



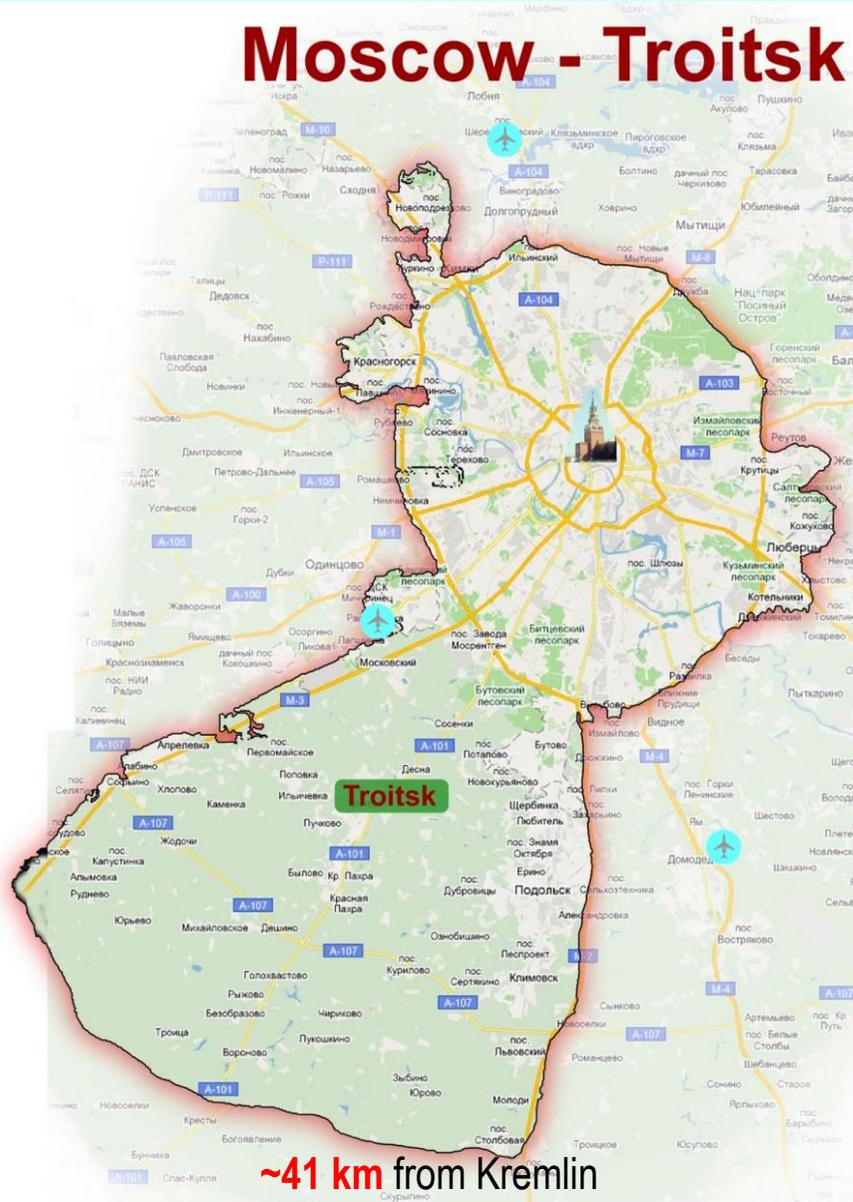
Quantum Computers and Quantum Computing: Dreams and Reality

Victor Zadkov

Institute of Spectroscopy, RAS

Where ISAN is located?

Moscow - Troitsk



~41 km from Kremlin

~15 km from 'old' Moscow border

Center of New Moscow



ISAN

Founded in XVII cent., from 1966 – Scientific center of RAS
from 1977 – city, from 2012 - urban okrug of Moscow, now ~45000 citizens

1. Institute of Earth Magnetism and Radiowaves Propagation (RAS)
2. Institute for High Pressure Physics (RAS)
3. Institute for Nuclear Researches (RAS)
4. Institute for Spectroscopy (RAS)
5. Lebedev Physical Institute - Branch (RAS)
6. Prokhorov General Physics Institute – Branch (RAS)
7. Institute on Laser and Information Technology (RAS)
8. Troitsk Institute of Innovation and Thermonuclear Investigation
9. Technological Institute for Superhard Novel Carbon Materials

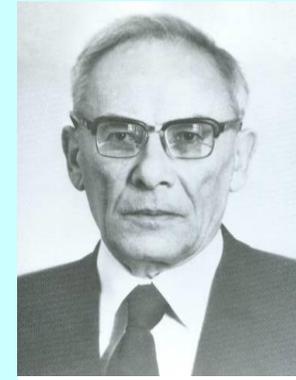
Foundation of ISAN

1960-th

- **A lot of new spectral data from space** -
(huge number of unknown spectral lines)
- **Laser light sources** -
(new effects of light-matter interaction)
- **High temperature plasma** -
(nuclear and thermonuclear research)
- **Technology demands for diagnostics** -
(material sciences, bio-, medical physics)



G.S. Landsberg



S.L. Mandelshtam



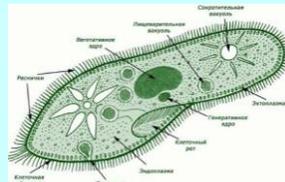
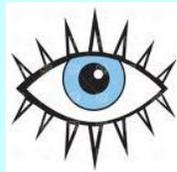
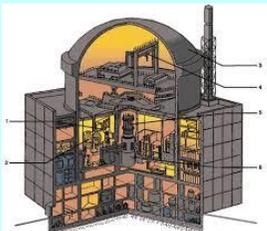
Lebedev Physical Institute of RAS



Commission of Spectroscopy



**Institute for Spectroscopy RAS
(1968)**

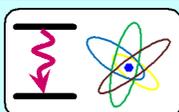


Staff: 200, including ~86 researchers (25 д.ф.-м.н., ~45 Ph.D.)

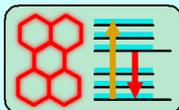
Published papers: ~120-150 papers/year (WoS)

ISAN rating: 3 rd to 5th place in all-Russian ranking table

ISAN is in the first top group of research institutes of the RAS after all-national rating



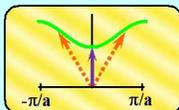
1. Atomic Spectroscopy Dept.



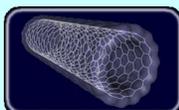
2. Molecular Spectroscopy Dept.



3. Laser Spectroscopy Dept.



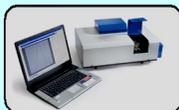
4. Solid State Spectroscopy Dept.



5. Nanostructure Spectroscopy Lab.



6. Theoretical Dept.

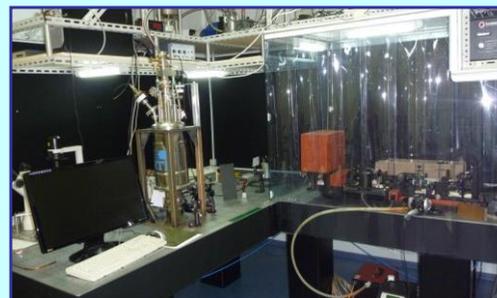


7. Laser Spectral Instrumentation Dept.

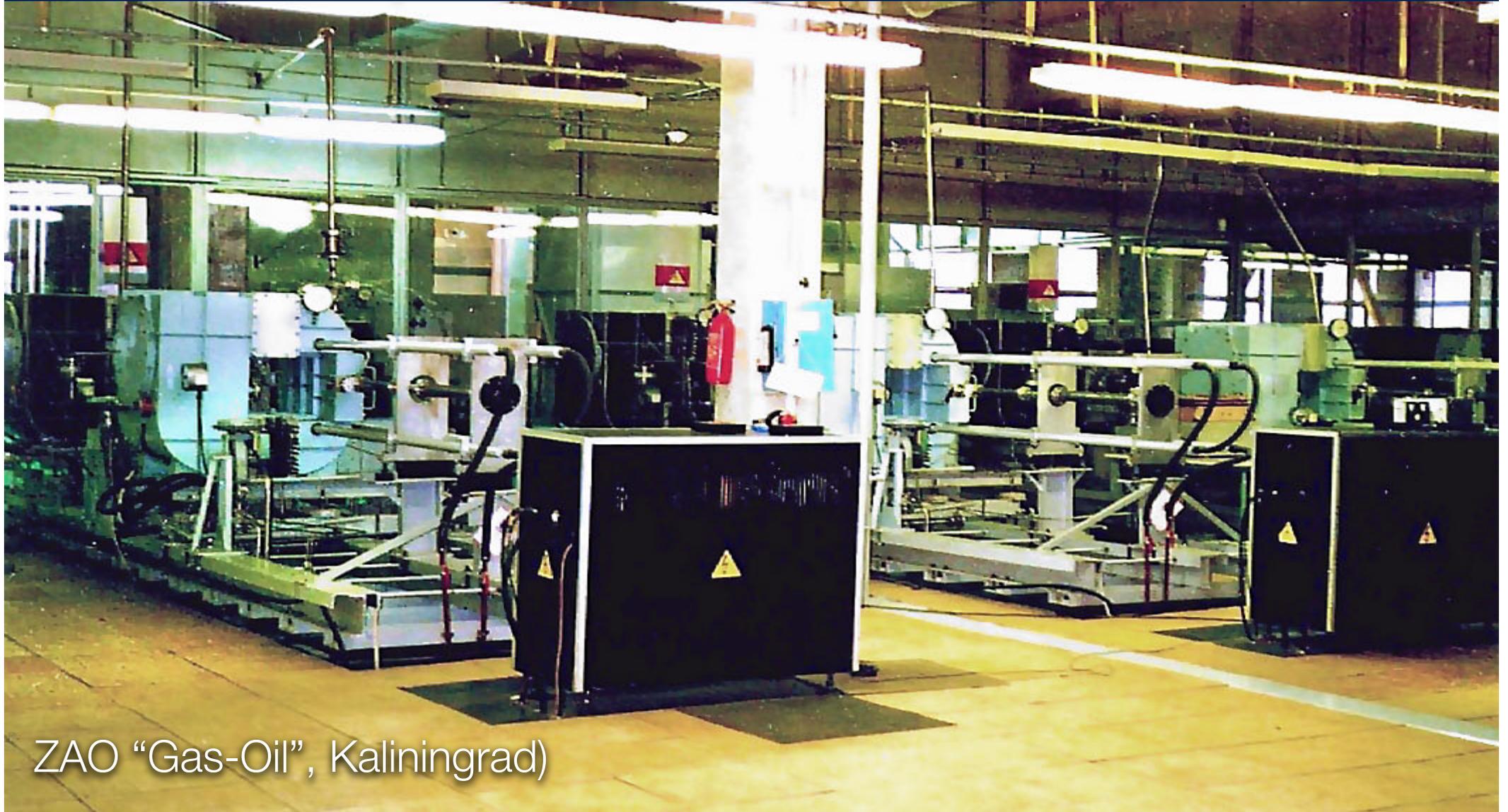


(* Research - Educational Center

- **Materials:** from atoms to biological
- **Spatial resolution:** up to single atoms size
- **Time:** from fs to months/years
- **Spectral range:** from UV to Microwave
- **Structure and dynamics**
- **Theory, experiment, instrumentation**
- **Basic research and applications**

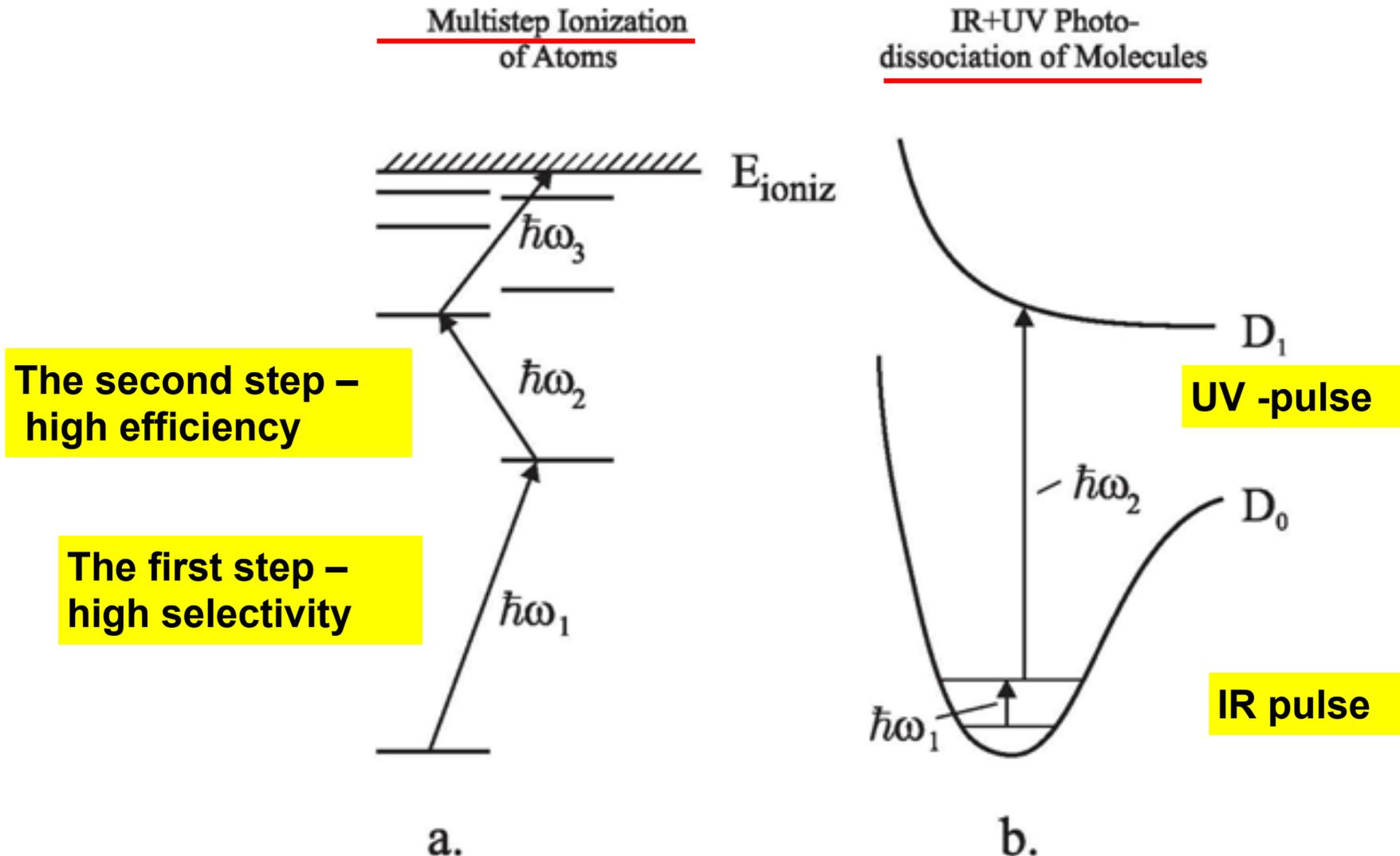


First worldwide factory on laser isotope separation (C13) (1997)



ZAO "Gas-Oil", Kaliningrad)

Increasing photoionization and photodissociation selectivity by using two laser pulses



Experiment with Rb and NH_3

Laser photon source @CERN was created [V.S. Letokhov, V.I. Mishin, V.N.Fedoseev et al (1991)]

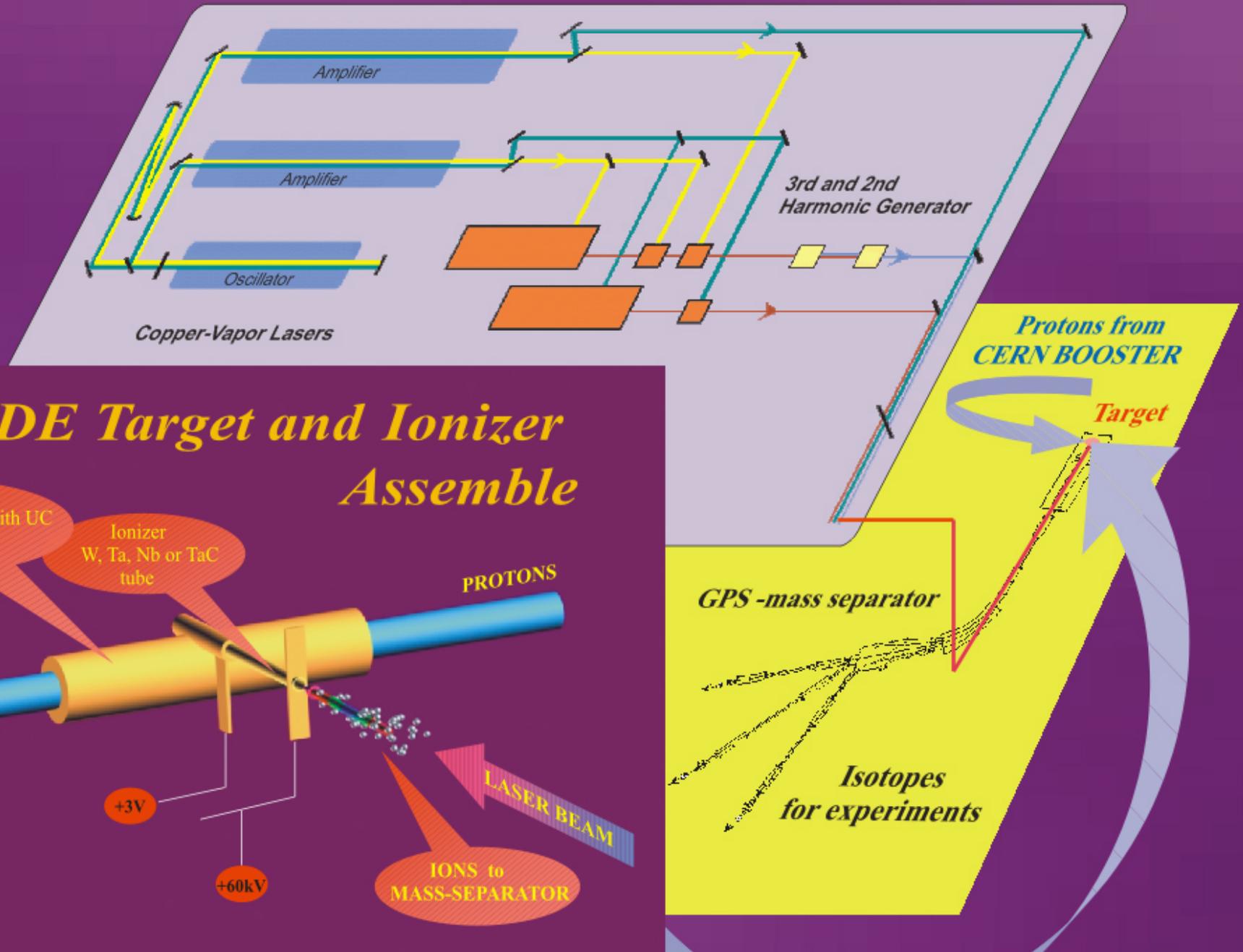
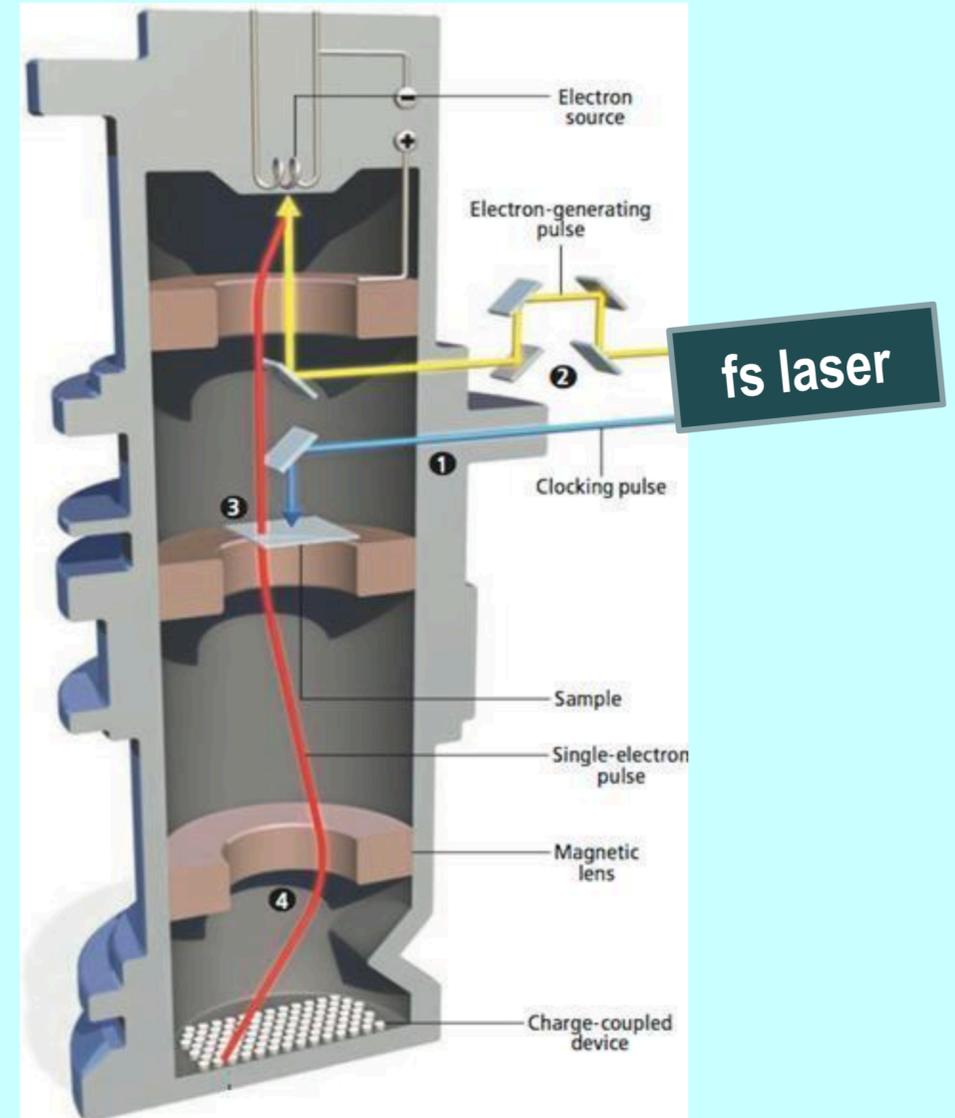
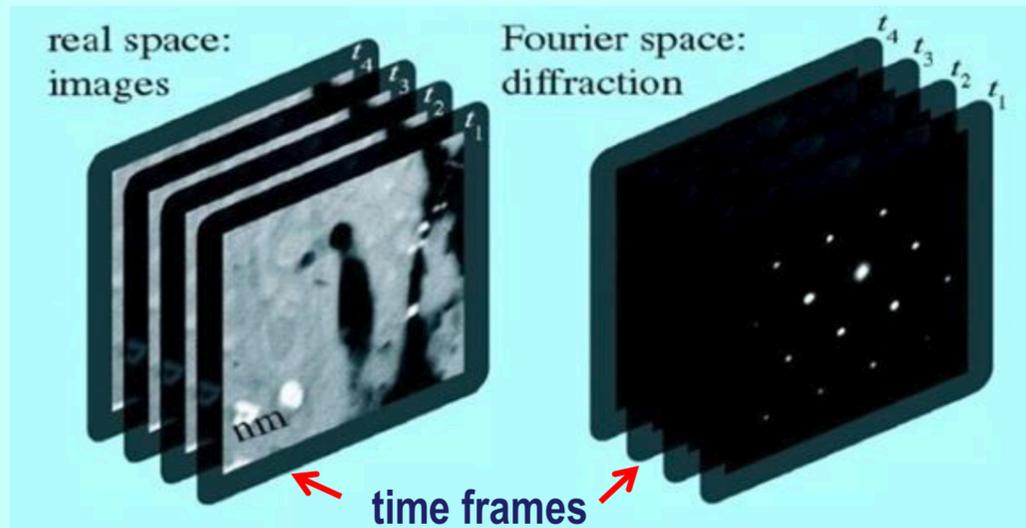


