L0 :
Why Science? Changing Paradigms in Computing

July 28, 2023

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Most of us are fascinated by ideas like the BIG BANG

Most of science is quieter

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compute

v. com·put·ed, com·put·ing, com·putes

v.tr. 1. To determine by mathematics, especially by numerical methods: *computed the tax due*. See Synonyms at calculate.

2. To determine by the use of a computer.

v.intr. 1. To determine an amount or number.

2. To use a computer.

3. Informal : To be reasonable, plausible, or consistent; make sense *Your alibi doesn't compute.*

n. Computation: *amounts beyond compute.*

[Fr. computer, from Old French, from Latin computre : com+putre, *to reckon*; Late Latin computus, ..., *to compute*]

com·puta·bili·ty *n.* com·puta·ble *adj.*

computing [kəm'pjuːtɪŋ] *n.* 1. the activity of using computers and writing programs for them

2. the study of computers and their implications

adj of or relating to computers *computing skills*

The revolution in literary form and aesthetic consciousness called modernism arose as the physical sciences were revising their most fundamental concepts: space, time, matter, and the concept of 'science itself. The coincidence has often been remarked upo in general terms, but rarely considered in detail. *Einstein's Wake* argues that the interaction of modern ism and the 'new physics' is best understood by reference to the metaphors which structured these developments. These metaphors, widely disseminated in the popular science writing of the period, provide a language with which modernist writers could articu late their responses to the experience of modernity. Beginning with influential aspects of nineteenth-century physics, *Einstein's Wake* qualifies the notion that Einstein alone was responsible for literary 'relativity'; it goes on to examine the fine detail of his legacy in literary appropriations of scientific metaphors, with particular attention to Virginia Woo D. H. Lawrence, Wyndham Lewis, and T. S. Eliot.

Michael H. Whitworth is Lecturer in English, University of Wales, Bangor

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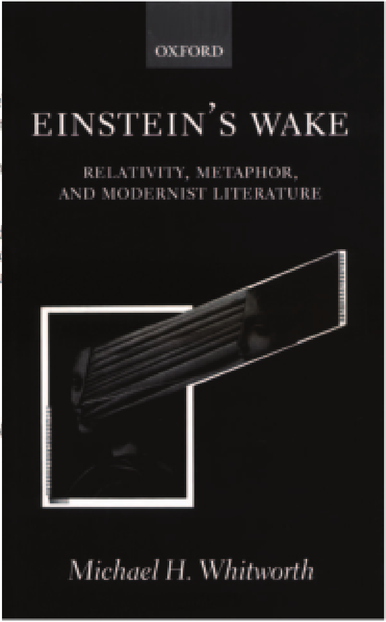
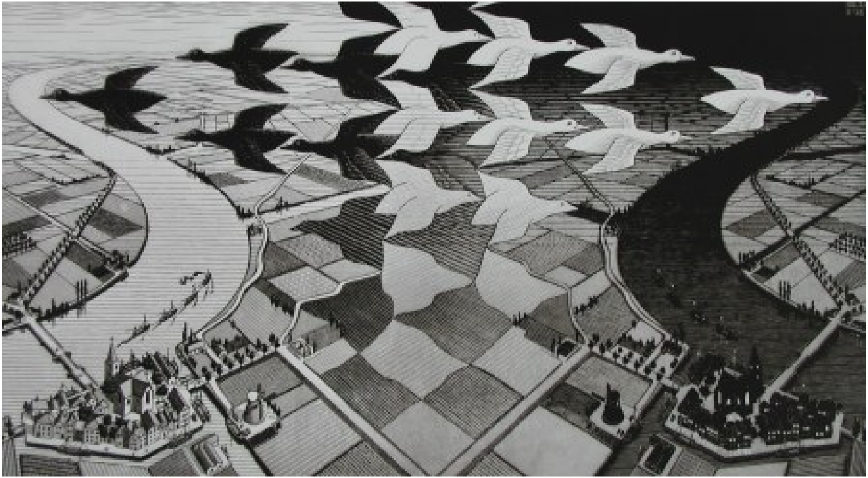
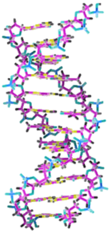
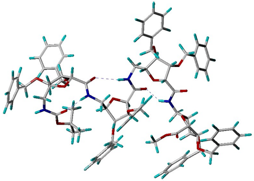


