Molecular-Dynamics Machines

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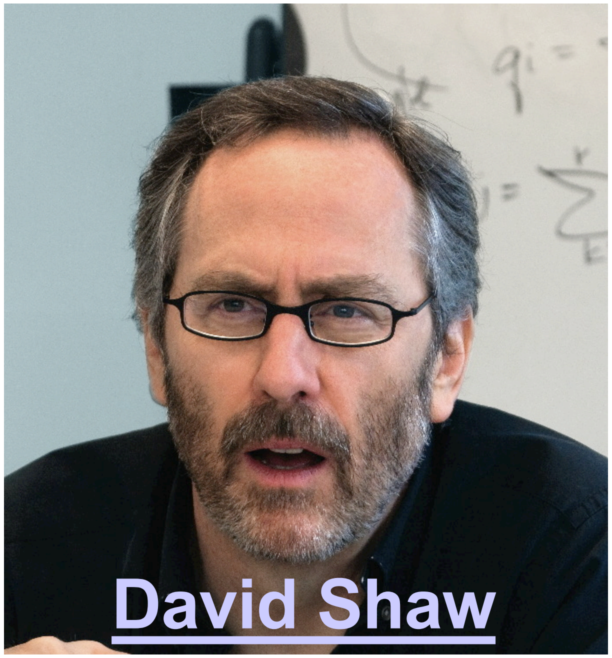
Why parallel MD? It's hot in computer science!

Anton: Computational Microscope



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

Named after Anton van Leeuwenhoek, who is often referred to as "the father of microscopy"

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

D E Shaw Research

"… 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)

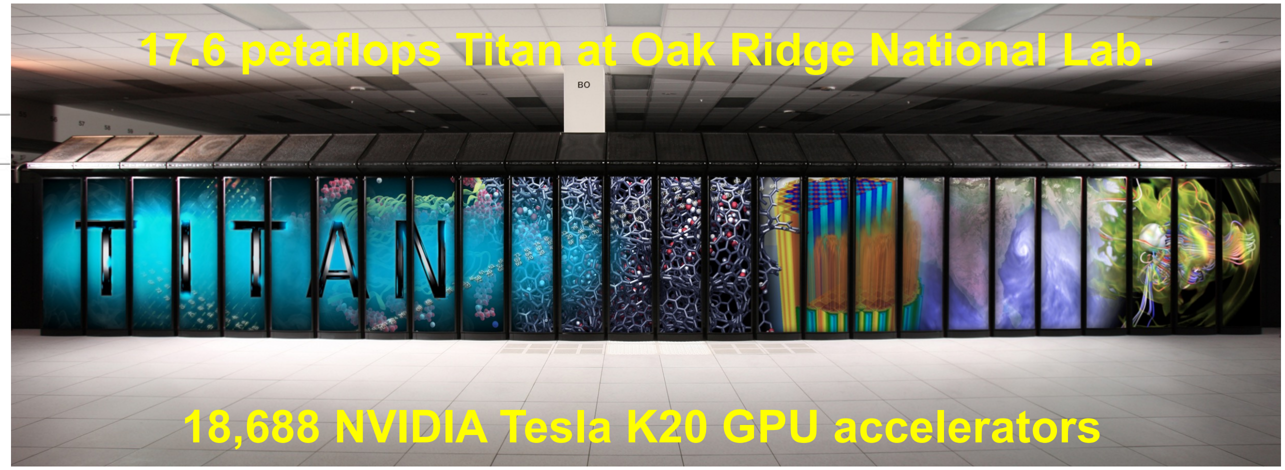
MD on GPU Clusters

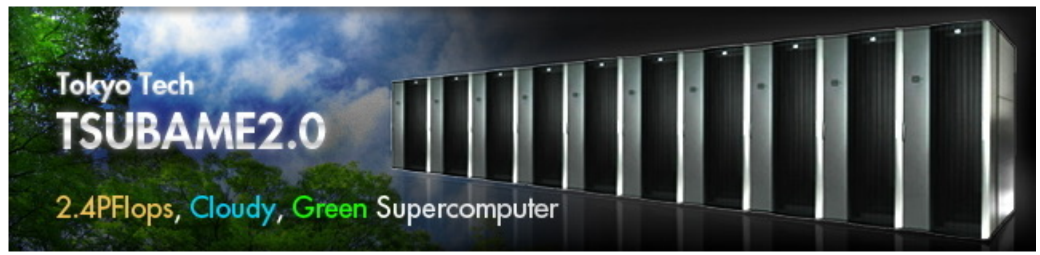
GPU acceleration and other computer performance increases will offer critical benefits to biomedical science.