Table-top realization of 4D microscopy @ISAN: the dream of Ahmed Zewail becomes a reality

Time-resolved electron microscopy - 4D-microscopy (new project under realization)



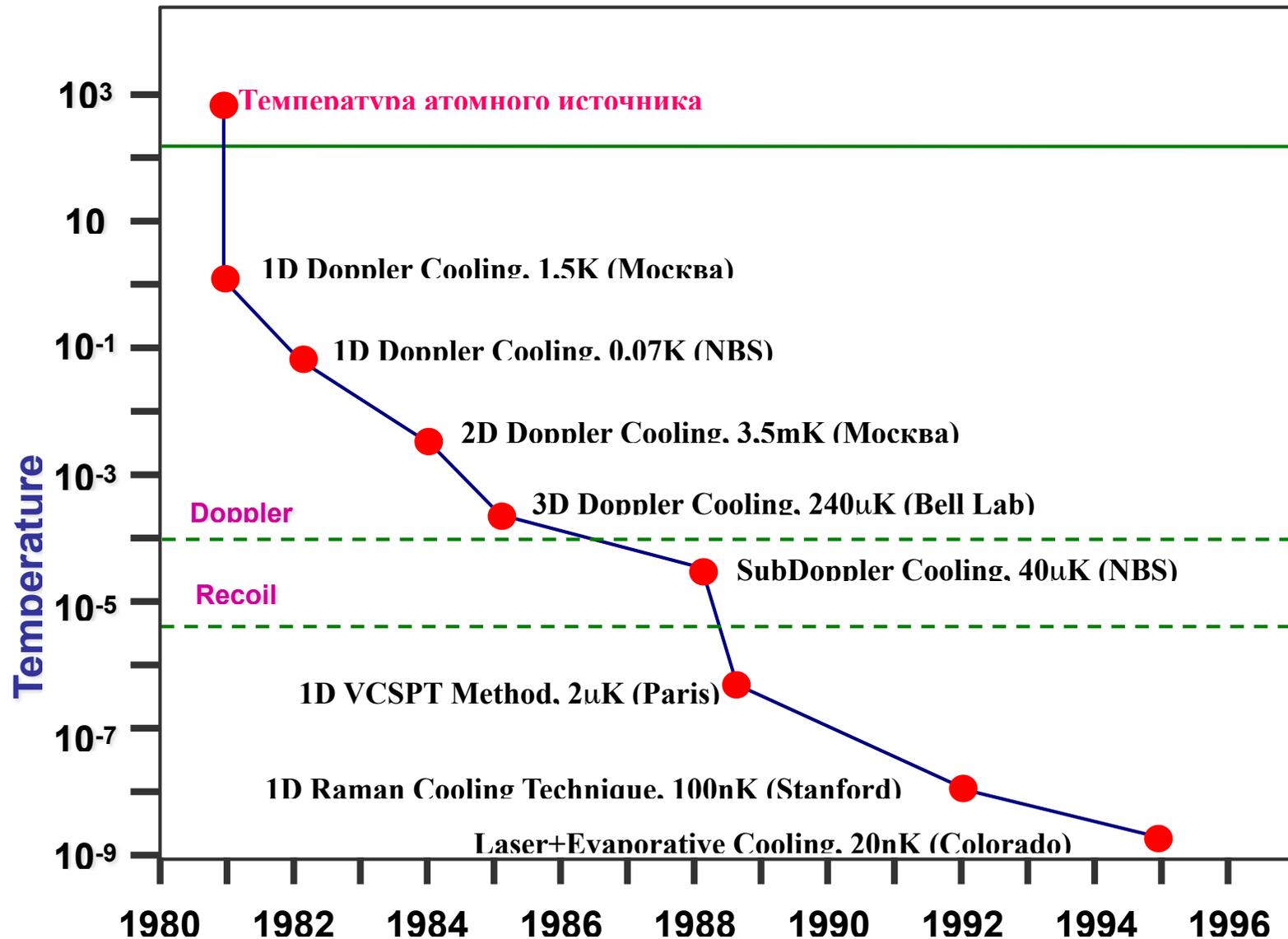
Tasks:

- **Material sciences:**
Dynamics of nuclei in solids, melting, etc.
- **Chemistry:**
Reaction dynamics - "Molecular movie"
- **Nanosciences:**
Dynamics in nanoparticles



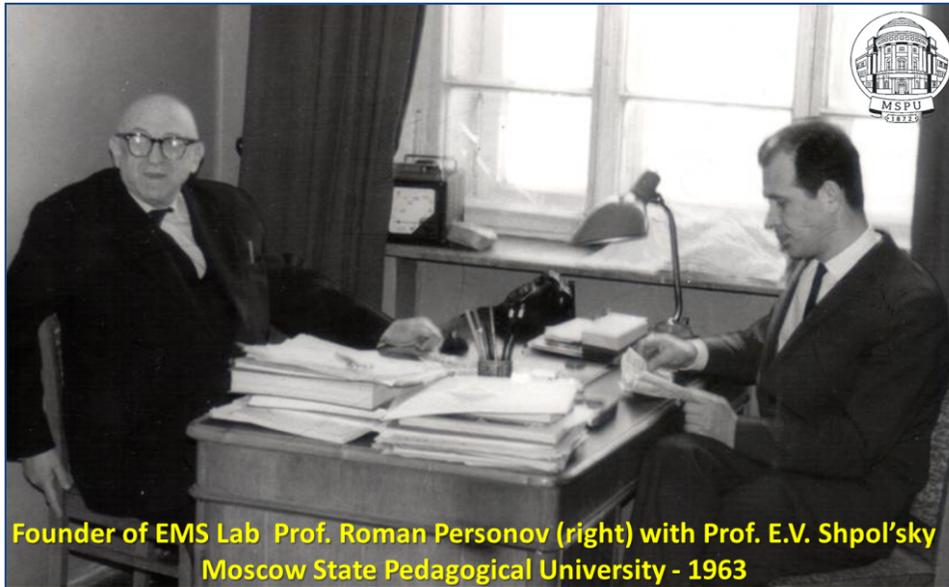
there are no small things in an experiment...

Progress in laser cooling of atoms (from the Nobel lecture of Claude Cohen-Tannoudji)



Laboratory of electronic spectra of molecules: Prof. A.V. Naumov (www.single-molecule.ru)

Laser Selective Spectroscopy of organic dye-molecules in complex solids



ПОСТАНОВЛЕНИЕМ ЦЕНТРАЛЬНОГО КОМИТЕТА КПСС
И СОВЕТА МИНИСТРОВ СССР
от 27 октября 1986 года
ПРИСУЖДЕНА
ГОСУДАРСТВЕННАЯ ПРЕМИЯ СССР

АВАРМАА Робин Арнольдовичу, доктору физико-математических наук, заведующему сектором Института физики Академии наук Эстонской ССР, ГОРОХОВСКОМУ Аннеле Александровичу; КИКАСУ Яну Вернеровичу, кандидату физико-математических наук, старшему научному сотруднику, работавшим в то же институте, ПЕРСОНОВУ Роману Ивановичу, доктору физико-математических наук, заведующему лабораторией Института спектроскопии Академии наук СССР, ХАРЛАМОВУ Борису Михайловичу, кандидату физико-математических наук, старшему научному сотруднику, АЛЬНИЦУ Евгению Иосифовичу, кандидату физико-математических наук, БЫКОВСКОЙ Людмиле Анатольевне, младшему научному сотруднику, работавшим в то же институте, МАСЛОВУ Владимиру Григорьевичу, кандидату физико-математических наук, старшему научному сотрудни-

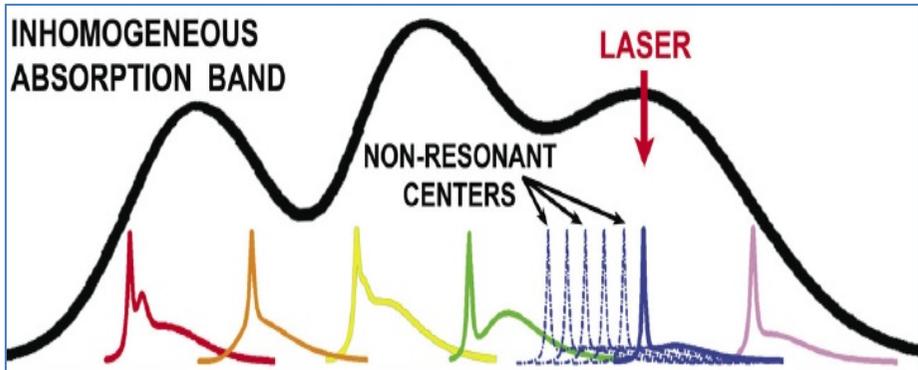


нику Государственного оптического института имени С. И. Вавилова, РЕБАНЕ Любови Александровне, доктору физико-математических наук, старшему научному сотруднику Института химической и биологической физики Академии наук Эстонской ССР, СОЛОВЬЕВУ Константину Николаевичу, доктору физико-математических наук, заведующему лабораторией Института физики Академии наук Белорусской ССР, — за цикл работ «Фотохимия и фотофизика стабильных спектральных ионов и селективная спектроскопия сложных молекул», опубликованных в 1972—1984 годах.

Данный диплом выдан
ПЕРСОНОВУ
Роману Ивановичу
№ 17985



Ученый секретарь Комитета по Ленинским и Государственным премиям СССР в области науки и техники при Совете Министров СССР
Климушкин
(В. ЧИВЕРКОВ)
МОСКВА



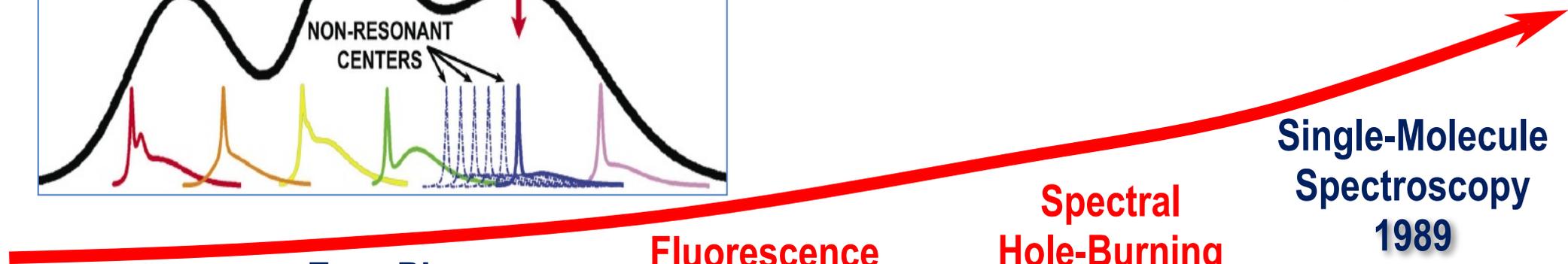
**Shpol'sky
Effect
1952**

**Zero-Phonon
Lines
1963**

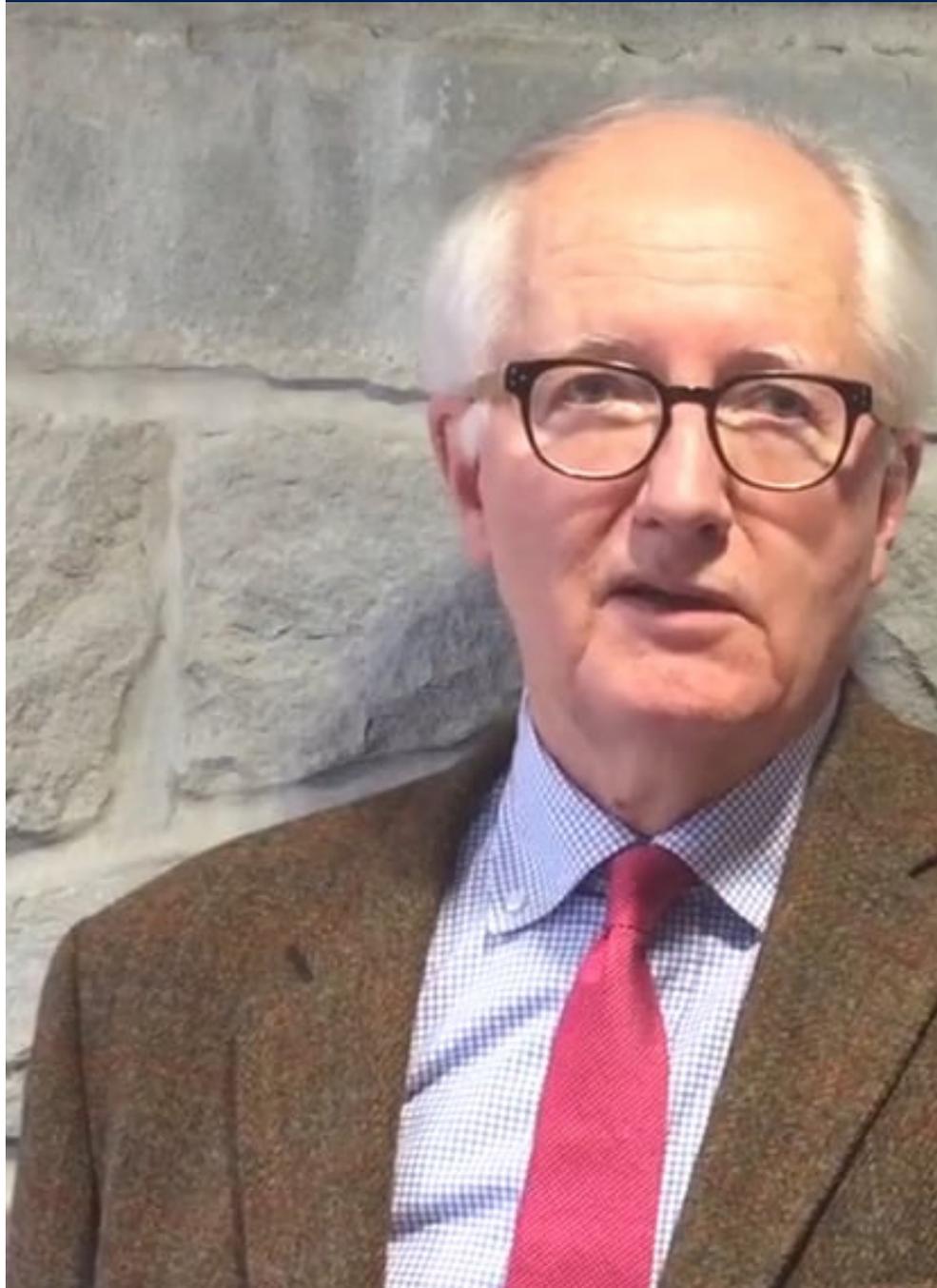
**Fluorescence
Line-Narrowing
ISAN - 1972**

**Spectral
Hole-Burning
ISAN - 1974
Tartu - 1974**

**Single-Molecule
Spectroscopy
1989
(USA, France)**



EPS Historic Site to ISAN in 2018



Rudiger Voss
EPS President

EUROPEAN PHYSICAL SOCIETY – EPS HISTORIC SITE

THE INSTITUTE OF SPECTROSCOPY OF THE RUSSIAN ACADEMY OF SCIENCES,
TROITSK, MOSCOW, RUSSIA

THIS INSTITUTE, THANKS TO THE APPLICATION OF ADVANCED OPTICAL AND LASER METHODS, INCLUDING THE SPECTROSCOPIC ONES, HAS BECOME AN INTERNATIONALLY RECOGNIZED LANDMARK OF RUSSIAN SCIENCE FOR RESEARCH ACROSS MANY FIELDS OF PHYSICS AND ASTROPHYSICS, CHEMISTRY, MATERIAL SCIENCES AND LIFE SCIENCES. GLORY AND WORLDWIDE FAME WERE BROUGHT TO THE INSTITUTE BY SERGEY MANDELSTAM (THEORY OF SPECTRA OF HIGHLY IONIZED ATOMS, ANALYTICAL SPECTROSCOPY), ROMAN PERSONOV (LASER FLUORESCENCE LINE NARROWING AND HOLE BURNING IN SPECTRA OF MOLECULES), VLADIMIR AGRANOVICH (THEORY OF EXCITONS, POLARITONS, AND OF RESONANT ORGANIC-INORGANIC NANOSTRUCTURES), AND OTHERS. THIS IS ALSO THE PLACE WHERE IN A CREATIVE ENVIRONMENT A TEAM OF TALENTED YOUNG RESEARCHERS INSPIRED BY VLADILEN LETOKHOV MADE PIONEERING EXPERIMENTS ON LASER TRAPPING AND COOLING OF ATOMS, WHICH PAVED THE WAY TO A WHOLE BUNCH OF NEW DIRECTIONS IN PHYSICS, AS WELL AS ON LASER ISOTOPE SEPARATION USING SELECTED LASER EXCITATION OF ATOMS AND MOLECULES, WHICH FINALLY LED TO THE DEVELOPMENT OF A NEW FIELD OF LASER CHEMISTRY.

Европейское Физическое Общество – Историческое место

Институт спектроскопии Российской академии наук (ИСАН),
Троицк, Москва, Россия

Институт спектроскопии РАН благодаря своим работам по применению оптических и лазерных методов, включая спектроскопические, получил всемирную известность за результаты исследований во многих областях физики и астрофизики, химии, материаловедения и науках о жизни. Признание ему принесли работы Сергея Манделштама (теория спектров высокоионизованных атомов, аналитическая спектроскопия), Романа Персонова (метод селективного лазерного возбуждения тонкоструктурных спектров и выжигание провалов в спектрах молекул), Владимира Аграновича (теория экситонов, поляритонов и резонансных наноструктур типа органика-полупроводник) и др. Здесь в творческой атмосфере группа молодых исследователей, возглавляемая Владиленом Летоховым, выполнила первые в мире эксперименты по лазерному захвату и охлаждению атомов, что привело к созданию новых направлений в физике, а также пионерские эксперименты по лазерному разделению изотопов с использованием методов селективного лазерного возбуждения атомов и молекул, что привело к созданию новой области лазерной химии.

