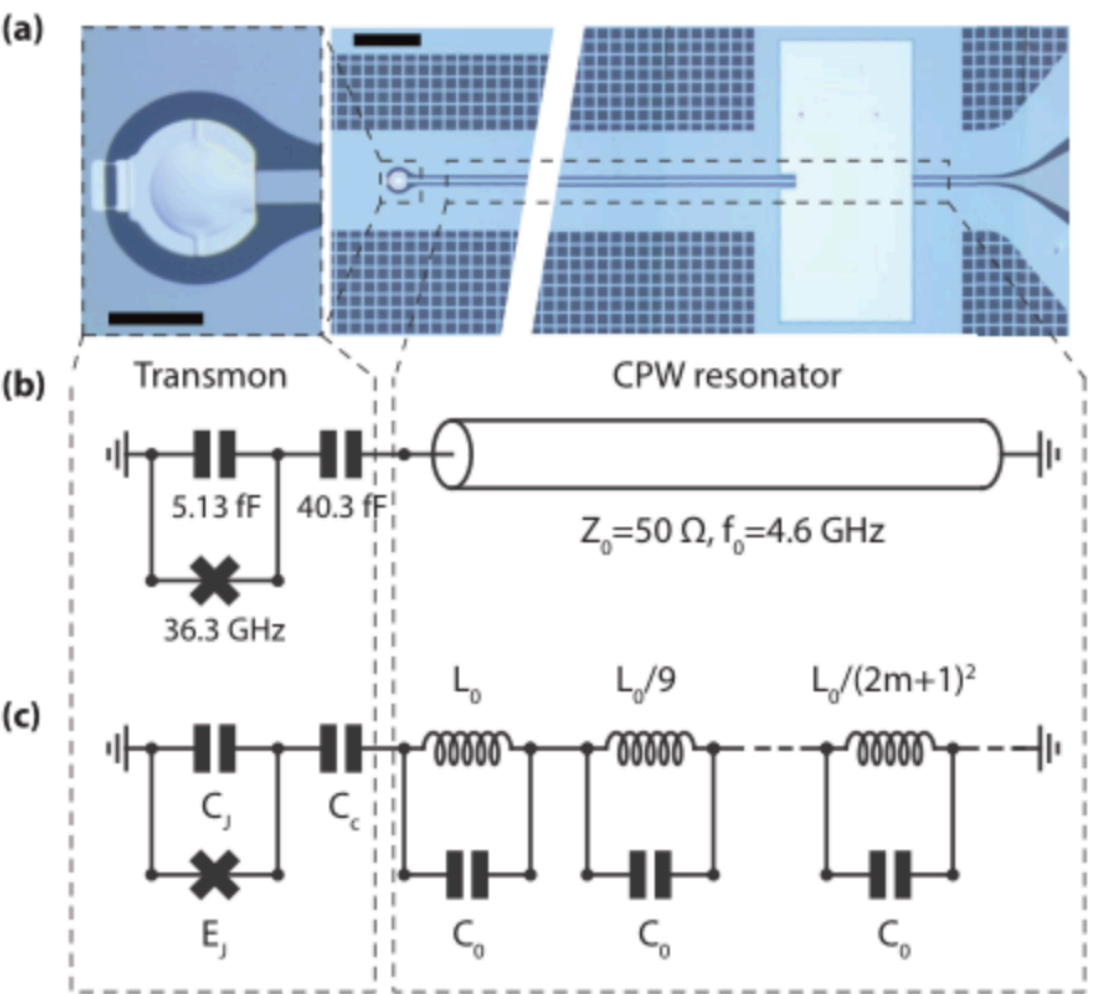
For Classical Cryptographic Systems

- (1) Identify their post-quantum security**
- (2) automate the procedure to upgrade its post-quantum security**
- (3) formal post-quantum security proofs**

Formally generated security analysis will provide not only efficient and high assurance proofs that can replace the tedious and error-prone analysis for experts, but also independently verifiable proofs that can be used by security practitioners without much quantum knowledge.

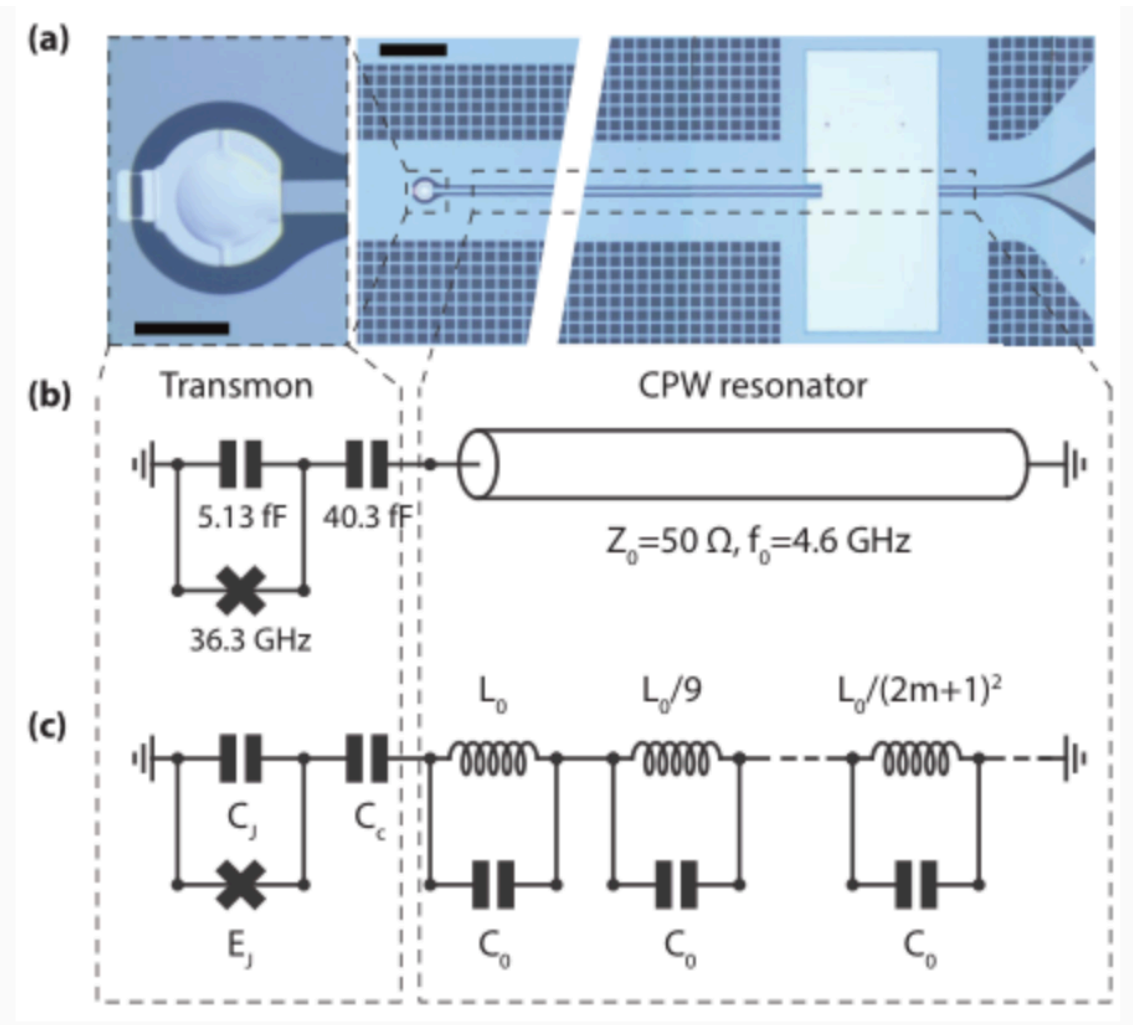


How to Scale and Automate the Design of Quantum Hardware ?

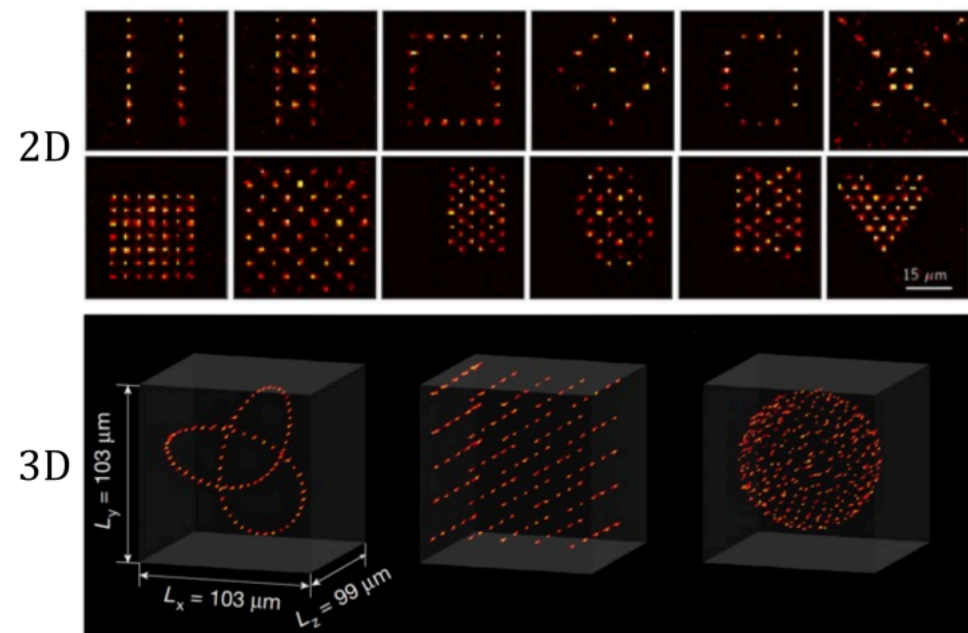


Superconducting Credit: arXiv:1704.06208

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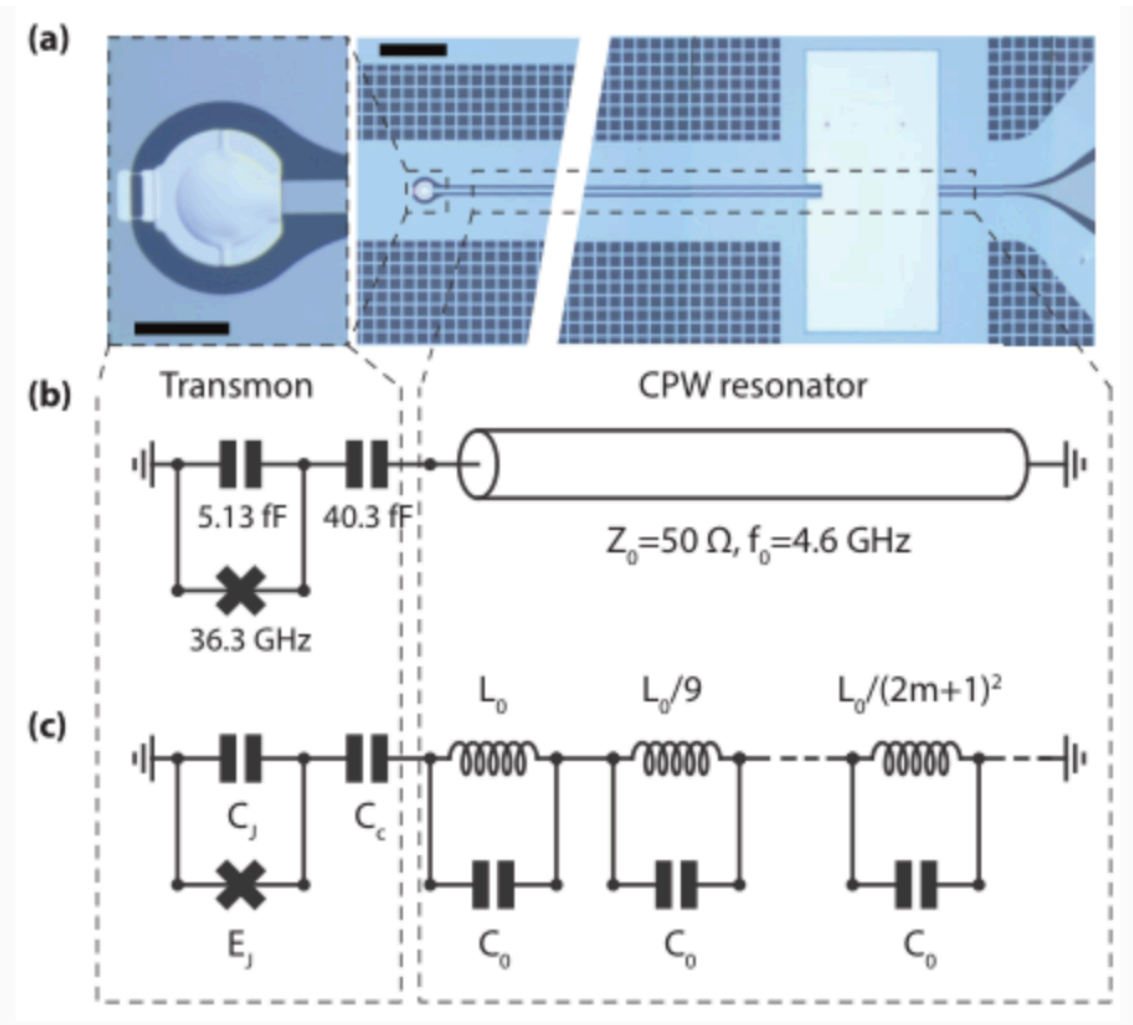


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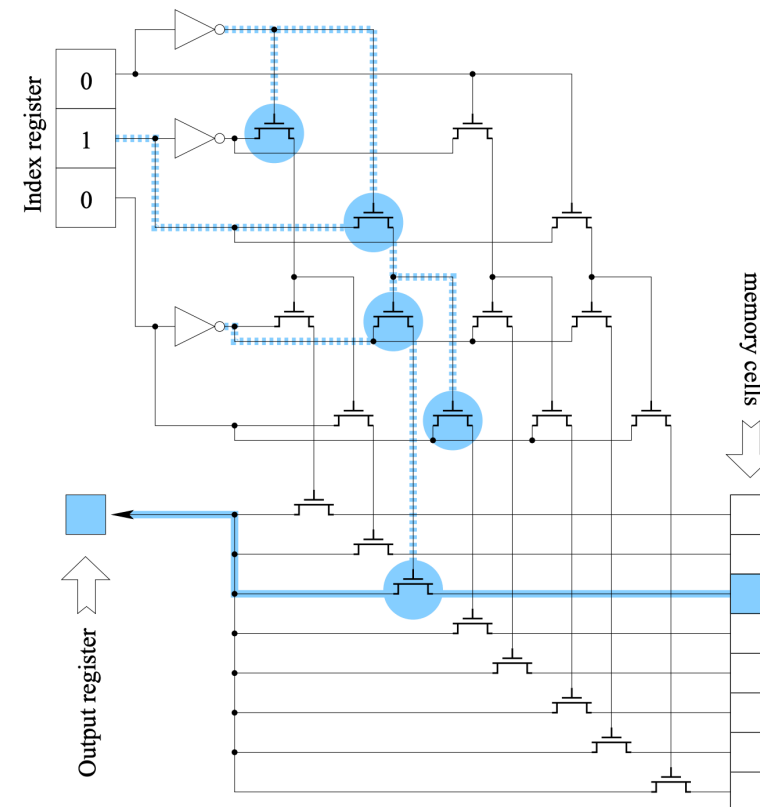


Neutral Atoms Credit: arXiv:2006.12326

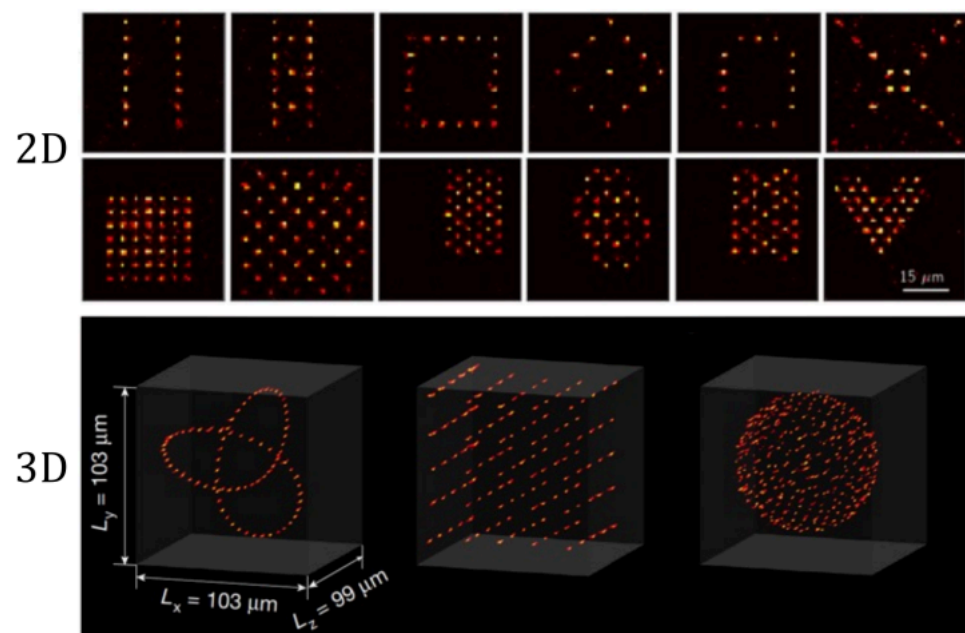
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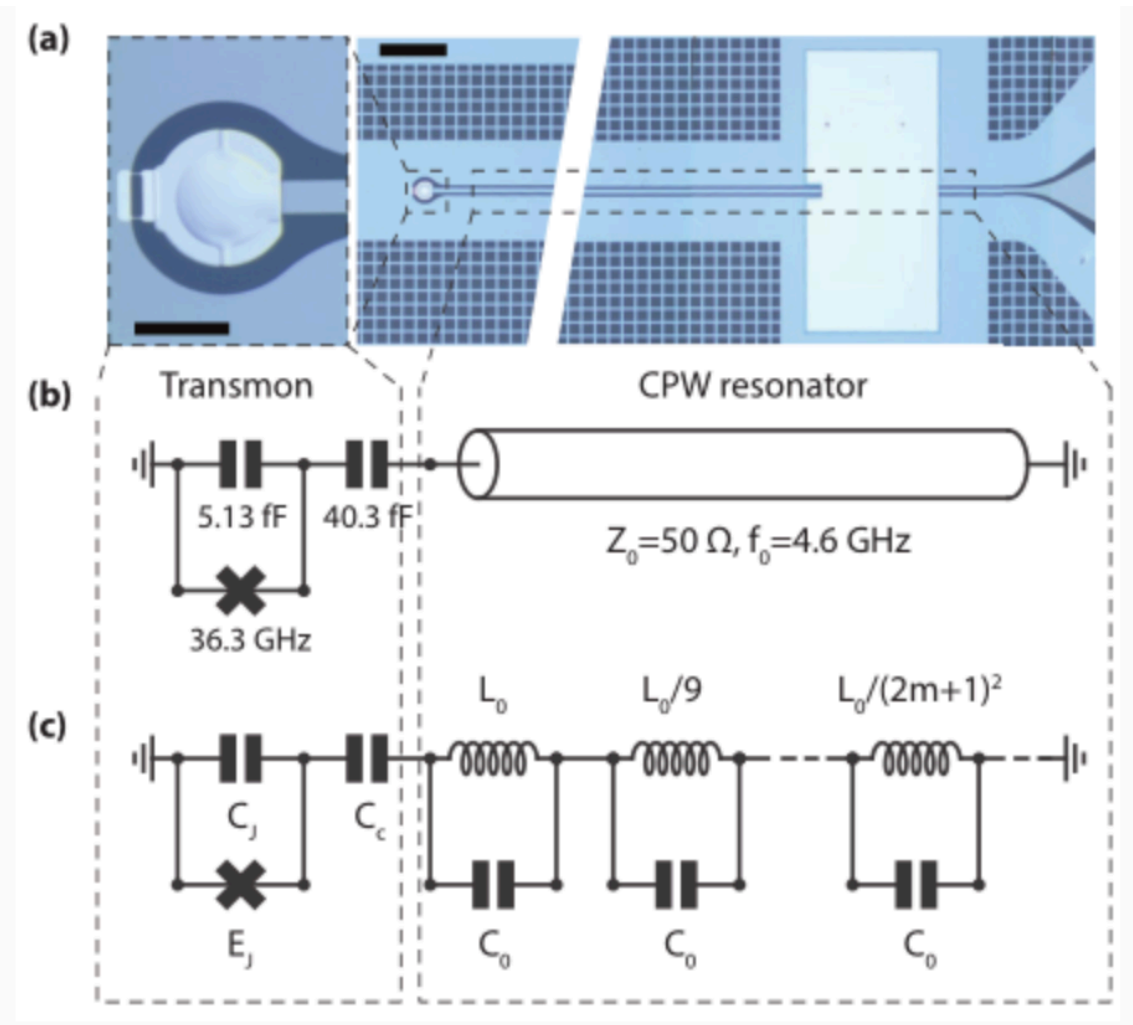


