Quantum Computation for Chemistry

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Quantum Information Science Workshop, Vienna, VA 2009
Does Our Universe Allow for Robust Quantum Computation?

Dave Bacon

Computers operating purely according to the laws of quantum theory might break modern cryptographic codes (1), revolutionize quantum chemical calculations (2), and overturn the most basic limits to computing (3). Standing in the way of creating these dream machines is the fact that quantum computers do not like to maintain their quantum nature, but instead have a propensity to decay into machines obeying the classical system. Left out, however, is the question of whether the theorem actually holds in an experimental setting: Does our universe allow for robust quantum computation?

This is a hard question because the cost (the number of experiments needed) of characterizing the properties of quantum systems useful for fault-tolerant computation rises exponentially with the number of quantum systems (9, 10). Emerson et al. have found a
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Antikythera device
Built around 150-100 B.C. (Ancient mechanical quantum simulator)
Without the computer-based simulation, the material culture of late-twentieth-century microphysics is not merely inconvenienced – it does not exist. Nor this is only true for particle detectors – machines including the huge plasma-heating Tokamaks, the complex fission-fusion nuclear weapons, the guidance systems of rockets are inseparable from their virtual counterparts – all are bound to simulations.

–Peter Galison
S. F. Boys, EDSAC and Gaussian orbitals

Boys, Cook, Reeves and Shavitt, Nature, 178, 1207 (1956)

AUTOMATIC FUNDAMENTAL CALCULATIONS OF MOLECULAR STRUCTURE

By Dr. S. F. BOYS, Dr. G. B. COOK, C. M. REEVES and I. SHAVITT

Theoretical Chemistry Department, University of Cambridge
Cell phone quantum chemistry: **mobimol**
High-performance quantum chemistry calculations

Spheroidene molecule QMC calculation (250,000 hours of CPU time), Usage allocation per area, NERSC Supercomputers (DOE), (2007)
Traditional Mexican ceramics and quantum chemistry methods

The tree of life
Traditional Computational Chemistry Roadmap
Martin Head-Gordon, *Physics Today* April, 2008
R. P. Feynman, *Simulating physics with computers*
Computational Chemistry vs. Quantum Simulation

Feynman’s Proposal

\[ |\psi^{\text{mol}}\rangle \rightarrow |\psi^{\text{QC}}\rangle \]

\[ \hat{U}^{\text{mol}}(t) = e^{-i\hat{H}^{\text{mol}}t} \rightarrow \hat{U}^{\text{QC}}(t) = e^{-i\hat{H}^{\text{QC}}t} \]

Quantum algorithms for simulation:
Zalka, Lloyd, Lidar, Cleve, Aharonov, Chuang, Brown, Love, Ortiz, Somma, Gubernatis, Kais, Nori, Aspuru-Guzik, ...
The quantum advantage

<table>
<thead>
<tr>
<th>Computational task</th>
<th>Classical cost</th>
<th>Quantum cost</th>
</tr>
</thead>
<tbody>
<tr>
<td>Factoring</td>
<td>$e^{O(n^{1/3} \log^{2/3} n)}$</td>
<td>$O(n^2 \log n \log \log n)$</td>
</tr>
<tr>
<td>Search</td>
<td>$O(n)$</td>
<td>$O(\sqrt{n})$</td>
</tr>
<tr>
<td>Full CI</td>
<td>$e^{O(n)}$</td>
<td>$O(n^5)$</td>
</tr>
<tr>
<td>Chemical dynamics</td>
<td>$e^{O(n)}$</td>
<td>$O(n^2)$</td>
</tr>
<tr>
<td>Protein folding</td>
<td>$e^{O(n)}$</td>
<td>?</td>
</tr>
</tbody>
</table>


Chemical reaction dynamics
Input

- The Hamiltonian of the system, \( \hat{H} = \hat{T} + \hat{V} = \frac{\hat{p}^2}{2m} + \hat{V}(\mathbf{x}) \)
- An initial condition for the wave packet

