

# Molecular-Dynamics Machines

---

---

Aiichiro Nakano

*Collaboratory for Advanced Computing & Simulations*

*Department of Computer Science*

*Department of Physics & Astronomy*

*Department of Chemical Engineering & Materials Science*

*Department of Biological Sciences*

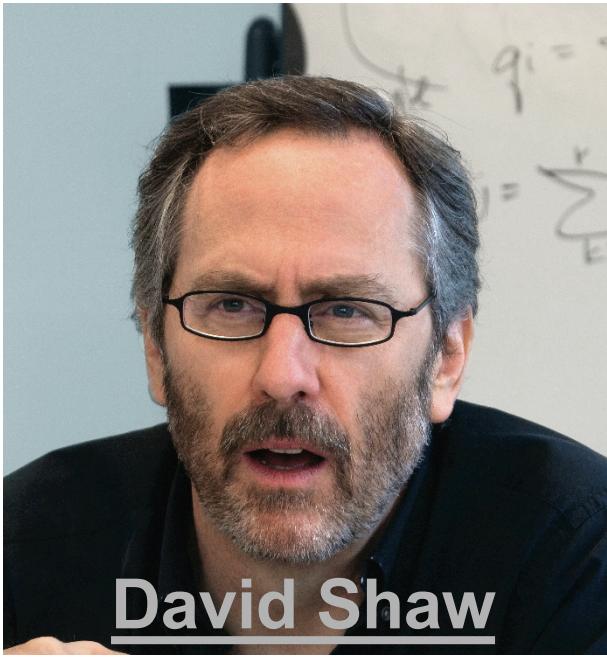
*University of Southern California*

Email: [anakano@usc.edu](mailto:anakano@usc.edu)

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



# Anton: Computational Microscope



David Shaw

“... 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”

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

16  $\mu$ s/day simulation on 512 nodes  
(5  $\mu$ s/step execution time)



D E Shaw Research

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

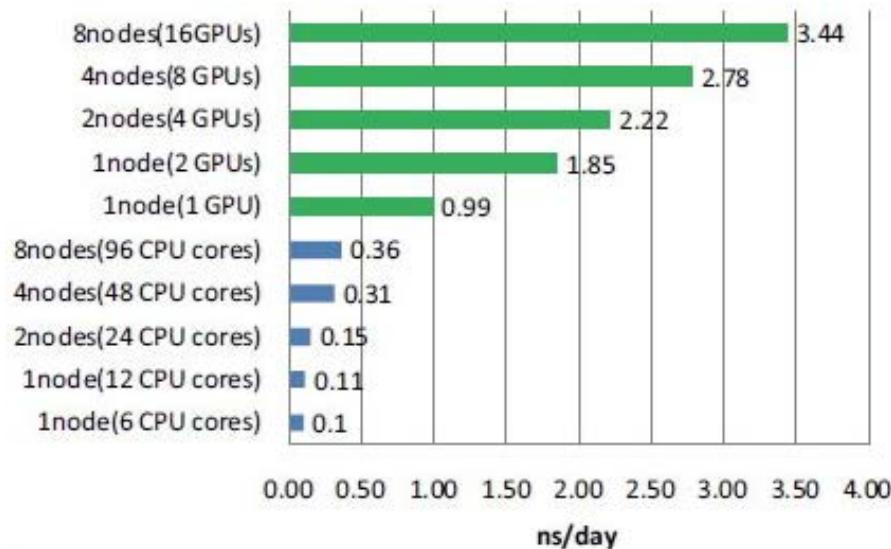
# MD on GPU Clusters

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

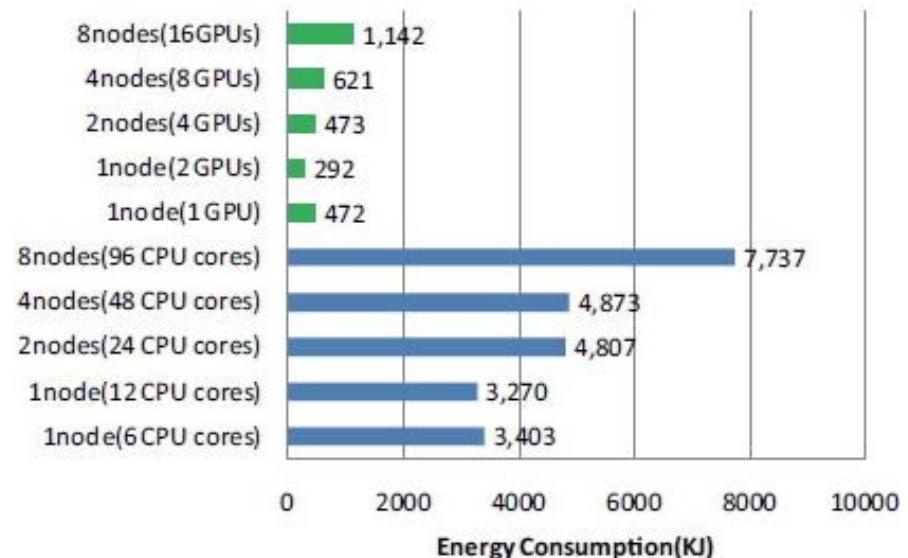
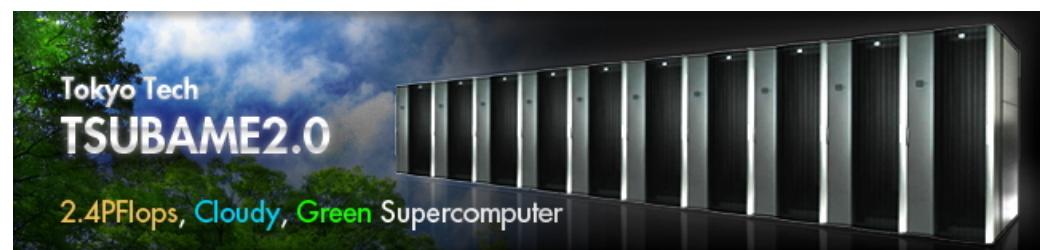
BY JAMES C. PHILLIPS AND JOHN E. STONE

