Simulating quantum mechanics with quantum computers

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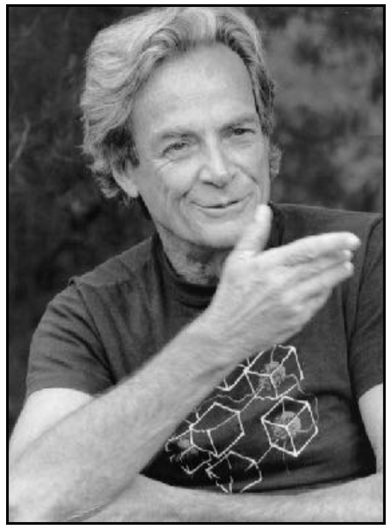


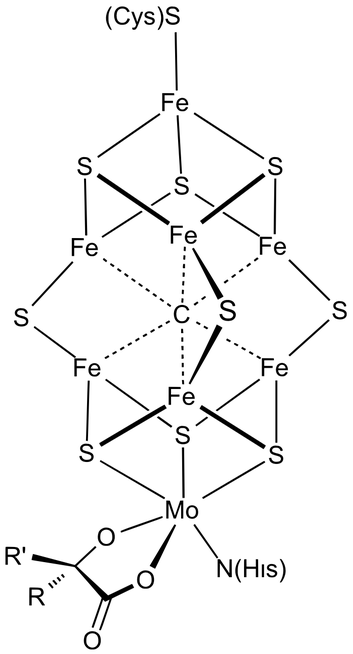
"… nature isn't classical, dammit, and if you want to make a simulation of nature, you'd better make it quantum mechanical, and by golly it's a wonderful problem, because it doesn't look so easy."

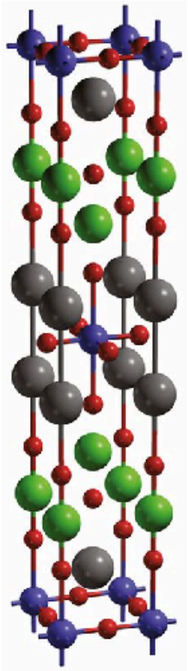
Richard Feynman
Simulating physics with computers (1981)

Why simulate quantum mechanics?

Computational chemistry/physics

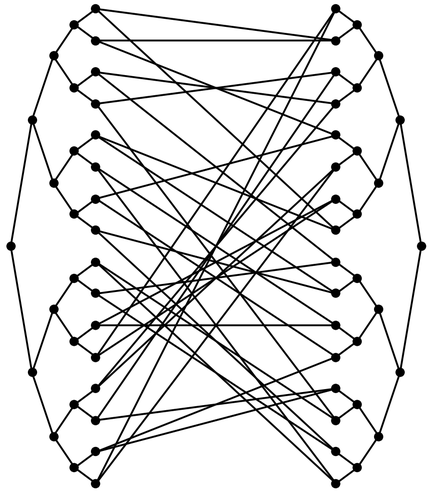
- chemical reactions (e.g., nitrogen fixation)
- properties of materials
- condensed matter physics

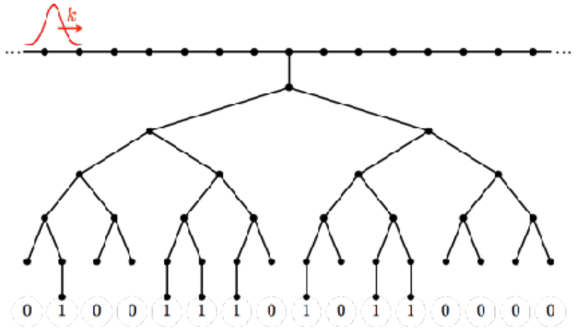




Implementing quantum algorithms

- continuous-time quantum walk (e.g., for formula evaluation, search, …)
- adiabatic quantum computation (e.g., for optimization or state generation)
- linear/differential equations





Simulating quantum mechanics with quantum computers

Algorithms

- Can we give an efficient algorithm?
- What is the best possible complexity as a function of various parameters?

Implementation

- What classically-hard simulations are easiest for a quantum computer?
- What simulation algorithm is best in practice for medium-scale problems?
- What optimizations can be applied to improve the implementation of algorithms?
- Are there resource tradeoffs (e.g., time vs. space)?
- Can we reliably do a classically-hard simulation without fault tolerance?
- How do the details of an experimental system (connectivity of qubits, timescales for different gates, etc.) interact with algorithmic issues?

Algorithms

Quantum dynamics

The dynamics of a quantum system are determined by its *Hamiltonian* H.

$$i\frac{\mathrm{d}}{\mathrm{d}t}|\psi(t)\rangle = H|\psi(t)\rangle \qquad \Rightarrow \qquad |\psi(t)\rangle = e^{-iHt}|\psi(0)\rangle$$

Quantum simulation problem: Given a description of the Hamiltonian H, an evolution time t, and an initial state $|\psi(0)\rangle$, produce the final state $|\psi(t)\rangle$ (to within some error tolerance ϵ)

A classical computer cannot even represent the state efficiently.

A quantum computer cannot produce a complete description of the state.

But given succinct descriptions of
- the initial state (suitable for a quantum computer to prepare it efficiently) and
- a final measurement (say, measurements of the individual qubits in some basis),

a quantum computer can efficiently answer questions that (apparently) a classical one cannot.

