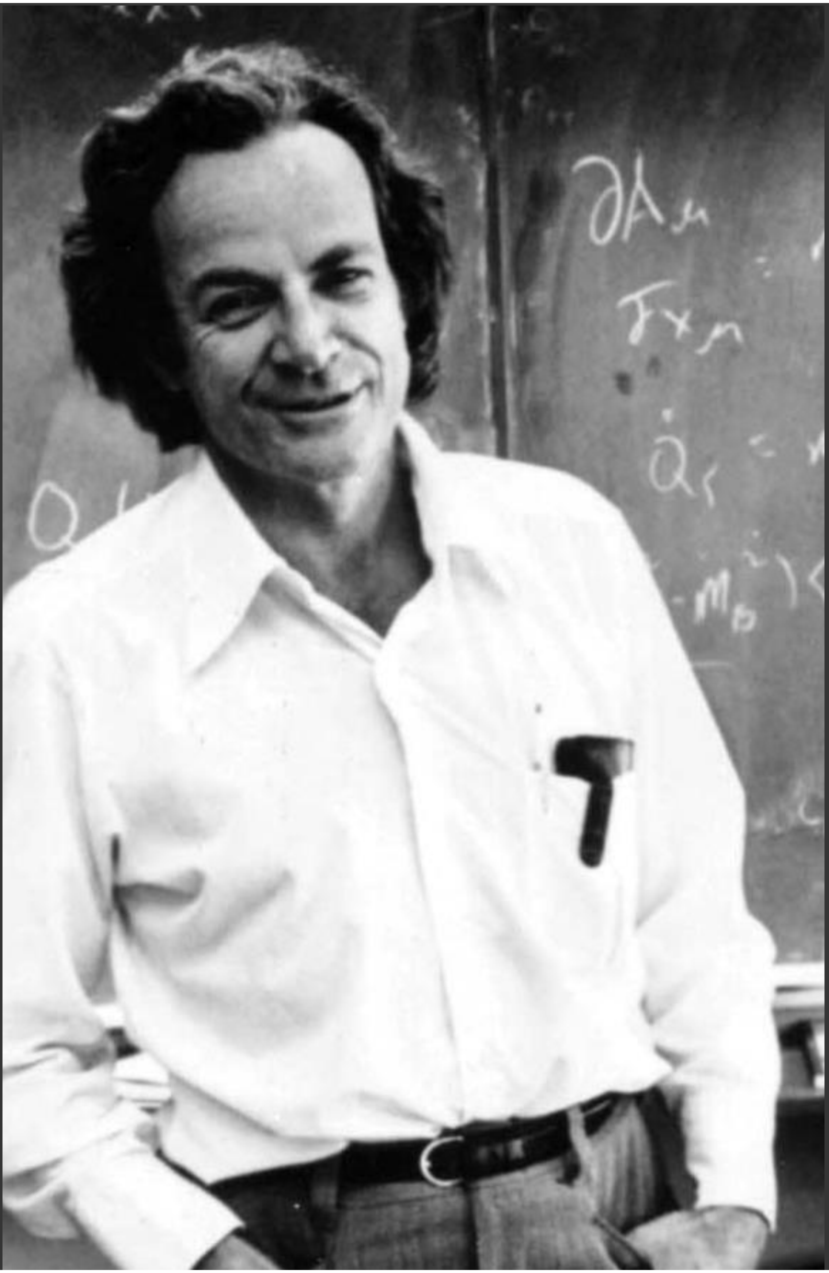
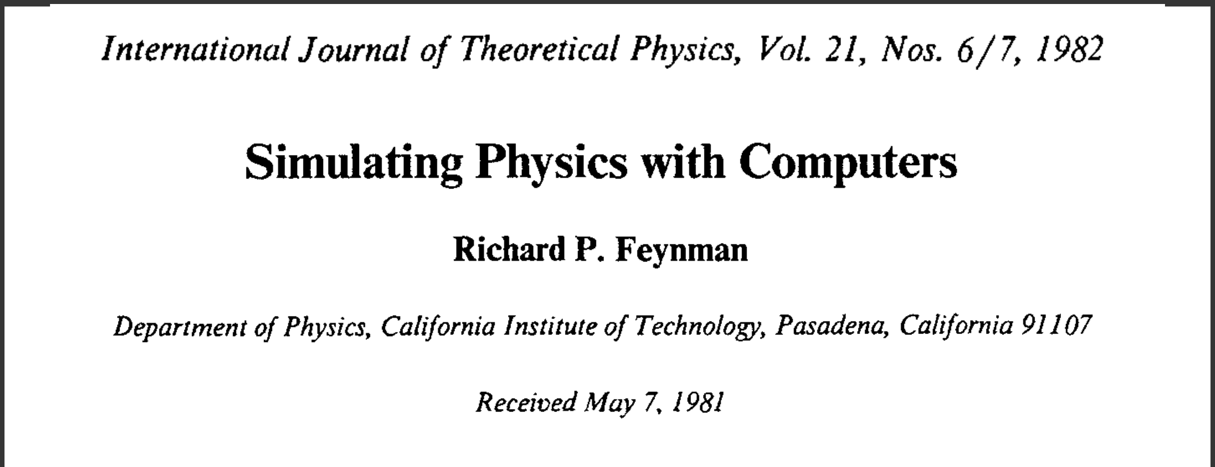
Microsoft

Quantum Algorithms for Many-Body Systems:

A chemistry and materials science perspective

Matthias Troyer





International Journal of Theoretical Physics, Vol. 21, Nos. 6/7, 1982

Simulating Physics with Computers

Richard P. Feynman

Department of Physics, California Institute of Technology, Pasadena, California 91107

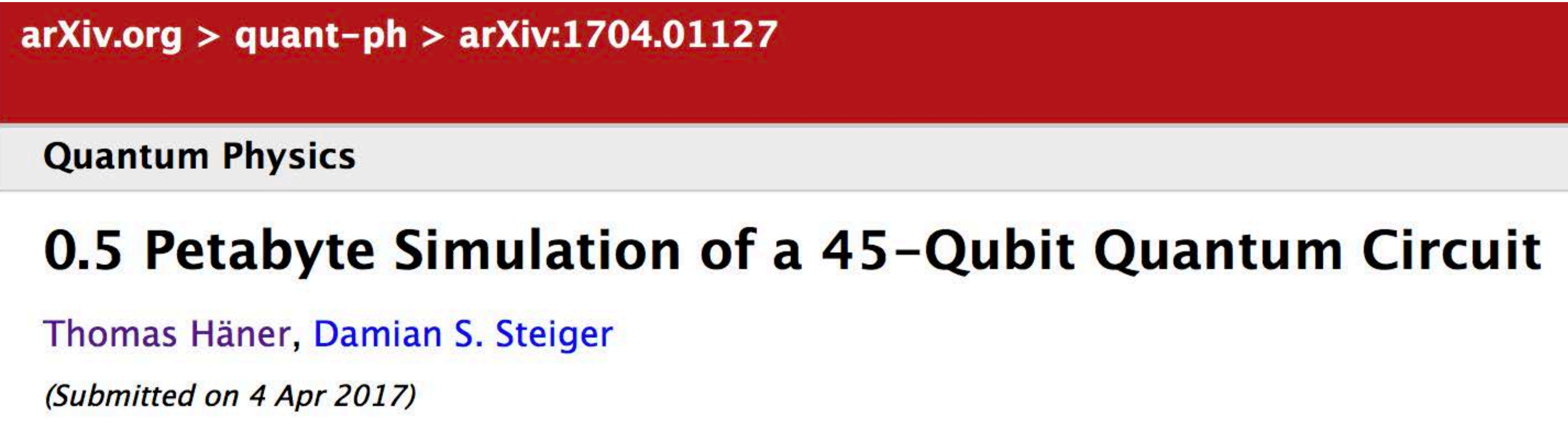
Received May 7, 1981

Feynman proposed to use quantum computers to simulate quantum physics

Simulating quantum computers on classical computers

Simulating a quantum gate acting on *N* qubits needs $O(2^N)$ memory and operations