## Probing Biomolecular Machines with Graphics Processors

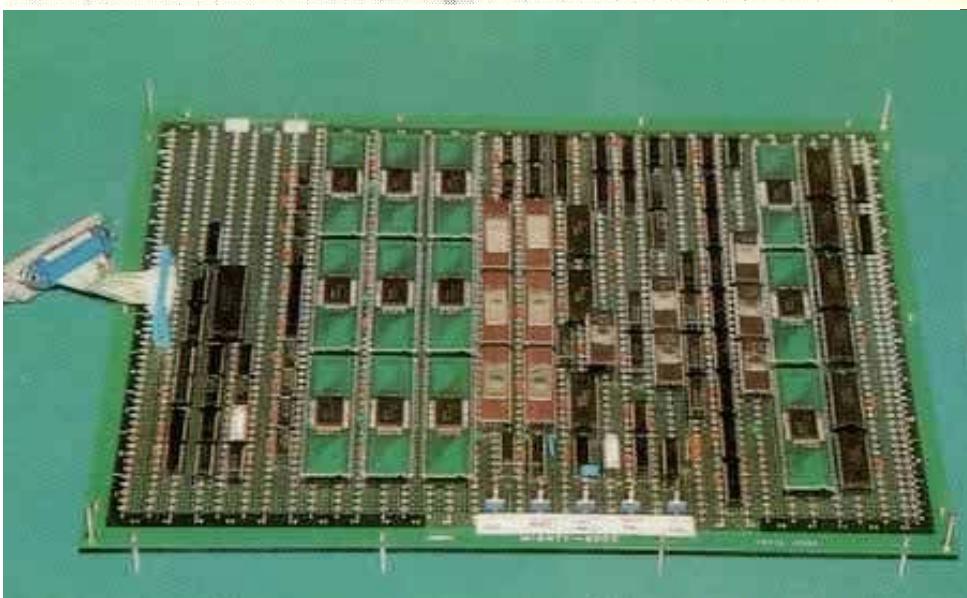
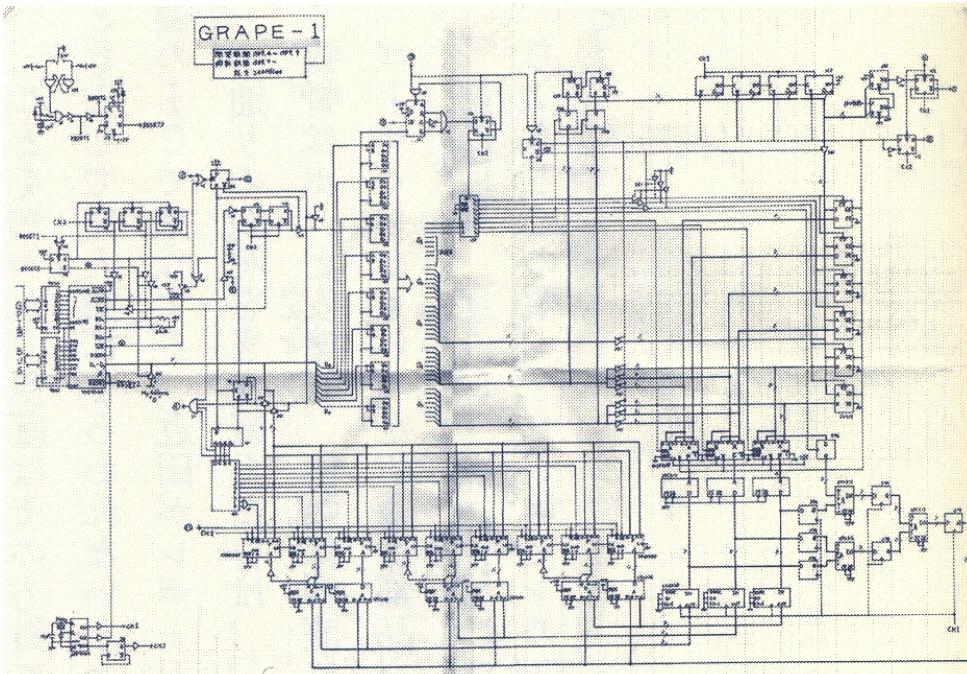
CACM 52(10), 34 ('09)



17.6 petaflops Titan at Oak Ridge National Lab.  
18,688 NVIDIA Tesla K20 GPU accelerators



