Advanced Monte Carlo

Aiichiro Nakano

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Department of Physics & Astronomy
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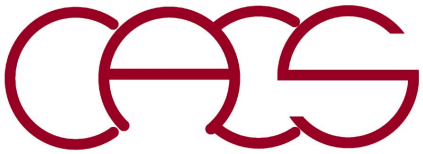
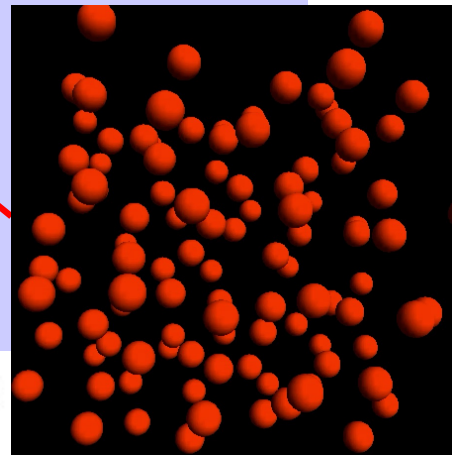


Hybrid MC

Combine collective motion of molecular dynamics (MD) with MC

- **MD mapping:** $g^{t,\delta t}: (\vec{r}^N, \vec{v}^N) \rightarrow: (\overrightarrow{r'^N}, \overrightarrow{v'^N})$
- **Energy nonconservation due to discretization error → apply Metropolis MC**

```
for step_MC = 1 to Max_step_MC
  Generate normal velocity distributions with temperature T
  Compute the total energy Hinit and forces for the initial state
  for step_MD = 1 ro Max_step_MD
    Velocity-Verlet update of coordinates and velocities for dt
  end for
  Compute the final energy Hfinal
  if DH = Hfinal - Hinit < 0 then
    Accept the state change, xinit → xfinal
  else if rand()/RAND_MAX < exp(-DH/kBT) then
    Accept the state change, xinit → xfinal
  end if
end for
```



Hybrid Monte Carlo method for condensed-matter systems

B. Mehlig, D. W. Heermann, and B. M. Forrest
Institut für Theoretische Physik, Universität Heidelberg, Philosophenweg 19, and Interdisziplinäres Zentrum für Wissenschaftliches Rechnen der Universität Heidelberg, 6900 Heidelberg, Germany
(Received 7 June 1991)

Phys. Rev. B **45**, 679 ('92)

Multigrid MC

PHYSICAL REVIEW

LETTERS

VOLUME 60 | 18 APRIL 1988 | NUMBER 16

Simulations without Critical Slowing Down

Daniel Kandel and Eytan Domany
Department of Electronics, Weizmann Institute of Science, Rehovot 76100, Israel

Dorit Ron and Achi Brandt
Department of Applied Mathematics, Weizmann Institute of Science, Rehovot 76100, Israel

and

Eugene Loh, Jr.
Theoretical Division and Center for Non-Linear Studies, Los Alamos National Laboratory, Los Alamos, New Mexico 87545
(Received 4 February 1988)

Phys. Rev. Lett. **60**, 1591 ('88)

