Molecular-Dynamics Machines

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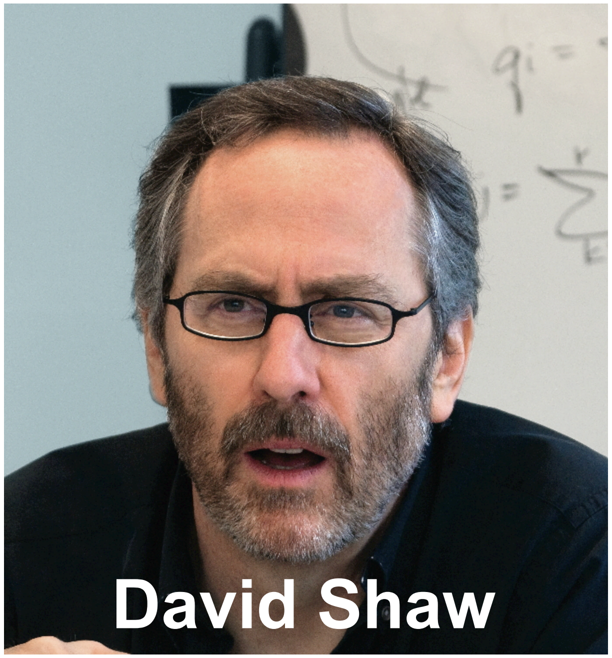
Anton: Computational Microscope



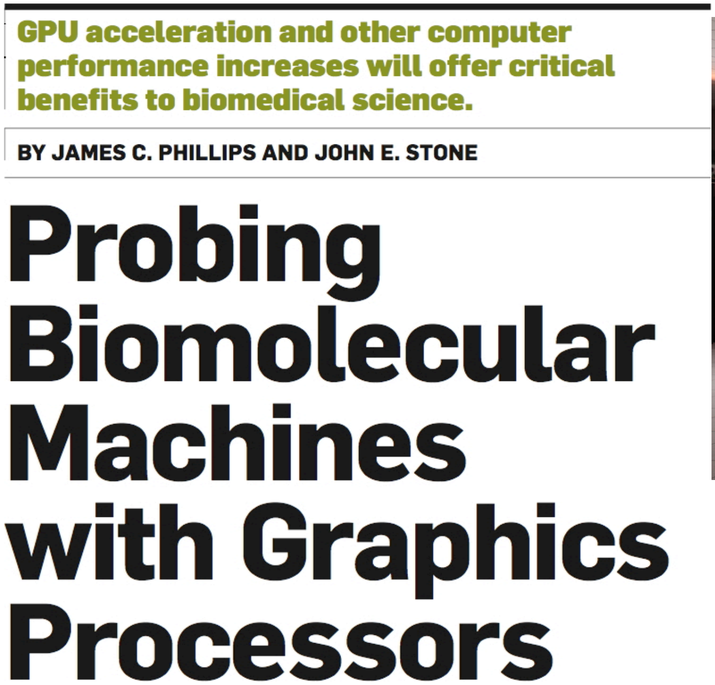
16 μs/day simulation on 512 nodes (5 μs/step execution time)

"... make all these discoveries because they were looking at the world in a different way."

"... there's still a lot of juicy, low-hanging fruit in this (molecular simulation) area ..."

"A conversation with David E. Shaw," *CACM* **52**(10), 49 ('09)

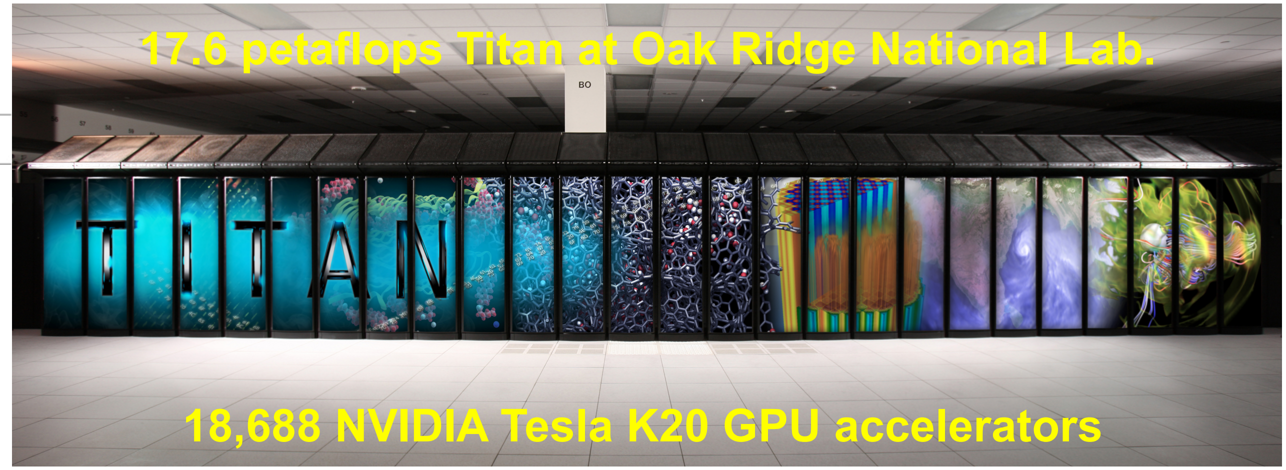
MD on GPU Clusters

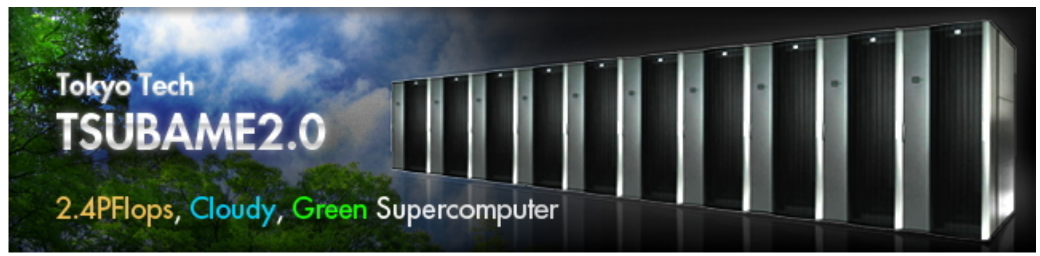

GPU acceleration and other computer performance increases will offer critical benefits to biomedical science.

