Applications: If we had a quantum computer, what would we do with it?

Francesco Evangelista | Emory University
Who Am I?

• Ph.D. in theoretical chemistry. Do research in electronic structure theory (quantum chemistry)
• I work on new methods to describe chemical reactions/photochemistry
• I develop open-source software

An open-source suite of quantum chemistry methods for strongly correlated electrons

Can find me at:

- www.evangelistalab.org
- github.com/evangelistalab
- fevange@emory.edu
How I Got Into Quantum Computing

Quantum Chemistry for Quantum Computing

Classic-quantum hybrid algorithms for small quantum computers

Quantum algorithms for strongly correlated electrons

Kenneth Brown (ion traps, Duke)

you should read Nielsen and Chuang

Evangelista, Chan, Scuseria (2019)

Stair, Huang, Evangelista (submitted)

Forte

BAGEL

Shiozaki

Whitfield

Scuseria

Aspuru-Guzik

Chan

Zgid

pyscf

Evangelista, Chan, Scuseria (2019)

Stair, Huang, Evangelista (submitted)
Quantum Computation Landmarks

- Shor's factoring algorithm
- Large investment by private companies and govern.
- Quantum advantage
- Applications of QC
- Error Corrected QC

1994

Noisy Intermediate-Scale Quantum

2019

Future
The Market for Quantum Computing Is Growing Rapidly

Quantum gold rush: the private funding pouring into quantum start-ups

A *Nature* analysis explores the investors betting on quantum technology.

Cash for qubits

A growing number of quantum technology firms are raising cash from private investors, particularly in the sectors of quantum computing and quantum software.

**TOTAL VALUE OF DEALS** (US$, millions)

![Circle chart showing total value of deals from 2012 to 2018: 46, 67, 67, 18, 86, 278, 173.]

**LOCATION OF INVESTMENTS 2012–18** (US$, millions)

![Map showing locations of investments with numbers and names of companies.]

So What Will Quantum Computing Be Useful for?

- Predicting molecular properties and simulating chemical reactions
- Discovering new materials, optimizing existing ones
- Physics of many-body systems
- Breaking cryptographic systems (RSA)
- Machine learning
- Solving hard optimization problems

Quantum computer promise to make problems that are impossible to solve become routine by bringing exponential speedup
What Is Computation?

Computation is any type of calculation that includes both arithmetical and non-arithmetical steps and follows a well-defined model, for example an algorithm.

Computation is a physical process!

- Digital computers
- Analog computers
- Mechanical computers
- Quantum computers
- DNA computers
- Molecular computers
- ...
Example: Atomic States From a Mechanical Computer

A *Meccano* differential analyzer

Hartree (left) and Porter computing atomic orbitals (1935)

A modern day version
Quantum, Quantum, Quantum

In quantum physics particles are described by a wave function.

A particle propagating through a double slit can interfere with itself and give patterns typical of a wave.
Motivation: Simulating Quantum Physics

The state of a $N$-particle quantum system is highly-dimensional function

$$\Psi(r_1, r_2, \ldots, r_N)$$

Stationary states are described by Schrödinger’s equation

$$\hat{H} \Psi = E \Psi$$

\[
\hat{H} = -\frac{1}{2} \sum_i \nabla_i^2 + \sum_i V(r_i) + \sum_{i<j} g(r_i, r_j)
\]

- Kinetic energy
- External potential
- Particle-particle interactions
The Curse of Dimensionality

Classical problem: 5 particles moving in 2D (on a $8 \times 8$ grid)

Need to store velocity and position vectors for 5 particles (20 variables)
The Curse of Dimensionality

Quantum problem: 5 particles in 2D

\[ |\Psi\rangle = c_1 + c_2 + c_3 + c_4 + c_5 + \ldots \]

The full quantum state is specified by \textbf{7624512} numbers

With ten particles the problem becomes more challenging

A grid twice as dense makes it intractable

\[ \binom{64}{5} \approx 8 \times 10^6 \]
\[ \binom{64}{10} \approx 1.5 \times 10^{11} \]
\[ \binom{256}{10} \approx 2.8 \times 10^{17} \]
Moore’s Law

Every two years the transistor count has doubled. This means at best the number of operations, however, has not increased exponentially, lately. Hardware has hit physical limitations!
Simulating Nature With Quantum Mechanical Elements

If nature is not classical, why try to simulate it with classical computers?