# GRAPE 1 (\$2K, 1989)

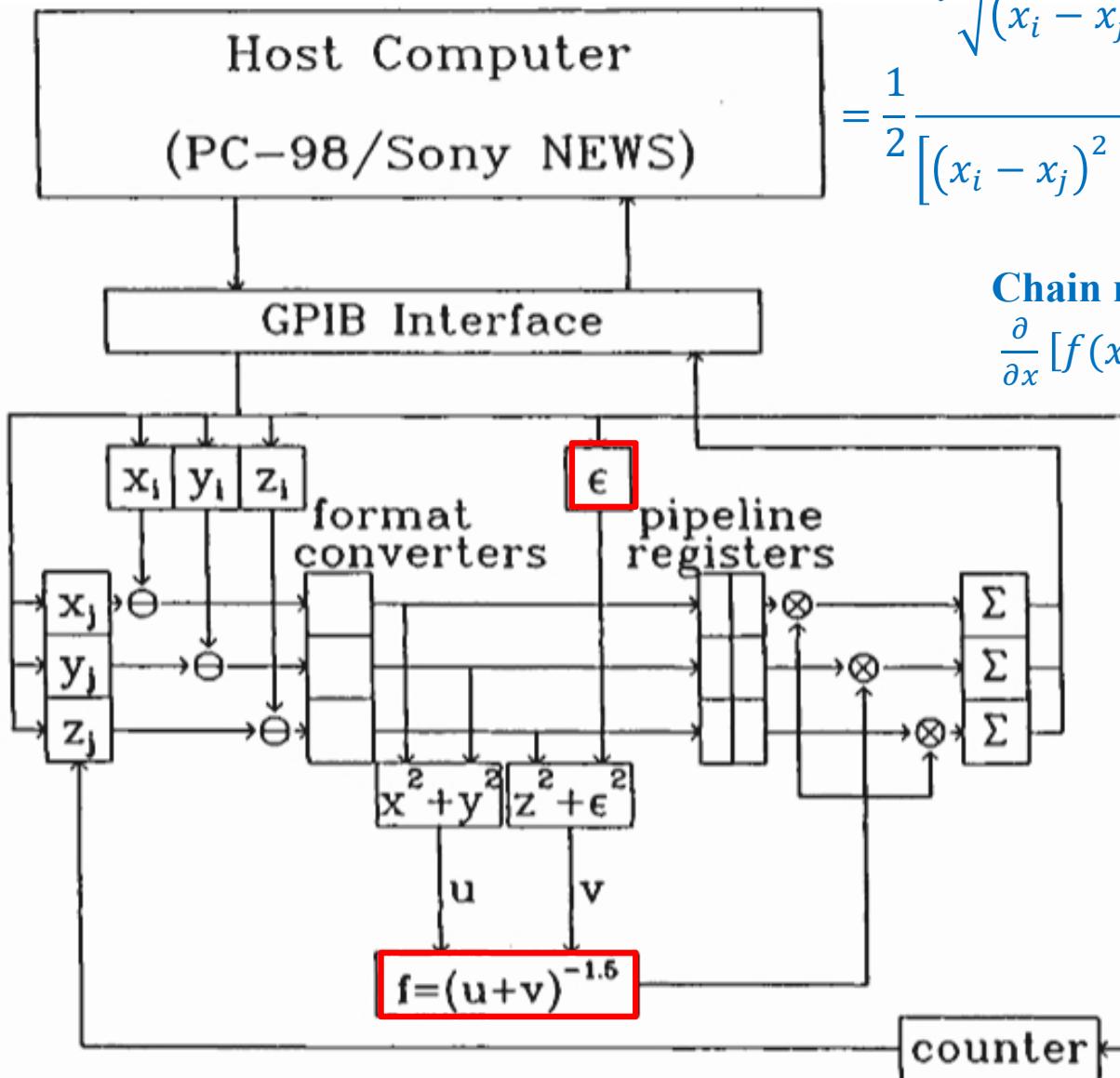


Tomoyoshi Ito & comics he authored

- **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

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



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

Chain rule:

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

- Small  $\varepsilon$  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

**SC2003 Gordon Bell Award**  
**Junichiro Makino**  
 University of Tokyo  
 Performance Evaluation and Tuning of GRAPE-6—Towards 40 "Real" Tflop/s

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

**SC2001**  
**GORDON BELL PRIZE**  
**Junichiro Makino**  
 Winner, Peak Performance  
 A 11.55 Tflops Simulation of Black Holes in a Galactic Center on GRAPE-6

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

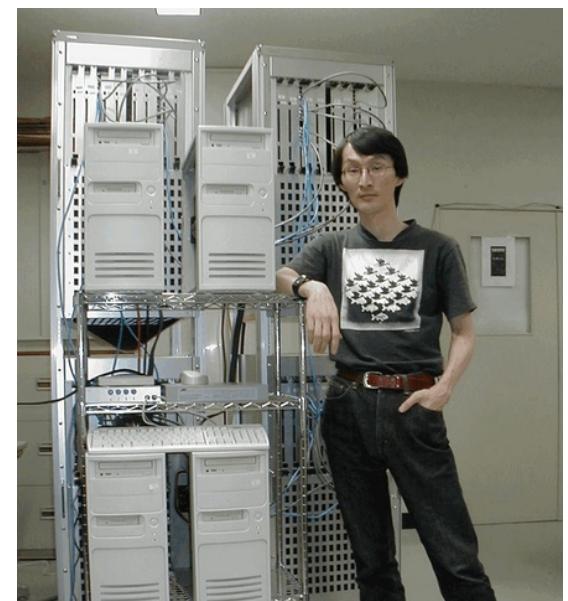
**SC2000**  
**GORDON BELL PRIZE**  
**Junichiro Makino**  
 Winner, Peak Performance Category  
 A 1.349 Tflops simulation of black holes in a galactic center on GRAPE-6

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

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

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



\$7.3Mflops Astrophysical N-Body Simulator with a netcode on GRAPE-6

Junichiro Makino  
 University of Tokyo

1999 Gordon Bell Prize, Price Performance, First Prize  
 Astrophysical N-body simulation  
 144 Glops / \$ 1 M on custom-built GRAPE-5 32-processor system