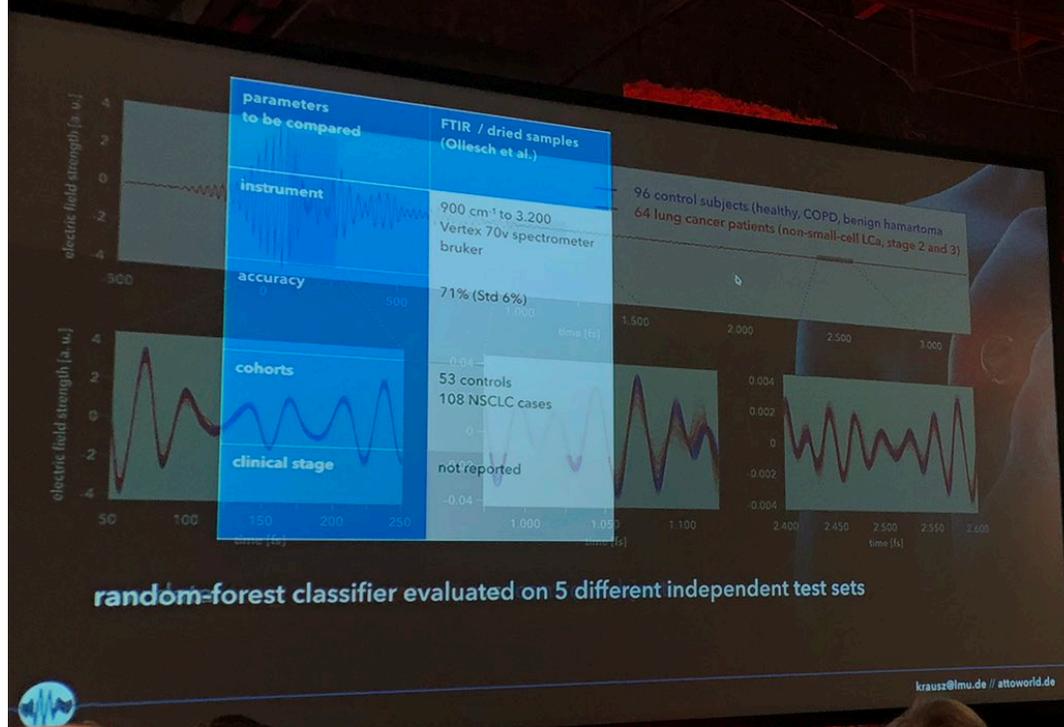
TROITSK, MOSCOW, RUSSIA, 2018

Троицк, Москва, Россия, 2018

EPS Vladilen Letokhov prize and medal
(launched in 2019)



Prof. Ferenz Kraus, first recipient of the EPS Letokhov medal delivers an inaugural talk at the ECAMP13 in Florence, Italy, in 2019



ECAMP13
13th EUROPEAN CONFERENCE ON ATOMIC MOLECULES AND PHOTONS
FLORENCE
APRIL 8-12
2019





Quantum Computers and Quantum Computing: Dreams and Reality

Victor Zadkov

*Institute of Spectroscopy of the Russian Academy of Sciences
Moscow, Troitsk, Russia*

Computers are **real** physical systems

Our goal is to make computers faster



The fact that a **real computer is a physical system** prompts us to think about the *space, time, and energy* implications of trying to make computers faster



Due to the signal speed limit we have to squeeze components closer together. Therefore, components have to be *smaller* to be packed closer

Limit: Atomic size



We have to drive components at a *higher clock speed*

Limit: ~ 40 GHz

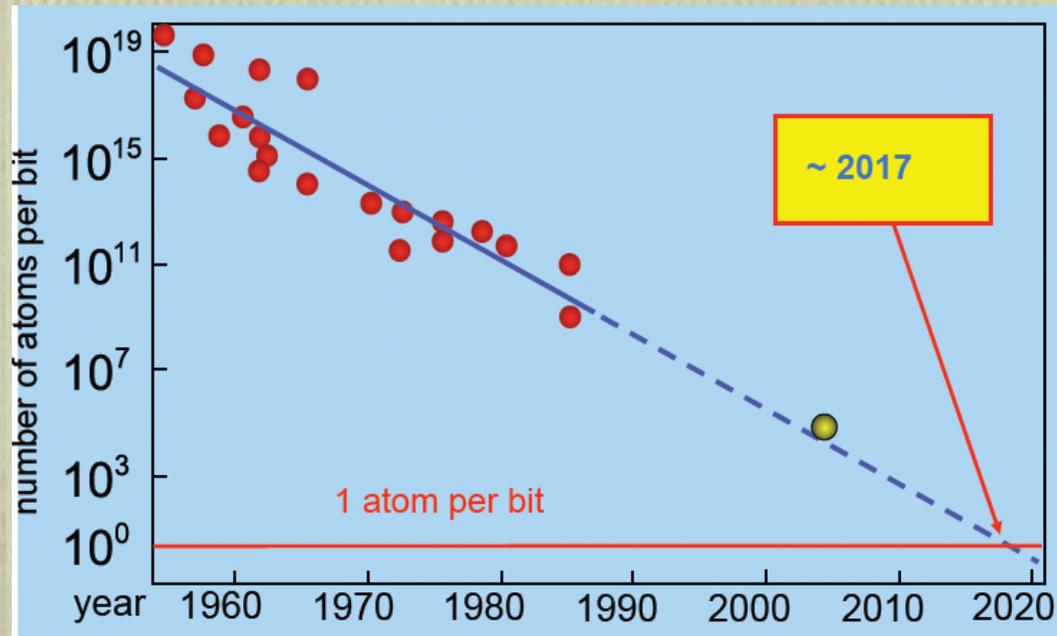


The components inside conventional computers give off a certain amount of heat as a side effect of their operation. Therefore, the components could not be packed closer with no improving their *energy efficiency*.

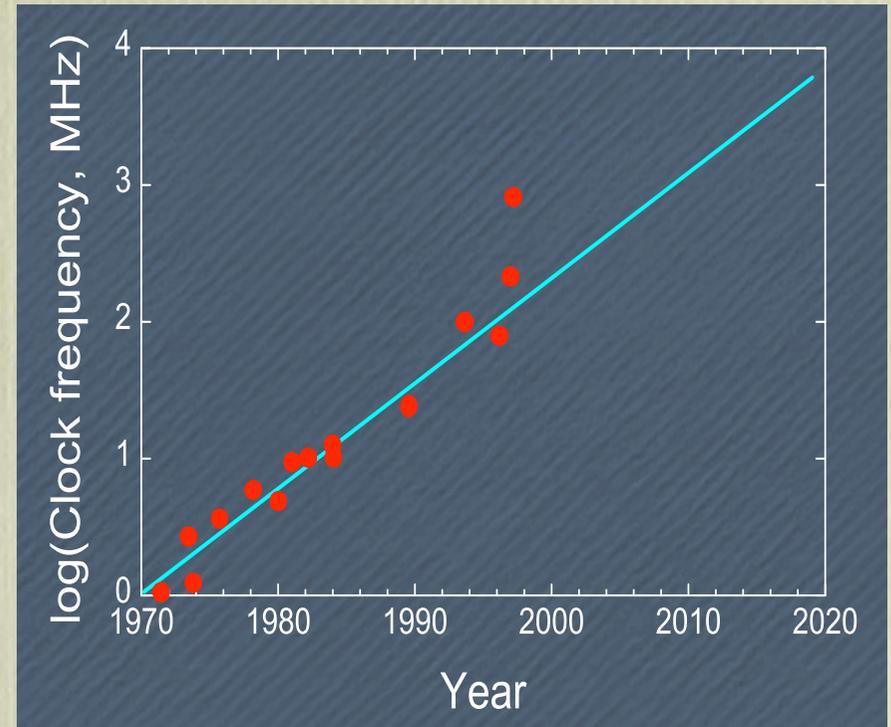
Example: in a PC ~ 10^8 kT
in DNA ~100 kT per bit
Limit: $kT \ln 2$ per operation

Moore's law (continued)

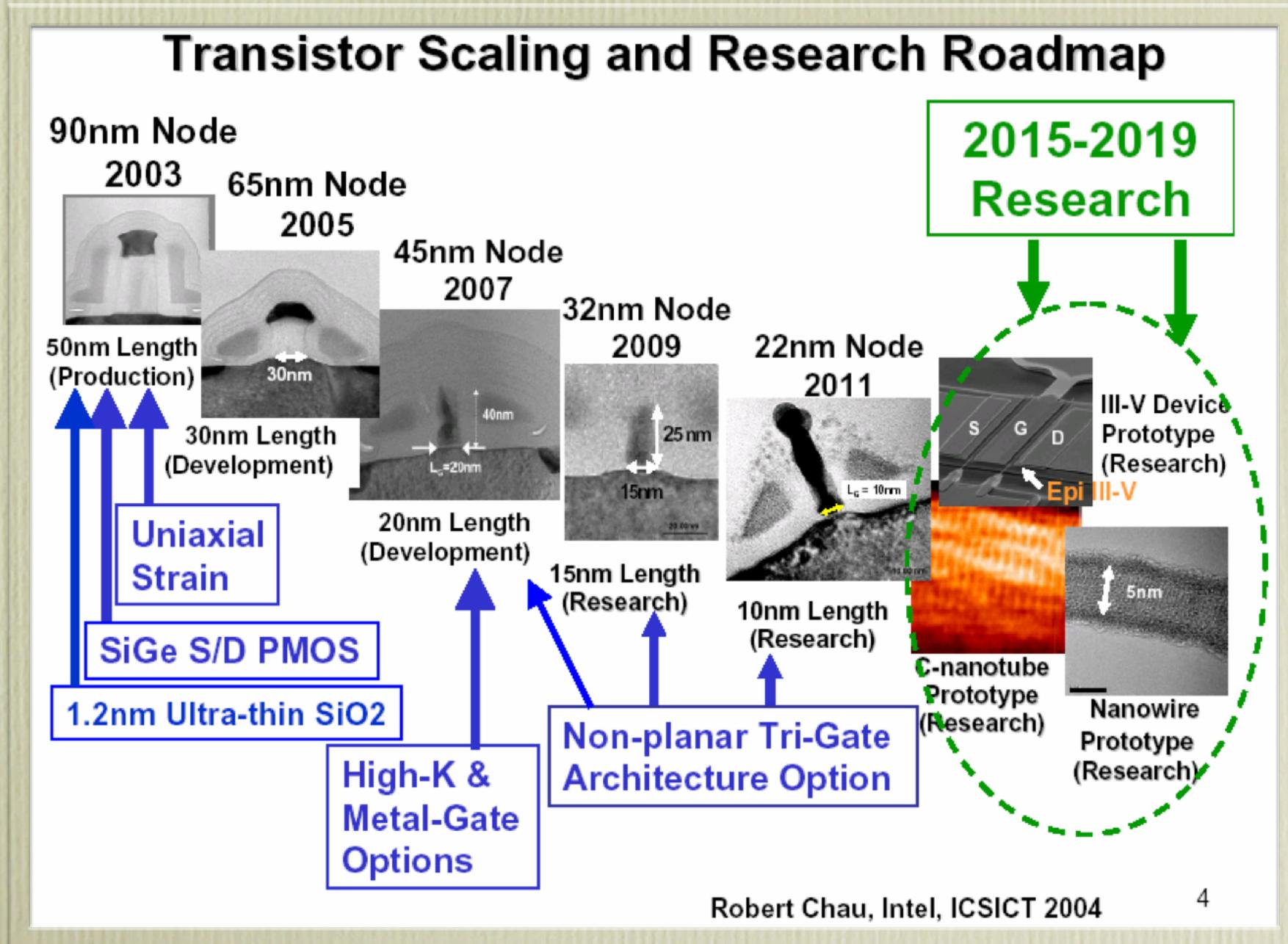
Atom limit



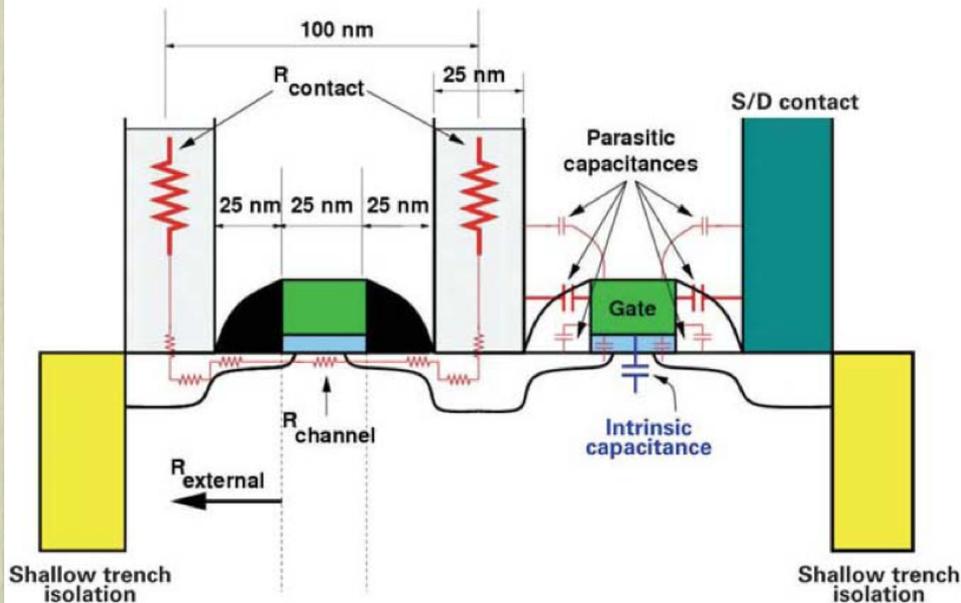
The smaller elements, the faster the clock frequency



Scaling of the size of logical elements leads to the violation of the Moore's law

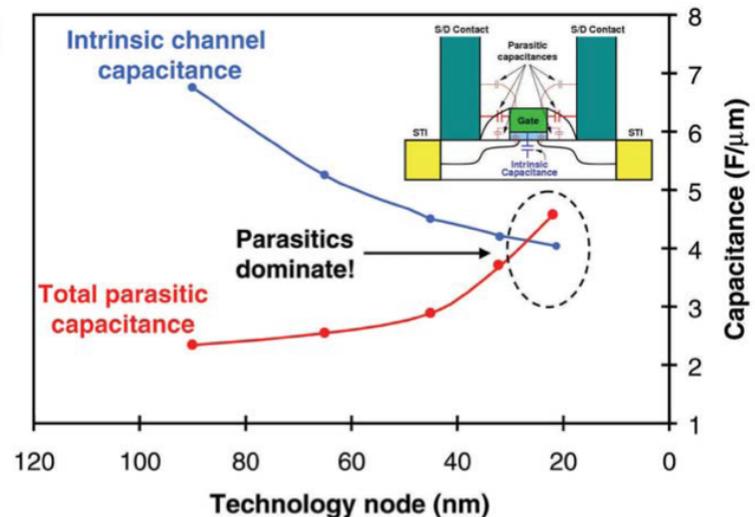
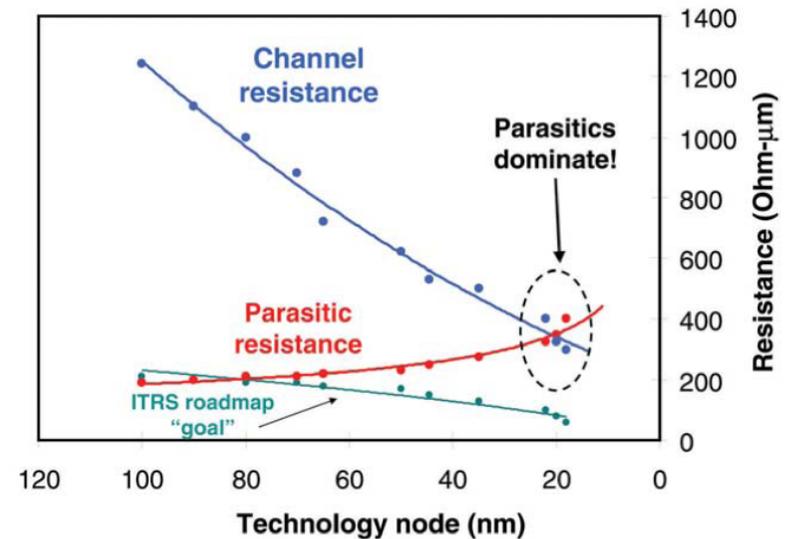


Existence of parasitic resistance and capacity

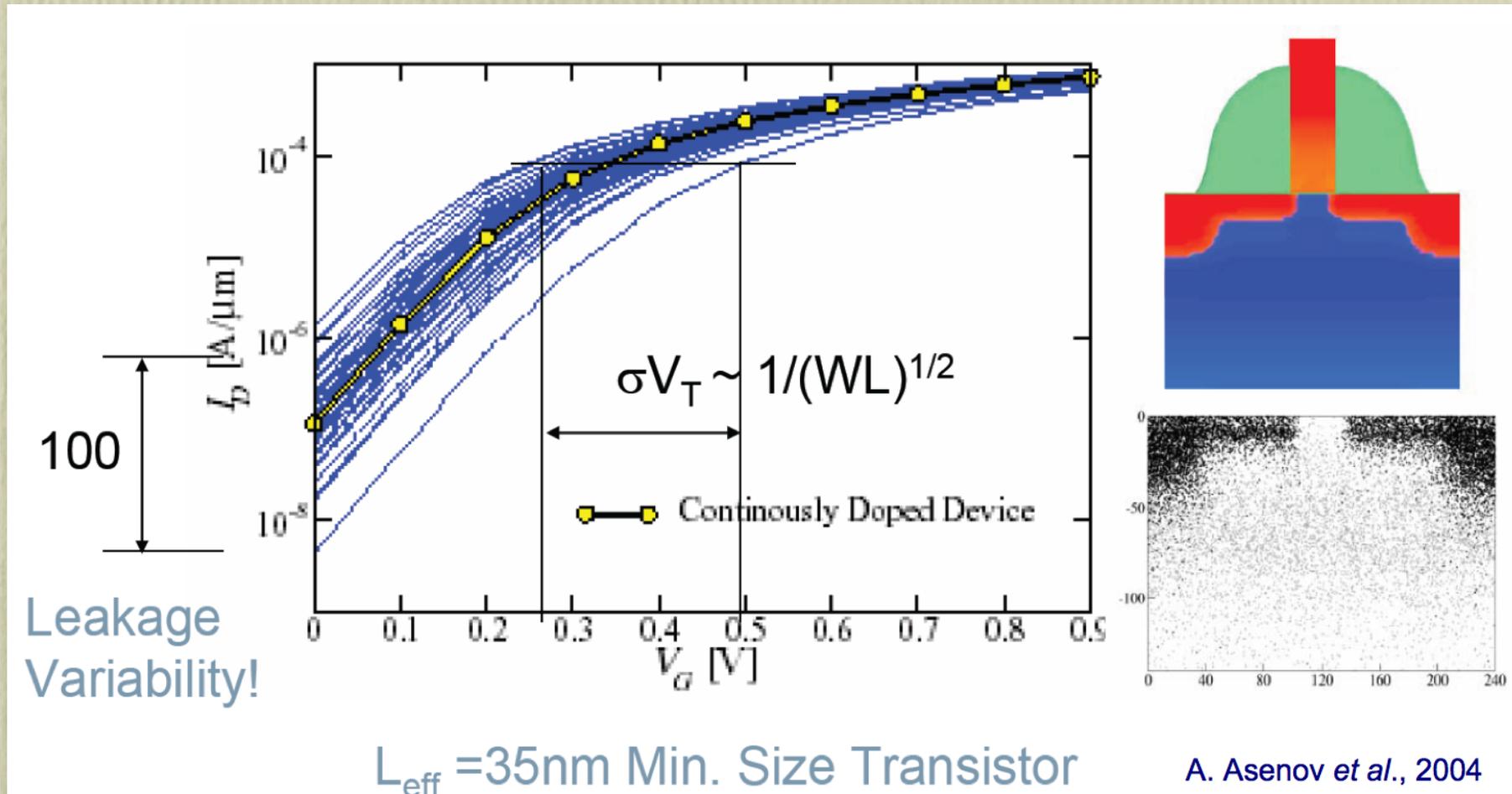


“Once the channel resistance becomes smaller than the external resistance, reducing the channel resistance further, even to zero, has little performance benefit (the same is true for capacitance).”

S. Thompson and S. Parthasarathy, 2006



Random doping



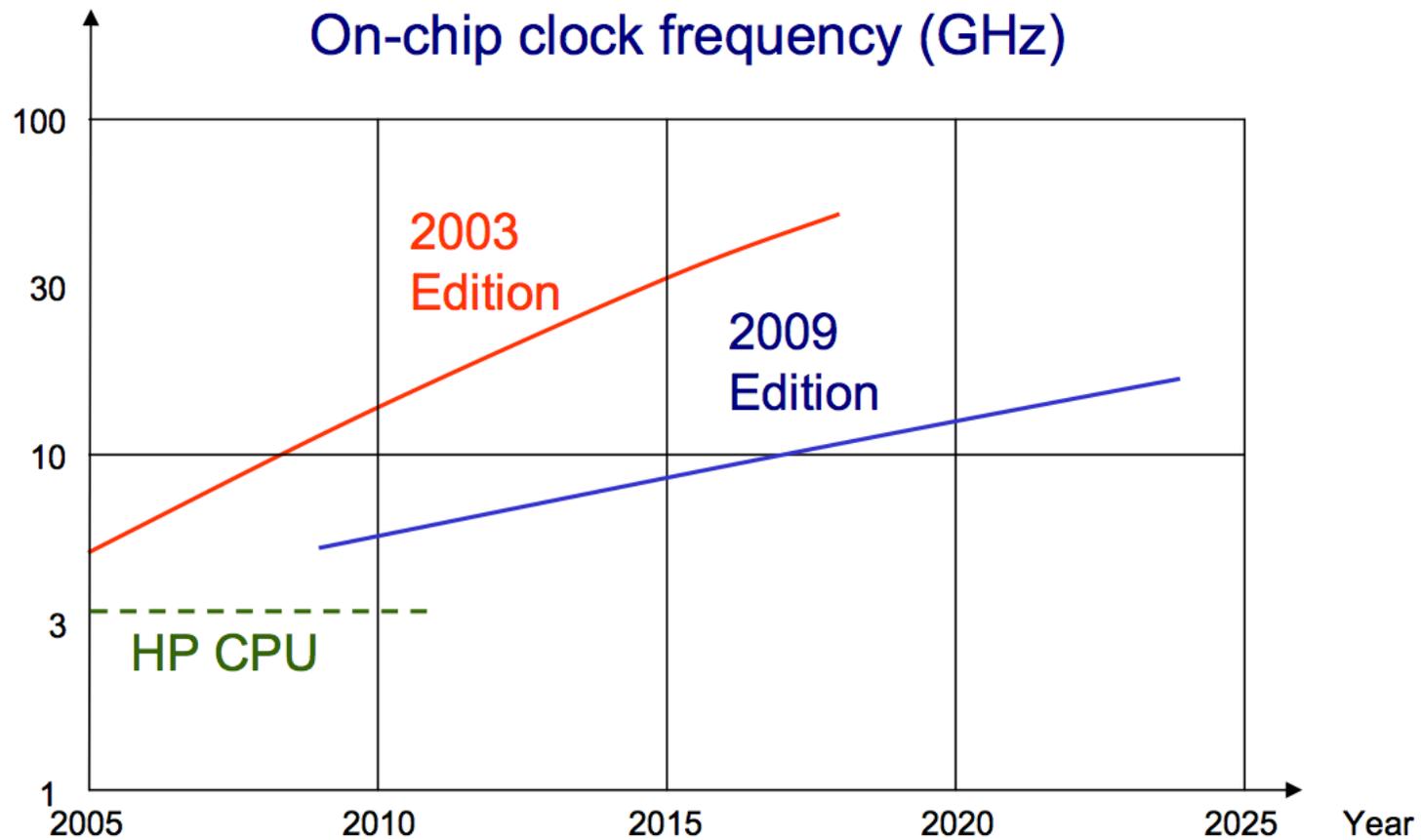
Identically fabricated logical elements essentially differ from each other!