Qubits	Memory	Time for one operation
10	16 kByte	microseconds on a smartwatch
20	16 MByte	milliseconds on smartphone
30	16 GByte	seconds on laptop
40	16 TByte	seconds on cluster
50	16 PByte	minutes on top supercomputers?
60	16 EByte	hours on exascale supercomputer?
70	16 ZByte	days on hypothetical future supercomputer?
…	…	…
250	size of visible universe	age of the universe



arXiv.org > quant-ph > arXiv:1704.01127

Quantum Physics

0.5 Petabyte Simulation of a 45-Qubit Quantum Circuit

Thomas Häner, Damian S. Steiger

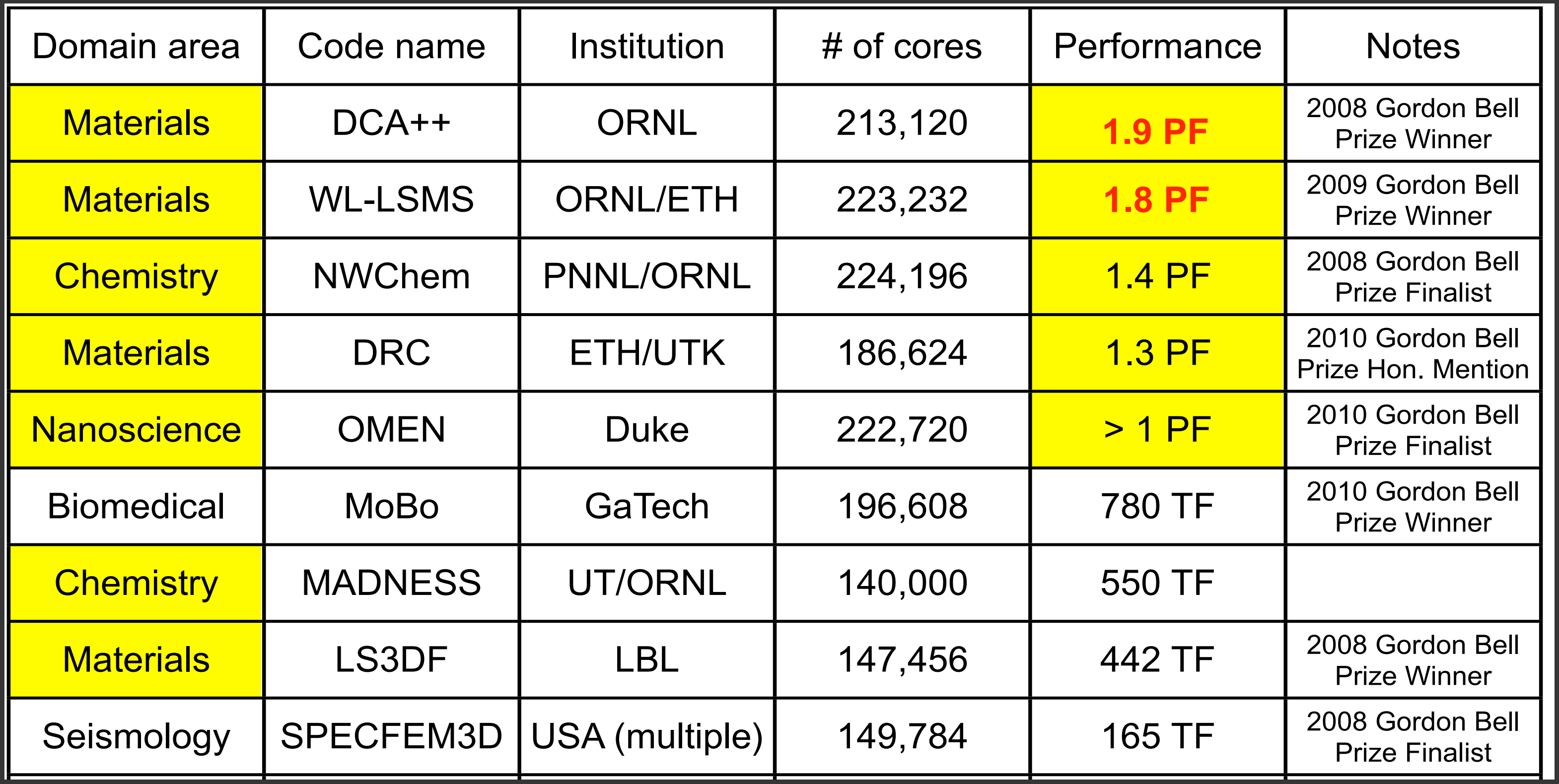
(Submitted on 4 Apr 2017)

HPC wire
Since 1987 - Covering the Fastest Computers in the World and the People Who Run Them
Home
Technologies
Sectors

DOE Supercomputer Achieves Record 45-Qubit Quantum Simulation

By Tiffany Trader

First applications that reached a petaflop on Jaguar @ ORNL



Domain area	Code name	Institution	# of cores	Performance	Notes
Materials	DCA++	ORNL	213,120	**1.9 PF**	2008 Gordon Bell Prize Winner
Materials	WL-LSMS	ORNL/ETH	223,232	**1.8 PF**	2009 Gordon Bell Prize Winner
Chemistry	NWChem	PNNL/ORNL	224,196	1.4 PF	2008 Gordon Bell Prize Finalist
Materials	DRC	ETH/UTK	186,624	1.3 PF	2010 Gordon Bell Prize Hon. Mention
Nanoscience	OMEN	Duke	222,720	> 1 PF	2010 Gordon Bell Prize Finalist
Biomedical	MoBo	GaTech	196,608	780 TF	2010 Gordon Bell Prize Winner
Chemistry	MADNESS	UT/ORNL	140,000	550 TF	
Materials	LS3DF	LBL	147,456	442 TF	2008 Gordon Bell Prize Winner
Seismology	SPECFEM3D	USA (multiple)	149,784	165 TF	2008 Gordon Bell Prize Finalist