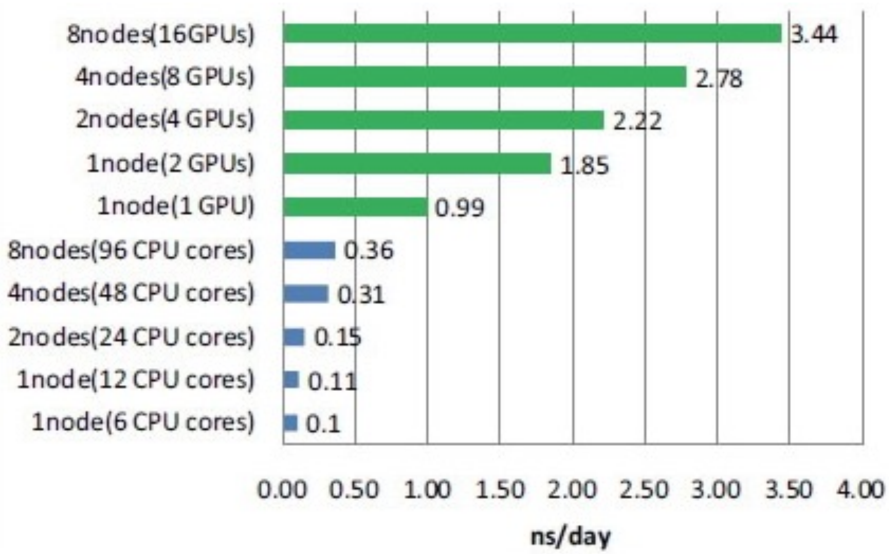
BY JAMES C. PHILLIPS AND JOHN E. STONE

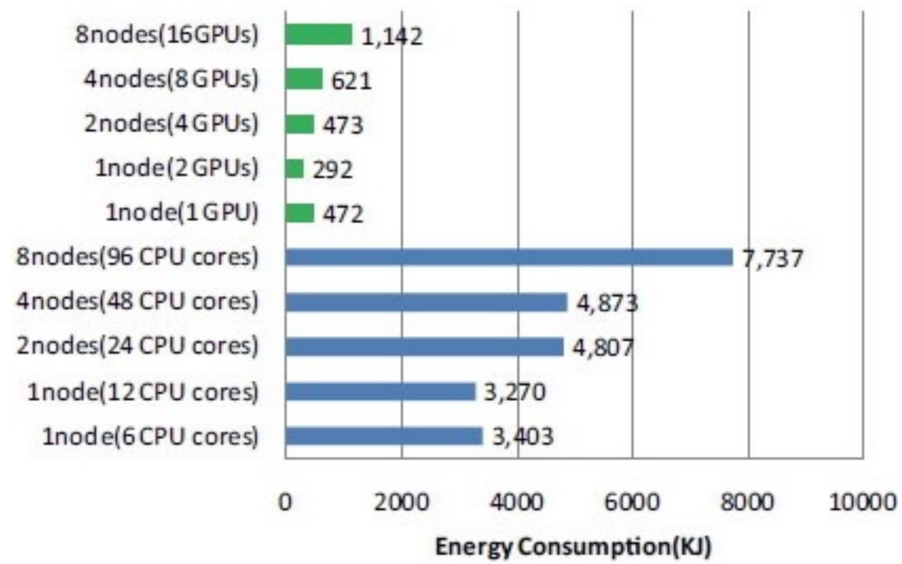
Probing Biomolecular Machines with Graphics Processors

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

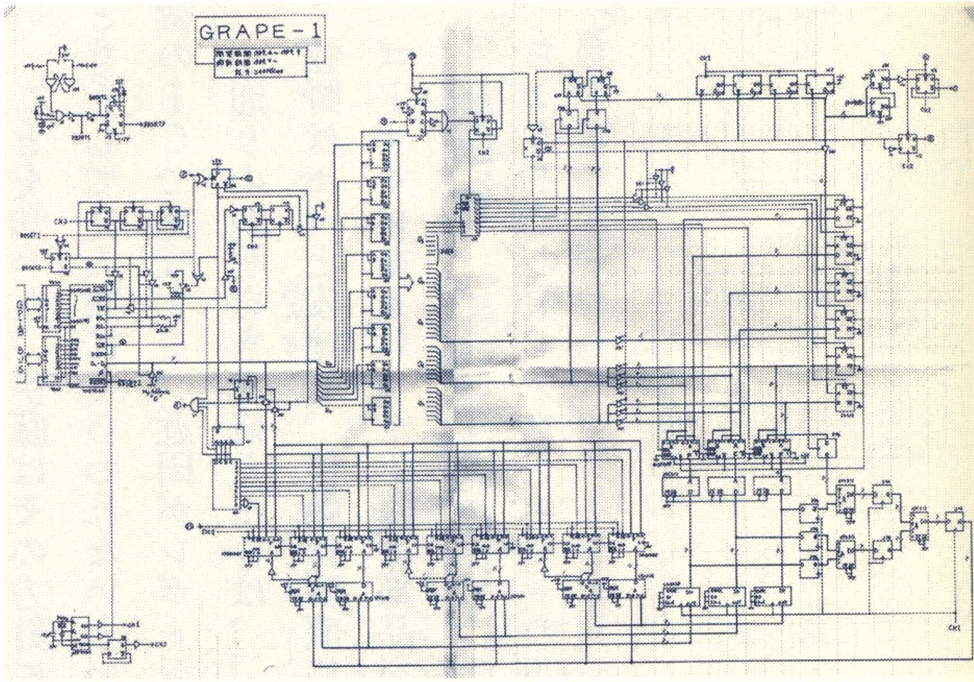


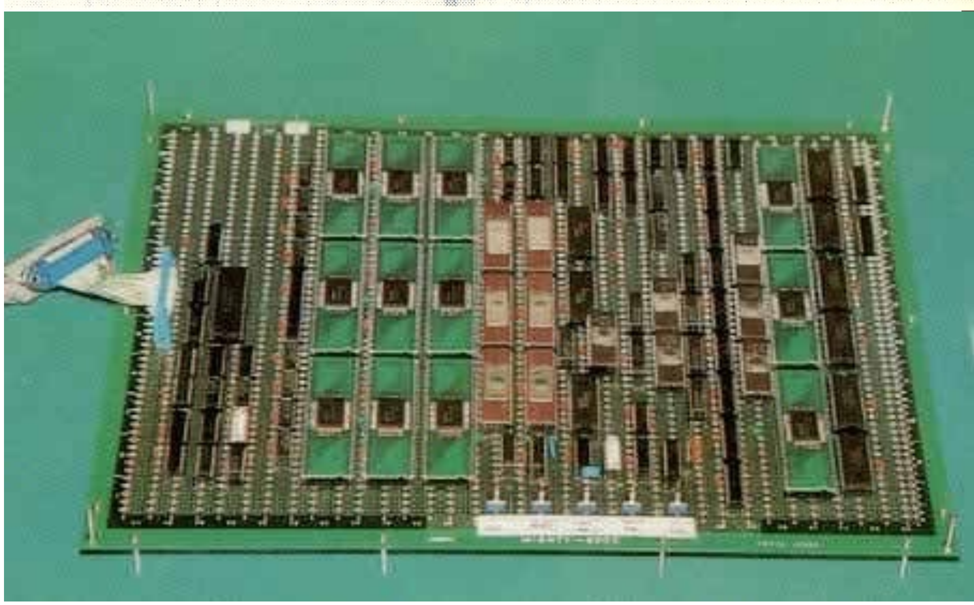






GRAPE 1 ($2K, 1989)