geometry and Escher



Chemical computations





Molecular mechanics
1,000,000 atoms

Semi-empirical quantum mechanics
10000 atoms

ab initio quantum mechanics
1000 electrons

Use empirically derived interactions

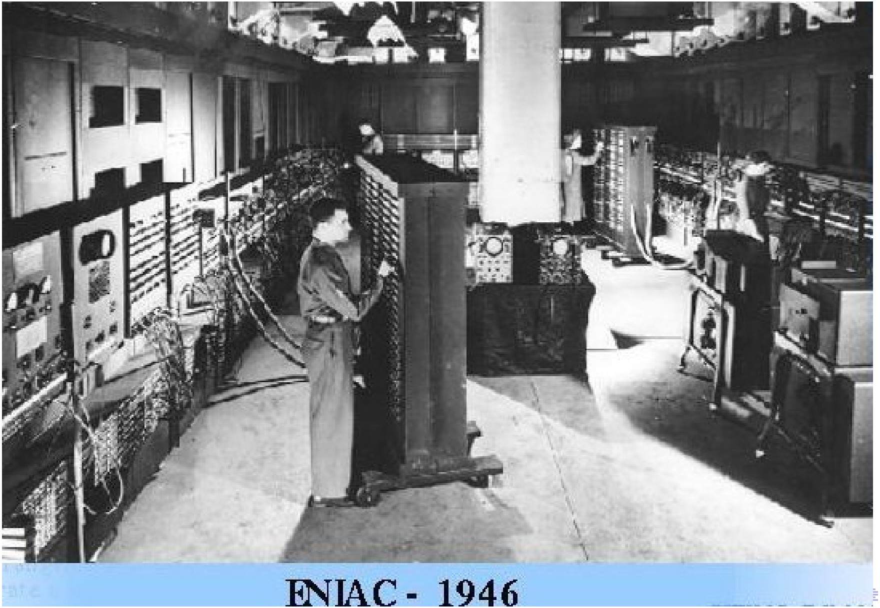
Solve approximate Schrödinger eqn

Solve exact Schrödinger eqn

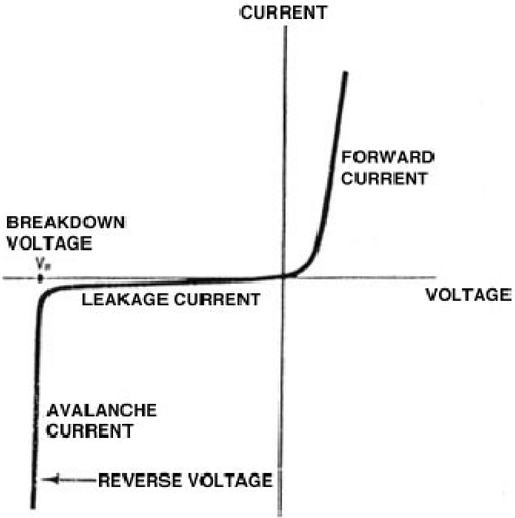
Empirical parameters needed

Computationally demanding

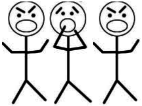
All significant developments in IT have originated from compelling questions in science or as a part of scientific research.



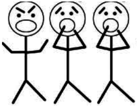
Past: The semiconductor technology: the magic curve



The digital logic



$\times$



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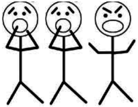
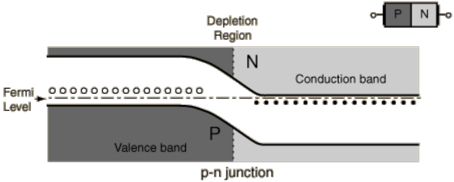
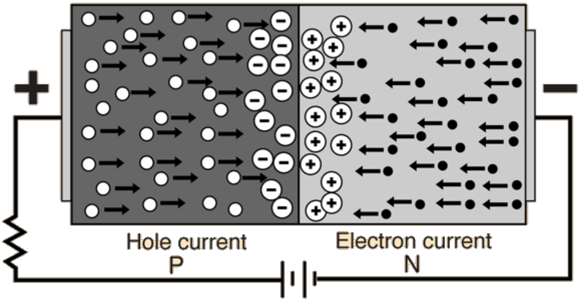
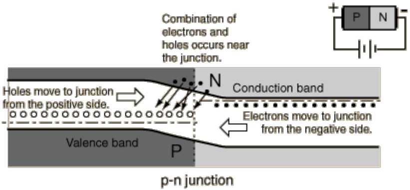


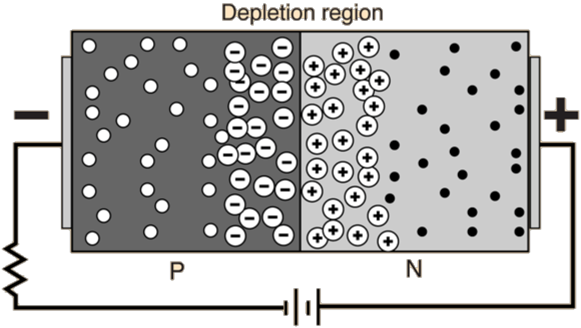
p-n junction equilibrium



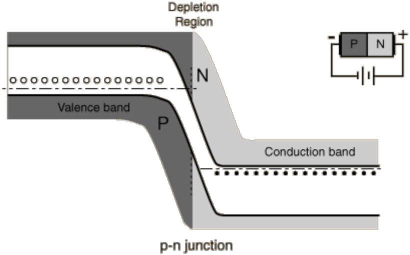


forward bias

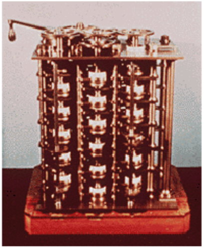


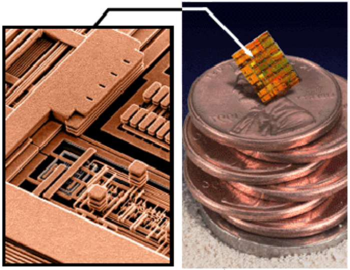


reverse bias



Macro to nano: from early computing machine built from mechanical gears to 2004 IBM chip with 0.25μ features





	Osborne Executive portable:1982:	Apple iPhone 14:2022
CPU	Zilog Z80 4MHz	3.23GHz A15 bionic hexacore
weight	100	1
size	500	1
cost	10	1
clock	1/810 (freq)	1

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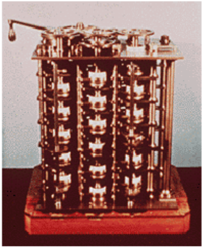

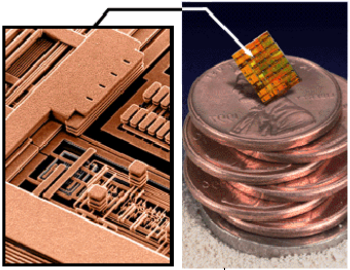

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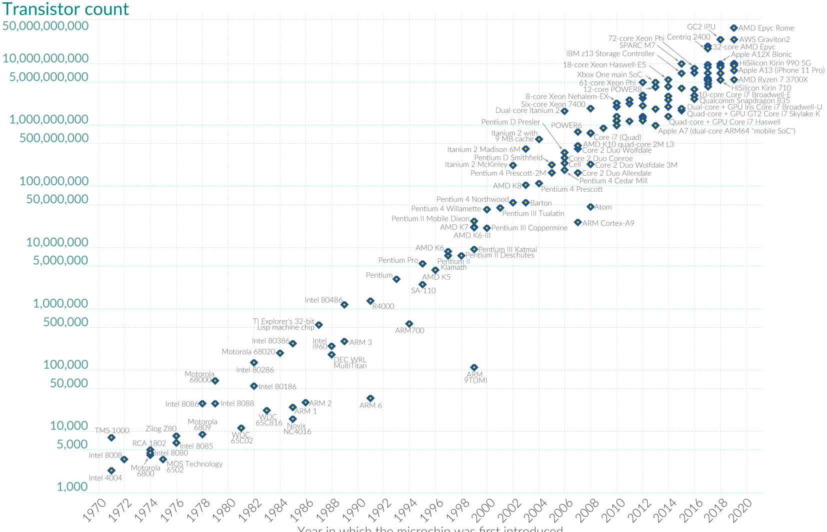
Moore's Law: The number of transistors on microchips doubles every two years

Our World in Data

Moore's law describes the empirical regularity that the number of transistors on integrated circuits doubles approximately every two years.
This advancement is important for other aspects of technological progress in computing – such as processing speed or the price of computers.



