Toward the first quantum simulation with quantum speedup

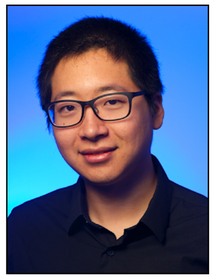
Andrew Childs
University of Maryland

COMPUTER SCIENCE
UNIVERSITY OF MARYLAND

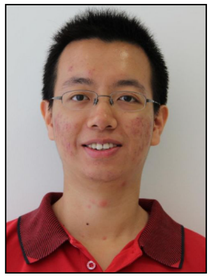
UMIACS
University of Maryland
Institute for Advanced
Computer Studies

JOINT CENTER FOR
QUANTUM INFORMATION
AND COMPUTER SCIENCE


Dmitri Maslov


Yunseong Nam


Neil Julien Ross


Yuan Su

arXiv:1711.10980

Simulating Hamiltonian dynamics on a small quantum computer

Andrew Childs

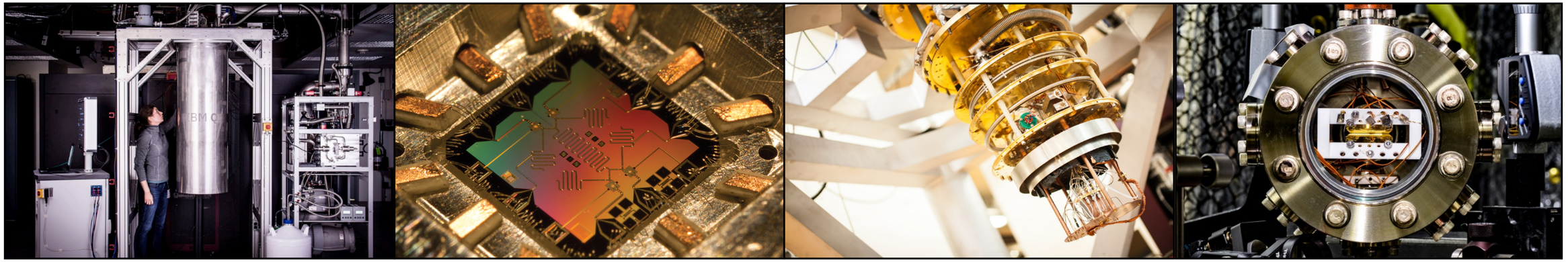
Department of Combinatorics & Optimization
and Institute for Quantum Computing
University of Waterloo

based in part on joint work with

Dominic Berry, Richard Cleve,
Robin Kothari, and Rolando Somma

Workshop on *What do we do with a small quantum computer?*
IBM Watson, 9 December 2013

Toward practical quantum speedup



IBM | Google/UCSB | Delft | Maryland

Important early goal: demonstrate quantum computational advantage

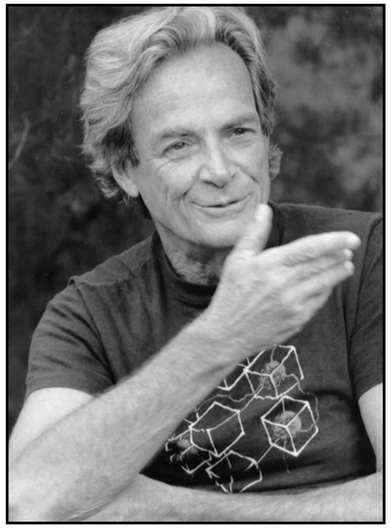
… but can we find a *practical* application of near-term devices?

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

Quantum simulation



"… 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 (1981)
Simulating physics with computers

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.

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]

Quantum walk simulation

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]

Taylor series simulation

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]

Quantum signal processing

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

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

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, performing the desired evolution.

[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!

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)	$O(t + \log(1/\epsilon))$	$O(n^3)$

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)	$O(t + \log(1/\epsilon))$	$O(n^3)$

