



So you've built a quantum computer...now what?

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Computer Systems Colloquium
4:14PM-5:30PM in Gates B01



Act I: Prologue

Working in the garage c.1938...

- Bill and Dave begin work in a garage at 367 Addison Avenue
- First product: The HP 200A, used to test sound equipment



The 200A audio oscillator

hp.com/hpinfo/abouthp/histnfacts/timeline/hist_30s.html

Working in the garage c.1938...

- Disney orders eight Model 200B oscillators, used to test the various channels, recording equipment and speaker systems in the twelve specially-equipped theaters that show Fantasia in 1940



Working in the garage c.1938...

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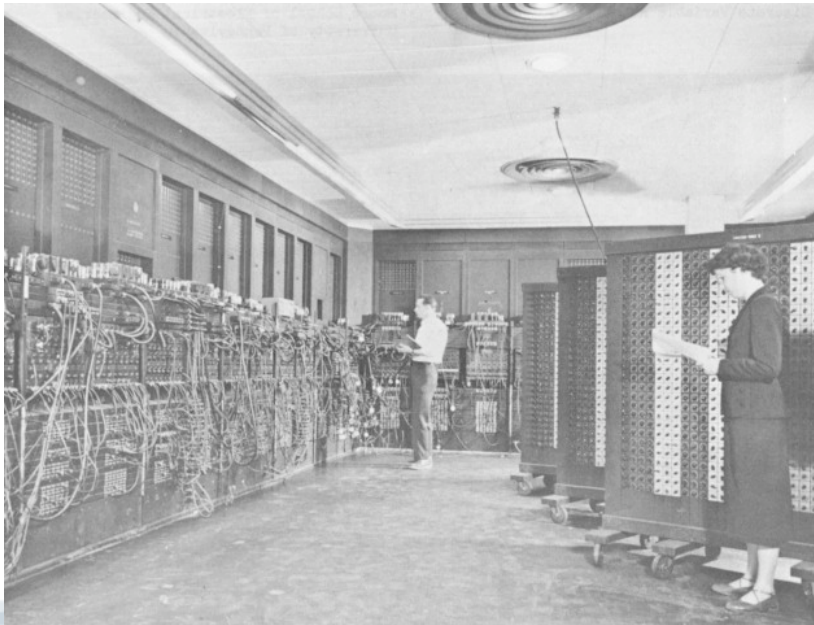


“...its popularity increased and its cult status was assured when the members of the 60's drug culture adopted it as a favorite hallucinatory experience”

filmsite.org/fant.html

Working in the garage c.2006...

- Alice and Bob begin work in a garage in Palo Alto
- AB's first product: The AB 200A, used to ?



The AB 200A quantum computer...
• 6 • (disclaimer: actually an ENIAC).

Why would Alice & Bob work on this?

- Very technically difficult
- Very thin supply chain & talent pool
- Has to be done in a “best practices” industrial environment
- Expensive
- Conventional computers are cheap, fast & can get much better

Act II: Quantum Computers

Context: \\what is a quantum computer?

- “Could you briefly describe how a quantum computer is fundamentally different from a conventional computer?”

Deep Thoughts: \computation and physics

- Computation and physics are deeply connected
- All of the stuff that makes up our world is constantly "computing" (i.e. evolving in time)
- When we build computers we tap into a very small part of that ongoing computation

Deep Thoughts: \computation and physics

- When a computer is built out of devices that behave according to the rules of classical physics, like Pentiums or balls rolling down hills, some of the computing resources that nature allows are not used
- Classical physics can be thought of as a highly restricted version of quantum physics
- This restriction removes computational capabilities that are allowed by quantum physics but not classical physics