Local and sparse Hamiltonians

Local Hamiltonians [Lloyd 96]

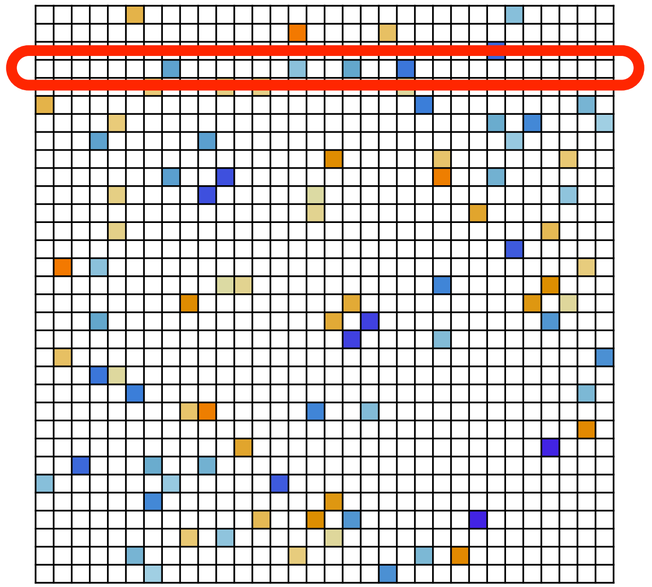
$H = \sum_{\ell=1}^{L} H_\ell$ where each H_ℓ acts on $k = O(1)$ qubits

Sparse Hamiltonians [Aharonov, Ta-Shma 03]

At most d nonzero entries per row, $d = \mathrm{poly}(\log N)$
(where H is $N \times N$)

In any given row, the location of the jth nonzero entry and its value can be computed efficiently

$H =$



Note: A k-local Hamiltonian with L terms is d-sparse with $d = 2^k L$

Product formula simulation

Suppose we want to simulate $H = \sum_{\ell=1}^{L} H_\ell$

Combine individual simulations with the Lie product formula. E.g., with two terms:

$$\lim_{r\to\infty} \left(e^{-iAt/r} e^{-iBt/r}\right)^r = e^{-i(A+B)t}$$

$$\left(e^{-iAt/r} e^{-iBt/r}\right)^r = e^{-i(A+B)t} + O(t^2/r)$$

To ensure error at most ϵ, take
$r = O\left((\|H\|t)^2/\epsilon\right)$

[Lloyd 96]

To get a better approximation, use higher-order formulas.

E.g., second order:

$$\left(e^{-iAt/2r} e^{-iBt} e^{-iAt/2r}\right)^r = e^{-i(A+B)t} + O(t^3/r^2)$$

Systematic expansions to arbitrary order are known [Suzuki 92]

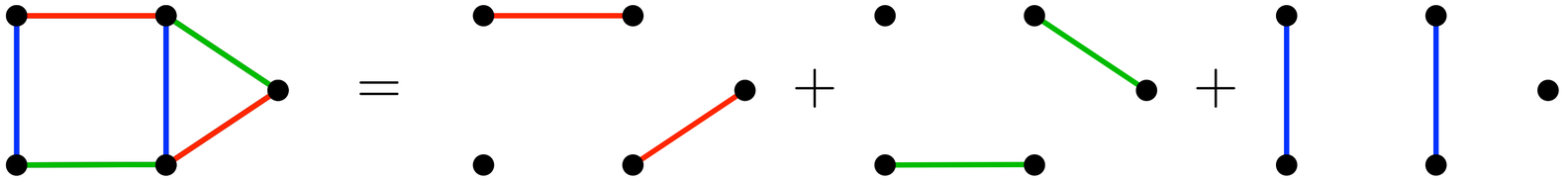
Using the $2k$th order expansion, the number of exponentials required for an approximation with error at most ϵ is at most

$$5^{2k} L^2 \|H\| t \left(\frac{L\|H\|t}{\epsilon}\right)^{1/2k}$$

[Berry, Ahokas, Cleve, Sanders 07]

Sparse Hamiltonians and coloring

Strategy: Color the edges of the graph of H. Then the simulation breaks into small pieces that are easy to handle.



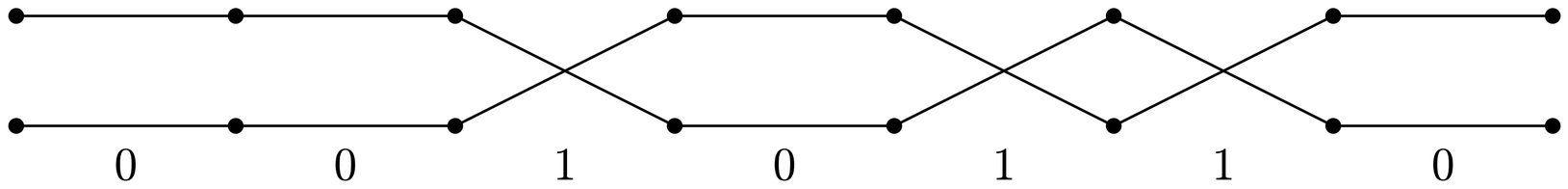
A sparse graph can be efficiently colored using only local information, so this gives efficient simulations.

Sometimes we can do better with different graph decompositions.

[Childs, Cleve, Deotto, Farhi, Gutmann, Spielman 03; Aharonov, Ta-Shma 03; Childs, Kothari 10]

Real-time simulation?

No fast-forwarding theorem: Simulating Hamiltonian dynamics for time t requires $\Omega(t)$ gates.



Complexity of kth order product formula simulation is $O(5^{2k}t^{1+1/2k})$.

Can we give an algorithm with complexity precisely $O(t)$?

Systems simulate their own dynamics in real time!

Hamiltonian simulation by quantum walk

Quantum walk corresponding to H

Alternately reflect about $\mathrm{span}\{|\psi_j\rangle\}_{j=1}^N$,

$$|\psi_j\rangle := |j\rangle \otimes \left(\nu \sum_{k=1}^{N} \sqrt{H_{jk}^*}|k\rangle + \nu_j |N+1\rangle \right),$$

and swap the two registers.

If H is sparse, this walk is easy to implement.

Spectral theorem: Each eigenvalue λ of H corresponds to two eigenvalues $\pm e^{\pm i \arcsin \lambda}$ of the walk operator (with eigenvectors closely related to those of H).