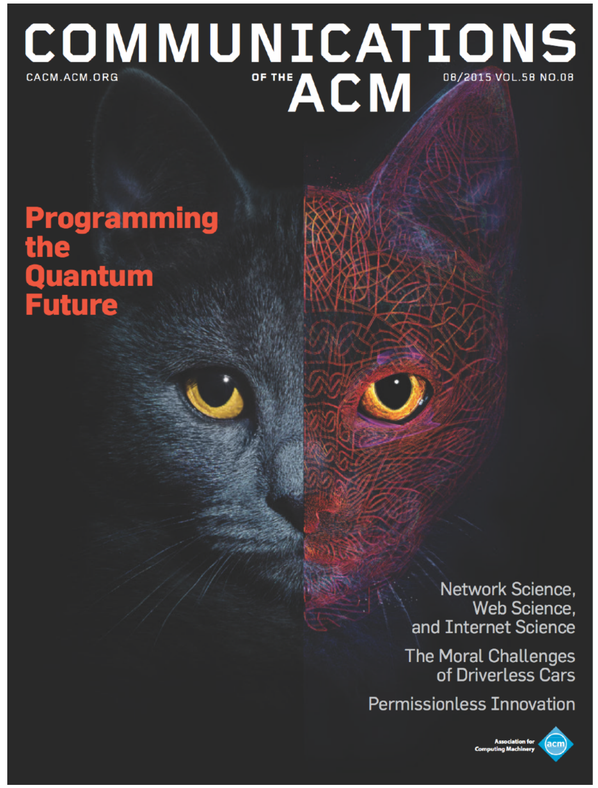
Circuit synthesis

We implemented 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 recent optimal synthesis algorithms [Kliuchnikov, Maslov, Mosca 13; Ross, Selinger 16].




```
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)
```

We verified correctness by simulating subroutines and small instances.

Implementation available at github.com/njross/simcount

We also applied an automated quantum circuit optimizer that we developed [arXiv:1710.07345]. CNOT/T gate counts improve by about 30% for PF. Less significant improvement for TS/QSP.

Product formula implementation

We consider four methods for choosing the parameters of the PF algorithm:

Analytic and **Minimized** error bounds: tightened versions of previous analysis

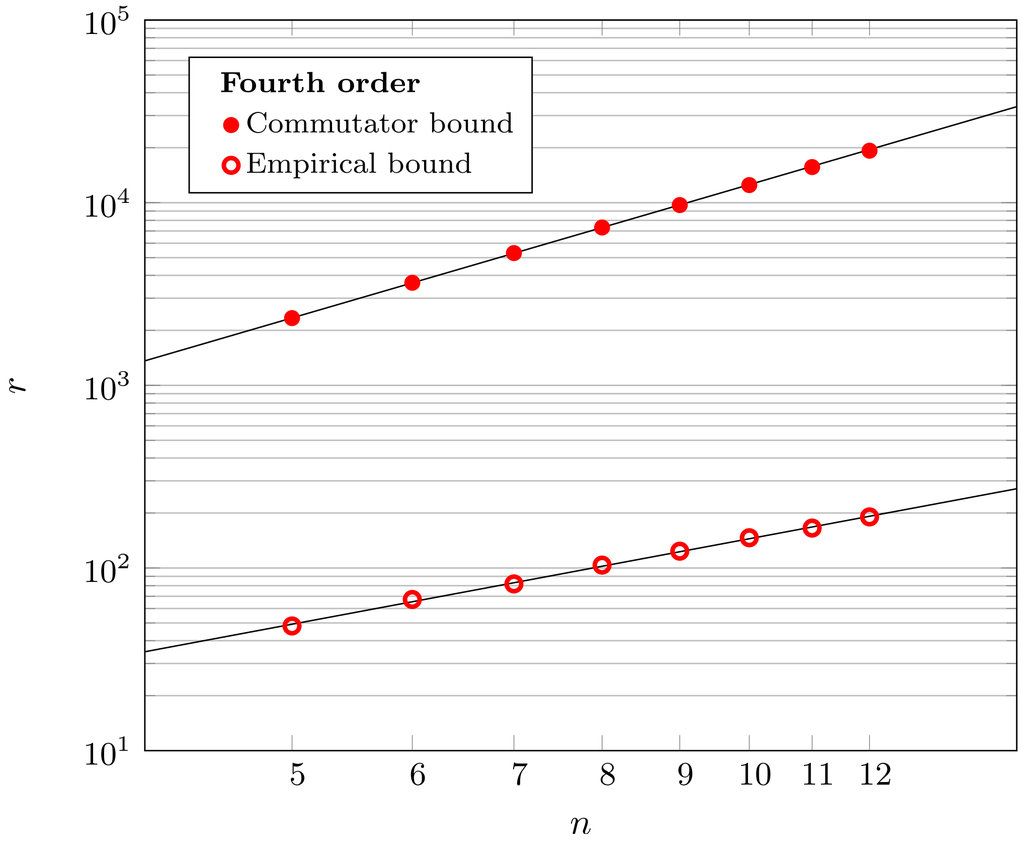
Commutator error bound: exploit commutation relations among terms in the Hamiltonian