Steps

- Initialize wavefunction using a proper mapping to qubits
- Propagate in time
- Measure observables

Output

- Reaction probability
- Thermal rate constant
- State-to-state distributions
Split-operator (Trotter) method

For a short timestep, $\delta t$,

$$U(\delta t) \approx e^{-iT\delta t} e^{-iV\delta t}.$$

Note that the potential operator $V$ is diagonal in position $R$ and $T$ is diagonal in momentum $P$. Use diagonal representation of operators.

$$|\psi(\delta t)\rangle = FT e^{-iT\delta t} FT^{-1} e^{-iV\delta t} |\psi(0)\rangle.$$

$$|\psi\rangle \rightarrow e^{-iV\delta t} |\psi\rangle = \sum_{x=0}^{2^n-1} a_x e^{-iV(x)\delta x} |x\rangle$$
A quantum architecture for an error correcting quantum computer
A. Steane. How to build a 300-bit, 1-gigaop quantum computer, Quantum Information and Computation, 7, 171 (2007)

- 300 logical qubits
- Encoded in $\approx 10,000$ physical qubits
- Ion-trap implementation
- Within error-correcting threshold and able to carry out $10^9$ quantum gates.

![Schematic diagram of the complete system. An optical chip contains laser sources, optical switches and r.f. control circuitry for the laser pulse; the multiple laser beams (2 of 1000 pairs are shown) are imaged onto an ‘ion chip’ (IC) in vacuum, containing the array of ion traps and the control circuitry for moving ions around. The detector registers optical fluorescence; its elements could alternatively be incorporated onto the IC. The optical chip could alternatively be placed inside the vacuum chamber, close to the IC, or else replaced by conventional methods of optical detection.](image-url)
$n = 10$, i.e., a grid of 1024 points per dimension

$(3N - 2)n$ qubits are required
Quantum gate requirements

\[ n = 10, \text{ i.e. a grid of } 2^{30} \text{ points} \]

Coloumb: \[ \frac{75}{4} n^3 + \frac{51}{2} n^2 \] elementary gates per step per pair of particles.

Lennard-Jones: \[ \frac{25}{2} n^3 + 12n^2 \] gates per step per pair of particles.
Determination of observables

Has the wave packet crossed the barrier?

\[ Q_0 \]

\[ Q_1 \]

\[ R_{AB} \]

\[ R_{BC} \]

Measuring the ancilla gives the transition probability.

\[ Q \left| x, y, 0 \right\rangle = \begin{cases} 
\left| x, y, 0 \right\rangle & \text{if } y < x \\
\left| x, y, 1 \right\rangle & \text{if } y \geq x 
\end{cases} \]
HF Determinants

1. HF GS: fill first $N$ orbitals and form Slater Determinant

2. There are $\binom{2K}{N}$ occupancy states (configurations)

3. These are organized into singles, doubles, triples, etc

4. The determinants formed from these configurations form an N-electron basis
**Full Configuration Interaction (FCI)**


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**Wavefunction representation**

Expand wavefunction in all HF determinants:

\[
\left| \psi \right\rangle = \alpha_0 \left| \psi^{HF} \right\rangle + \sum \alpha_b^a \left| \psi^b \right\rangle + \sum \alpha_{cd}^{ab} \left| \psi^{cd} \right\rangle + \ldots
\]

---

**Hamiltonian: CI Matrix**

Hamiltonian is given by all matrix elements between determinants. Solving the matrix eigenvalue problem for this \(\binom{2K}{N} \times \binom{2K}{N}\) matrix gives exact results within the given basis.
Time Evolution