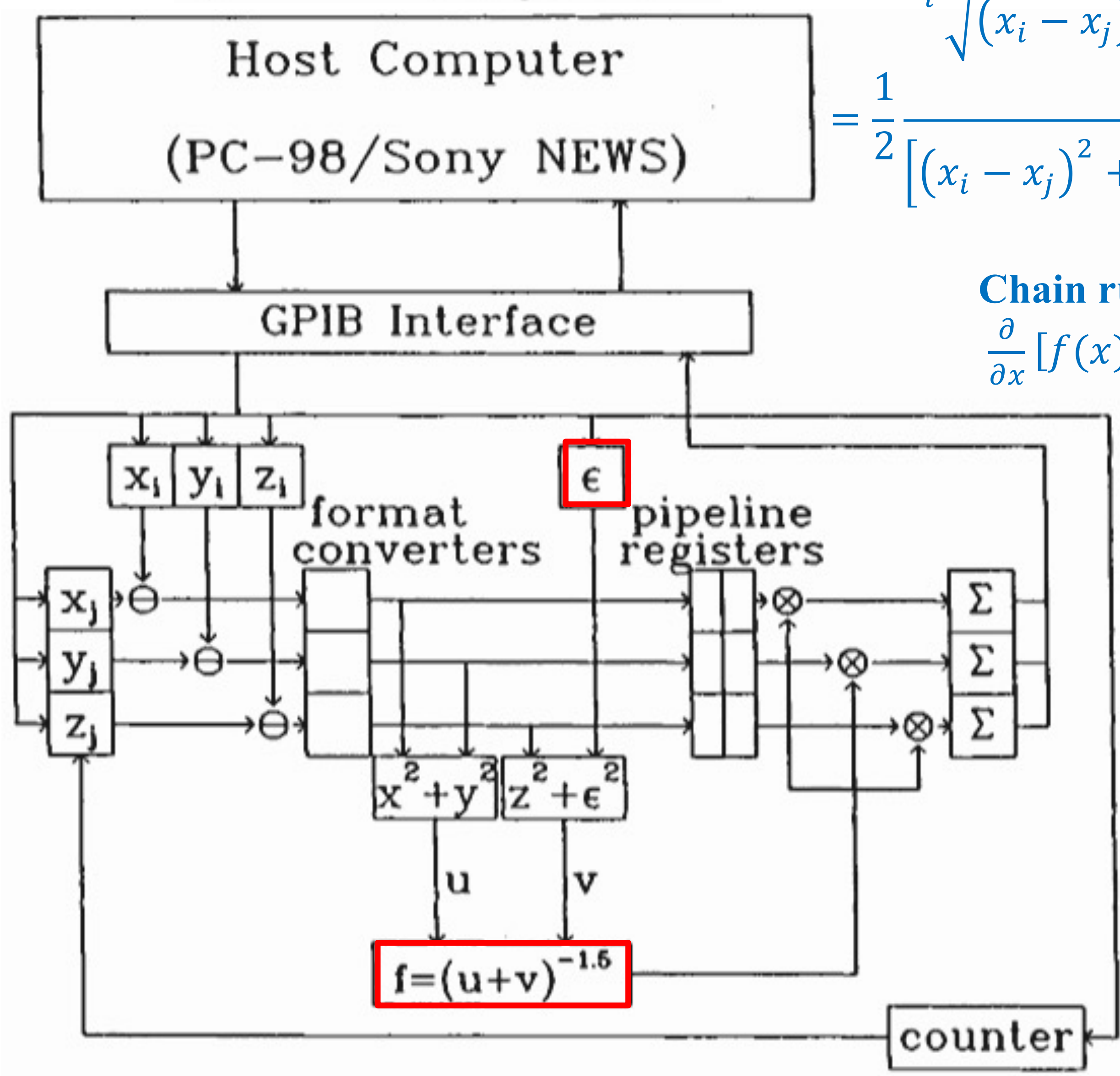


Tomoyoshi Ito & comics he authored

- **GRAPE (GRAvity PipE) = special-purpose computer 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

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



$$-\frac{\partial}{\partial x_i} \frac{1}{\sqrt{(x_i - x_j)^2 + (y_i - y_j)^2 + (y_i - y_j)^2 + \varepsilon^2}}$$

$$= \frac{1}{2} \frac{2(x_i - x_j)}{\left[(x_i - x_j)^2 + (y_i - y_j)^2 + (y_i - y_j)^2 + \varepsilon^2\right]^{3/2}}$$

Chain rule:

$$\frac{\partial}{\partial x}[f(x)]^{-1/2} = -\frac{1}{2}[f(x)]^{-3/2}\frac{\partial f}{\partial x}$$

- **Small ε to avoid if $(i \neq j)$ & pipeline stall**
- **$x^{-3/2}$ was implemented as table look-up using read-only memory (ROM)**

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

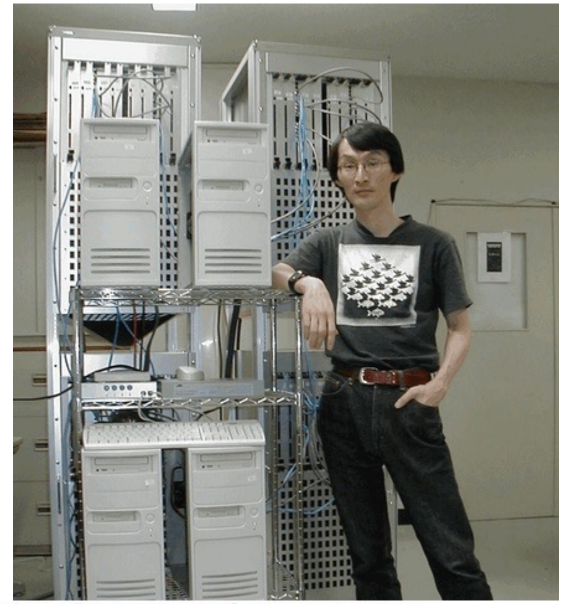
2000 Gordon Bell Prize, Winner, Peak Performance Category
A 1.349 Tflops simulation of black holes in a galactic center on GRAPE-6

Junichiro Makino, Toshiyuki Fukushige, Masaki Koga

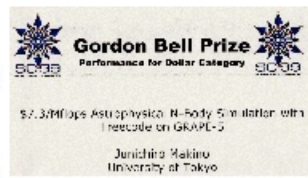
2000 Gordon Bell Prize, Winner, Peak Performance Category (tie with above)
1.34 Tflops Molecular Dynamic simulation for NaCl with a Special Purpose Computer: MDM
(MD-GRAPE system)

Tetsu Narumi, Ryutaro Susukita, Takahiro Koishi, Kenji Yasuoka, Hideaki Furusawa, Atsushi Kawai, Toshikazu Ebisuzaki

Gordon Bell Prize, commonly referred to as the Nobel Prize of Supercomputing [Wikipedia].



J. Makino & Grape 6 (2001)



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

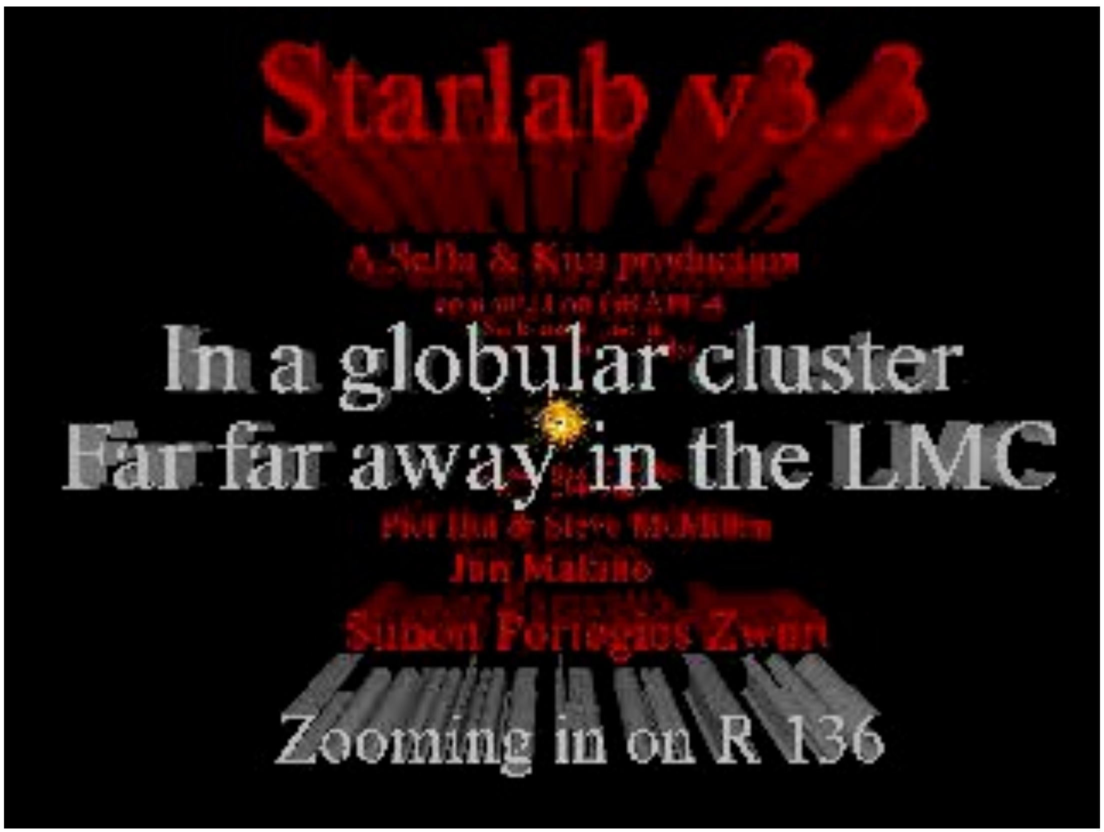
www.green500.org (Nov. '10)