Involves extensive analysis to derive the bound and compute it for our model system

Improved asymptotic performance:

$$O(n^{3+1/k}) \rightarrow O(n^{3+2/(2k+1)})$$

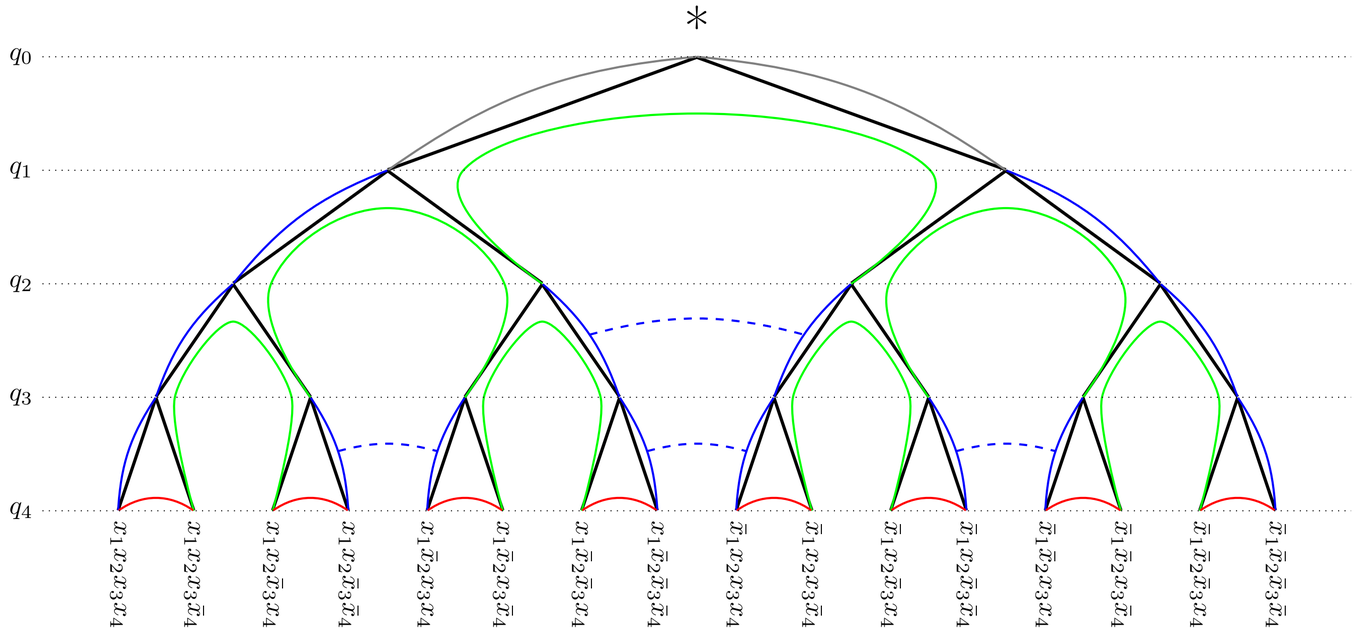
Empirical error bound: extrapolate performance from small instances



Taylor series implementation

Main implementation issue: construct circuits for the operation $\mathrm{select}(V) = \sum_{j=1}^{\Gamma} |j\rangle\langle j| \otimes V_j$

We construct an optimized walk on a binary tree that encodes the control into a single qubit, saving a factor of about $\log \Gamma$ (between 5 and 9 in our instances).



Also give concrete error analysis. Empirical error bounds are infeasible but probably not helpful.

Quantum signal processing implementation

QSP is built from the same basic subroutines as TS (state preparation, reflection, $\mathrm{select}(\mathrm{V})$).

To compute a sequence of rotation angles that define the algorithm, 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.