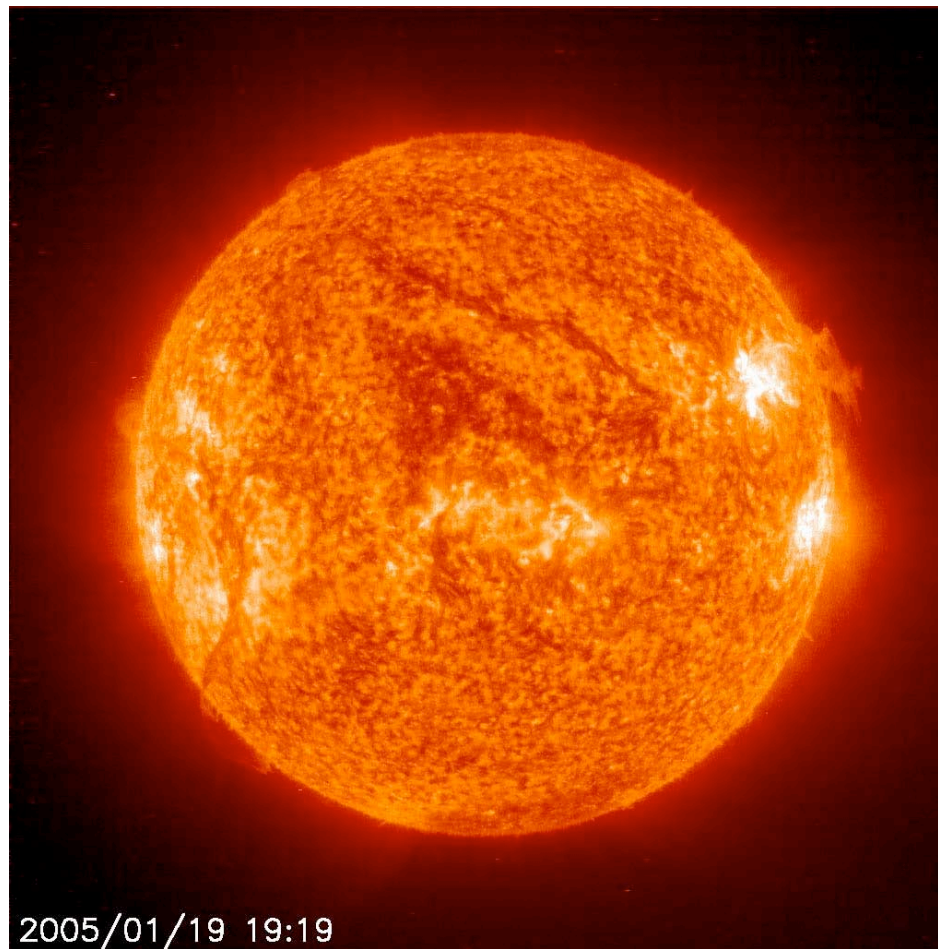
Deep Thoughts: \computation and physics

- When computers are built out of components that can harness the resources made available by quantum mechanics, they gain access to computational resources that are not available to conventional computers