QRAM Architecture
Credit: ArXiv 0807.4994

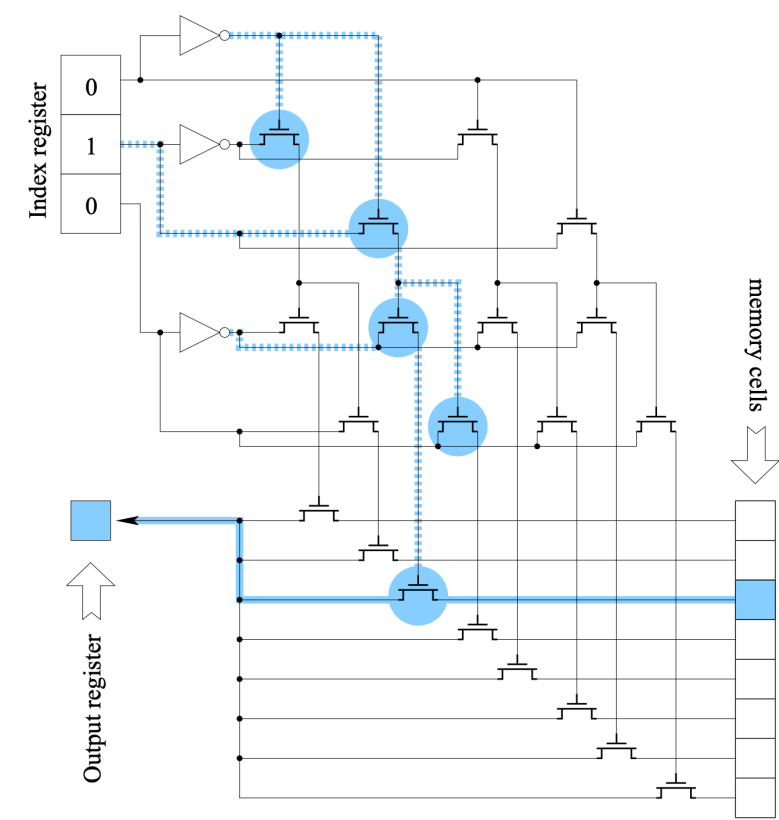


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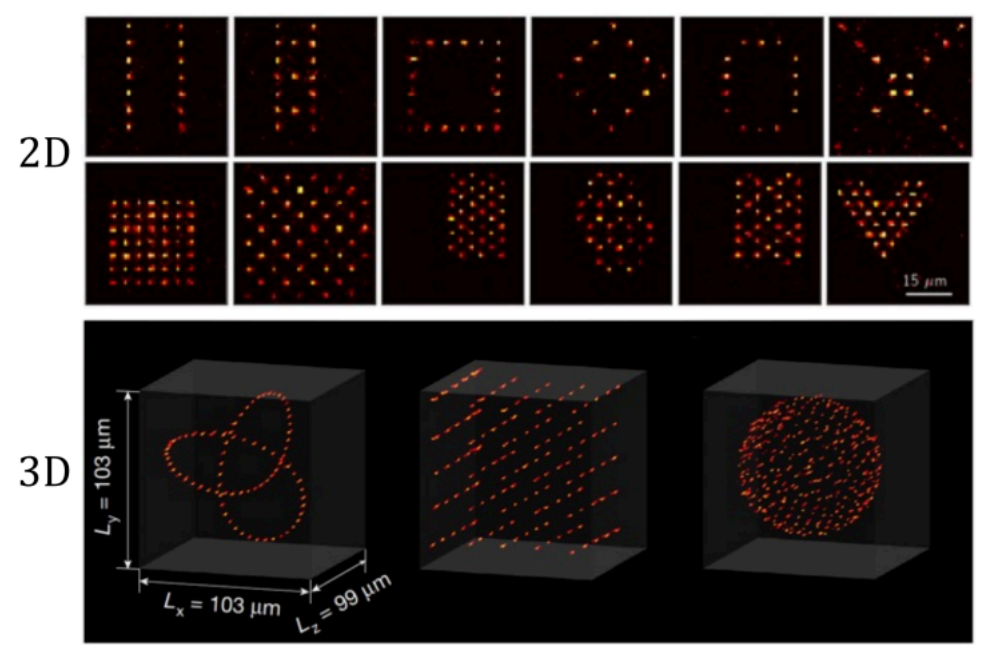


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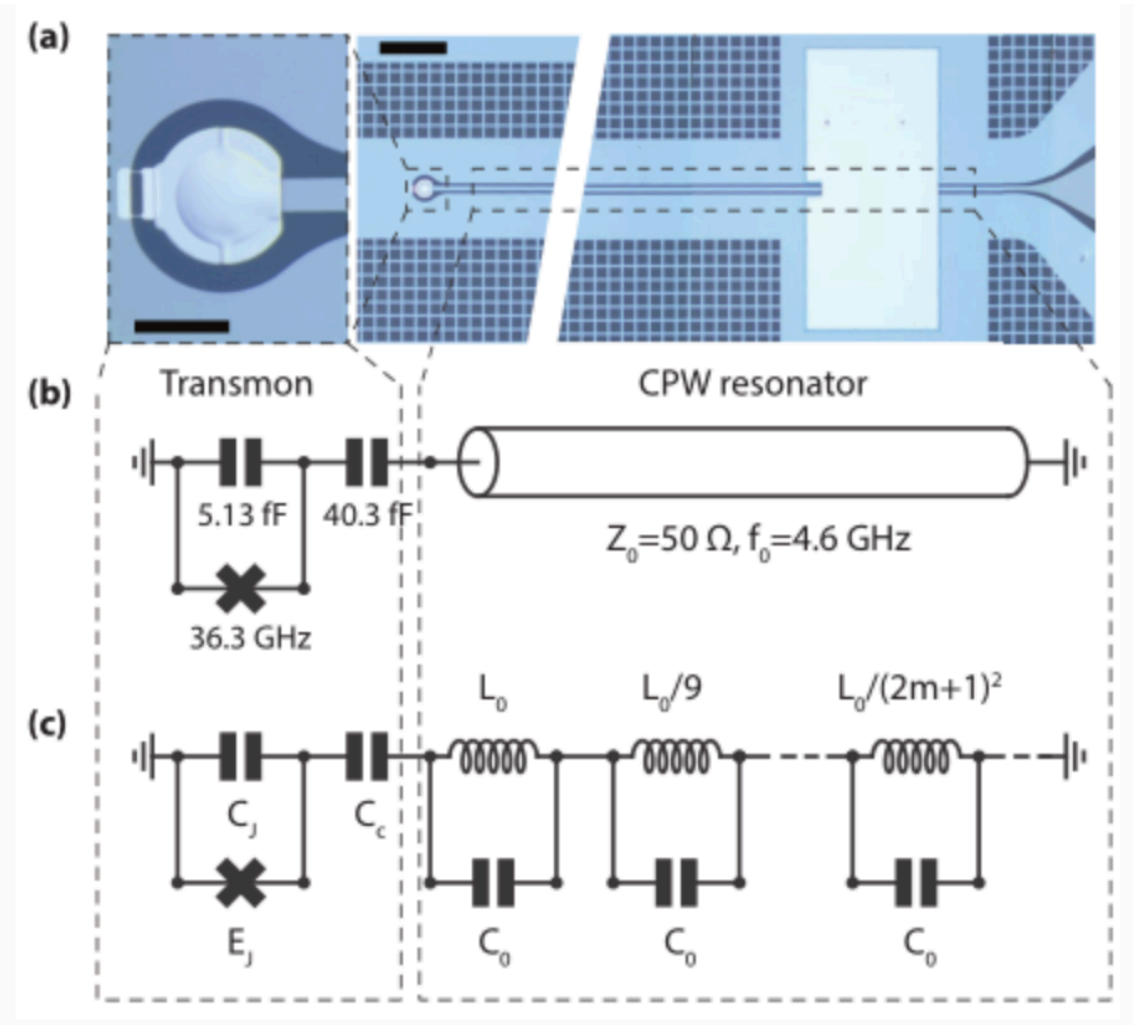
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Demonstrate A Lot of Design Choices
Hard to Scale without **Automatic Tools**

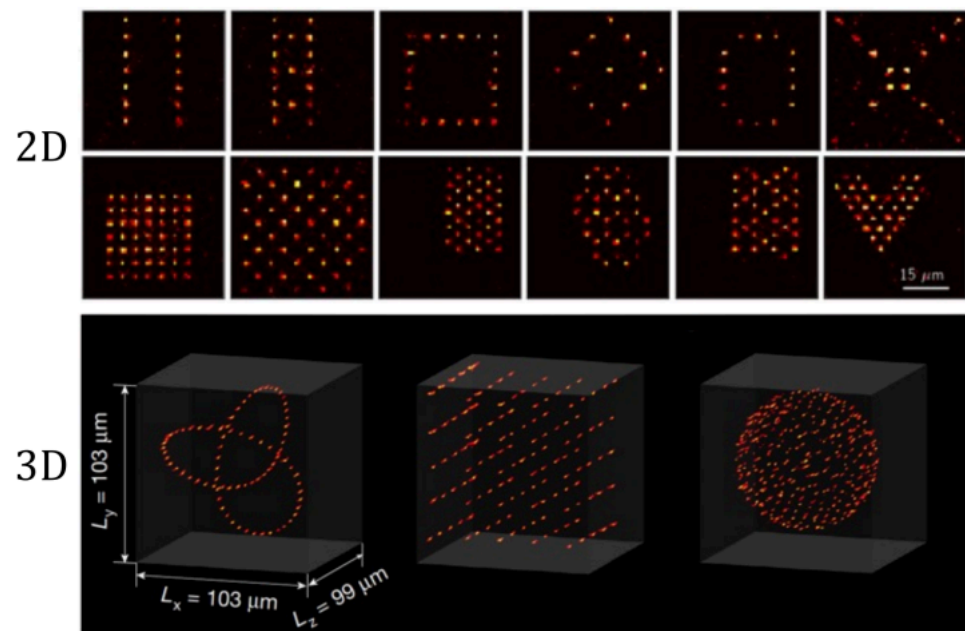


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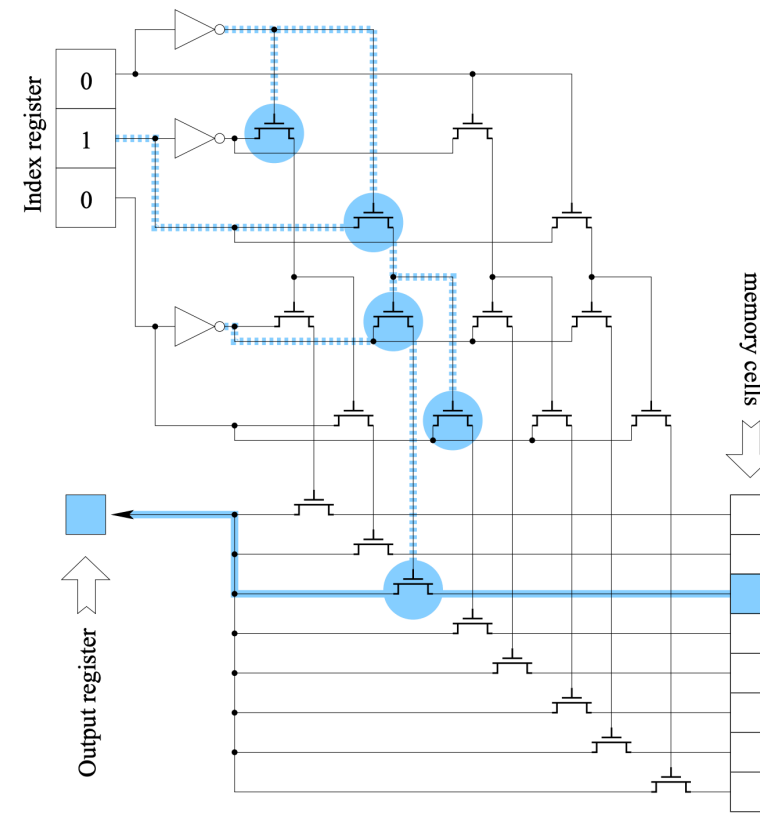
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**A Golden Age of Hardware Description Languages:
Applying Programming Language Techniques to
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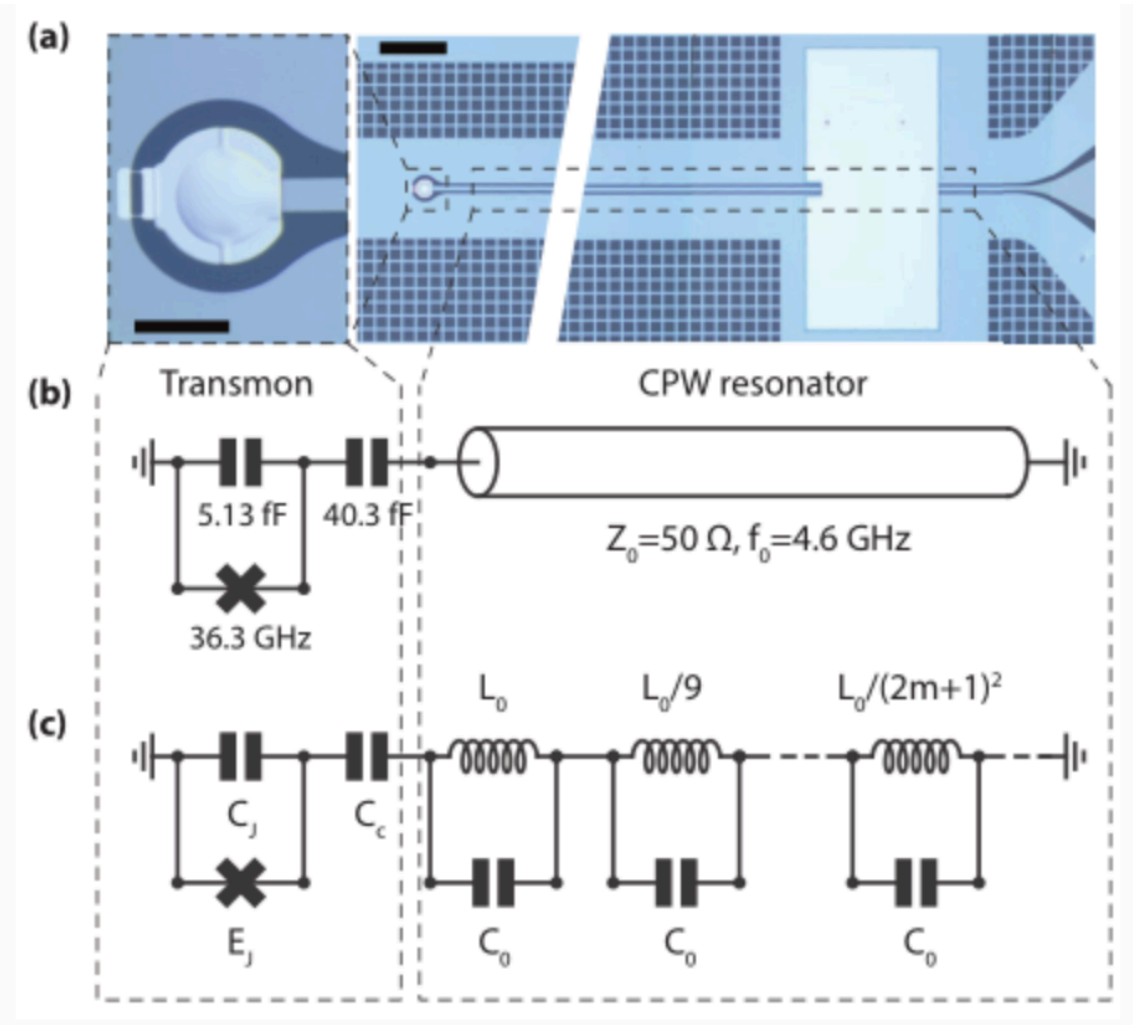
Lenny Truong
Stanford University, USA
lenny@cs.stanford.edu

Pat Hanrahan
Stanford University, USA
hanrahan@cs.stanford.edu

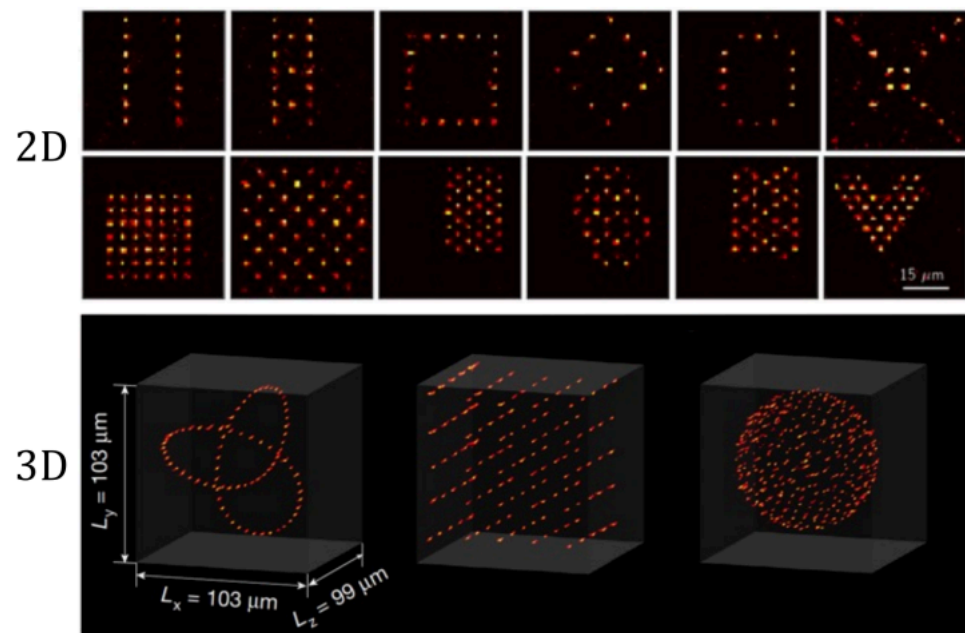
SNAPL 2019



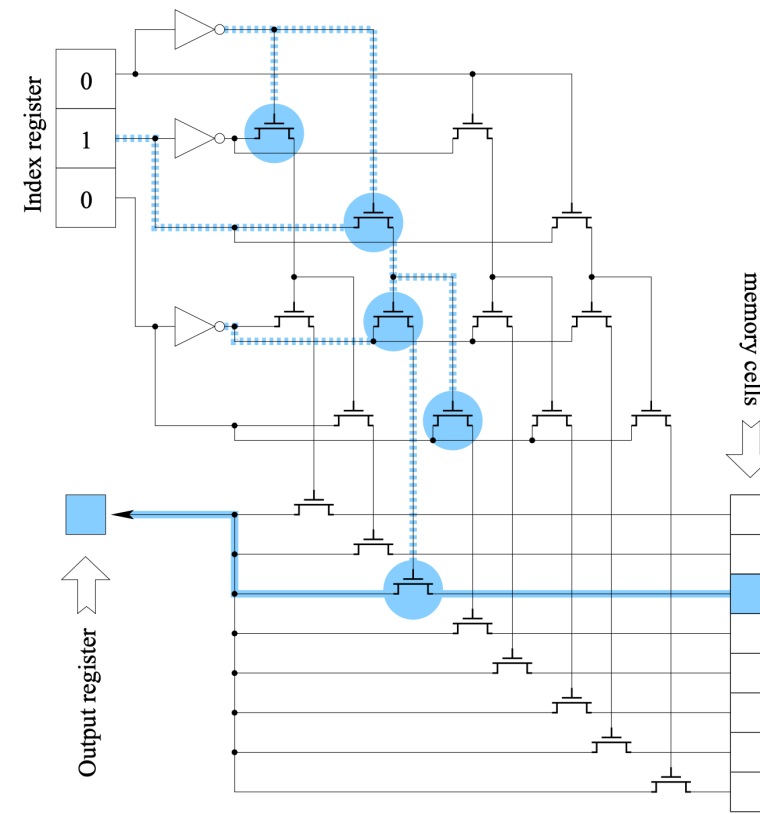
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SNAPL 2019



Applies to Quantum Hardware too!

Summary

Quantum PLs



Software Tool-chain



Architecture



Security



Hardware Design



Summary

Satisfactory

Quantum PLs



Software Tool-chain



Architecture



Security



Hardware Design



Summary

Satisfactory

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Software Tool-chain



Architecture



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Hardware Design



More questions could be asked !



Summary

Satisfactory

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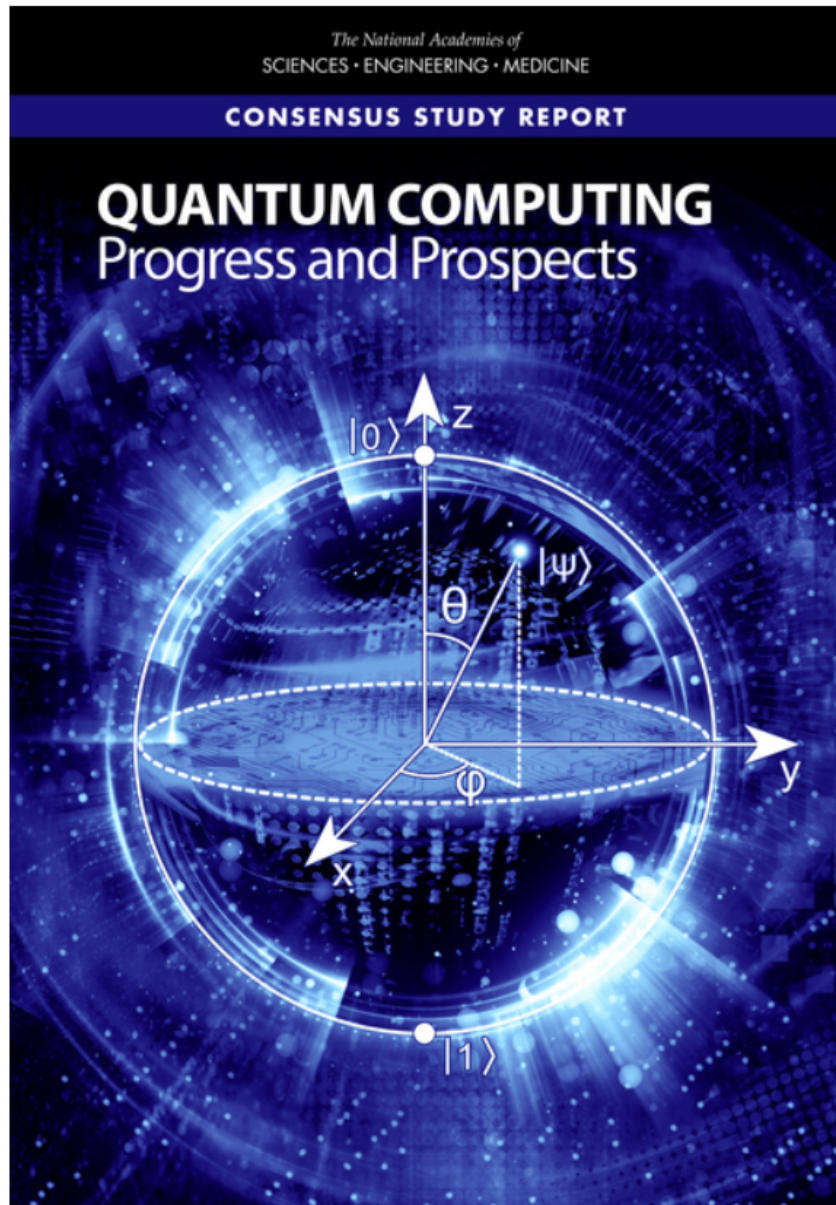
Hardware Design



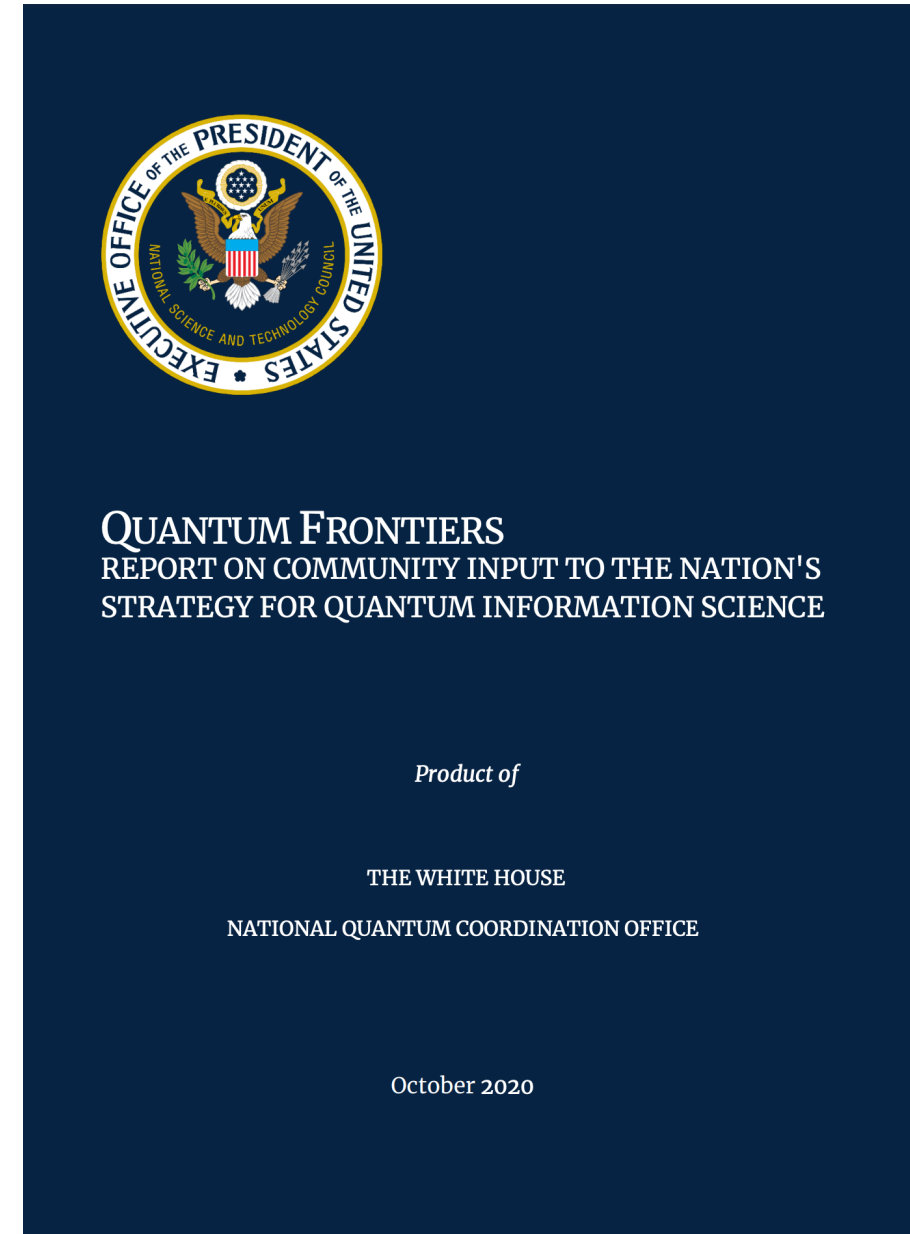
More questions could be asked !