Source: T. Schulthess

The Theory of Everything

Laughlin & Pines
PNAS 2000

The N-body Schrödinger equation

$$i\hbar\frac{\partial\Psi(\vec{r}_1,\ldots,\vec{r}_N,t)}{\partial t}=H\Psi(\vec{r}_1,\ldots,\vec{r}_N,t)$$

Describes (almost) everything we encounter in daily life with a very simple Hamilton

$$H=\sum_i\left(-\frac{1}{2m_i}\Delta_i+V^{ext}(\vec{r}_i)\right)+\sum_{i,j}\frac{q_iq_j}{|\vec{r}_i-\vec{r}_j|}$$

It is a simple linear partial differential equation (PDE)

But is exponentially complex since it lives in 3N dimensions

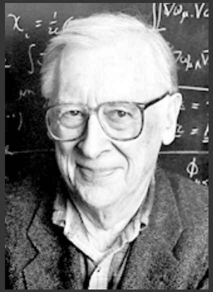
Density functional theory and quantum chemistry

Approximates the *N*-body Schrödinger by a tractable 1-body problem

$$E_0 = \min_{\rho(\vec{r})}\left(F[\rho] + \int d^3\vec{r}\,V(\vec{r})\rho(\vec{r})\right)$$

Successful in calculating properties
many metals, insulators, semiconductors

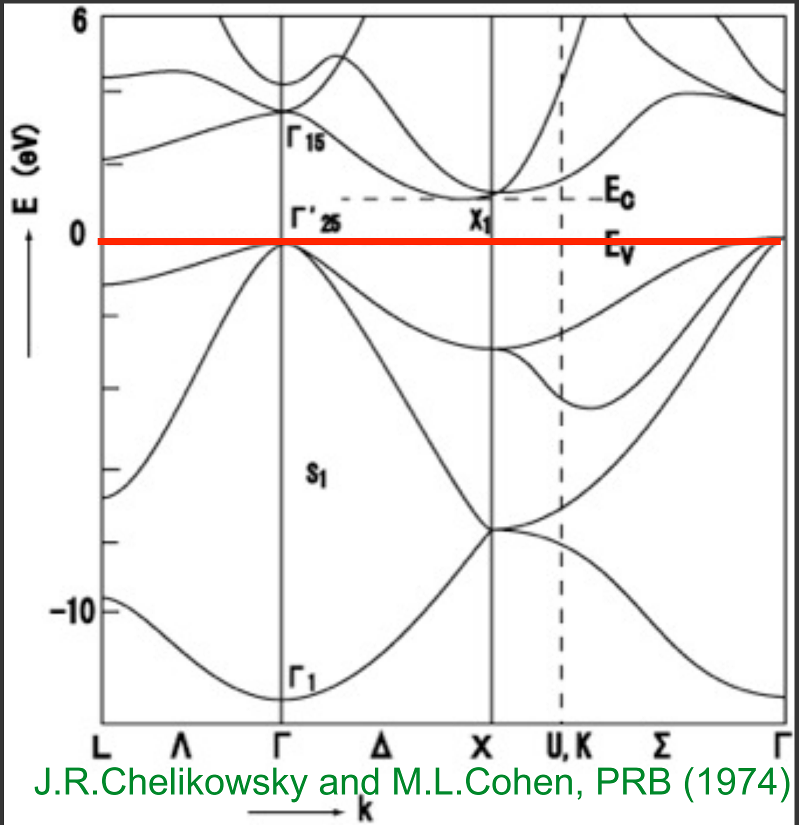
Walter Kohn



John A. Pople

1998 Nobel prize in chemistry

Band structure of silicon



J.R.Chelikowsky and M.L.Cohen, PRB (1974)

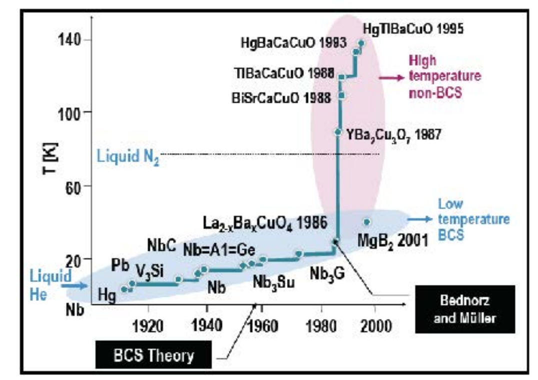
Cuprate high temperature superconductors

Undoped materials:

half-filled band and metal according to DFT

but antiferromagnetic insulator in experiment!

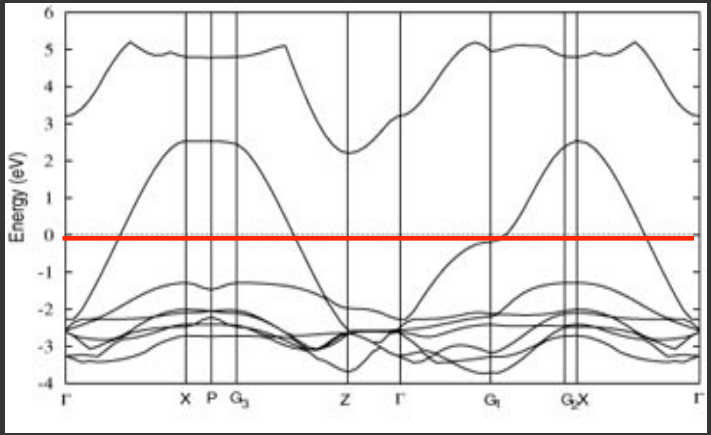
Band structure calculation breaks down!



Doped materials:
high-temperature superconductors

What causes superconductivity?

Are there room temperature superconductors?



Fermi level

Band structure of La_2CuO_4

Preparing the ground state

On a classical computer

Imaginary time projection

Power method or other iterative eigensolver

$$|\Psi_{GS}\rangle = \lim_{\tau\to\infty} e^{-\tau H}|\Psi_T\rangle$$

$$|\Psi_{GS}\rangle = \lim_{n\to\infty}(H-\Lambda)^n|\Psi_T\rangle$$

On a quantum computer

~~Imaginary time evolution~~

~~Power method~~

Unitary operations + measurements:

prepare trial state

projectively measure energy

obtain the ground state if
the ground state energy was measured

$$|\Psi_T\rangle$$

$$|\Psi_T\rangle \to |\phi_n\rangle \text{ with } H|\phi_n\rangle = E_n|\phi_n\rangle$$

$$|\phi_n\rangle \text{ picked with propability } |\langle\phi_n|\Psi_T\rangle|^2$$

Quantum phase estimation

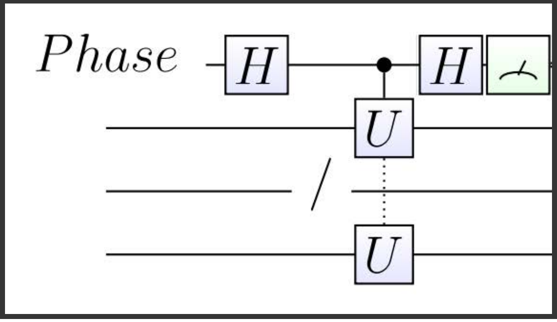
Energy can be measured through the phase of a wave function after unitary time evolution

$$U\left|\phi_n\right\rangle \equiv e^{-iHt}\left|\phi_n\right\rangle = e^{-iE_n t}\left|\phi_n\right\rangle = e^{-i\phi}\left|\phi_n\right\rangle$$