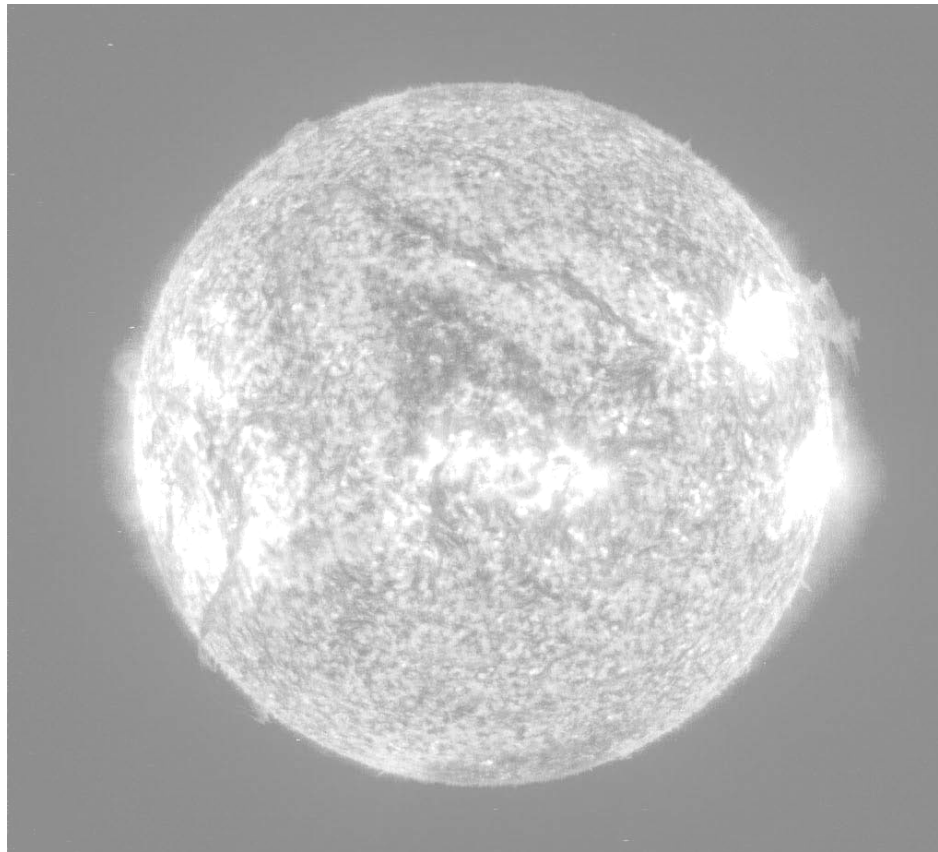
Deep Thoughts: A painting analogy

- Two artists drawing the same object
- Artist #1 only gets to use black and white; artist #2 gets to use all colors
- If the job is to paint a picture of the sun, artist #1 can never get it right, no matter how skilled, because he doesn't have access to the right resources (i.e. red and yellow paint don't exist for him); artist #2 has a big advantage

This is a photograph of the “real” sun



This is a black and white model of the sun



This is a red and yellow model of the sun



A clue: look for apps where these “colors” are important



Context: \\what is a quantum computer?

- “Could you briefly describe how a quantum computer is fundamentally different from a conventional computer?”

Quantum computers harness one or more of the **resources** available to quantum systems

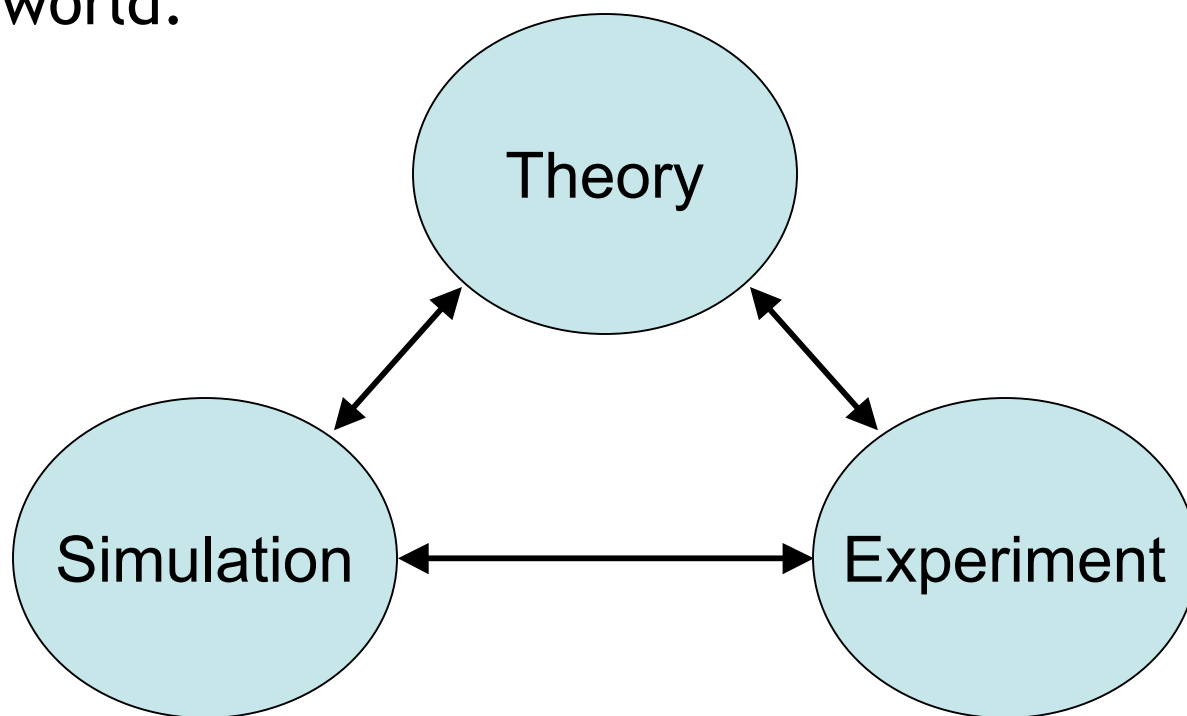
Act III: Chemistry

Quantum computers: \\what's the “killer app”?