More details will come back in Part III of the tutorial.

Further Readings: Thank You! Q & A



Next Steps in Quantum Computing: Computer Science's Role



Reference: links are available at [https://www.cs.umd.edu/~xwu/mini lib.html](https://www.cs.umd.edu/~xwu/mini_lib.html)



Outline

(1) Introduction to Quantum Computing and Potential Roles of Programming Languages (25 min + 5 Q & A)

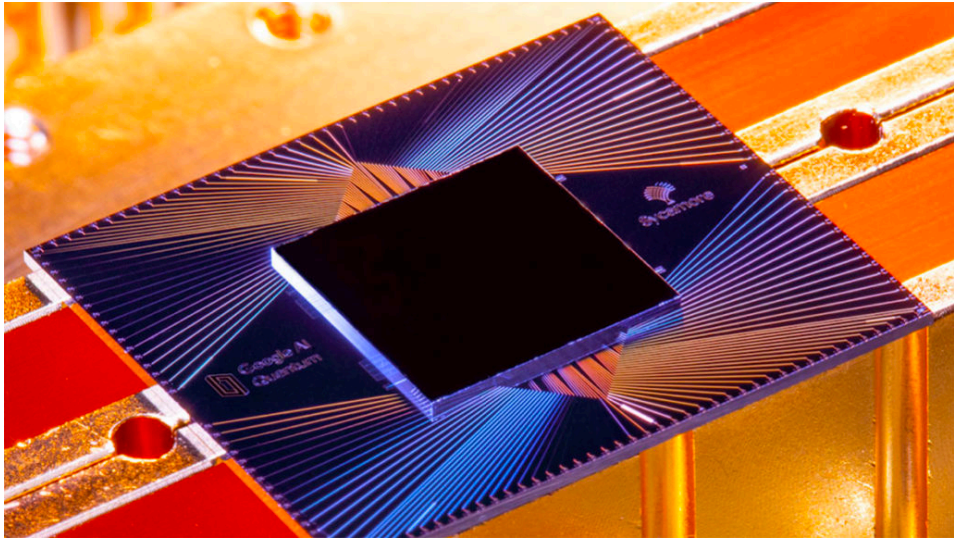
(2) A Mini-Course of Quantum Hoare Logic on Quantum While Language (30 min + 5 Q & A)

(3) Discussion on existing and potential Programming Language research opportunities (20 min + 5 Q & A)

Reference: tutorial slides and some references are available at https://www.cs.umd.edu/~xwu/mini_lib.html



What is Quantum Computing?



A Quantum Computer

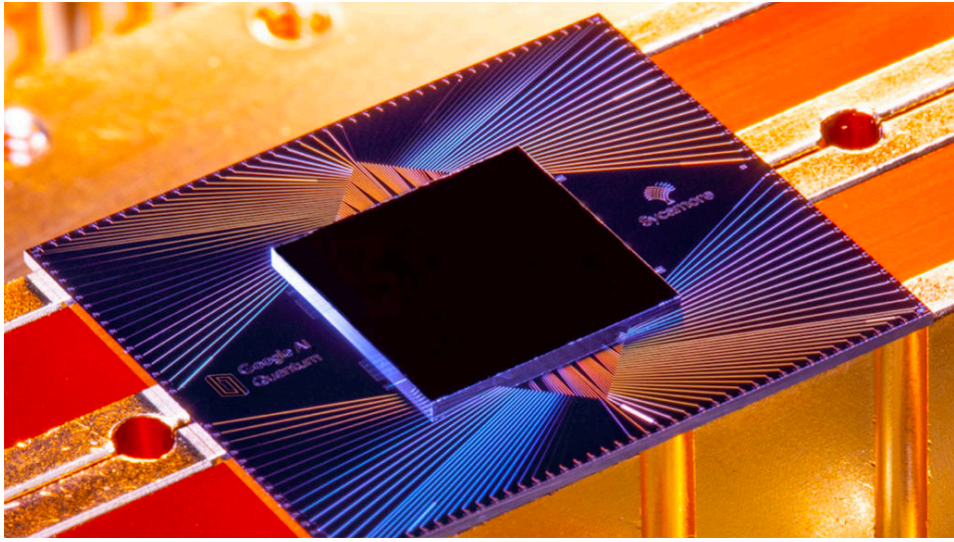
An Operation $O \rightarrow$ A **Quantum** Physical Evolution Q

Computation:

Evolution of the Machine: Q_1, Q_2, Q_3, \dots

The accumulative evolution carries some computation!

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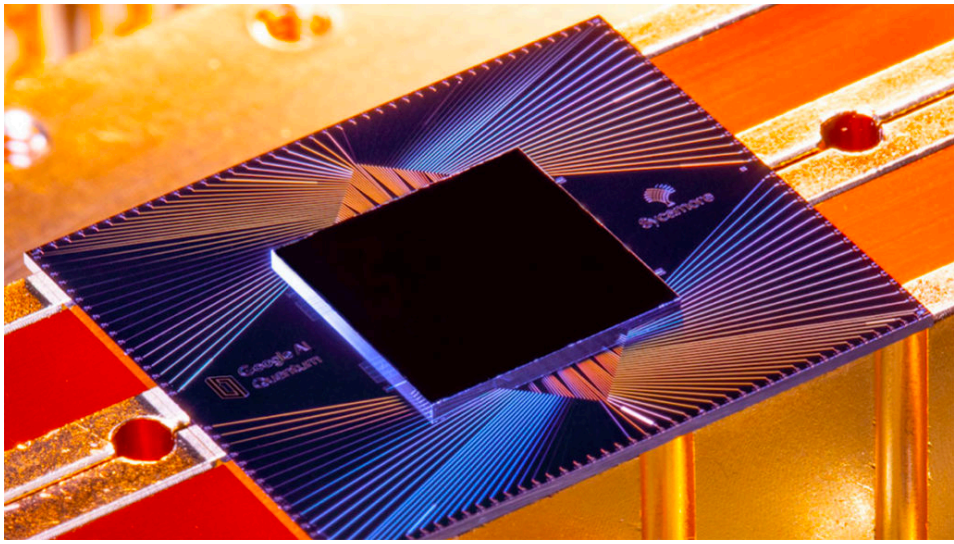
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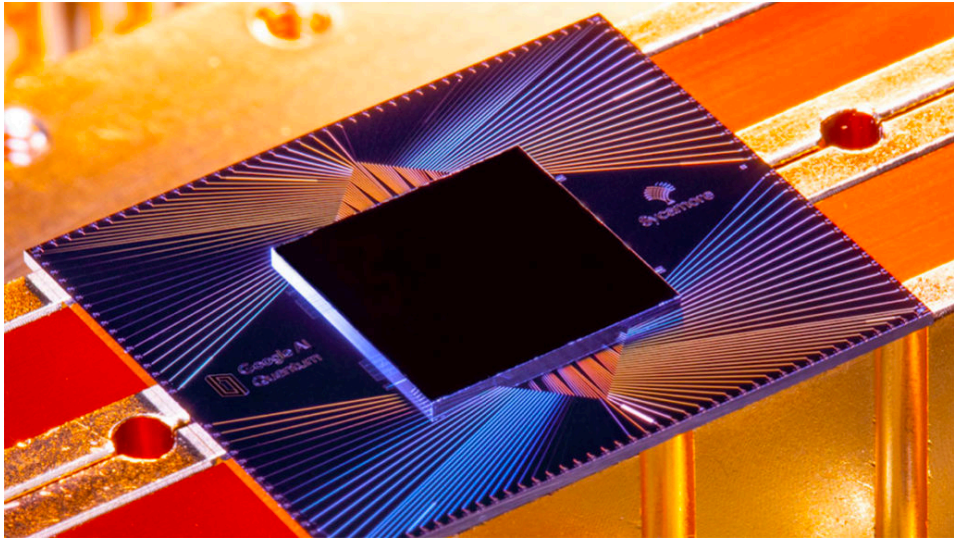
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The **Math Model** of Quantum Machines comes from the math model of Q_i s.
(semantics)

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Four Postulates for Quantum Mechanics:

State Space postulate

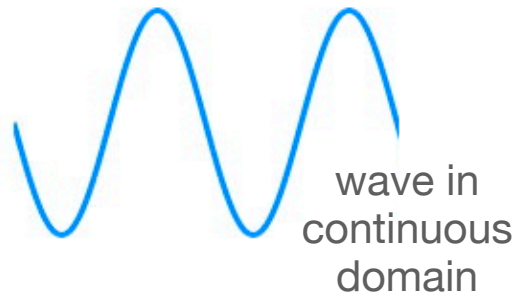
Evolution postulate — **No-Cloning** theorem

Composite System postulate

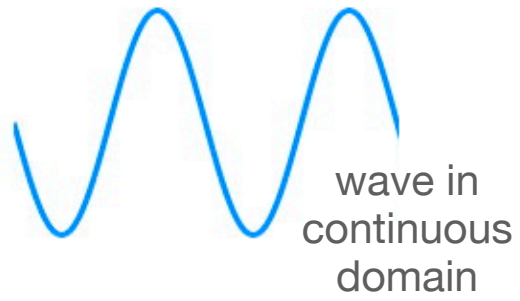
Measurement postulate

State Space postulate: (pure) quantum state represented by **unit complex vectors**

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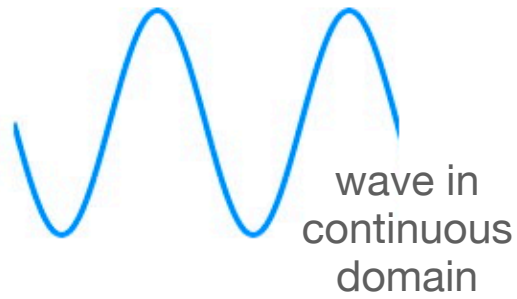


State Space postulate: (pure) quantum state represented by **unit complex vectors**



A *quantum bit* (**qubit**) refers to a quantum system of dimension 2

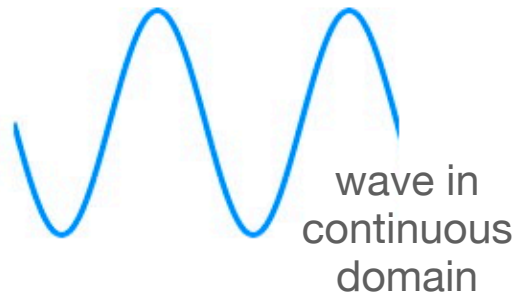
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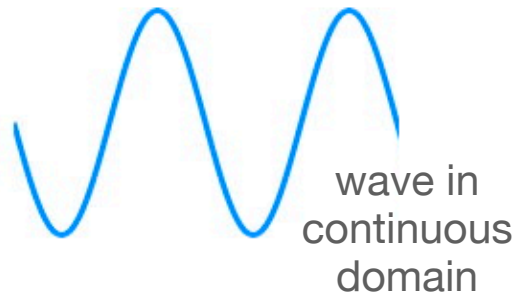


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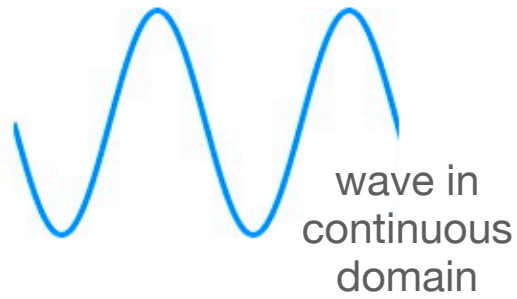
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A general qubit:

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α, β are general **complex** numbers.
Constraint due to Born's **probability amplitude** interpretation.

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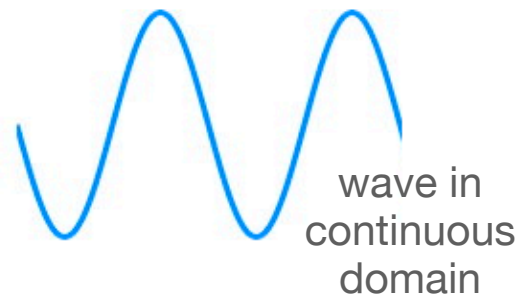
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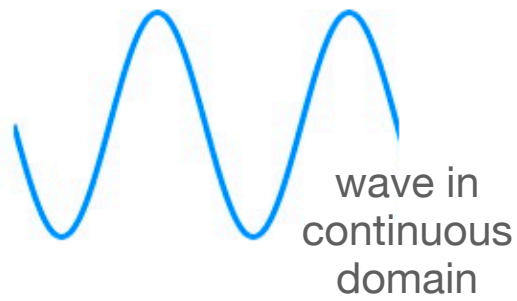
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Unitary evolution is a simple consequence of being linear and preserving ℓ_2 norm

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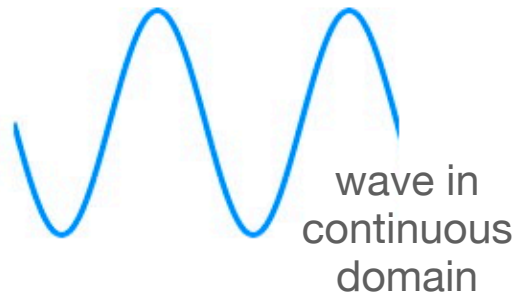
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The representation of two qubits lies in $\mathbb{C}^2 \otimes \mathbb{C}^2$ (dim-4), where \mathbb{C}^2 (dim-2) is for a qubit.

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So $|00\rangle = |0\rangle \otimes |0\rangle$

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A **n**-qubit system requires 2^n dimensional space. **Exponential cost in classical simulation!**

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Examples of Common Quantum Gates

► Pauli gates: **Single-qubit Gate**

$$X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad Y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad Z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

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► The controlled-NOT (CNOT) gate: **Two-qubit Gate**

$$CNOT = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}$$

Composite System postulate: joint system (A,B) in the **tensor-product** of A and B

The representation of two qubits lies in $\mathbb{C}^2 \otimes \mathbb{C}^2$ (dim-4), where \mathbb{C}^2 (dim-2) is for a qubit.

So $|00\rangle = |0\rangle \otimes |0\rangle$ $|01\rangle$ $|10\rangle$ $|11\rangle$

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Consider an arbitrary state $|\psi\rangle = \alpha|0\rangle + \beta|1\rangle$

$$U|\psi\rangle|0\rangle = \alpha|0\rangle|0\rangle + \beta|1\rangle|1\rangle \\ \neq |\psi\rangle|\psi\rangle$$

CONTRADICTION!

Measurement postulate: how to **read** classical info out of q. system?

This information reading procedure will **distribute/collapse** the underlying q. systems.

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- ▶ A *measurement* is modelled as a set of operators $M = \{M_m\}$ with $\sum_m M_m^\dagger M_m = I$.

- ▶ If a quantum system was in pure state $|\psi\rangle$ before the measurement, then:

- ▶ the probability that measurement outcome is λ :

$$p(m) = \|M_m|\psi\rangle\|^2$$

where $\|\cdot\|$ is the length of vector.

- ▶ the state of the system after the measurement:

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More advanced math formulation of ensemble of quantum states

Density matrices

- ▶ In the n -dimensional Hilbert space \mathbb{C}^n , an operator is represented by an $n \times n$ complex matrix A .
- ▶ The trace of an operator A is $tr(A) = \sum_i A_{ii}$ (the sum of the entries on the main diagonal).
- ▶ A positive semidefinite matrix ρ is called a *partial density matrix* if $tr(\rho) \leq 1$; in particular, a *density matrix* ρ is a partial density matrix with $tr(\rho) = 1$.

▶ For any mixed state $\{(p_1, |\psi_1\rangle), \dots, (p_k, |\psi_k\rangle)\}$,

$$\rho = \sum_i p_i |\psi_i\rangle\langle\psi_i|$$

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Example:

$$\left\{ \left(\frac{2}{3}, |0\rangle \right), \left(\frac{1}{3}, |-\rangle \right) \right\} \longrightarrow \rho = \frac{2}{3}|0\rangle\langle 0| + \frac{1}{3}|-\rangle\langle -| = \frac{1}{6} \begin{pmatrix} 5 & -1 \\ -1 & 1 \end{pmatrix}$$

Quantum While-Language

Syntax

A *core* language for imperative quantum programming

$$\begin{aligned} S ::= & \mathbf{skip} \mid q := |0\rangle \\ & \mid S_1; S_2 \\ & \mid \bar{q} := U[\bar{q}] \\ & \mid \mathbf{if} (\square m \cdot M[\bar{q}] = m \rightarrow S_m) \mathbf{fi} \\ & \mid \mathbf{while} M[\bar{q}] = 1 \mathbf{do} S \mathbf{od} \end{aligned}$$

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Classically, one has

$u := t$ $t \sim$ expression.

However, due to no-cloning,

1) initialization

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Classical control requires reading information out of quantum systems.