We can only measure relative phases, thus do a controlled evolution

$$|0\rangle|\phi_n\rangle \to \frac{1}{\sqrt{2}}\left(|0\rangle+|1\rangle\right)|\phi_n\rangle \to \frac{1}{\sqrt{2}}\left(|0\rangle|\phi_n\rangle+U|1\rangle|\phi_n\rangle\right)=\frac{1}{\sqrt{2}}\left(|0\rangle+e^{-i\phi}|1\rangle\right)|\phi_n\rangle \to \frac{1}{2}\left((1+e^{-i\phi})|0\rangle+(1-e^{-i\phi})|1\rangle\right)|\phi_n\rangle$$

Measure the ancilla qubit to obtain the phase



Solving quantum chemistry on a quantum computer

1. Select a finite (generally non-orthogonal) basis set

2. Perform a Hartree-Fock calculation to

   get an approximate solution

   get an orthogonal basis set

3. Find the true ground state of the Hamiltonian in this new basis set

$$H = \sum_{pq} t_{pq} c_p^\dagger c_q + \sum_{pqrs} V_{pqrs} c_p^\dagger c_q^\dagger c_r c_r$$

exact classical approach: full-configuration interaction

exponential complexity!

Solving quantum chemistry on a quantum computer

1. Select a finite (generally non-orthogonal) basis set

2. Perform a Hartree-Fock calculation to

   get an approximate solution

   get an orthogonal basis set

3. Find the true ground state of the Hamiltonian in this new basis set

$$H = \sum_{pq} t_{pq} c_p^\dagger c_q + \sum_{pqrs} V_{pqrs} c_p^\dagger c_q^\dagger c_r c_r$$

4. Prepare a good guess for the ground state

5. Perform quantum phase estimation to

   get the ground state wave function and energy

Representing fermion terms by quantum circuits

Map the occupation of each spin-orbital to the states of one qubit

$$|0\rangle = |\uparrow\rangle \qquad |1\rangle = |\downarrow\rangle$$

Density operators get mapped to Pauli matrices

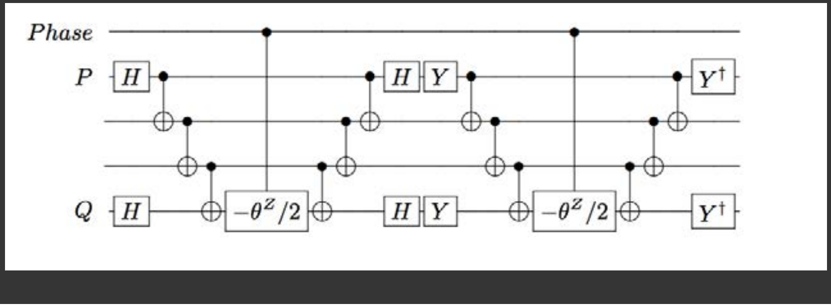
$$n_i = \frac{1}{2}\left(1-\sigma_i^z\right)$$

Hopping terms get mapped to spin flips with Jordan-Wigner strings

$$c_p^\dagger c_q = \sigma_p^- \prod_{i=p+1}^{q-1} \sigma_i^z \sigma_p^+$$

Time evolution gets mapped to circuits built from unitary gates

$$e^{-i\theta\left(c_p^\dagger c_q + c_q^\dagger c_p\right)} =$$



Guessing a good trial state

Mean field approximation

- Hartree-Fock
- Density functional theory

Variational approaches: fit parameters in variational ansatz

- Configuration-Interaction
- Variational Monte Carlo — McMillan, Phys. Rev (1965)
- Tensor network methods (e.g. DMRG) — White, Phys. Rev. Lett. (1992)
- Neural network states — Carleo & Troyer, Science (2017)

Preparing a good trial state

Adiabatic evolution from a simple initial Hamiltonian H_0 with known ground state to the desired Hamiltonian H_1

$$H(s) = (1 - s)H_0 + sH_1$$

Good starting Hamiltonians

- Mean-field approximation (with right broken symmetry)
- Non-interacting particles (in the right symmetry sector)

Cooling into a good trial state

Evolve the system coupled to a heat bath that is being cooled

See e.g. Kaplan, Klco, Roggero, arXiv:1709.08250

Monte Carlo sampling with the quantum Metropolis algorithm

- Use a unitary update + phase estimation to propose a new energy eigenstate
- Accept or reject according to the Metropolis algorithm
- Solves the sign problem of QMC by working with energy eigenstates

Temme et al, Nature (2011)

Simulating time evolution on quantum computers

There are O(N^4) interaction terms in an *N*-electron system

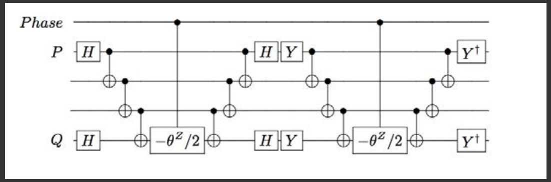
$$H = \sum_{pq} t_{pq} c_p^\dagger c_q + \sum_{pqrs} V_{pqrs} c_p^\dagger c_q^\dagger c_r c_r \equiv \sum_{m=1}^{M} H_m$$

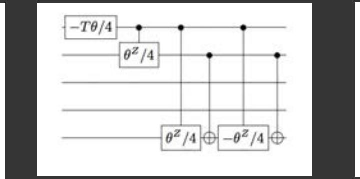
$M = O(N^4)$ terms

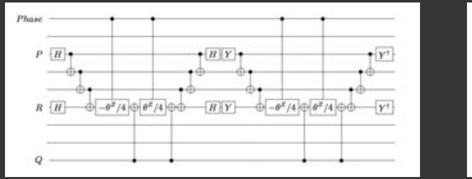
We need to evolve separately under each of them

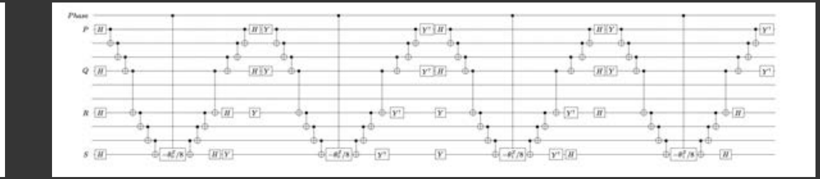
$$e^{-i\Delta t H} \approx \prod_{m=1}^{M} e^{-i\Delta\tau H_m}$$

Efficient circuits available for each of the N^4 terms









Runtime estimates turn out to be O(NM^2) = $O(N^9)$

It's efficient since it's polynomial!