Atsushi Kawai, Toshiyuki Fukushige, and Junichiro Makino

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



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

# Enabling Science by Hardware

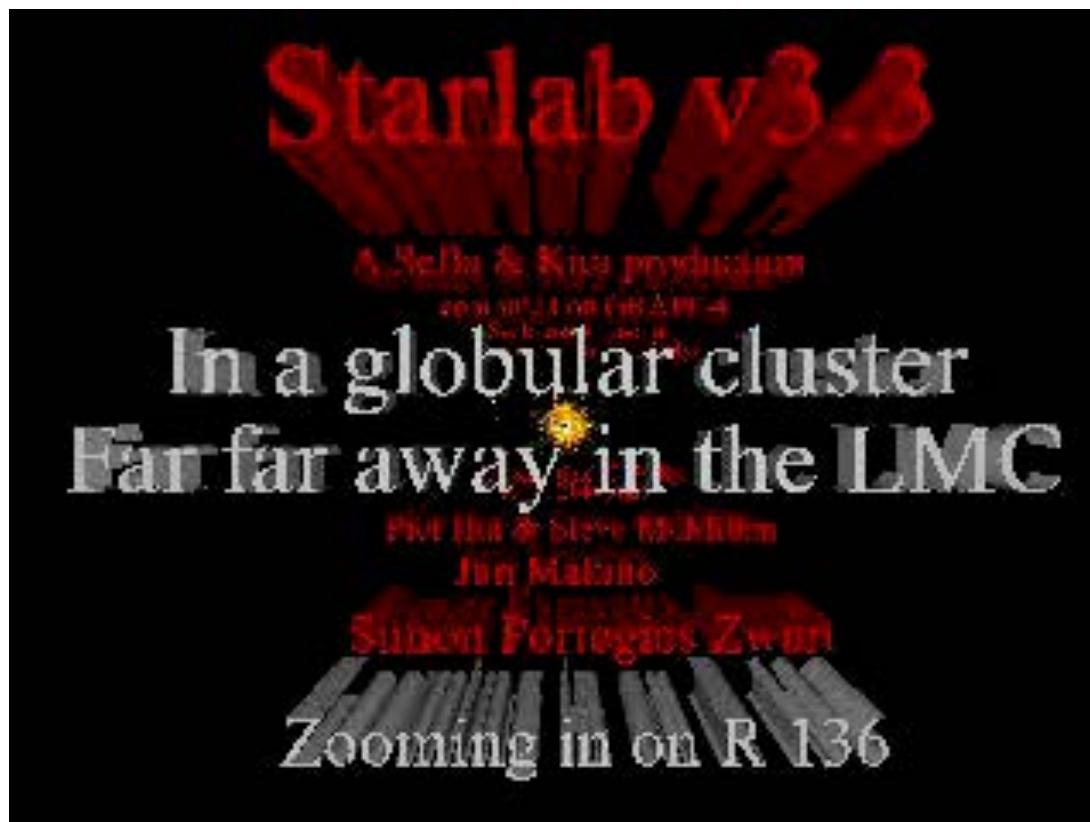
## A special-purpose computer for gravitational many-body problems

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

NATURE · VOL 345 · 3 MAY 1990

33

© 1990 Nature Publishing Group



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!

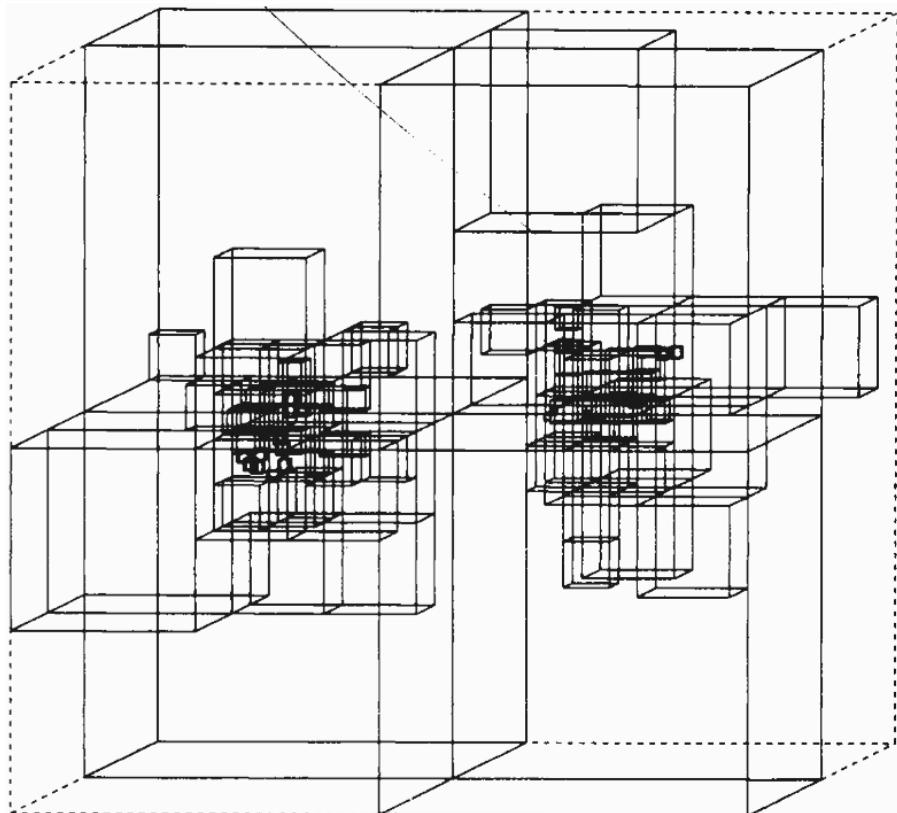
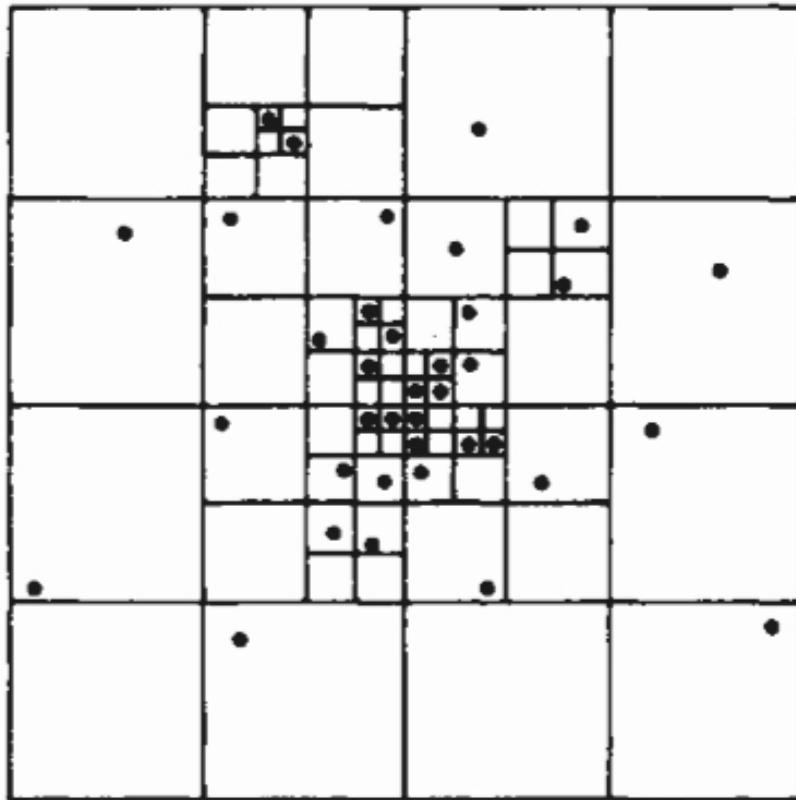
# Enabling Science by Algorithm