“[...], how can we simulate quantum mechanics? [...] Let the computer itself be built of quantum mechanical elements which obey quantum mechanical laws.”

Richard P. Feynman

Department of Physics, California Institute of Technology, Pasadena, California 91107
Translating Feynman’s Idea: Quantum Simulation

Use cold atomic gasses trapped in an external potential to do quantum simulations

Material with interesting properties → \( \hat{H}_{\text{model}} \) → Interactions are tuned to reproduce the model.
Qubits and the *Digital* Quantum Computing Model

One qubit

\[ \{0,1\} \rightarrow |\Psi\rangle = \alpha |0\rangle + \beta |1\rangle \]

Classic bit  Quantum bit (qubit)

Two qubits

\[ \{00,01,10,11\} \rightarrow |\Psi\rangle = c_1 |00\rangle + c_2 |01\rangle + c_3 |10\rangle + c_4 |11\rangle \]

Two classic bits  Two quantum bits
The Digital Quantum Computer Model

Classical digital computer

Quantum gates

|101⟩ → Classical gates → |110⟩

3 bits = 1 state

Quantum digital computer

Quantum gates

|Ψ⟩ = C₀|000⟩ + C₁|001⟩ + C₂|010⟩ + C₃|011⟩ + C₄|100⟩ + C₅|101⟩ + C₆|110⟩ + C₇|111⟩

3 qubits = 2³ = 8 states

Classical gates

Quantum gates

|Ψ’⟩ = C₀'|000⟩ + C₁'|001⟩ + C₂'|010⟩ + C₃'|011⟩ + C₄'|100⟩ + C₅'|101⟩ + C₆'|110⟩ + C₇'|111⟩

The Quantum Advantage

- Quantum algorithms are discrete unitary circuits
- The purpose is general, can implement any quantum algorithm

- Can represent a vector in a state of 2ⁿ elements with n quantum bits
- Can apply operations to all of these elements in fixed amount of time
- Ways exist to control error
Quantum Computing and Exponential Speedup

A quantum computer with $K$ qubits (spins, two-level states)

$$|\Psi_{QC}\rangle = \sum_{q_1 q_2 \cdots q_K} \{0,1\} C_{q_1 \cdots q_K} |q_1 \cdots q_K\rangle$$

Spans a space of $2^K$ configurations

How precisely does this property translate into a computational advantage?

http://www.smbc-comics.com/comic/the-talk-3
Quantum Computation Workflow

Prepare an initial state

\[ |\Psi_{\text{initial}}\rangle \]

Apply quantum gates

A series of unitary operations that modify the state. Parameters of the problem will enter here (e.g. strength of interactions of electrons)

Apply quantum gates

\[ q_1 \]
\[ \vdots \]
\[ q_K \]

Perform a measurement on the registers

The quantum state “collapses” to one classical configuration of qubits

\[ |\Psi_{\text{measure}}\rangle = |10\ldots11\rangle \]

This is where we extract information. Measurement destroys the state we produced 😞
Quantum Computing and Exponential Speedup

A quantum computer with $K$ qubits (spins, two-level states)

$$|\Psi_{QC}\rangle = \sum_{q_1 q_2 \cdots q_K} \{0,1\} C_{q_1 \cdots q_K} |q_1 \cdots q_K\rangle$$

Spans a space of $2^K$ configurations

In quantum computing, the whole idea is just to choreograph a pattern of interference where the paths leading to each wrong answer interfere destructively and cancel out, while the paths leading to the right answer reinforce each other.