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



In Univ. of Tokyo, computer science started as part of physics department (not math or CS)

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

CPC homepage

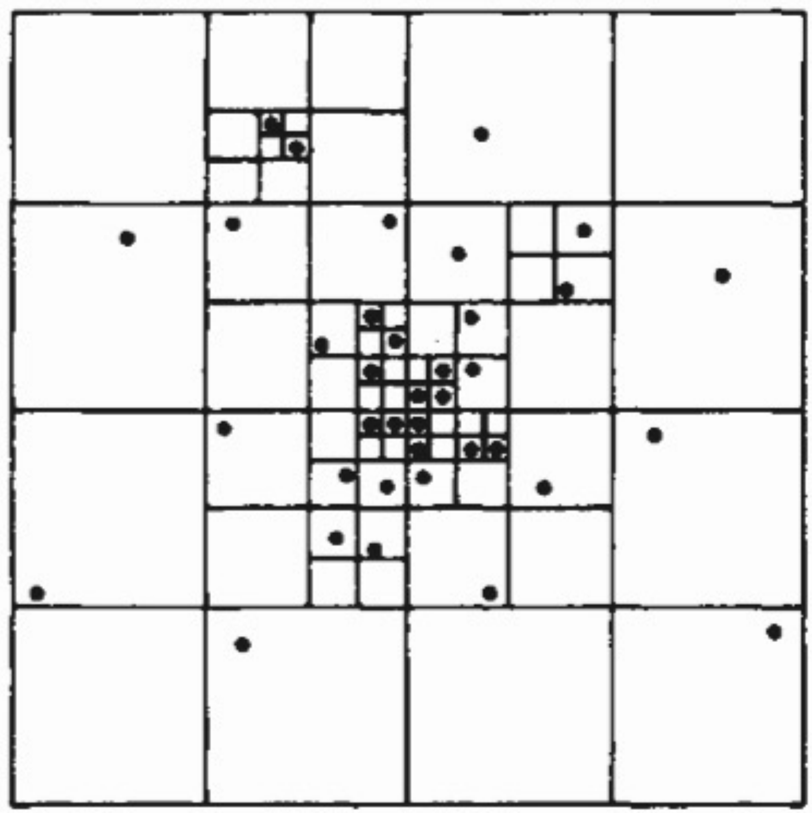
Submit your first paper to *CPC*!