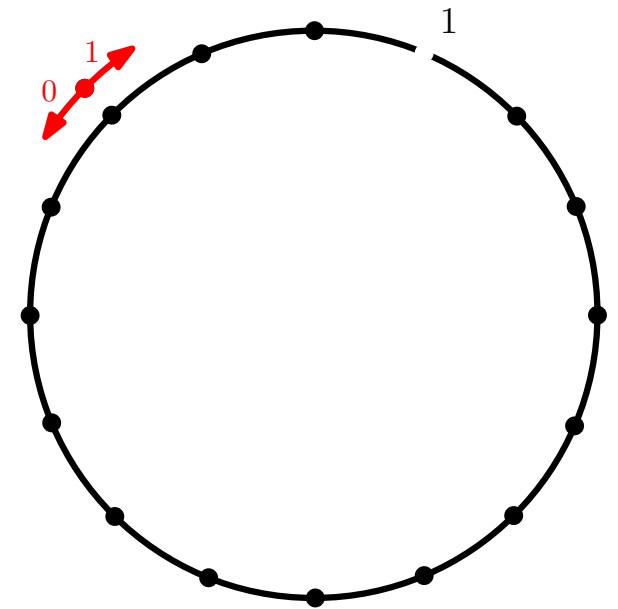
However, by measuring the guard, it leads to

(1) a probabilistic choice of branches

(2) a collapse of the guard state before entering each branch

Quantum 1-D Loop Walk

```
 $QW \equiv c := |L\rangle;$   
 $p := |0\rangle;$   
while  $M[p] = no$  do  
   $c := H[c];$   
   $c, p := S[c, p]$   
od
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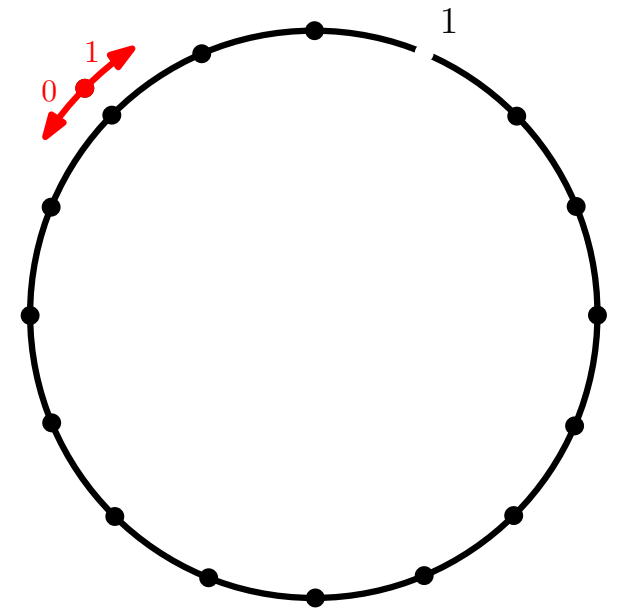


Operator Definition

$$S = \sum_{i=0}^{n-1} |L\rangle\langle L| \otimes |i \ominus 1\rangle\langle i| + \sum_{i=0}^{n-1} |R\rangle\langle R| \otimes |i \oplus 1\rangle\langle i|.$$

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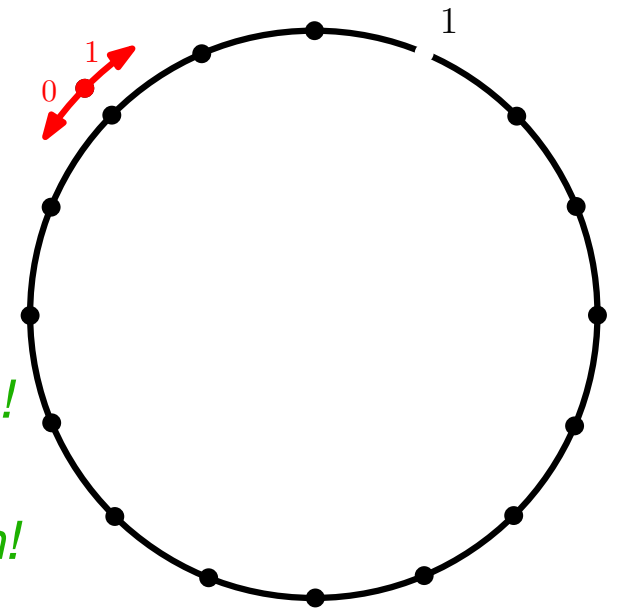


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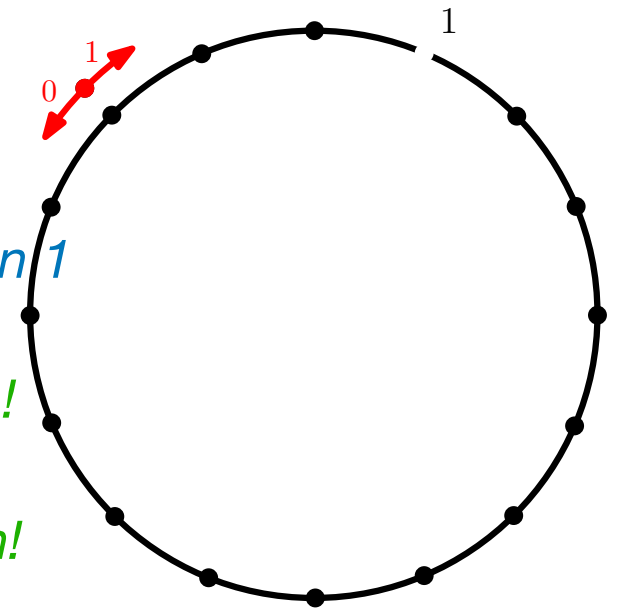


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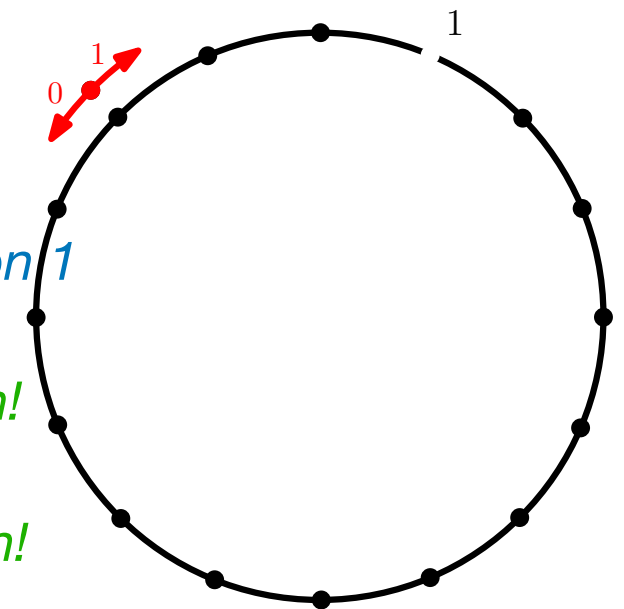
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Quantum 1-D Loop Walk

Goal: reason about this program

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Semantics of Quantum While-Language

Operational Semantics

A *configuration*: $\langle S, \rho \rangle$

- ▶ S is a quantum program or E (the empty program)
- ▶ ρ is a partial density operator in

$$\mathcal{H}_{\text{all}} = \bigotimes_{\text{all } q} \mathcal{H}_q$$

$$(Sk) \quad \overline{\langle \text{skip}, \rho \rangle} \rightarrow \langle E, \rho \rangle$$

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Capture the **Collapse** of the **Guard** state.

Semantics of Quantum While-Language

Denotational Semantics

Semantic function of quantum program S :

$$\llbracket S \rrbracket : \mathcal{D}(\mathcal{H}_{\text{all}}) \rightarrow \mathcal{D}(\mathcal{H}_{\text{all}})$$

$$\llbracket S \rrbracket(\rho) = \sum \{ |\rho'\rangle : \langle S, \rho \rangle \rightarrow^* \langle E, \rho' \rangle | \} \text{ for all } \rho \in \mathcal{D}(\mathcal{H}_{\text{all}})$$

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Observation:

$$\text{tr}(\llbracket S \rrbracket(\rho)) \leq \text{tr}(\rho)$$

for any quantum program S and all $\rho \in \mathcal{D}(\mathcal{H}_{\text{all}})$.

- ▶ $\text{tr}(\rho) - \text{tr}(\llbracket S \rrbracket(\rho))$ is the probability that program S diverges from input state ρ .

Quantum Predicate & Hoare Triple

- ▶ A *quantum predicate* is a Hermitian operator (observable) P such that $0 \sqsubseteq P \sqsubseteq I$.

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- ▶ A *correctness formula* is a statement of the form:

$$\{P\}S\{Q\}$$

where:

- ▶ S is a quantum program
- ▶ P and Q are quantum predicates.
- ▶ Operator P is called the *precondition* and Q the *postcondition*.

Quantum Predicate & Hoare Triple

- ▶ A *quantum predicate* is a Hermitian operator (observable) P such that $0 \sqsubseteq P \sqsubseteq I$.

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Continuous logic
[0, 1]
Matrix Upgrade

- ▶ A *correctness formula* is a statement of the form:

$$\{P\}S\{Q\}$$

where:

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$$\text{tr}(P\rho) \leq \text{tr}(Q[S](\rho)) \text{ for all } \rho.$$

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↑
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Semantics

2. $\{P\}S\{Q\}$ is true in the sense of *partial correctness*:

$$\models_{\text{par}} \{P\}S\{Q\},$$

if

$$\text{tr}(P\rho) \leq \text{tr}(Q[[S]](\rho)) + [\text{tr}(\rho) - \text{tr}([S](\rho))]$$

Quantum Predicate & Hoare Triple

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Similar as Classical
Hoare triple w/
different semantics

1. $\{P\}S\{Q\}$ is true in the sense of *total correctness*:

2. $\{P\}S\{Q\}$ is true in the sense of *partial correctness*:

$$\models_{\text{tot}} \{P\}S\{Q\}$$

$$\models_{\text{par}} \{P\}S\{Q\},$$

if

$$\text{if } \begin{array}{cc} \text{Pre-S State} & \text{Post-S State} \\ \text{tr}(P\rho) \leq \text{tr}(Q[[S]](\rho)) & \text{for all } \rho. \end{array}$$

if

$$\text{tr}(P\rho) \leq \text{tr}(Q[[S]](\rho)) + [\text{tr}(\rho) - \text{tr}([S](\rho))]$$


Semantics


Divergence

Quantum Hoare logic for Partial Correctness

(Axiom Sk) $\{P\} \mathbf{Skip} \{P\}$

(Axiom Ini)

$type(q) = \mathbf{Boolean} :$

$$\{|0\rangle_q \langle 0| P |0\rangle_q \langle 0| + |1\rangle_q \langle 0| P |0\rangle_q \langle 1|\} q := |0\rangle \{P\}$$

$type(q) = \mathbf{integer} :$

$$\left\{ \sum_{n=-\infty}^{\infty} |n\rangle_q \langle 0| P |0\rangle_q \langle n| \right\} q := |0\rangle \{P\}$$

(Axiom Uni) $\{U^\dagger P U\} \bar{q} := U[\bar{q}] \{P\}$

(Rule Seq)

$$\frac{\{P\} S_1 \{Q\} \quad \{Q\} S_2 \{R\}}{\{P\} S_1; S_2 \{R\}}$$

(Rule IF)

$$\frac{\{P_m\} S_m \{Q\} \text{ for all } m}{\{\sum_m M_m^\dagger P_m M_m\} \mathbf{if} (\square m \cdot M[\bar{q}] = m \rightarrow S_m) \mathbf{fi} \{Q\}}$$

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$$\frac{\{Q\} S \{M_0^\dagger P M_0 + M_1^\dagger Q M_1\}}{\{M_0^\dagger P M_0 + M_1^\dagger Q M_1\} \mathbf{while} M[\bar{q}] = 1 \mathbf{do} S \{P\}}$$

(Rule Ord)

$$\frac{P \sqsubseteq P' \quad \{P'\} S \{Q'\} \quad Q' \sqsubseteq Q}{\{P\} S \{Q\}}$$

Quantum Hoare logic for Partial Correctness

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Parts of Classical Hoare Logic

AXIOM 2: ASSIGNMENT

$$\{p[u := t]\} u := t \{p\}$$

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RULE 4: CONDITIONAL

$$\frac{\{p \wedge B\} S_1 \{q\}, \{p \wedge \neg B\} S_2 \{q\}}{\{p\} \text{if } B \text{ then } S_1 \text{ else } S_2 \text{ fi} \{q\}}$$

RULE 5: LOOP

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Theorem (Soundness and Completeness)

For any quantum program S and quantum predicates P, Q ,

$$\models_{\text{par}} \{P\} S \{Q\} \text{ if and only if } \vdash_{PD} \{P\} S \{Q\}.$$

Quantum Hoare logic for Total Correctness

Proof System for Total Correctness

Let P be a quantum predicate and $\epsilon > 0$. A function

$$t : \mathcal{D}(\mathcal{H}_{\text{all}}) \text{ (density operators)} \rightarrow \mathbb{N}$$

is called a (P, ϵ) -*ranking function* of quantum loop:

while $M[\bar{q}] = 1$ **do** S **od**

$$(1) \{Q\}S\{M_0^\dagger P M_0 + M_1^\dagger Q M_1\}$$

(2) for any $\epsilon > 0$, t_ϵ is a $(M_1^\dagger Q M_1, \epsilon)$ -ranking function of loop

if for all ρ :

1. $t(\llbracket S \rrbracket(M_1 \rho M_1^\dagger)) \leq t(\rho)$;
2. $\text{tr}(P\rho) \geq \epsilon$ implies $t(\llbracket S \rrbracket(M_1 \rho M_1^\dagger)) < t(\rho)$

(Rule LT)

$$\frac{\text{function of loop}}{\{M_0^\dagger P M_0 + M_1^\dagger Q M_1\} \mathbf{while} M[\bar{q}] = 1 \mathbf{do} S \mathbf{od} \{P\}}$$

Theorem (Soundness and Completeness)

For any quantum program S and quantum predicates $P Q$,

$$\models_{\text{tot}} \{P\}S\{Q\} \text{ if and only if } \vdash_{TD} \{P\}S\{Q\}.$$

Quantum Hoare logic and Invariants : POPL17

$QW \equiv c := |L\rangle;$ *coin space = {L, R}*

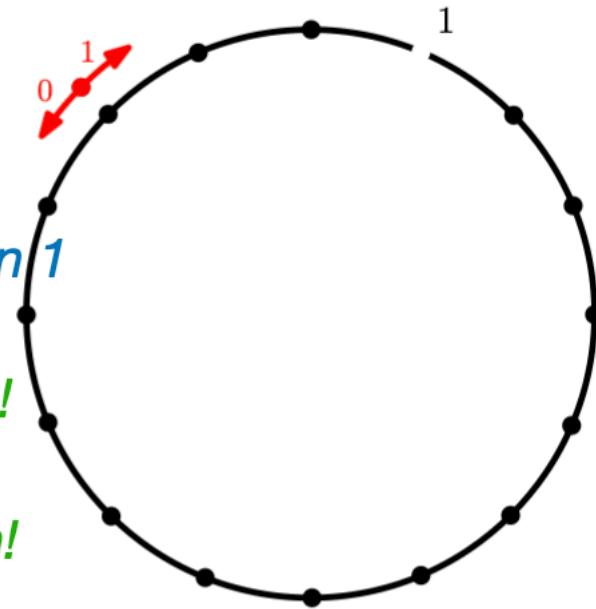
$p := |0\rangle;$ *position space = {0, ..., n-1}*

while $M[p] = no$ **do** *Terminal of loop: position 1*

$c := H[c];$ *Create a new coin in superposition!*

$c, p := S[c, p]$ *Random walk based on that coin!*

od



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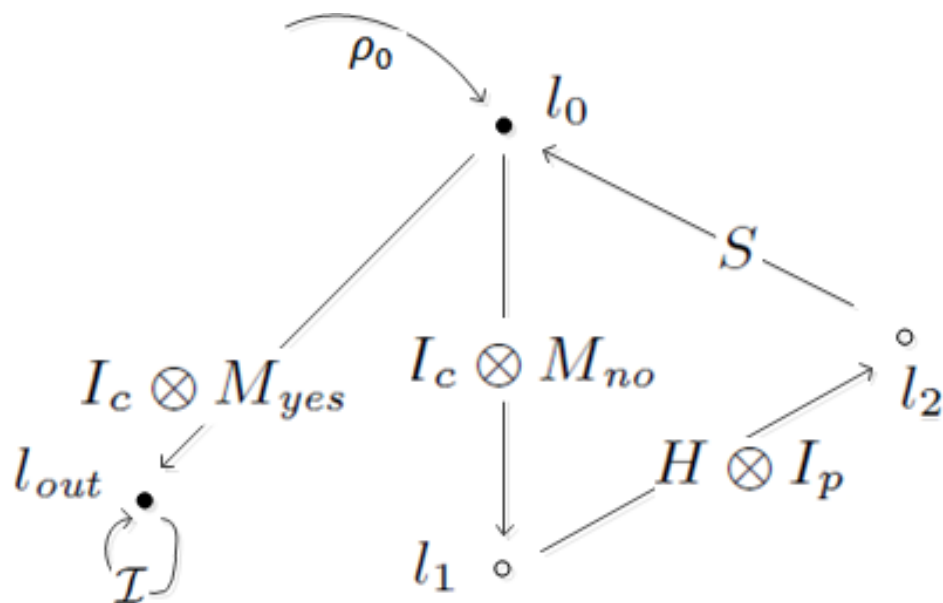
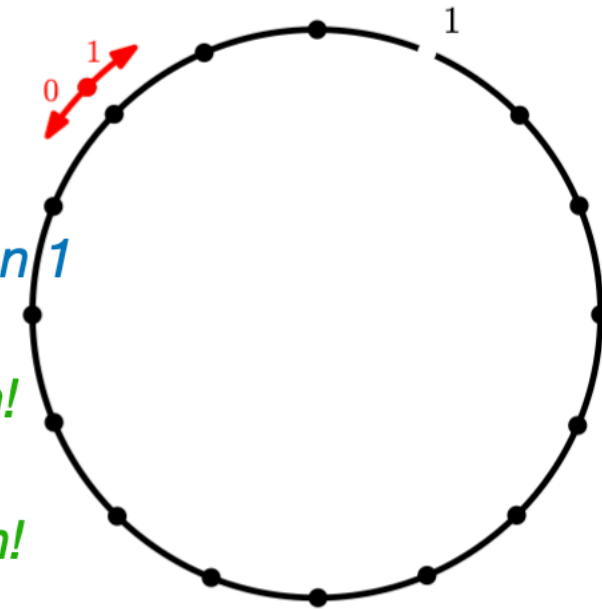
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Control - Flow - Graph

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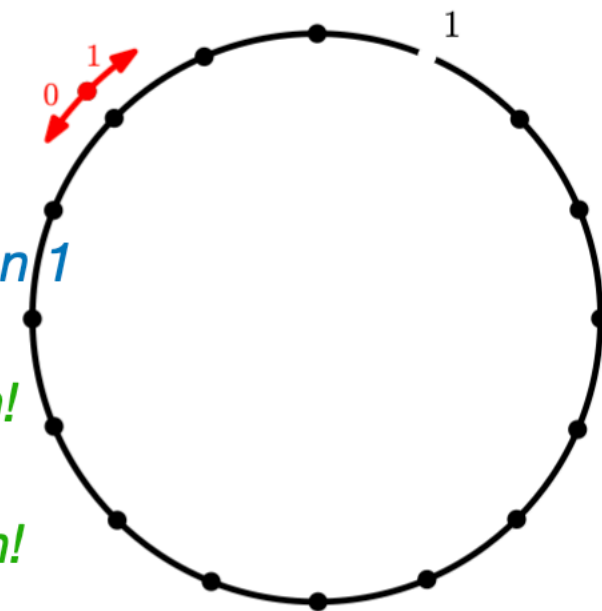
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Invariants

- ▶ A set Π of paths is *prime* if for each

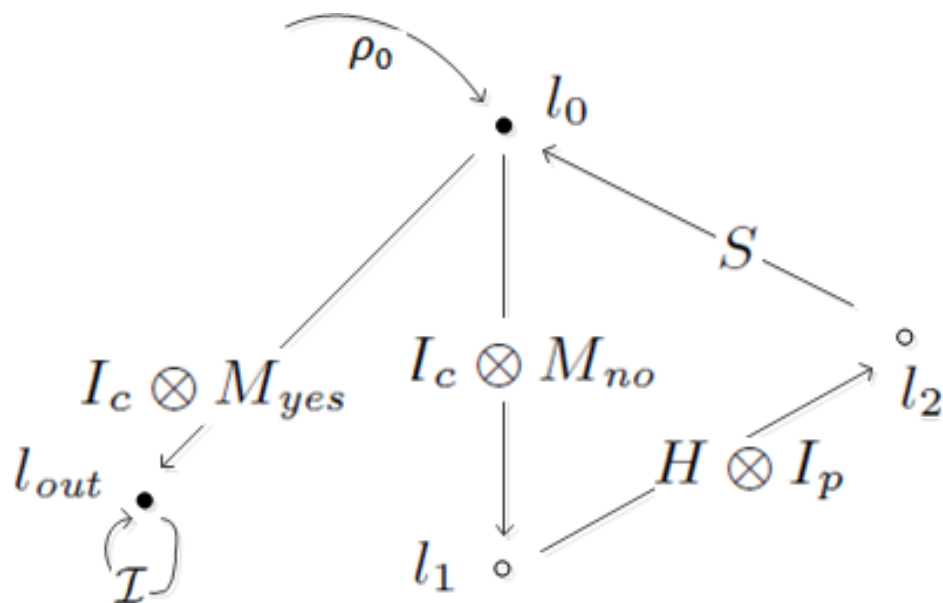
$$\pi = l_1 \xrightarrow{\mathcal{E}_1} \dots \xrightarrow{\mathcal{E}_{n-1}} l_n \in \Pi$$

its proper initial segments $l_1 \xrightarrow{\mathcal{E}_1} \dots \xrightarrow{\mathcal{E}_{k-1}} l_k \notin \Pi$ for all $k < n$.

- ▶ Let $\mathcal{G} = \langle \mathcal{H}, L, l_0, \rightarrow \rangle$, Θ a quantum predicate (initial condition), $l \in L$. An *invariant* at l is a quantum predicate O such that for any density operator ρ , any prime set Π of paths from l_0 to l :

$$tr(\Theta\rho) \leq 1 - tr(\mathcal{E}_\Pi(\rho)) + tr(O\mathcal{E}_\Pi(\rho))$$

where $\mathcal{E}_\Pi = \sum \{|\mathcal{E}_\pi : \pi \in \Pi|\}$.



Control - Flow - Graph

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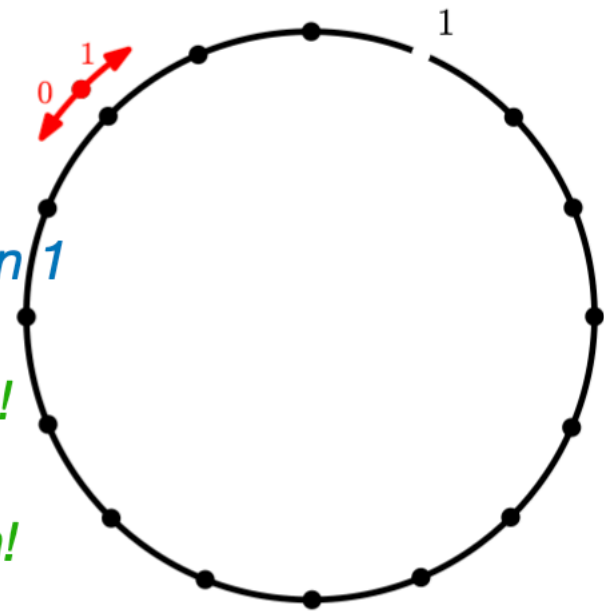
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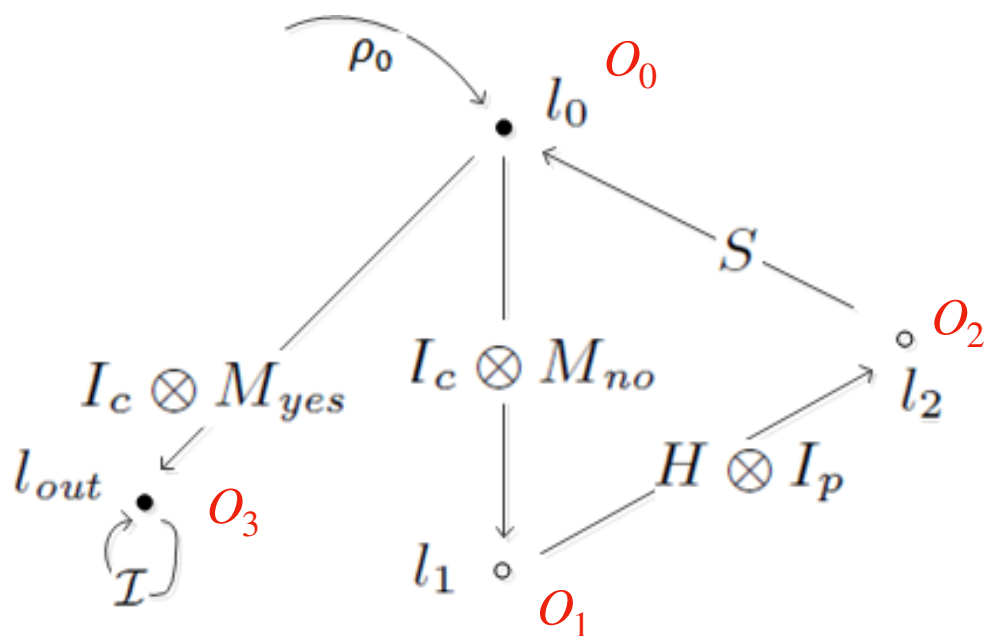
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Control - Flow - Graph

Finding Quantum Invariants

Theorem (Partial Correctness)

Let P be a quantum program. If O is an invariant at l_{out}^P in \mathcal{S}_P , then

$$\models_{par} \{\Theta\}P\{O\}$$

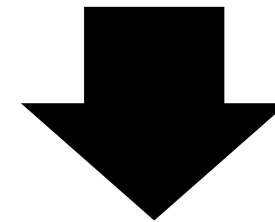
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Inductive Assertion Maps



Reducing **Global** Constraints
Into **Local** Ones

- ▶ Given $\mathcal{G} = \langle \mathcal{H}, L, l_0, \rightarrow \rangle$ with a cutset C and initial condition Θ .
- ▶ An *assertion map* is a mapping η from each cutpoint $l \in C$ to a quantum predicate $\eta(l)$.
- ▶ Π_l : the set of all basic paths from l to some cutpoint.
- ▶ l_π : the last location in a path π .
- ▶ An assertion map η is *inductive* if:
 - ▶ **Initiation**: for any density operator ρ :

$$\text{tr}(\Theta\rho) \leq 1 - \text{tr}(\mathcal{E}_{\Pi_{l_0}}(\rho)) + \sum_{\pi \in \Pi_{l_0}} \text{tr}(\eta(l_\pi)\mathcal{E}_\pi(\rho));$$

- ▶ **Consecution**: for any density operator ρ , each cutpoint $l \in C$:

$$\text{tr}(\eta(l)\rho) \leq 1 - \text{tr}(\mathcal{E}_{\Pi_l}(\rho)) + \sum_{\pi \in \Pi_l} \text{tr}(\eta(l_\pi)\mathcal{E}_\pi(\rho)).$$

Finding Quantum Invariants

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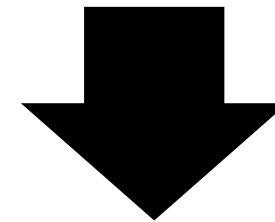
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Reducing **Global** Constraints
Into **Local** Ones

Reduce to a SDP (Semi-Definite Programming) Problem

- ▶ Assume $C = \{l_0, l_1, \dots, l_m\}$.
- ▶ Write $O_i = \eta(l_i)$ for $i = 0, 1, \dots, m$.
- ▶ $\mathcal{E}_{ij}^* = \sum\{|\mathcal{E}_\pi^* : \text{basic path } l_i \xrightarrow{\pi} l_j\}$ for $i, j = 0, 1, \dots, m$.

SDPs for Quantum Invariants

Theorem

Invariant Generation Problem is equivalent to find complex matrices O_0, O_1, \dots, O_m satisfying the constraints:

$$0 \sqsubseteq \sum_j \mathcal{E}_{0j}^*(O_j) + A,$$

$$0 \sqsubseteq \sum_{j \neq i} \mathcal{E}_{ij}^*(O_j) + (\mathcal{E}_{ii}^* - \mathcal{I})(O_i) + A_i \quad (i = 0, 1, \dots, m),$$

$$0 \sqsubseteq O_i \sqsubseteq I \quad (i = 0, 1, \dots, m),$$

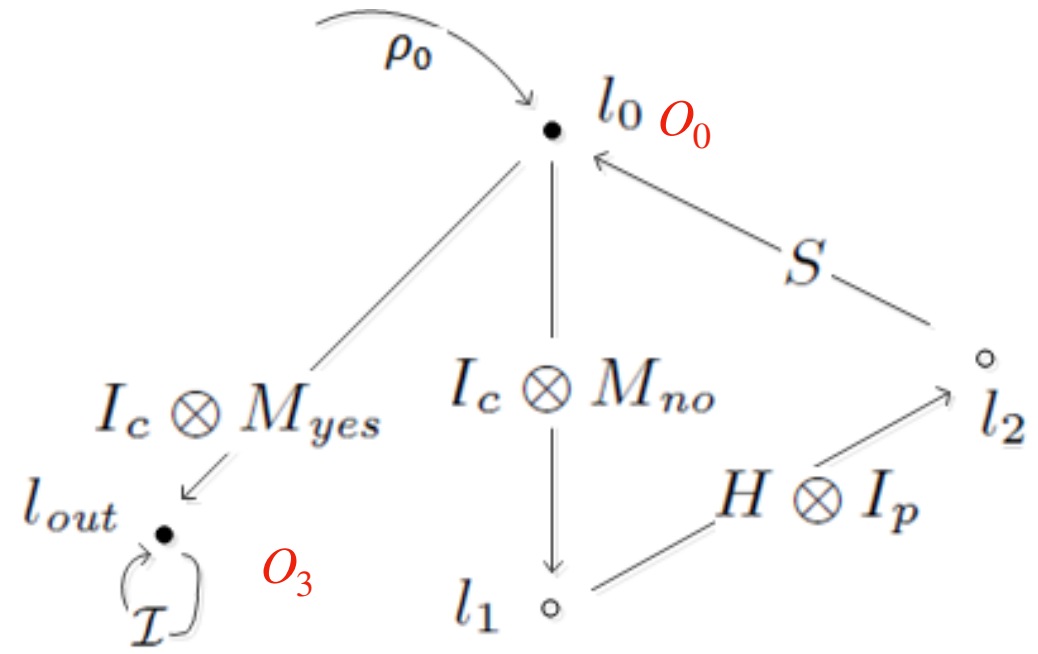
where:

$$\begin{cases} A = I - \sum_j \mathcal{E}_{0j}^*(I) - \Theta, \\ A_i = I - \sum_j \mathcal{E}_{ij}^*(I) \quad (i = 0, 1, \dots, m). \end{cases}$$

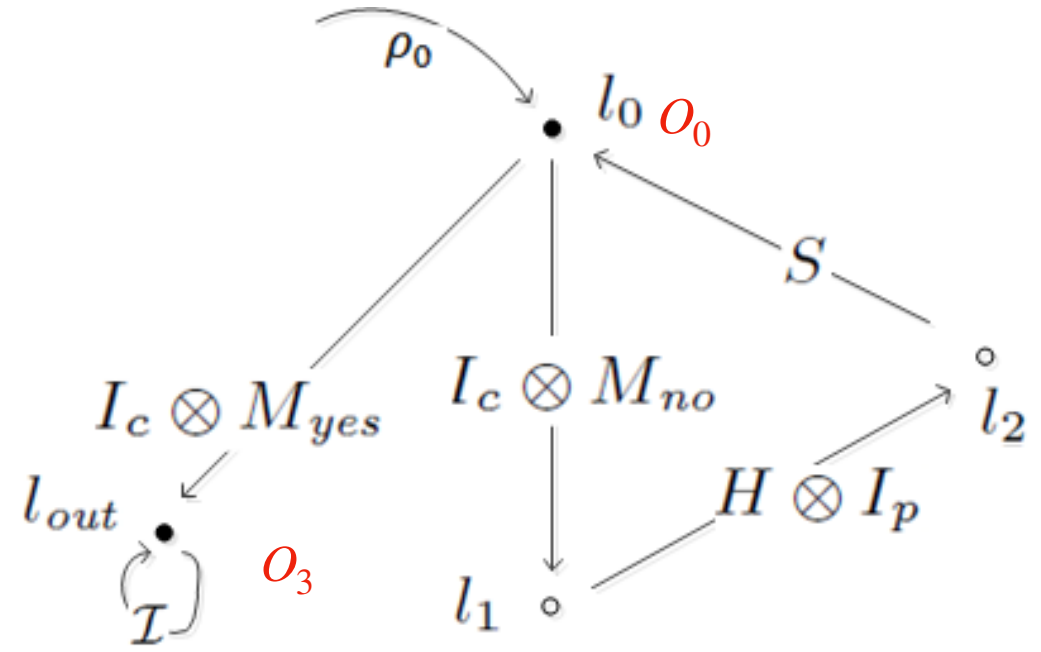
```

