Molecular-Dynamics Machines

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“... 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)
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

\[ \frac{d^2 x_i}{dt^2} = f_i = \sum_j \frac{m_j (x_j - x_i)}{(r_{ij}^2 + \epsilon^2)^{3/2}} \]

Host Computer
(PC-98/Sony NEWS)

GPIB Interface

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' TFlops/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 Kohshi, 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
Atsushi Kawai, Toshiyuki Fushuishi, 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 Tagai

Green500

<table>
<thead>
<tr>
<th>Rank</th>
<th>MFLOPS/W</th>
<th>Site*</th>
<th>Computer*</th>
<th>Total Power (KW)</th>
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<tbody>
<tr>
<td>1</td>
<td>1844.20</td>
<td>IBM Thomas J. Watson Research Center</td>
<td>NNS/60 Blue Gene/Q Prototype</td>
<td>38.80</td>
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<tr>
<td>2</td>
<td>1448.93</td>
<td>National Astronomical Observatory of Japan</td>
<td>GRAPE-OR Accelerator Cluster, Infiband</td>
<td>24.59</td>
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<td>2</td>
<td>908.36</td>
<td>GSIC Center, Tokyo Institute of Technology</td>
<td>HP ProLiant SL390s G7 Xeon 8C X970, Nvidia GPU, Linux/Windows</td>
<td>1243.80</td>
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<td>3</td>
<td>933.06</td>
<td>NCIA</td>
<td>Hybrid Cluster Com 12 2.29GHz Dual Core, NVIDIA C2050, Infiniband</td>
<td>36.00</td>
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<tr>
<td>4</td>
<td>828.67</td>
<td>RIKEN Advanced Institute for Computational Science</td>
<td>K computer, SPARC64 VIIIfx 2.0GHz, Topl interconnect</td>
<td>57.95</td>
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</tbody>
</table>

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

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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

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

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

For his dissertation "The Rapid Evaluation of Potential Fields in Particle Systems."
Enabling Science by Online Game

LETTERS

Predicting protein structures with a multiplayer online game

Seth Cooper¹, Firas Khatib², Adrien Treuille¹,³, Janos Barbero¹, Jeehyung Lee³, Michael Beenen¹, Andrew Leaver-Fay², David Baker²,³, Zoran Popović¹ & Foldit players
Ising Machine: A Special Purpose Computer for 1-bit Worlds

TAIJI Makoto
(Received 3 March 1994)

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)

Evidence for quantum annealing with more than one hundred qubits

Sergio Boixo¹, Troels F. Rønnow², Sergei V. Isakov², Zhihui Wang³, David Wecker⁴, Daniel A. Lidar⁵, John M. Martinis⁵ and Matthias Troyer²*

- **Adiabatic quantum optimization**

\[
H(t) = \sum_i \Delta(t) \sigma_x^i + \sum_i h_i \sigma_z^i + \sum_{i,j} J_{ij} \sigma_z^i \sigma_z^j
\]

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