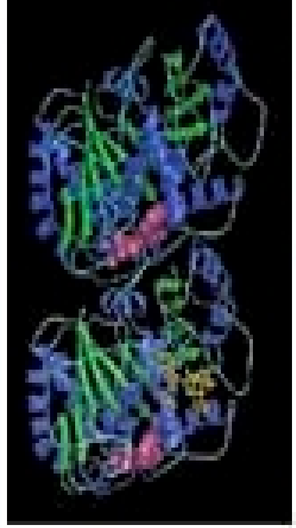
Lecture 2 (cont)

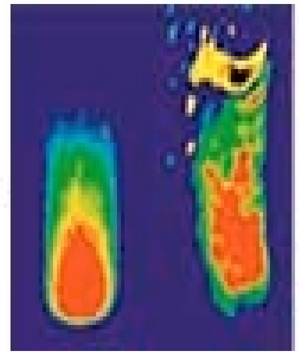
Trends in Computational Science

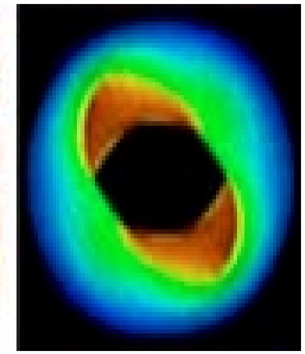
DNA and Quantum Computers

Sources

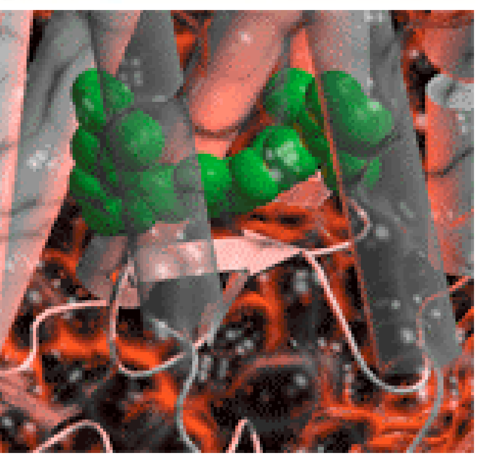
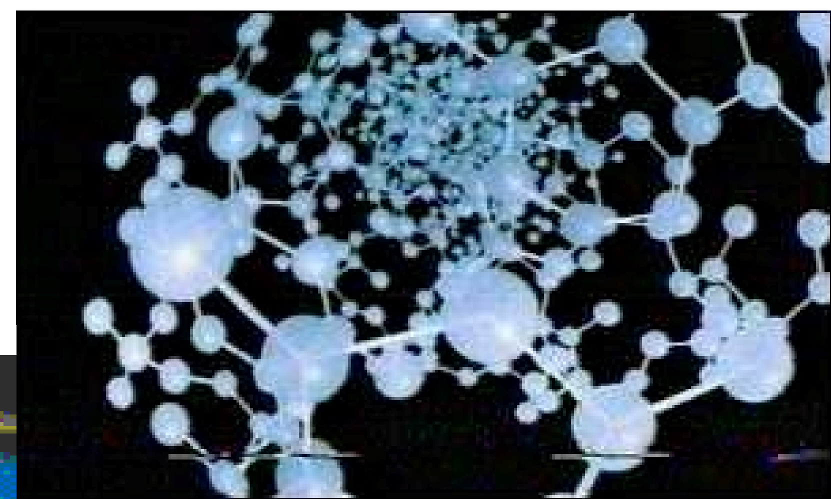
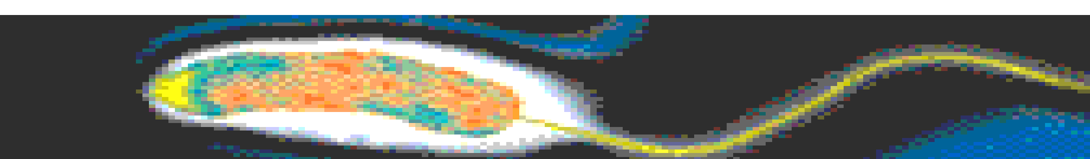
- •1. Nicholas Carter
- •2. Andrea Mantler, University of North Carolina
- •3. Michael M. Crow, Executive Vice Provost , Columbia University.
- •4. Russell Deaton, Computer Science and Engineering, University of Arkansas
- •5. Petra Farm, John Hayes, Steven Levitan, Anas Al-Rabadi, Marek Perkowski, Mikael Kerttu, Andrei Khlopotine, Misha Pivtoraiko, Svetlana Yanushkevich, C. N. Sze, Pawel Kerntopf, Elena Dubrova





Dominating role of biology and system science

Outline

- Trends in Science
- Programmability/Evolvability Trade-Off
- DNA Computing
- Quantum Computing
- DNA and Quantum Computers

Introduction

- What's beyond today's computers based on solid state electronics?
- Biomolecular Computers (DNA, RNA, Proteins)
- Quantum Computers
- Might DNA and Quantum computers be combined? Role of evolutionary methods.

Scientific questions are growing more complex and interconnected.

We know that the greatest excitement in research often occurs at the borders of disciplines, where they interface with each other.

Computers and Information Technology

No field of research will be left untouched by the current explosion of information--and of information technologies. Science used to be composed of two endeavors--theory and experiment. Now it has a third component: computer simulation, which links the other two.

- Rita Colwell

Government Initiatives on Information Technology

- Interdisciplinary teams to exploit advances in computing
  - Involves computer science, mathematics, physics, psychology, social sciences, education
- **Focus on**:
  - Role of entirely new concepts, mostly from biology
  - New technologies are for linking computing with real world - nano-robots, robots, intelligent homes, communication.
  - Developing architecture to scale up information infrastructure
  - Incorporating different representations of information (visual, audio, text)
  - Research on social, economic and cultural factors affected by and affecting IT usage
  - Ethical issues.