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**

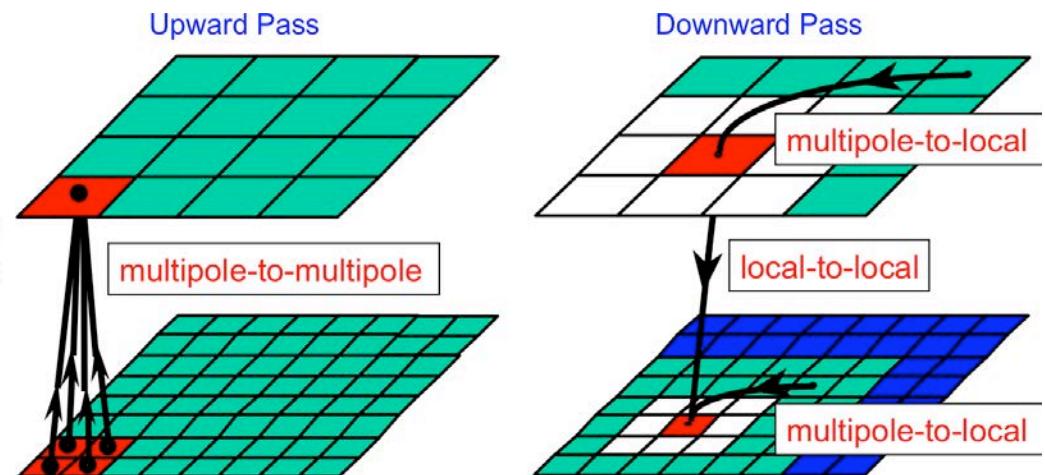
<http://longnow.org/essays/richard-feynman-connection-machine/>

## 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 Rouge, Louisiana 70803-4001*

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

Molecular dynamics simulations of porous silica in the density range  $2.2\text{--}0.1 \text{ g/cm}^3$  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

Tsuyoshi Hamada  
Department of Computer and Information Sciences  
Nagasaki University  
Nagasaki, Japan  
hamada@cis.nagasaki-u.ac.jp

Tetsu Narumi  
Department of Computer Science  
University of Electro-Communications  
Tokyo, Japan  
narumi@cs.uec.ac.jp

Rio Yokota  
Department of Mathematics  
University of Bristol  
Bristol, United Kingdom  
rio.yokota@bristol.ac.uk

Kenji Yasuoka  
Department of Mechanical Engineering  
Keio University  
Yokohama, Japan  
yasuoka@mech.keio.ac.jp

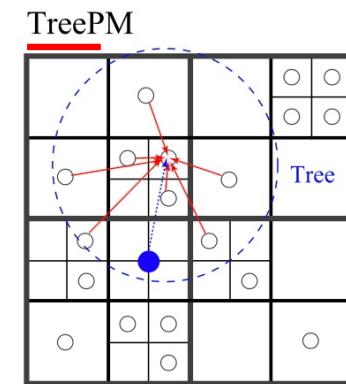
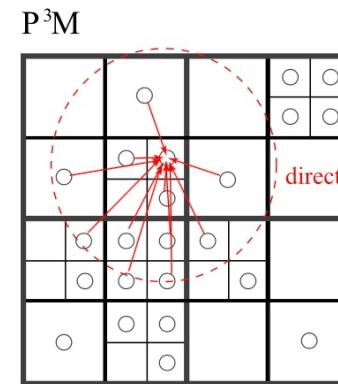
Keigo Nitadori  
High-Performance Molecular Simulation Team  
RIKEN Advanced Science Institute  
Wako, Japan  
keigo@riken.jp

Makoto Taiji  
High-Performance Molecular Simulation Team  
RIKEN Advanced Science Institute  
Wako, Japan  
taiji@riken.jp

## 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		<b>23,520,832</b>	<b>\$ 228,912</b>



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

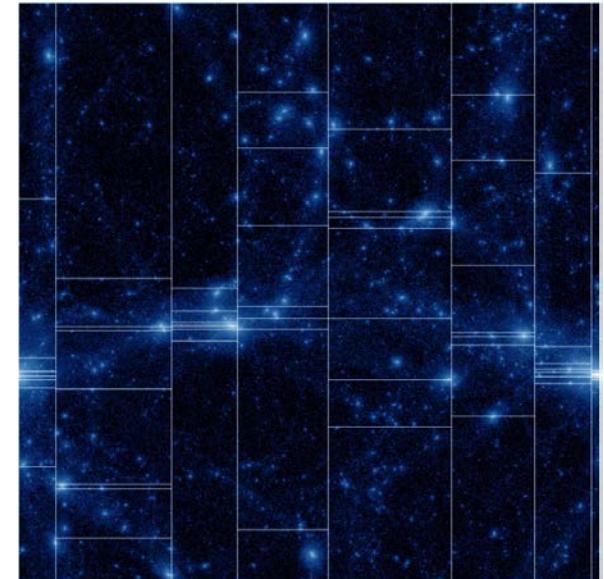
Tomoaki Ishiyama  
Center for Computational Science  
University of Tsukuba  
ishiyma@ccs.tsukuba.ac.jp