Plus to this, quantum physics started to play an essential role!

Radical forecast change in semiconductor chips production

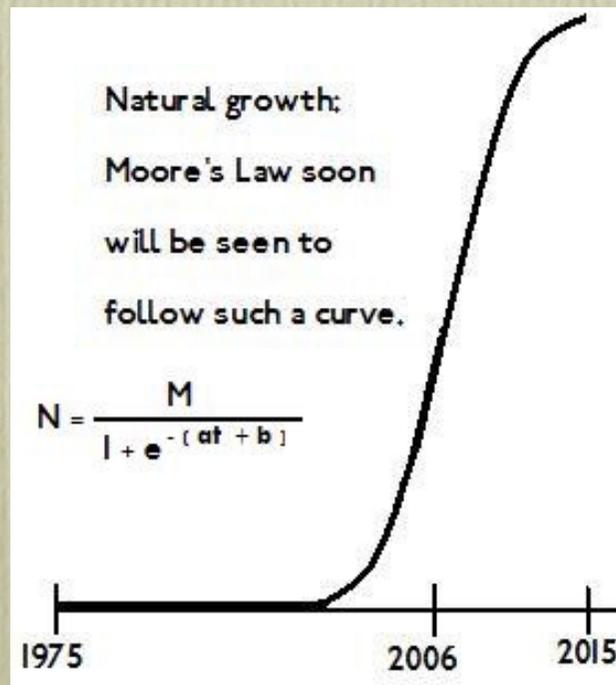


International Technology Roadmap for Semiconductors

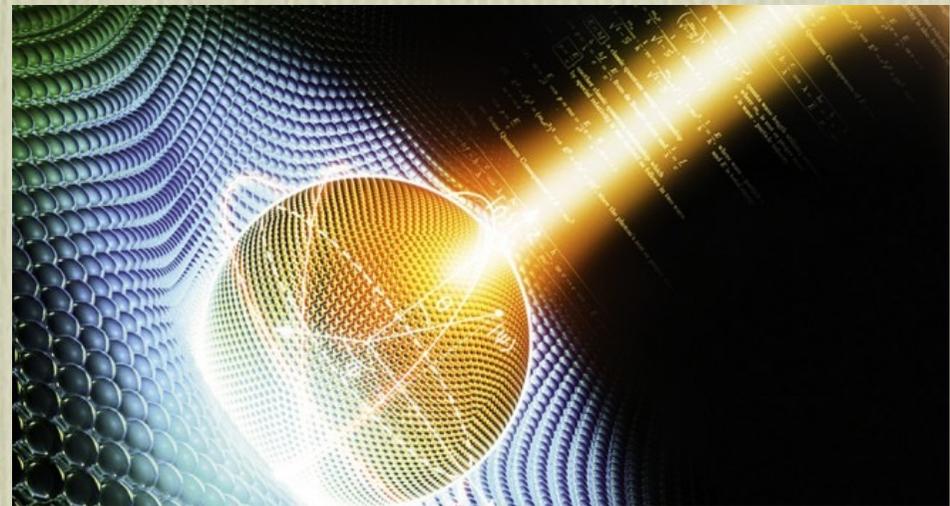


Two ways to go further...

Cope with the quantum effects



Use quantum effects



“Quantum technologies is a radical change in nowadays technologies. They differ from them more than a digital computer differs from an abacus”.

Bill Philips, Nobel laureate (1997)

New era of quantum computers



The idea of quantum calculations was first published by Russian mathematician Yuri Manin in 1980, however it received its further development after independent works by Richard Feynman.

“There’s plenty of room at the bottom.”

— *Richard Feynman**

“...it seems that the laws of physics present no barrier to reducing the size of computers until bits are the size of atoms, and quantum behavior holds dominant sway.”

— *Richard Feynman***

*) R.P.Feynman, “There’s plenty of room at the bottom,” *Engineering and Science*, vol. 23, pp.22-36 (1960).

**) R.P.Feynman, “Quantum mechanical computers,” *Optics News*, vol. 11, pp. 11-20 (1985).

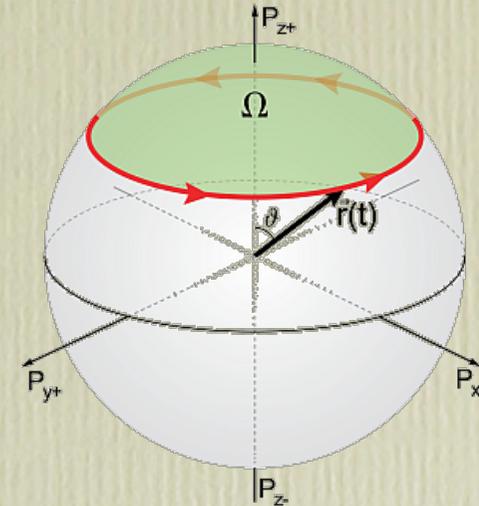


Richard P. Feynman

Key advantages of quantum computers vs classical ones



Analogous computational machine (ACM) is a physical system, which models its own dynamics



Operators in Hilbert space

$$|\psi\rangle = \begin{bmatrix} a_n \\ a_y \end{bmatrix}$$

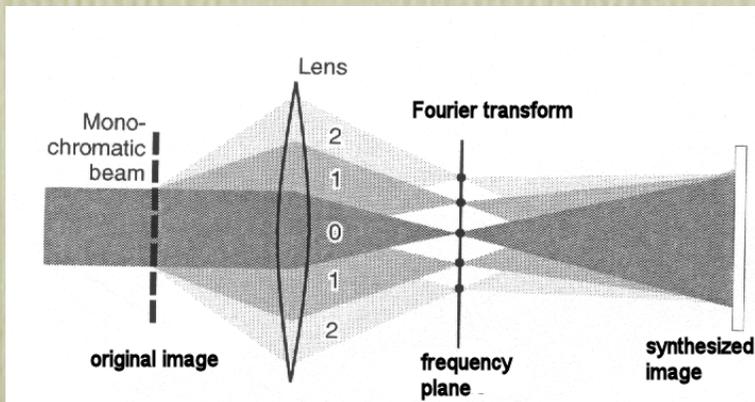
$$O|\psi\rangle = [R] \begin{bmatrix} a_n \\ a_y \end{bmatrix}$$

$$\langle \phi | O | \psi \rangle = [b_n \ b_y] [R] \begin{bmatrix} a_n \\ a_y \end{bmatrix}$$

Linear Operator

$$A(a|\psi\rangle + b|\phi\rangle)$$

$$= aA|\psi\rangle + bA|\phi\rangle$$



Lens performs a parallel Fourier transform

For which problems quantum computers have advantages vs classical ones?

APPLICATIONS	QUANTUM COMPUTERS	CLASSICAL COMPUTERS
Cryptographic applications	<i>Shor's algorithm (1994)</i> finds prime factors of an N-digit number in a time of order N^3 .	Any factoring algorithm that runs on a classical computer require a time that increases with N faster than any power.
Searching an unsorted database	In a database containing N items, the one item that meets a specific criterion can be found with the help of <i>Grover's algorithm (1996)</i> in a time of order $N^{1/2}$.	The database search would take a time of order N.
Simulation behavior of quantum systems (material science, chemistry, etc.)	Quantum device can store quantum information far more efficiently than any classical device (Feynman, 1982). N qubits live in a Hilbert space of dimension 2^N and operations on them are massively parallel.	A classical device would record $2^N - 1$ complex numbers to describe N qubits. Operations on them also require exponential resources.

Which fundamental problems are expected to be solved using QCs

One of the key problems is to understand how the quantum materials work and learn how to develop new materials with pre-selected properties (one of the key problems in XXI century)

Magnetism (storing of XXXL-scale data bases)

High temperature superconductivity
(electrical energy)

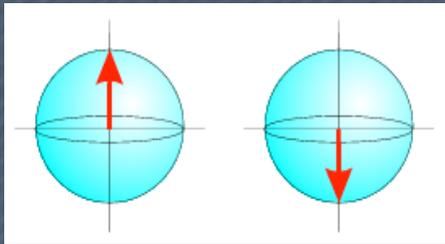


10-20% of electrical energy is lost during its transfer. \this problem can be solved by implementing the energy-transfer lines based on High temperature superconductivity.

Bits and qubits

Classical bit

Has only two states
“0” and “1”



Quantum bit (qubit*)

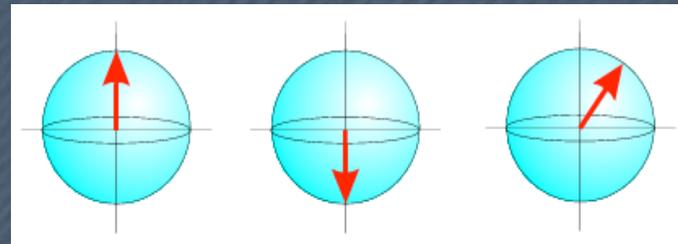
$$|\Psi\rangle = a|0\rangle + b|1\rangle$$

has two “classical” states:

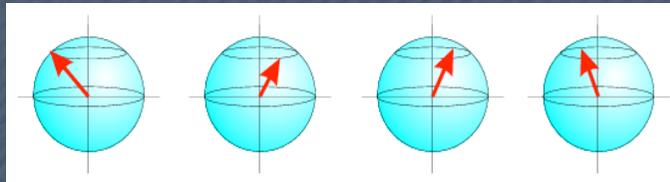
$$\text{“0”}: |\Psi\rangle_0 = 1|0\rangle + 0|1\rangle = |0\rangle$$

$$\text{“1”}: |\Psi\rangle_1 = 0|0\rangle + 1|1\rangle = |1\rangle$$

and all the states “in between”



The phase factors do not affect the relative contributions of the eigenstates to the whole state, but they are crucially important in quantum interference effects



*)This term was coined by Schumacher (Phys. Rev. A51, 2738 (1995))

Classical logical elements

NO

a	NOT a
0	1
1	0

AND

a	b	a AND b
0	0	0
0	1	0
1	0	0
1	1	1

OR

a	b	a OR b
0	0	0
0	1	1
1	0	1
1	1	1

Reversible OR

a	b	a	a OR b
0	0	0	0
0	1	0	1
1	0	1	1
1	1	1	1

- * Fundamental set of gates (NOT, AND, and OR)
- * These gates (except NOT) are logically irreversible
- * Irreversible gates generate energy as they run
- * Irreversible gates can be converted into reversible ones

Quantum logical elements

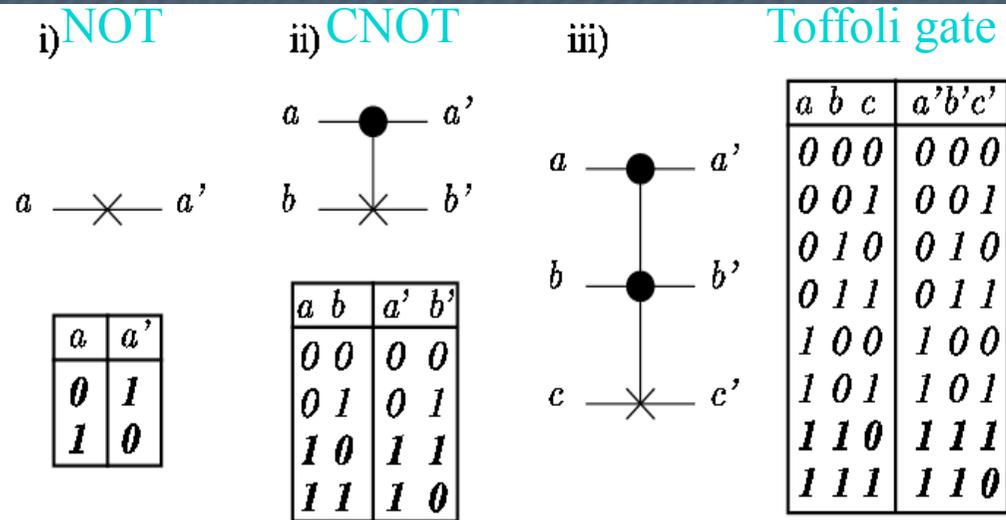


FIG. 5. Truth tables and graphical representations of the elementary quantum gates used for the construction of more complicated quantum networks. The control qubits are graphically represented by a dot, the target qubits by a cross. i) NOT operation. ii) Control-NOT. This gate can be seen as a “copy operation” in the sense that a target qubit (b) initially in the state 0 will be after the action of the gate in the same state as the control qubit. iii) Toffoli gate. This gate can also be seen as a Control-control-NOT: the target bit (c) undergoes a NOT operation only when the two controls (a and b) are in state 1.

A quantum network is a quantum computing device consisting of quantum logical gates whose computational steps are synchronized in time

Simple quantum computational device

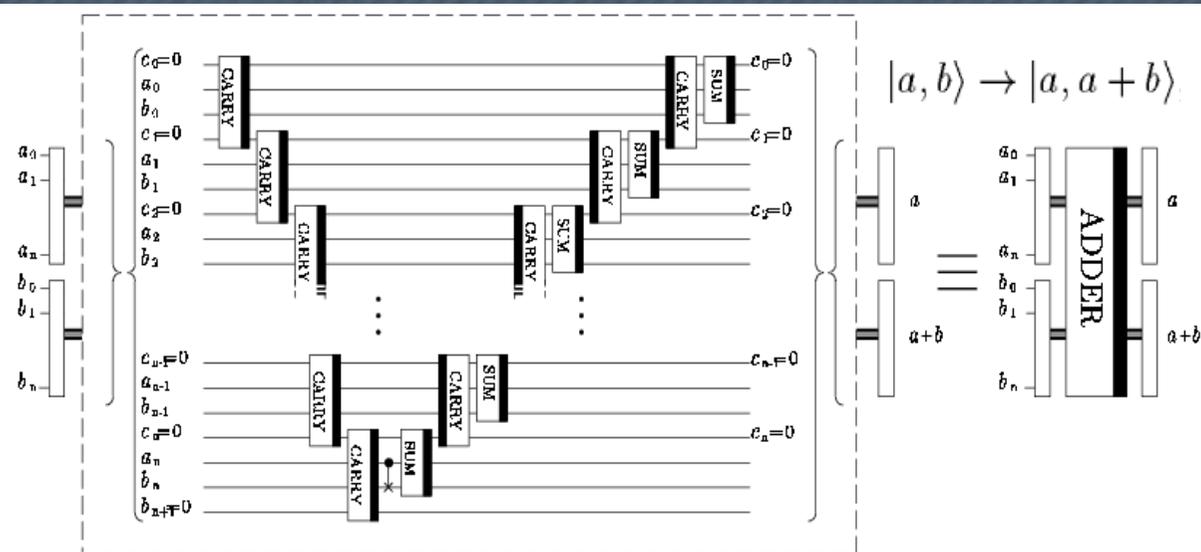
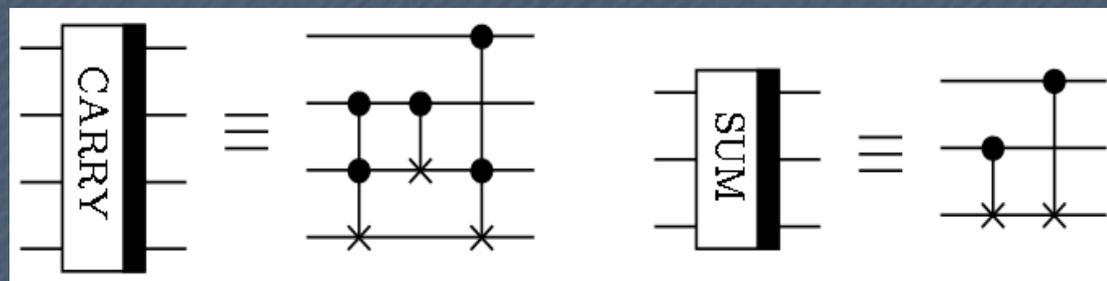


FIG. 6. Plain adder network. In a first step, all the carries are calculated until the last carry gives the most significant digit of the result. Then all these operations apart from the last one are undone in reverse order, and the sum of the digits is performed correspondingly. Note the position of a thick black bar on the right or left hand side of basic carry and sum networks. A network with a bar on the left side represents the reversed sequence of elementary gates embedded in the same network with the bar on the right side.



Factorization time on a classical computer

Size of modulus (bits)	1,024	2,048	4,096
Factoring time in 1997	10^7 years	3×10^{17} years	2×10^{31} years
Factoring time in 2006	10^5 years	5×10^{15} years	3×10^{29} years
Factoring time in 2015	2,500 years	7×10^{13} years	4×10^{27} years
Factoring time in 2024	38 years	10^{12} years	7×10^{25} years
Factoring time in 2033	7 months	2×10^{10} years	10^{24} years
Factoring time in 2042	3 days	3×10^8 years	2×10^{22} years

Table 2: Projected future factoring times using the GNFS for various moduli using 1,000 workstations.

Source: R.J.Hnughes, e-print, quant-ph/9801006

(We assume that each workstation in 1997 is rated at 200 MIPS and there are no algorithmic developments beyond the General Number Field Sieve (GNFS) algorithm.)

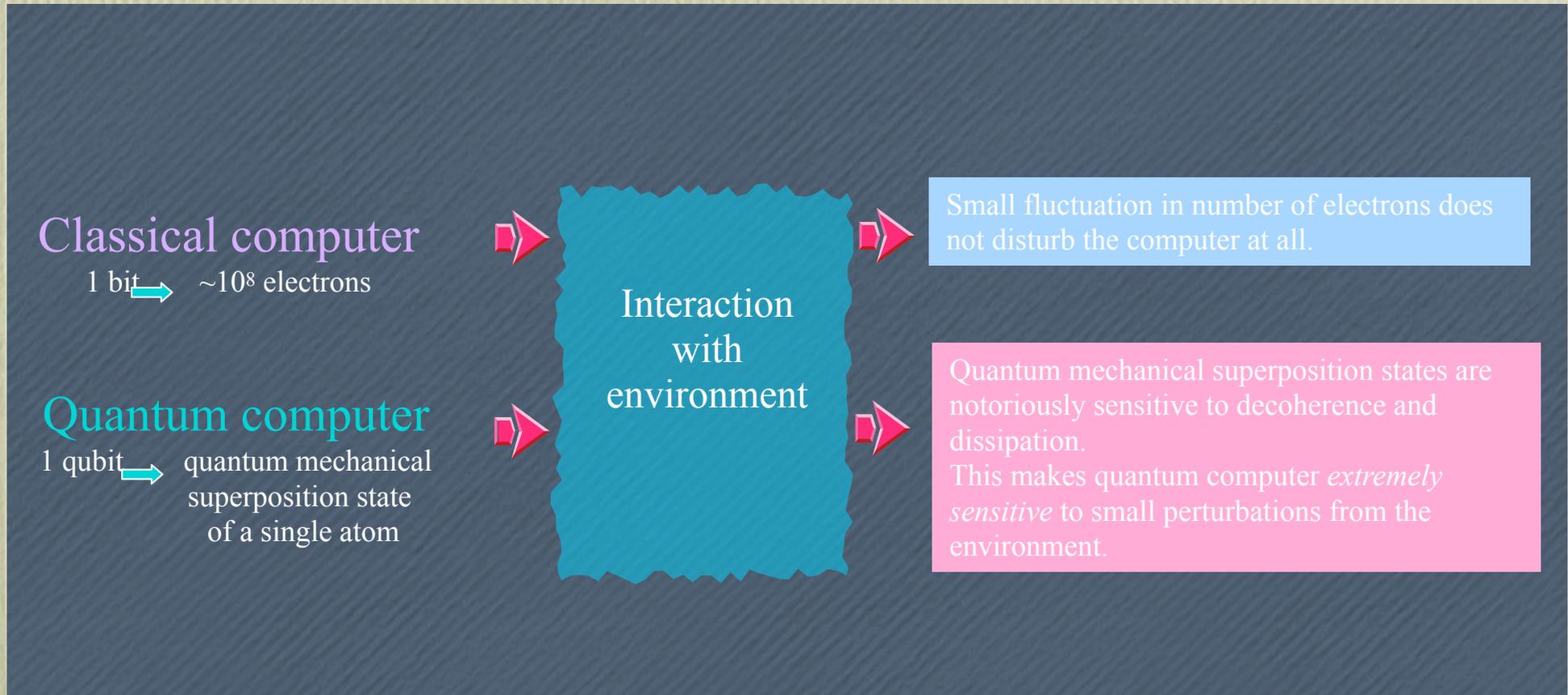
Shor algorithm

Size of modulus (bits)	512	1,024	2,048	4,096
Quantum memory (qubits)	2,564	5,124	10,244	20,484
Number of quantum gates	3×10^9	3×10^{10}	2×10^{11}	2×10^{12}
Quantum factoring time	33 seconds	4.5 minutes	36 minutes	4.8 hours

Table 3: Quantum factoring times of various moduli on a hypothetical 100-MHz QC.

Source: R.J.Hnughes, e-print, quant-ph/9801006

Problem of decoherence



QCs require algorithms which correct the errors during calculations!