- “Could you give some real-world examples of problems that can be addressed by quantum computers but are impossible to solve with conventional computers?”

Nature at the molecular scale: **chemistry**

Chemistry takes the fundamental laws of physics and makes them applicable for the description and understanding of the molecular world.

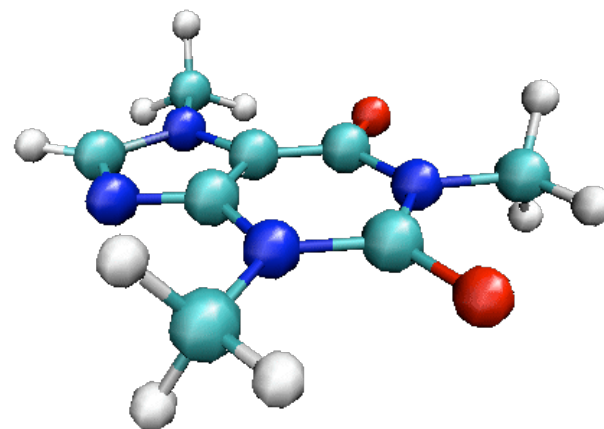
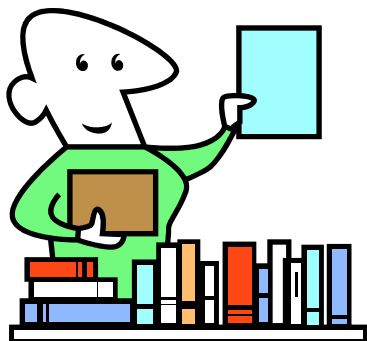


Nature at the molecular scale: **chemistry**

The fundamental laws necessary for the mathematical treatment of a large part of physics and the whole of chemistry are thus **completely known**, and the difficulty lies only in the fact that application of these laws lead to equations that are **too complex to be solved**.

- Paul Dirac
1933 Nobel Laureate in Physics

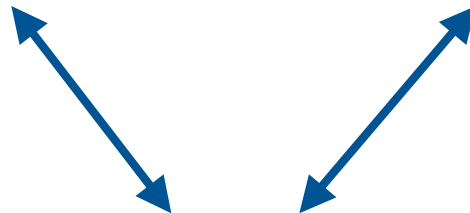
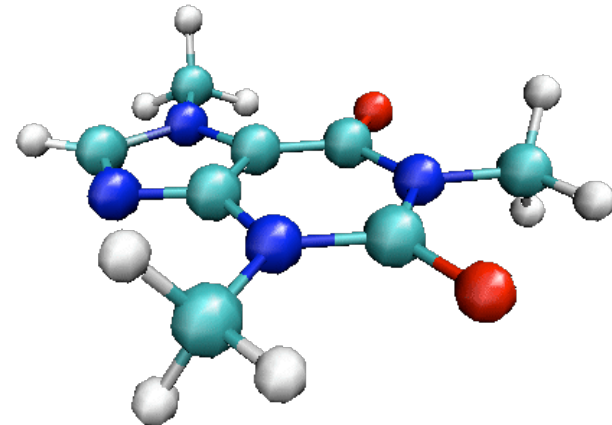
Nature at the molecular scale: \\chemistry