Molecular Hamiltonian

\[ \hat{H} = \sum_x \hat{h}_x = \sum_{p,q} \langle p| \hat{T} + \hat{V}_N|q\rangle \hat{a}_p^\dagger \hat{a}_q - \frac{1}{2} \sum_{p,q,r,s} \langle p|\langle q|\hat{V}_e|r\rangle|s\rangle \hat{a}_p^\dagger \hat{a}_q^\dagger \hat{a}_r \hat{a}_s \]

Trotter Expansion and Jordan-Wigner Transformation

\[ e^{-i\hat{H}t} \approx \left[ \prod_x e^{-i\hat{h}_x t/M} \right]^M \]

\[ \hat{a}_p^\dagger \hat{a}_q \rightarrow \hat{X}_p \hat{X}_q \left[ \prod_{i=p+1}^{q-1} \hat{\sigma}_z^i \right] \hat{P}_0 \hat{P}_1 \]

- Number of Terms in \( \hat{H} \) grows as \( N_{\text{basis}}^4 \)
- Each term involves a controlled action on at most 4 qubits
- Few gates required by term
Time Evolution

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Phase Estimation: A Recursive Algorithm

Get a lower bound and measure the difference ... repeatedly ... as much as you want.

\[
\hat{V}_0 = \hat{U} \quad \hat{V}_k = \left[ \exp(-i2\pi\phi_{k-1})\hat{V}_{k-1} \right]^2
\]
Qubit Requirements

![Graph showing the relationship between spatial basis functions and qubits with data points labeled a, b, and c for benzene, caffeine, and cholesterol.]

- **Compact, 6-31G* (approximate)**
- **Compact, cc-pVTZ (approximate)**
- **Direct**
- **Compact, 6-31G* (examples)**
- **Compact, cc-pVTZ (examples)**
Two-qubit gates required for simulating molecules
Whitfield, Biamonte, AAG, In Preparation

Number of CNOTs required for molecular simulation (Trotter step=1 au)

Two qubit operations

Qubits

Benzene
Caffeine
Cholesterol
Challenges

- Hardware is unreliable
  - Passive Error Prevention
  - Active Error Correction

- Simulating systems with protected subspaces.
  *Energy protection arguments fail in the interaction picture*

- Quantum simulation on a fault-tolerant quantum computer.
  *Resource requirements for fault-tolerant quantum simulation: the transverse Ising model ground state*  
  C.R. Clark and KRB, Georgia Tech  
  T.S. Metodi and S.D. Gasster, Aerospace Corporation  
Tile Based Architecture
Communication by qubit movement
Specifically designed based on ion traps.
Extendable to other models

- Quantum Dots
Parallelize and Decompose

Cat States for Parallelization
(|0000...>+|1111...>)

1. Decompose into one and two qubit gates.
2. Use Solovay-Kitaev algorithm to decompose single qubit gates into H, T, X, Z, Y

Phase Bit Precision > Trotter Error > Solovay-Kitaev Error
Ken Brown (GA Tech): Quantum Resources
Quantum simulation of Ising Model in a Transverse magnetic field

Precision and Time

Universal Gate Set + Solovay-Kitaev
Change in Error Correction Level
N=100 TIM
Quantum optics for quantum chemistry
First quantum chemistry quantum computing experiment, 2008
Lanyon et al.. In review.

Quantum Technology Lab - Brisbane, Australia
Ben Lanyon
Andrew White
M. DeAlmeida
Geoff Gillet

Aspuru-Guzik research group - Harvard, USA
James Whitfield
Ivan Kassal
Alejandro Perdomo
Masoud Mohseni
The hydrogen molecule

\[ V = \sum P^* V_p \]

\[ V = V_0 - \sum V_{\text{IA}} \left\{ 1 - \frac{\sigma_a}{\sigma} \right\} \]

\[ \text{sym} \]

\[ \text{Impulse at (x)} \]

\{plau, antiong\}
$H_2$ STO-3G Basis set Full CI
$H_2$ FCI Quantum computer experiment
Experimental setup