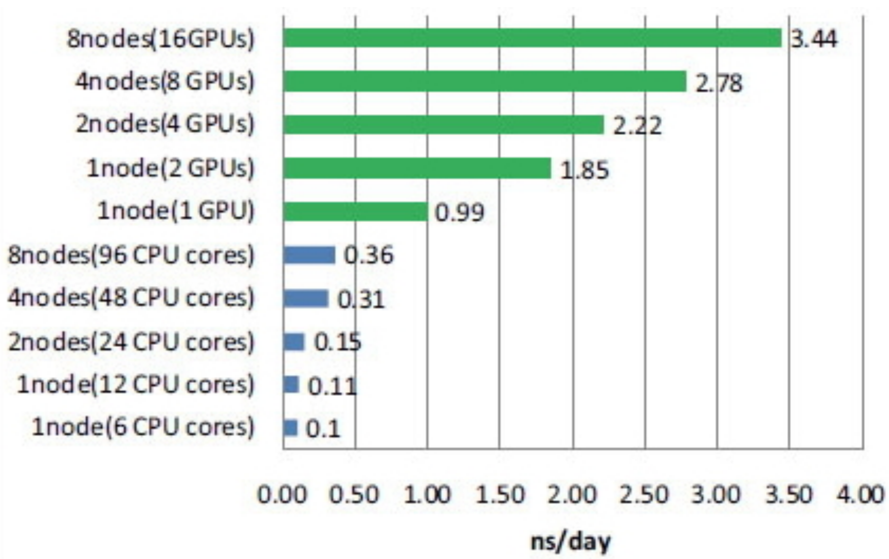
BY JAMES C. PHILLIPS AND JOHN E. STONE

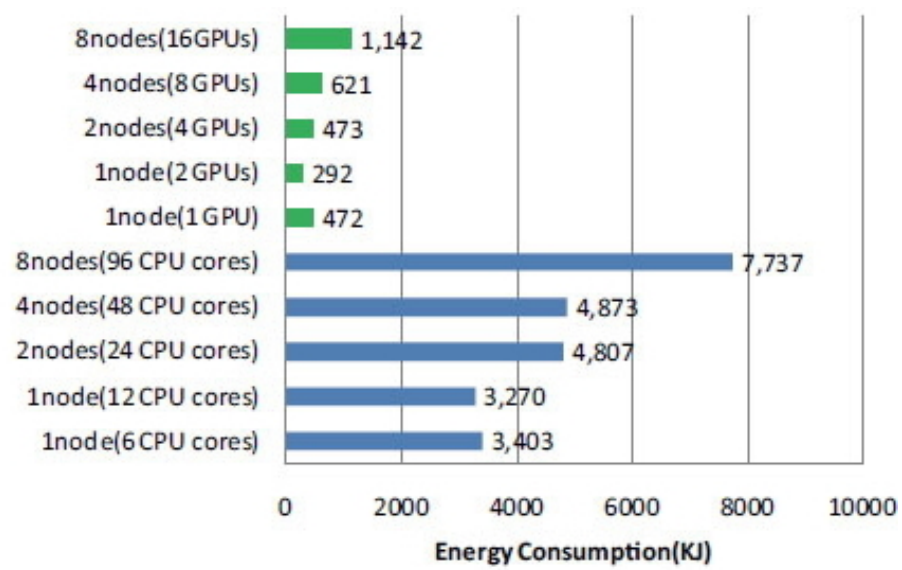
Probing Biomolecular Machines with Graphics Processors

CACM **52**(10), 34 ('09)

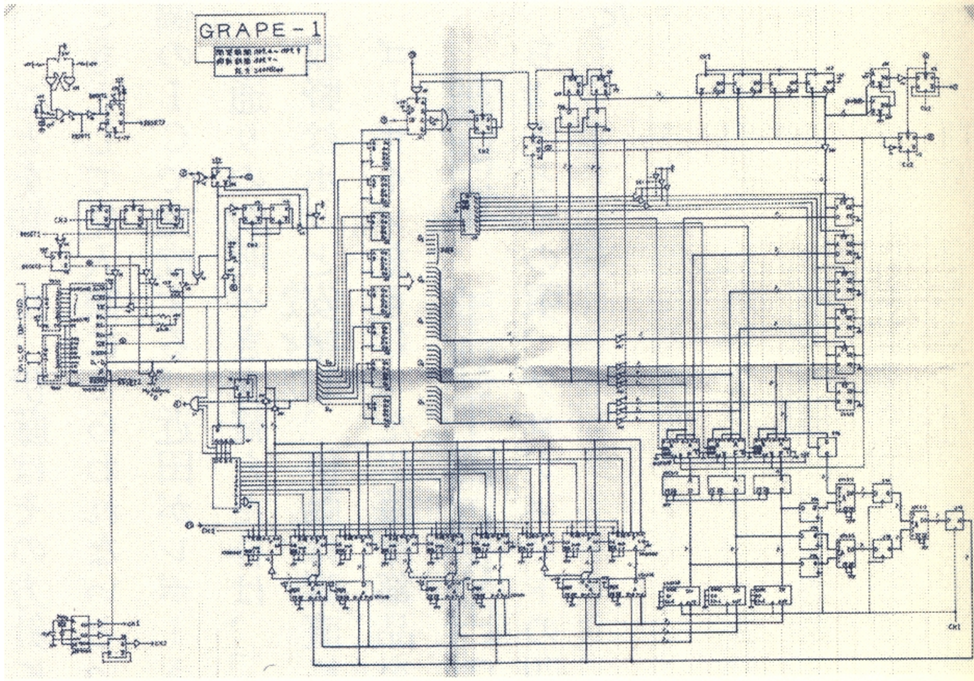


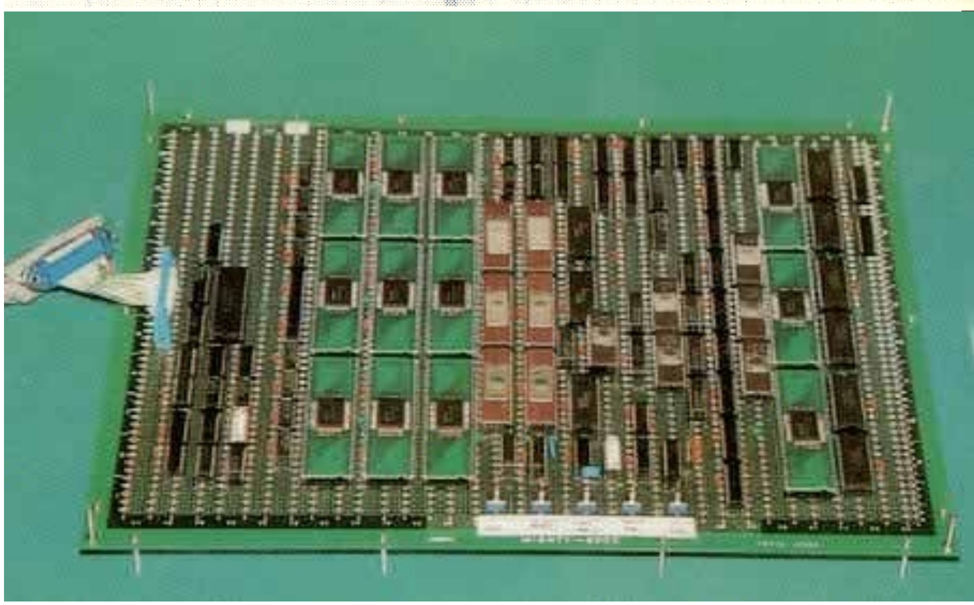






GRAPE 1 ($2K, 1989)