The Price of Programmability

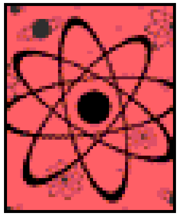
- Michael Conrad
- Programmability: Instructions can be exactly and effectively communicated
- Efficiency: Interactions in system that contribute to computation
- Adaptability: Ability to function in changing and unknown environments

CAD problems in nanotechnology

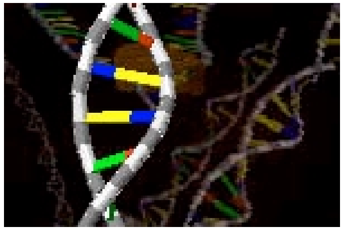
- What is nanotechnology?
  - Any technology below nano-meter scale
    - Carbon nano-tubes
    - Molecular computing
    - Quantum computing
- Are we going there?
  - Yes, a technology compatible with existing silicon process would be the best candidate.
- Is it too early for architecture and CAD?
  - No

Nanotechnology

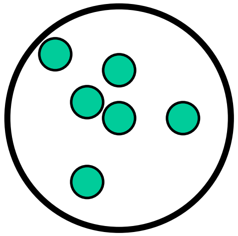
We are at the point of connecting machines to individual cells



Atoms
<1 nm



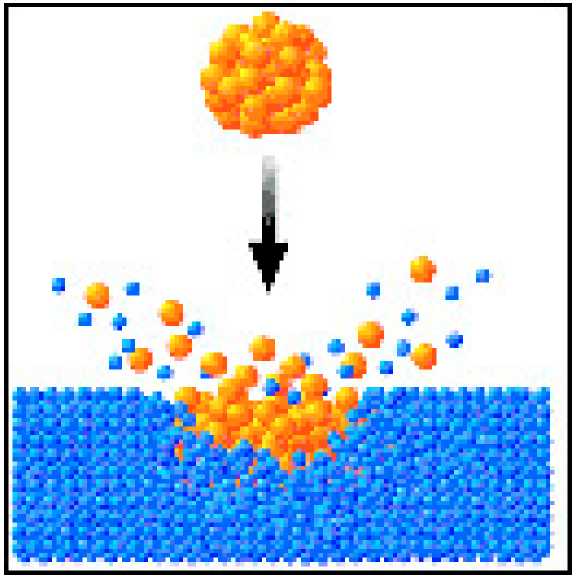
DNA
~2.5 nm



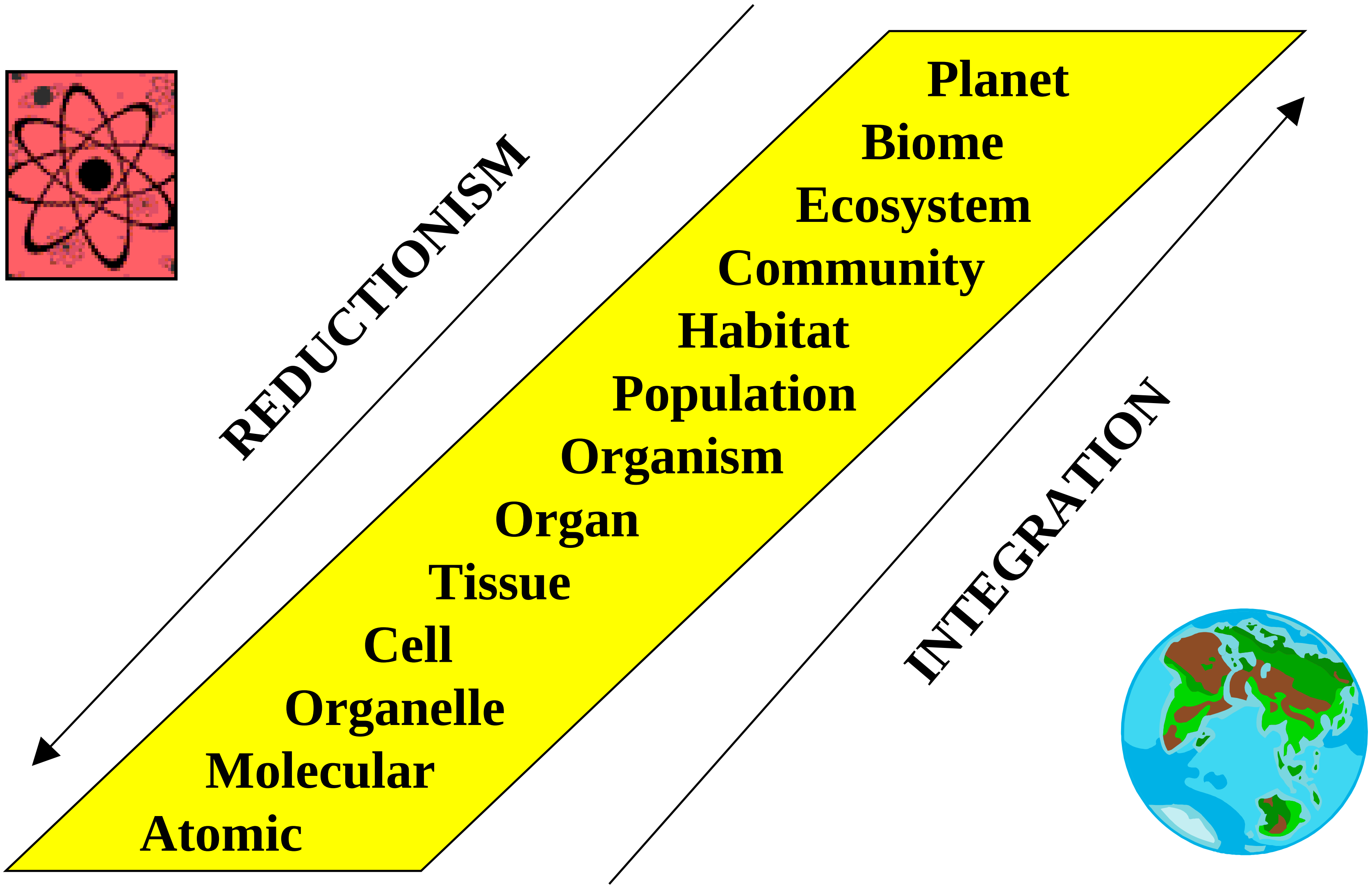
Cells
thousands of nm

Federal Initiative: Nanotechnology

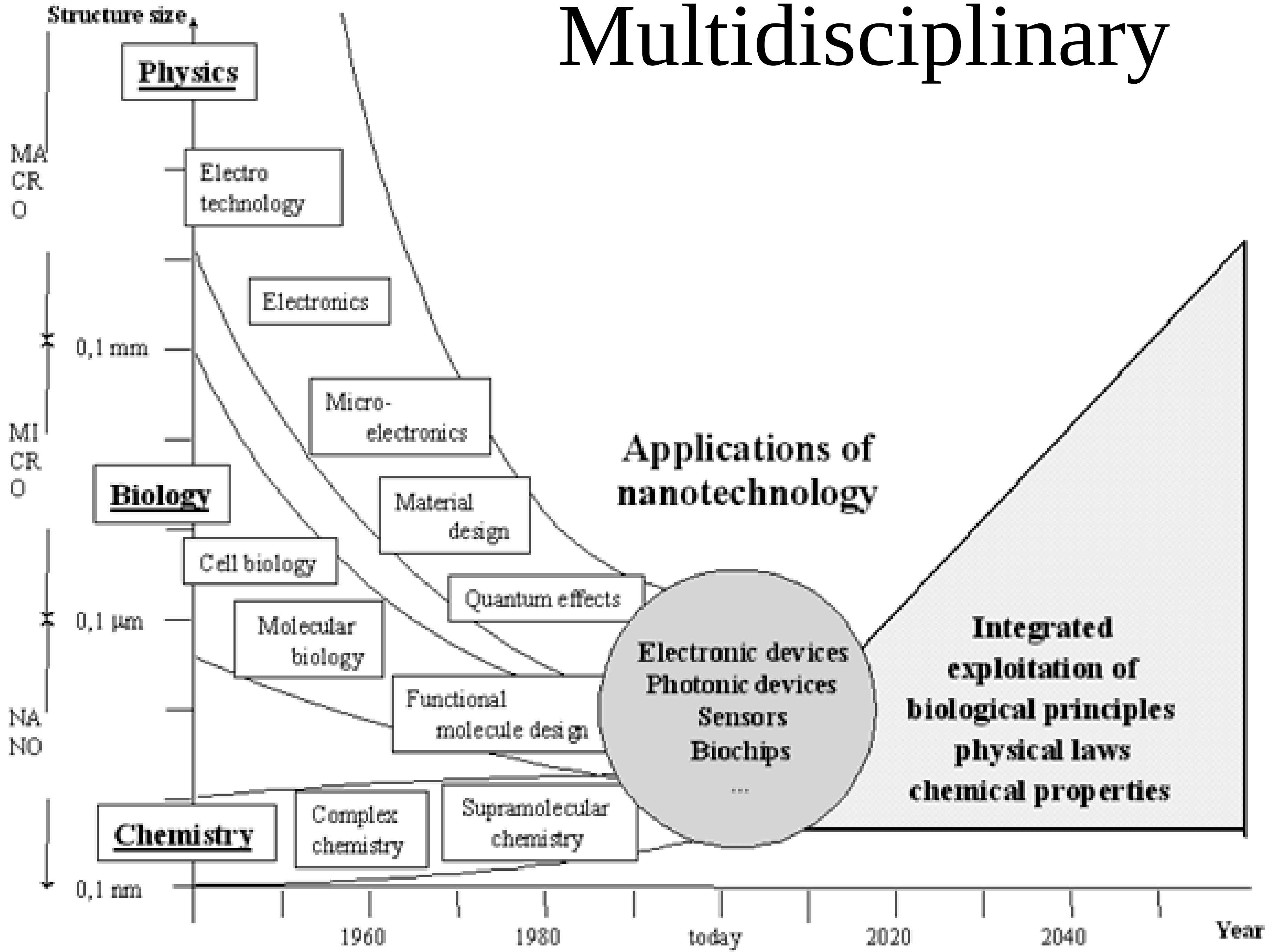
- Interdisciplinary ability to systematically control and manipulate matter at very small scales
  - Involves biology, math, physics, chemistry, materials, engineering, information technology
- Focus on:
  - Biosystems, structures of quantum control, device and system architecture, environmental processes, modeling and simulation



Biocomplexity



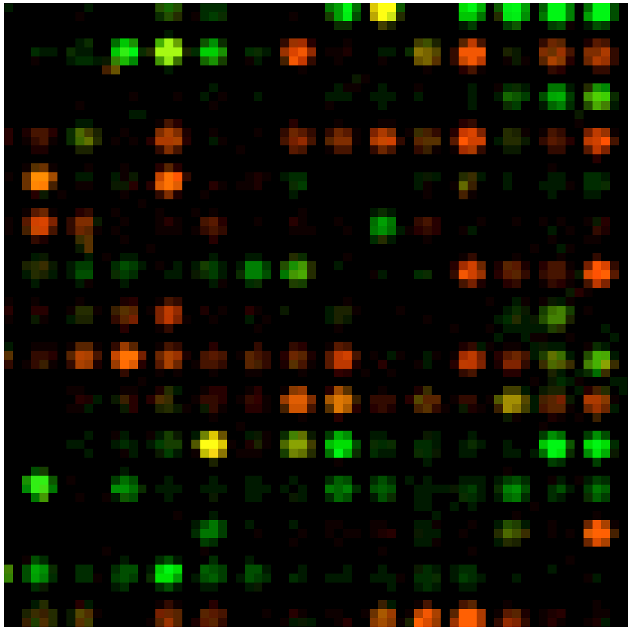
Multidisciplinary



Human Genome Sequence

- Next race: annotation
  - Pinpoint genes