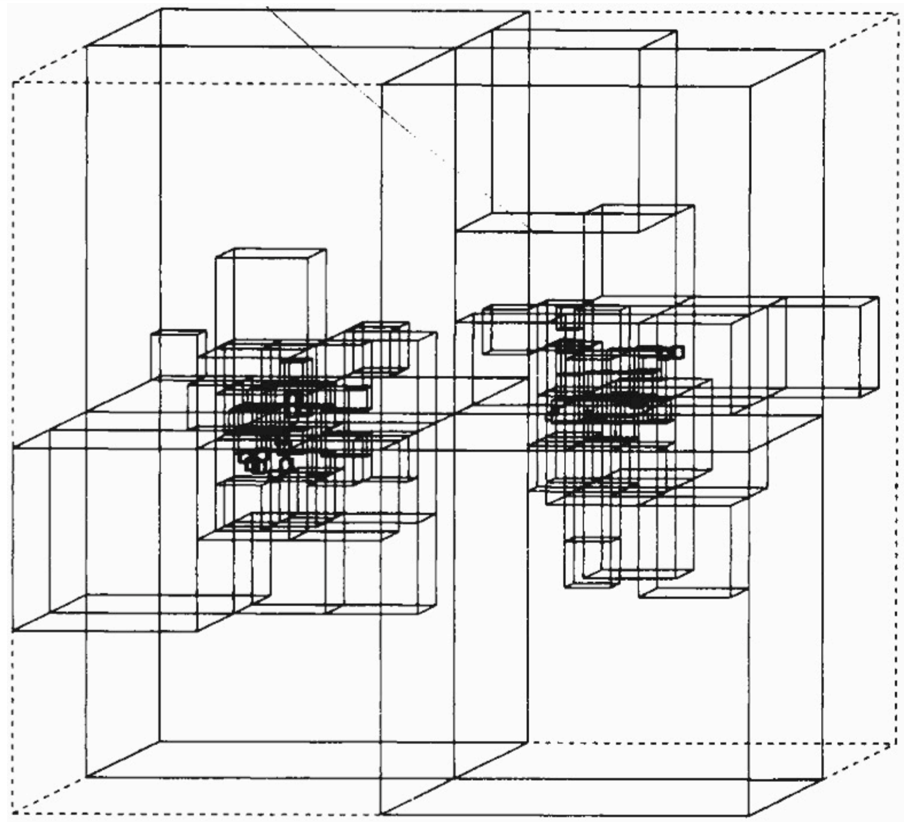
Enabling Science by Algorithm

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/

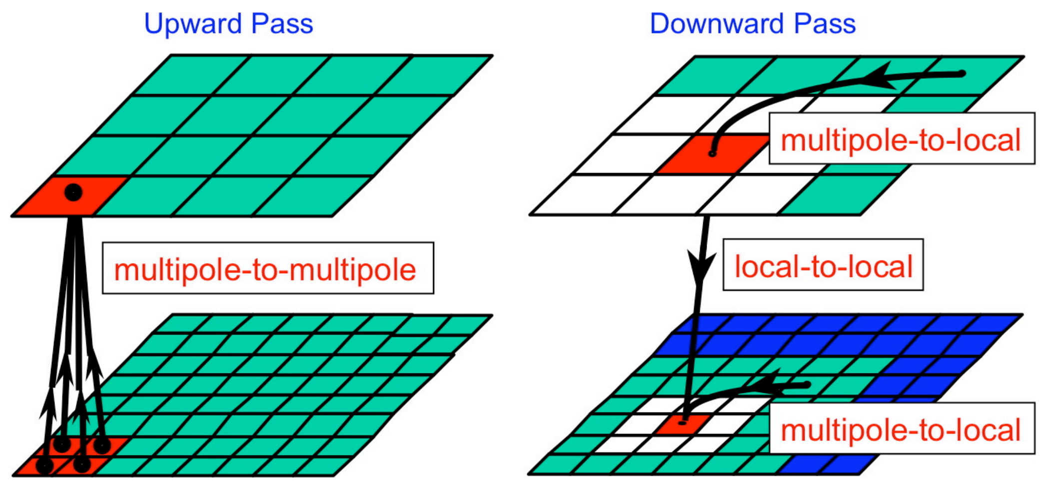
LESLIE GREENGARD

Doctoral Dissertation Award

United States – 1987

CITATION

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



See lecture notes at https://aiichironakano.github.io/cs653.html

A Small Step in Parallel MD

VOLUME 71, NUMBER 1 PHYSICAL REVIEW LETTERS 5 JULY 1993

Structural Correlations in Porous Silica: Molecular Dynamics Simulation on a Parallel Computer

Aiichiro Nakano, Lingsong Bi, Rajiv K. Kalia, and Priya Vashishta

Concurrent Computing Laboratory for Materials Simulations, Department of Physics and Astronomy, Department of Computer Science, Louisiana State University, Baton Route, Louisiana 70803-4001

(Received 9 November 1992; revised manuscript received 2 April 1993)

Molecular dynamics simulations of porous silica in the density range 2.2–0.1 g/cm^3 are carried out on a 41 472 particle system using a multiple instruction multiple data computer. The internal surface area, pore surface-to-volume ratio, pore size distribution fractal dimension, correlation length, and mean particle size are determined as a function of the density. Structural transition between a condensed amorphous phase and a low-density porous phase is characterized by these quantities. Various dissimilar porous structures with different fractal dimensions are obtained by controlling the preparation schedule and temperature.

This work was supported by the U.S. Department of Energy, Office of Energy Research, Basic Energy Science, Materials Science Division, Grant No. DE-FG05-92ER45477. The computations were performed using the eight-node iPSC/860 in the Concurrent Computing Laboratory for Materials Simulations (CCLMS) at Louisiana State University. The facilities in the CCLMS were acquired with the Equipment Enhancement Grants awarded by the Louisiana Board of Regents through Louisiana

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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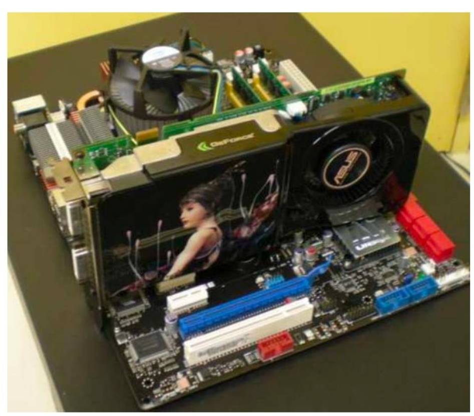
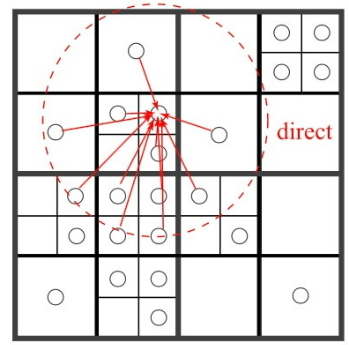
2009 Gordon Bell Prize
Price/Performance Category

Table 2: Price of the GPU cluster

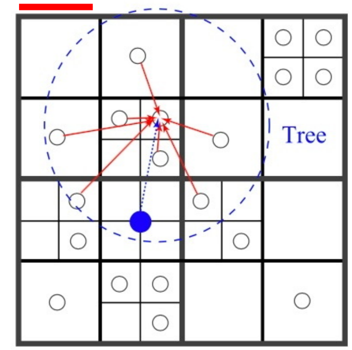
Elements	Quantity	Price (JPY)	Price ($)
GPUs	256	12,160,000	$ 118,345
Host PCs	128	10,716,032	$ 104,292
Network switch	4	644,800	$ 6,275
Total		**23,520,832**	**$ 228,912**



P^{3}M



TreePM



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

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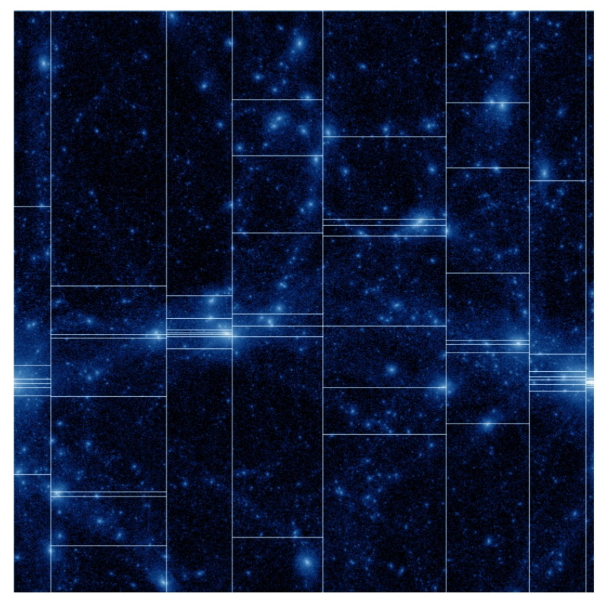
makino@geo.titech.ac.jp

IEEE/ACM supercomputing, SC12

Machine & algorithm!