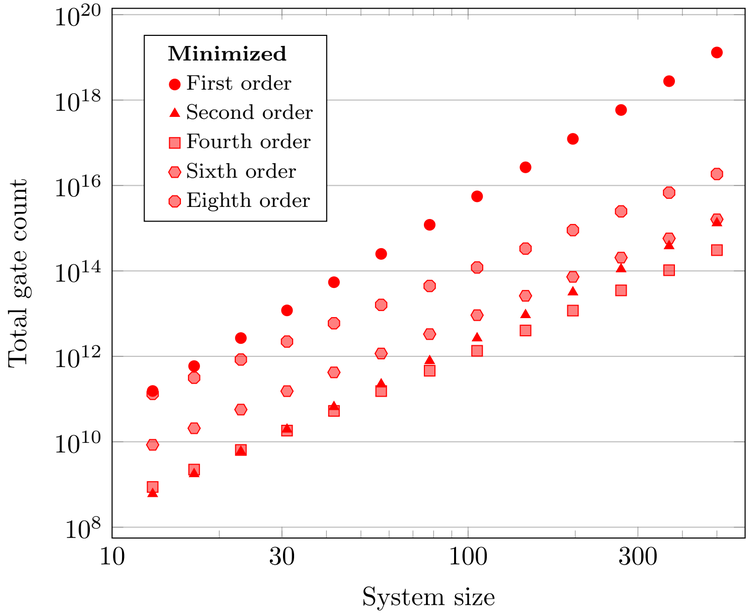
Workarounds:

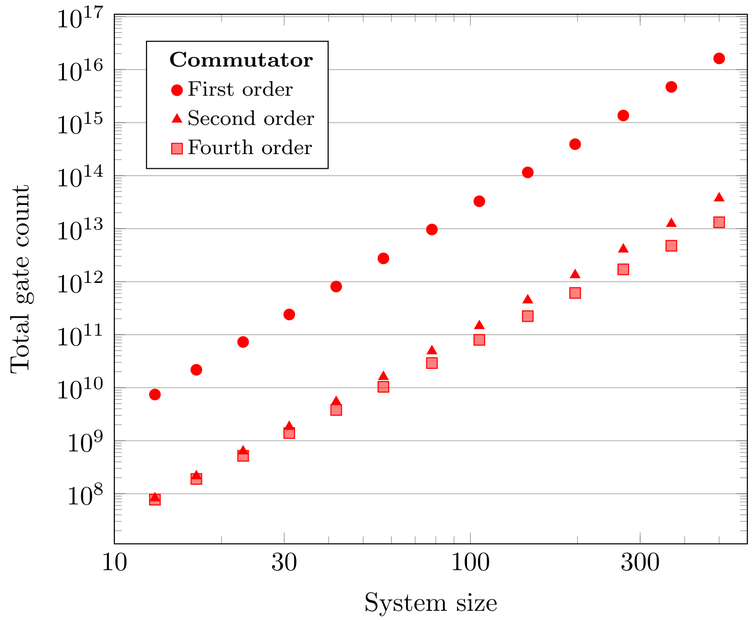
- Compute the gate count using placeholder angles
- Consider a *segmented* version of the algorithm: concatenate segments that are short enough to be simulated. Modest overhead: with M angles, $O(n^{3+4/M})$ vs. $O(n^3)$ for full QSP.

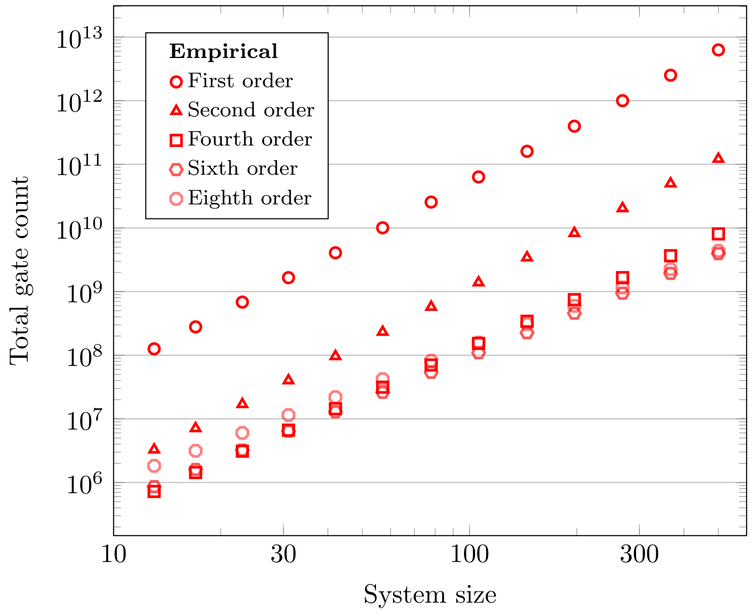
Empirical error bounds:

- Empirical estimate of the error in the Jacobi-Anger expansion saves about 30-45%.
- Comprehensive empirical error bounds are just barefly feasible and probably not helpful.