The polynomial time quantum shock

Estimates for a benchmark molecule: Fe_2S_2 with 118 spin-orbitals

Gate count	10^{18}
Parallel circuit depth	10^{17}
Run time @ 100ns gate time	300 years

We cannot declare victory proving the existence of polynomial time algorithms

We need quantum software engineers to develop better algorithms and implementations

The result of quantum software optimization

Estimates for a benchmark molecule: Fe_2S_2 with 118 spin-orbitals

Gate count	10^{18}
Parallel circuit depth	10^{17}
Run time @ 100ns gate time	300 years

Reduced gate count	10^{11}
Parallel circuit depth	10^{10}
Run time @ 100ns gate time	20 minutes

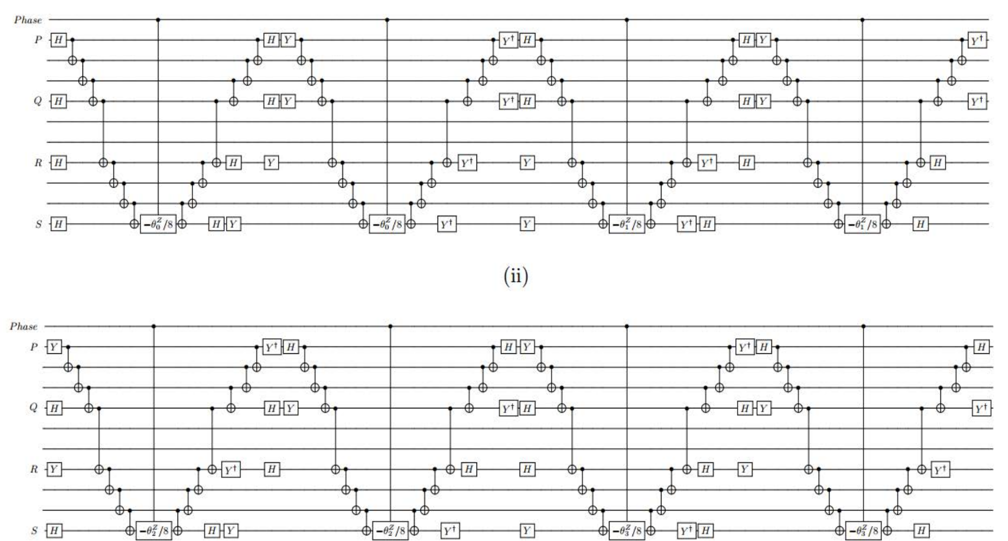
Attempting to reduce the horrendous runtime estimates we achieved
Wecker *et al*., PRA (2014), Hastings *et al*., QIC (2015), Poulin *et al*., QIC (2015)

Reuse of computations:	O(*N*) reduction in gates
Parallelization of terms:	O(*N*) reduction in circuit depth
Optimizing circuits:	4x reduction in gates
Smart interleaving of terms:	10x reduction in time steps
Multi-resolution time evolution:	10x reduction in gates
Better phase estimation algorithms:	4x reduction in rotation gates

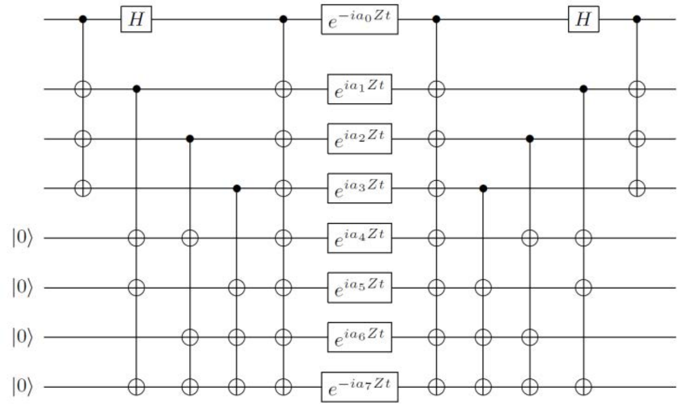
Improvements in algorithms

Original circuit

Improved circuit



(ii)



Reducing the number of terms

Reduce the number of terms in the evolution from O(N^4) to O(N^2) by using real-space representations and quantum Fourier transforms

First quantized formulation

Kivlichan, Wiebe, et al, J. Phys. A (2017)

requires expensive quantum arithmetic

Plane wave basis

Babbush, Wiebe, et al, arXiv:1706.00023

requires much larger number of basis states

Can the asymptotic advantages be realized with reasonable runtimes?

Avoiding the Trotter breakup

New quantum algorithms based on series expansions into sums of unitary operators have exponentially better error scaling

$$e^{-iH} \approx \sum_{-K}^{K} \alpha_k U^k$$

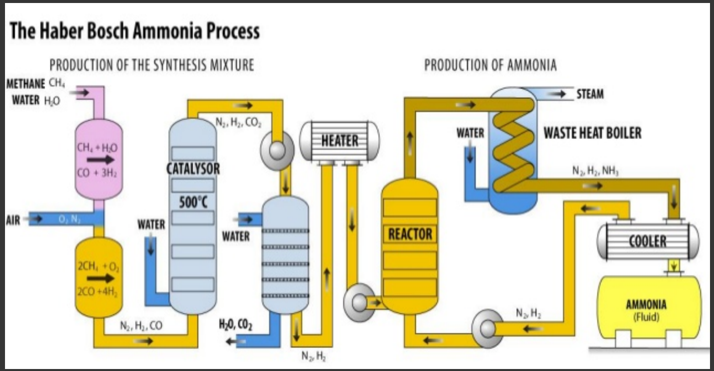
$$U = \sum_{m=1}^{M} \beta_m V_m$$

Childs & Wiebe, QIC (2012)
Berry *et al*, STOC'14
Low & Chuang, PRL (2017)
....

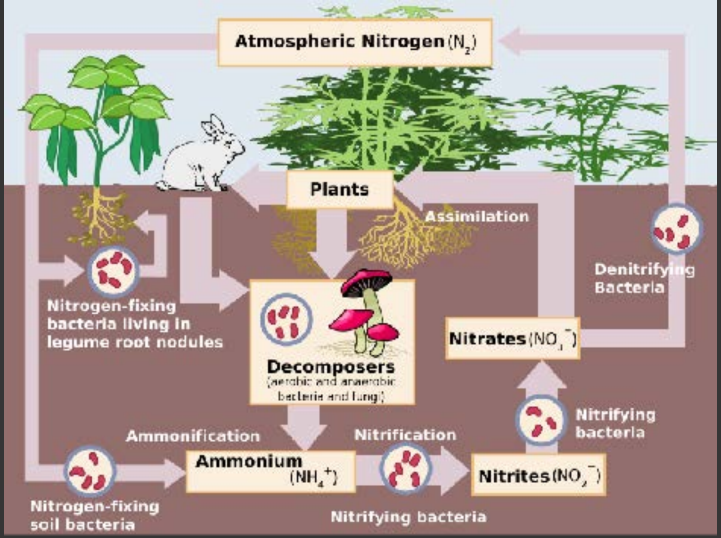
Are these methods advantageous given the unavoidable errors due to finite basis sets/lattice spacings?