Simulation by phase estimation

$$\begin{aligned} |\lambda\rangle &\mapsto |\lambda\rangle|\widetilde{\arcsin \lambda}\rangle && \text{(phase estimation)} \\ &\mapsto e^{-i\lambda t}|\lambda\rangle|\widetilde{\arcsin \lambda}\rangle \\ &\mapsto e^{-i\lambda t}|\lambda\rangle && \text{(inverse phase est)} \end{aligned}$$

Theorem: $O(t/\sqrt{\epsilon})$ steps of this walk suffice to simulate H for time t with error at most ϵ.

[Childs10; Berry, Childs 12]

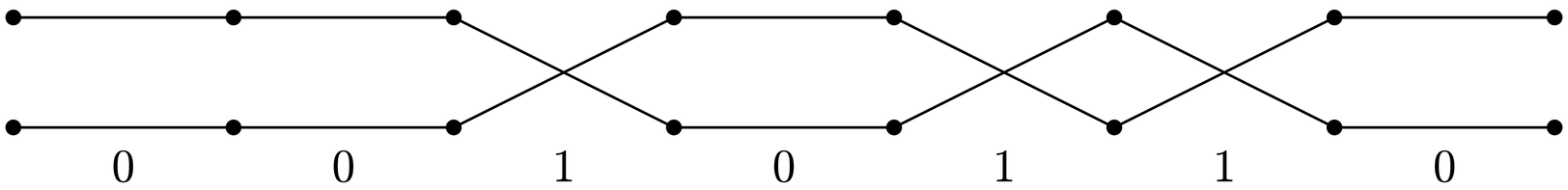
High-precision simulation?

Can we improve the dependence on ϵ?

Many approximate computations can be done with complexity $\mathrm{poly}(\log(1/\epsilon))$:

- computing π
- boosting a bounded-error subroutine
- Solovay-Kitaev circuit synthesis
- and more…

Lower bound (based on the *unbounded-error* query complexity of parity): $\Omega\left(\frac{\log(1/\epsilon)}{\log\log(1/\epsilon)}\right)$



Quantum walk simulation: $O(1/\sqrt{\epsilon})$

Product formulas ($2k$th order): $O(5^{2k}\epsilon^{-2k})$

Can we do better?

Hamiltonian simulation by linear combinations of unitaries

Main idea: Directly implement the series

$$e^{-iHt} = \sum_{k=0}^{\infty} \frac{(-iHt)^k}{k!}$$

$$\approx \sum_{k=0}^{K} \frac{(-iHt)^k}{k!}$$

Write $H = \sum_\ell \alpha_\ell H_\ell$ with H_ℓ unitary.

Then

$$\sum_{k=0}^{K} \sum_{\ell_1,\ldots,\ell_k} \frac{(-it)^k}{k!} \alpha_{\ell_1} \cdots \alpha_{\ell_k} H_{\ell_1} \cdots H_{\ell_k}$$

is a linear combination of unitaries.

LCU Lemma: Given the ability to perform unitaries V_j with unit complexity, one can perform the operation $U = \sum_j \beta_j V_j$ with complexity $O(\sum_j |\beta_j|)$. Furthermore, if U is (nearly) unitary then this implementation can be made (nearly) deterministic.

Main ideas:

- Implement U with some amplitude:

$$|0\rangle|\psi\rangle \mapsto \sin\theta|0\rangle U|\psi\rangle + \cos\theta|\Phi\rangle$$

- Boost the amplitude for success by *oblivious amplitude amplification*

Query complexity: $O\big(t \frac{\log(t/\epsilon)}{\log\log(t/\epsilon)}\big)$

[Berry, Childs, Cleve, Kothari, Somma 14 & 15]

Tradeoff between t and ϵ

Combining known lower bounds on the complexity of simulation as a function of t and ϵ gives

$$\Omega\left(t + \frac{\log \frac{1}{\epsilon}}{\log\log \frac{1}{\epsilon}}\right) \quad \text{vs. upper bound of} \quad O\left(t \frac{\log \frac{t}{\epsilon}}{\log\log \frac{t}{\epsilon}}\right)$$

Very recent work, using an alternative method for implementing a linear combination of quantum walk steps, gives an optimal tradeoff.

Main idea: Encode the eigenvalues of H in a two-dimensional subspace; use a carefully-chosen sequence of single-qubit rotations to manipulate those eigenvalues.

To compute the rotation angles, we must find the roots of a high-degree polynomial to high precision. This can be done in polynomial time (classically), but it's expensive in practice.

[Low, Chuang 16]