  - Translate genes into proteins
  - Assign functions to proteins
- Genomic tool example: DNA chip
  - Array of genetic building blocks
    - acts as "bait" to find matching DNA sequences from human samples

Entire yeast genome on a chip



DNA Computers

- **Massive Parallelism** through simultaneous biochemical reactions
- Huge information storage **density**
- ***In Vitro*** Selection and Evolution
- **Satisfiability** and **Hamiltonian Path**

DNA Computers

DNA Computing (Adleman, 1994)

DNA is the hereditary molecule in every biological cell.

Its shape is like a twisted rubber ladder (i.e. a double helix).

The rungs of the ladder consist of two bonded molecules called **bases,** of 4 possible types, labeled **G, C, A, T.**

G can only bond (pair off) with C, and A with T.

If a single **strand (string)** of DNA is placed in a solution with isolated bases of A, G, C, T, then those bases will **pair off** with the bases in the string, and form a complementary string, e.g.

G A T T C A G A G A T T A T

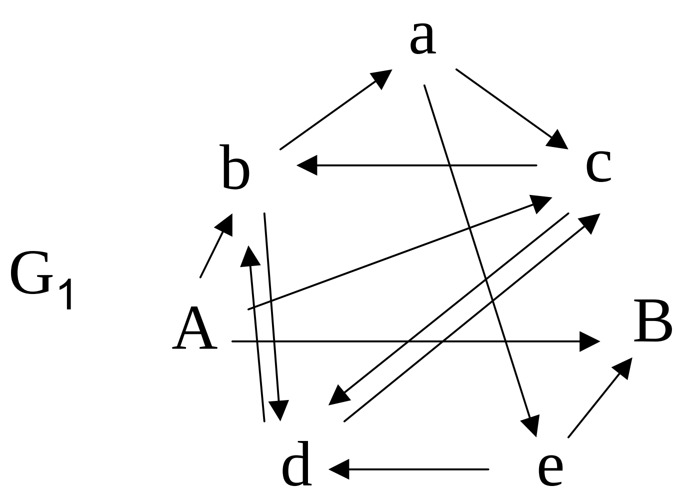
C T A A G T C T C T ← A

This **complementary bonding** can be used to perform computation, e.g. a version of the traveling salesperson problem (TSP), called the **Hamiltonian Path** problem

This problem is stated as follows :-

Start with a **directed graph** G (i.e. the edges between nodes are arrows) at node A, and end at node B. The graph G has a Hamiltonian Path from A to B if one **enters every other node** *exactly once*.