*We are stardust, we are golden //
We are billion year old carbon*

Woodstock, Joni Mitchell

Nature at the molecular scale: chemistry



$$i\hbar \frac{d}{dt} |\Psi\rangle = H |\Psi\rangle$$

Nature at the molecular scale: **quantum simulation**

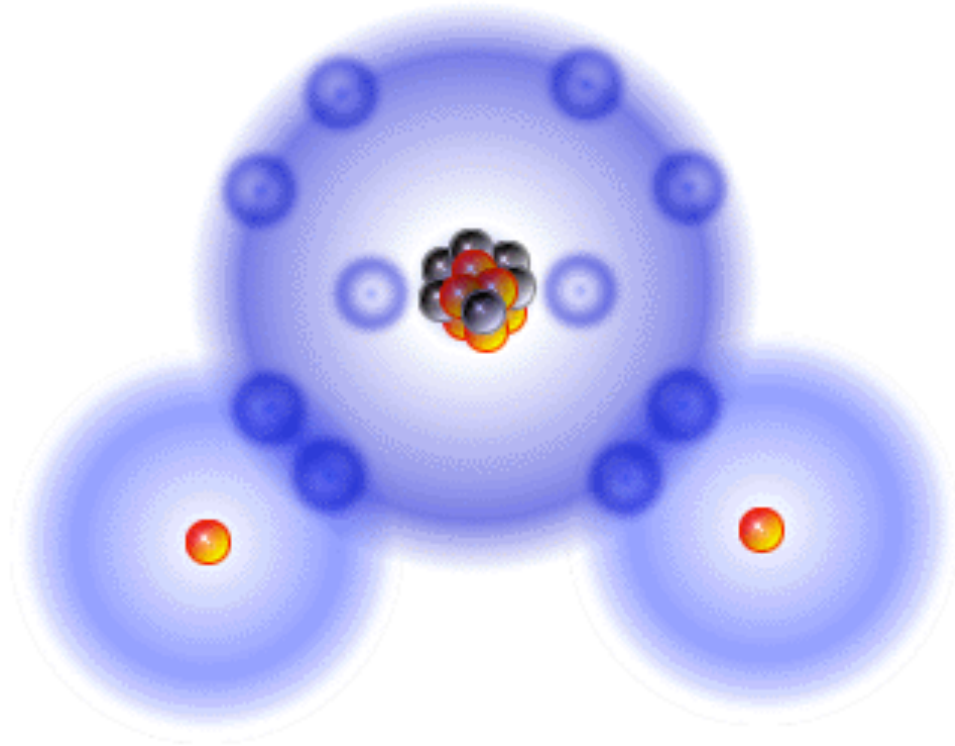
Simulated quantum computation of molecular energies

A. Aspuru-Guzik, A.D. Dutoi, P.J. Love and M. Head-Gordon,
Science 309 p. 5741, 2005

Nature at the molecular scale: \\\quantum simulation

Water Molecule

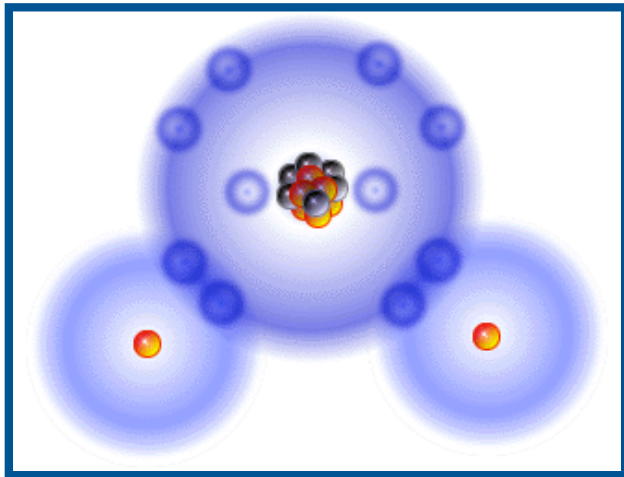
Key: protons neutrons electrons



From www.brooklyn.cuny.edu

A “Turing Test” for simulation

Real water molecule



Mathematical model of a water molecule

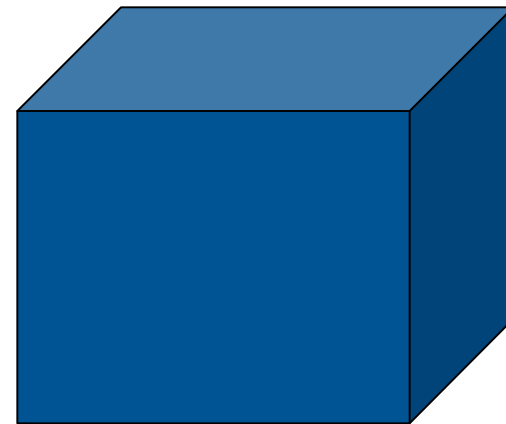
$$i\hbar \frac{d}{dt} |\Psi\rangle = H |\Psi\rangle$$