Data source: Wikipedia (wikipedia.org/wiki/Transistor_count)
OurWorldinData.org – Research and data to make progress against the world's largest problems.

Intel Process Roadmap

PROCESS NAME	INTEL 10NM SUPERFIN	INTEL 7	INTEL 4	INTEL 3	INTEL 20A	INTEL 18A
Production	In High-Volume (Now)	In Volume (Now)	2H 2022	2H 2023	2H 2024	2H 2025
Perf/Watt (over 10nm ESF)	N/A	10-15%	20%	18%	>20%?	TBA

May '23

intel processors:

Raptor lake 10 nm

$>$ 4+ bn transistors

As transistors became smaller more could be integrated into a single microchip, and so the computational power increased.

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Feynman (1959) lecture: *There's Plenty of Room at the Bottom: an invitation to enter a new field of physics*

• problem of manipulating

and controlling on a small scale • staggeringly small world that is below

- "in 2000, they will wonder why until 1960 nobody began to move in this direction"

Feynman offered 2 prizes each $1000

•...who makes an electric motor ... [which is] only $\frac{1}{64}$ inch cube

• ...who can take information on a page of a book and put it on area $\frac{1}{25000}$ smaller in linear scale so that it can be read by an electron microscope

updated talk (1983): predicted that with today's technology we can easily...construct motors a fortieth of `that size in each dimension, 64000 times smaller...`

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- Processor miniaturization is now reaching a limit, a quantum threshold below which transistors will cease to function. Present 'state-of-the-art' components possess features only a few tens of nm across
- *At the scale of tens of nm, their operation is disrupted by emergence of quantum phenomena, such as electrons tunneling through barriers between wires.*
- what more can be done with 'silicon' based technology?
  - parallelisation
  - peripherals development
- This sophisitication has given rise to interesting pseudoscience: http://www.youtube.com/watch?v=ApQlMm39xr0

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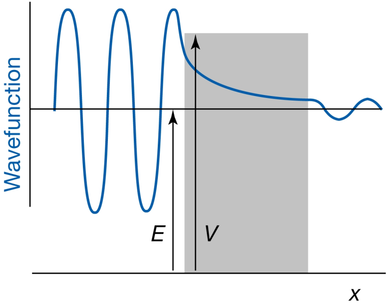
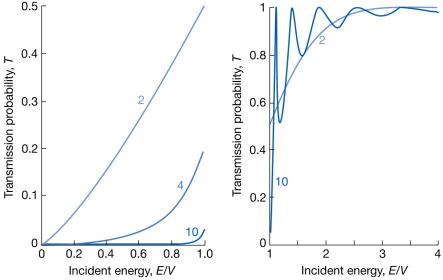
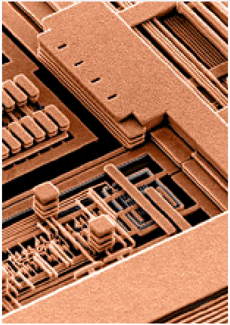
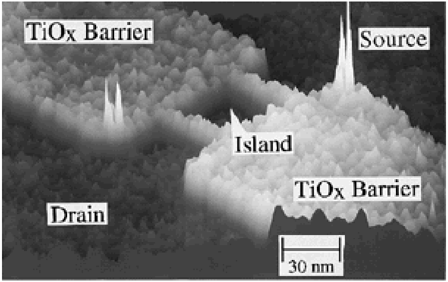
Tunneling:


Wavefunction
E
V
x


Transmission probability, T
Incident energy, E/V
0.5
0.4
0.3
0.2
0.1
0
0.2
0.4
0.6
0.8
1.0
2
4
10
1
0.8
0.6
0.4
0.2
0
1
2
3
4
2
10

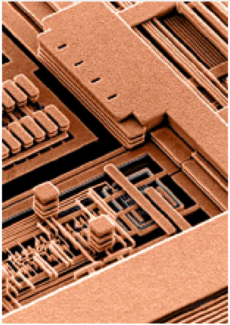


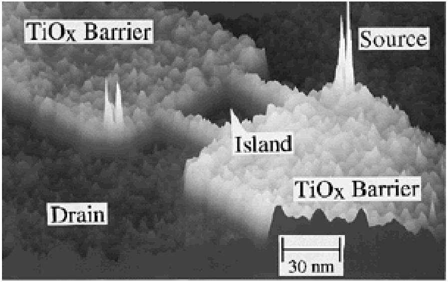


Microtechnology $\Longrightarrow$ Nanotechnology.

- Right: a single-electron transistor (SET) which was carved by the tip of a scanning tunneling microscope (STM).
- According to classical physics, there is no way that electrons can get from the 'source' to the 'drain', because of the two barrier walls either side of the 'island'. But the structure is so small that quantum effects occur, and electrons can tunnel through the barriers (but only one electron at a time can do this!).

SET wouldn't work without quantum mechanics.