E.G. for the directed graph G_1 shown,



A solution, (G_1's Hamiltonian Path) is

A => c => d => b => a => e => B

DNA Computers

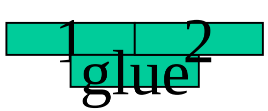
The following (nondeterministic) algorithm solves the directed Hamiltonian path problem:

- **Step 1**: Generate random paths through the graph.
- **Step 2**: Keep only those paths that begin with A and end with B.
- **Step 3**: If the graph has n nodes, then keep only those paths that enter exactly n nodes.
- **Step 4**: Keep only those paths that enter all of the nodes of the graph at least once.
- **Step 5**: If any paths remain, say "Yes"; otherwise, say "No."

DNA Computers

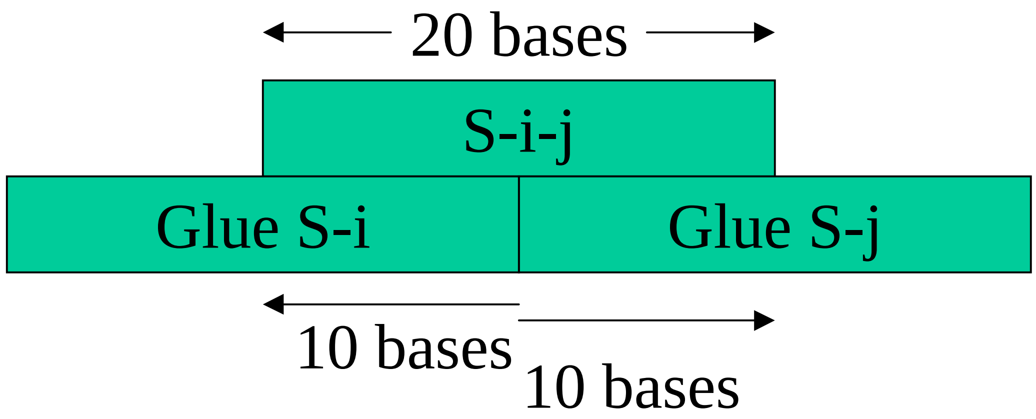
DNA can implement this algorithm! (Uses 10^{15} DNA strings)

Step 1 : To each node "i" of the graph is associated a *random* 20 base string (of the 4 bases A,G,C,T), e.g. TATCGGATCGGTATATCCGA Call this string "S-i".
(It is used to "glue" 2 other strings, like LEGO bricks).



For each directed (arrowed) edge (node “i” to node “j”) of the graph, associate a 20 base DNA string, called “S-i-j” whose -

a) **left half** is the DNA complement (i.e. c) of the **right half of S-i**,
b) **right half** is the DNA complement of the **left half of S-j**.



Step 2 : The product of Step 1 was amplified by “Polymerase Chain Reaction (**PCR**) using primers O-A and (complement) cO-B. Thus, only those molecules encoding paths that began with node A and ended with node B were amplified.

DNA Computers

PCR is a technique in molecular biology that makes zillions of copies of a given DNA (starter) string.

Step 3 : The product of Step 2 was run on an gel, and the 140-base pair (bp) band (corresponding to double-stranded DNA encoding paths entering exactly seven nodes) was extracted.

Step 4 : Generate single-stranded DNA from the double-stranded DNA product of Step 3 and incubate the single-stranded DNA with cO-i stuck to magnetic beads.

Only those single-stranded DNA molecules that contained the sequence cO-a (and hence encoded paths that entered node a at least once) annealed to the bound cO-a and were retained.

DNA Computers

This process was repeated successively with cO-b, cO-c, cO-d, and cO-e.

Step 5 : The product of Step 4 was amplified by PCR and run on a gel (to see if there was a solution found at all).

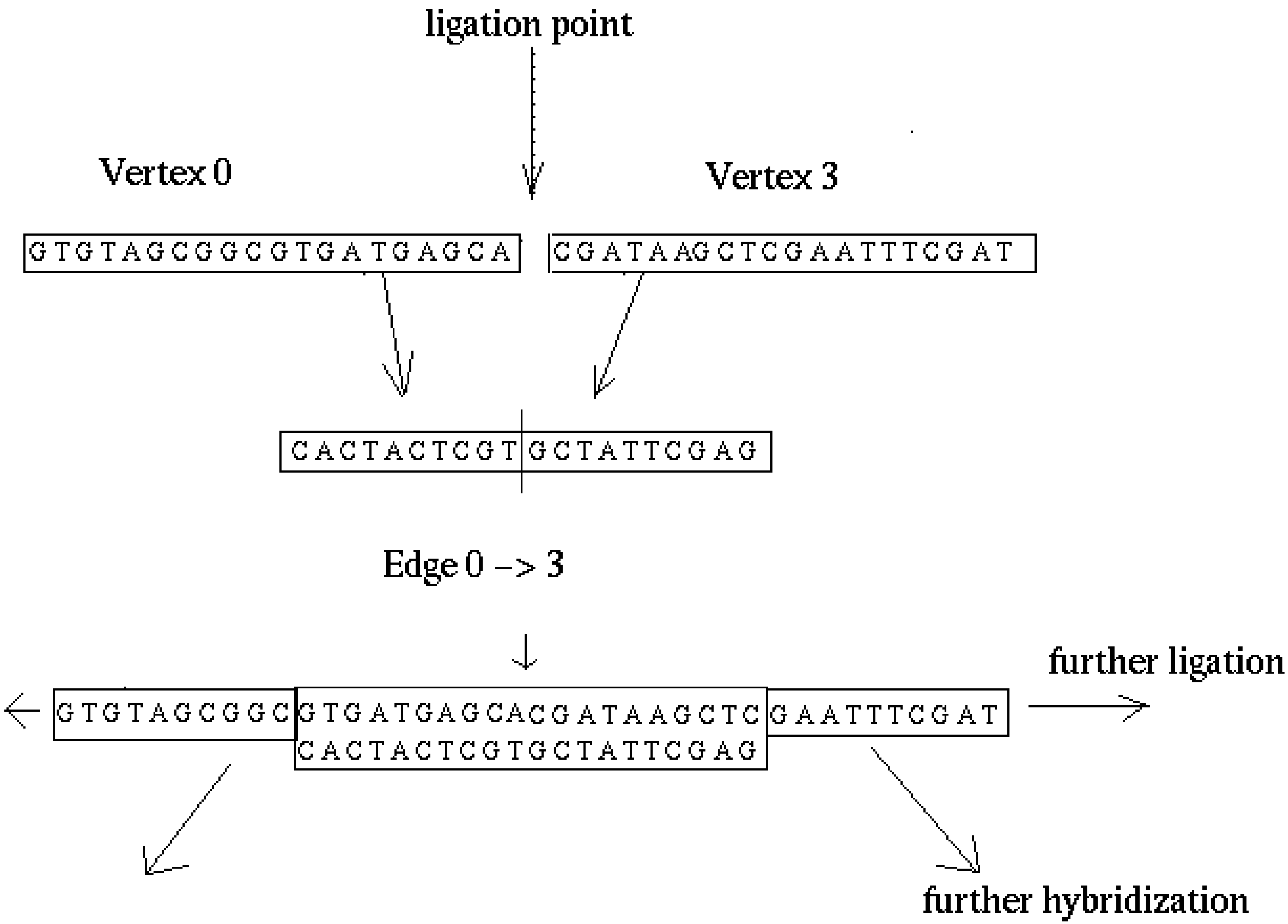
This work took Adleman (the inventor of DNA computing, 1994) a week.