And that gives your computer a huge speed boost!

Well, we only know how to do that for a few special problems.

The important thing for you to understand is that quantum computing isn’t just a matter of trying all the answers in parallel.
Quantum algorithm for the recommendation problem (a ML problem) achieves exponential speedup.

Tang “de-quantized” it and produced a classical randomized algorithm that is only polynomially slower.

A quantum-inspired classical algorithm for recommendation systems

Ewin Tang

May 10, 2019

Abstract

We give a classical analogue to Koremidis and Prakash’s quantum recommendation system, previously believed to be one of the strongest candidates for provably exponential speedups in quantum machine learning. Our main result is an algorithm that, given an $m \times n$ matrix in a data structure supporting certain $\ell^p$-norm sampling operations, outputs an $\ell^2$-norm sample from a rank-$k$ approximation of that matrix in time $O(\text{poly}(k)\log(mn))$, only polynomially slower than the quantum algorithm. As a consequence, Koremidis and Prakash’s algorithm does not in fact give an exponential speedup over classical algorithms. Further, under strong input assumptions, the classical recommendation system resulting from our algorithm produces recommendations exponentially faster than previous classical systems, which run in time linear in $m$ and $n$.
What Are Good Problems for Quantum Computing?

Prepare an initial state $|\Psi_{\text{initial}}\rangle$

Apply quantum gates

Perform a measurement on the registers

Computational cost is determined by the number of gates applied. The gate count reflects the number of parameters in the problem (e.g. elements of a matrix)

Good problems require few measurements
An Example of a Quantum-Friendly Problem

Solving a linear system with a classical algorithm

\[ Ax = b \]

Quantum version of the problem

\[ \hat{A} |x\rangle = |b\rangle \]

Readout of the components of \( x \) is expensive on a quantum computer

\[ x_i \]

On a quantum computer it is easier to find the component of \( x \) with the largest magnitude

\[ \arg \max_i |x_i| \]
How Many Qubits To Make a Difference?

Nitrogen fixation in bacteria (catalysis)

Nitrogenase FeMo cofactor (Fe$_7$MoS$_9$C)

> 100 qubits

Table 1. Simulation time estimates

<table>
<thead>
<tr>
<th>Structure</th>
<th>T gates</th>
<th>Cl. gates</th>
<th>$\Delta t$ (10 ns)</th>
<th>$\Delta t$ (100 ns)</th>
<th>Qubits</th>
</tr>
</thead>
<tbody>
<tr>
<td>Quantitatively accurate simulation (0.1 mHa)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Structure 1</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Serial</td>
<td>$1.1 \times 10^{15}$</td>
<td>$1.7 \times 10^{15}$</td>
<td>130 d</td>
<td>3.6 y</td>
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<tr>
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<td>$3.5 \times 10^{15}$</td>
<td>$5.7 \times 10^{15}$</td>
<td>15 d</td>
<td>4.9 mo</td>
<td>135</td>
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<tr>
<td>PAR</td>
<td>$3.1 \times 10^{16}$</td>
<td>$3.1 \times 10^{16}$</td>
<td>110 h</td>
<td>1.5 mo</td>
<td>1,982</td>
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<tr>
<td>Structure 2</td>
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<td></td>
<td></td>
<td></td>
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<td>210 h</td>
<td>2.9 mo</td>
<td>2,024</td>
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<tr>
<td>Qualitatively accurate simulation (1 mHa)</td>
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<tr>
<td>Structure 1</td>
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<tr>
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<tr>
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<td>1.4 d</td>
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<td>$3.0 \times 10^{15}$</td>
<td>11 h</td>
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<td>1,982</td>
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<tr>
<td>PAR</td>
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<td>$5.5 \times 10^{15}$</td>
<td>20 h</td>
<td>8.3 d</td>
<td>2,024</td>
</tr>
</tbody>
</table>

Assuming perfect qubits
So, When Will Be Able To Start?