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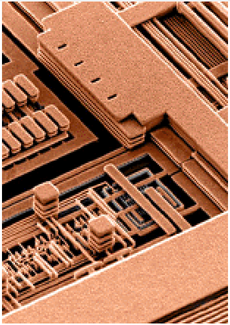

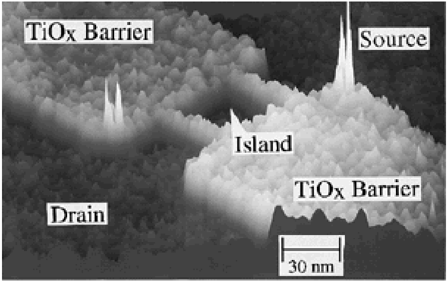

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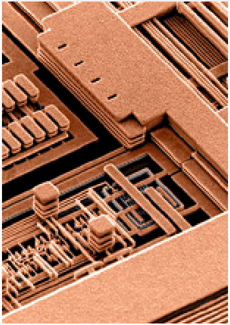

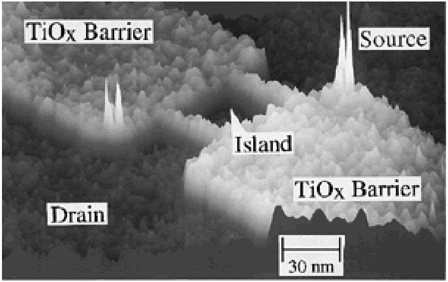

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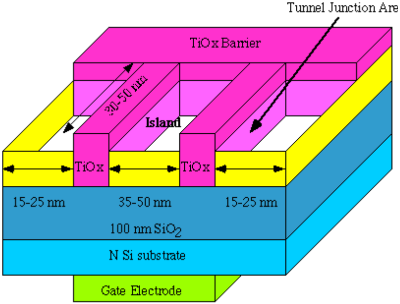
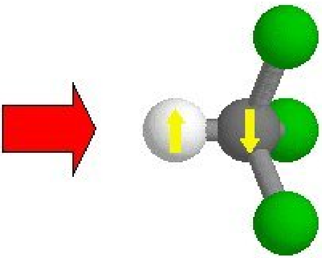
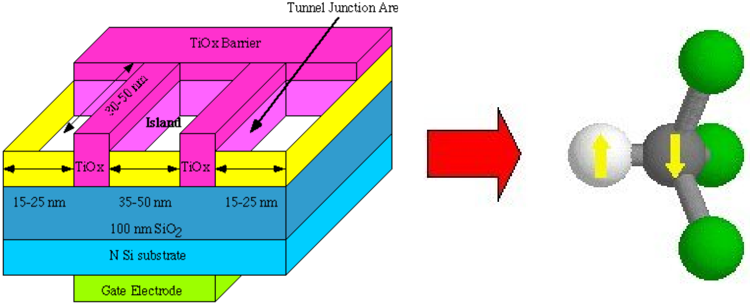
- The first generation of nanocomputers have components that behave according to quantum mechanics, but the algorithms that they run do not involve quantum mechanics.
- There is another, more exciting possibility - quantum mechanics might be used in an entirely new kind of algorithm that would be fundamentally more powerful than any classical scheme. A computer that runs such an algorithm is a true 'quantum computer'.





From an SET (on the left) to the ultimate computer element: a molecule

Although both these structures use quantum mechanics, only the one on the right could be employed in a true '*quantum computer*'. The 1H and 13C nuclei in isotopically labeled chloroform behave like small magnets, and interact with an external magnetic field. Nuclear spins can store and process information in "*quantum superpositions*".



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Quantum mechanics timeline

19th century :
1859 – Kirchhoff: blackbody spectrum depends only on its temperature
1860–1900 – Boltzmann, Maxwell and others: statistical mechanics. Entropy is a measure of disorder.
1877 – Boltzmann: energy levels of a physical system could be discrete based on stat mech and mathematical arguments; the first atomic model of a molecule (e.g., an I_2 molecule), later (in 1928) called MOs, of the constituting atoms.

1887 – Hertz: photoelectric effect, shown by Einstein in 1905 to involve quanta of light.
1888 – Hertz demonstrates experimentally that electromagnetic waves exist, as predicted by Maxwell.
1888 – Rydberg modifies Balmer formula to include all spectral series of lines for the H atom, producing Rydberg formula which is employed later by Bohr and others (1912) to verify first quantum model of atom.
1895 – Röntgen: X-rays in experiments with electron beams in plasma.
1896 – Becquerel : radioactivity

1896 – Zeeman splitting
1896–1897 Marie Curie : charge on α and β particles (names coined later)
1899 to 1903 – Rutherford : coins the terms α and β rays in 1899
Rutherford and Soddy: nuclear transmutation (1902)

1900–1909

1900 – Planck suggests that electromagnetic energy could only be emitted in quantized form, $E = h\nu$

1902 – Lewis: the "cubical atom" theory in which electrons in the form of dots are positioned at the corner of a cube. Single, double, or triple "bonds" : two atoms are held together by multiple pairs of electrons

1903 – Becquerel, Curie and Curie : 1903 Nobel Prize in Physics

1905 – Einstein : photoelectric effect (1887 : Hertz)

1905 – Einstein : Brownian motion

1905 – Einstein : Special Theory of Relativity.

1905 – Einstein : equivalence of matter and energy.
1907 to 1917 – Rutherford: α particle scattering and nuclear structure.
1908 : Nobel Prize in Chemistry
1911: Rutherford explained the Geiger–Marsden experiment
1909 – Taylor demonstrates that interference patterns of light were generated even when the light energy introduced consisted of only one photon. This discovery of the wave–particle duality of matter and energy is fundamental to the later development of quantum field theory.
1909 and 1916 – Einstein : if Planck's law of black-body radiation is accepted, the energy quanta must also carry momentum $p = \frac{h}{\lambda}$, making them full-fledged particles

1913 – Bohr model of atom.
1914 – Franck and Hertz : experiment on electron collisions with mercury atoms - new test of Bohr's model of atomic energy levels.
1922 – Compton effect or scattering
1922 – Stern–Gerlach experiment
1922 – Bohr updates his model - "closed shells", presaging orbital theory
1923 – Auger effect
1923 – de Broglie : wave–particle duality for particles: $\lambda = \frac{h}{p}$