See *November 11, 1994 Science*, *(Vol. 266*, *page 1021)*

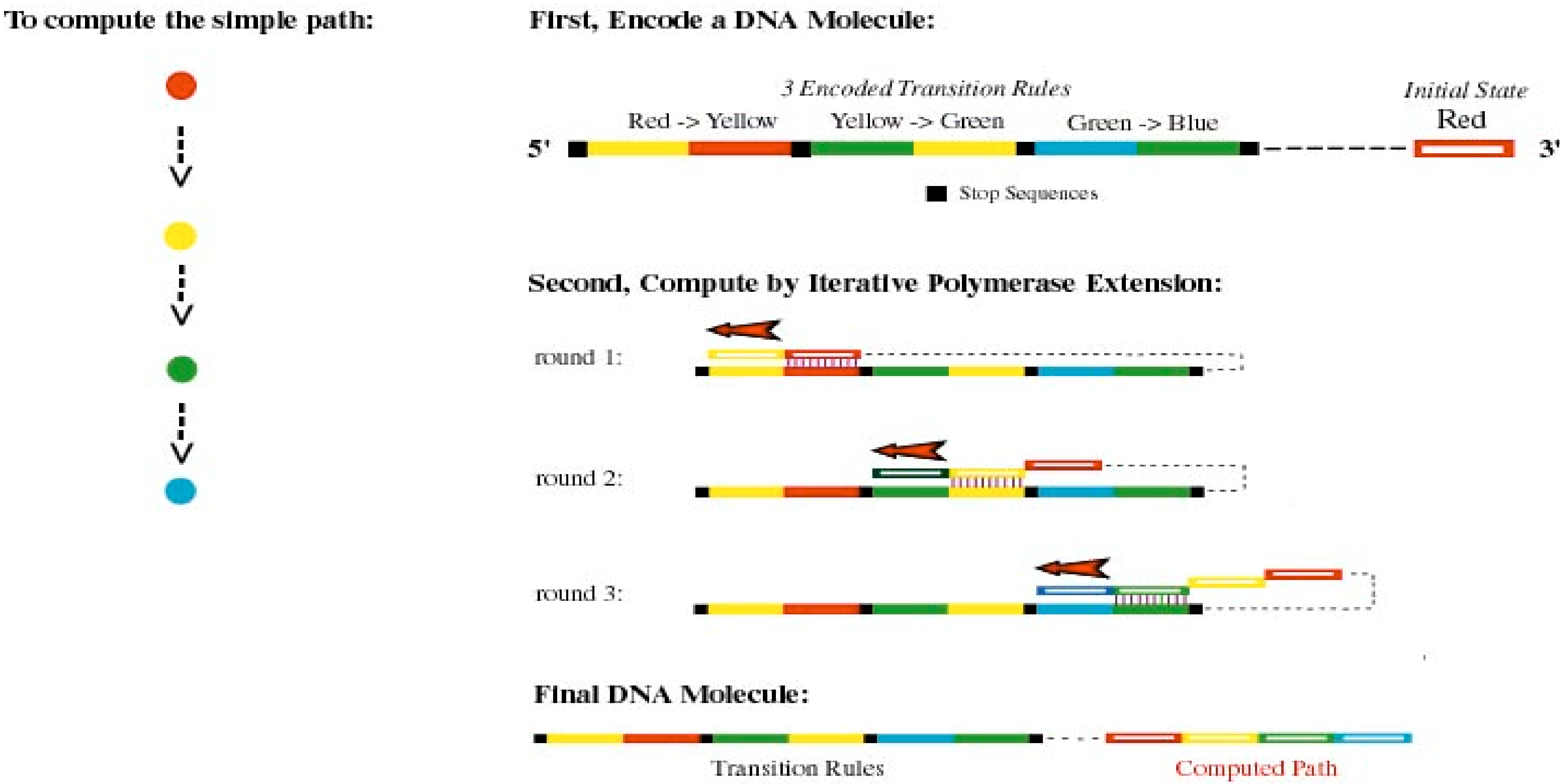
As the number of nodes increases, the quantity of DNA needed rises exponentially, so the DNA approach does not scale well. The problem is NP-complete.

But for N nodes, where N is not too large, the 10^{15} DNA molecules offer the advantages of **massive parallelism**.