A “Turing Test” for simulation

Dr. Peter J. Love



Black Box

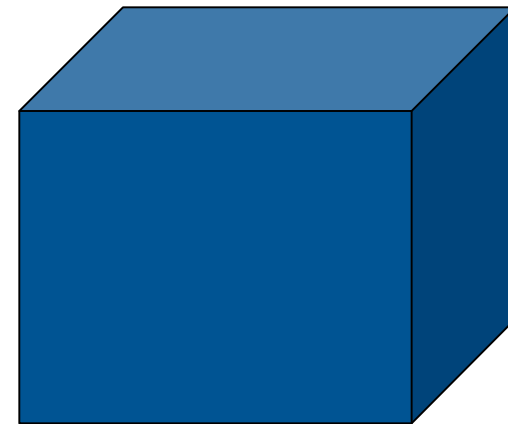


Peter can ask for the value of any “observable”.

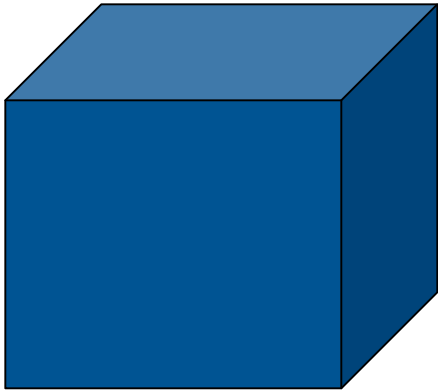
Dr. Peter J. Love



Black Box



Two Different Strategies: Simulation vs. Emulation



Strategy #1: Simulation

- Represent the system using a supercomputer
- Exact algorithm scales factorially with the number of electrons
- Approximate algorithms (HF, DFT, QMC, wave function methods) scale polynomially

The Tree of Life

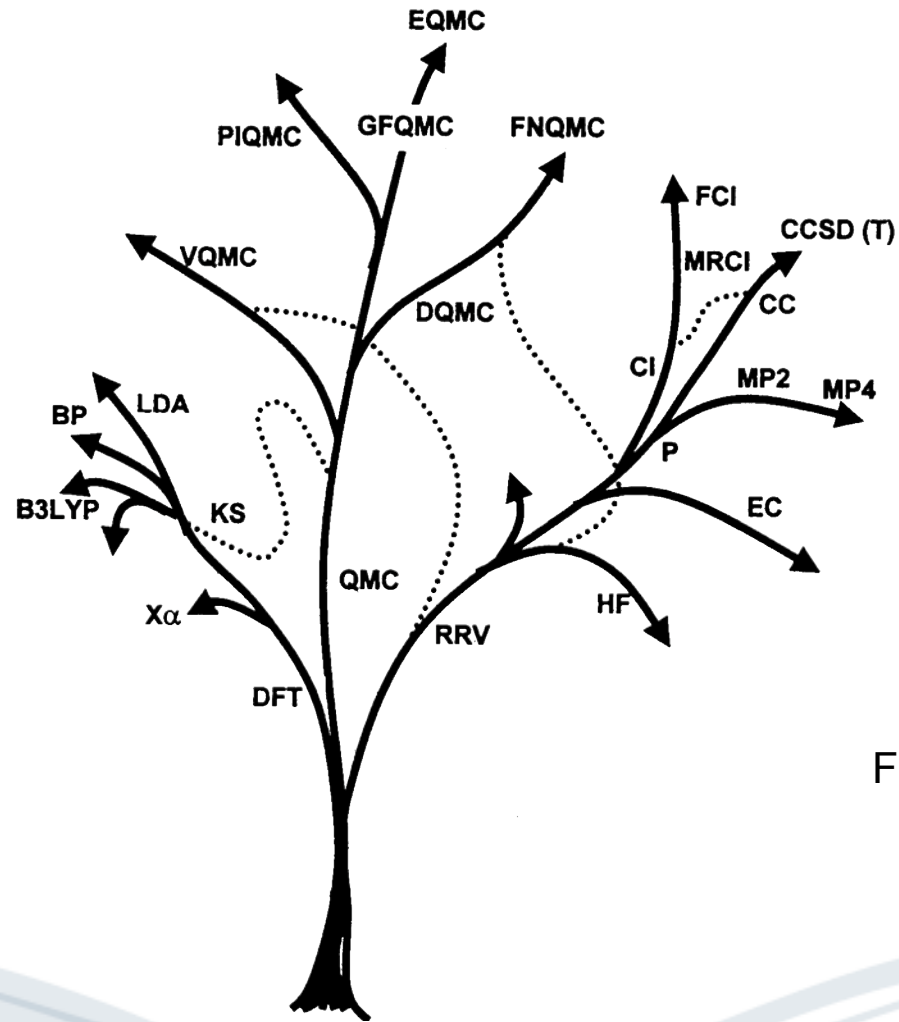
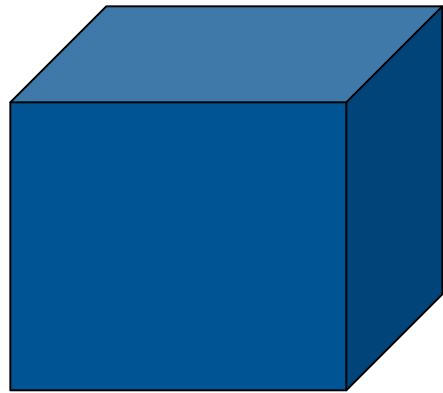
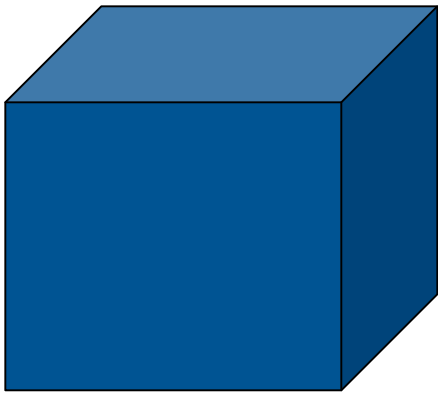