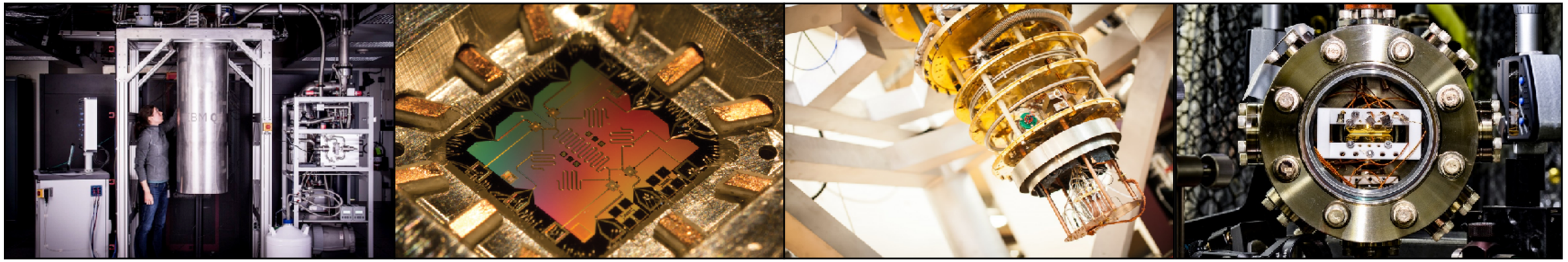
Algorithm comparison

Algorithm	Query complexity	Gate complexity
Product formula, 1st order	$O(d^4t^2/\epsilon)$	$O(d^4t^2/\epsilon)$
Product formula, (2k)th order	$O\left(5^{2k}d^3t(\frac{dt}{\epsilon})^{1/2k}\right)$	$O\left(5^{2k}d^3t(\frac{dt}{\epsilon})^{1/2k}\right)$
Quantum walk	$O(dt/\sqrt{\epsilon})$	$O(dt/\sqrt{\epsilon})$
Fractional-query simulation	$O\left(d^2t\frac{\log(dt/\epsilon)}{\log\log(dt/\epsilon)}\right)$	$O\left(d^2t\frac{\log^2(dt/\epsilon)}{\log\log(dt/\epsilon)}\right)$
Taylor series	$O\left(d^2t\frac{\log(dt/\epsilon)}{\log\log(dt/\epsilon)}\right)$	$O\left(d^2t\frac{\log^2(dt/\epsilon)}{\log\log(dt/\epsilon)}\right)$
Linear combination of q. walk steps	$O\left(dt\frac{\log(dt/\epsilon)}{\log\log(dt/\epsilon)}\right)$	$O\left(dt\frac{\log^{3.5}(dt/\epsilon)}{\log\log(dt/\epsilon)}\right)$
Quantum signal processing	$O\left(dt+\frac{\log(1/\epsilon)}{\log\log(1/\epsilon)}\right)$	$O\left(dt+\frac{\log(1/\epsilon)}{\log\log(1/\epsilon)}\right)$

OPTIMAL!

Implementation

Toward practical quantum speedup



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Important early goal: demonstrate quantum computational advantage

… but can we find a *practical* application of near-term devices?

Challenges

- Improve experimental systems
- Improve algorithms and their implementation, making the best use of available hardware

Our goal: Produce concrete resource estimates for the simplest possible practical application of quantum computers

What to simulate?

~~Quantum chemistry?~~ Spin systems!

Heisenberg model on a ring: $H = \sum_{j=1}^{n} \left(\vec{\sigma}_j \cdot \vec{\sigma}_{j+1} + h_j \sigma_j^z \right)$ $h_j \in [-h, h]$ uniformly random

This provides a model of *self-thermalization* and *many-body localization*.

The transition between thermalized and localized phases (as a function of h) is poorly understood. Most extensive numerical study: fewer than 25 spins. [Luitz, Laflorencie, Alet 15]

Could explore the transition by preparing a simple initial state, evolving, and performing a simple final measurement. Focus on the cost of simulating dynamics.

For concreteness: $h = 1, \quad t = n, \quad \epsilon = 10^{-3}, \quad 20 \leq n \leq 100$

Algorithms

Algorithm	Gate complexity (t, ϵ)	Gate complexity (n)
Product formula (PF), 1st order	$O(t^2/\epsilon)$	$O(n^5)$
Product formula (PF), (2k)th order	$O(5^{2k} t^{1+1/2k}/\epsilon^{1/2k})$	$O(5^{2k} n^{3+1/k})$
Quantum walk	$O(t/\sqrt{\epsilon})$	$O(n^4 \log n)$
Fractional-query simulation	$O\big(t \frac{\log^2(t/\epsilon)}{\log\log(t/\epsilon)}\big)$	$O\big(n^4 \frac{\log^2 n}{\log\log n}\big)$
Taylor series (TS)	$O\big(t \frac{\log^2(t/\epsilon)}{\log\log(t/\epsilon)}\big)$	$O\big(n^3 \frac{\log^2 n}{\log\log n}\big)$
Linear combination of q. walk steps	$O\big(t \frac{\log^{3.5}(t/\epsilon)}{\log\log(t/\epsilon)}\big)$	$O\big(n^4 \frac{\log^2 n}{\log\log n}\big)$
Quantum signal processing (QSP)	$O(t + \log(1/\epsilon))$	$O(n^3)$
Segmented QSP, q iterates per segment	$O(t^{1+2/q}/\epsilon^{2/q})$	$O\big(n^{3+4/q}\big)$

Algorithms

Algorithm	Gate complexity (t, ϵ)	Gate complexity (n)
Product formula (PF), 1st order	$O(t^2/\epsilon)$	$O(n^5)$
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Circuit synthesis

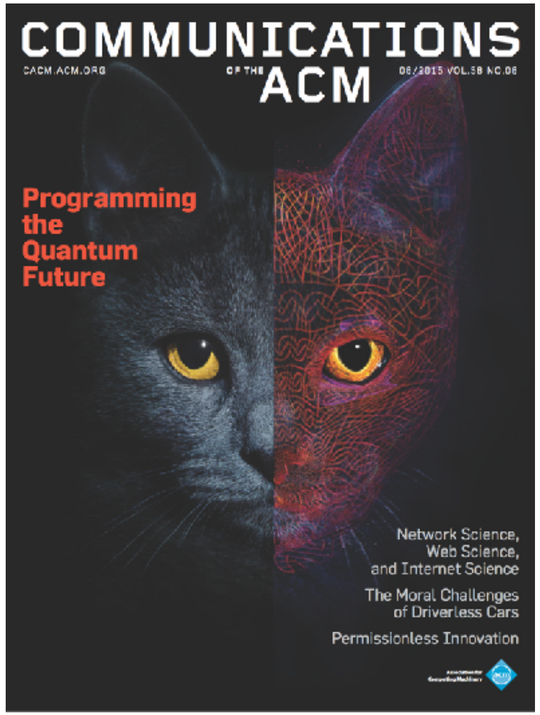
We implemented each of these algorithms using Quipper, a quantum circuit description language that facilitates concrete resource counts

Gate sets:

- Clifford+R_z
- Clifford+T

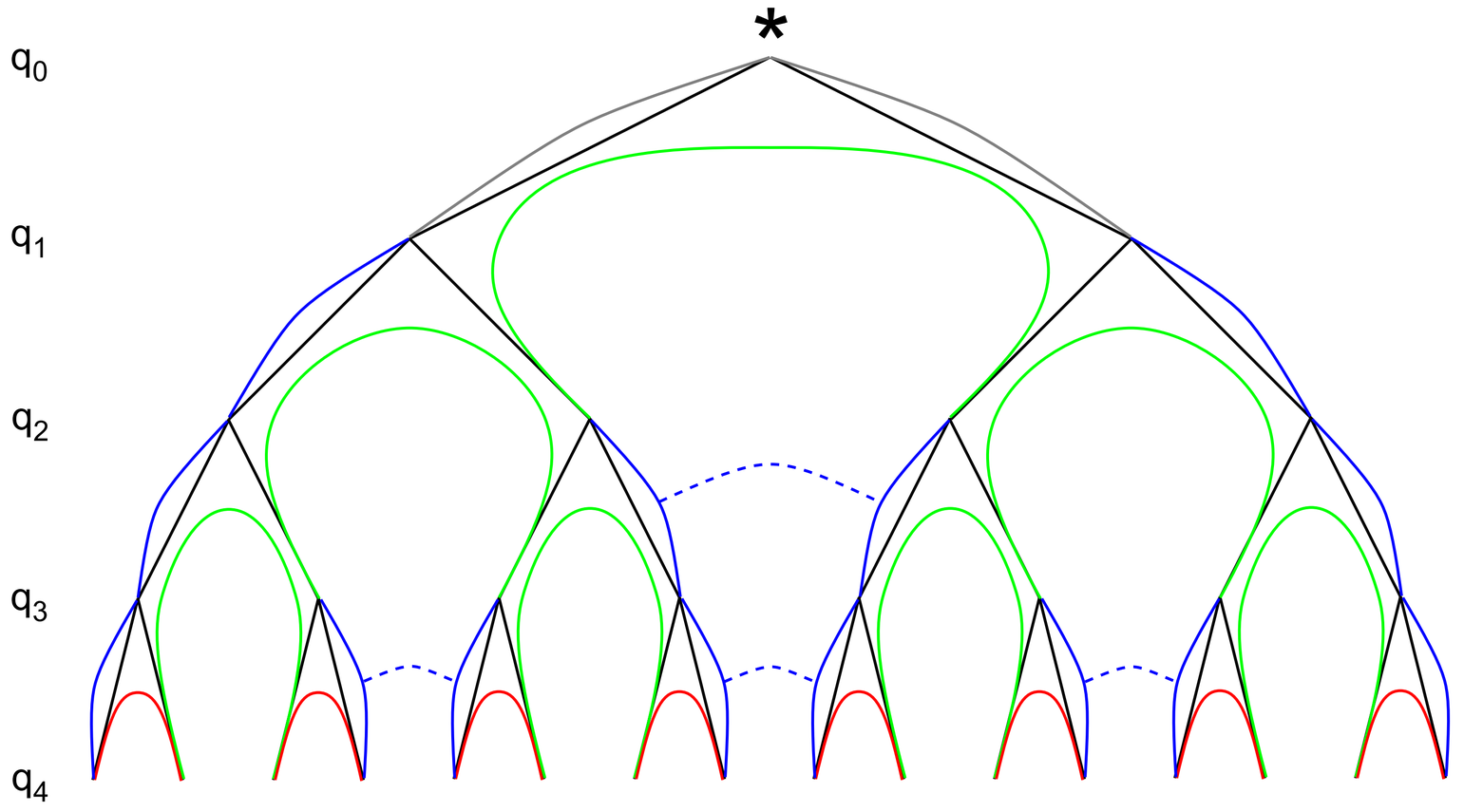
Quipper can produce Clifford+T circuits using recently-developed optimal synthesis algorithms [Kliuchnikov, Maslov, Mosca 13; Ross, Selinger 16]

We verified correctness using simulations of subroutines and small instances.