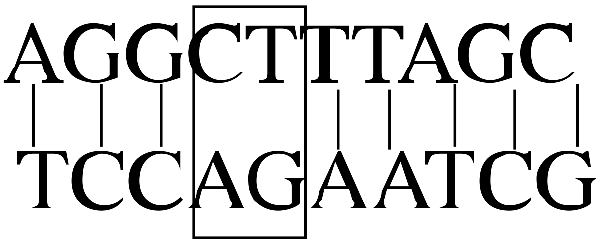
DNA Computers



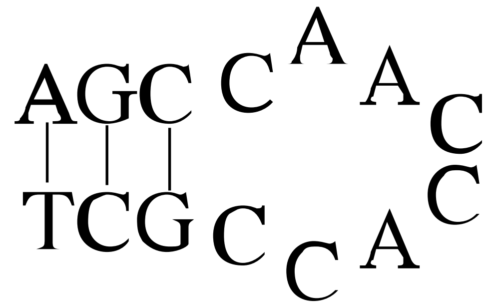
DNA Computers



DNA Computers



Mismatched Hybridization



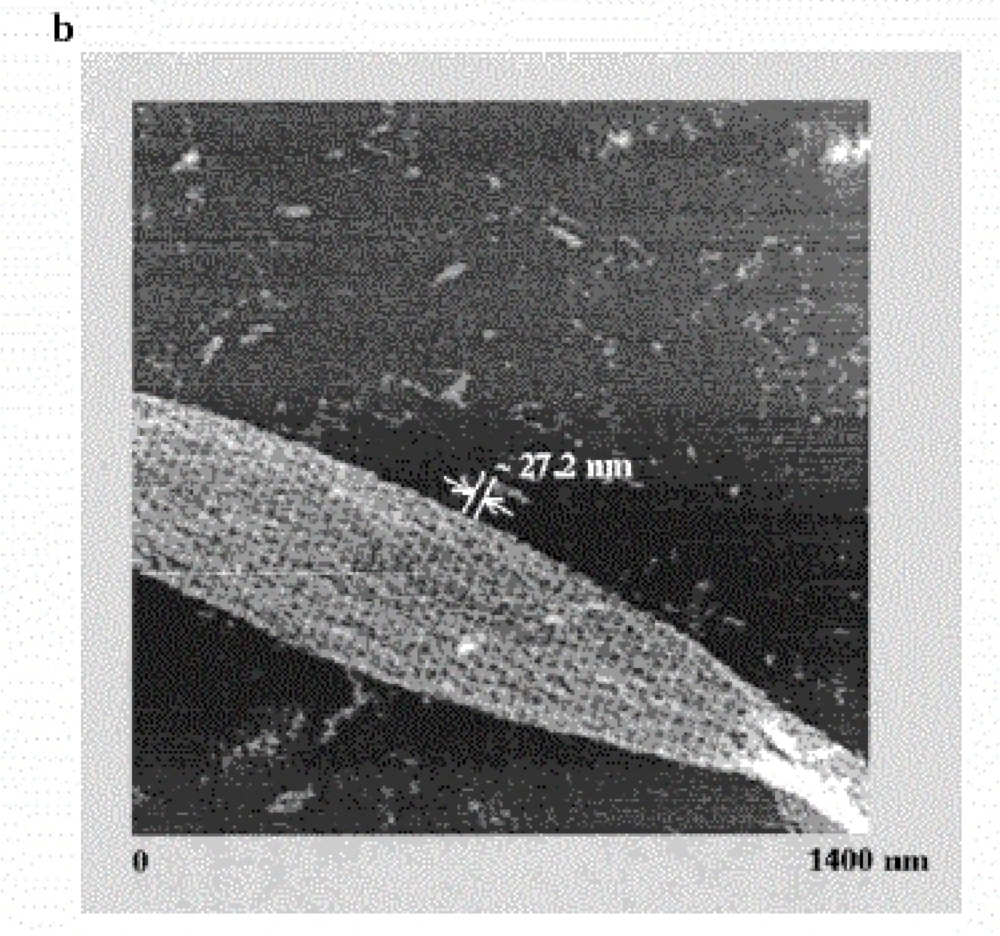
Hairpin Hybridization

Shifted Hybridization

DNA Computers

- Can be adaptable through enzymatic action
- Hard to program because of hybridization errors
- Not very efficient because of space complexity

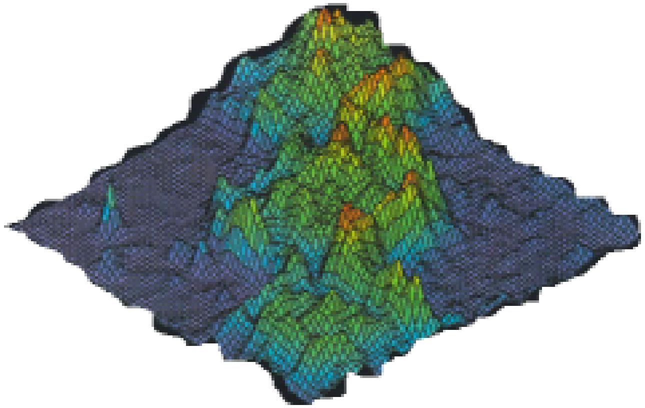
DNA Self-Assembly



Molecular Computing

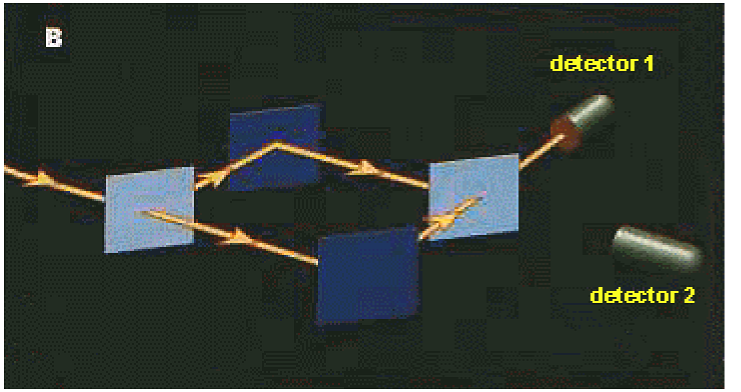
- Building electronic circuits from the bottom up, beginning at the molecular level

Single monolayer of organically functionalized silver quantum dots
Journal of Physical Chemistry, May 6, 1999



- Molecular computers will be the size of a tear drop with the power of today's fastest supercomputers

Molecular Computing as an Emerging Field



Observing quantum interference

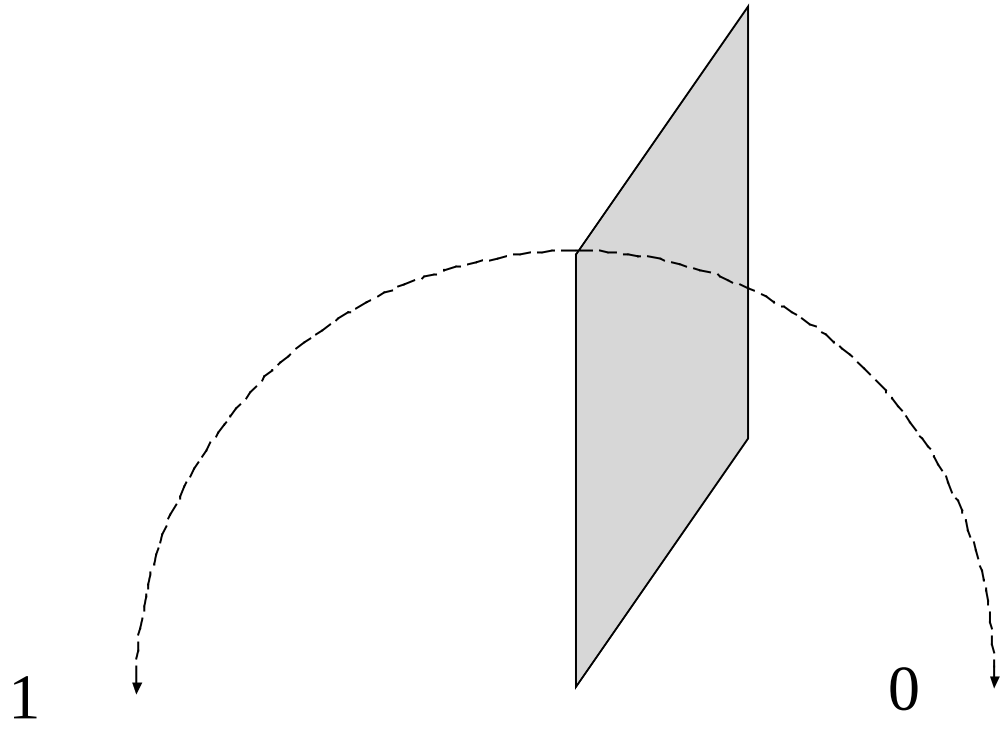
- Interdisciplinary field of quantum information science addresses atomic system (vs. classical system) efficiency and ability to handle complexity
  - Involves physics, chemistry, mathematics, computer science and engineering
- Quantum information can be exploited to perform tasks that would be nearly impossible in a classical world