Nobel prize in Physics (2012)



Photo: U. Montan
Serge Haroche
Prize share: 1/2

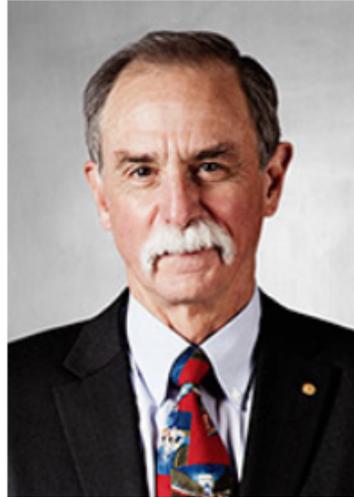
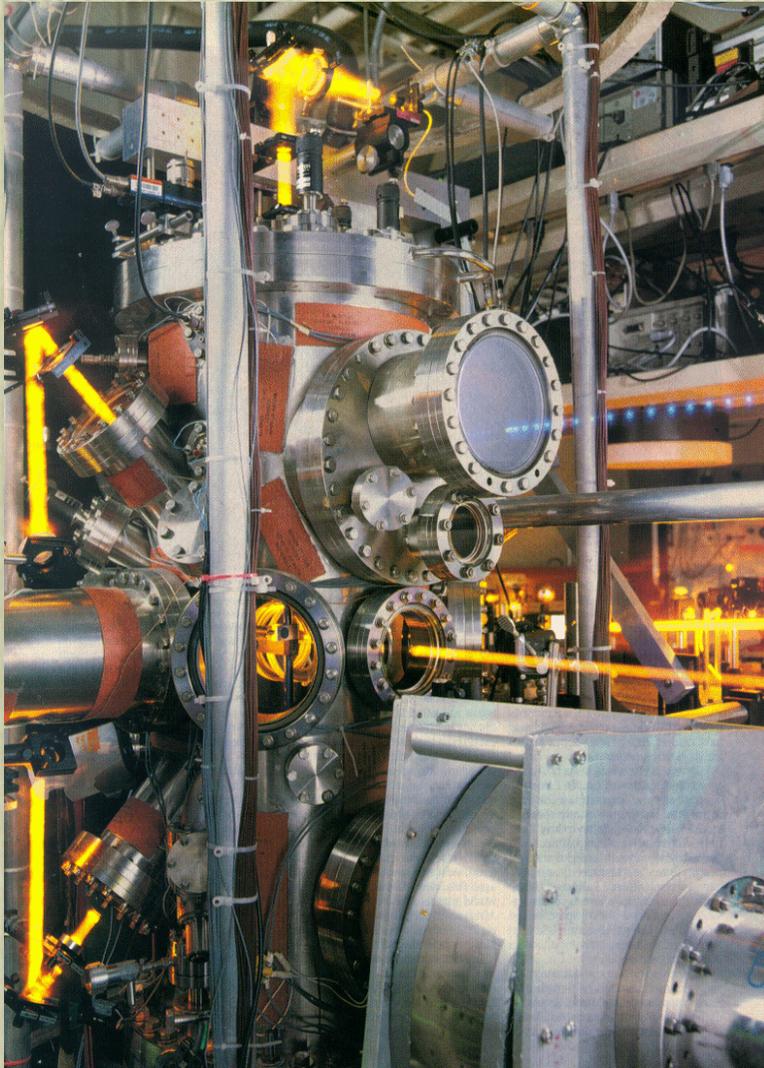


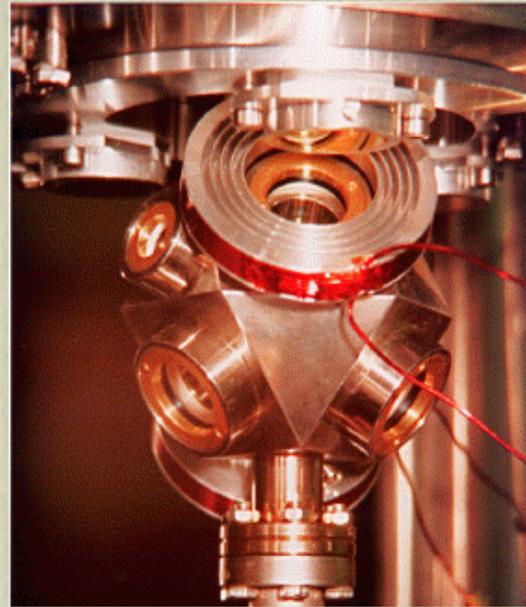
Photo: U. Montan
David J. Wineland
Prize share: 1/2

The [2012 Nobel Prize in Physics](#) was awarded jointly to [Serge Haroche](#) and [David J. Wineland](#) *"for ground-breaking experimental methods that enable measuring and manipulation of individual quantum systems"*.

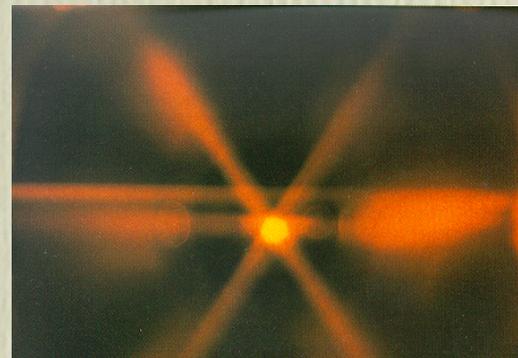
Traps for atoms and ions



Source: *S.Chu, Scientific American, February 1992, p.48*

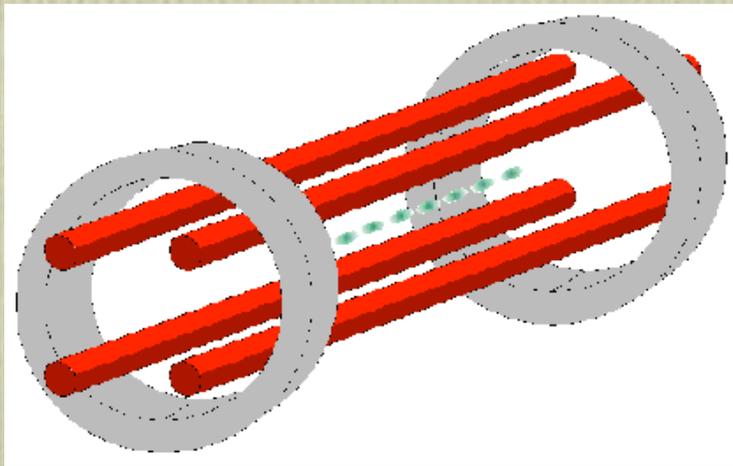


Source: *H.Bachor et al., Australian National University*

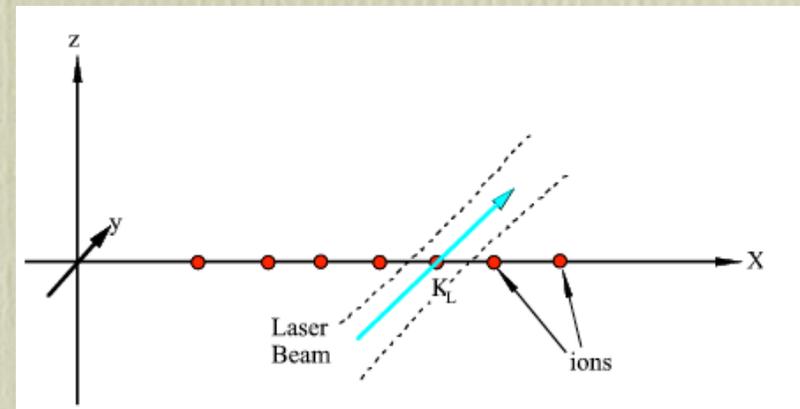


Source: *C.Cohen-Tannoudji, W.Phillips, Physics Today, October 1990, p. 35*

QC prototype based ions in the ion trap



Source: V.Vedral, M.B.Plenio, Progr. Quant. Electron., vol. 22, pp. 1–40 (1998)



Source: D.F.V.James, et. Al. Proc. NASA-QCQC'98 (1998)

Proposal: J.I.Cirac, P.Zoller, Phys. Rev. Lett., vol. 74, p.4091 (1995)

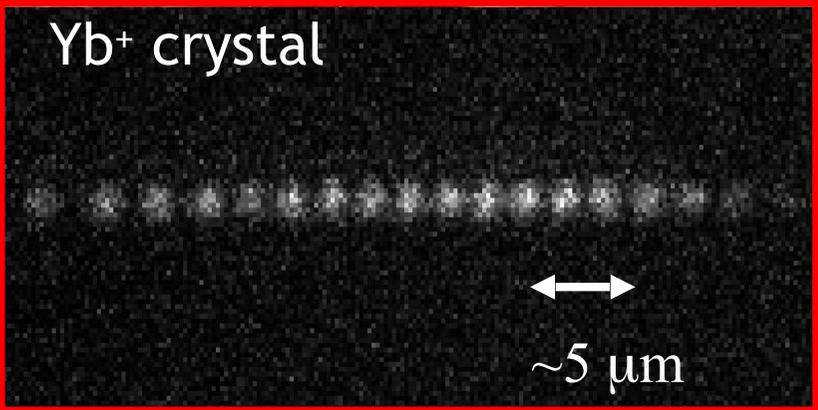
Ions in the trap

Superconducting Circuits for Quantum Information: An Outlook

M. H. Devoret^{1,2} and R. J. Schoelkopf^{1*}

The performance of superconducting qubits has improved by several orders of magnitude in the past decade. These circuits benefit from the robustness of superconductivity and the Josephson effect, and at present they have not encountered any hard physical limits. However, building an error-corrected information processor with many such qubits will require solving specific architecture problems that constitute a new field of research. For the first time, physicists will have to master quantum error correction to design and operate complex active systems that are dissipative in nature, yet remain coherent indefinitely. We offer a view on some directions for the field and speculate on its future.

Science, 339, 8 March 2013



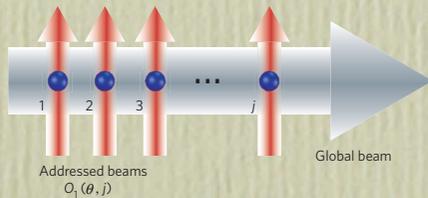
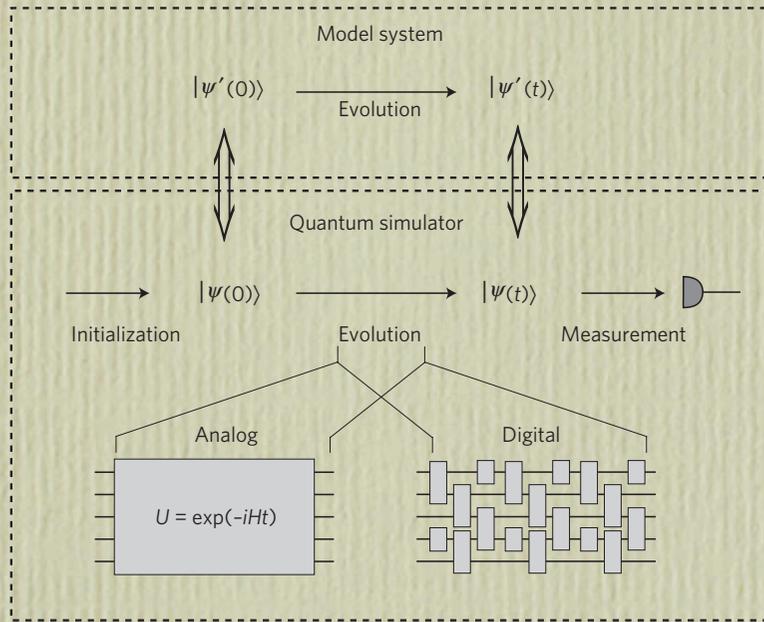
Yb⁺ crystal



~5 μm

8 qubits in 2006, expected up to 30

Modeling of Izing model on an ion-based QC (ions in the trap)



NATURE PHYSICS | VOL 8 | APRIL 2012

Quantum simulations with trapped ions

R. Blatt^{1,2*} and C. F. Roos^{1,2}

In the field of quantum simulation, methods and tools are explored for simulating the dynamics of a quantum system of interest with another system that is easier to control and measure. Systems of trapped atomic ions can be accurately controlled and manipulated, a large variety of interactions can be engineered with high precision and measurements of relevant observables can be obtained with nearly 100% efficiency. Here, we discuss prospects for quantum simulations using systems of trapped ions, and review the available set of quantum operations and first proof-of-principle experiments for both analog and digital quantum simulations with trapped ions.

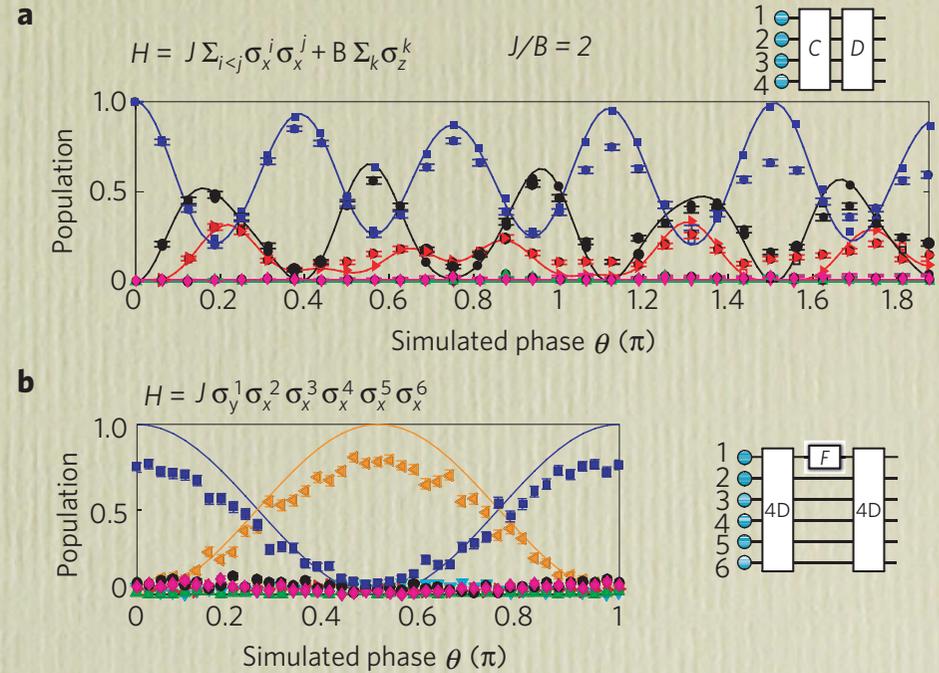
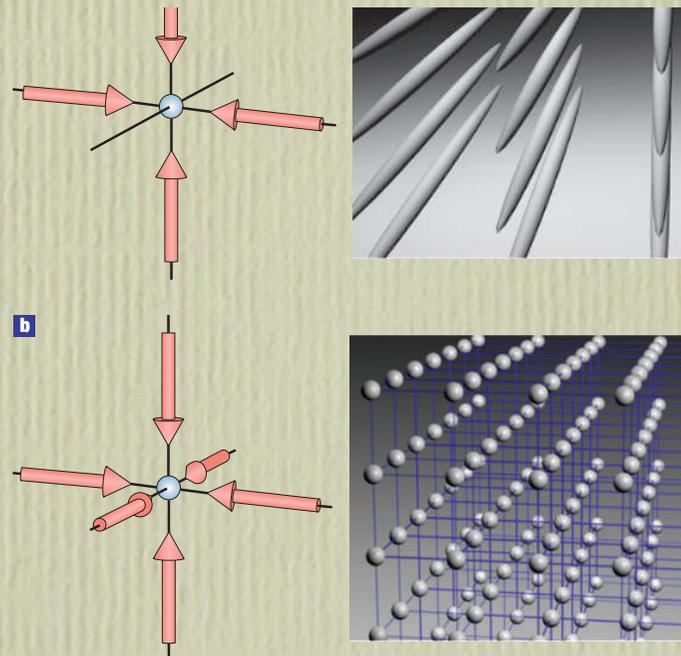


Figure 7 | Digital simulations of four- and six-spin systems. Dynamics of the initial state where all spins point up. **a**, Four-spin long-range Ising system. Each digital step is $D.C = O_4(\pi/16, 0).O_2(\pi/32)$. Error bars are smaller than the point size. **b**, Six-spin six-body interaction. $F = O_1(\theta, 1)$, $4D = O_4(\pi/4, 0)$. Lines, exact dynamics. Open symbols, ideal digitized. Filled symbols, data (blue square, P_0 ; magenta diamond, P_1 ; black circle, P_2 ; green triangle, P_3 ; red right triangle, P_4 ; cyan down triangle, P_5 ; orange left triangle, P_6 , where P_i is the total probability of finding i spins pointing down). Figure reproduced with permission from ref. 77, © 2011 AAAS.

QCs based on the cold atoms in molasses



Immanuel Bloch, Nature Physics, 2005

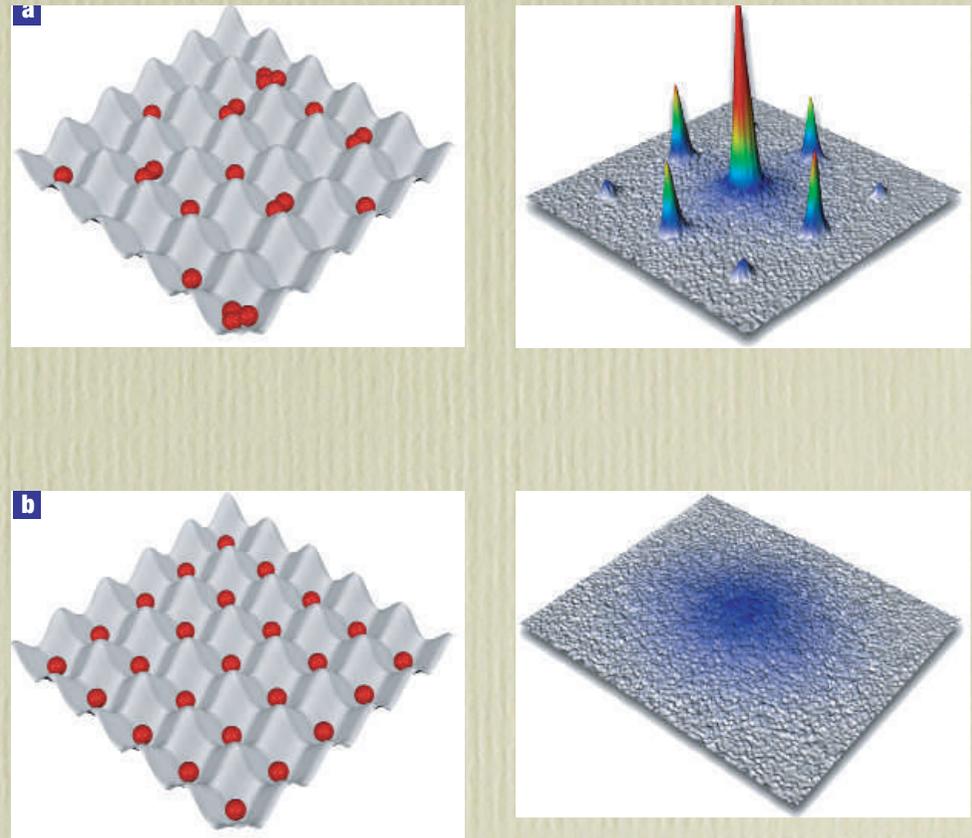


Figure 6 Transition from a superfluid to a Mott insulator. **a**, In the superfluid state of a BEC, the underlying atoms can be described as a giant macroscopic matter wave. When such a condensate is released from the periodic potential, a multiple matter-wave interference pattern appears, owing to the phase coherence between the atomic wavefunctions on different lattice sites. In this case, the phase of the macroscopic matter wave is well defined. However, the atom number on each lattice site fluctuates. **b**, In the other limit of a Mott insulating state of matter, each lattice site is filled with a fixed number of atoms but the phase of the matter-wave field remains uncertain. No matter-wave interference can be seen in this case when the quantum gases are released from the lattice potential (see for example, ref. 3).

QCs based on the circuits of linear optics

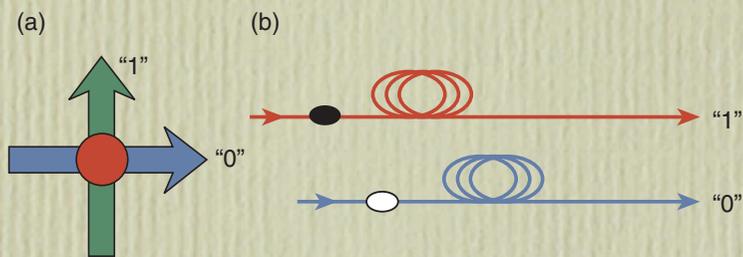


Figure 1. Two methods for implementing quantum bits, or “qubits,” using the quantum states of single photons.⁴ (a) Polarization encoding in which a horizontally polarized single photon represents a logical value of 0 and a vertically polarized single photon represents a logical value of 1. (b) Path encoding, where the presence of a single photon in one of two optical fibers represents a logical value of 0 or 1.

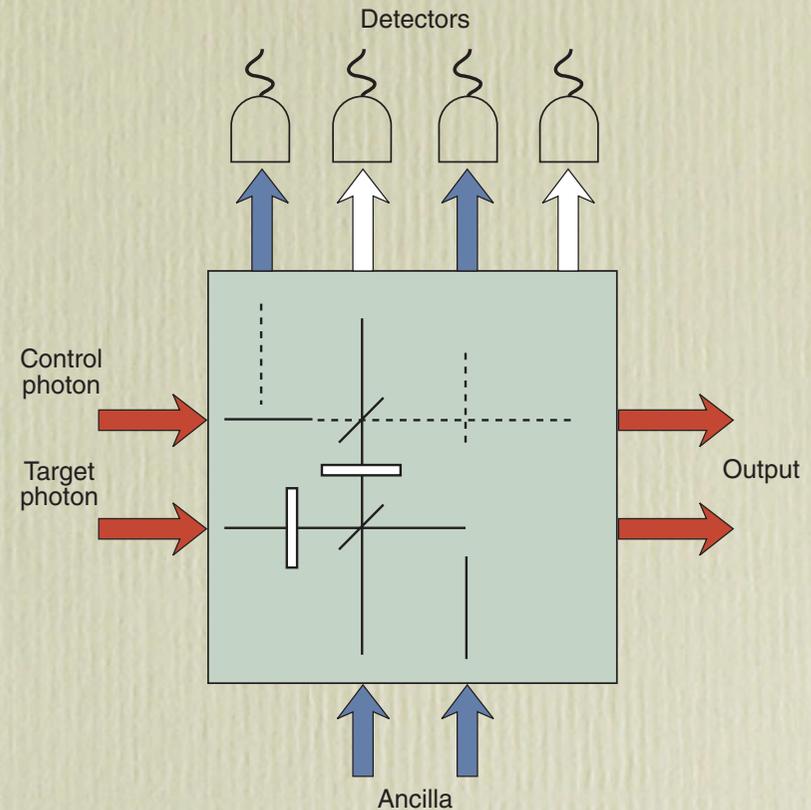


Figure 2. Basic idea of a two-input quantum logic gate constructed using linear optical elements, additional resource (ancilla) photons, and single-photon detectors. The ancilla photons are combined with the logical qubits using linear elements such as beamsplitters and phase shifters. The quantum state of the ancilla photons is measured after they leave the device. The correct logical output is known to have been produced when measurements on the ancilla photons produce certain results. The output can be corrected for other measurement results.