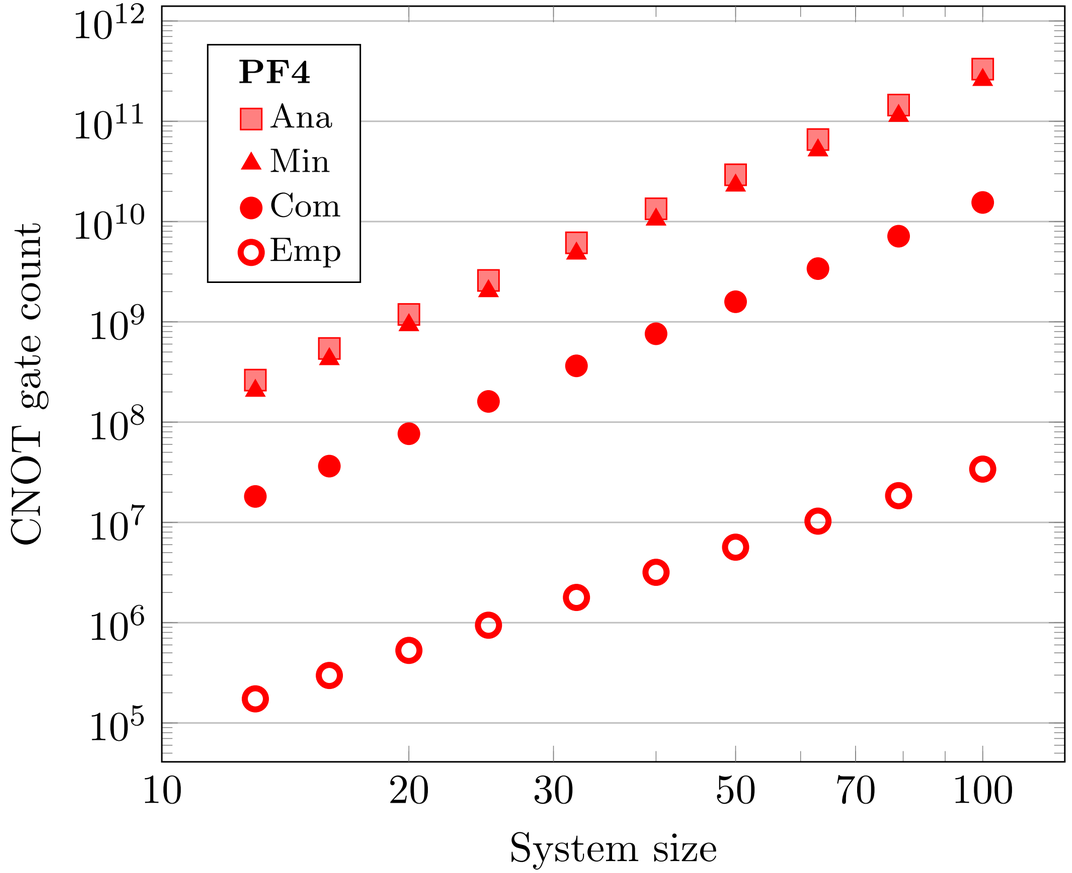


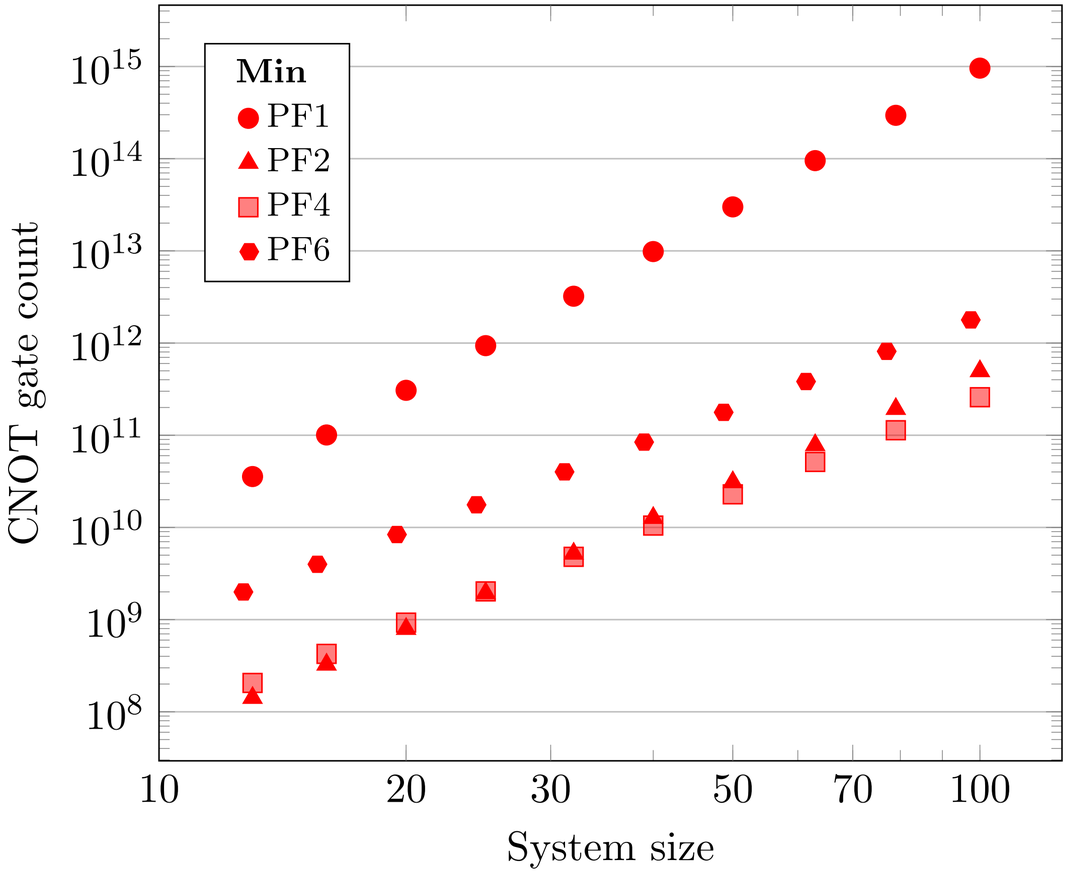

```
multiplexor :: [Double] -> [Qubit] -> Qubit -> Circ ([Qubit], Qubit)
multiplexor as controls target = case controls of
  -- No controls.
  [] -> do
    let angle = as !! 0
    expYt (- angle) target
    return ([], target)

  -- One control.
  [q0] -> do
    let (as0, as1) = split_angles as
    ([], target) <- multiplexor as0 [] target
    target <- qnot target `controlled` q0
    ([], target) <- multiplexor as1 [] target
    target <- qnot target `controlled` q0
    return ([q0], target)

  -- Two controls.
  [q0,q1] -> do
    let (as0, as1) =  split_angles as
    ([q1], target) <- multiplexor as0 [q1] target
    target <- qnot target `controlled` q0
    ([q1], target) <- multiplexor as1 [q1] target
    target <- qnot target `controlled` q0
    return ([q0,q1], target)

  -- Three controls.
  [q0,q1,q2] -> do
    let (as0, as1, as2, as3) = split_angles_3 as
    ([q2], target) <- multiplexor as0 [q2] target
    target <- qnot target `controlled` q1
    ([q2], target) <- multiplexor as1 [q2] target
    target <- qnot target `controlled` q0
    ([q2], target) <- multiplexor as3 [q2] target
    target <- qnot target `controlled` q1
    ([q2], target) <- multiplexor as2 [q2] target
    target <- qnot target `controlled` q0
    return ([q0,q1,q2], target)

  -- Four or more controls.
  qs -> do
    let (as0, as1) =  split_angles as
    let (qhead:qtail) = qs
    (qtail, target) <- multiplexor as0 qtail target
    target <- qnot target `controlled` qhead
    (qtail, target) <- multiplexor as1 qtail target
    target <- qnot target `controlled` qhead
    return (qs, target)

  where
    -- Compute angles for recursive decomposition of a multiplexor.
    split_angles :: [Double] -> ([Double], [Double])
    split_angles l =
      let (l1, l2) = splitIn2 l in
        let p w x  = (w + x) / 2 in
          let m w x = (w - x) / 2 in
            (zipWith p l1 l2, zipWith m l1 l2)

    -- Compute the angles for recursive decomposition of a multiplexor
    -- with three controls, saving 2 CNOT gates, as in the
    -- optimization in Fig. 2 of Shende et.al.
    split_angles_3 :: [Double] -> ([Double],[Double],[Double],[Double])
    split_angles_3 l =
      let (l1, l2, l3, l4) = splitIn4 l in
        let pp w x y z = (w + x + y + z) / 4 in
          let pm w x y z = (w + x - y - z) / 4 in
            let mp w x y z = (w - x - y + z) / 4 in
              let mm w x y z = (w - x + y - z) / 4 in
                let lpp = zipWith4 pp l1 l2 l3 l4 in
                  let lpm = zipWith4 pm l1 l2 l3 l4 in
                    let lmp = zipWith4 mp l1 l2 l3 l4 in
                      let lmm = zipWith4 mm l1 l2 l3 l4 in
                        (lpp, lmm, lpm, lmp)
```