Keigo Nitadori  
Center for Computational Science  
University of Tsukuba  
keigo@ccs.tsukuba.ac.jp

Junichiro Makino  
Graduate School of Science and Engineering  
Tokyo Institute of Technology  
makino@geo.titech.ac.jp

IEEE/ACM supercomputing, SC12

*Machine  
&  
algorithm!*

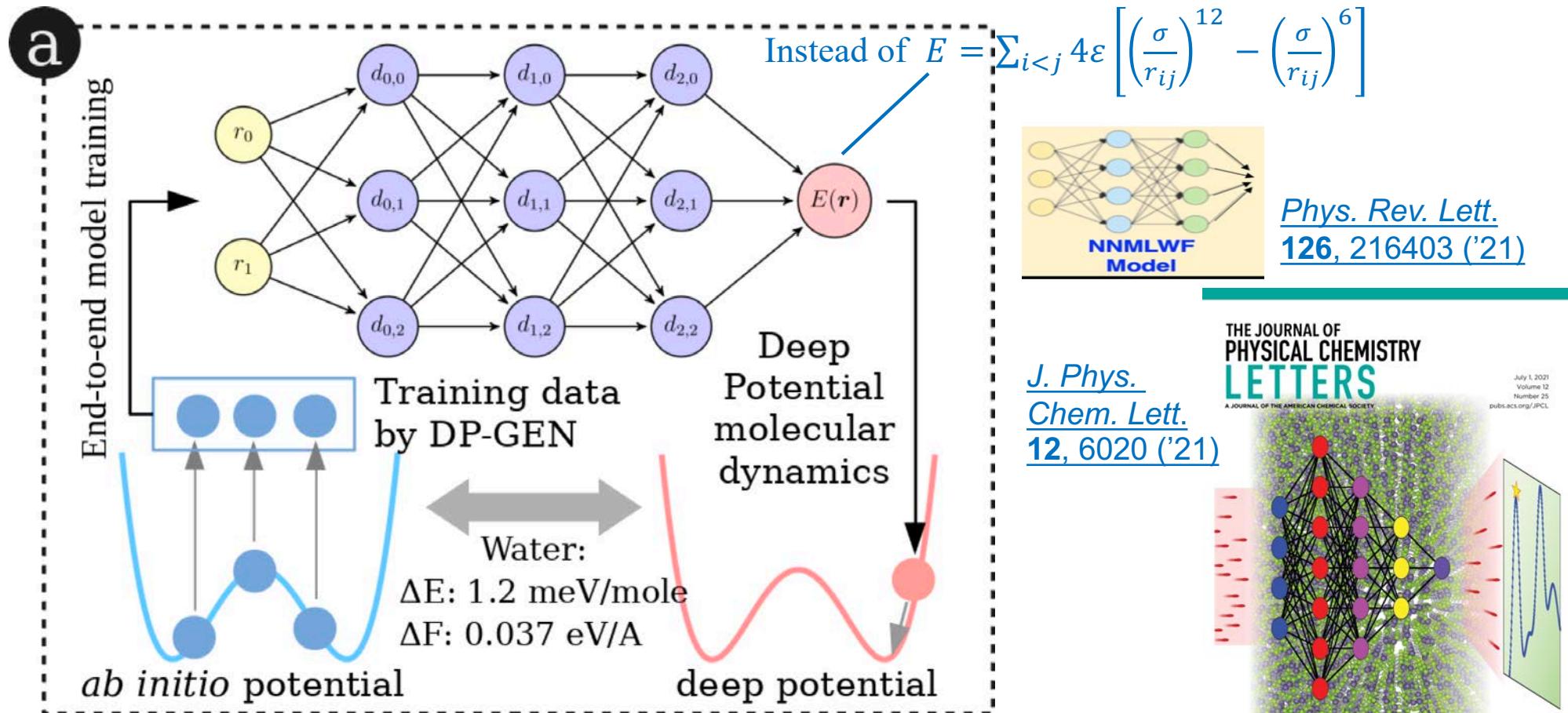


# Now It's Deep MD

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*



<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<sup>1</sup>, Firas Khatib<sup>2</sup>, Adrien Treuille<sup>1,3</sup>, Janos Barbero<sup>1</sup>, Jeehyung Lee<sup>3</sup>, Michael Beenen<sup>1</sup>, Andrew Leaver-Fay<sup>2</sup>†, David Baker<sup>2,4</sup>, Zoran Popović<sup>1</sup> & Foldit players

The image shows two screenshots of the Foldit game interface. The left screenshot displays a green ribbon logo and the text "foldit BETA". Below it is a protein structure with a central message: "Click to learn how you contribute to science by playing Foldit." The right screenshot shows a more detailed view of a protein structure with numbered arrows pointing to specific residues or features. The top bar indicates "Rank: 317" and "Score: 2534". A sidebar on the right lists "Group Competition" and "Soloist Competition" results, including names like "Rice Biochemistry" and "Team Commonwealth". The bottom navigation bar includes buttons for "Actions" (Shake Sidechains, Wiggle All, Wiggle Backbone, Wiggle Sidechains, Freeze Protein, Remove Bands, Disable Bands, Align Guide, Reset Structures), "Modes" (Social, Behavior), "View" (Reset Puzzle, Help, Glossary, Notifications), and "Menu".

Rank: 317 Score: 2534

BLOG PUZZLES FEEDBACK

Click to learn how you contribute to science by playing Foldit.