1923 – Theory of Lewis acids and bases
1924 – Bose–Einstein statistics
1924 – Pauli exclusion principle
1925 – Uhlenbeck and Goudsmit postulate the existence of electron spin.
1925 – Hund's rule of Maximum
1925 – Heisenberg, Born, and Jordan : matrix mechanics formulation of QM
1925-26: Schrödinger eqn
1926 – Lewis coins the term photon, which he derives from the Greek word for light

Quantum Computers

A synthesis of classical information theory, computer science and quantum physics

A bit - 0 or 1

- the voltage between the plates in a capacitor
- two different polarisations of light
- two different electronic states of an atom.

the state of an atom/molecule as a physical bit

quantum mechanics $\Longrightarrow$ apart from the two distinct electronic states the atom can be also prepared in a coherent superposition of the two states.

superposition $\leftrightarrow$ a quantum mechanical phenomenon:

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Quantum Computers

A synthesis of classical information theory, computer science and quantum physics

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- the voltage between the plates in a capacitor
- two different polarisations of light
- two different electronic states of an atom.

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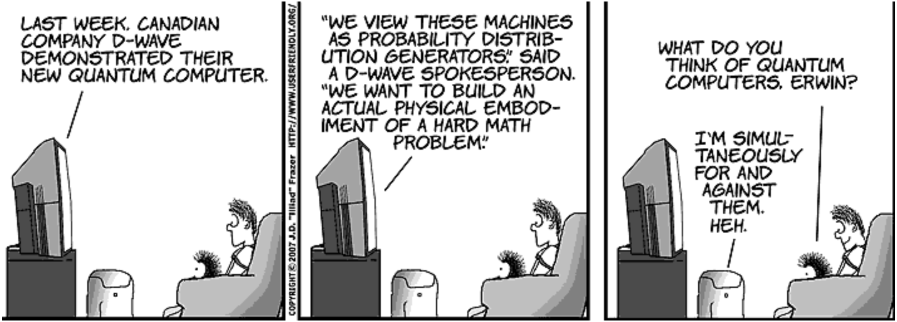

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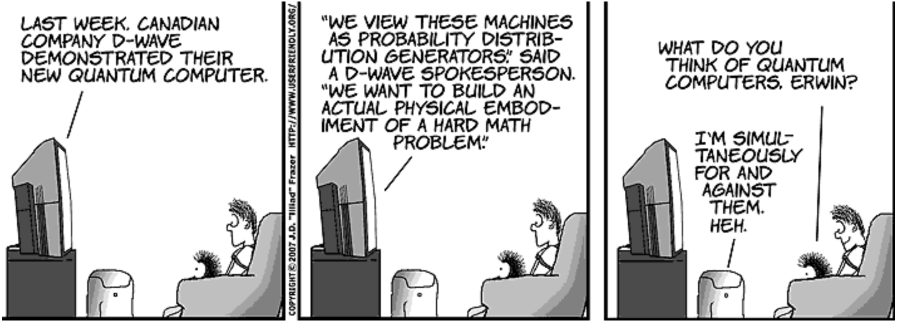

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Consider 3 physical bits.

classical register ⇒ can store at a given moment of time only one out of eight different numbers,

• it can be in only one out of eight possible configurations such as 000, 001, 010, ... 111.

quantum register ⇒ composed of three qubits can store at a given moment of time all eight numbers in a quantum superposition.

$$|x\rangle = \alpha_1|000\rangle + \alpha_2|001\rangle + \alpha_3|010\rangle + \cdots ; \quad \sum_i \alpha_i^2 = 1$$

If we keep adding qubits to the register we increase its storage capacity exponentially i.e. three qubits can store 8 different numbers at once, four qubits can store 16 different numbers at once, and so on; in general L qubits can store 2^L numbers at once.

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two main quantum computing methods :

1. analog quantum computing : prepare initial set of qubits representing all possible solutions to a problem
   exploit properties of superposition and entanglement, such that the set of qubits evolves and identifies an optimal solution
   most mature version of an analog quantum computer is quantum annealing machine :
   designed to solve certain optimization problems
   - may have uses in optimizing **drug design**, donor matching, traffic flows, and transportation routes
2. gate-based quantum computing, which breaks a problem down into a sequence of basic operations, or gates which perform operations on bits or store bit values
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physical qubits are created from a variety of systems including:

- Particles such as atoms, ions, and photons
- Objects that mimic particles, such as superconducting circuits, quantum dots (small semiconducting crystals that resemble transistors), and defects in a crystal (e.g., a nitrogen atom within a diamond's carbon lattice, known as a color center)

multiple qubits can be entangled with one another

- accomplished with lasers, microwaves, electric or magnetic fields, and other ways to control qubits
- However, Quantum information is fragile and can be irreversibly lost through interactions with the environment, in a process called decoherence
- coherence time : how long a qubit maintains a superposition or entangled state before decoherence, a factor that limits how long a qubit can be used for an operation
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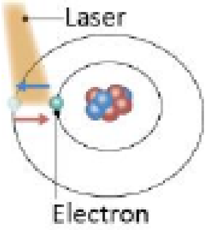


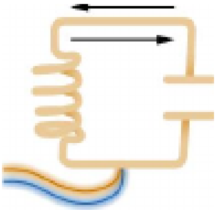
Trapped Ion :

Single ions trapped in electric/magnetic fields and laser-cooled to $\approx$ 0K

Trapped ion qubits manipulated with lasers or microwave pulses

a few dozen noisy qubits

platforms : IonQ, Honeywell, and Sandia National Laboratory's Quantum Scientific Computing Open User Testbed ...