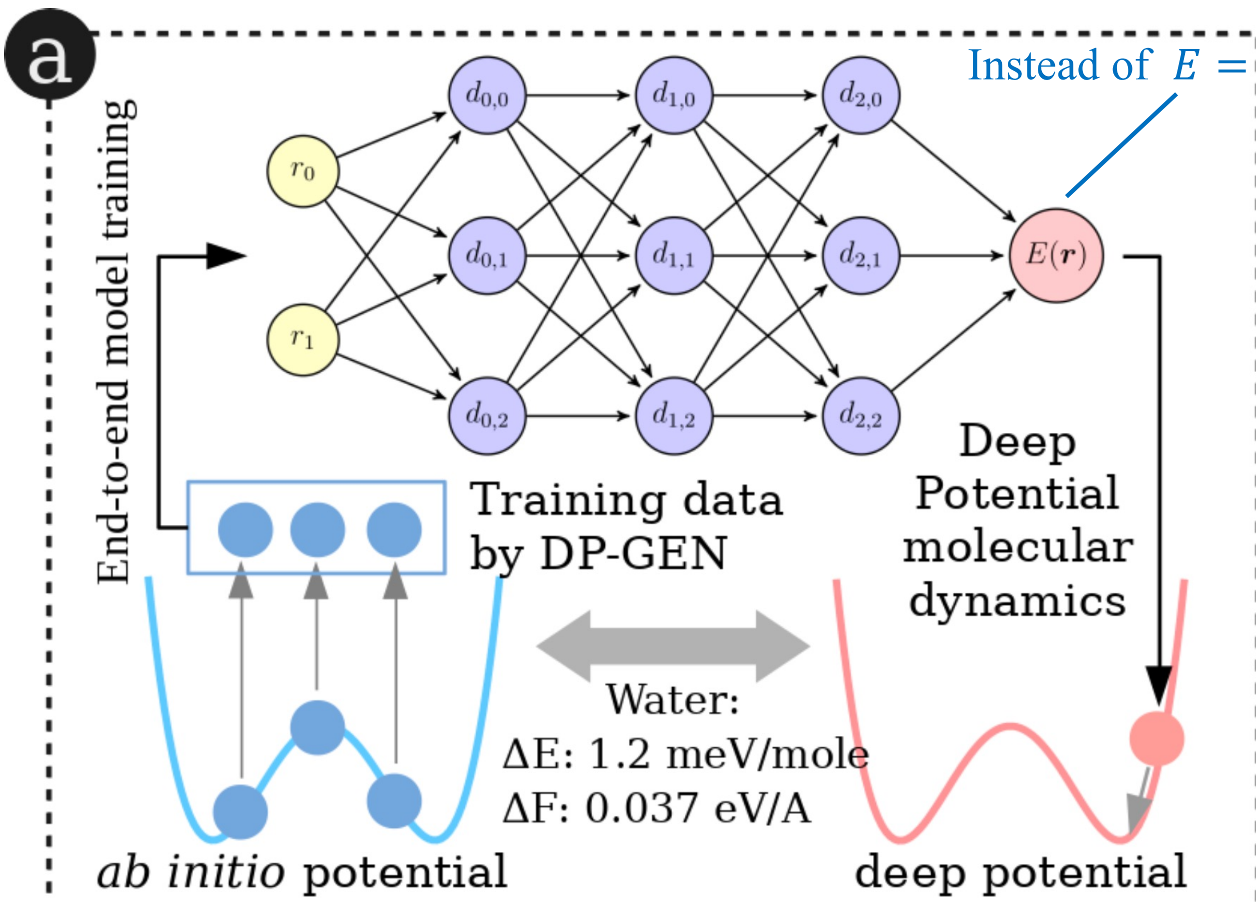


Now It's Deep MD

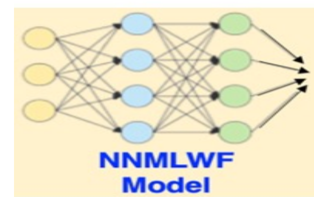
Pushing the limit of molecular dynamics with ab initio accuracy to 100 million atoms with machine learning

Weile Jia, Han Wang, Mohan Chen, Denghui Lu, Jiduan Liu, Lin Lin, Roberto Car, Weinan E, Linfeng Zhang

Proc. Supercomputing, SC20, Gordon Bell prize

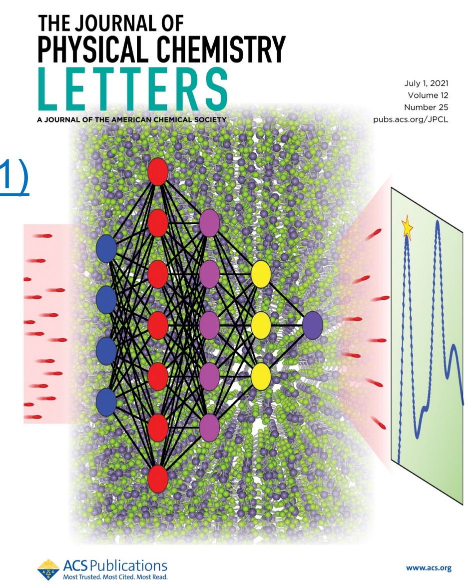


Instead of $E = \sum_{i<j} 4\varepsilon \left[\left(\frac{\sigma}{r_{ij}} \right)^{12} - \left(\frac{\sigma}{r_{ij}} \right)^{6} \right]$



Phys. Rev. Lett. **126**, 216403 ('21)