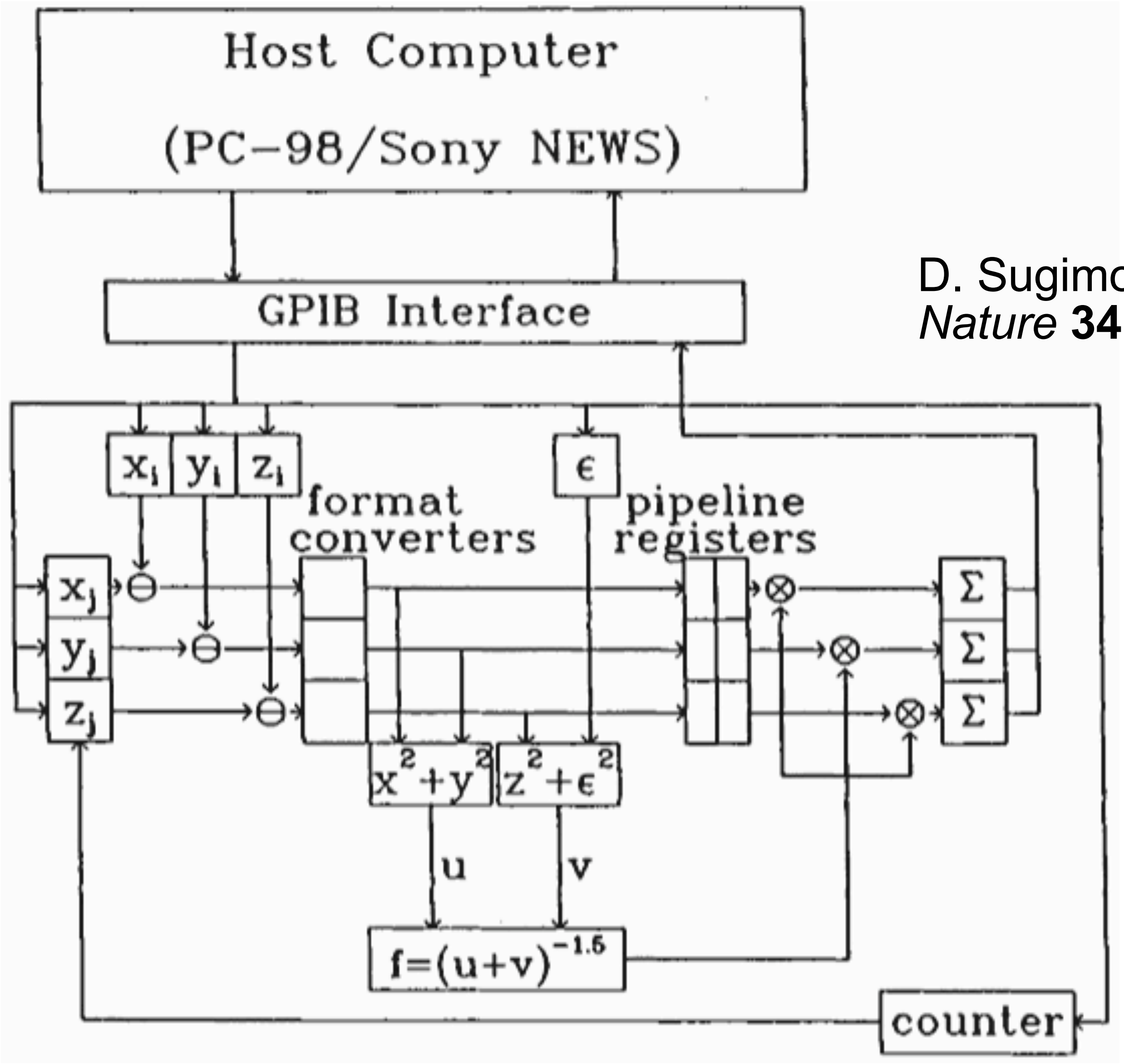


Tomoyoshi Ito & comics he authored

- **GRAPE (GRAvity PipE) = special-purpose computers for the gravitational *N*-body problem built by astrophysicists at Univ. of Tokyo**
- **GRAPE 1 designed by a 1st-year Ph.D. student (with $140K/year income)**

Gravitational Pipeline

$$\frac{d^2\mathbf{x}_i}{dt^2} = \mathbf{f}_i = \sum_j \frac{m_j(\mathbf{x}_j - \mathbf{x}_i)}{(r_{ij}^2 + \varepsilon^2)^{3/2}}$$



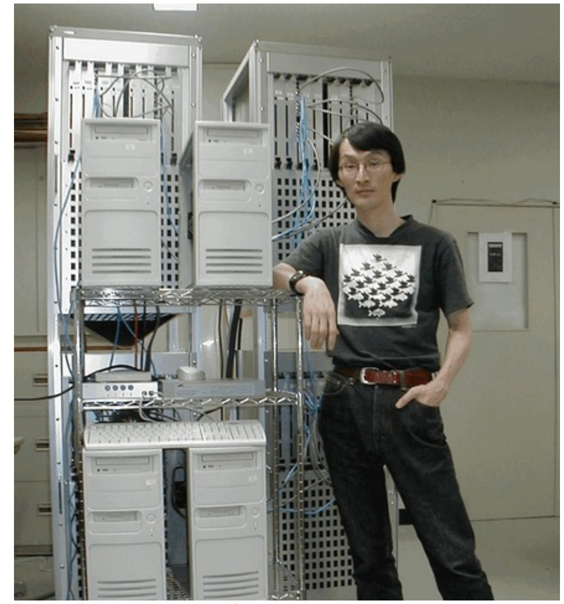
D. Sugimoto *et al*., *Nature* **345**, 33 ('90)

GRAPE & Gordon Bell Prizes

2003 Gordon Bell Prize, Special Achievement
Performance Evaluation and Tuning of GRAPE-6—Towards 40 'Real' Tflop/s
Junichiro Makino, Hiroshi Daisaka, Eiichiro Kokubo, Toshiyuki Fukushige