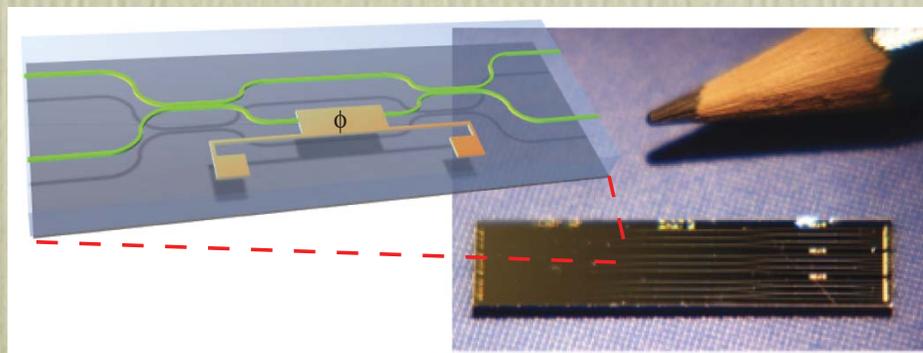


Figure 2 | Photonic quantum computer. A microchip containing several silica-based waveguide interferometers with thermo-optic controlled phase shifts for photonic quantum gates²⁰. Green lines show optical waveguides; yellow components are metallic contacts. Pencil tip shown for scale.

From: T.B.Pittman, B.C.Jacobs, J.D. Franson,
Johns Hopkins APL Technical Digest (2004)

QCs based on the circuits of linear optics (modeling H₂ molecule)

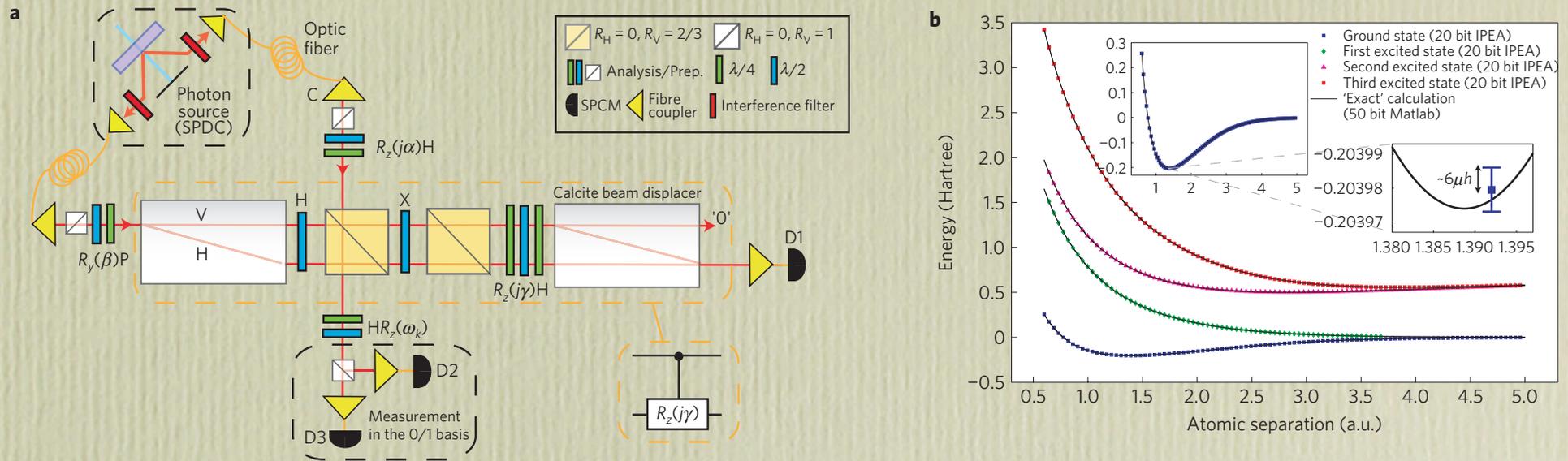


Figure 1 | First quantum chemistry experiment on a quantum information processor. **a**, Quantum optics experiment for simulating the energy of the hydrogen molecule in the minimal basis set. A pair of entangled photons generated via the spontaneous parametric down-conversion (SPDC) process implements an iterative phase-estimation scheme where one of the photons represents two 2×2 blocks of the 6×6 full configuration interaction matrix of H₂ in the minimal quantum chemistry basis set²⁰. The photons are coupled into free space optical modes C (control) and R (register) and manipulated by using half-wave plates ($\lambda/2$) and quarter-wave plates ($\lambda/4$) to implement single-qubit rotations around the Bloch axes, R_y and R_z , as well as Hadamard (H) and Pauli X gate (X) operations. Coincident detection events between single photon counting modules (SPCMs) D1 and D3 (D2 and D3) herald a successful run of the circuit. Panel reproduced from ref. 20. **b**, Plot of the molecular energies of the different electronic states as a function of interatomic distance obtained with the device to 20 bits of precision using an iterative phase-estimation procedure (IPEA) and a majority-voting scheme as a simple error correction protocol.

Quantum Chemistry in the Age of Quantum Computing

Yudong Cao, Jonathan Romero, Jonathan P. Olson, Matthias Degroote, Peter D. Johnson, Mária Kieferová, Ian D. Kivlichan, Tim Menke, Borja Peropadre, Nicolas P. D. Sawaya, Sukin Sim, Libor Veis, and Alán Aspuru-Guzik*

Cite this: *Chem. Rev.* 2019, 119, 19, 10856–10915

Publication Date: August 30, 2019

<https://doi.org/10.1021/acs.chemrev.8b00803>

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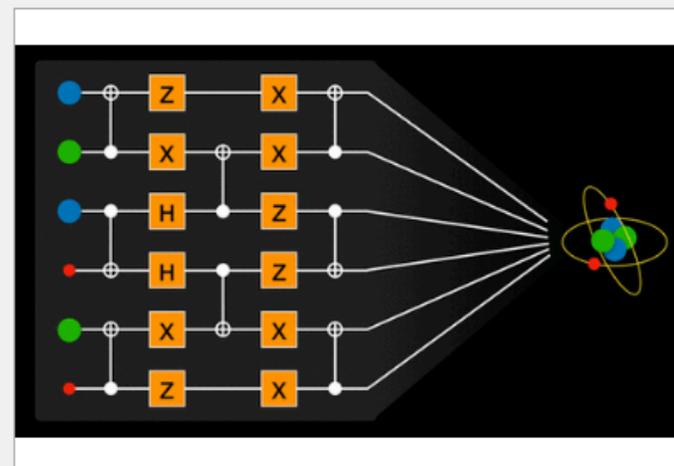
Read Online

PDF (4 MB)

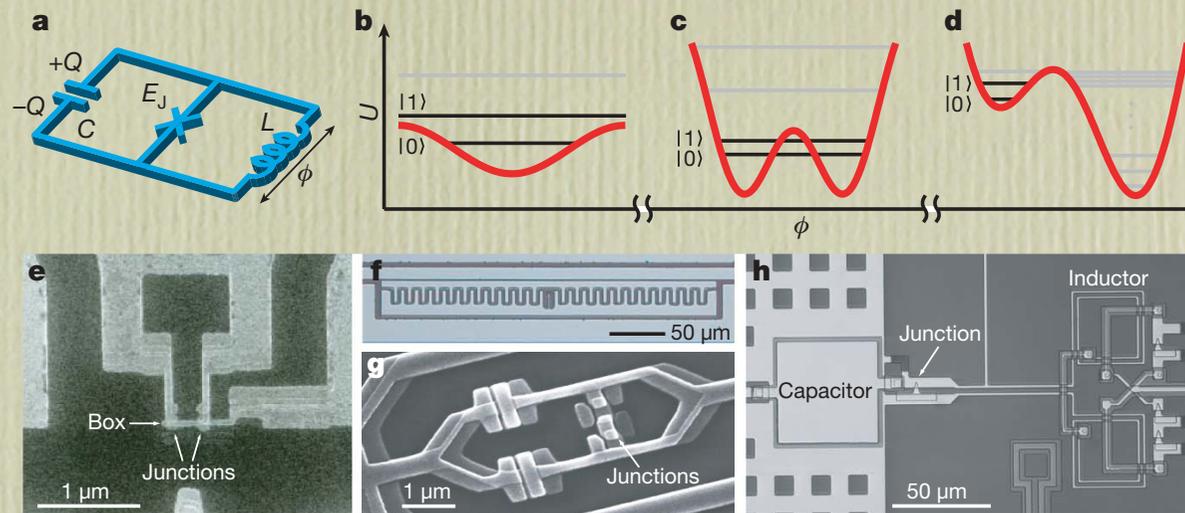
SUBJECTS: Algorithms, Wave function, Quantum mechanics, Mathematical methods, Hamiltonians

Abstract

Practical challenges in simulating quantum systems on classical computers have been widely recognized in the quantum physics and quantum chemistry communities over the past century. Although many approximation methods have been introduced, the complexity of quantum mechanics remains hard to appease. The advent of quantum computation brings new pathways to navigate this challenging and complex landscape. By manipulating quantum states of matter and taking advantage of their unique features such as superposition and entanglement, quantum computers promise to efficiently deliver accurate results for many important problems in quantum chemistry, such as the electronic structure of molecules. In the past two decades, significant advances have been made in developing algorithms and physical hardware for quantum computing, heralding a revolution in simulation of quantum systems. This Review provides an overview of the algorithms and results that are relevant for quantum chemistry. The intended audience is both quantum chemists who seek to learn more about quantum computing and quantum computing researchers who would like to explore applications in quantum chemistry.



QCs on superconducting elements



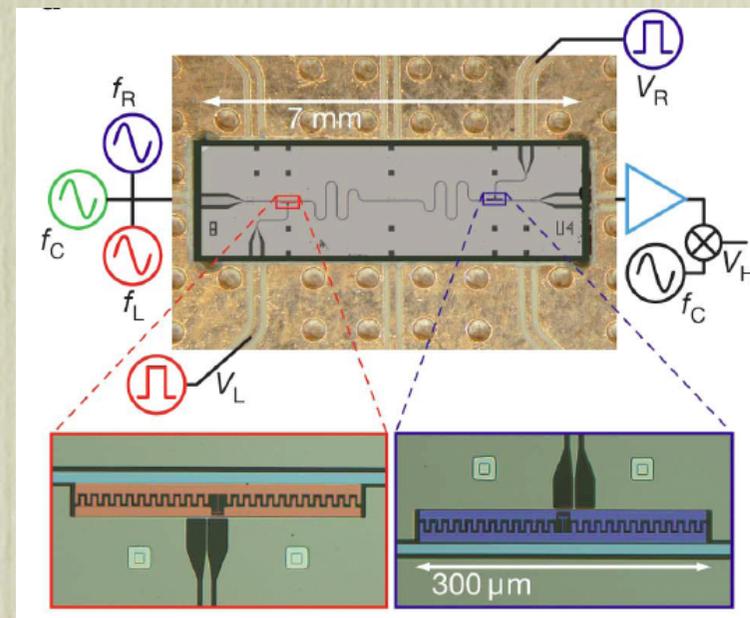
NATURE | Vol 464 | 4 March 2010

Figure 5 | Superconducting qubits. **a**, Minimal circuit model of superconducting qubits. The Josephson junction is denoted by the blue 'X'. **b-d**, Potential energy $U(\Phi)$ (red) and qubit energy levels (black) for charge (**b**), flux (**c**), and phase qubits (**d**), respectively. **e-h**, Micrographs of superconducting qubits. The circuits are made of Al films. The Josephson

junctions consist of Al_2O_3 tunnel barriers between two layers of Al. **e**, Charge qubit, or a Cooper pair box. **f**, Transmon, a derivative of charge qubit with large E_J/E_C (courtesy of R. J. Schoelkopf). The Josephson junction in the middle is not visible at this scale. **g**, Flux qubit (courtesy of J. E. Mooij). **h**, Phase qubit (courtesy of J. M. Martinis).

Demonstration of two-qubit algorithms with a superconducting quantum processor Nature 2009

L. DiCarlo¹, J. M. Chow¹, J. M. Gambetta², Lev S. Bishop¹, B. R. Johnson¹, D. I. Schuster¹, J. Majer³, A. Blais⁴, L. Frunzio¹, S. M. Girvin¹ & R. J. Schoelkopf¹

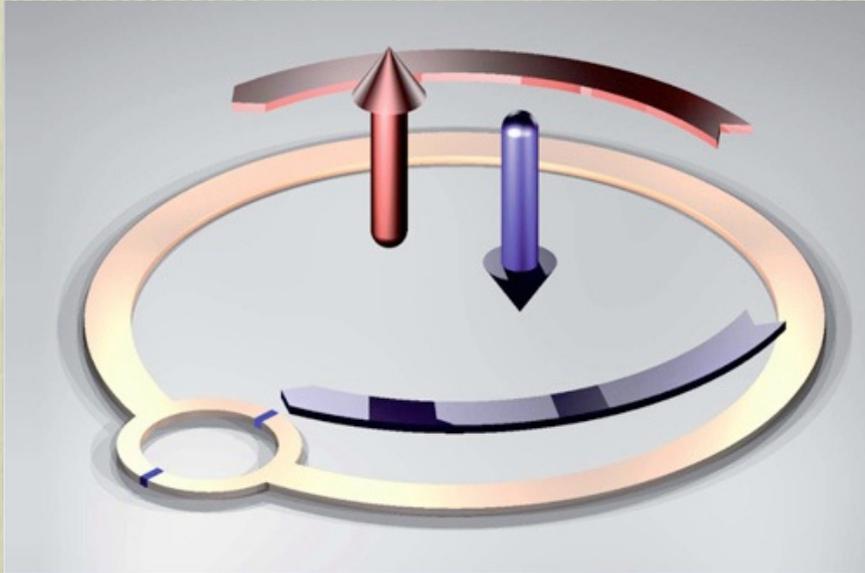


D-Wave quantum simulator



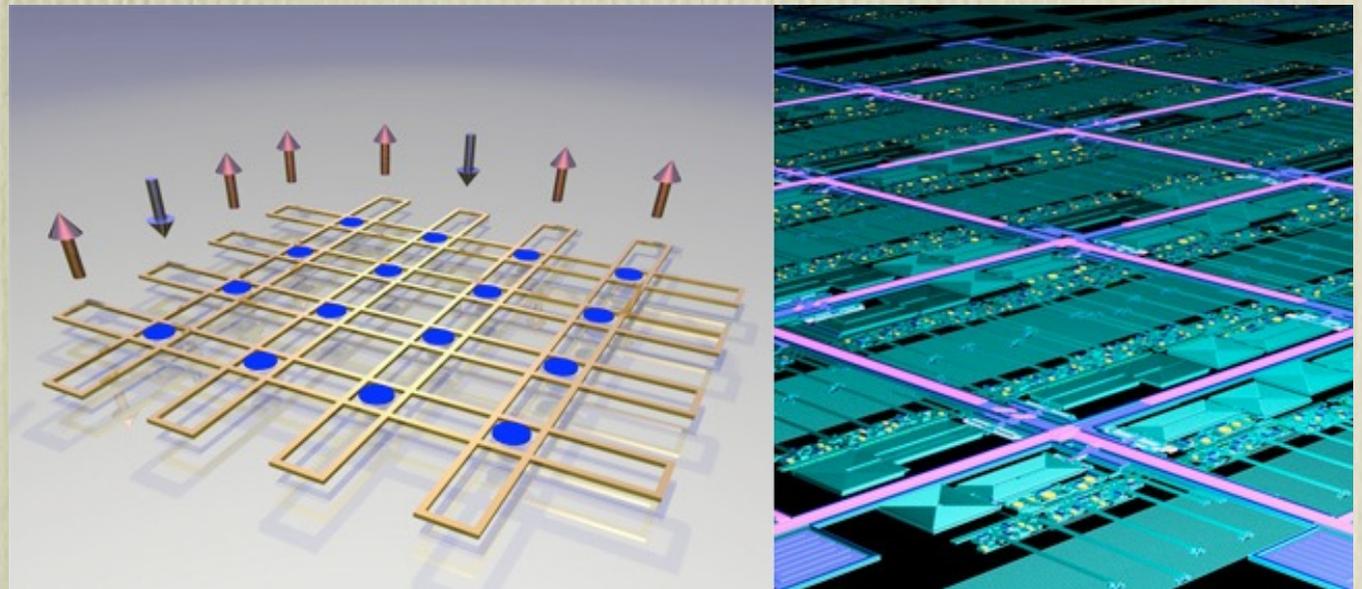
D-Wave Systems, Inc. is a quantum computing company, based in Burnaby, British Columbia. On May 11, 2011, D-Wave System announced D-Wave One, labeled "the world's first commercially available quantum computer," and also referred to it as an adiabatic quantum computer using quantum annealing to solve optimization problems operating on an **128 qubit** chip-set. [www.dwavesys.com]

The building blocks of D-Wave One quantum simulator

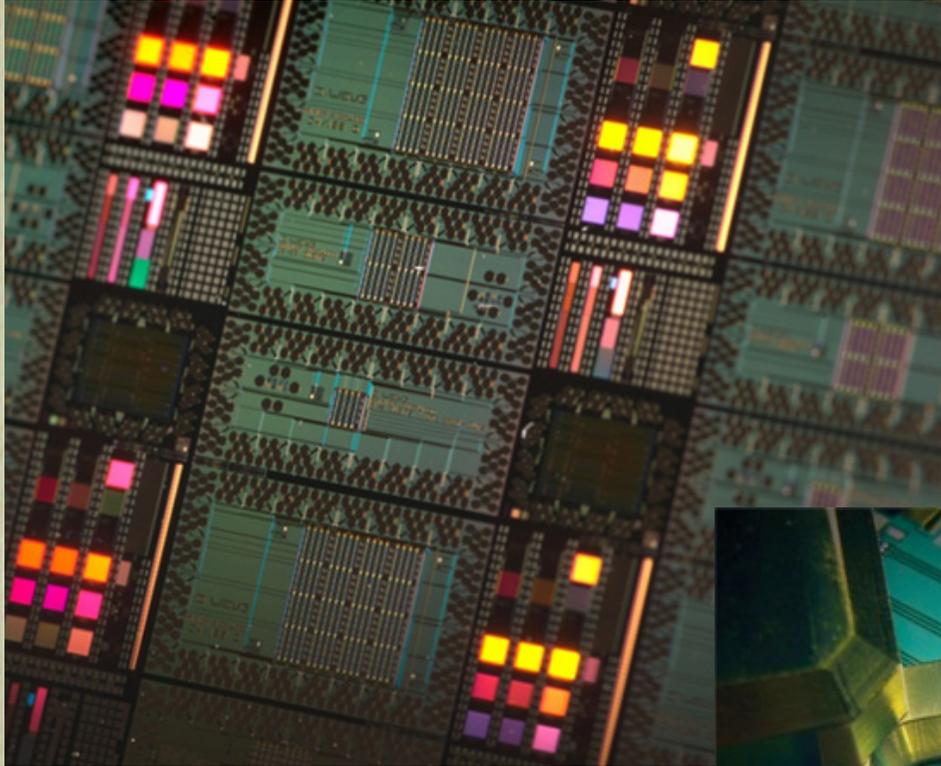


Schematic of a superconducting qubit, the basic building block of the D-Wave One Quantum Computer. The arrows indicate the magnetic spin states which encode the bits of information as $+1$ and -1 values. Unlike regular bits of information, these states can be put into quantum mechanical superposition.

Left: A schematic illustration of 8 qubit loops (gold) connected by 16 coupling devices (blue). Right: A CAD layout of the full chip architecture. Qubit loops are now shown in pink and the control circuitry is indicated by the blue and yellow features.