J. Phys. Chem. Lett. **12**, 6020 ('21)



https://aiichironakano.github.io/cs596/Jia-DeePMD-SC20.pdf

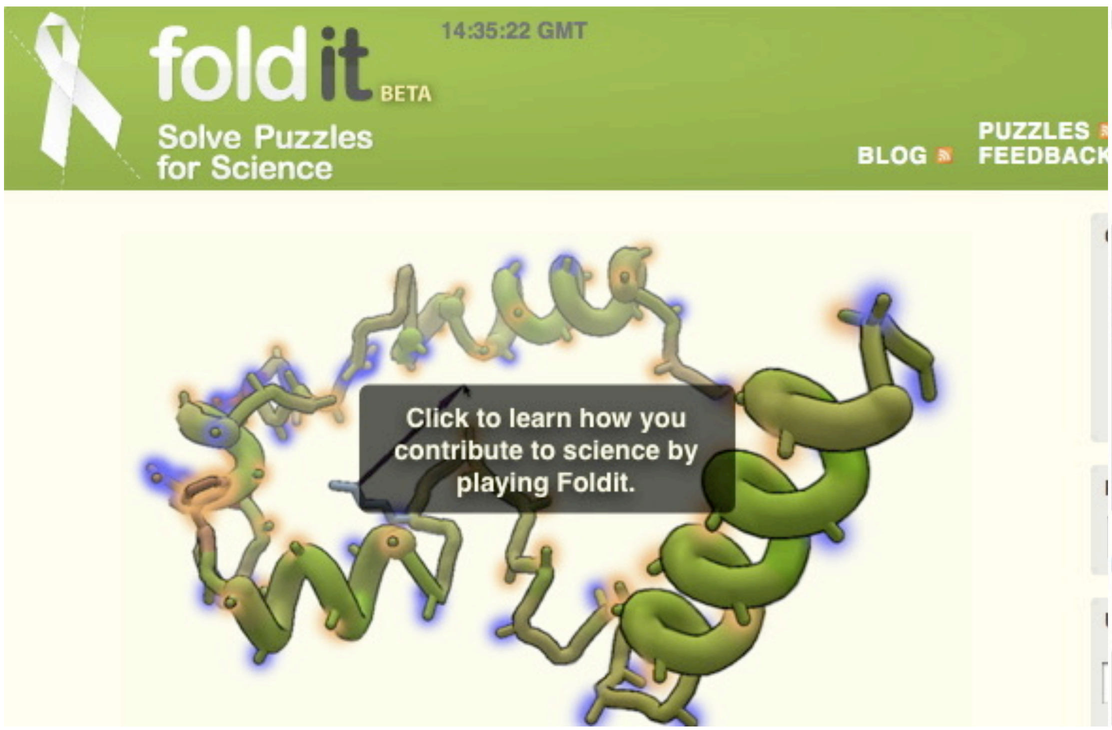
Enabling Science by Online Game

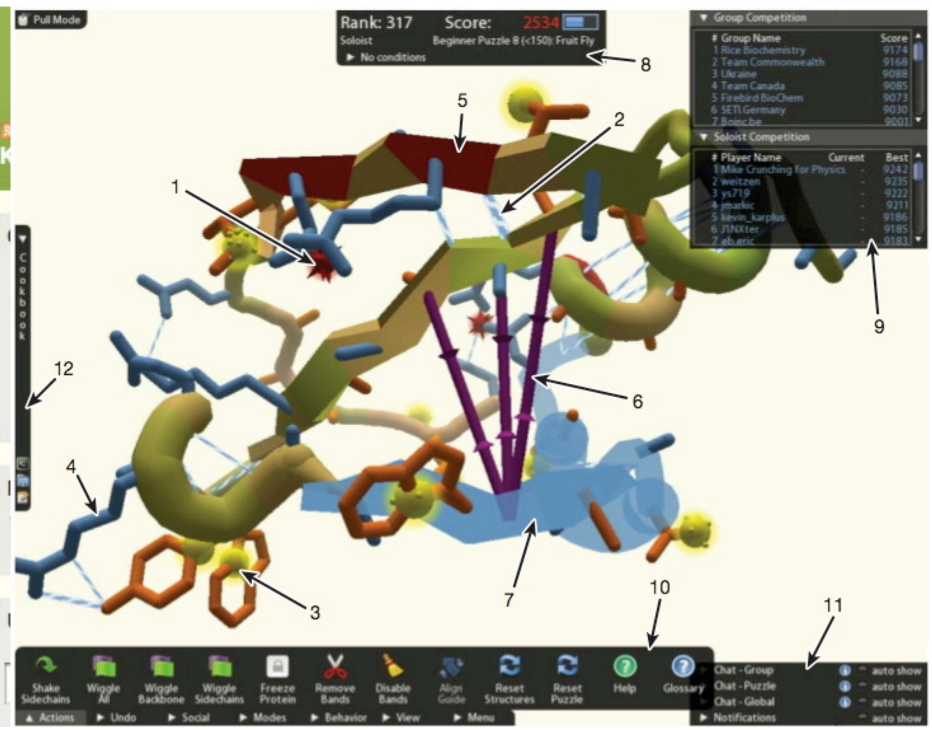
nature Vol 466 | 5 August 2010 | doi:10.1038/nature09304

LETTERS

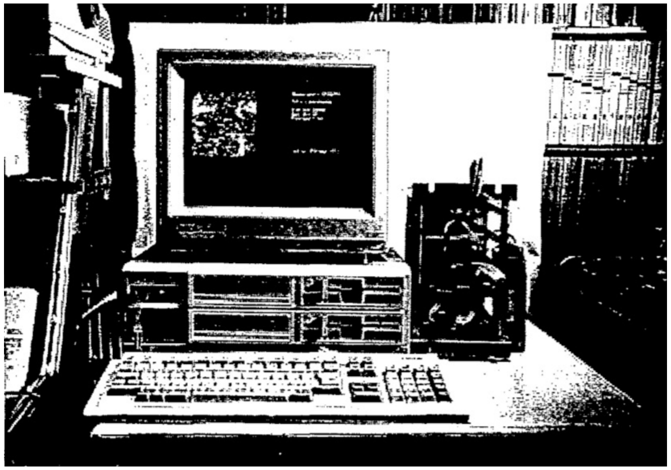
Predicting protein structures with a multiplayer online game

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

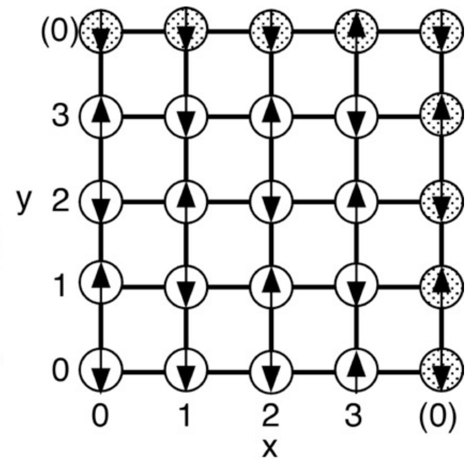
——イジング・マシーン——

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

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)

https://aiichironakano.github.io/phys516-lecture.html

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)

cf. **Original GRAPE was a 48-bit machine**

USC Quantum Computation Center

- **D-Wave 2X system with 1,098-quantum bits (qubits)**

Phase transitions in a programmable quantum spin glass simulator

R. Harris[1*], Y. Sato[1], A. J. Berkley[1], M. Reis[1], F. Altomare[1], M. H. Amin[1,2], K. Boothby[1], P. Bunyk[1], C. Deng[1], C. Enderud[1], S. Huang[1], E. Hoskinson[1], M. W. Johnson[1], E. Ladizinsky[1], N. Ladizinsky[1], T. Lanting[1], R. Li[1], T. Medina[1], R. Molavi[1,3], R. Neufeld[1], T. Oh[1], I. Pavlov[1], I. Perminov[1], G. Poulin-Lamarre[1], C. Rich[1], A. Smirnov[1], L. Swenson[1], N. Tsai[1], M. Volkmann[1], J. Whittaker[1], J. Yao[1]