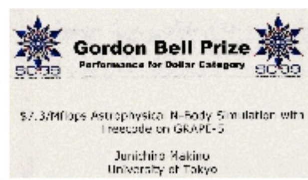
2001 Gordon Bell Prize, Winner, Peak Performance
A 11.55 Tflops simulation of black holes in a galactic center on GRAPE-6
Junichiro Makino, Toshiyuki Fukushige

2000 Gordon Bell Prize, Winner, Peak Performance Category
A 1.349 Tflops simulation of black holes in a galactic center on GRAPE-6
Junichiro Makino, Toshiyuki Fukushige, Masaki Koga



J. Makino & Grape 6 (2001)

2000 Gordon Bell Prize, Winner, Peak Performance Category (tie with above)
1.34 Tflops Molecular Dynamic simulation for NaCl with a Special Purpose Computer: MDM
(MD-GRAPE system)
Tetsu Narumi, Ryutaro Susukita, Takahiro Koishi, Kenji Yasuoka, Hideaki Furusawa, Atsushi Kawai, Toshikazu Ebisuzaki



1999 Gordon Bell Prize, Price Performance, First Prize
Astrophysical N-body simulation
144 Glops / $ 1 M on custom-built GRAPE-5 32-processor system
Atsuchi Kawai, Toshiyuki Fushushige, and Junichiro Makino

1996 Gordon Bell Prize, Performance, Honorable Mention
Simulation of the motion of 780,000 stars
333 Gflops using the Grape-4 machine w/ 1,269 processors
Junichiro Makino, Toshiyuki Fukushige

1995 Gordon Bell Prize, First Place, Special Purpose Machines
Simulation of the Motion of 10,000 Stars
112 Gflops using the Grape-4 machine with 288 processors
Astrophysical N-body Simulations on GRAPE-4 Special-Purpose Computer
Junichiro Makino, Makoto Taiji

Green500 Rank	MFLOPS/W	Site*	Computer*	Total Power (kW)
1	1684.20	IBM Thomas J. Watson Research Center	NNSA/SC Blue Gene/Q Prototype	38.80
2+	1448.03	National Astronomical Observatory of Japan	GRAPE-DR accelerator Cluster, Infiniband	24.59
2	958.35	GSIC Center, Tokyo Institute of Technology	HP ProLiant SL390s G7 Xeon 6C X5670, Nvidia GPU, Linux/Windows	1243.80
3	933.06	NCSA	Hybrid Cluster Core i3 2.93Ghz Dual Core, NVIDIA C2050, Infiniband	36.00
4	828.67	RIKEN Advanced Institute for Computational Science	K computer, SPARC64 VIIIfx 2.0GHz, Tofu interconnect	57.96

www.green500.org (Nov. '10)

Enabling Science by Hardware

A special-purpose computer for gravitational many-body problems

Daiichiro Sugimoto*, Yoshihiro Chikada†, Junichiro Makino*, Tomoyoshi Ito*, Toshikazu Ebisuzaki* & Masayuki Umemura‡

NATURE · VOL 345 · 3 MAY 1990 33

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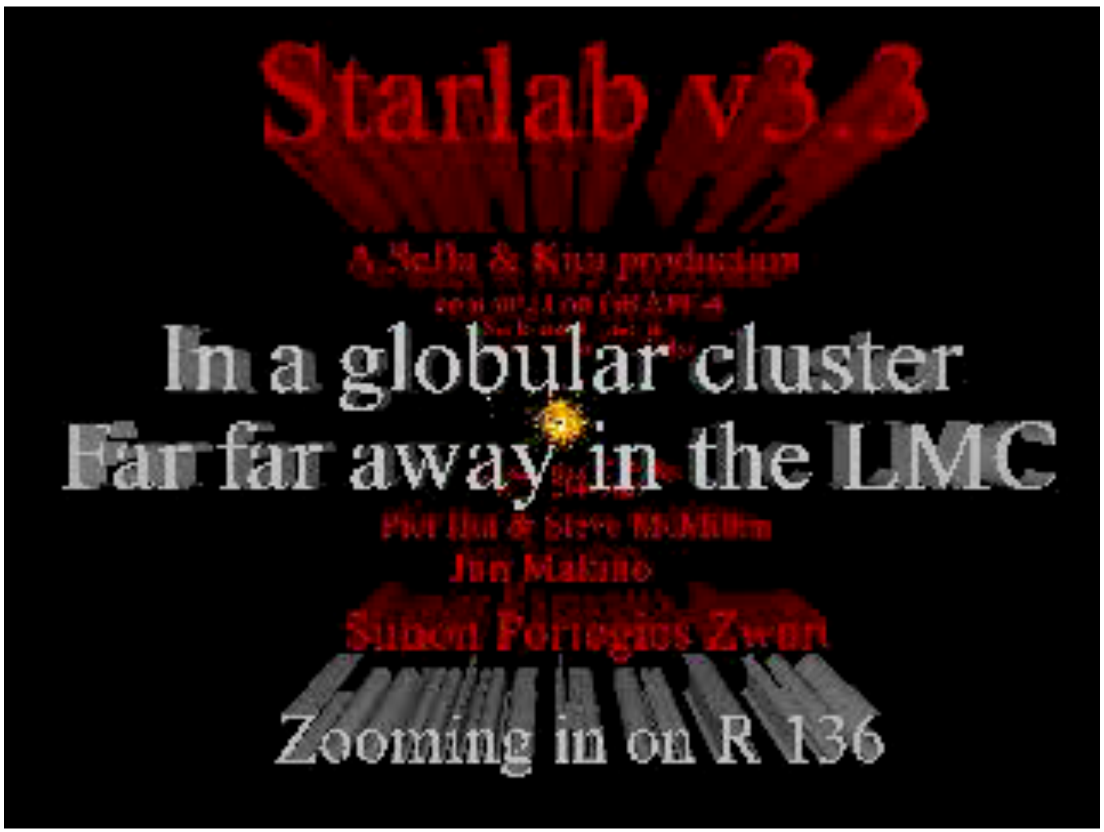


Computer Physics Communications 60 (1990) 187–194

A special-purpose *N*-body machine GRAPE-1

Tomoyoshi Ito, Junichiro Makino, Toshikazu Ebisuzaki and Daiichiro Sugimoto
Department of Earth Science and Astronomy, College of Arts and Sciences, University of Tokyo, Tokyo 153, Japan