Superconducting :

artificial atom circuit loop made of superconductors cooled to $\approx$ 0K

qubits controlled with microwave electronics and can operate quickly

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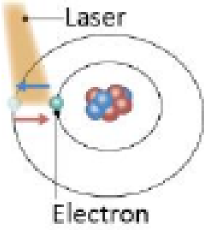

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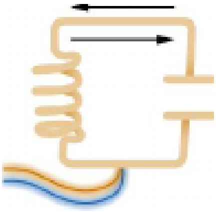

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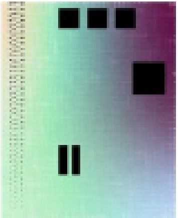

Photonic :

Encodes qubits in light that travels through optical chips or fiber

qubit systems can operate at room temperature but some may require technologies at ≈ 0K to detect qubits

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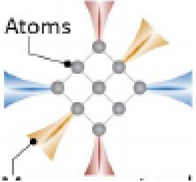
platforms : Xanadu



measurement and control lasers

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Neutral atoms similar to trapped ions and controlled by lasers or microwave pulses

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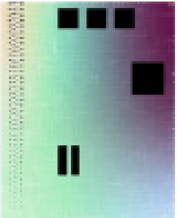
Platform availability: appearing now



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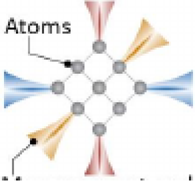

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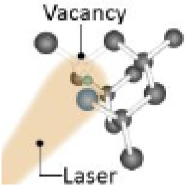

Color Centers : artificial atom in diamond or another crystal with defect created by an added atom or a vacant space

qubits controlled with light and optically detected

$\approx$ two dozen qubits

Platform :

not yet

Quantum Dot :

artificial atom, similar to a transistor, consisting of small semiconducting crystal controlled with microwaves or electrical signals

qubits require temperatures of ≈ 1K to operate

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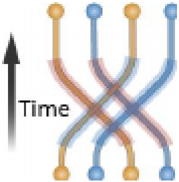
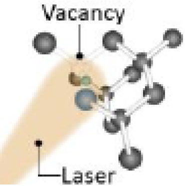


Topological :

channeling electrons along the boundary between two different materials

qubits composed of "quantum braids" in time

Not demonstrated



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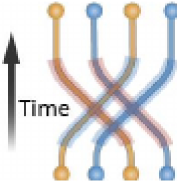

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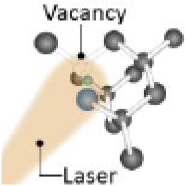

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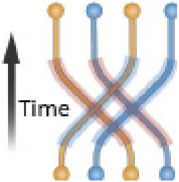

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Various physical realisations of interacting systems of quantum bits
-Nielsen and Chuang: 1995

System	$\tau_Q(s)$	$\tau_{op}(s)$	$n_{op} = \lambda^{-1} = \frac{\tau_Q}{\tau_{op}}$
Nuclear spin	$10^2 - 10^8$	$10^{-3} - 10^{-6}$	$10^5 - 10^{14}$
Electron spin	10^{-3}	10^{-7}	10^4
Ion trap	10^{-1}	10^{-14}	10^{13}
Electron-Au	10^{-8}	10^{-14}	10^6
Electron-GaAs	10^{-10}	10^{-13}	10^3
Quantum Dot	10^{-6}	10^{-9}	10^3
Optical Cavity	10^{-5}	10^{-14}	10^9
Microwave cavity	10^0	10^{-4}	10^4