Nitrogen fixation

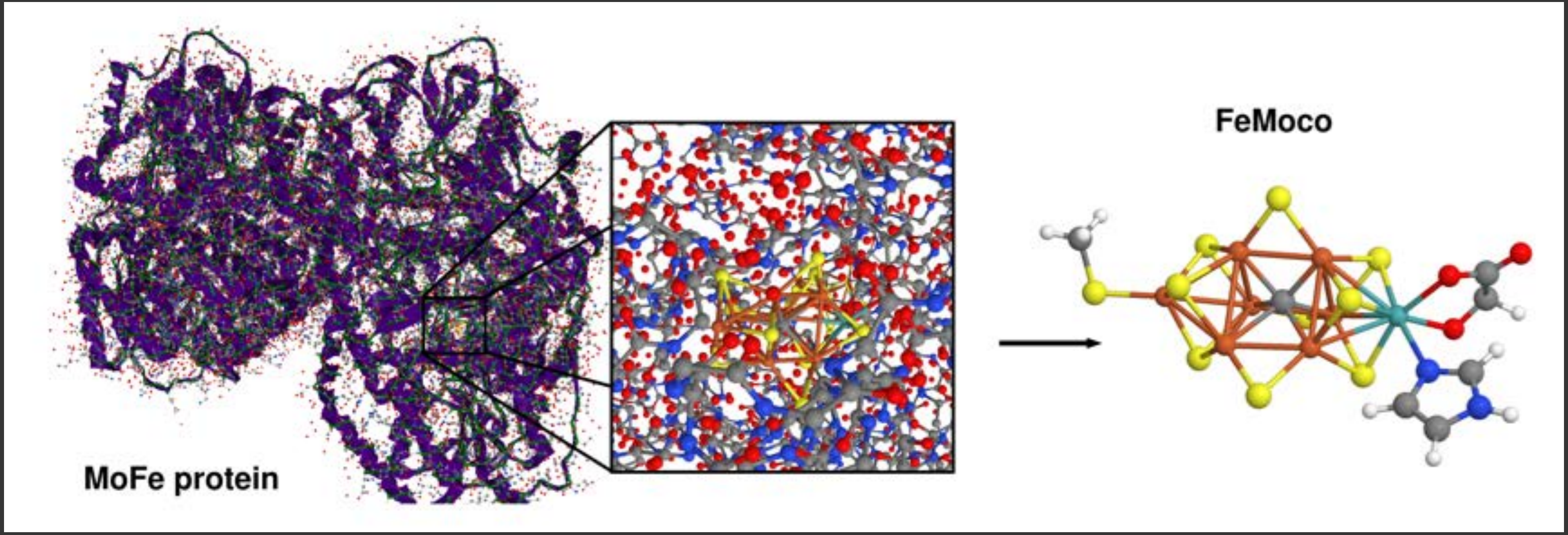
Fertilizer production using Haber-Bosch process needs 3% of the world’s natural gas production



But bacteria can do it in the soil without a huge factory!



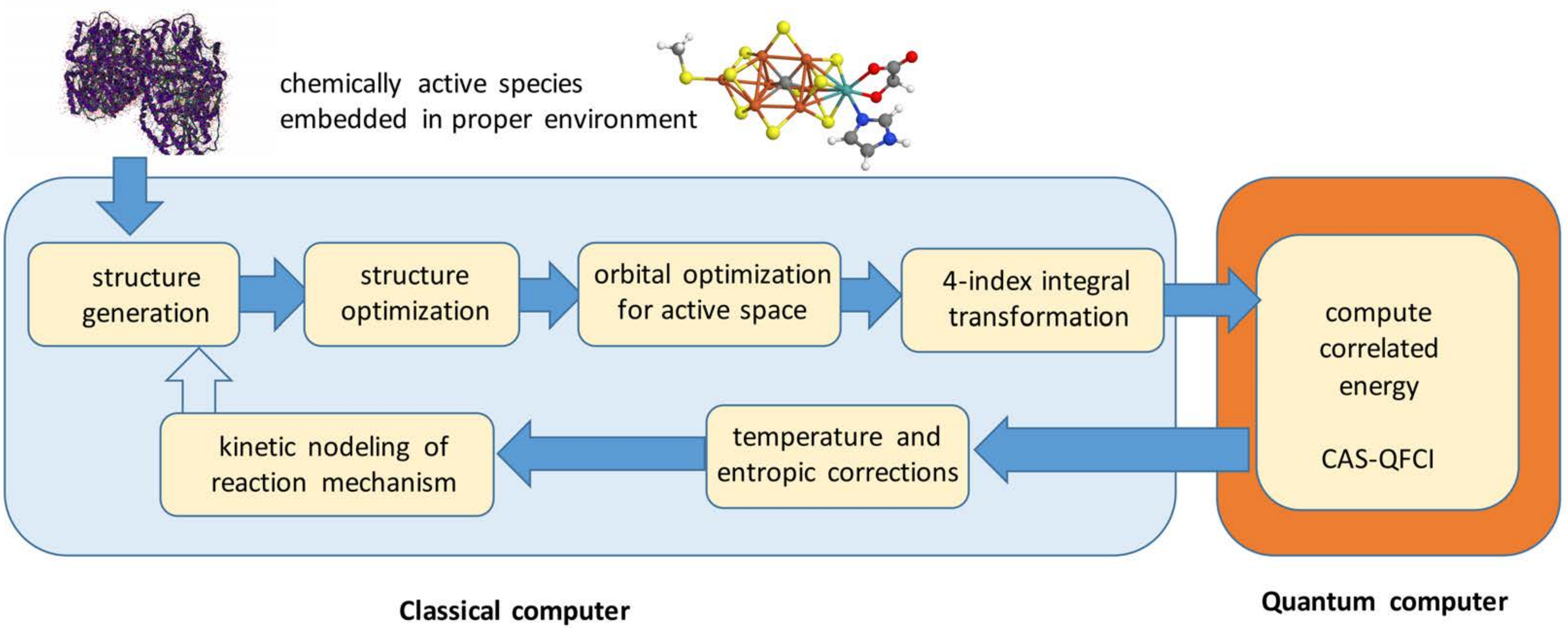
Understanding biological nitrogen fixation