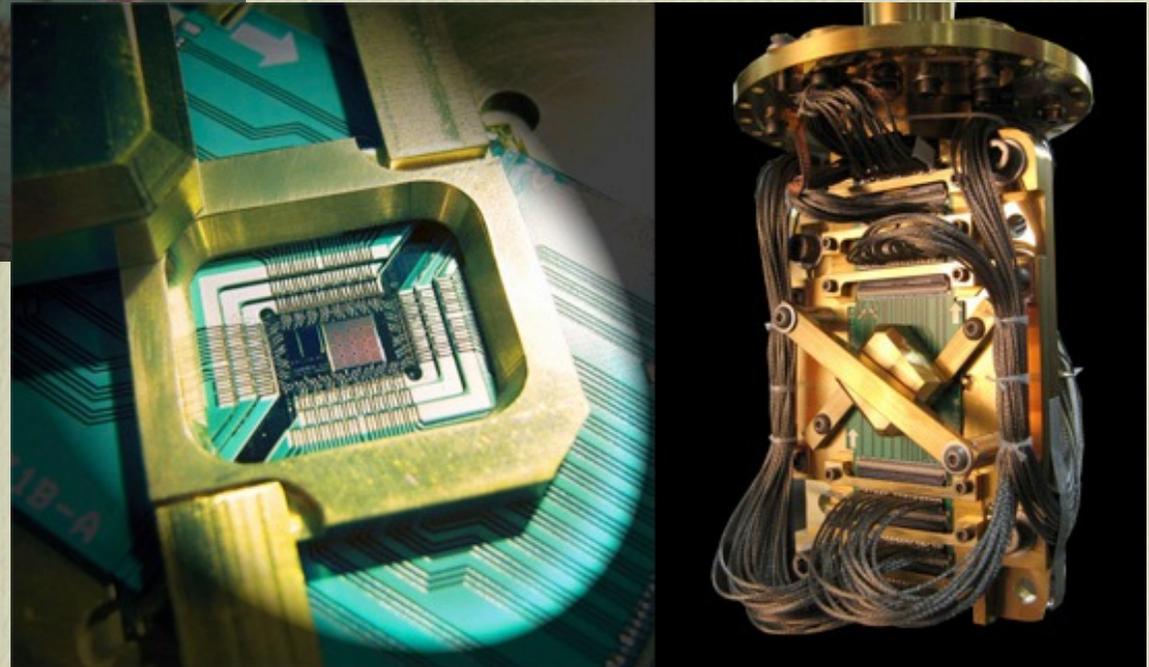


The building blocks of D-Wave One quantum simulator

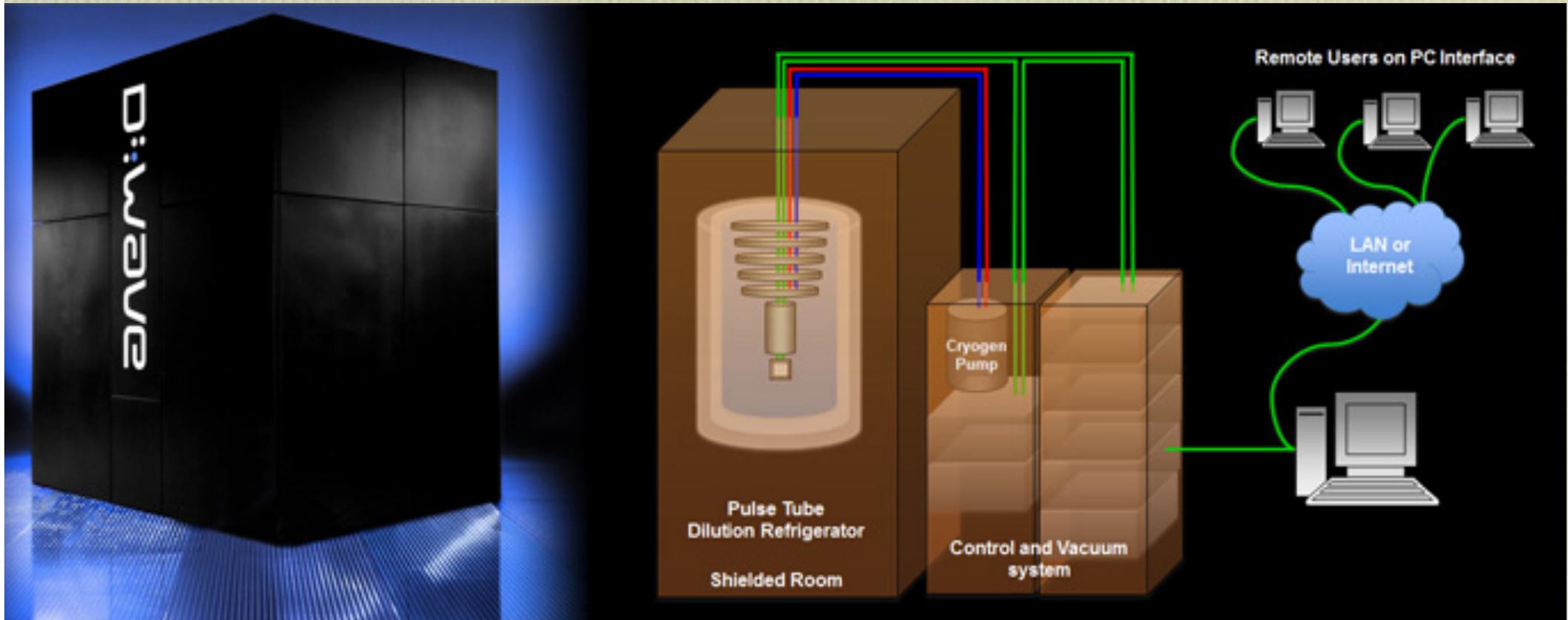


Photograph of a wafer of Rainier processors, including the 128-qubit processor used in the D-Wave One.

Left: A photograph of the chip after being bonded to the computer motherboard. Right: The motherboard is attached to the ultra-low temperature refrigeration system.

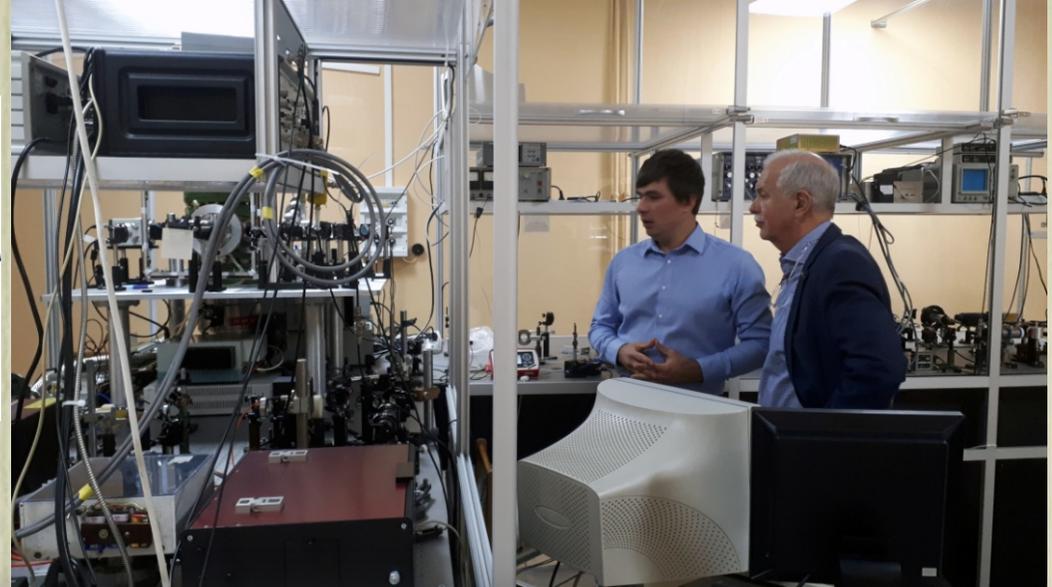


The building blocks of D-Wave One quantum simulator



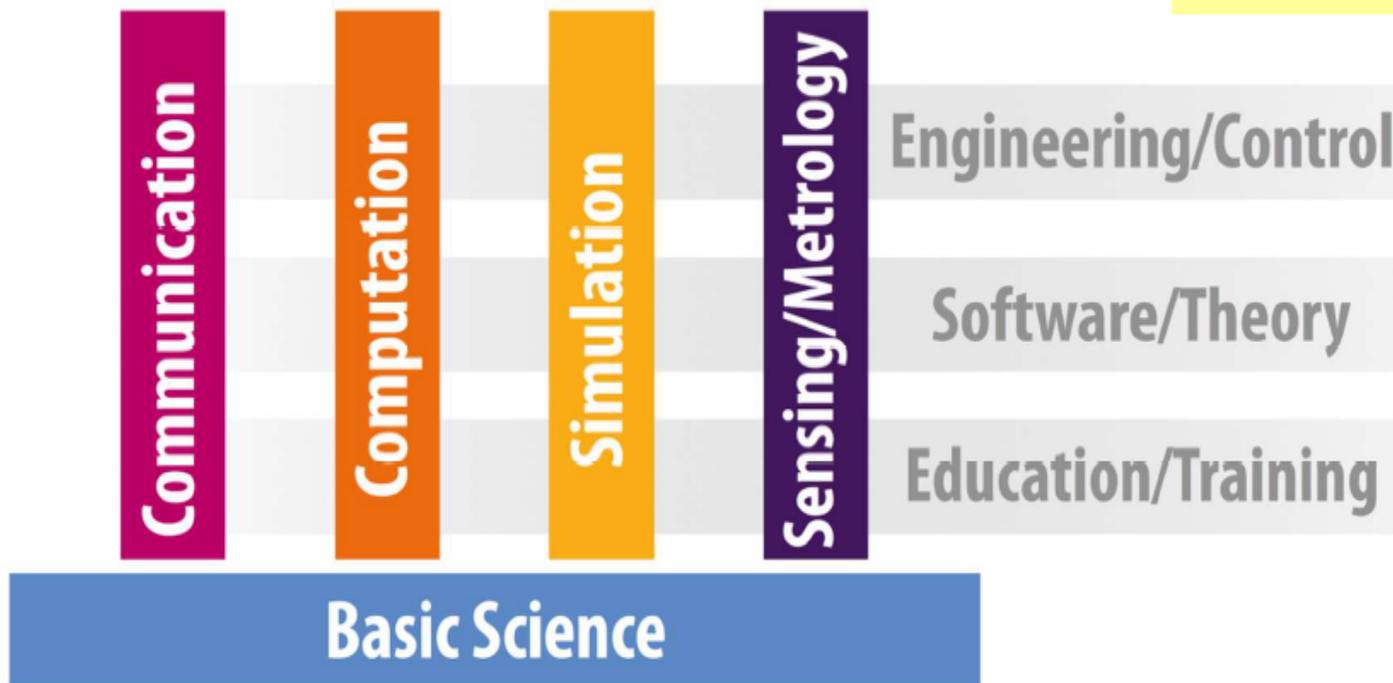
Left: Photograph of the D-Wave One Quantum Computing system. Right: Schematic of the system infrastructure and connection to LAN/internet

Quantum technologies in Europe



Ультрахолодные атомы

The chairman - Prof. Dr. Jürgen Mlynek



How can we make then
regular calculations orders
of magnitude faster for the
problems that do not allow
paralleling?

Rapid Single Flux Quantum Logic (RSFQ)

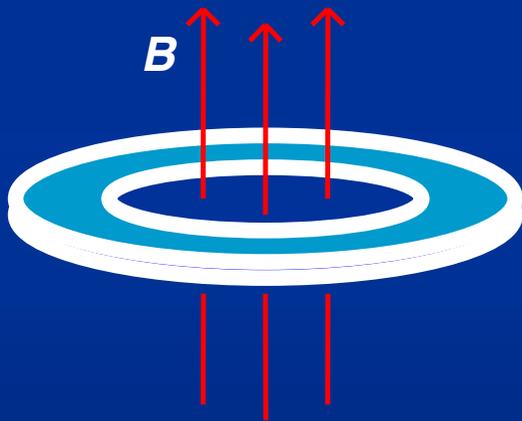


Prof. Konstantin Likharev

Rapid Single Flux Quantum logic (RSFQ) was proposed and developed in detail in the early 80's by then Soviet physicists Konstantin Likharev, Vasily Semenov and Oleg Mukhanov and others, who were with Physics Dept. at Lomonosov Moscow State University. Technologically it was realized at Moscow Institute of Radioelectronics and Automation of the Russian Academy of Sciences (group of Prof. Valery Koshelets).

Rapid Single Flux Quantum Logic (RSFQ)

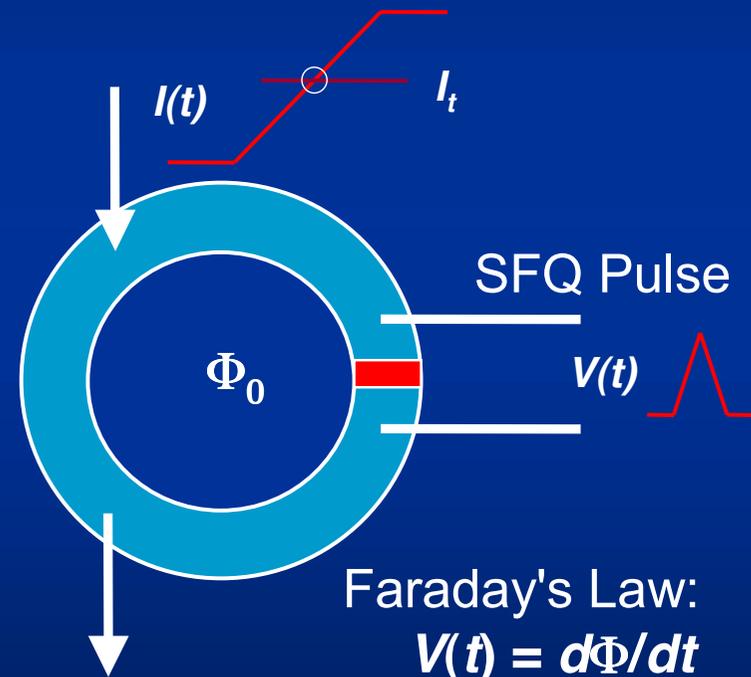
Magnetic flux quantization in a superconductor loop:



$$\Phi = \int B_n dA = n \Phi_0$$

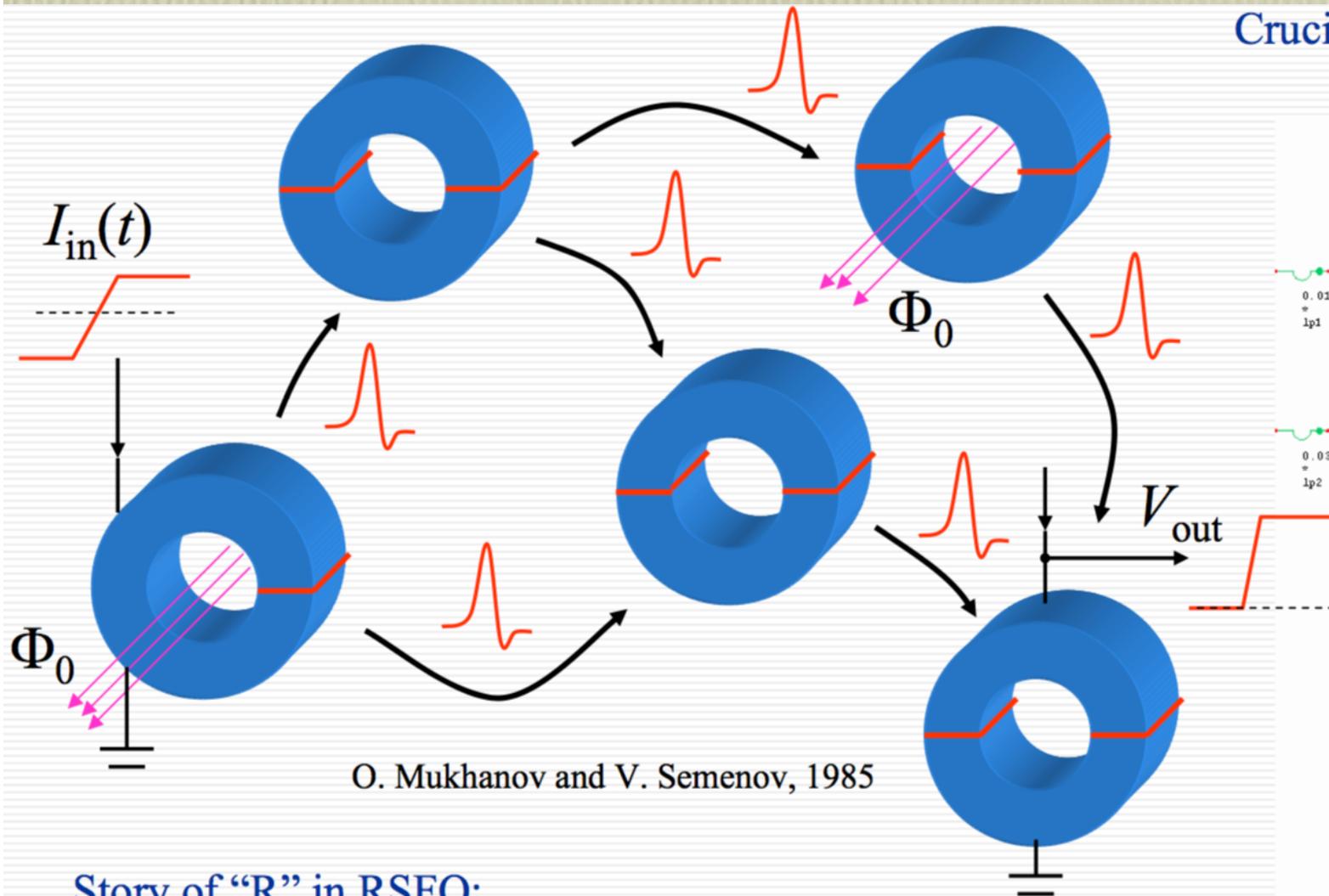
$$\Phi_0 = h/2e \approx 2.07 \times 10^{-15} \text{ Wb}$$

Josephson junction loop as an SFQ pulse generator:

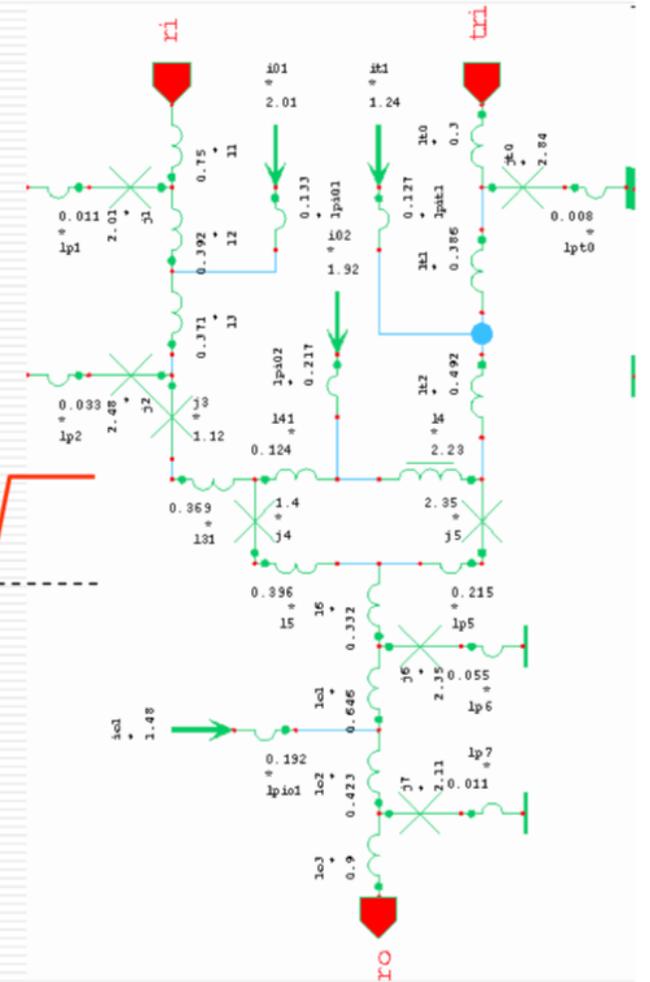


For the SFQ pulse:
 $\int V(t) dt = \Phi_0 \approx 2 \text{ mV-ps}$

Rapid Single Flux Quantum Logic (RSFQ) devices



Crucial new circuit:
latching inverter

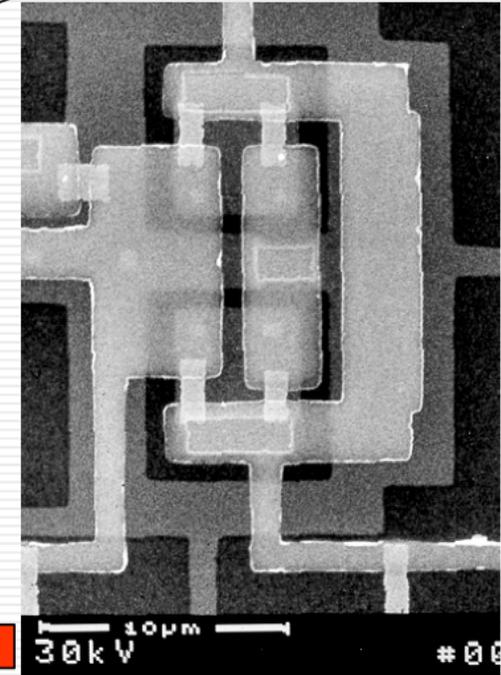
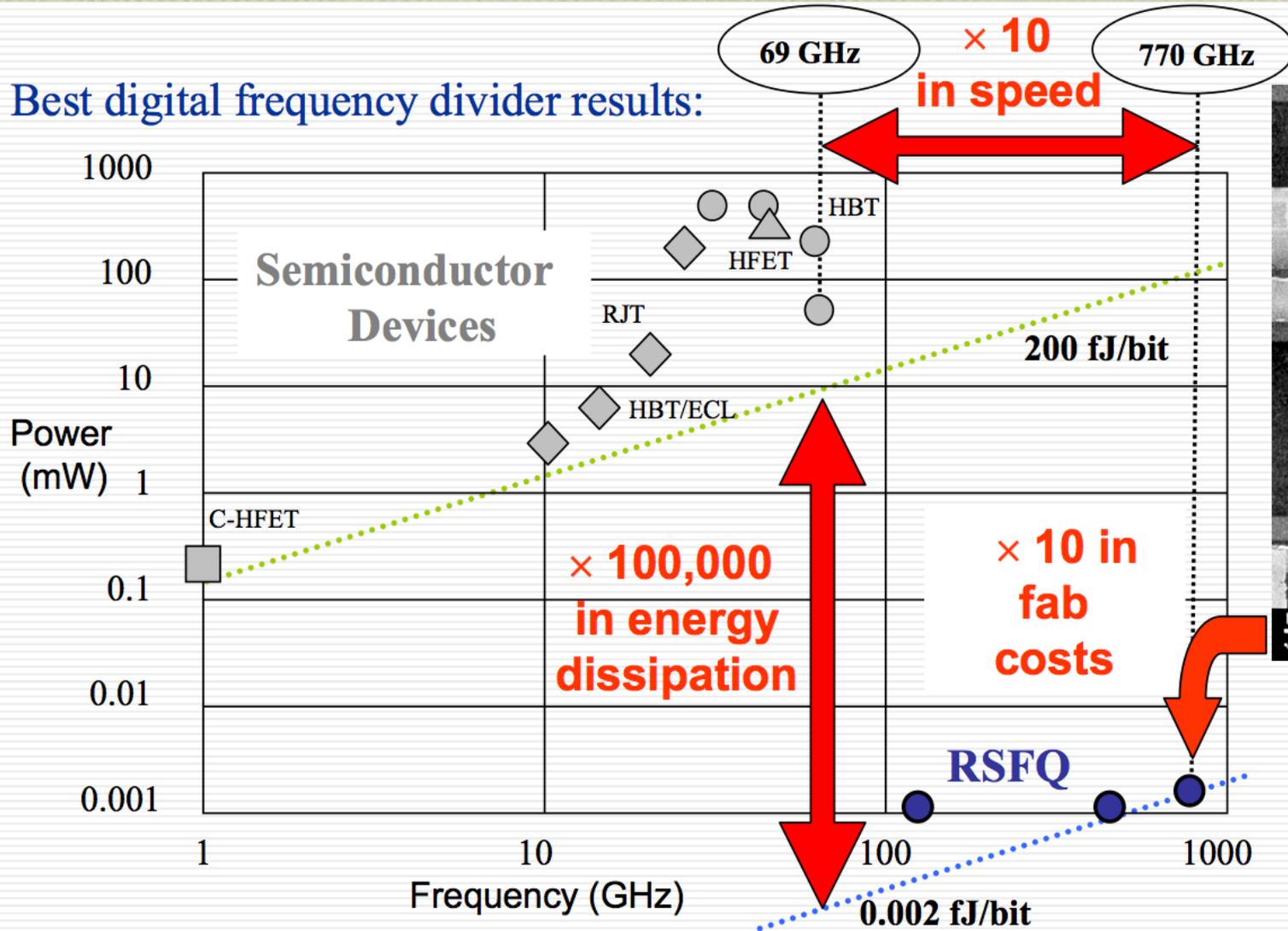