τ_Q=decoherence time; τ_{op}=operation time; n_{op}=max. no. of operations

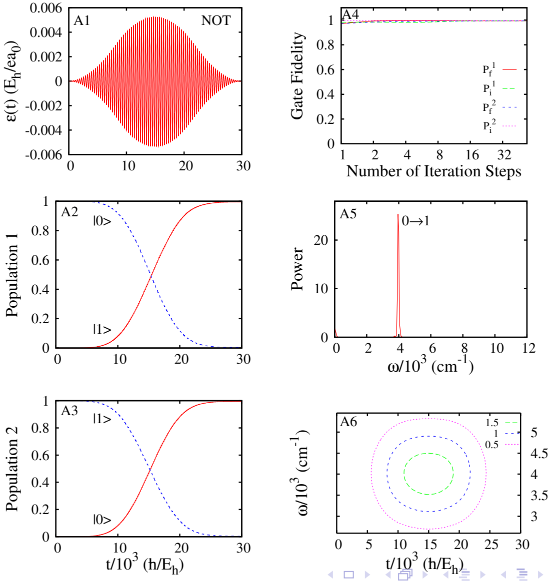
single qubit quantum gates

NOT

$$\begin{pmatrix} |0\rangle \\ |1\rangle \end{pmatrix}$$

$$\Downarrow$$

$$\begin{pmatrix} |1\rangle \\ |0\rangle \end{pmatrix}$$

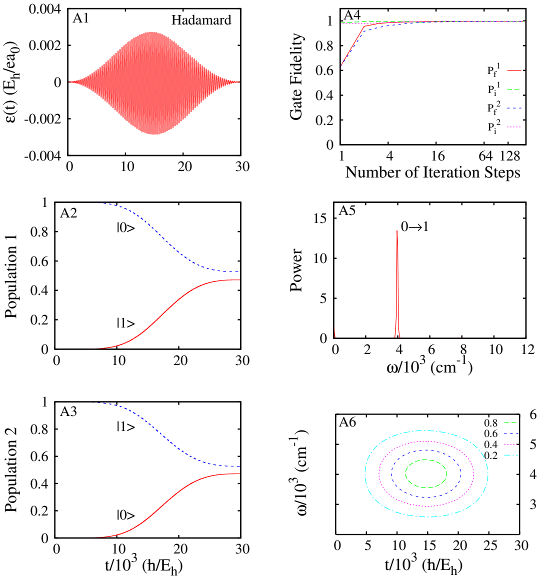


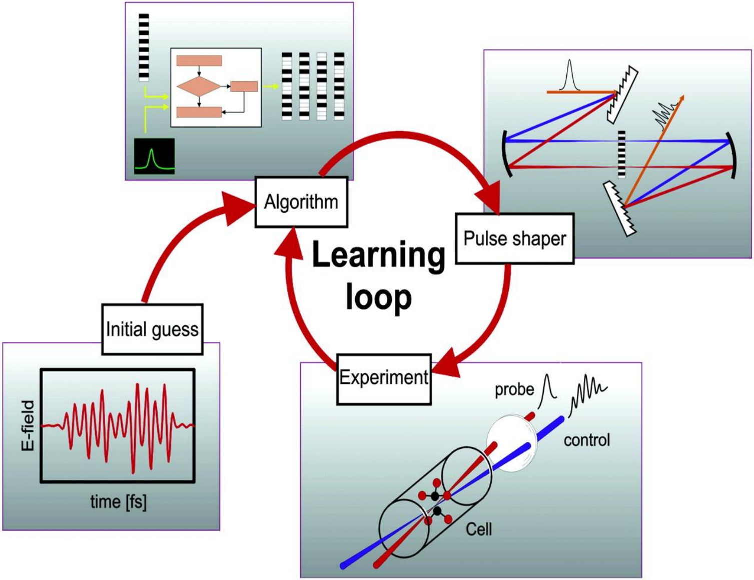
HADAMARD

$$\begin{pmatrix} |0\rangle \\ |1\rangle \end{pmatrix}$$

$$\Downarrow$$

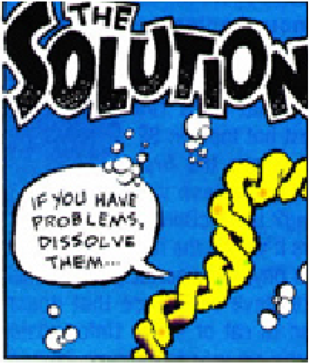
$$\begin{pmatrix} \frac{|0\rangle+|1\rangle}{\sqrt{2}} \\ \frac{|0\rangle-|1\rangle}{\sqrt{2}} \end{pmatrix}$$




Algorithm
Pulse shaper
Learning loop
Initial guess
E-field
time [fs]
Experiment
probe
control
Cell

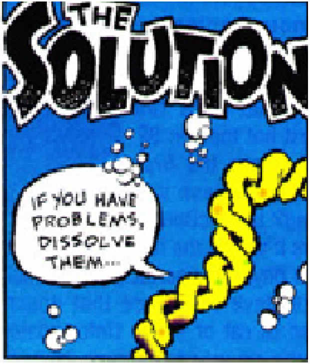
Computational task	Classical cost	Quantum cost
Factoring	$e^{O(n^{1/3} \log^{2/3} n)}$	$O(n^2 \log n \log l$
Search	$O(n)$	$O(\sqrt{n})$
Full CI	$e^{O(n)}$	$O(n^5)$
Chemical dynamics	$e^{O(n)}$	$O(n^2)$
Protein folding	$e^{O(n)}$	?

"IF YOU HAVE PROBLEMS, DISSOLVE THEM"
(Larry Gonick cartoons)



A chemical computer with individual molecules as working parts

"IF YOU HAVE PROBLEMS, DISSOLVE THEM" (Larry Gonick cartoons)



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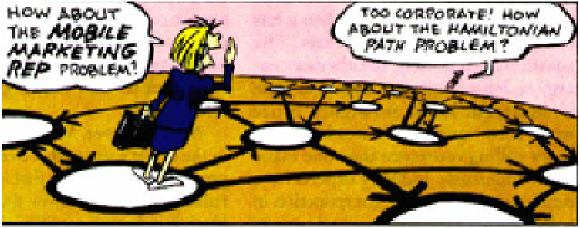
Computation using DNA

Leonard Adleman: (*Science* **1994**, 266(5187):1021-4)
Traveling Salesman problem (Hamiltonian Path problem)

A Marketing Rep has a map of several cities with one-way streets between some of them.
Task: Find a route that passes through each city exactly once, with a designated beginning and end.



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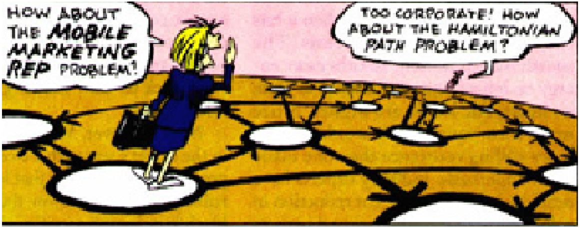
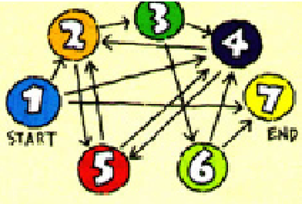
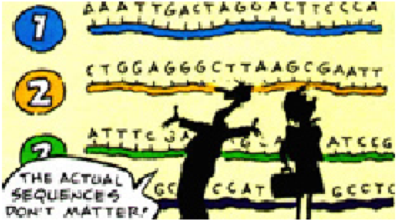


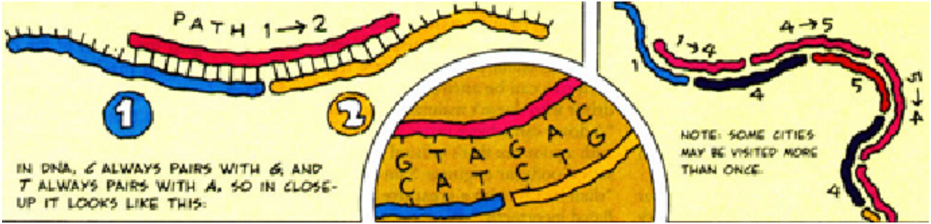
Adleman chose 7 cities and 13 streets.



Each city is represented by a ssDNA 20 bases long.



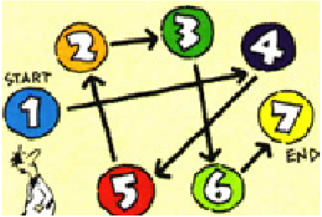
A street between two cities is the complementary 20-base strand that overlaps each city's strand halfway.
A multicity tour becomes a piece of dsDNA.



A few grams of DNA has over 10^{15} molecules. With all combinations of city and street put together multiple copies of every path are created. The task is to find the paths that satisfy the conditions stated earlier.

For this, Chemical techniques are used:

- Extract all paths going from 'START' to 'END'.
- Of those, find the ones passing through 7 cities.
- Of those, isolate paths with 7 different cities.