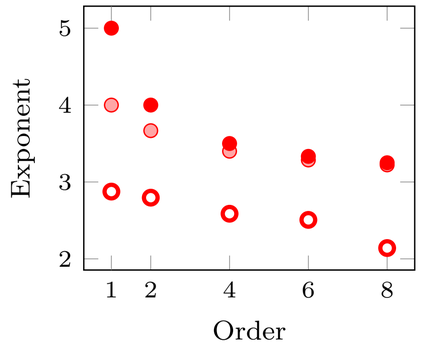
Product formula comparisons



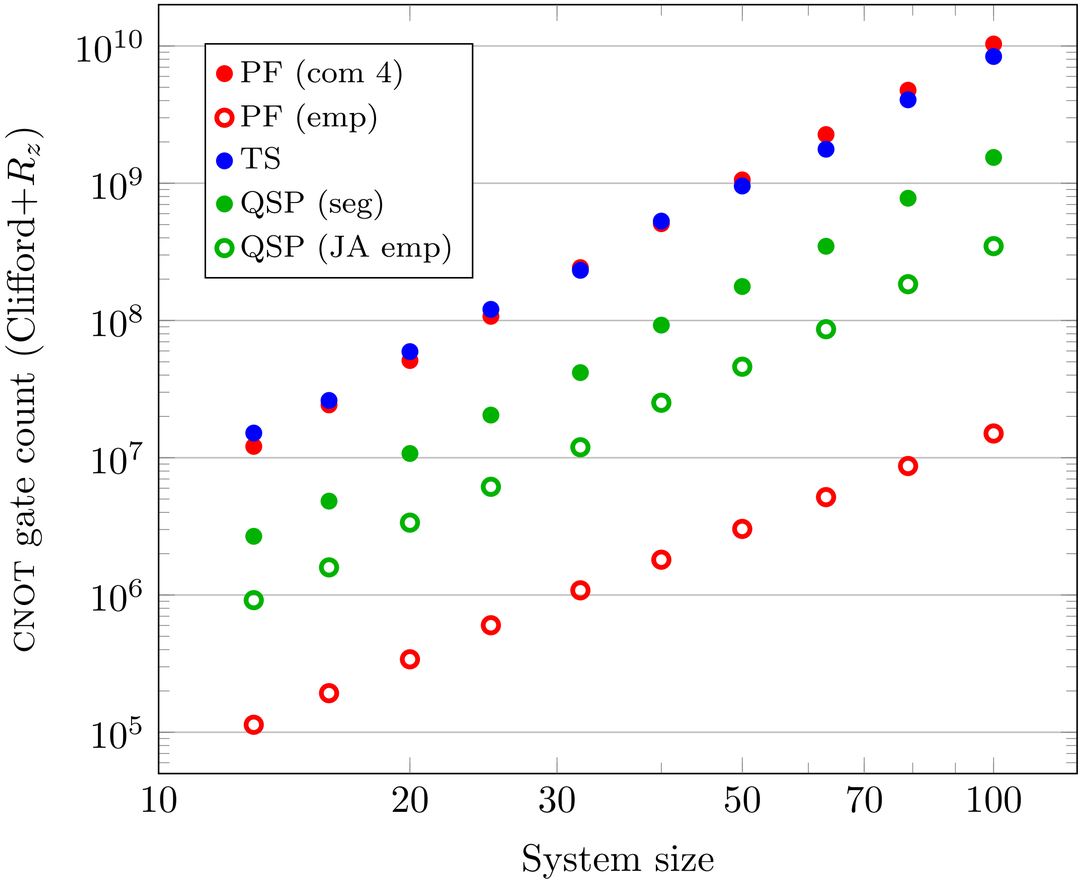


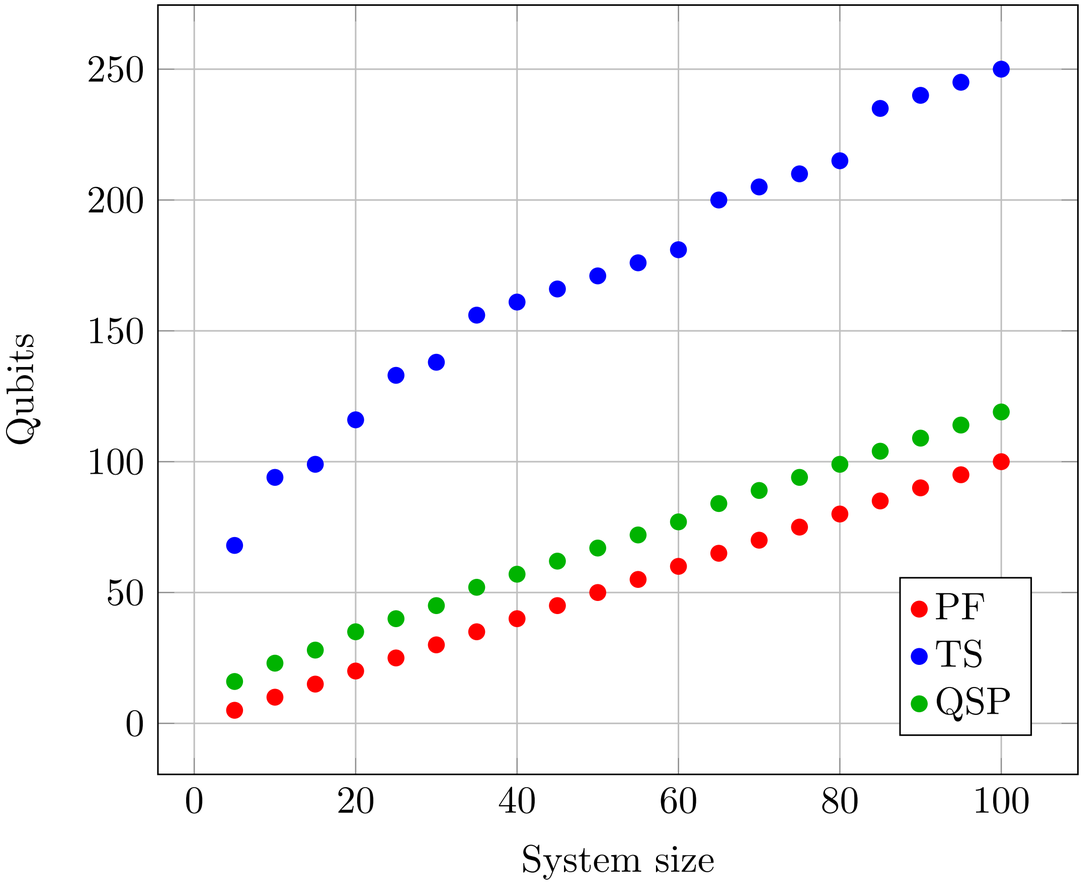


Bound	Order 1	2	4	6	8
● Analytic/Minimized	5	4	3.5	3.333	3.25
◌ Commutator	4	3.667	3.4	3.286	3.222
○ Empirical	2.964	2.883	2.555	2.311	2.141