Intractable on classical supercomputers

But a 200-qubit quantum computer will let us understand it

Simulation strategy



chemically active species embedded in proper environment

structure generation

structure optimization

orbital optimization for active space

4-index integral transformation

compute correlated energy

CAS-QFCI

temperature and entropic corrections

kinetic nodeling of reaction mechanism

Classical computer

Quantum computer

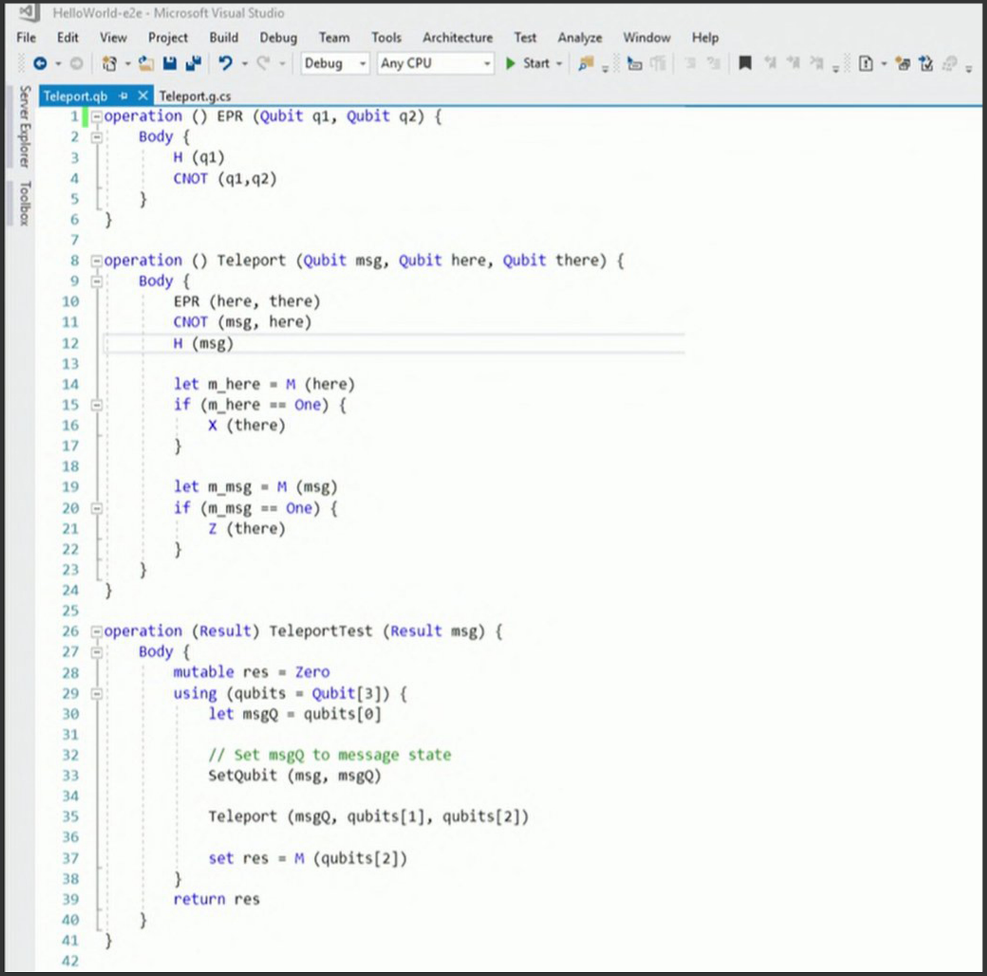
Quantum developer tools

Learn quantum programming

Develop quantum algorithms

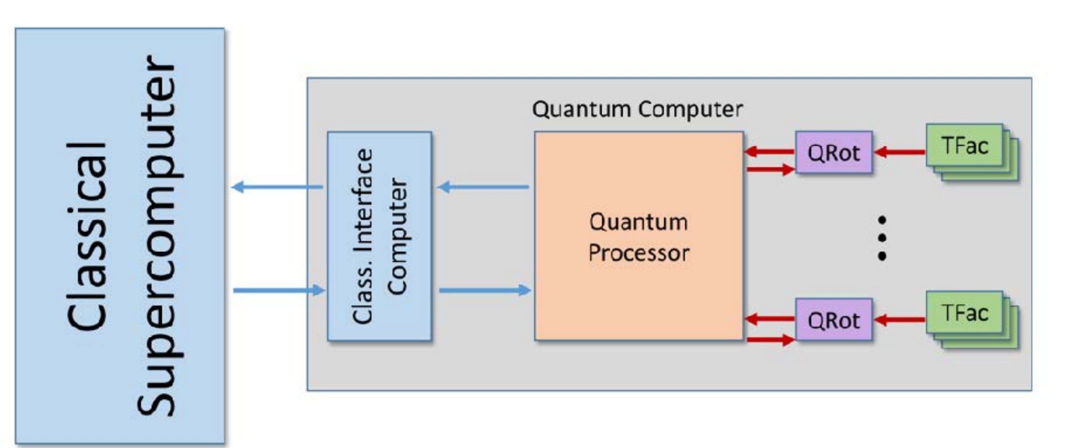
Estimate runtime and memory needs

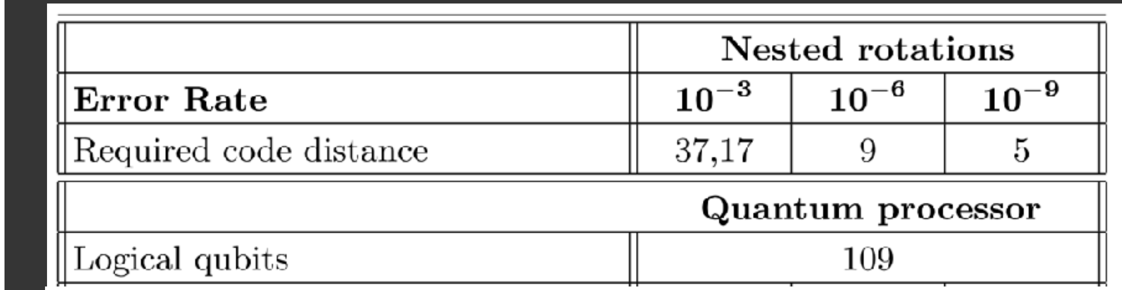
MICROSOFT.COM/QUANTUM



```
operation () EPR (Qubit q1, Qubit q2) {
    Body {
        H (q1)
        CNOT (q1,q2)
    }
}

operation () Teleport (Qubit msg, Qubit here, Qubit there) {
    Body {
        EPR (here, there)
        CNOT (msg, here)
        H (msg)

        let m_here = M (here)
        if (m_here == One) {
            X (there)
        }

        let m_msg = M (msg)
        if (m_msg == One) {
            Z (there)
        }
    }
}

operation (Result) TeleportTest (Result msg) {
    Body {
        mutable res = Zero
        using (qubits = Qubit[3]) {
            let msgQ = qubits[0]

            // Set msgQ to message state
            SetQubit (msg, msgQ)

            Teleport (msgQ, qubits[1], qubits[2])

            set res = M (qubits[2])
        }
        return res
    }
}