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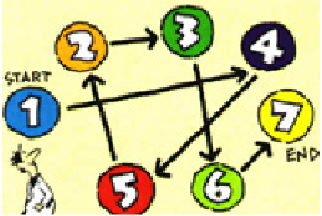

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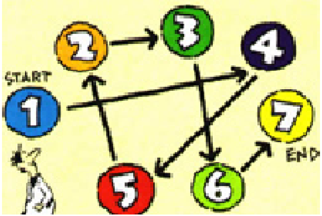

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TECHNOLOGY

First sale for quantum computing

But critics say that D-Wave's system is still something of a black box.

BY ZEEYA MERALI

It could turn out to be a milestone for quantum computing. Last week, D-Wave Systems of Burnaby in British Columbia, Canada, announced the first sale of a commercial quantum computer, to global security firm Lockheed Martin, based in Bethesda, Maryland.

Yet perhaps fittingly for a quantum device, uncertainty persists around how the impressive black monolith known as D-Wave One actually works. Computer scientists have long questioned whether D-Wave's systems truly exploit quantum physics, and although the company last month published a paper in *Nature* (M. W. Johnson *et al. Nature* **473,** 194–198; 2011) to help verify its quantum credentials, some say that the technique used is still in doubt.

Quantum computers could revolutionize the way we tackle problems that stump even the best classical computers, which store and process their data as 'bits' — essentially a series of switches that can be either on or off.

The power of quantum bits — or qubits

reviewing the D-Wave One computer before purchasing it. Although D-Wave has been cagey about specific applications, Lockheed Martin plans to use the technology to help it build "cyber-physical systems", which integrate software with environmental sensors, says Madden.

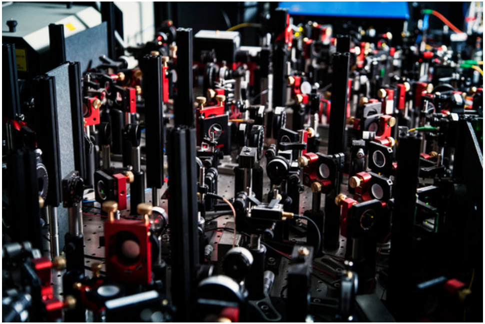
D-Wave's co-founder, Geordie Rose, says that the sale demonstrates that quantum computing is finally living up to its decades-long promise. Aaronson, however, thinks that the computer-science community will need more

DOMINIC SCHAEFER PHOTOGRAPHY

driven by plain old classical physics. At the time, D-Wave did not respond with any publications ruling out this possibility.

But the company's paper in *Nature* demonstrated definitive quantum behaviour in a system with eight qubits, made from superconducting niobium loops. Magnetic fields manipulate the combined energy state of the qubits until the system defines the parameters of the problem to be solved. Because the system exists in a quantum superposition, it can simultaneously 'search' through multiple energy states that each represent different solutions, explains Rose. Cooling the system snaps it out of the superposition, so that it settles into a single, low-energy state that represents the final answer, an approach known as quantum annealing (W. D. Oliver *Nature* **473,** 164–165; 2011). D-Wave One uses sixteen of these eight-qubit cells.

Sceptics had argued that the system could actually work by using thermal fluctuations — rather than quantum effects — to jostle the qubits through various energy states. However, because



http://www.nytimes.com/2014/05/30/science/scientists-report-finding-reliable-way-to-teleport-data.html

Scientists Report Finding Reliable Way to Teleport Data

By JOHN MARKOFFMAY 29, 2014

Scientists in the Netherlands have moved a step closer to overriding one of Albert Einstein's most famous objections to the implications of quantum mechanics, which he described as "spooky action at a distance."

In a paper published on Thursday in the journal Science, physicists at the Kavli Institute of Nanoscience at the Delft University of Technology reported that they were able to reliably teleport information between two

Quantum technologies continue to improve

- 3-qubit magnetic resonance machine in 1998
- 14- qubit entangled state using a trapped ion quantum computing system in 2010
- 53- qubit superconducting quantum computing system in 2019
- 76-qubit, photon-based system in 2020
- possible : 1,000-plus qubit device by 2023

Grand challenges today

1. Control processes at the level of electrons
2. Design and perfect atom- and energy-efficient syntheses of new forms of matter with tailored properties.
3. Understand and control the remarkable properties of matter that emerge from complex correlations of atomic and electronic constituents
4. Master energy and information on the nanoscale to create new technologies with capabilities rivaling those of living things
5. Characterize and control matter away “especially far away” from equilibrium
6. Synthesizing Life-Like Systems
7. Understanding the Brain : Consciousness
8. Predicting Individual Organisms Characteristics from Their DNA Sequence (Genomes to Phenomes)
9. Interactions of the Earth, Its Climate, and the Biosphere
10. Understanding Biological Diversity

It from Bit

Hypothesis: every item of the physical world, be it particle or field of force, ultimately derives its very existence from apparatus-solicited answers to binary, yes /no questions

-John Wheeler

Parts of a poem by Prof Don Anderson, Professor of Geophysics, Caltech

The First Ten Million Millenia or So

In the "beginning" nothing
No time, no space, no matter.
No energy, no strings
nothing
not even a point, not even a void
nothing

No laws of physics
no myths, no Gods;
nothing, absolutely nothing
Then a singularity...
Call it a bang, call it a Big Bang, call it light, call it God
Perhaps a thought
In the beginning, the Laws of Logic begat the Laws of Physics.
The rules.
From Nothing, expansion
false vacuums, phase changes, befinning the time and space.
Potential for something, Everything Energy, potential
Waves, strings,
monopoles, sheets,threads
webs.

From the void, chaos
out of vacuum, Genesis.
Condensation, knots, cosmic freezing.
wrinkles in time, defects
Bubbles, foams. A detergent universe

Strong force, weak force,
symmetry breaking; machos, wimps, tubes of energy, gigantic loops.
A pasta universe
....
Look at Earth
crust
oceans air Life Cool!
a trivial speck, an afterthought
But all we got.
So here we are,
simple and meek,
Now how do we get through the rest of the week?

Thank You