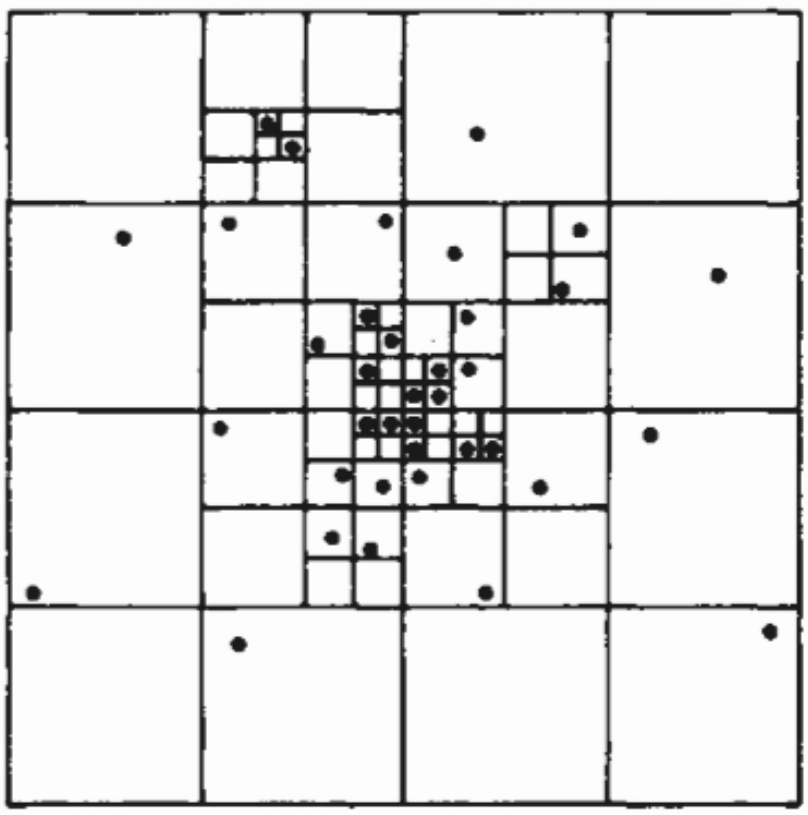
Enabling Science by Algorithm

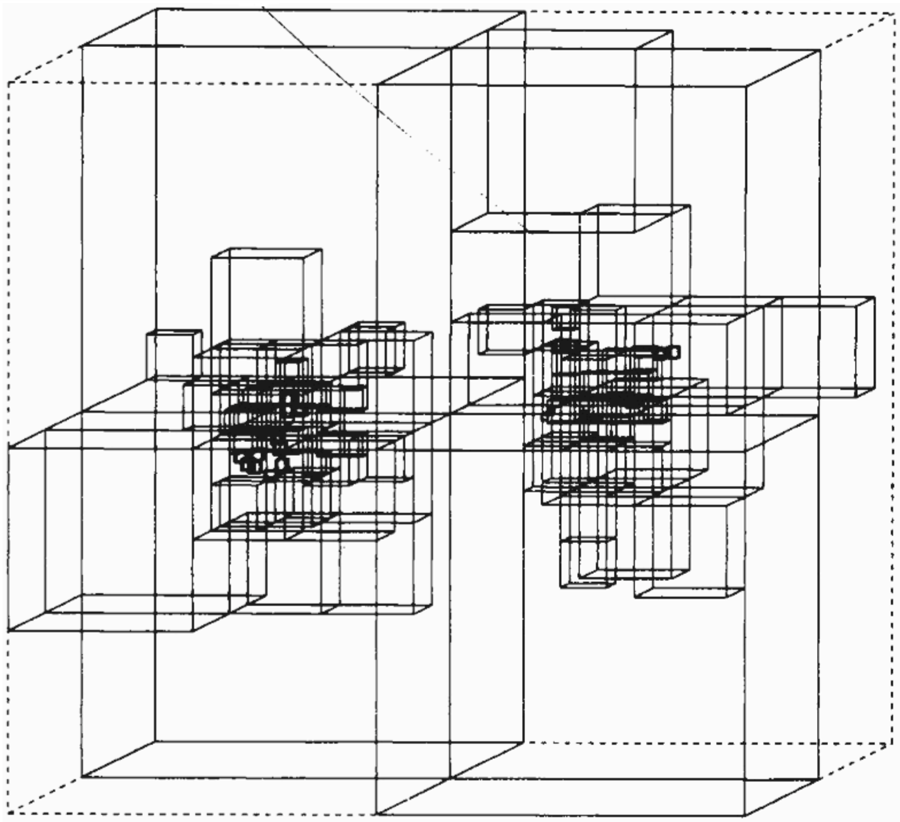
NATURE

NATURE VOL. 324 4 DECEMBER 1986

A hierarchical $O(N \log N)$ force-calculation algorithm

Josh Barnes & Piet Hut





ACM Best Theses: Machine *vs*. Algorithm

DANNY HILLIS

Doctoral Dissertation Award

United States – 1985

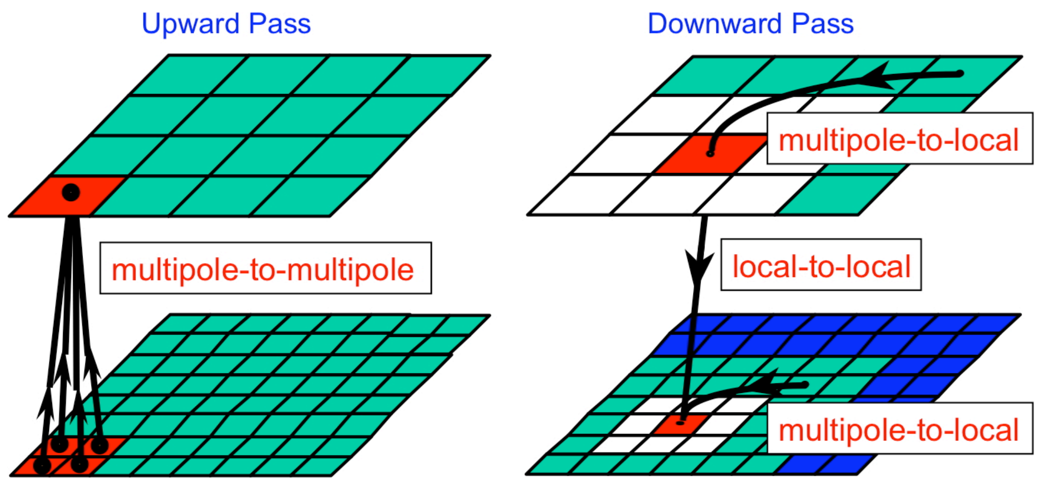
CITATION

For his dissertation "The Connection Machine."

Watch: Hillis on Richard Feynman

http://longnow.org/essays/richard-feynman-connection-machine/

LESLIE GREENGARD



Doctoral Dissertation Award

United States – 1987

CITATION

For his dissertation "The Rapid Evaluation of Potential Fields in Particle Systems."