Harris *et al.*, *Science* **361**, 162–165 (2018) 13 July 2018

- **Adiabatic quantum optimization**

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

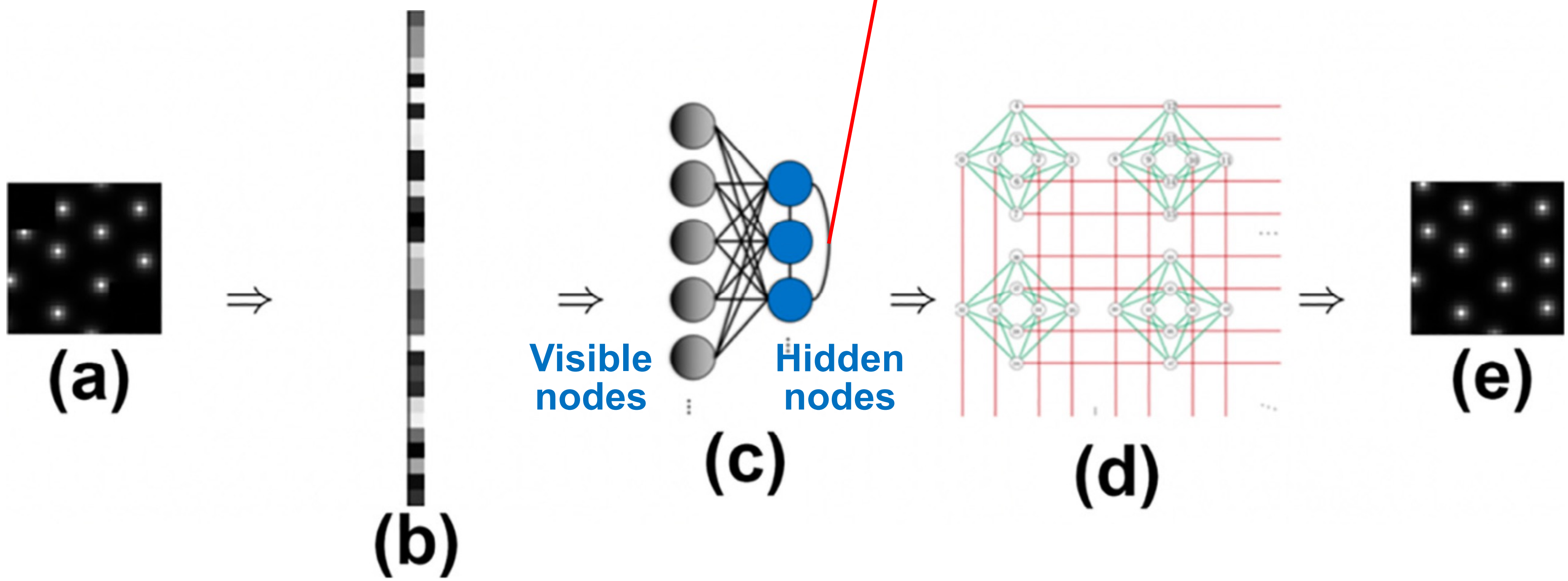
Machine Learning on D-Wave

Boltzmann machine modeling of layered MoS_2 synthesis on a quantum annealer

J. Liu, A. Mohan, R. K. Kalia, A. Nakano, K. Nomura, P. Vashishta, and K.T. Yao

Comput. Mater. Sci. **173**, 109429 ('20)

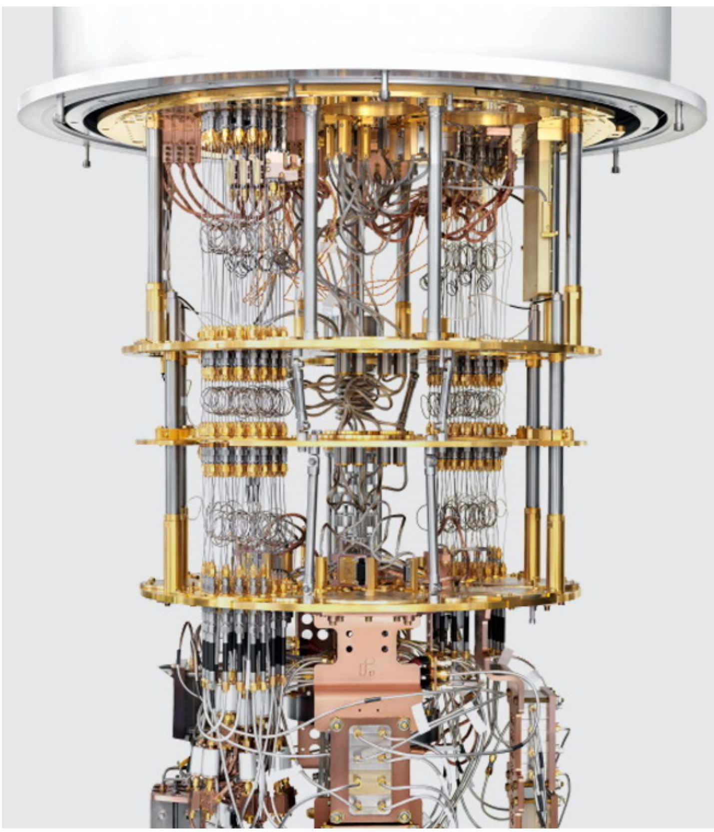
- **Computing power of D-Wave allows unrestricted Boltzmann Machine to enhance machine learning performance**



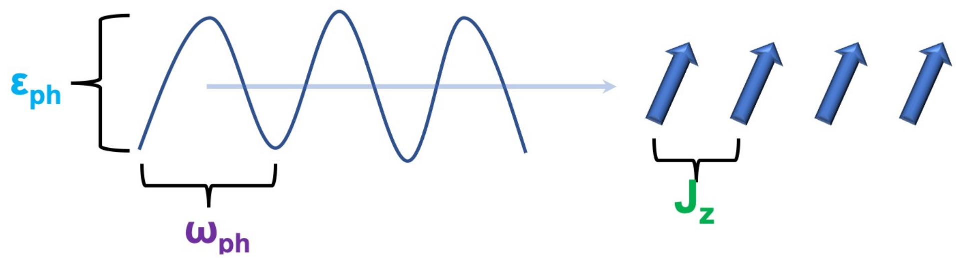
Final project by Ankith Mohan (MSCS) with Jeremy Liu (PhD-CS)

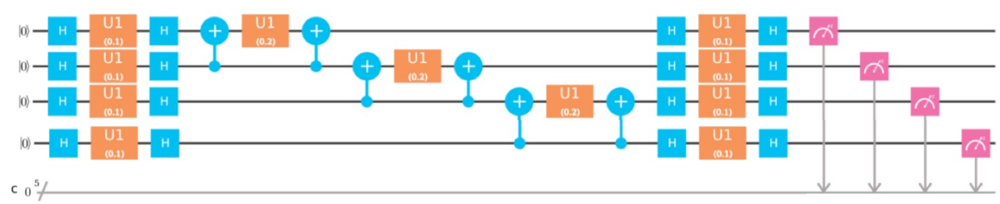
Quantum Computational Science

- **Quantum computing for science: *Universal simulator of quantum many-body systems*** [R. P. Feynman, *Int. J. Theo. Phys.* **21**, 467 ('82); S. Lloyd, *Science* **273**, 1073 ('96)]
- **Successfully simulated quantum many-body dynamics on publicly-available IBM's Q16 Melbourne & Rigetti's Aspen quantum computers** [L. Bassman *et al.*, *Phys. Rev. B* **101**, 184305 ('20)]
- **AI-inspired domain-specific quantum compiler has reduced the circuit size by 30% below that by the vendor's native compiler** [L. Bassman *et al.*, *Quant. Sci. Tech.* **6**, 014007 ('21)]



$$H(t) = -J_z \sum_{i=1}^{N-1} \boldsymbol{\sigma}_z^i \boldsymbol{\sigma}_z^{i+1} - \varepsilon_{ph} \sin(\omega_{ph} t) \sum_{i=1}^{N} \boldsymbol{\sigma}_x^i$$






```
    #define the two non-commuting terms that comprise the Hamiltonian
    Hz = PauliTerm("Z", 0, epsilon_0)
    Hy = PauliTerm("Y", 0, epsilon_ph*np.sin(w_ph*t))
    #exponentiate the terms of the Hamiltonian for use in Trotter approx
    exp_Hz = exponential_map(Hz)(delta_t/(2.0*hbar))
    exp_Hy = exponential_map(Hy)(delta_t/hbar)
```