QW  $\equiv$   $c := |L\rangle;$ 
       $p := |0\rangle;$ 
      while  $M[p] = no$  do
         $c := H[c];$ 
         $c, p := S[c, p]$ 
      od

```



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Invariant SDPs for Quantum 1-D Loop Walk

Choose cut-set $C = \{l_0, l_3\}$ with $l_3 = l_{out}$. $\Theta = I$. Invariants O_0 and O_3 satisfy the following constraints:

$$0 \sqsubseteq \mathcal{E}_{00}^*(O_0) + \mathcal{E}_{03}^*(O_3) - \Theta, \quad (1)$$

$$0 \sqsubseteq (\mathcal{E}_{00}^* - \mathcal{I})(O_0) + \mathcal{E}_{03}^*(O_3), \quad (2)$$

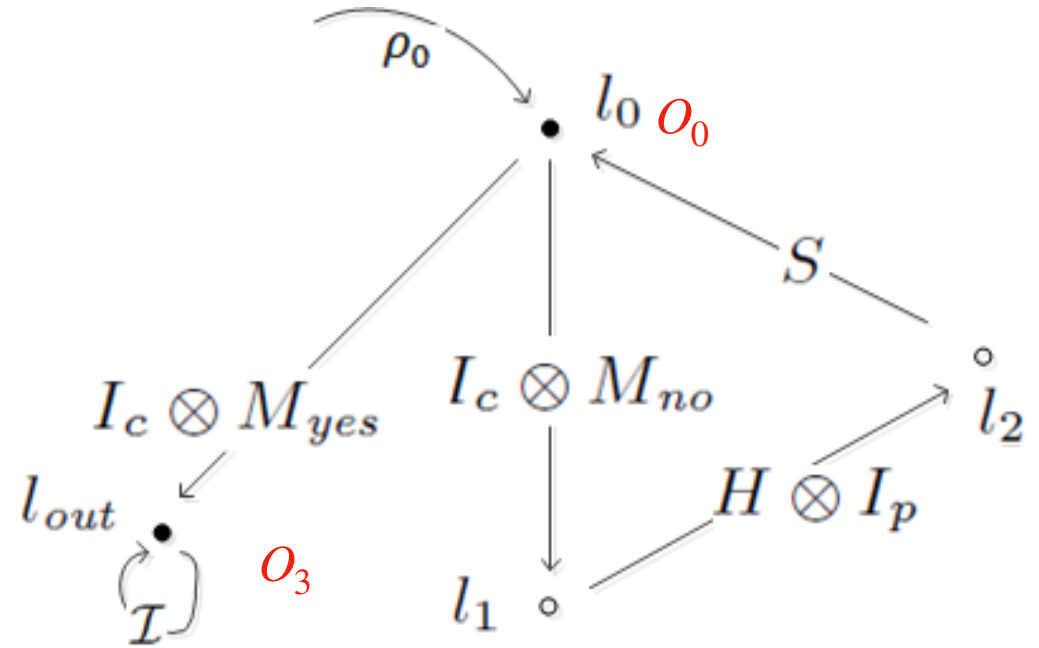
$$0 \sqsubseteq (\mathcal{E}_{33}^* - \mathcal{I})(O_3) - (I - \mathcal{E}_{33}^*(I)), \quad (3)$$

$$0 \sqsubseteq O_0, O_3 \sqsubseteq I \quad (4)$$

$$\mathbb{E}_{00} = E_{00} \circ E_{00}^\dagger, \mathbb{E}_{03} = E_{03} \circ E_{03}^\dagger, \mathbb{E}_{33} = \mathcal{I},$$

$$E_{00} = S(H \otimes I_p)(I_c \otimes M_{no}), E_{03} = I_c \otimes M_{yes}, \text{ and } I_c, I_p \text{ identities.}$$

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 $p := |0\rangle;$
while $M[p] = no$ **do**
 $c := H[c];$
 $c, p := S[c, p]$
od



Invariant SDPs for Quantum 1-D Loop Walk

Choose cut-set $C = \{l_0, l_3\}$ with $l_3 = l_{out}$. $\Theta = I$. Invariants O_0 and O_3 satisfy the following constraints:

$$0 \sqsubseteq \mathcal{E}_{00}^*(O_0) + \mathcal{E}_{03}^*(O_3) - \Theta, \quad (1)$$

$$0 \sqsubseteq (\mathcal{E}_{00}^* - \mathcal{I})(O_0) + \mathcal{E}_{03}^*(O_3), \quad (2)$$

$$0 \sqsubseteq (\mathcal{E}_{33}^* - \mathcal{I})(O_3) - (I - \mathcal{E}_{33}^*(I)), \quad (3)$$

$$0 \sqsubseteq O_0, O_3 \sqsubseteq I \quad (4)$$

$\mathbb{E}_{00} = E_{00} \circ E_{00}^\dagger, \mathbb{E}_{03} = E_{03} \circ E_{03}^\dagger, \mathbb{E}_{33} = \mathcal{I},$
 $E_{00} = S(H \otimes I_p)(I_c \otimes M_{no}), E_{03} = I_c \otimes M_{yes},$ and I_c, I_p identities.

Using SDP Solver

$$O_3 = I_c \otimes |1\rangle\langle 1|$$



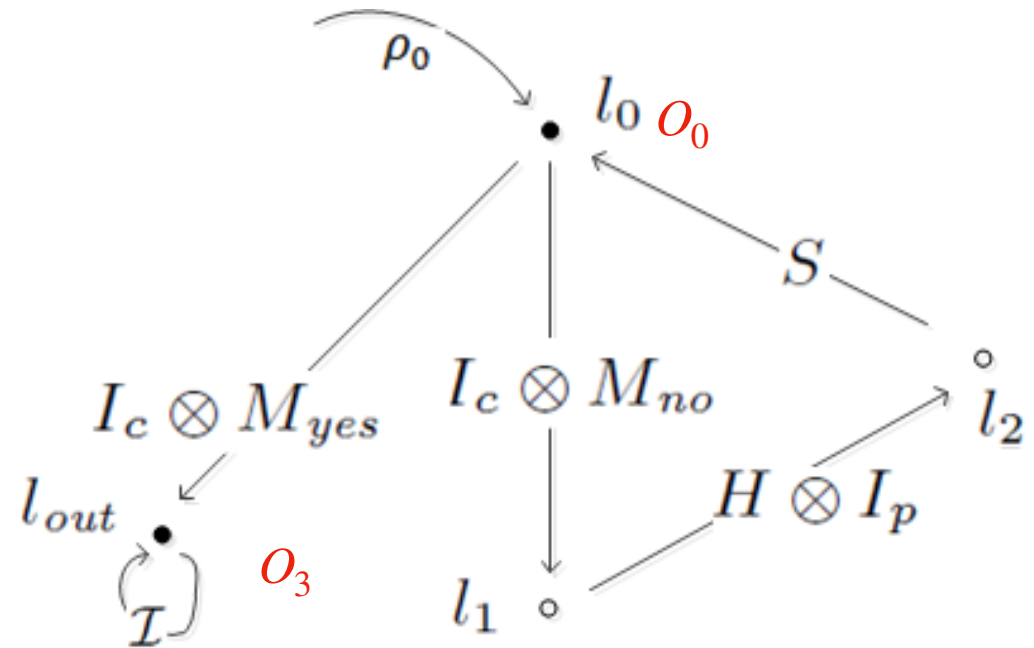
$$\text{tr}(O_3 \rho_{out}) \geq \text{tr}(\Theta \rho_{in}) = 1.$$

Namely, QW always terminates at the position $|1\rangle$ regardless of the input state ρ_0 .


```

QW  $\equiv$   $c := |L\rangle;$ 
       $p := |0\rangle;$ 
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Drawback: all these matrices are *exponentially* large.

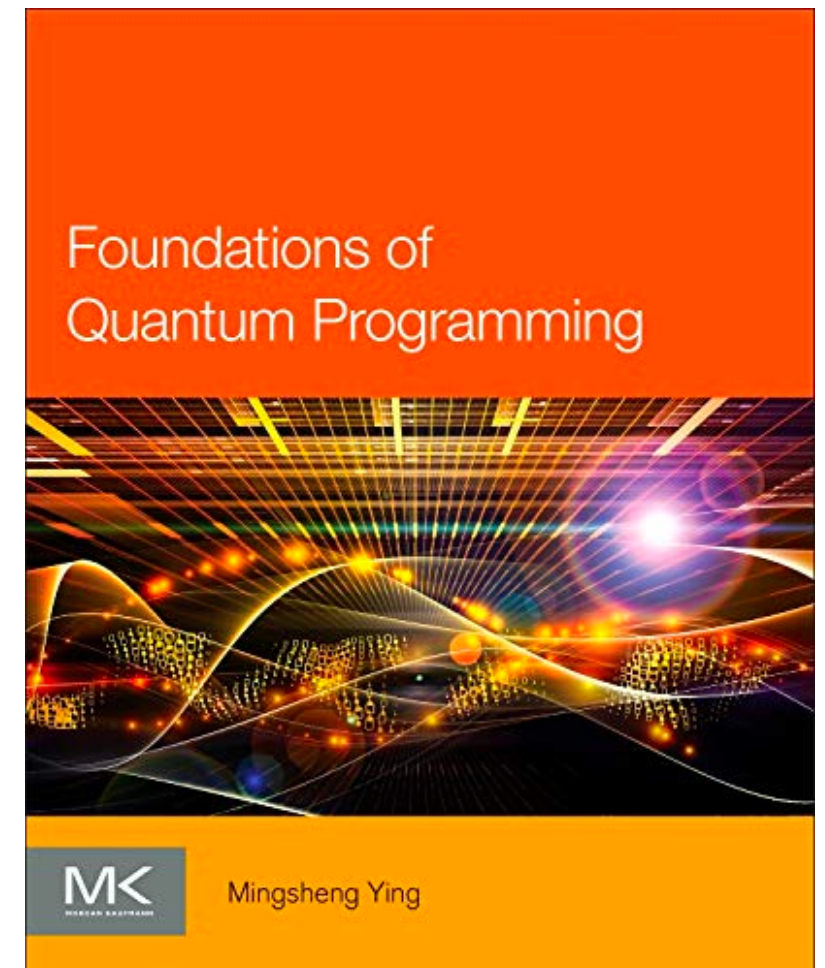
Further Readings: Thank You! Q & A

Applications

- ▶ Quantum walk on an n -circle.
- ▶ Quantum Metropolis sampling on n -qubits.
- ▶ Repeat-Until-Success.
- ▶ Quantum Search.
- ▶ Quantum Bernoulli Factory.
- ▶ Recursively written Quantum Fourier Transformation.

References

- ▶ M. S. Ying. Floyd-Hoare Logic for Quantum Programs, *TOPLAS*, 2011.
- ▶ M. S. Ying. Foundations of Quantum Programming, Morgan Kaufmann, 2016.
- ▶ M. S. Ying, S. G. Ying and X. Wu, Invariants of quantum programs: characterizations and generation, *POPL* 2017.
- ▶ Y. Li, and M. S. Ying. Algorithmic Analysis of Termination Problems for Quantum Programs, *POPL*, 2018.
- ▶ L. Zhou, N. Yu, and M. S. Ying. An Applied Quantum Hoare Logic, *PLDI*, 2019.
- ▶ S. H. Hung, Y. Peng, X. Wang, S. Zhu, and X. Wu. On the Theory and Practice of Invariant-based Verification of Quantum Programs, manuscript, 2020.