More *N*-body Simulations at SC

42 TFlops Hierarchical *N*-body Simulations on GPUs with Applications in both Astrophysics and Turbulence

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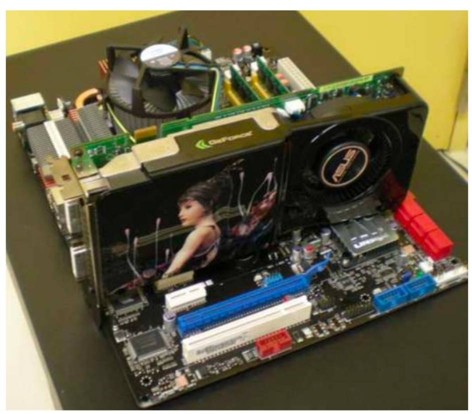
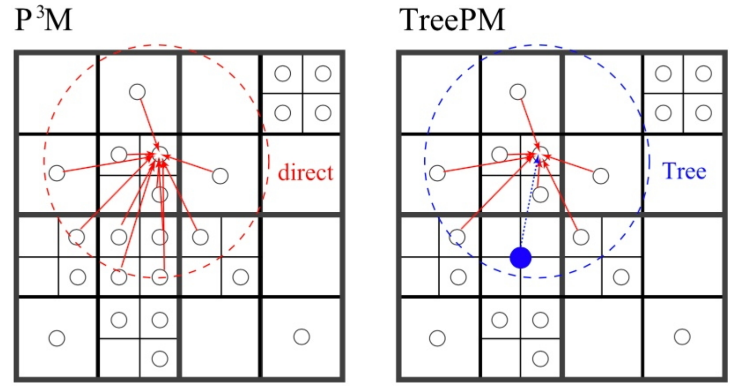
2009 Gordon Bell Prize
Price/Performance Category

Table 2: Price of the GPU cluster

Elements	Quantity	Price (JPY)	Price ($)
GPUs	256	12,160,000	$ 118,345
Host PCs	128	10,716,032	$ 104,292
Network switch	4	644,800	$ 6,275
Total		**23,520,832**	**$ 228,912**





4.45 Pflops Astrophysical N-Body Simulation on K computer - The Gravitational Trillion-Body Problem

Tomoaki Ishiyama
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Keigo Nitadori
Center for Computational Science
University of Tsukuba
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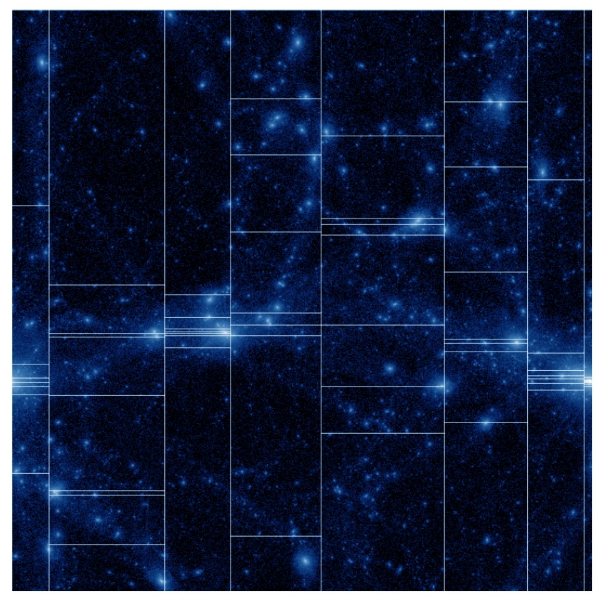
Junichiro Makino
Graduate School of Science and Engineering
Tokyo Institute of Technology
makino@geo.titech.ac.jp

IEEE/ACM supercomputing, SC12

Machine & algorithm!