1 2 3 4 5 6 7 8 9 10 11 12

Group Competition

# Group Name	Score
1 Rice Biochemistry	9174
2 Team Commonwealth	9168
3 Team Canada	9165
4 Team Canada	9085
5 Firebird BioChem	9073
6 SETI Germany	9030
7 Bonche	9001

Soloist Competition

# Player Name	Current	Best
1 Mike Crunching for Physics	-	9242
2 weitzan	-	9222
3 ys719	-	9235
4 pharic	-	9211
5 kevin_karpilas	-	9196
6 JINXter	-	9193
7 abruce	-	9181

Actions: Shake Sidechains, Wiggle All, Wiggle Backbone, Wiggle Sidechains, Freeze Protein, Remove Bands, Disable Bands, Align Guide, Reset Structures, Undo, Social, Behavior, View, Help, Glossary, Menu.

# Ising Machine



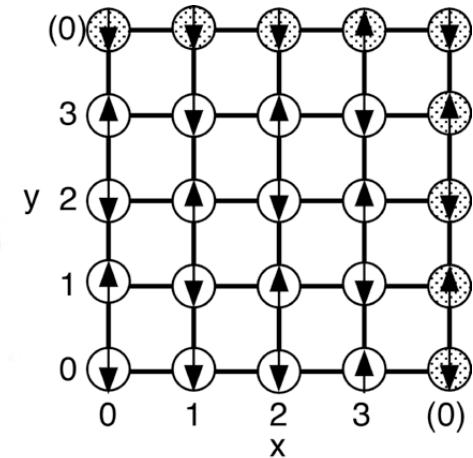
## 1bit の世界の専用計算機 —イジング・マシーン—

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)

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



<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)

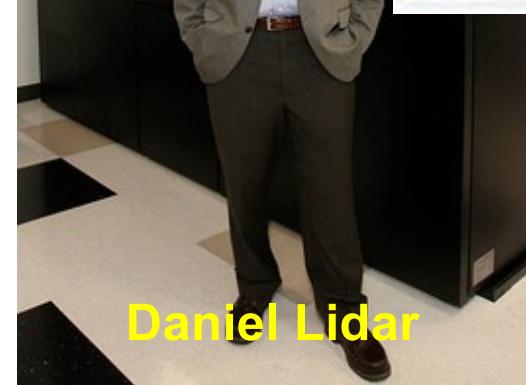
## Phase transitions in a programmable quantum spin glass simulator