Outline

(1) Introduction to Quantum Computing and Potential Roles of Programming Languages (25 min + 5 Q & A)

(2) A Mini-Course of Quantum Hoare Logic on Quantum While Language (30 min + 5 Q & A)

(3) Discussion on existing and potential Programming Language research opportunities (20 min + 5 Q & A)

Reference: tutorial slides and some references are available at https://www.cs.umd.edu/~xwu/mini_lib.html



Summary from Part I

Satisfactory

Quantum PLs

Software Tool-chain

Architecture



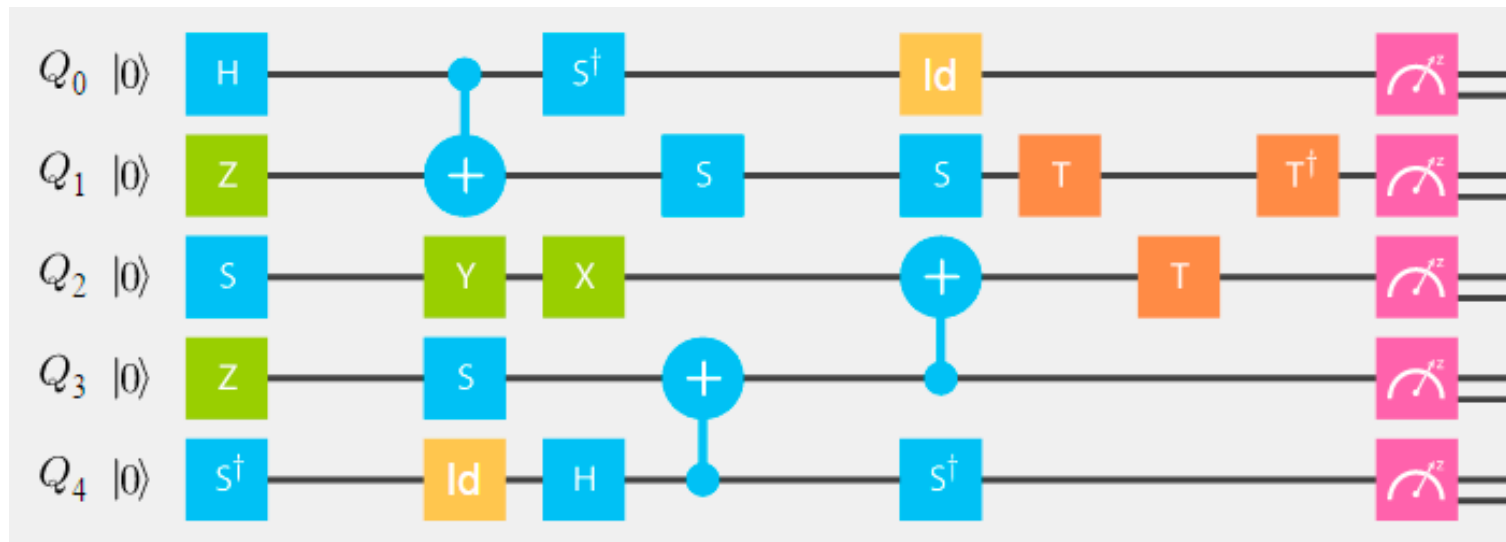
From the implementation perspective

Highlight some concrete problems! (Not a survey)



Design of Quantum Programming Languages

- Gap:** (1) **too-low-level-abstraction**: very hard to write **complex** programs
(2) **lack of scalable verification**: very hard to write **correct** programs

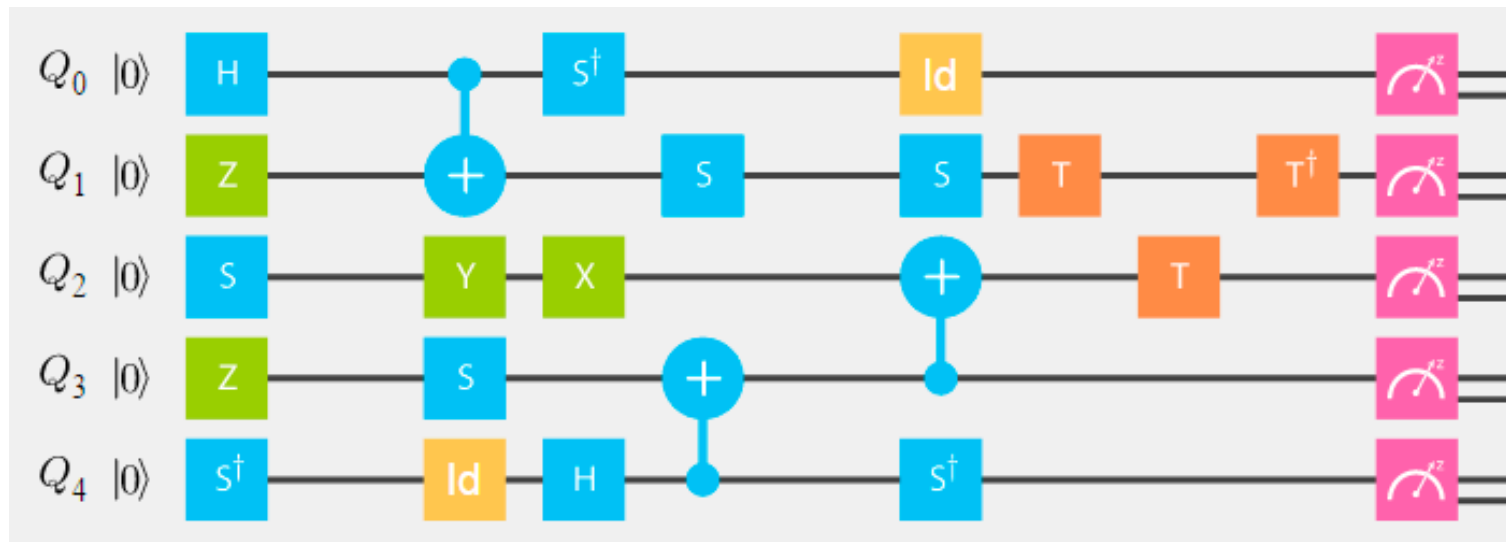


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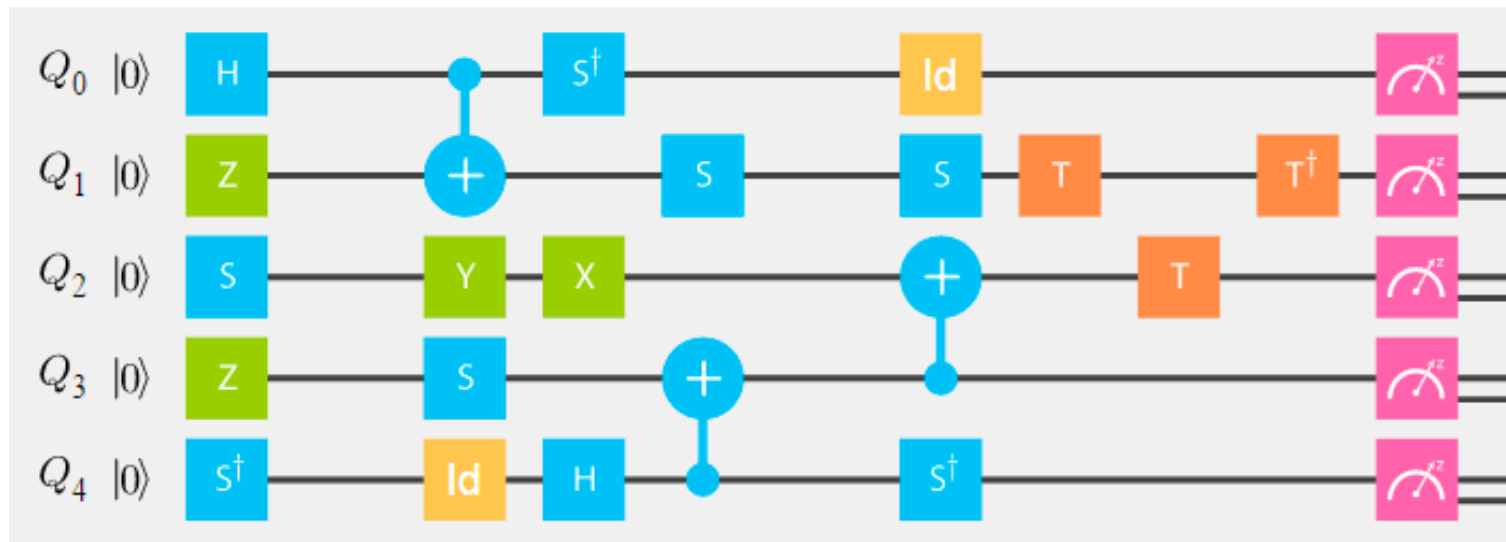
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Ancilla: keep track of the scope of ancilla qubits (Quipper)

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Consider **quantum stack** ~ truly quantum recursion ~ quantum apps

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Develop Q Hoare logic for *parallel, concurrent, distributed* programs.

Some preliminary results exist. Essential difficulty exists due to quantum correlations.

Debugging Quantum Programs for NISQ

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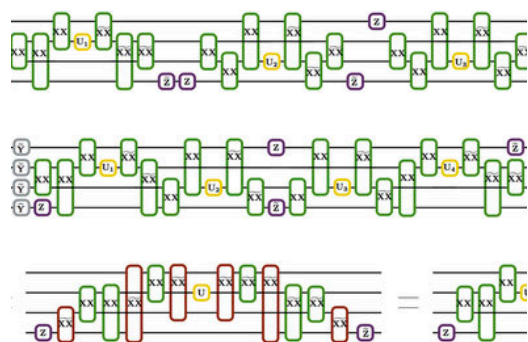
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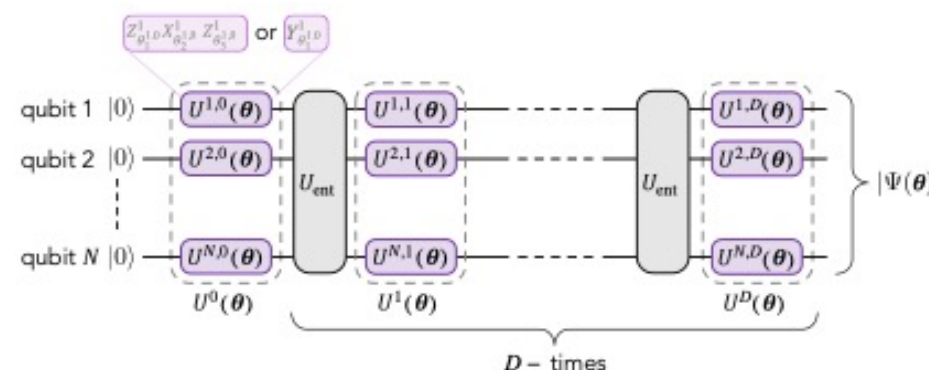
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Likely to be application-specific



Quantum Simulation



Variational Quantum Methods

Compilation of Quantum Application: Analog Machines

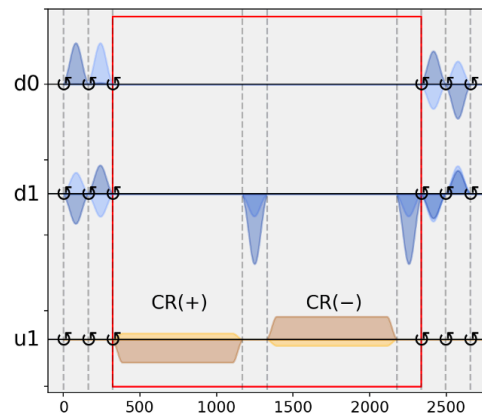
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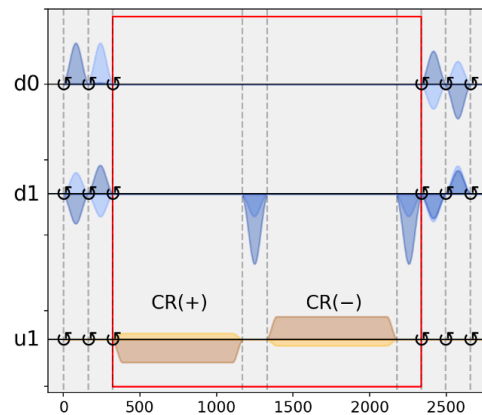


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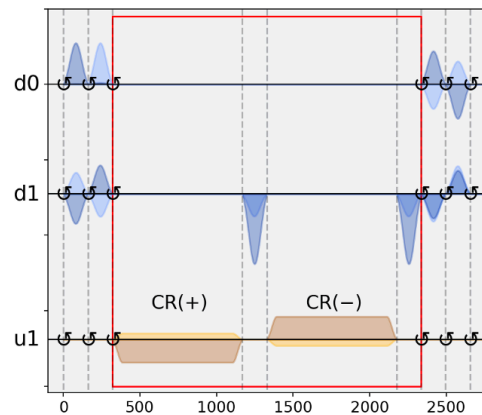
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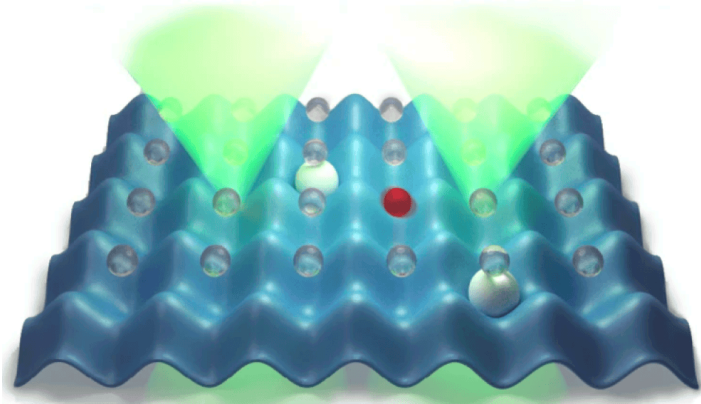


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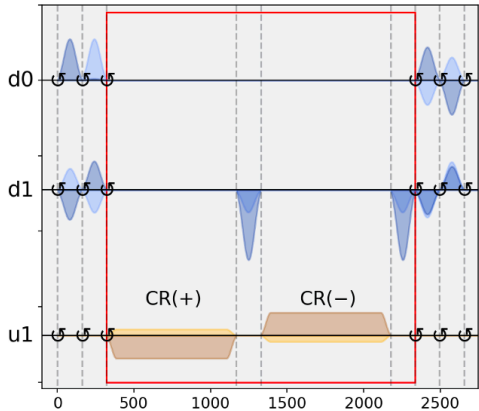
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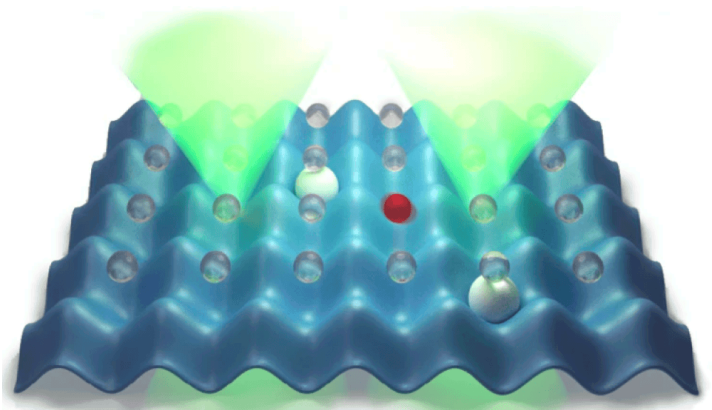
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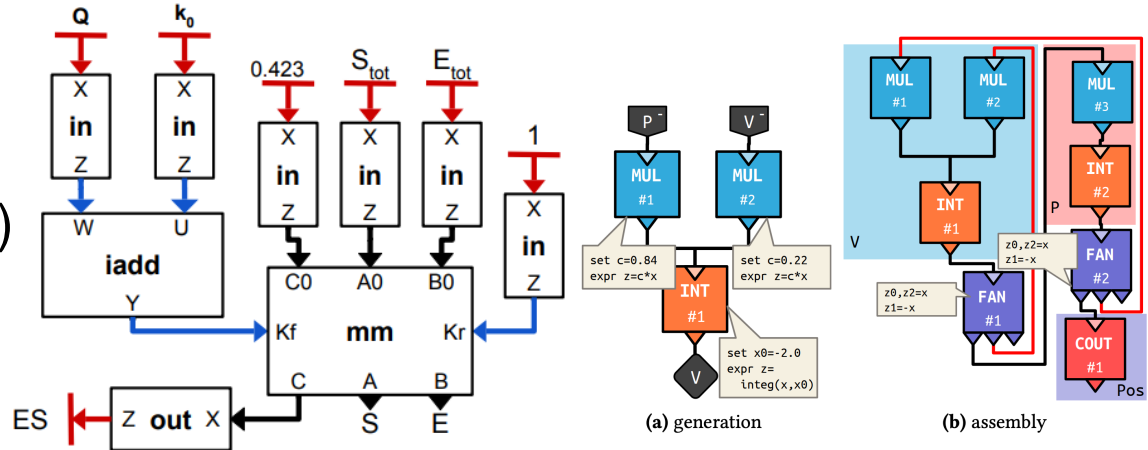


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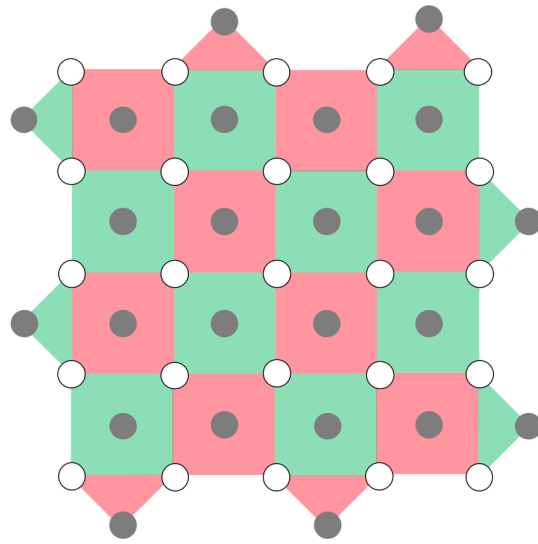
Classical Examples:

- Achour et al. (PLDI16)
- Achour & Rinard (ASPLOS 20)



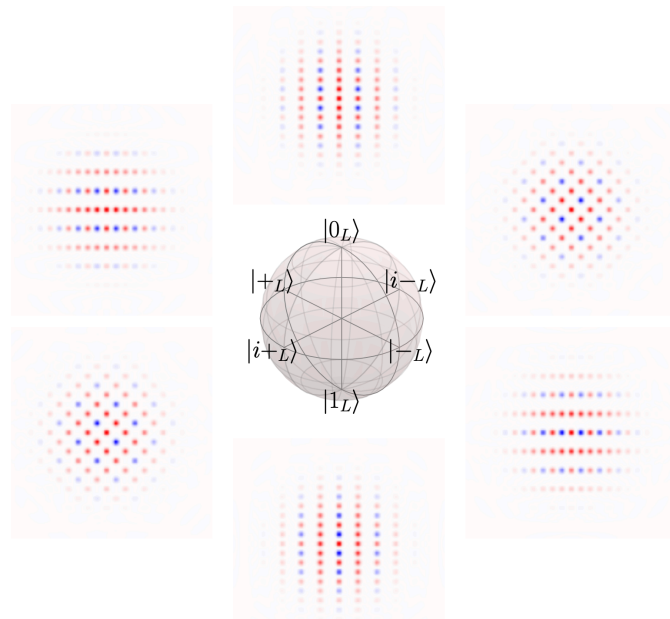
ERROR

Nature



Quantum Error Correction
Fight
Quantum Decoherence

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Approximate Computing & Quantum Computing

- General-purpose fault-tolerant quantum computers are *impractical* in the near term.
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- Automatic error-resource-optimization on a per-program basis!

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 - *vision, machine learning; also with guarantees for critical data*

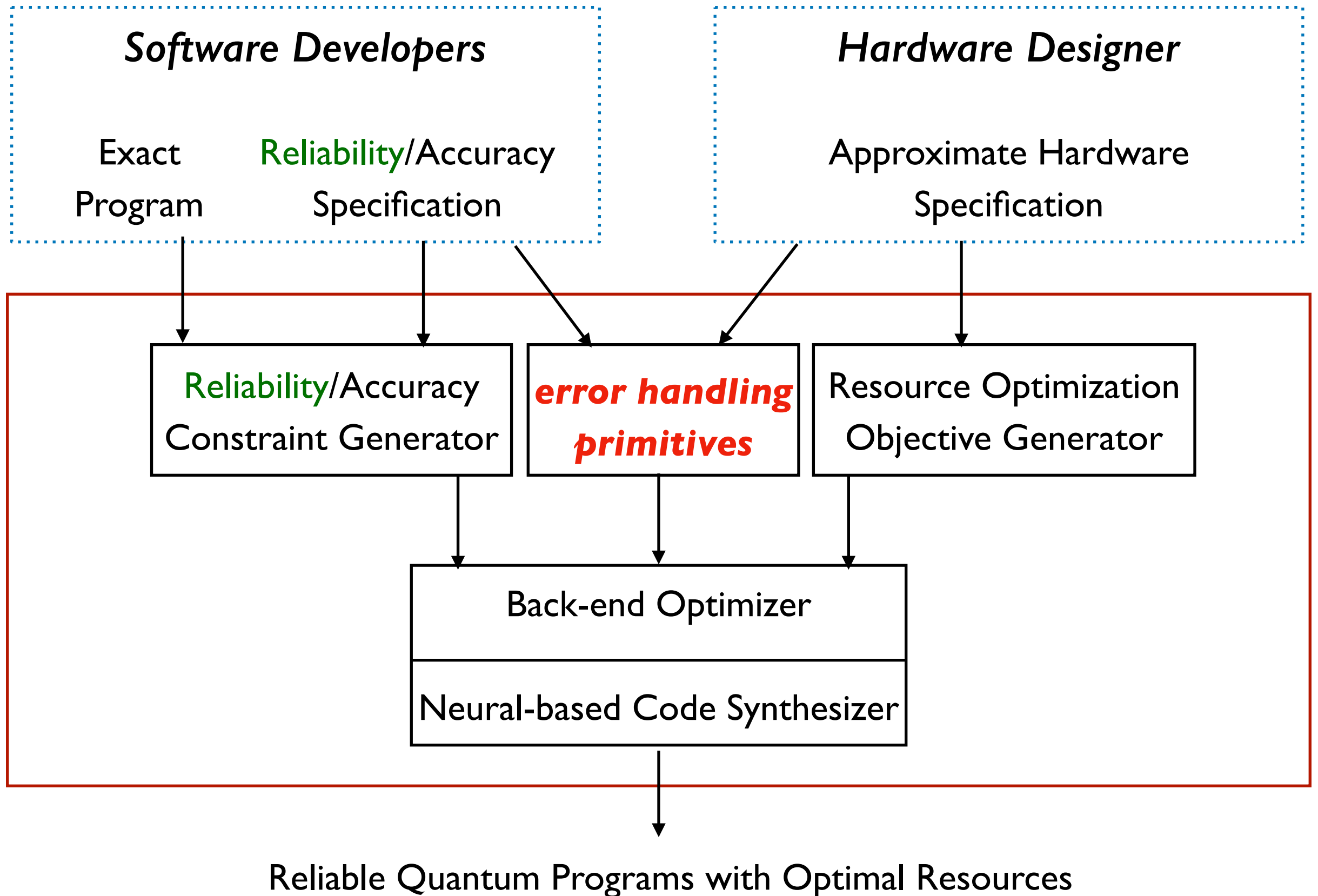
Methodology

- Elevate the handling of errors to the level of programming language.
- Reason *reliability/accuracy* of quantum programs via *static* analysis.
- Conduct *resource optimization* via *code synthesis* of quantum programs.

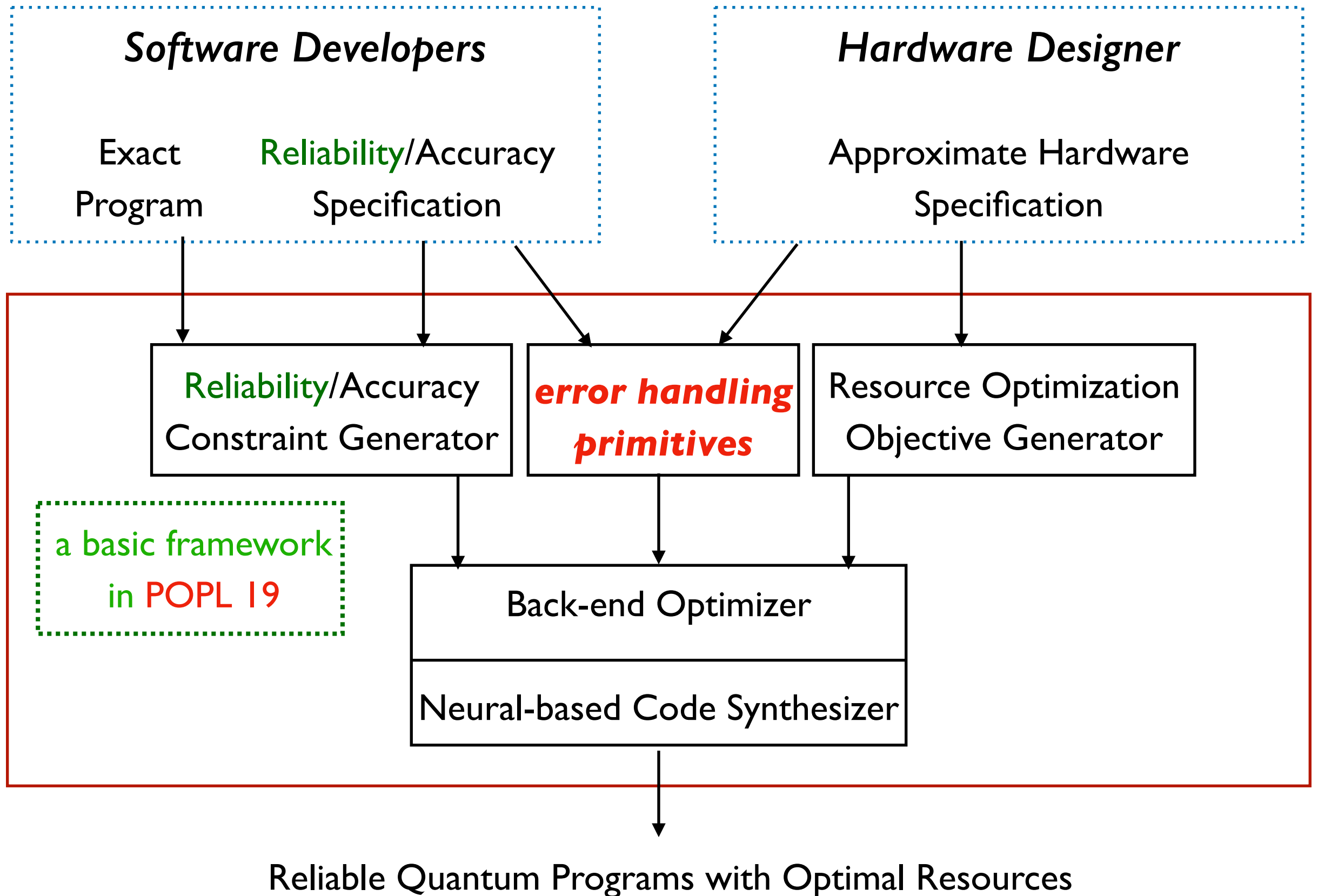
An important classical tool: *approximate computing* !