1. HOW’S YOUR QUANTUM COMPUTER PROTOTYPE COMING ALONG?
   GREAT!

2. THE PROJECT EXISTS IN A SIMULTANEOUS STATE OF BEING BOTH TOTALLY SUCCESSFUL AND NOT EVEN STARTED.

3. CAN I OBSERVE IT?
   THAT’S A TRICKY QUESTION.
Molecular Modeling (Chemistry) and Materials Science

We want to predict properties and understand chemical reactivity

Outcomes
- Design catalysts to perform new reactions
- Optimize existing catalytic processes

Design molecular structures with specific functionality

Outcomes
- Drug design
- Use earth abundant metals to perform catalysis
- Reduce the energy footprint of chemical processes
- Increase energy conversion efficiency in solar cells
Haber-Bosch reaction (production of ammonia)

\[ \text{N}_2 + 3\text{H}_2 \rightarrow 2\text{NH}_3 \]

Catalyst: Iron with K$_2$O, CaO, SiO$_2$, and Al$_2$O$_3$
Pressure: 150–250 atm
Temperature: 400–500 °C (752–932 °F)
Consumes 1-2% of world energy production

Nitrogen fixing bacteria

\[ \text{N}_2 + 16 \text{ATP} + 8 \text{e}^- + 8\text{H}^+ \rightarrow 2\text{NH}_3 + \text{H}_2 + 16 \text{ADP} + 16 \text{P}_i \]
Pressure: 1 bar
Temperature: 0-40
Chemistry and the Quantum Many-Body Problem

Coulomb repulsion between electrons makes the wave function quite complicated!

One electron

\[ \Psi(x_1) : \mathbb{R}^3 \rightarrow \mathbb{C} \]

Orbitals

\[ \Psi(x_1, x_2, \ldots, x_N) : \mathbb{R}^{3N} \rightarrow \mathbb{C} \]

\[ e^- \quad e^- \quad e^- \quad e^- \]

\[ \gamma \]

electron 1
electron 2
nucleus
Mapping the Complexity/Size Landscape

- **Complexity of electronic structure**
- **Photochemistry of small molecules** (near-degenerate states)
- **Transition metal complexes** (spin states)
- **Chemistry on nanoparticles** (many states)
- **Conjugated polymers**
- **Astrochemistry/Combustion**
- **Metalloenzymes (catalysis)**
- **Protein folding**

### Examples
- 

\[
\begin{align*}
\text{CT lifetime} & \approx 100 \text{ ps} \\
[\text{Fe(btz)}_3]^{3+}
\end{align*}
\]
Mapping the Complexity/Size Landscape

- **Complexity of electronic structure**
  - Photochemistry of small molecules (near-degenerate states)
  - Transition metal complexes (spin states)
  - Chemistry on nanoparticles (many states)
  - Conjugated polymers
  - Protein folding

- **Methods**
  - Exact (FCI)
  - Tensor Network States
  - Many-body methods
  - Astrochemistry/Combustion
  - DFT

- **Chemistry on nanoparticles (many states)**
  - Metalloenzymes (catalysis)

- **Photochemistry of small molecules (near-degenerate states)**
  - Near-degenerate states

- **Transition metal complexes (spin states)**
  - Spin states

- **Conjugated polymers**
  - Polymers

- **Protein folding**
  - Folding states

- **Metalloenzymes (catalysis)**
  - Catalysis
An equivalent representation is as a (linear) combination of configurations of electrons in orbitals

$$|\Psi\rangle = \sum_{I} C_{I} |\Phi_{I}\rangle = \sum_{i_1<i_2<\ldots<i_N}^{K} C_{i_1i_2\ldots i_N} |\varphi_{i_1}\varphi_{i_2}\ldots \varphi_{i_N}\rangle$$