```

Total cost with error correction





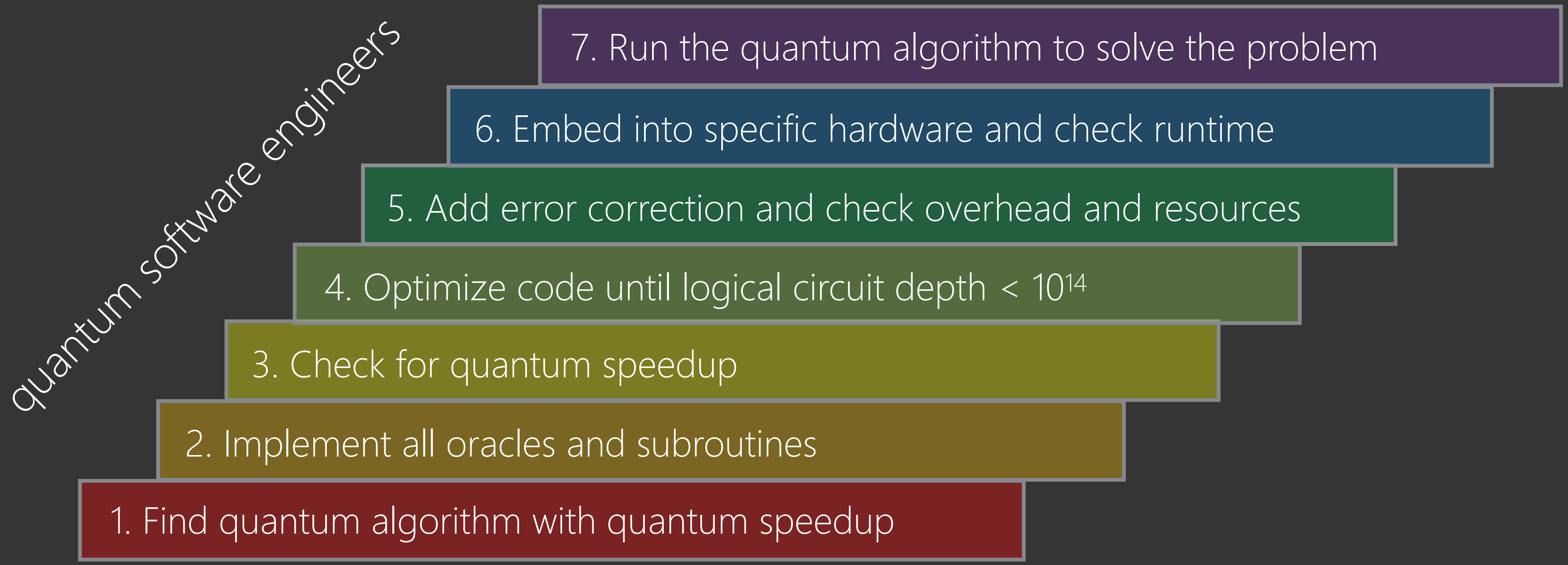
	Nested rotations		
Error Rate	**10^{-3}**	**10^{-6}**	**10^{-9}**
Required code distance	37,17	9	5
	Quantum processor		
Logical qubits	109		

We want very good qubits!

Better algorithms!

Better error correction and gate synthesis

Steps in software development for quantum applications



quantum software engineers

7. Run the quantum algorithm to solve the problem

6. Embed into specific hardware and check runtime

5. Add error correction and check overhead and resources

4. Optimize code until logical circuit depth < 10^{14}

3. Check for quantum speedup

2. Implement all oracles and subroutines

1. Find quantum algorithm with quantum speedup

Coming soon:

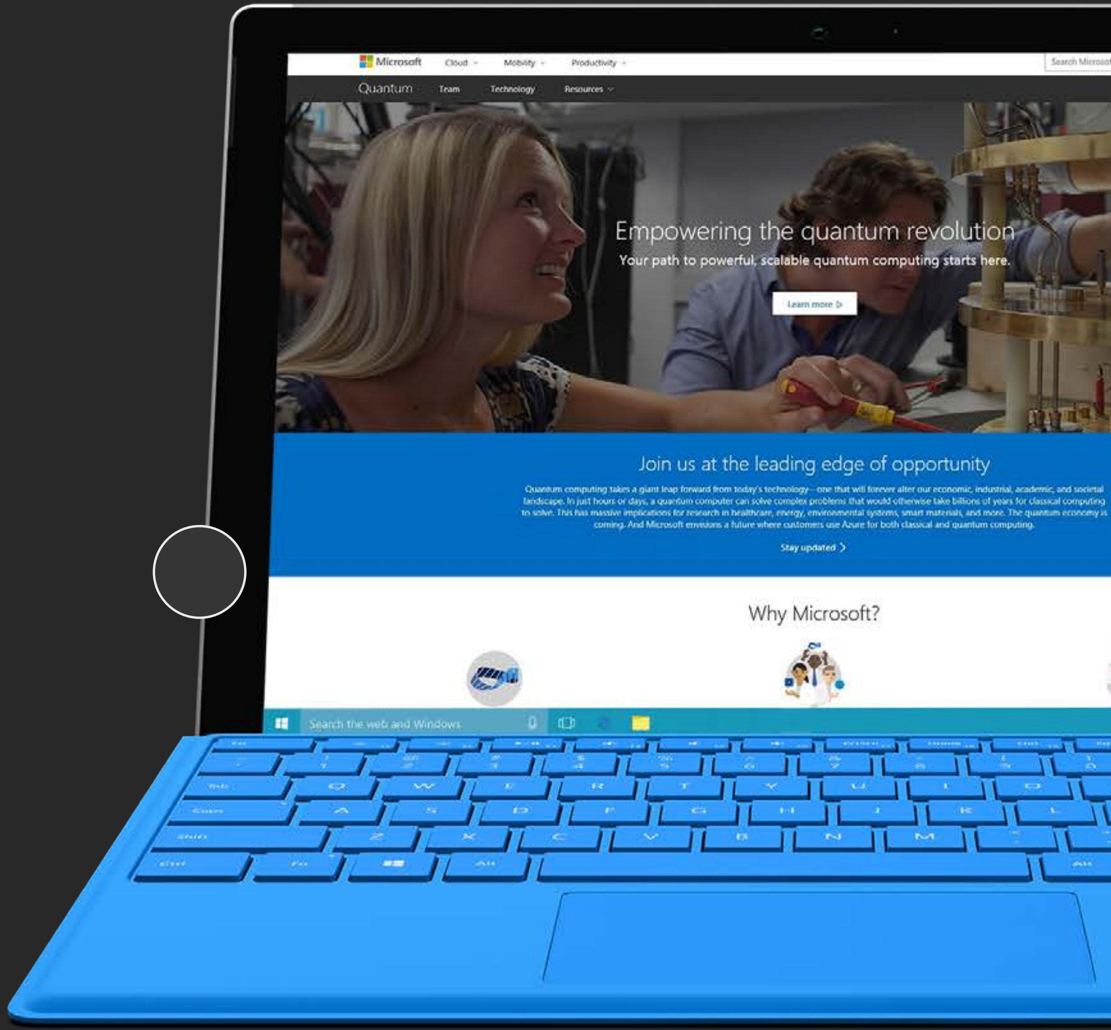
Quantum programming language

Visual Studio extensions

Quantum simulator

Learn more & sign up at:

MICROSOFT.COM/QUANTUM



Empowering the quantum revolution

Your path to powerful, scalable quantum computing starts here.

Join us at the leading edge of opportunity

Quantum computing takes a giant leap forward from today's technology—one that will forever alter our economic, industrial, academic, and societal landscape. In just hours or days, a quantum computer can solve complex problems that would otherwise take billions of years for classical computing to solve. This has massive implications for research in healthcare, energy, environmental systems, smart materials, and more. The quantum economy is coming. And Microsoft envisions a future where customers use Azure for both classical and quantum computing.

Why Microsoft?