- Return possibly inaccurate/approximate results!
 - *unreliable hardware*
 - *limited computational resource*
- **Good** when *approximate results* are sufficient for applications!
 - *vision, machine learning; also with guarantees for critical data*
- Various techniques developed in classical PL literature.

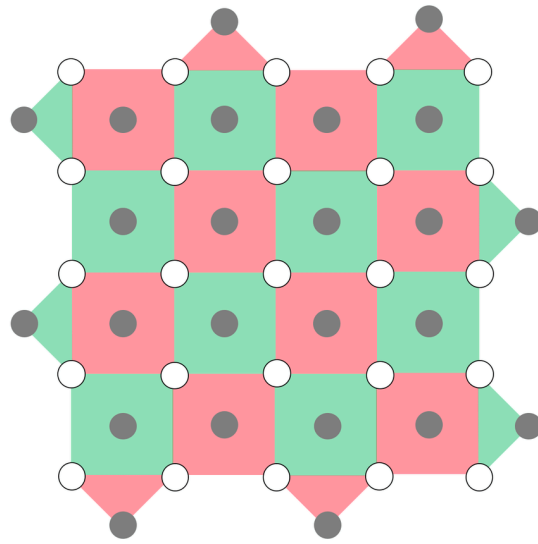
Overview



Overview

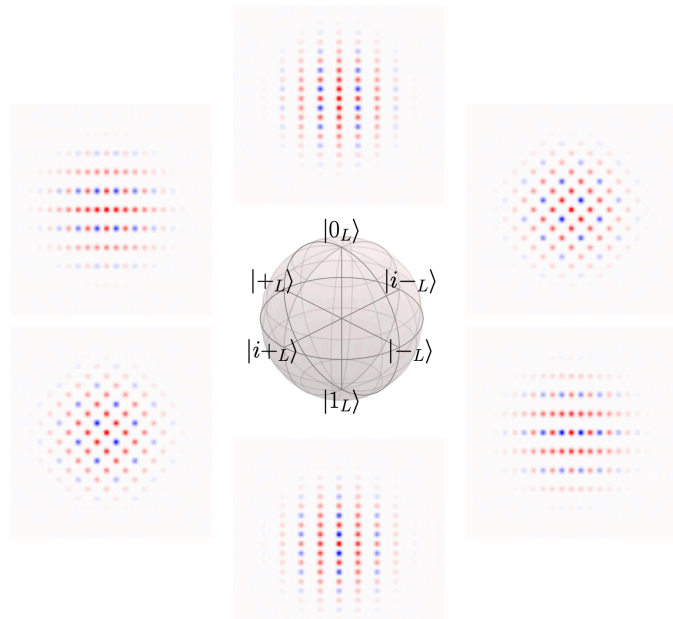


Nature

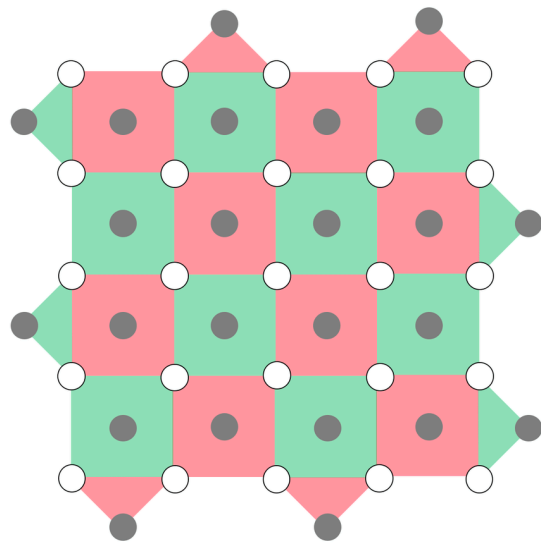


Quantum Error Correction
Fight
Quantum Decoherence

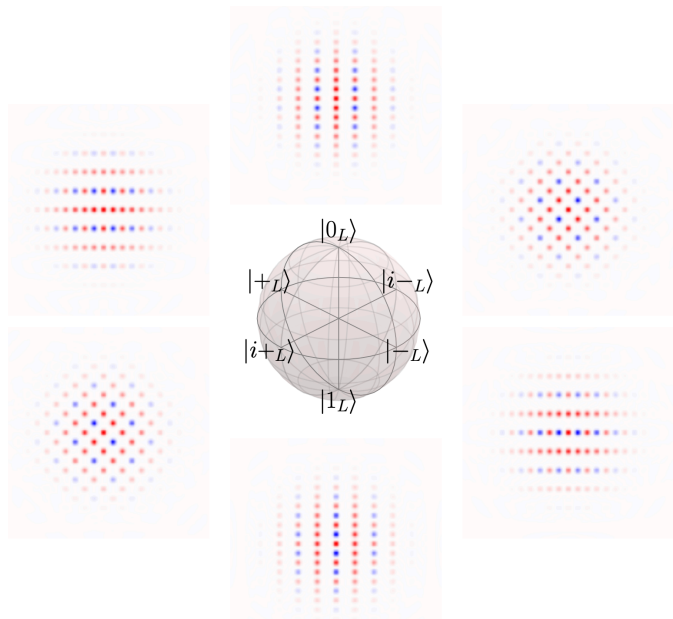
ERROR



Nature

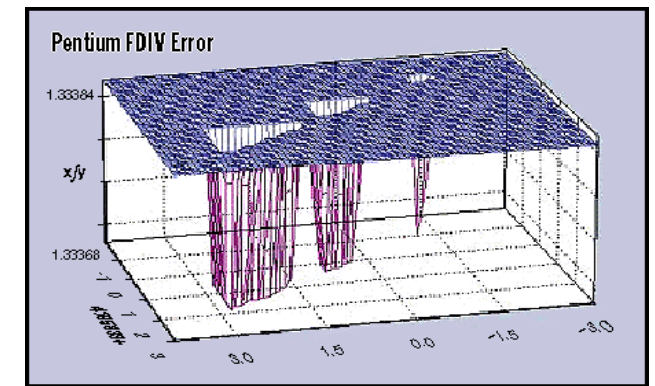


Quantum Error Correction
Fight
Quantum Decoherence



ERROR

Human

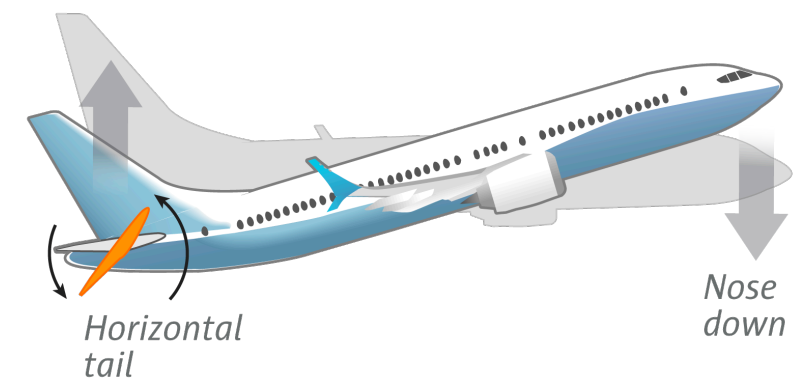


Intel Pentium FPU error



Ariane 5

MCAS safety system engages



Human Errors in Quantum Software Engineering

Being careful cannot solve the human error problem in either classical or quantum.

Quantum case : Significantly More **CHALLENGING** than Classical

- standard software assurance techniques, e.g., black-box / unit test, expensive in q.
- quantum mechanics prohibits certain testing, e.g., assertions

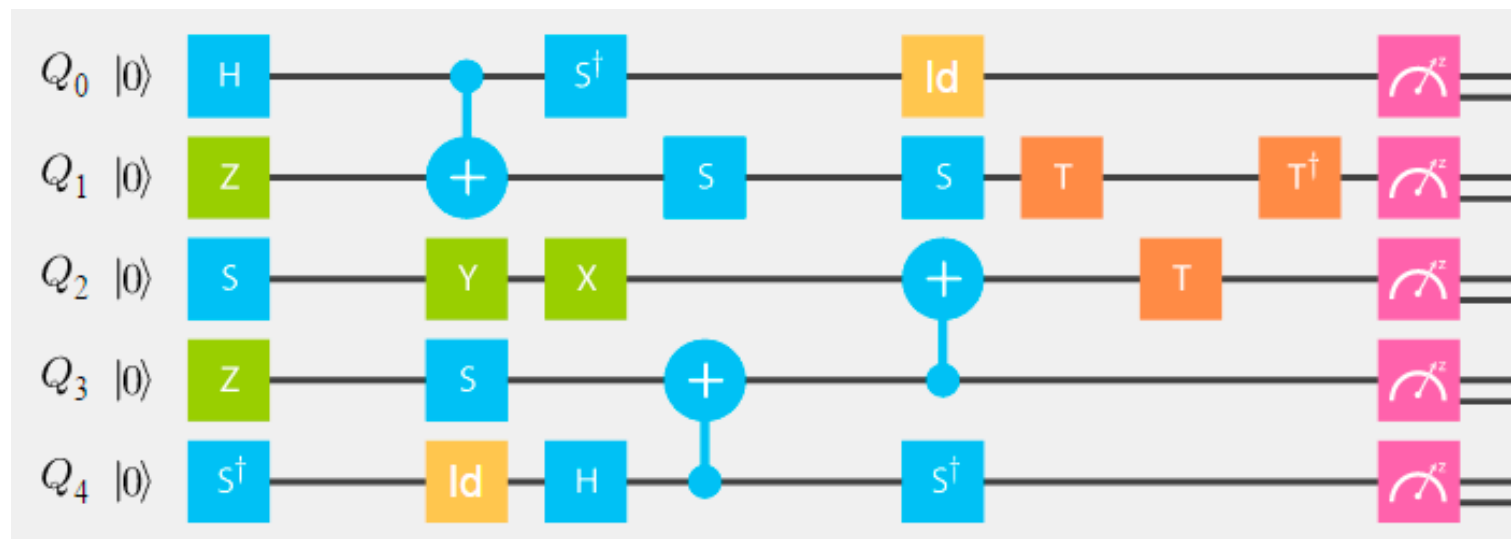
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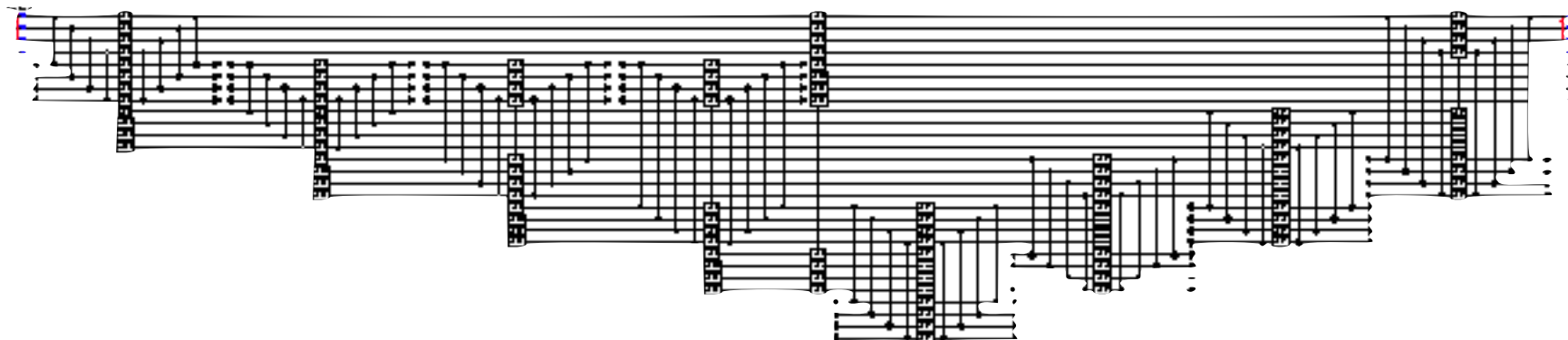
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Reality: testing in quantum today



confirming the circuit by observation.... not scalable...



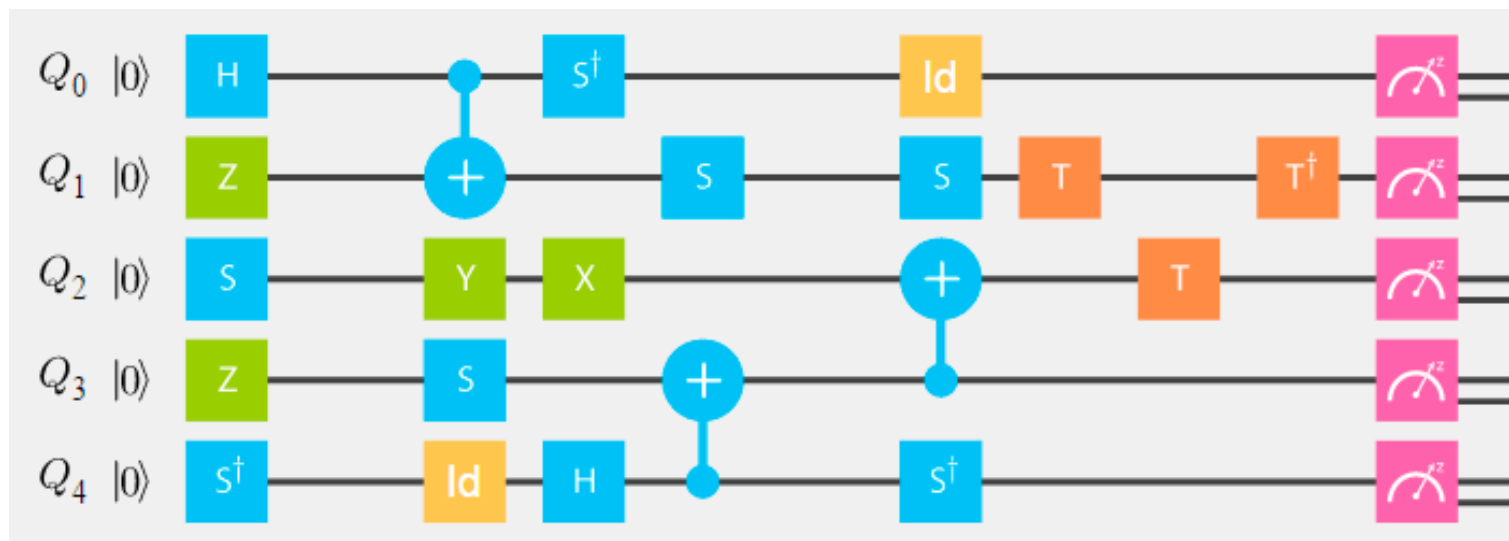
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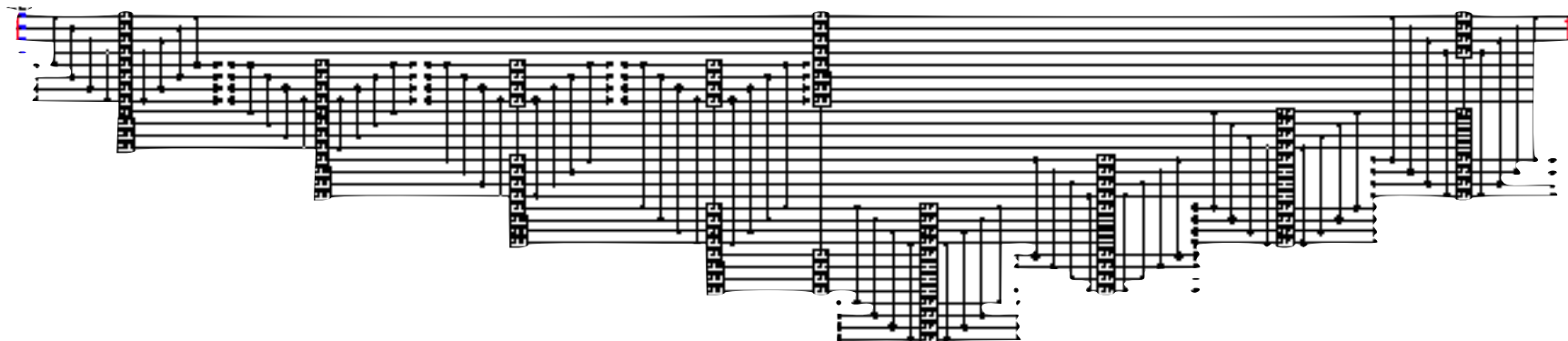


QISKIT Compiler **ERRORS**

Much **HARDER** to detect!

Serious Consequences!

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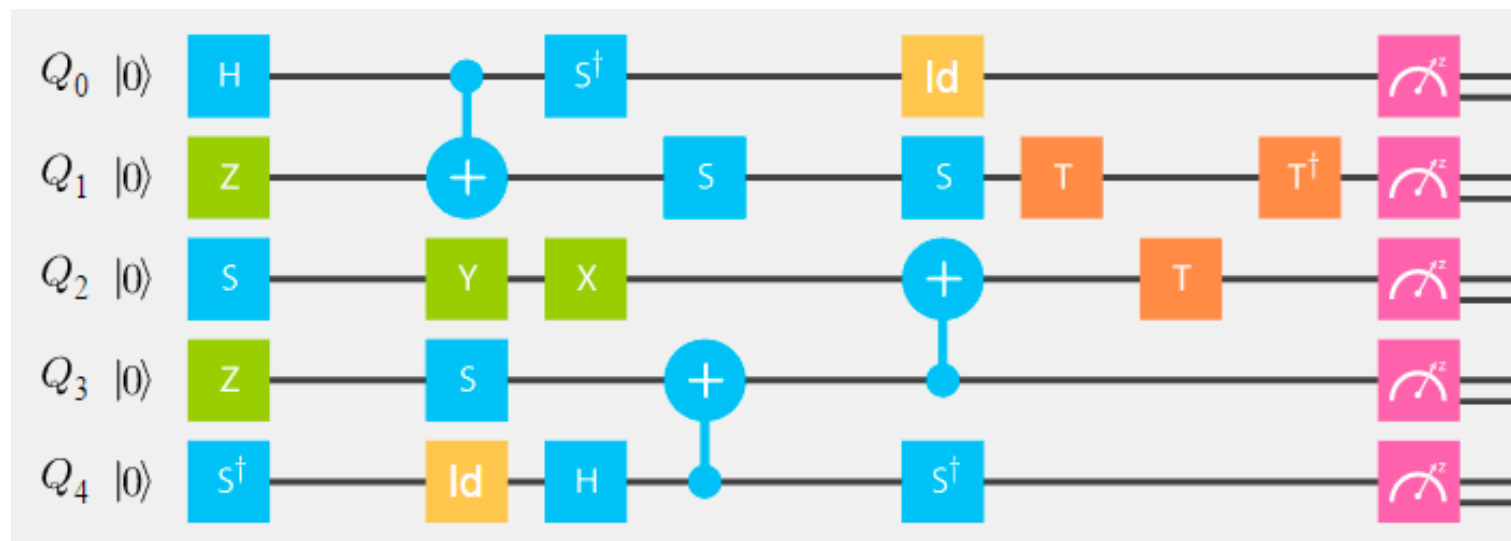
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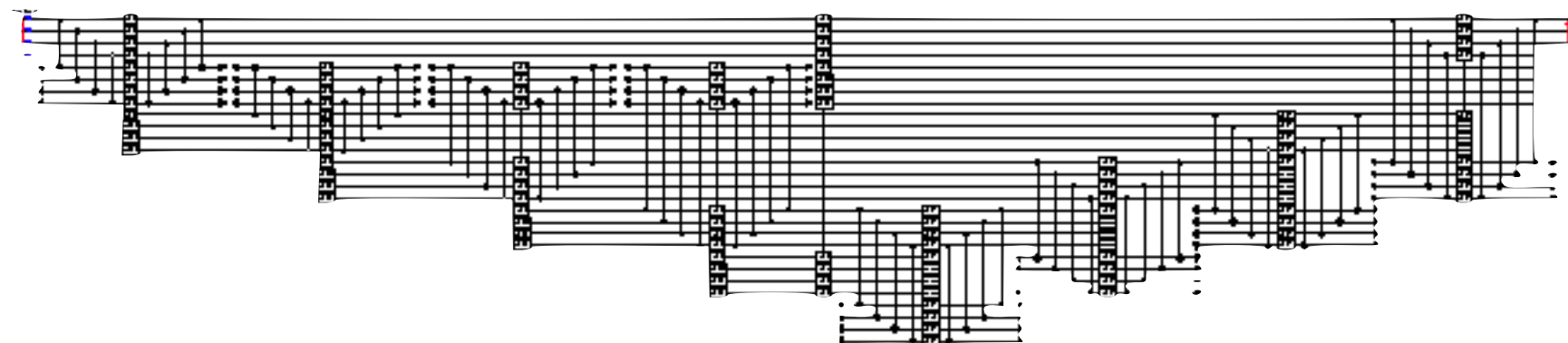
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confirming the circuit by observation.... not scalable...



Similar Concerns
in classical !

More **SERIOUS**
in quantum !