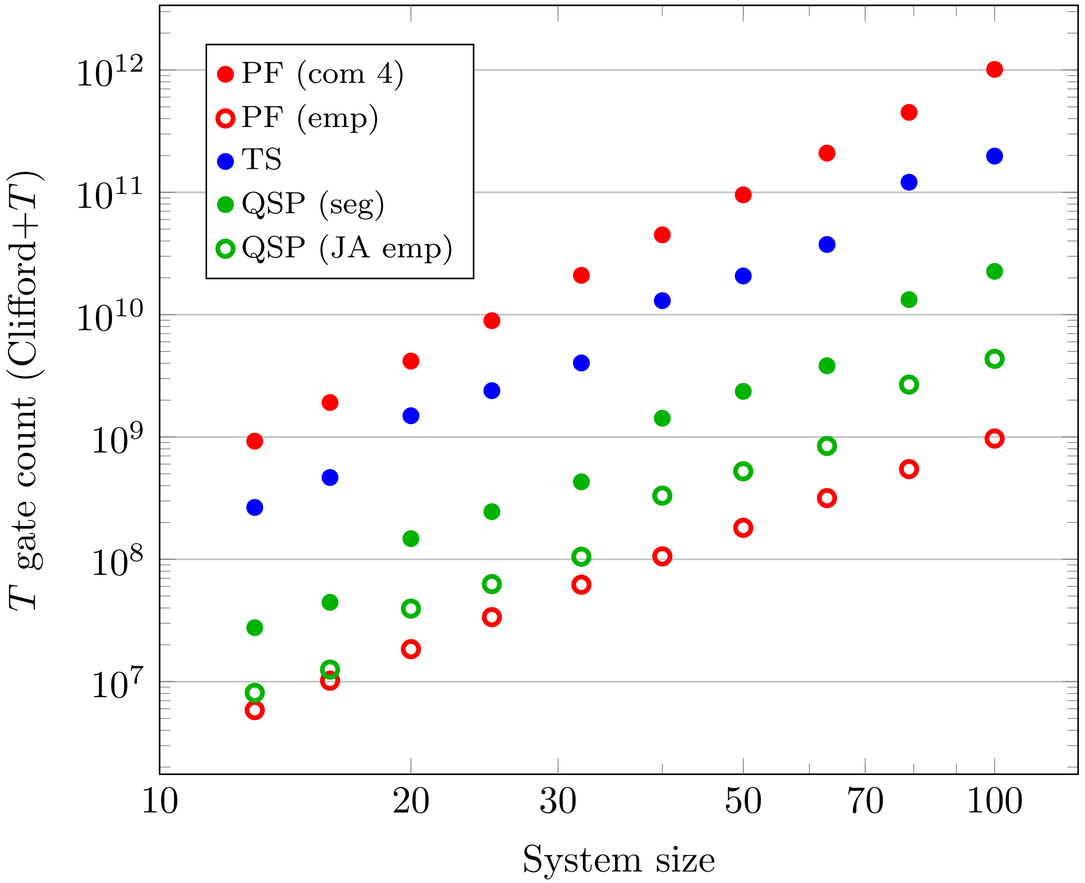


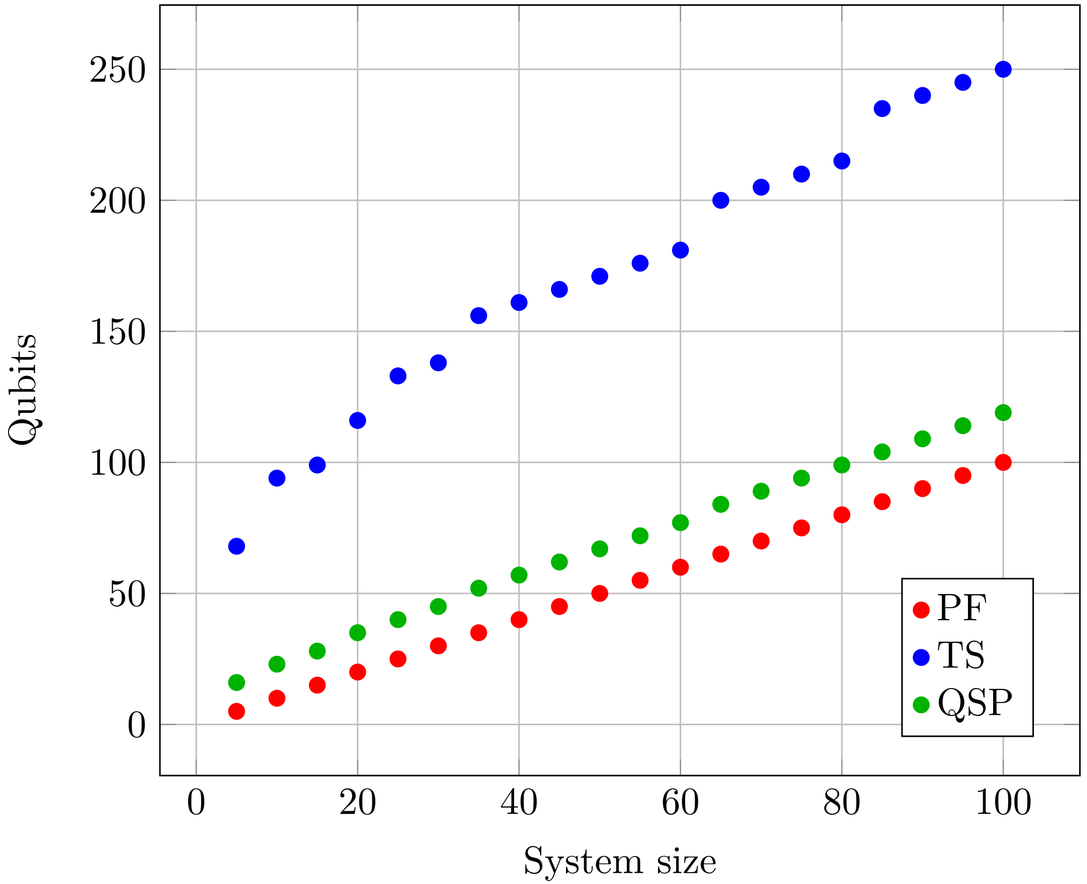
Resource estimates (physical level)