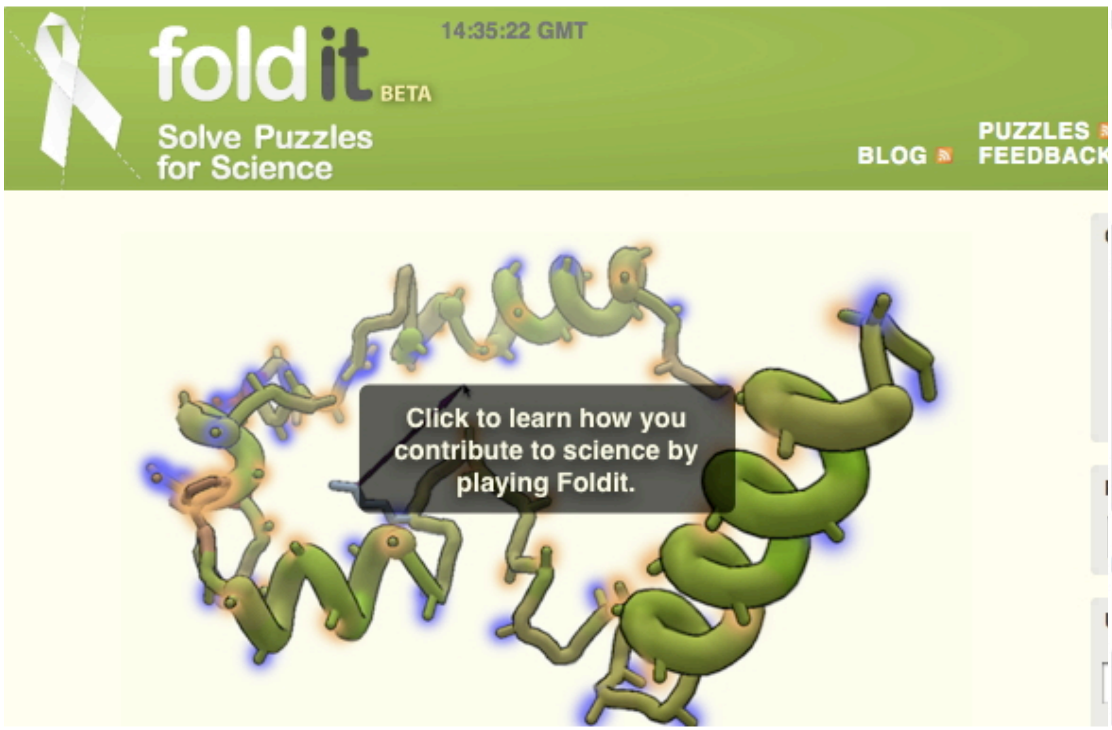
Enabling Science by Online Game

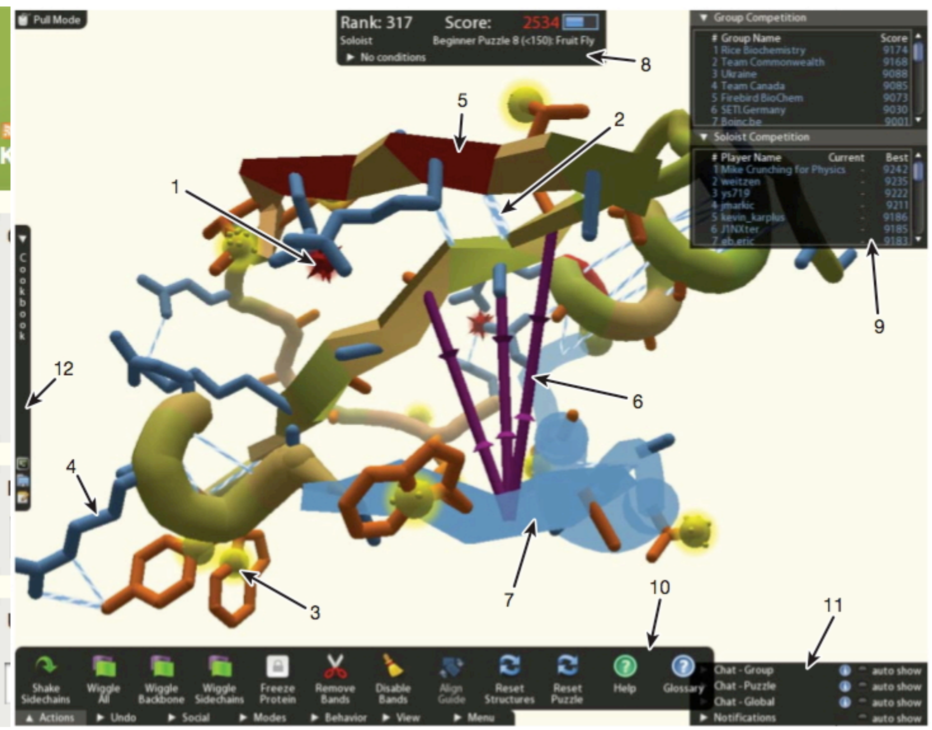
nature Vol 466 | 5 August 2010 | doi:10.1038/nature09304

LETTERS

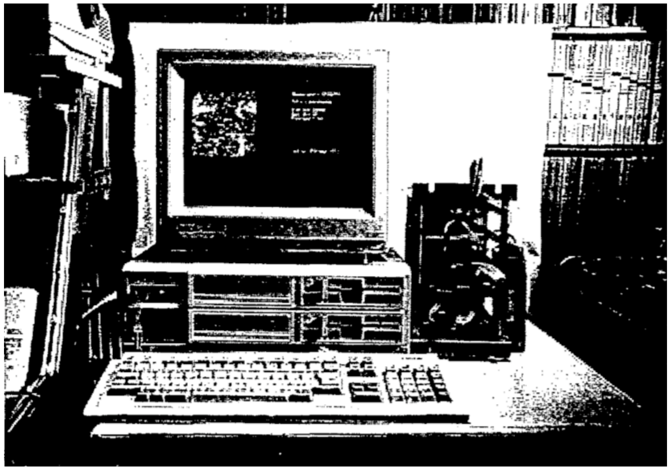
Predicting protein structures with a multiplayer online game

Seth Cooper[1], Firas Khatib[2], Adrien Treuille[1,3], Janos Barbero[1], Jeehyung Lee[3], Michael Beenen[1], Andrew Leaver-Fay[2]†, David Baker[2,4], Zoran Popović[1] & Foldit players





Ising Machine

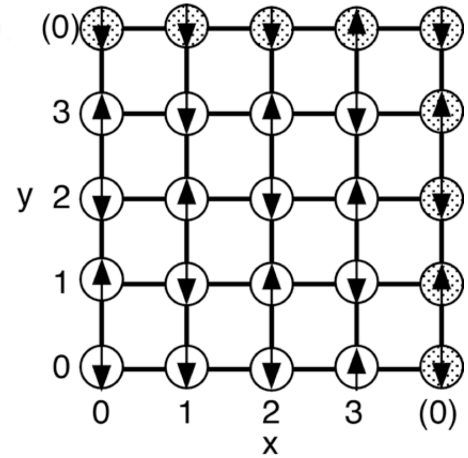


1bit の世界の専用計算機
——イジング・マシーン——

泰地　真弘人

（東京大学教養学部）

（1994年 3 月 2 日受理）



Ising Machine: A Special Purpose Computer for 1-bit Worlds

TAIJI Makoto

(Received 3 March 1994)

$$V(s^N) = -J \sum_{(k,l)} s_k s_l - H \sum_k s_k, \quad s_k = \pm 1$$

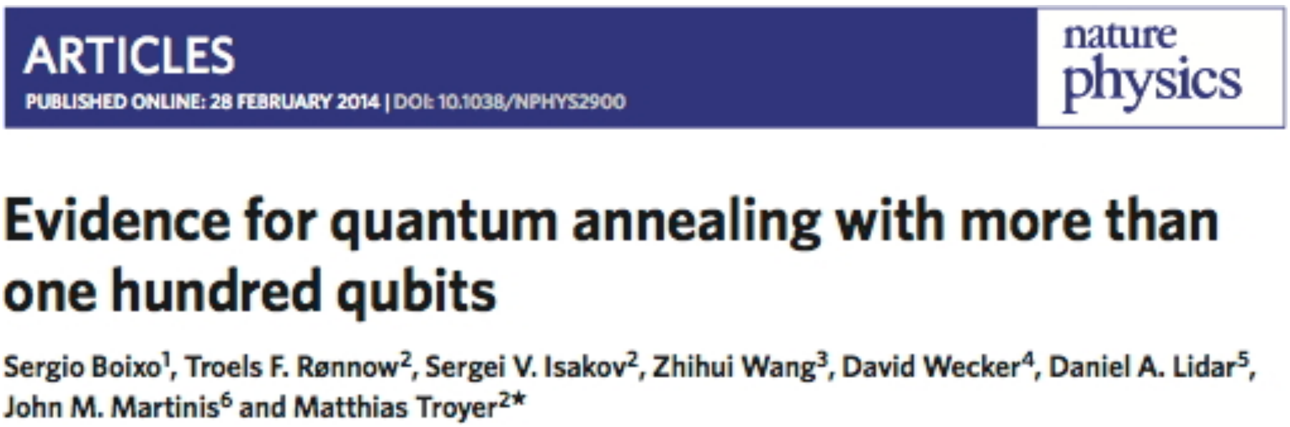
Abstract

This paper describes the development of special-purpose computer systems for Ising models, "Ising Machine" m-TIS 1 and 2. The first two sections explain Ising models and their Monte Carlo simulations. In section 3 and 4, I describe my motivation to build a special-purpose computer and the development of m-TIS 1. In section 5 and 6, the use of field-programmable gate arrays in a special-purpose computer is discussed. In the last two sections I discuss the potential abilities and future prospects of both Ising machine and a special-purpose computer in general.