Quantum Computers

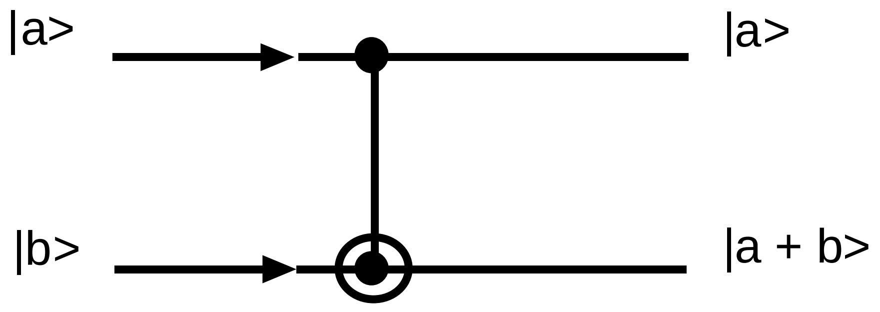
- Different operating principles than either DNA or conventional computers
- Coherent superposition of states produces massive parallelism
- Explores all possible solutions simultaneously
- Prime Factorization, Searching Unsorted List

Quantum Computers

- Qubits: |Q> = A |0> + B |1>
- $|A|^2 + |B|^2 = 1$
- $P(0) = |A|^2$, $P(1) = |B|^2$