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

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

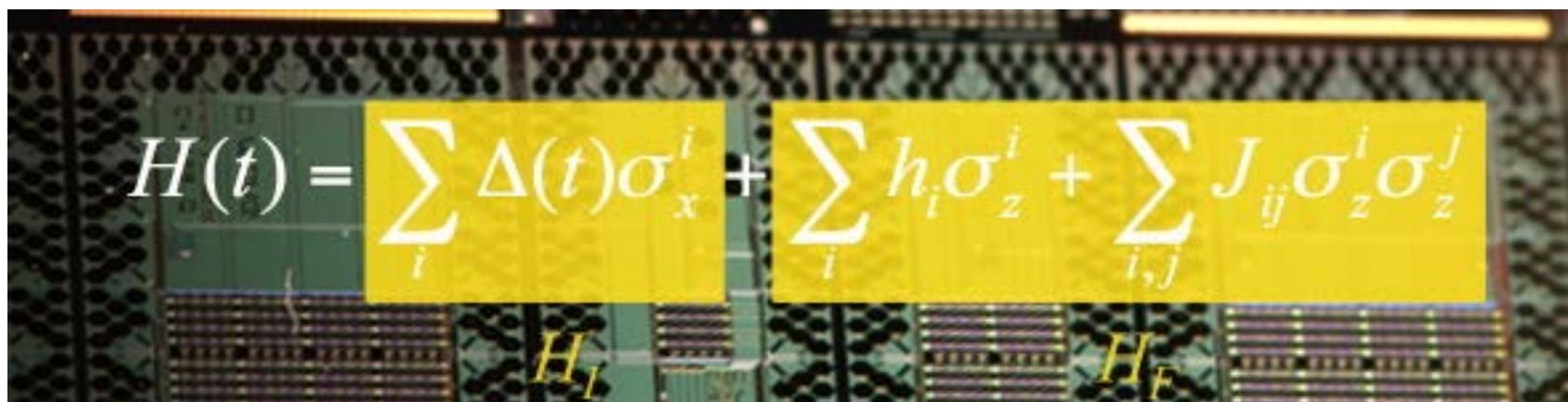


Bob Lucas



Daniel Lidar

- Adiabatic quantum optimization



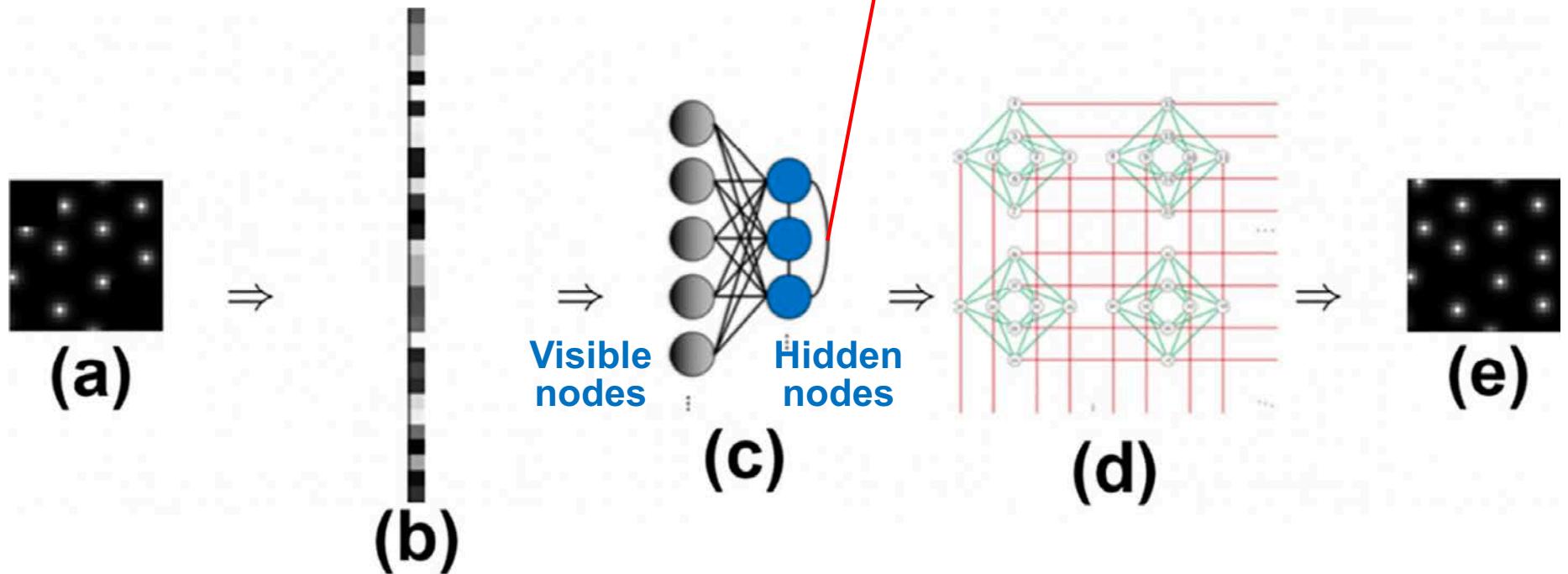
# Machine Learning on D-Wave

## Boltzmann machine modeling of layered MoS<sub>2</sub> 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)

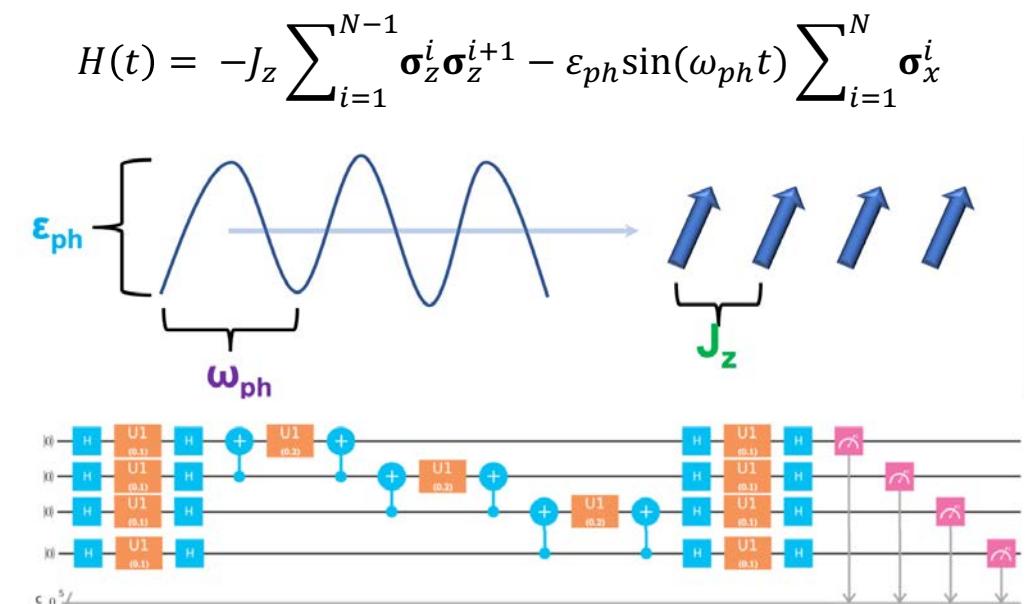
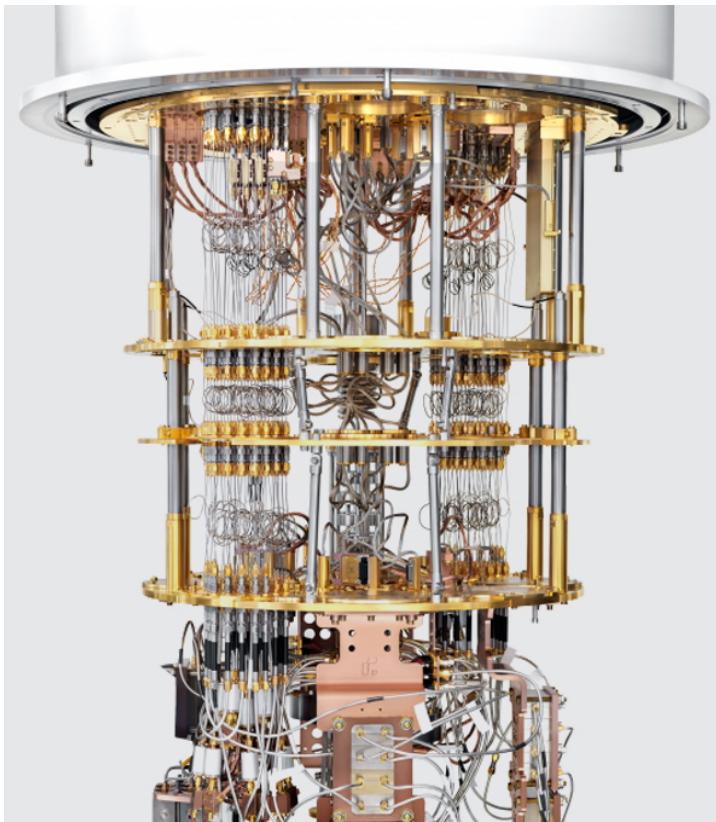
- Computing power of D-Wave allows unrestricted Boltzmann Machine to enhance machine learning performance



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 \('21\)](#)]



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