Coefficient of an electron configuration (unknown)
An equivalent representation is as a (linear) combination of configurations of electrons in orbitals

$$|\Psi\rangle = \sum_{I} C_I |\Phi_I\rangle = \sum_{i_1<i_2<\ldots<i_N} C_{i_1 i_2 \ldots i_N} |\varphi_{i_1} \varphi_{i_2} \ldots \varphi_{i_N}\rangle$$

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Coefficient of an electron configuration (unknown)
Chemistry and the Quantum Many-Body Problem

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\]

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$$|\Psi\rangle = \sum_I C_I |\Phi_I\rangle = \sum_{i_1<i_2<...<i_N}^{K} C_{i_1i_2...i_N} |\varphi_{i_1}\varphi_{i_2}...\varphi_{i_N}\rangle$$

Coefficient of an electron configuration (unknown)
An equivalent representation is as a (linear) combination of configurations of electrons in orbitals

$$|\Psi\rangle = \sum_{I} C_I |\Phi_I\rangle = \sum_{i_1<i_2<\ldots<i_N}^{K} C_{i_1i_2\ldots i_N} |\varphi_{i_1}\varphi_{i_2}\ldots\varphi_{i_N}\rangle$$

Coefficient of an electron configuration (unknown)

$$|\Psi\rangle = c_0 + c_S \ldots + c_D \ldots$$

Mean field (MO picture)  Orbital relaxation  2-electron correlation

# of configurations = $\binom{K}{N}$
Quantum Algorithms for Quantum Field Theories

Stephen P. Jordan,1,4 Keith S. M. Lee,2 John Preskill3

Quantum field theory reconciles quantum mechanics and special relativity, and plays a central role in many areas of physics. We developed a quantum algorithm to compute relativistic scattering probabilities in a massive quantum field theory with quartic self-interactions (φ4 theory) in spacetime of four and fewer dimensions. Its run time is polynomial in the number of particles, their energy, and the desired precision, and applies at both weak and strong coupling. In the strong-coupling and high-precision regimes, our quantum algorithm achieves exponential speedup over the fastest known classical algorithm.

Editors' Suggestion: Featured in Physics

Cloud Quantum Computing of an Atomic Nucleus

E. F. Dumitrescu,1 A. J. McCauley,2 G. Hagen,1,4 G. R. Jansen,1,3 T. D. Morris,1,3 T. Papenbrock,1,3,5 R. C. Pooser,1,4 D. J. Dean,1 and P. Longowski1,3

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(Received 12 January 2018; published 23 May 2018)

We report a quantum simulation of the deuteron binding energy on quantum processors accessed via cloud servers. We use a Hamiltonian mean-field effective field theory at leading order. We design a low-depth version of the unitary coupled-cluster ansatz, use the variational quantum eigensolver algorithm, and compute the binding energy to within a few percent. Our work is the first step towards scalable nuclear structure computations on a quantum processor via the cloud, and it sheds light on how to map scientific computing applications onto near-term quantum devices.

DOI: 10.1103/PhysRevLett.120.210501
Quantum computing offers a different way to tackle certain types of hard computational problems.

Quantum advantage is not trivial and might require formulating a problem in a different way.

Quantum computing is likely to have the largest impact on problems related to quantum simulations, optimization, and machine learning.

There is still so much we do not know about the potential and limitations of quantum computing.

Thank You for Your Attention! I Look Forward to Your Questions
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Zgid
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Chan

Quantum Algorithms for Quantum Chemistry
Thrust III
Evangelista
(Lead)
Shiozaki
Whitfield
Scuseria
Zgid
Aspuru-Guzik
Chan

BAGEL

Forté

Funding

Software
And Many More ...

Optimization

Monte Carlo Simulations

Machine Learning

Cryptography
Slide Title

Subtitle
Header
Body and **body (with accent)**

Caption

References