Certified software: a solution to validation of q. software

The Verifying Compiler: A Grand Challenge for Computing Research

TONY HOARE

Microsoft Research Ltd., Cambridge, UK

Journal of the ACM, Vol 50, 2003

Certified software: a solution to validation of q. software

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CompCert: a certified “GCC”, bug-free

Certified software: a solution to validation of q. software

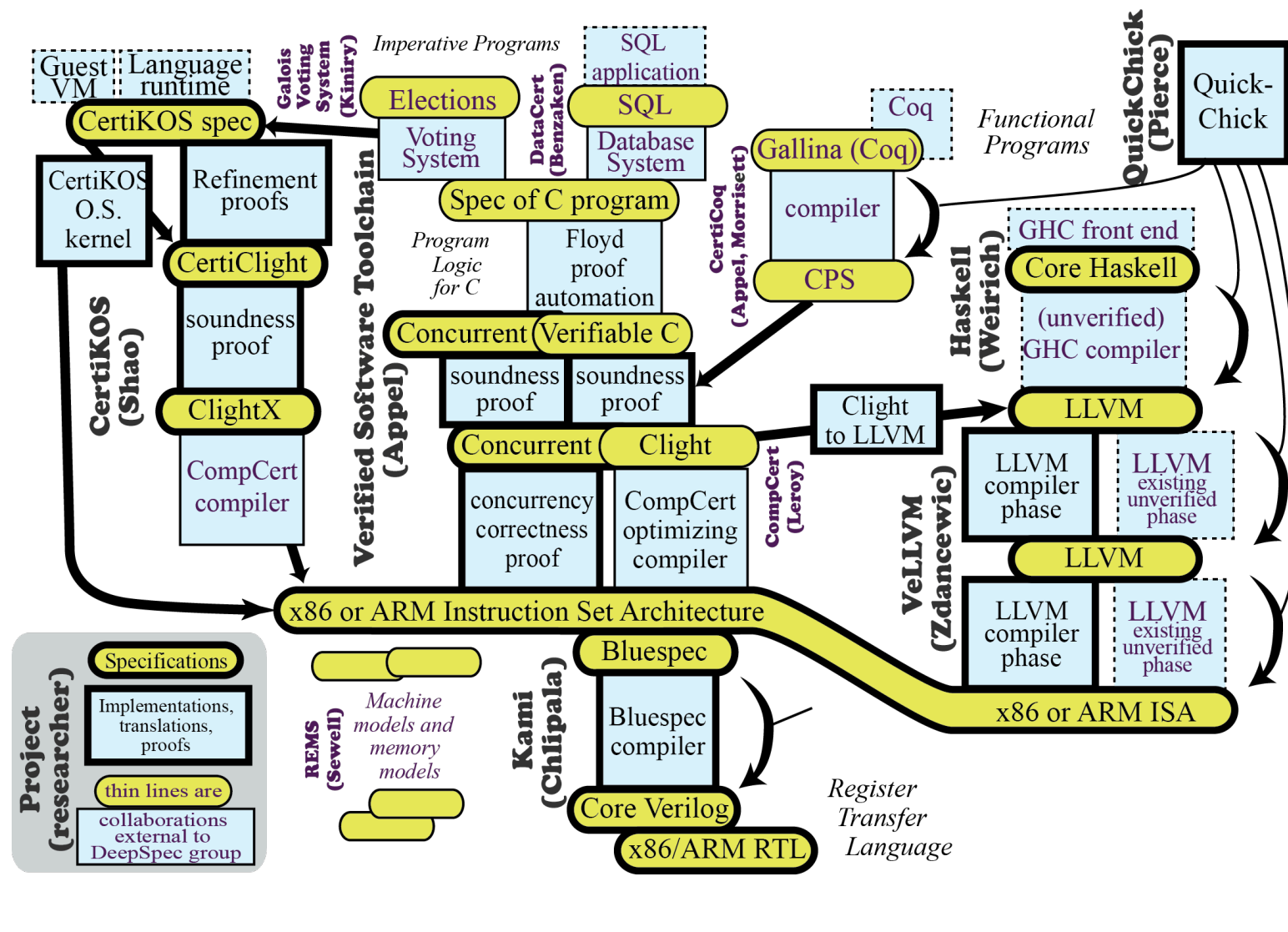
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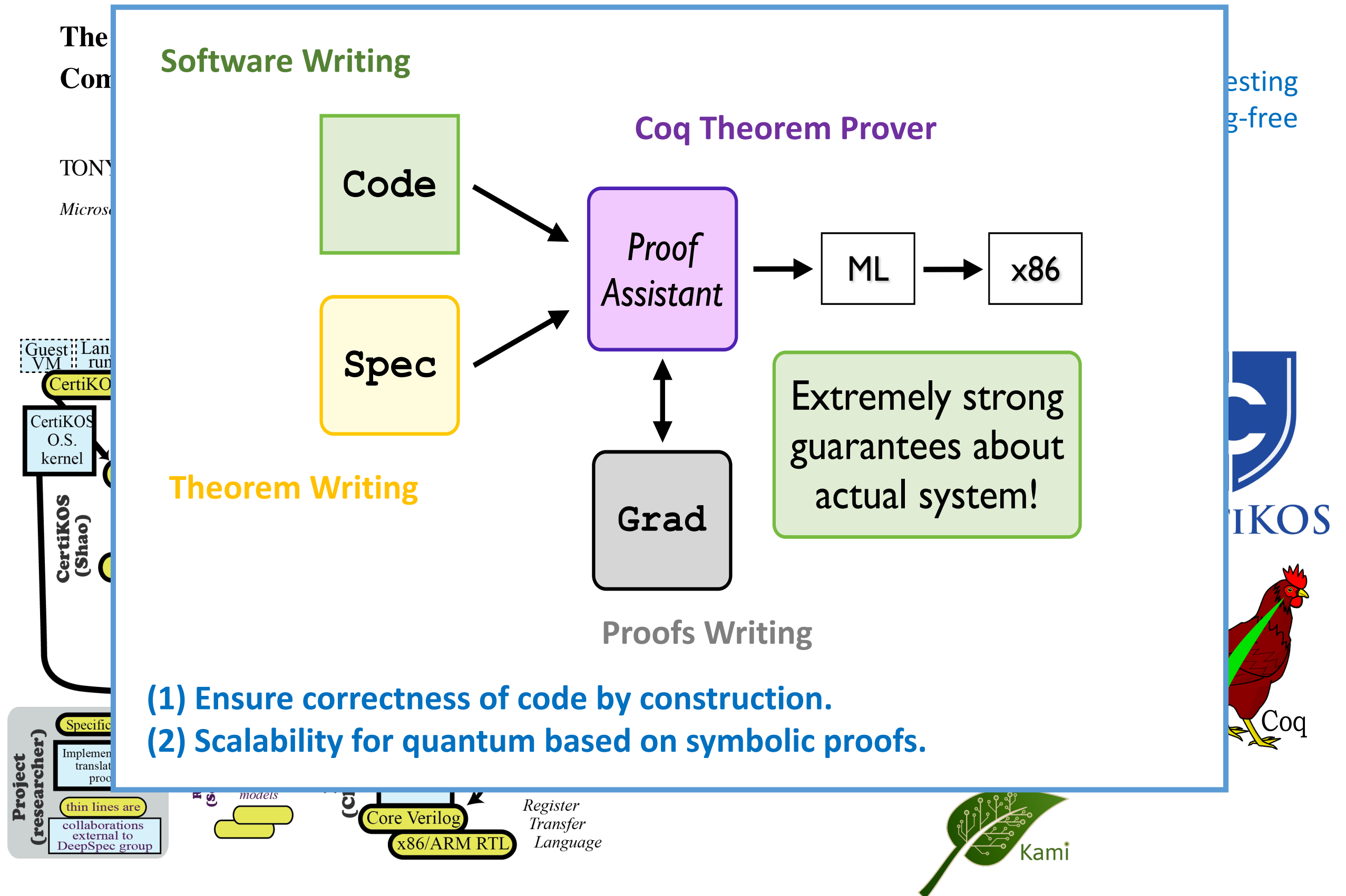
Microsoft Research Ltd., Cambridge, UK

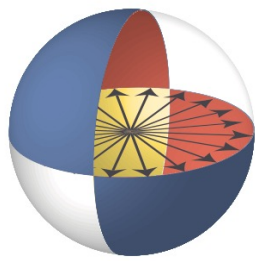
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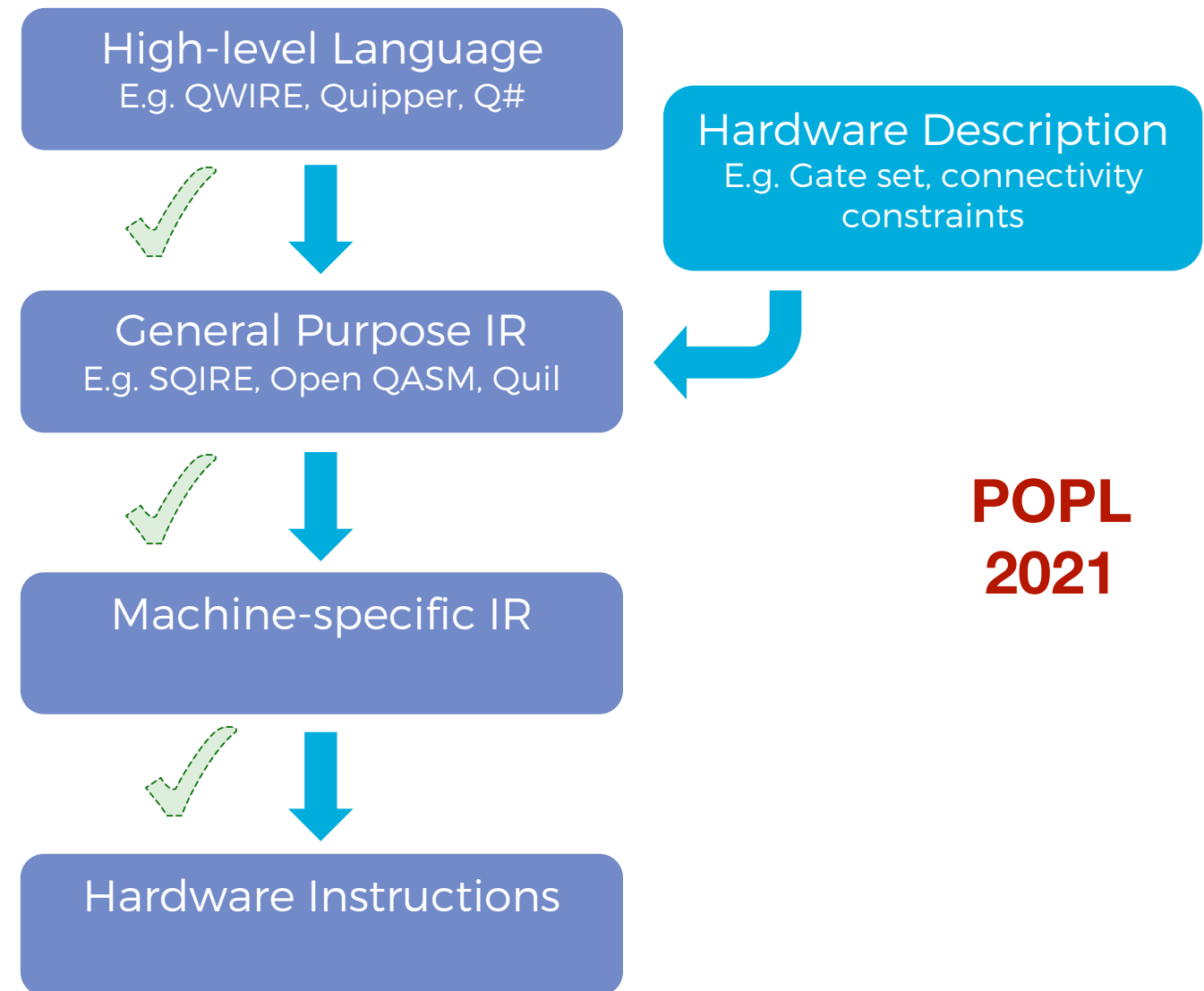
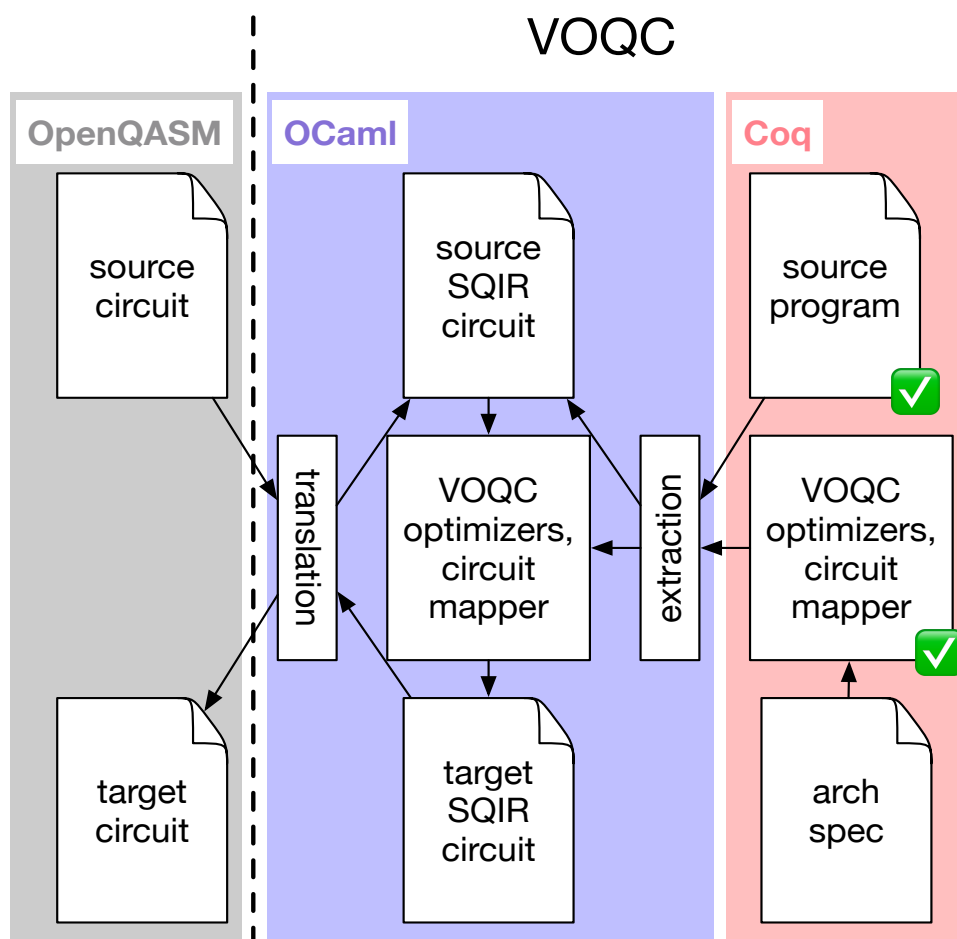


Certified software: a solution to validation of q. software



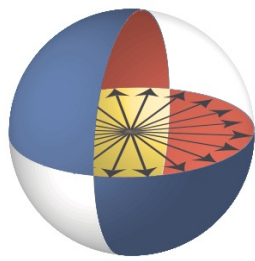


(Verified Optimizer for Quantum Circuits)

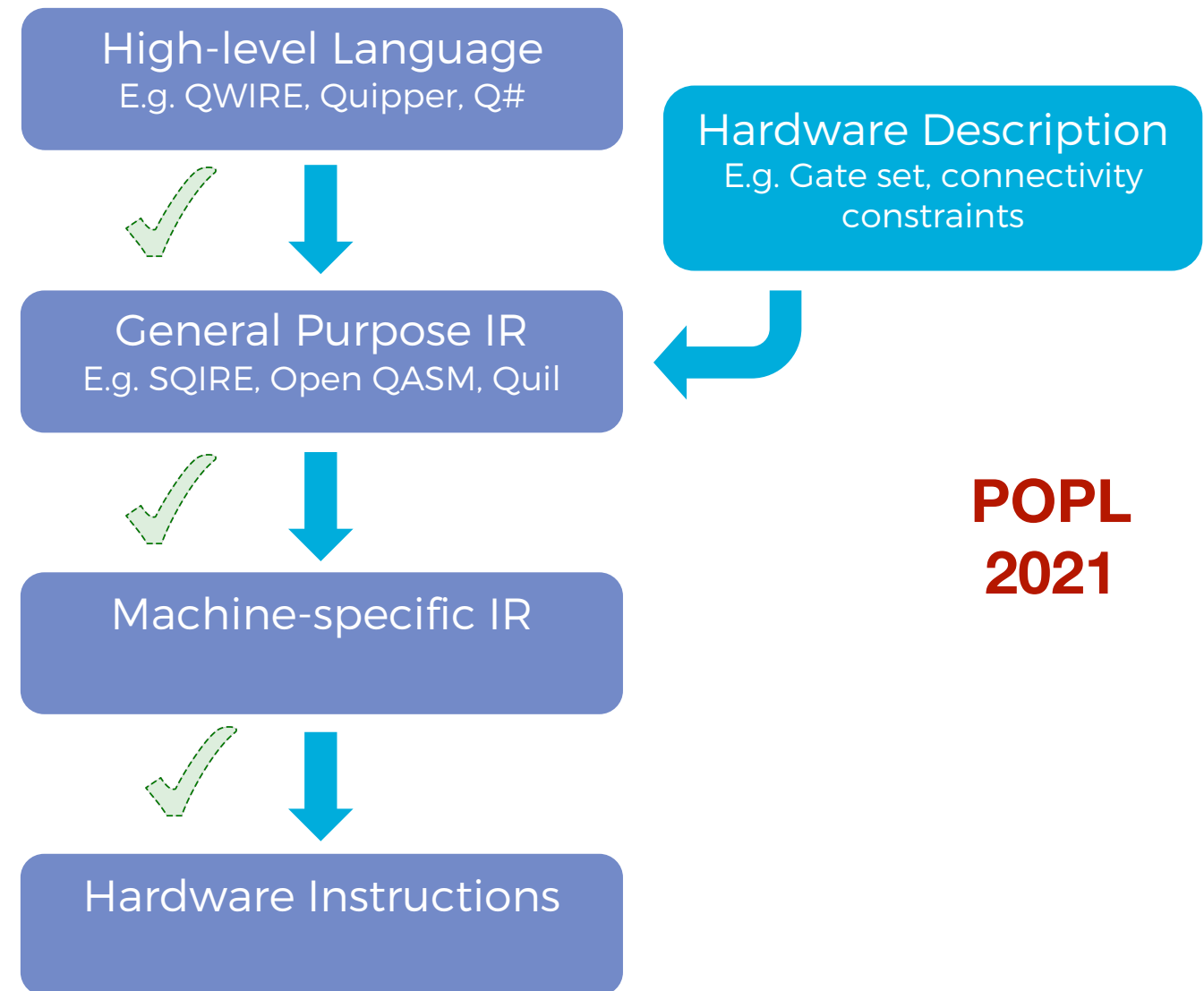
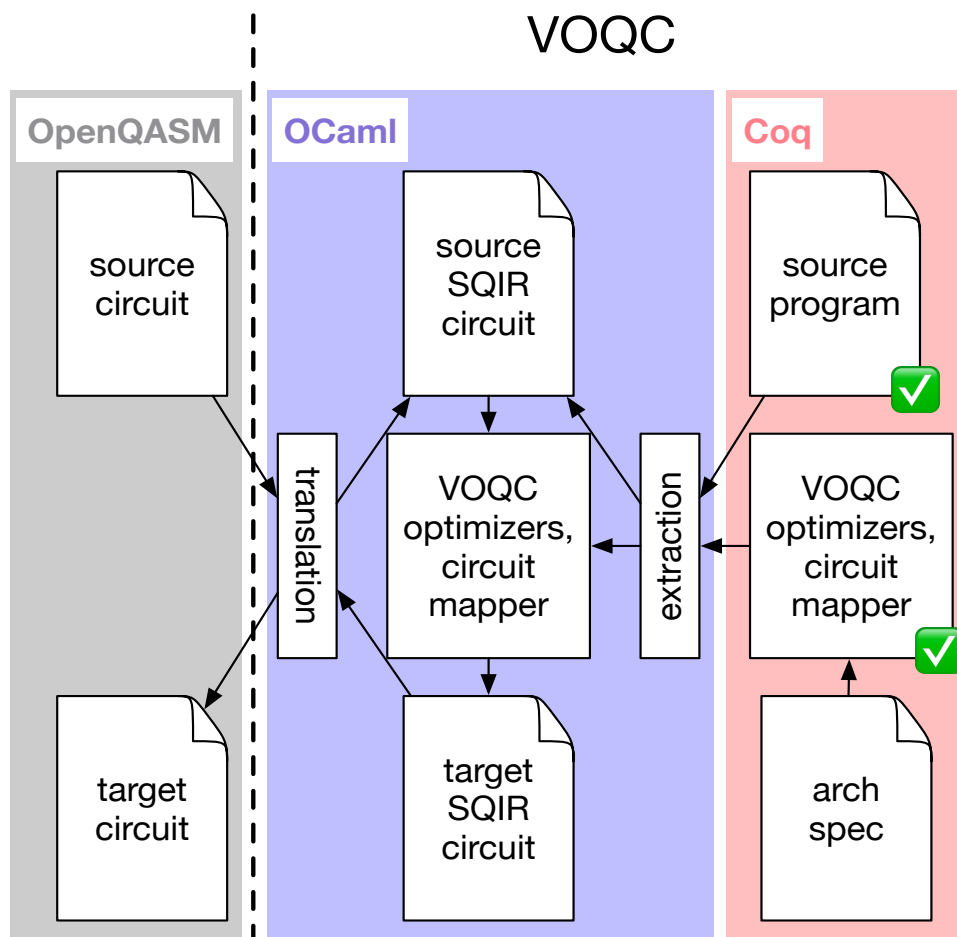


VOQC: a first step towards a fully certified quantum compiler.

SQIRE: a simple quantum intermediate-representation embedded in Coq.



(Verified Optimizer for Quantum Circuits)



VOQC: a first step towards a fully certified quantum compiler.

SQIRE: a simple quantum intermediate-representation embedded in Coq.

Our infrastructure powerful enough:

an end-to-end implementation of **Shor's algorithm** & its correctness proof.

About Today's Tutorial:



Goal: Some Basic Quantum Computing & PL + References

(1) Introduction to Quantum Computing and Potential Roles of Programming Languages (25 min + **5 Q & A**)

(2) A Mini-Course of Quantum Hoare Logic on Quantum While Language (30 min + **5 Q & A**)

(3) Discussion on existing and potential Programming Language research opportunities (20 min + **5 Q & A**)

Reference: tutorial slides and some references are available at https://www.cs.umd.edu/~xwu/mini_lib.html