$$\mathrm{select}(V) = \sum_j |j\rangle\langle j| \otimes V_j$$

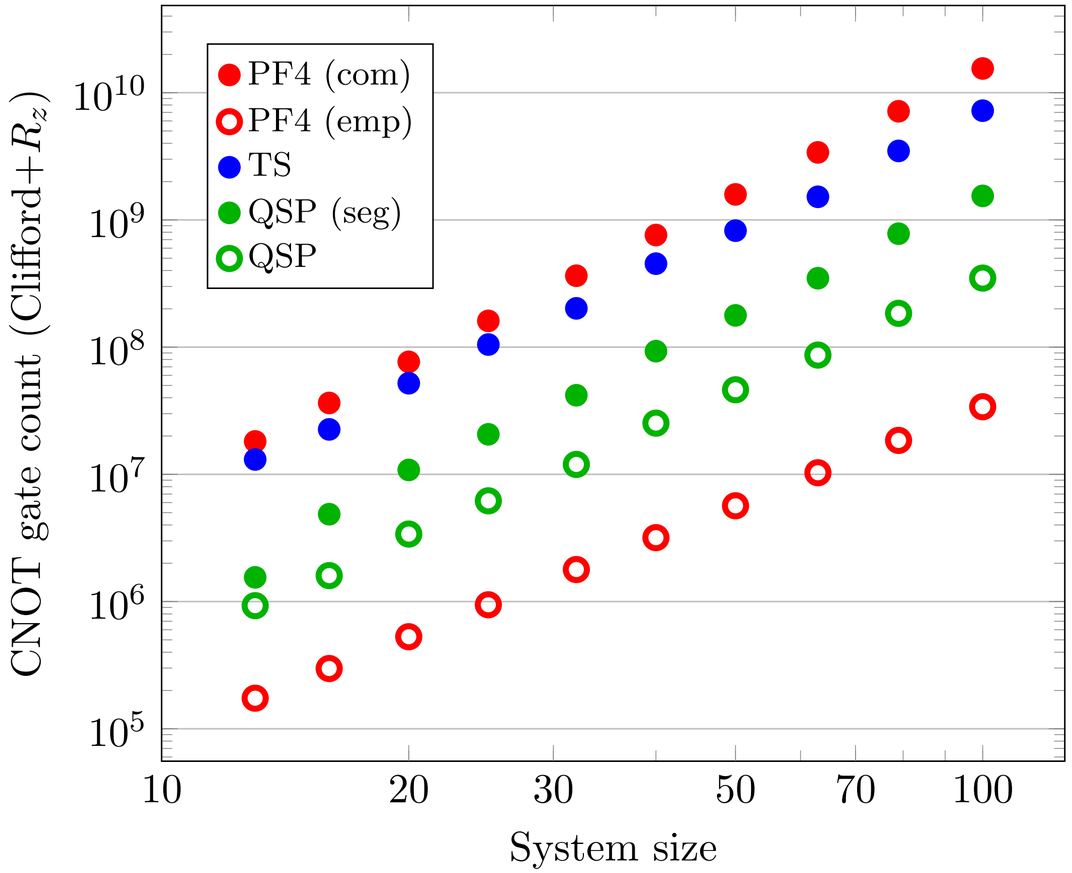


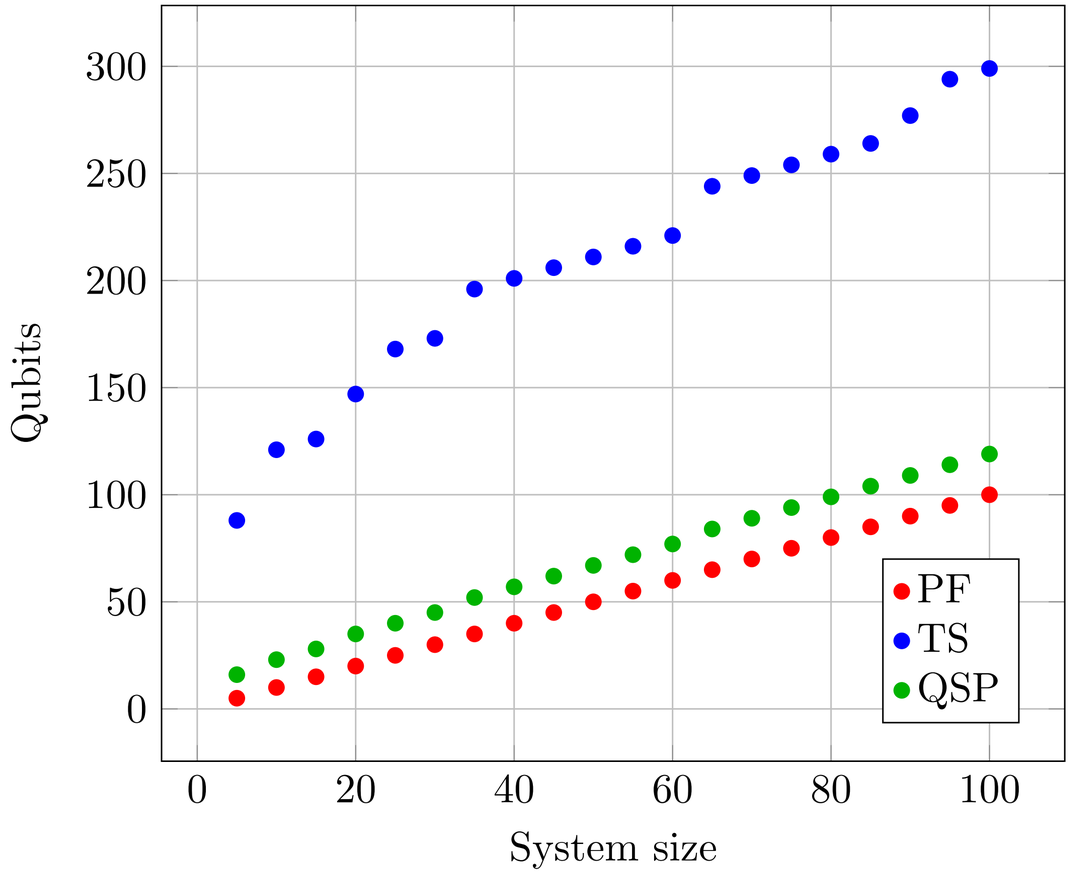
Product formula comparisons



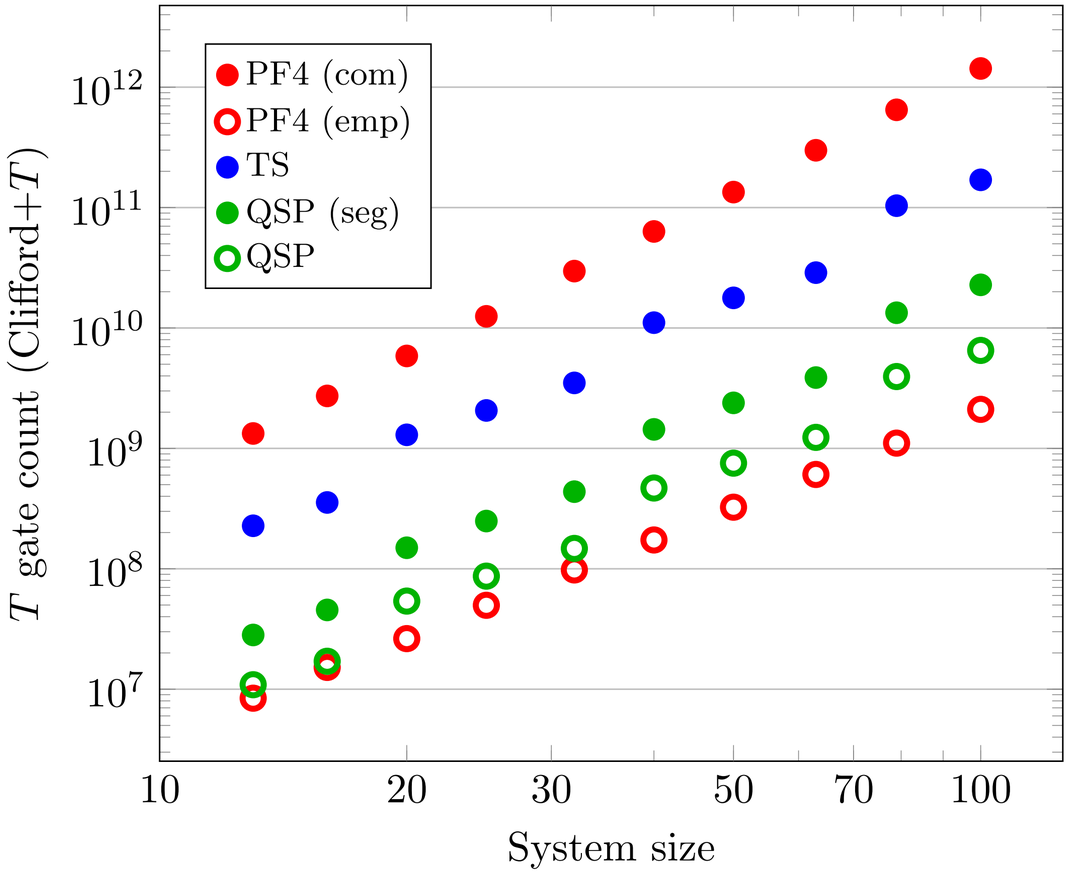


Resource estimates





Resource estimates



Simulating a 50-qubit system (PF4, empirical):

- 50 qubits
- 3.2×10^8 T gates

Factoring a 1024-bit number [Kutin 06]:

- 3132 qubits
- 5.7×10^9 T gates

Simulating FeMoco [Reiher et al. 16]:

- 111 qubits
- 1.0×10^{14} T gates

Outlook

Super-classical quantum simulation without invoking fault tolerance?

- Improved error bounds (e.g., empirical error bound for QSP algorithm?)
- Optimized implementations
- Alternative target systems
- New simulation algorithms
- Experiments!

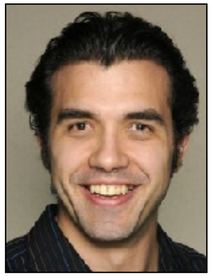
Resource estimates for more practical models

- Architectural constraints, parallelism
- Fault-tolerant implementations

Better provable bounds for simulation algorithms

- Product formula error bounds beyond the triangle inequality
- Efficient synthesis of the QSP circuit

Algorithms


Dominic Berry


Richard Cleve


Robin Kothari

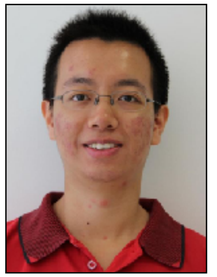

Rolando Somma

Implementation


Dmitri Maslov


Yunseong Nam


Neil Julien Ross


Yuan Su

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Product formula error extrapolation (4th order)