O. Mukhanov and V. Semenov, 1985

Story of "R" in RSFQ:
from *Resistive* to *Rapid*

RSFQ-based devices vs semiconductor electronics

Best digital frequency divider results:

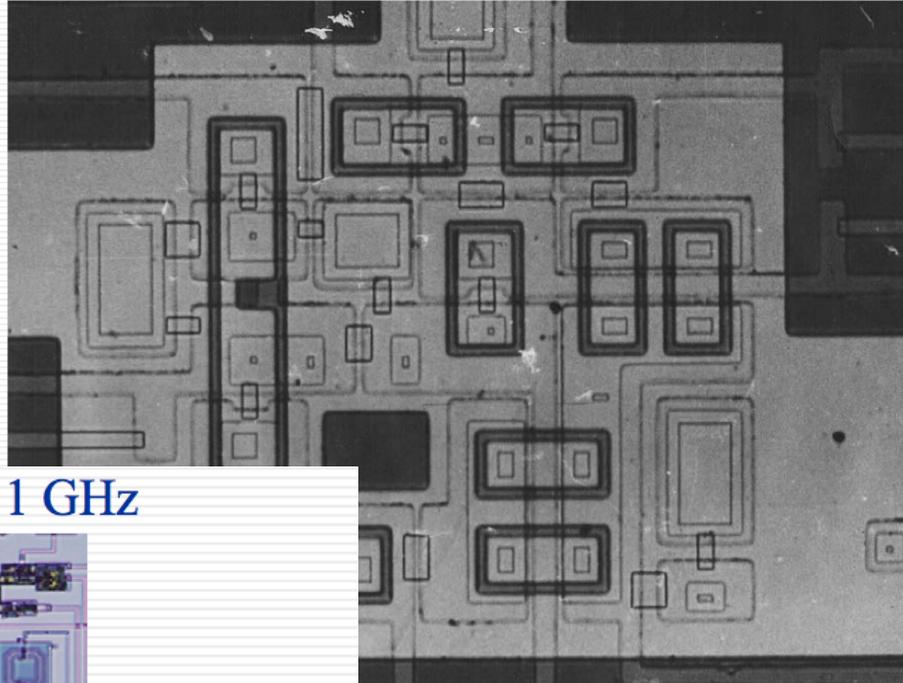


W. Chen *et al.*, 1999

Factor of $\sim 10^3$ in energy advantage even including the Carnot factor

RSFQ-electronics: First demonstrations

TFF operating up to 30 GHz (IRE + MSU):

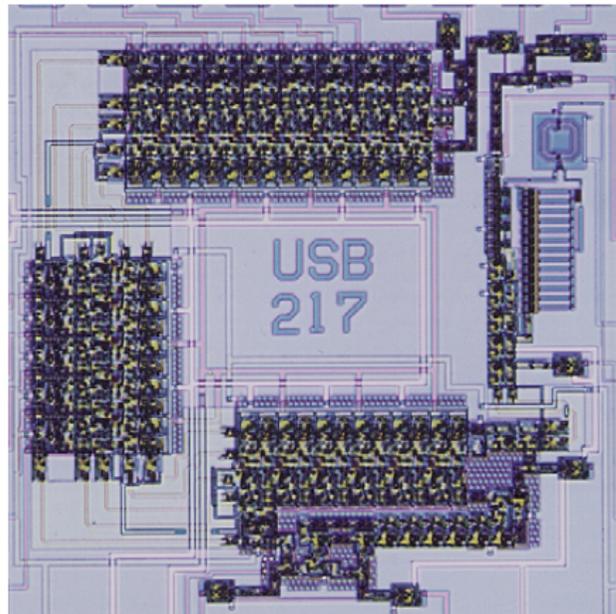


V. Koshelets *et al.*, 1987



MSU, Moscow, 1982

ADC, ~2K JJs, tested at 11 GHz



J. Lin *et al.*,
1995 (design)

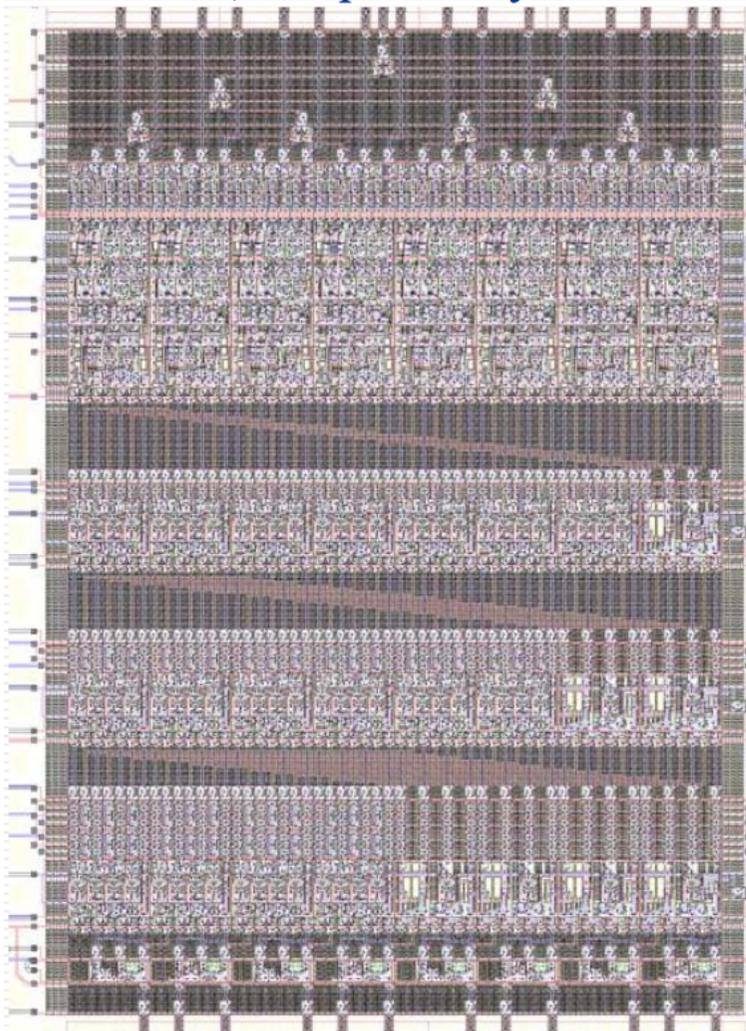
V. Semenov
et al., 1997
(expt)

Project "Contact" (~\$5M/yr):

- proposal filed: late 1987
- Politburo ordeal: Apr. 1988
- funding granted: mid-1988
- financing ended: June 1990

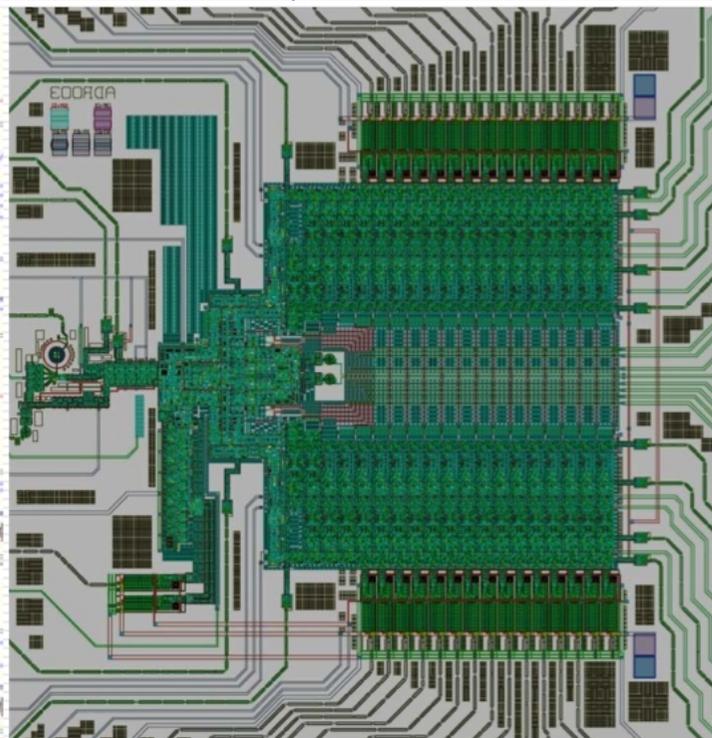
RSFQ-electronics: Further realizations

8-bit asynchronous ALU:
8K JJs, 390 ps latency



T. Filippov *et al.*, 2011

X-band digital RF receiver:
11K JJs, 37 GHz clock

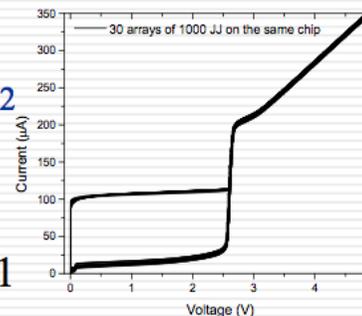


D. Gupta *et al.*, 2011

LTS JJ fab improved:

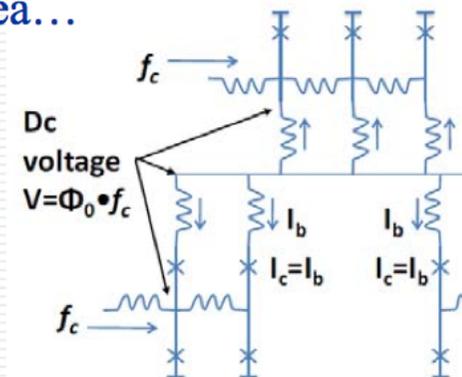
- transfer to 4.5 kA/cm²
- variability decreased

S. Tolpygo, 2011

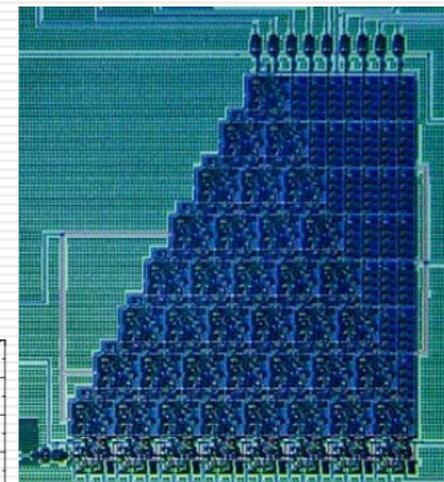


Static power reduction
scheme (“ERSFQ”):

- idea...



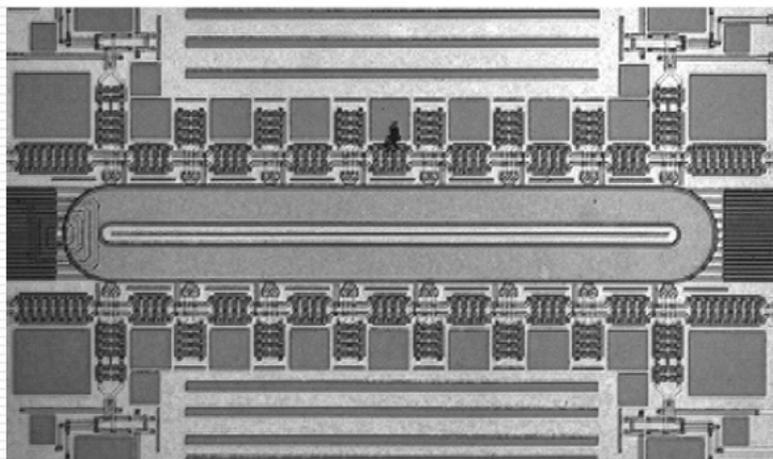
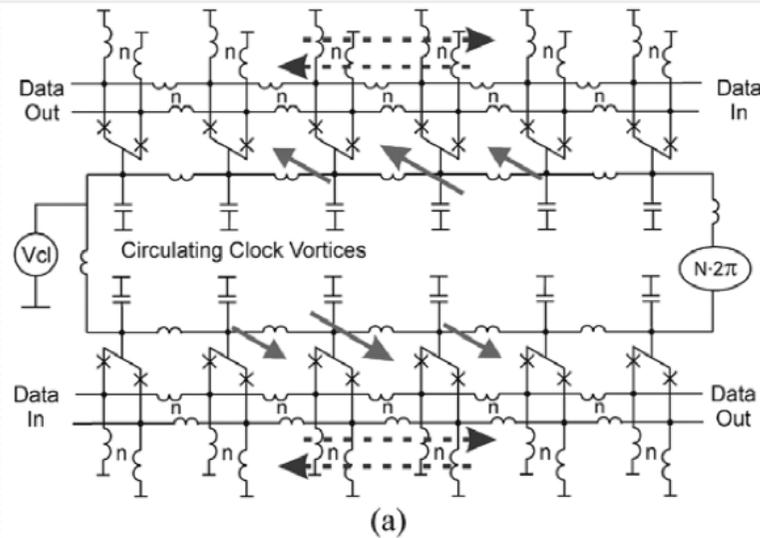
... and demonstration:



D. Kirichenko *et al.*, 2011
A. Kirichenko, private
Communication (2011)

RSFQ-devices can easily be made using reversible logic

Toward experimental demo:



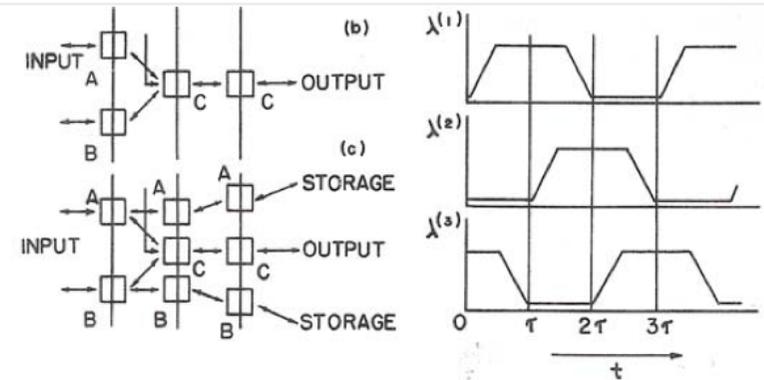
(b)

J. Ren and V. Semenov, 2011

Circuits:

- irreversible:

- reversible:



KL, 1982

Constructive example:

fast convolver:

$$y(n) = \sum_k x(n) \times h(n-k)$$

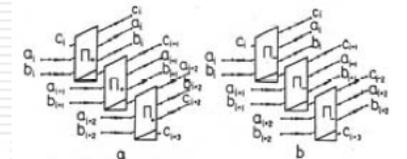
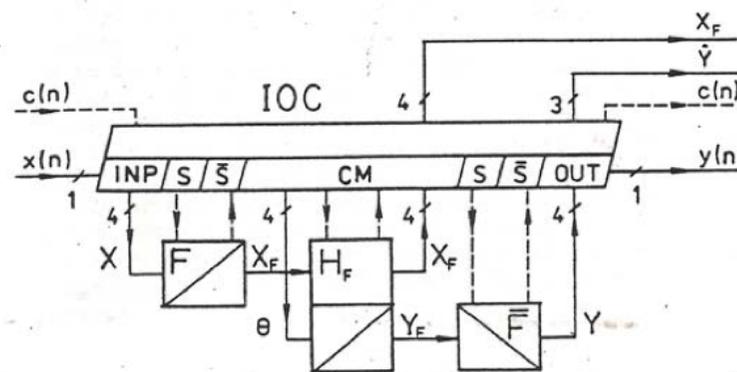
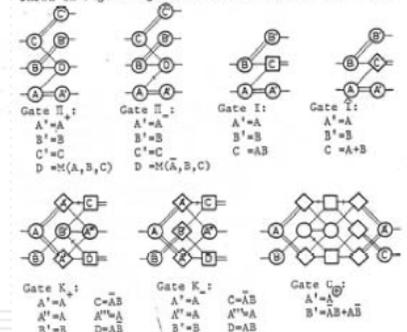


Figure 7. Fragments of the diagonal logic structures DII_+ and DII_- .

A complete set of such gates used in our device is shown in Fig. 8 together with the logic functions per-

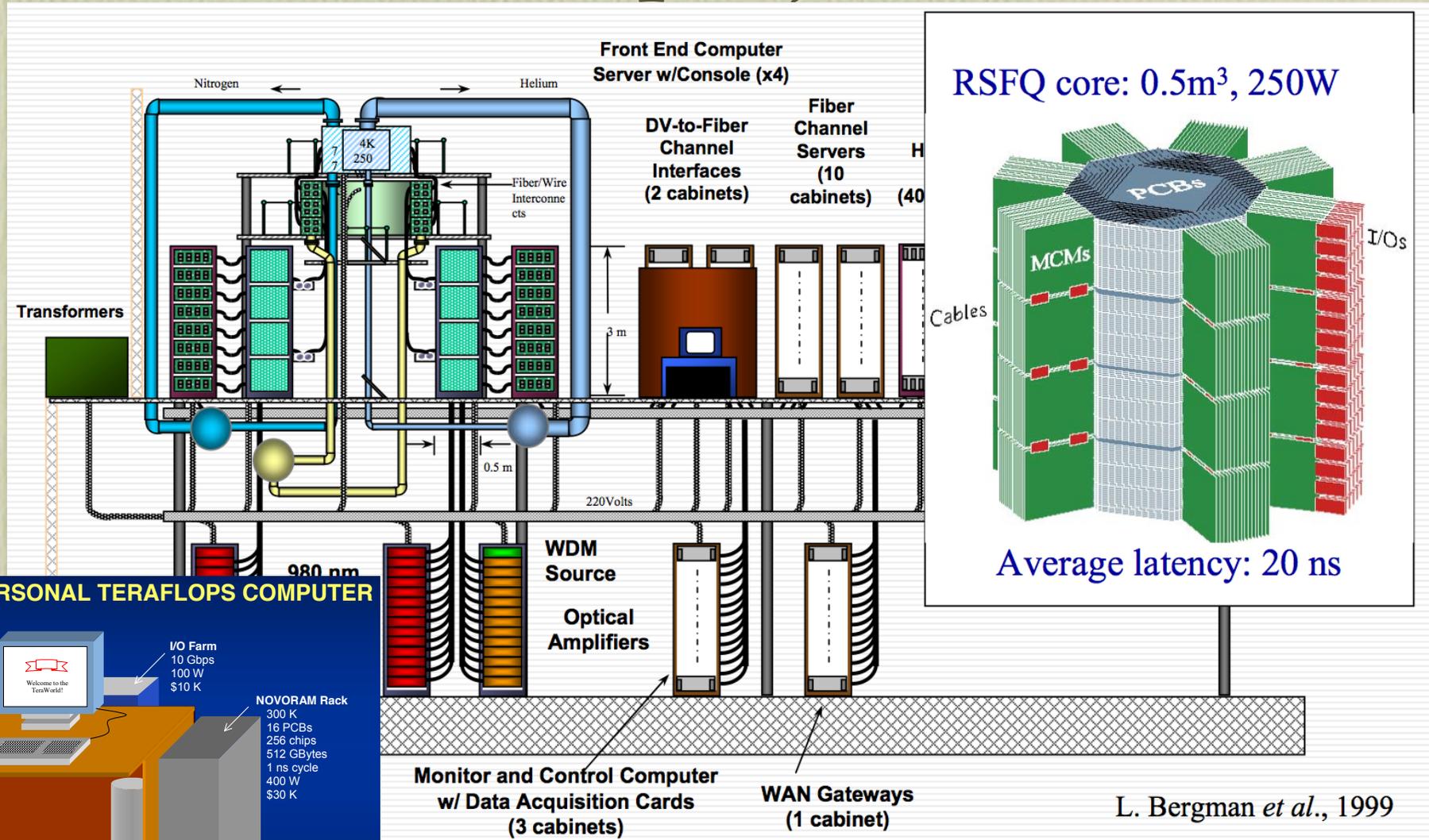


For 8 bits, 1024 points:

30 nW @ 1 GHz & 4.2 K; but: 9.2×10^6 PQs

S. Rylov et al., 1987

PetaFLOPS personal computer (HTMT project)



PeT CONCEPT: PERSONAL TERAFLOPS COMPUTER

- RSFQ Tower**
 - 4 K
 - 1 MCM
 - 100 chips
 - 4 SPELLs
 - 100 GHz
 - 300 W
 - \$30 K
- I/O Farm**
 - 10 Gbps
 - 100 W
 - \$10 K
- NOVORAM Rack**
 - 300 K
 - 16 PCBs
 - 256 chips
 - 512 GBytes
 - 1 ns cycle
 - 400 W
 - \$30 K
- SET Hard Disk Case**
 - 256 disks
 - 8 TBytes
 - 200 W
 - \$10 K

GRAND TOTAL: 1 TF FOR \$100K & 1kW

L. Bergman *et al.*, 1999

What can we learn from
this story?

Thank you for your
attention!