(a) \[ |0\rangle \xrightarrow{H} R_z(\omega_k) \xrightarrow{H} \xrightarrow{ Classical feedback } \]

(b) SPDC

(c) \[ U^j = R_z(j\alpha) R_y(\beta) R_z(j\gamma) R_y(\delta) \]
Experimental curves and number of photons per point

H2 potential energy surfaces

Energy (Hartrees) vs. atomic separation (au)

- Ground
- Excited 1
- Excited 2
- Excited 3
- Theory

1 photon per bit

Attempts before success

11 photons per bit
Coherence Dynamics in Photosynthesis: Protein Protection of Excitonic Coherence

Hohjai Lee, Yuan-Chung Cheng, Graham R. Fleming*

The role of quantum coherence in promoting the efficiency of the initial stages of photosynthesis is an open and intriguing question. We performed a two-color photon echo experiment on a bacterial reaction center that enabled direct visualization of the coherence dynamics in the reaction center. The data revealed long-lasting coherence between two electronic states that are formed by mixing of the bacteriochlorophyll and accessory bacteriochlorophyll excited states. This coherence can only be explained by strong correlation between the protein-induced fluctuations in the transition energy of neighboring chromophores. Our results suggest that correlated protein environments preserve electronic coherence in photosynthetic complexes and allow the excitation to move coherently in space, enabling highly efficient energy harvesting and trapping in photosynthesis.

Room temperature coherence observed in a conjugated polymer at room temperature for hundreds of femtoseconds.

Dendrimers

Quantum walks on “perfect” trees have exponential speedup. What about “imperfect” light-harvesting molecules?

Image: Takuzo Aida, University of Tokyo
Environment Assisted Quantum Transport (ENAQT)

P. Rebentrost, M. Mohseni, S. Lloyd, A. Aspuru-Guzik
M. Plenio and Huelga, arxiv:0807.4902
Emergence of “quantum biology”?

- Other quantum information scientists involved or interested (not exhaustive): M. Plenio (Imperial College), B. Whaley (UC Berkeley), Gerald Milburn (Queensland), Hans Briegel (Innsbruck), Vlatko Vedral (Leeds/Singapore), A. Olaya-Castro (UC London), Keye Martin (NRL), M. Lanzagorta (ITT), . . .
- Conferences. DARPA (2008), Singapore (2008), Lisbon (this Summer, 2009)
Protein Folding
Protein Energy Landscapes
Funnel idea (P. Wolynes)
Lattice Protein Models
Mapping to 2D Ising Model in a Magnetic Field

Protein Lattice Model
Image: Prof. Backofen, Uni. Freiburg

Classical Ising Model
The hydrophobic-polar (HP) model

Mapping to 2D Ising Model in a Magnetic Field

Slide Credit: Ken Dill
Adiabatic evolution to simplest HP model ground state
Energy Landscape: Lennard-Jones Cluster example
David Wales, Cambridge, UK
Finding low-energy conformations of Lennard-Jones clusters using Grover Search

Grover’s Algorithm for optimized Lennard-Jones Cluster

- 9 qubits total. 5 for the bond length, 4 for the bond angle
- The final optimized structure are shown in the picture, it is the same as the classical simulation result
- Our next project is try to extend the simulations to N=4, 5, 6,…

Figure 6.8. Final probability distribution of the wave function for LJ (N=3) cluster. The global minimum located at $B_1 = 1.032, B_2 = 1.032$ and $A_1 = 60^\circ$. The left inner panel is the distribution of total iteration number before reach the global minimum for 100 search experiments. The right inner panel is the total measure step before reach the global minimum.
Conclusions and Outlook

- Quantum computing provides exponential speedups for electronic structure and quantum dynamics
- Interesting quantum algorithms for structure optimization that might exhibit polynomial (quadratic) speedup.
- Quantum information providing insight into photosynthesis and solar energy harvesting
- Other physical chemistry / quantum information connections awaiting to be explored.