Figure by Jim Anderson

Two Different Strategies: Simulation vs. Emulation



Strategy #2: Emulation

- Map the wavefunction and evolution operator onto a programmable quantum system (quantum computer)
- Exploit the quantum resources of the emulator to achieve **polynomial-scaling exact** algorithms

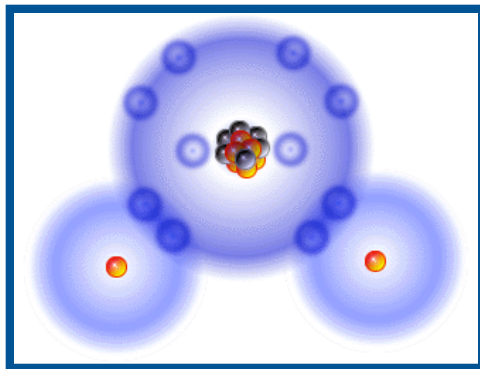
There's Something About Molecules...

**That you just can't capture using conventional computers.
Ever.
Even in principle.**

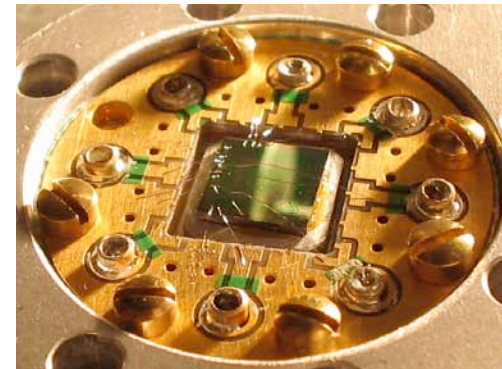
Ever.