J. Plasma Fusion Res. **70**, 332 ('94)

USC Quantum Computation Center

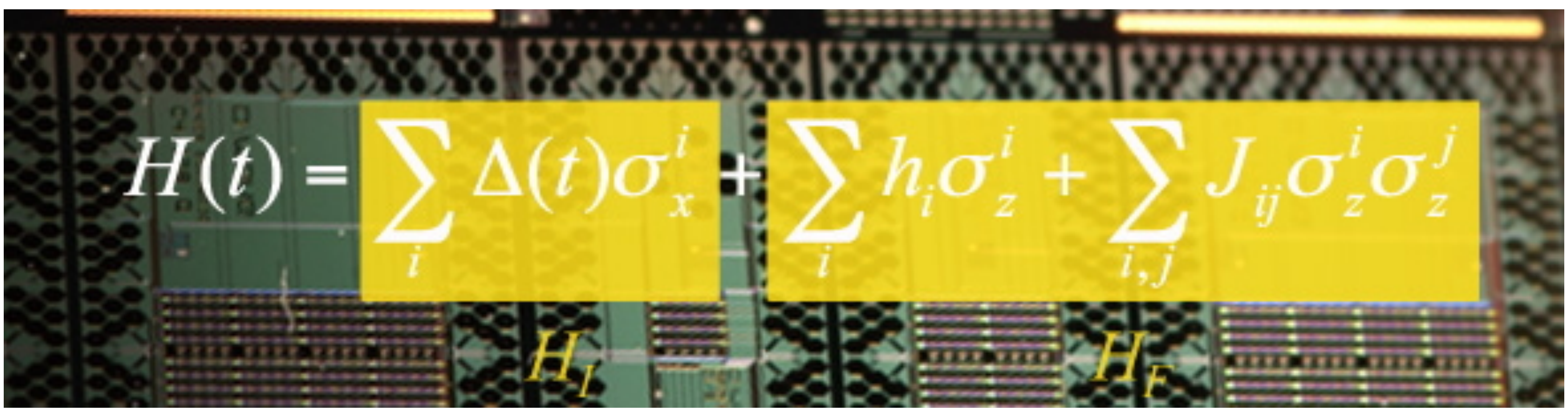
- **D-Wave One system with a 128-quantum bit (qubit) Rainier processor (*cf*. 512-bit D-Wave Two)**


ARTICLES
PUBLISHED ONLINE: 28 FEBRUARY 2014 | DOI: 10.1038/NPHYS2900
nature physics

Evidence for quantum annealing with more than one hundred qubits

Sergio Boixo[1], Troels F. Rønnow[2], Sergei V. Isakov[2], Zhihui Wang[3], David Wecker[4], Daniel A. Lidar[5], John M. Martinis[6] and Matthias Troyer[2*]

- **Adiabatic quantum optimization**



http://www.isi.edu/research_groups/quantum_computing/home

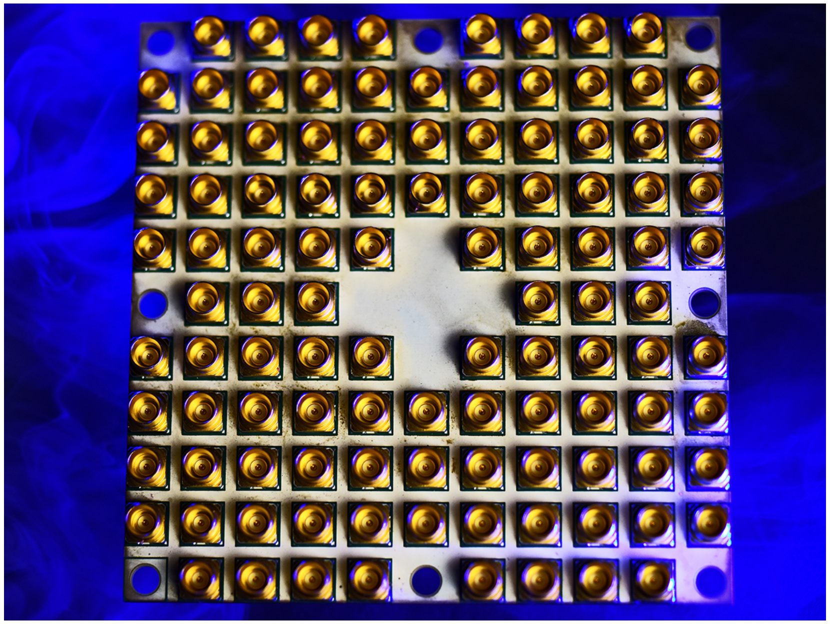
Quantum Simulation on Quantum Computer

- **Quantum computer as a universal simulator of quantum many-body systems** [R. P. Feynman, *Int. J. Theor. Phys*. **21**, 467 ('82); S. Lloyd, *Science* **273**, 1073 ('96)]
- ***Quantum parallelism*: Quantum gates operating on quantum bits (qubits) allow function evaluation for exponentially-large arguments; key = how to minimize measurements (or I/O), *cf*. distributed parallel computing**
- **Successful quantum computing for *static* simulation—ground state energy of small molecules** [A. Aspuru-Guzik *et al*., *Science* **309**, 1704 ('05)]
- **Variational eigensolver** [A. Aspuru-Guzik *et al*., *Science* **309**, 1704 ('05)] **utilizes noisy intermediate-scale quantum (NISQ) computer** [J. Preskill, *Quantum* **2**, 79 ('18)]
- **Remains a challenge to simulate quantum many-body *dynamics* on current-to-near-future NISQ computers comprised of 10-100 qubits** [H. Lamm & S. Lawrence, *Phys. Rev. Lett*. **121**, 170501 ('18)]
- **Demonstrated successful simulation of nontrivial quantum dynamics on currently-available few qubits—ultrafast control of emergent magnetism by THz radiation in atomically-thin 2D material** [L. Bassman *et al*. ('19)]
- **Volunteer to boost quantum dynamics simulation to *O*(10) qubits *via* more efficient compilation** [*cf*. E. Campbell, *Phys. Rev. Lett*. **123**, 070503 ('19)]

Intel's Future Computing

1. **Quantum computing**

49-qubit chip



2. **Neuromorphic computing**