A presentation for Quantum Computation A Glimpse Into the Future of Computing Frances C. Arrillaga Alumni Center, Stanford University, June 16 2004

Computational Nanotechnology

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This is a caffeine molecule.





Molecules are (mostly) made of electrons.





"If we are interested in describing the electron distribution in detail, there is no substitute for quantum mechanics. Electrons are very light particles, and they cannot be described even qualitatively correctly by classical mechanics."

Introduction to Computational Chemistry

Frank Jensen



The two slit experiment





(b) After 100 electrons



(c) After 3000 electrons



(d) After 70 000 electrons

100 electrons

3,000 electrons

70,000 electrons

The two slit experiment





"The fundamental laws necessary for the mathematical treatment of large parts of physics and the whole of chemistry are thus fully known, and the difficulty lies only in the fact that application of these laws leads to equations that are too complex to be solved."

Paul Dirac

Nobel Prize Winner, 1929



"Chemistry is knowing the energy as a function of the nuclear coordinates."

Introduction to Computational Chemistry Frank Jensen



Name: Caffeine Molecular Formula: C₈H₁₀N₄O₂ Number of electrons: 102



Schrodinger Equation:

- Set of coupled ordinary differential equations
- Total number 4^N
- N is number of electrons



Name:CaffeineMolecular Formula: $C_8H_{10}N_4O_2$ Number of electrons:102Number of equations: 4^{102}





Name:CaffeineMolecular Formula: $C_8H_{10}N_4O_2$ Number of electrons:102Number of equations: 4^{102}

4¹⁰² is:

- .26 * 10⁶²
- 25,711,008,708,143,844,408,671,393,477,458,601,640,355,
 247, 900,524,685,364,822,016
- Mass of visible universe in micrograms
- Width of visible universe in Planck lengths (10-35 m)



Solving the underlying equations of nature would allow us to predict the properties of nanostructures without having to do experiments.

Unfortunately, for conventional (classical) computers, this is an impossible task.



"...when Boeing builds an airplane, it doesn't build seven and see which one flies. That would be a pretty expensive process. But the pharmaceutical industry does that, because it's the only way they can do it."

> Jim Karis CEO, Entelos Inc.



"...to describe say a hundred atoms, would require 10¹⁰⁰ bits. So to put this in perspective...there are only about 10⁹⁰ elementary particles in the whole universe. You could solve that same problem on a quantum computer with just a few hundred bits."

Dr. Seth Lloyd

Professor, Department of Mechanical Engineering, MIT



Schrodinger Equation on a quantum computer:

- Design hardware that solves SAME Schrodinger Equation
- Total number of electrons N
- Total number of qubits linear in N [$(3N \log_2 G + R)*E$]
- Output is an R-bit digital number encoding energy as a function of given nuclear coordinates

Schrodinger Equation on a quantum computer:

- Design hardware that solves SAME Schrodinger Equation
- Total number of electrons N
- Total number of qubits linear in N [$(3N \log_2 G + R)^*E$]
- Output is an R-bit digital number encoding energy as a function of given nuclear coordinates



What does a quantum computer look like?







QC Chip Goes Here





How do I use a quantum computer?



Think Mainframe Model



ENIAC, the first all-electronic digital computer



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