Emulating one quantum system with another

A molecule



A programmable quantum system



Maps

Wavefunction #1



Wavefunction #2

Evolution Operator #1



Evolution Operator #2

Observable Operators #1

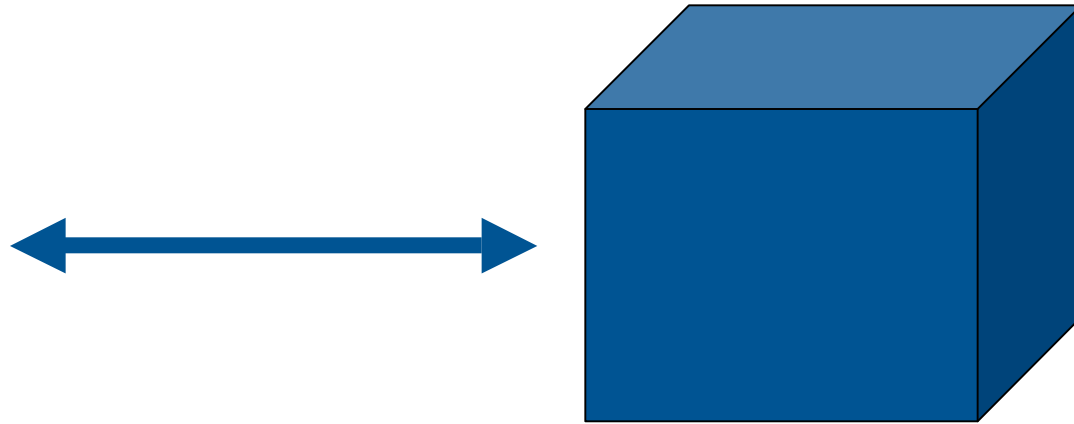


Observable Operators #2

Dr. Peter J. Love



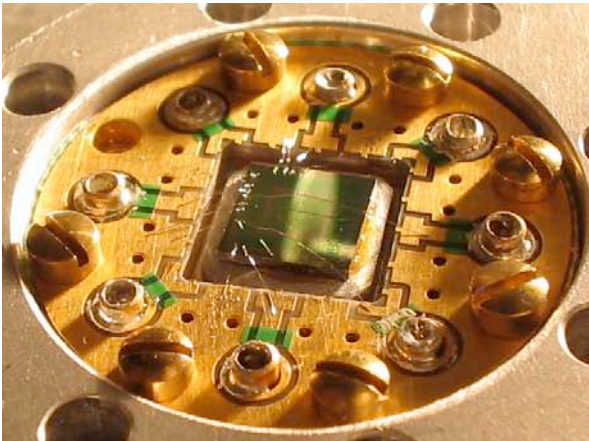
Black Box



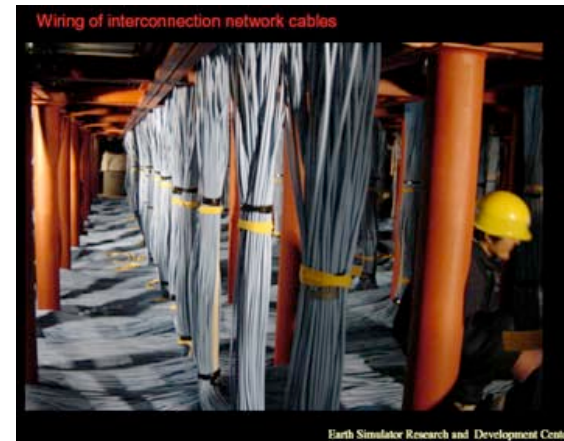
- There is no way to tell the difference between a chip mimicking the molecule and the “actual” molecule
- They are, to the outside world, entirely indistinguishable
- This is not possible with conventional computers; it is easy with quantum computers

Running the killer app: \\what does the AB 200A need?

- Classically intractable chemical calculations can be performed on quantum computers with 50 qubits



- Runs on 6V batteries
- Takes up 100 square feet
- Costs a lot less



- Consumes 6MW of power
- 1700 miles of network cables
- Cost \$300M + ~\$30M/year

Running the killer app: \\who cares?

- Chemical companies: BASF, Dow, Dupont, ...
- Biotechnology companies: Amgen, Genentech, Monsanto, ...
- Pharmaceutical companies: Big 7 (Pfizer, Merck, etc.)
- “Nanotechnology” companies

Success means://a chance to fundamentally change three trillion dollar industries?

Total market cap of pharma, chemical and biotech industries:
 $US\$964B + US\$1153B + US\$979B = US\$3.1T$

**GDP of US in 2004:
\$11.75 trillion**

GDP: The total dollar value of all final goods and services produced in the country in a year. Canada ranked 11th at \$1.023T in 2004. US was 1st.

Act IV: Epilogue

Recap://so you've built a quantum computer...now what?

- QCs will only be built if there is a VERY good reason (& code-breaking isn't it)
- Killer application #1: simulating nature at the molecular scale
- This app has the potential to change the way three trillion dollar industries create value

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