Quantum Computers: CNOT Gate

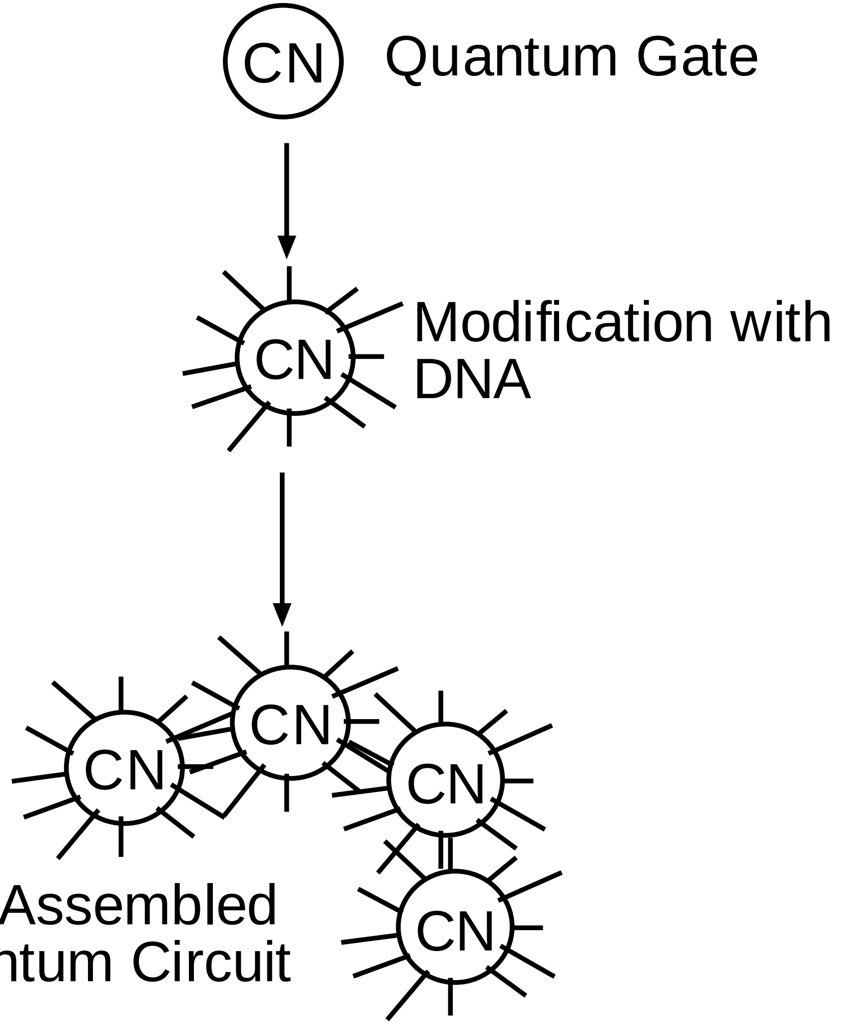


|a>	|b>	|a'>	|a+b>
0	0	0	0
0	1	0	1
1	0	1	1
1	1	1	0

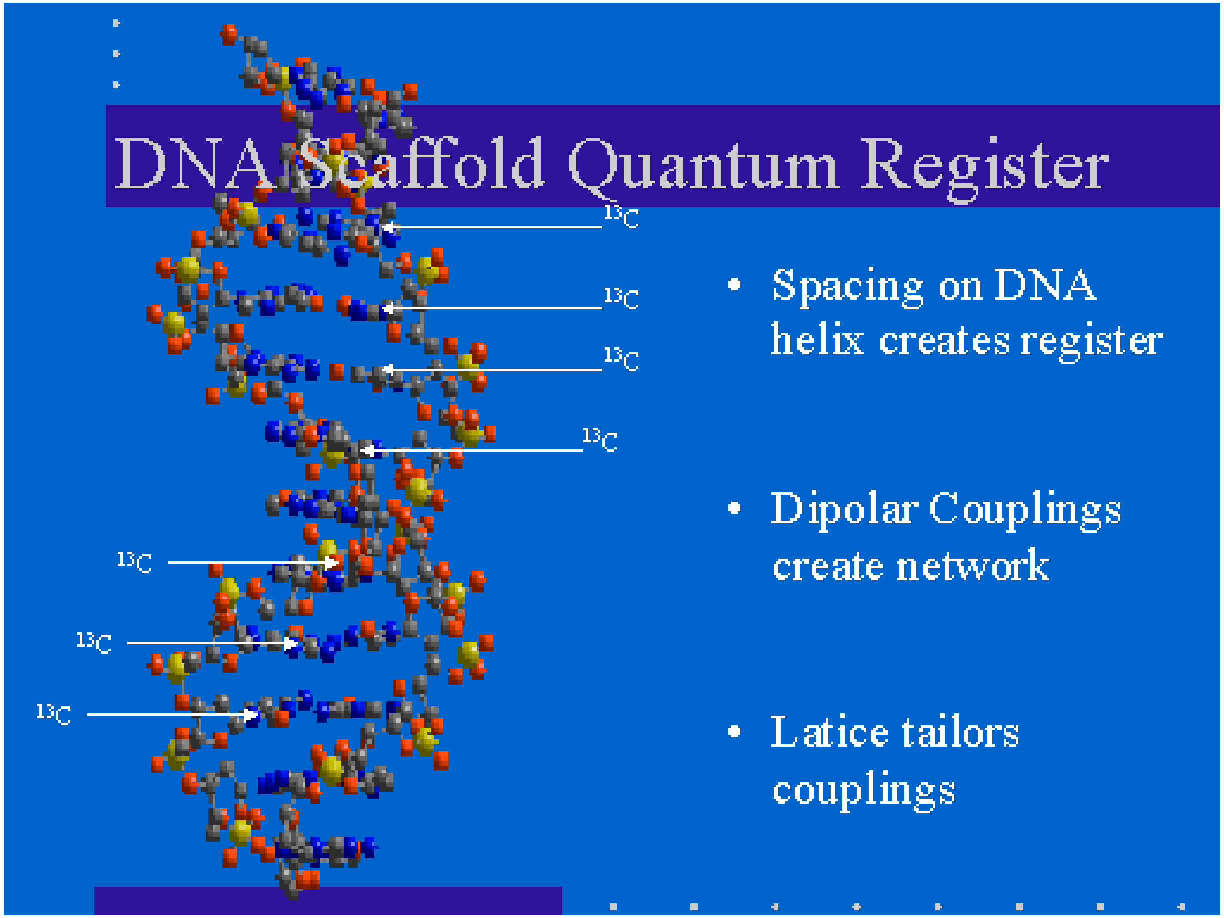
Quantum Computers

- Very efficient because of superposition of exponential number of states
- Can be programmed
- Not adaptable
- Must be isolated from the environment

DNA Assembly of Quantum Circuits

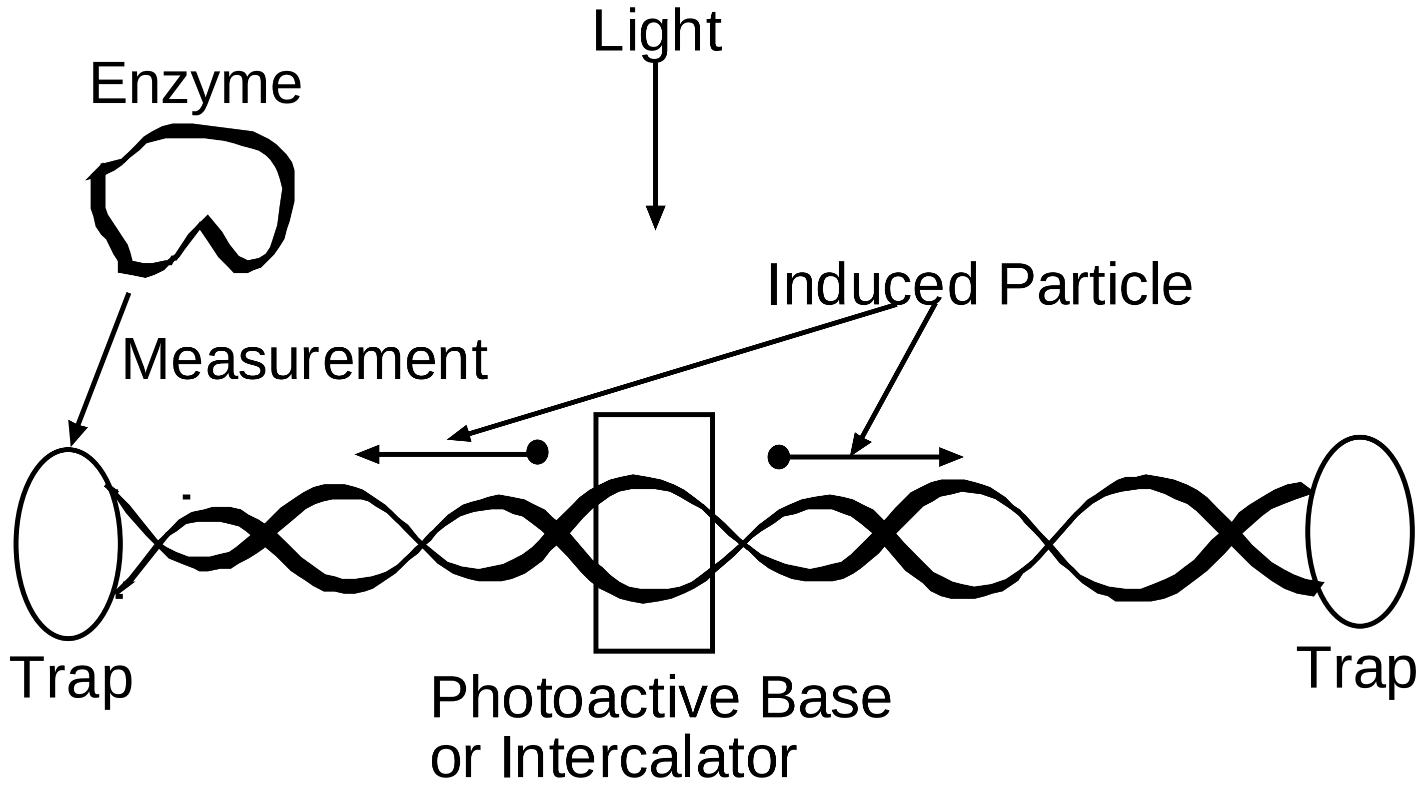


DNA NMR Computers



http://rabi.cchem.berkeley.edu/~kubinec/slideshow1/slideshow/sld013.htm

DNA Qubit


Light
Enzyme
Induced Particle
Measurement
Trap
Trap
Photoactive Base
or Intercalator

Research Issues

- What is the state-of-art?
  - A lot of funding available!
  - Lots of experimental research on device level
    - Molecular RAMs
    - Carbon-film memories
  - Limited activity of higher levels of design
  - Lack of communication between physicists/chemists and architecture/CAD engineers

What could the CAD community contribute at this stage?

- Identifying which properties we need to build circuits
  - Composability/cascadability: (x')' = x
  - Gain for signal restoration
    - Restoring logic (molecular amplifiers)
    - Error-correcting techniques in quantum computing
- Techniques for building reliable circuits from unreliable components
  - What logic abstractions do we need for that?
  - How much can be borrowed from the existing fault-tolerant design techniques?

Conclusions

- DNA, Quantum Computers and other nano-technologies have great potential.
- Serious technical barriers need to be overcome.
- These technologies have complementary properties.
- Work together to have programmability, efficiency, and adaptability
- It is not too early to think about CAD, architectures, and algorithms.
- Past (thousands), present (50 years) and future (few years) technologies of computing.
- **Be brave**, have a perspective.

Reading Assignment

- 1. Read slides to lectures 1, 2 and 3 from my WebPage.
- 2. Read Chapter three (Introduction to Computer Science) from Nielsen and Chuang.
- 3. Read Chapter 1. Sections 1.1, 1.2, 1.3, 1.4.1, and 1.4.2.
- You may expect a very short quizz next week.

This is the end of Lecture 2.