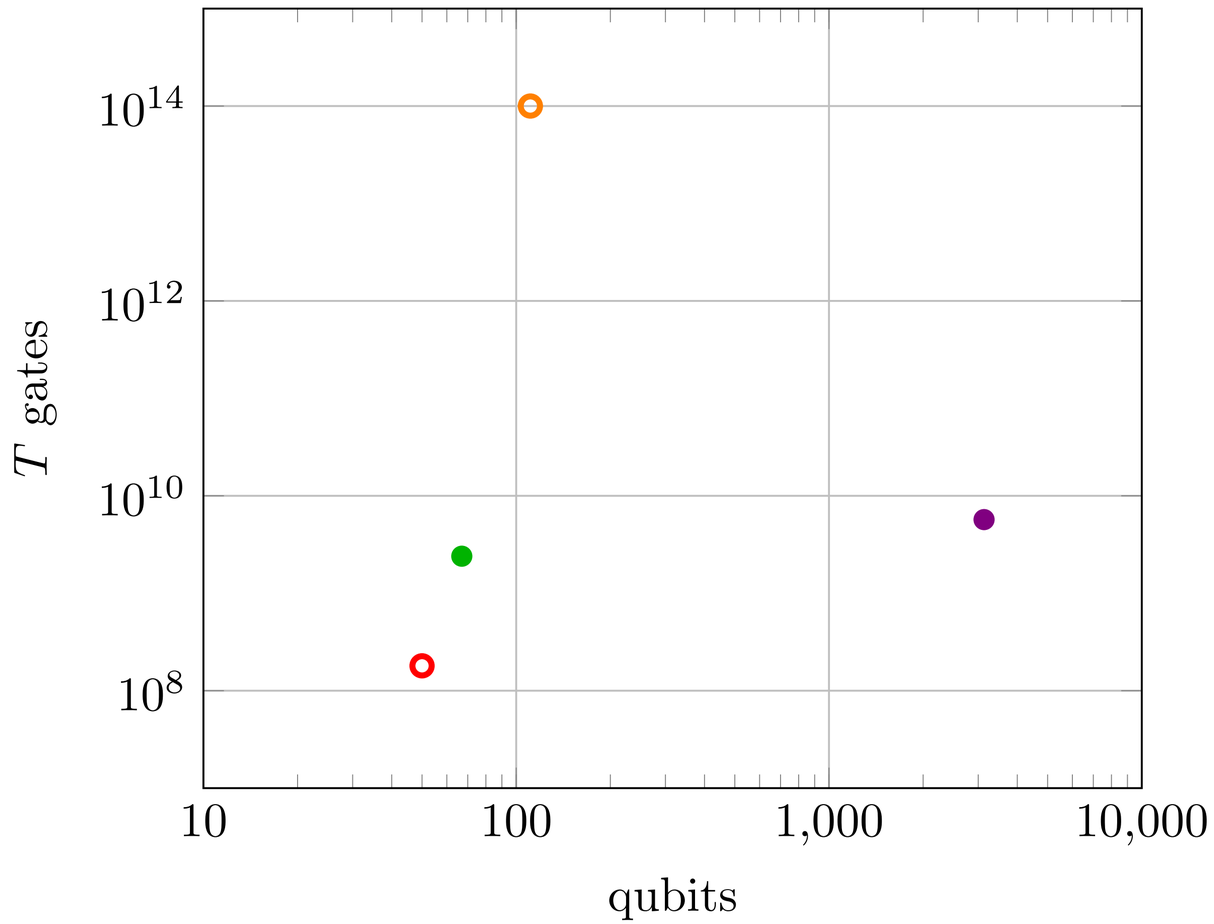


Resource estimates (logical level)





Comparisons



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

Simulating 50 spins (segmented QSP)

- 67 qubits
- 2.4×10^9 T gates

Simulating 50 spins (PF6 empirical)

- 50 qubits
- 1.8×10^8 T gates

Summary

This work establishes benchmarks for a simple quantum simulation that would be useful and that is classically hard.

Spin systems are much easier than factoring or quantum chemistry…

… but may still be out of reach of pre-fault tolerant digital quantum computers.

Higher-order product formulas are useful even at very small sizes.

Exisiting analysis of product formulas is very loose.

More sophisticated algorithms (especially quantum signal processing) are competitive at surprisingly small sizes and give the best approach with rigorous guarantees.

Outlook

Super-classical quantum simulation without invoking fault tolerance?

- Improved error bounds
- 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