Correlation time

$$\tau \propto L^z$$

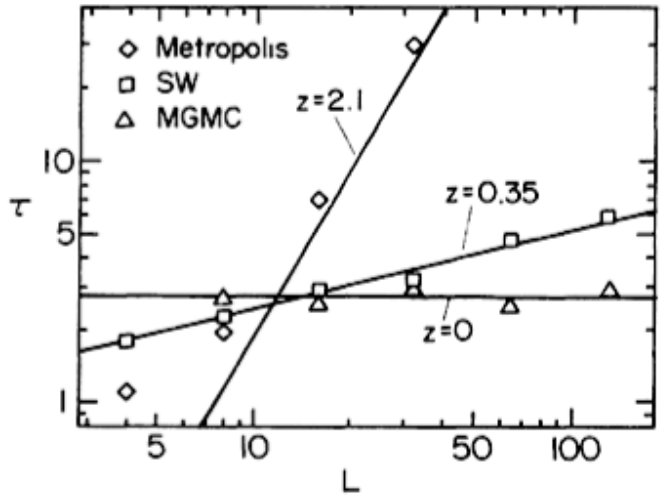
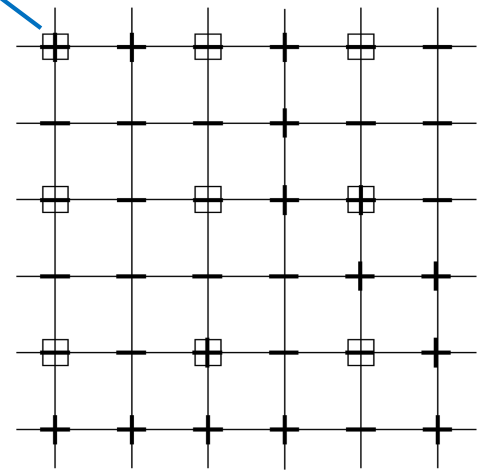


FIG. 1. Relaxation time τ vs (linear) system size L. Three methods are compared: Metropolis algorithm (Ref. 7), Swendsen and Wang's method (Ref. 6) (SW), and the multigrid Monte Carlo technique (MGMC).

Multigrid MC

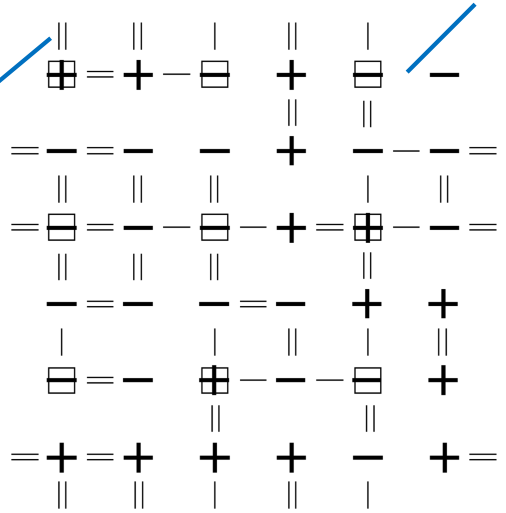
Cluster of clusters: Coarsening

Representative spin

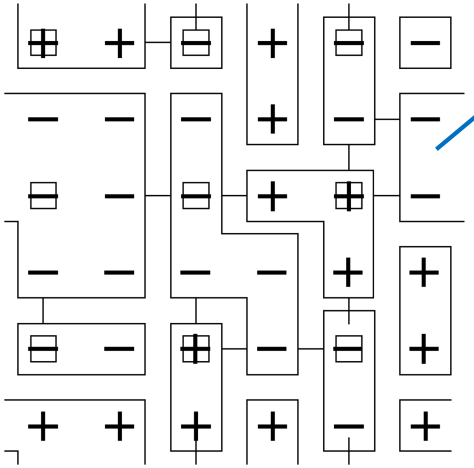


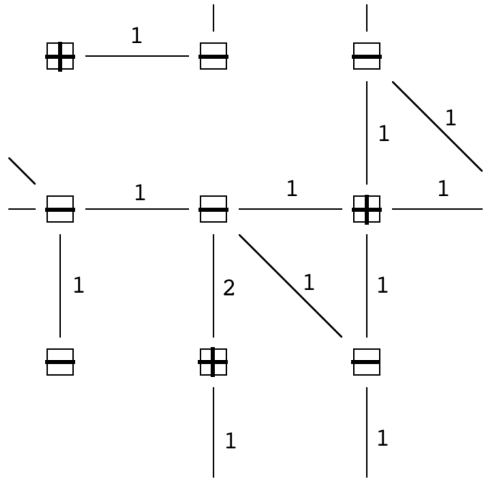
Deleted bond

Frozen bond



Cluster

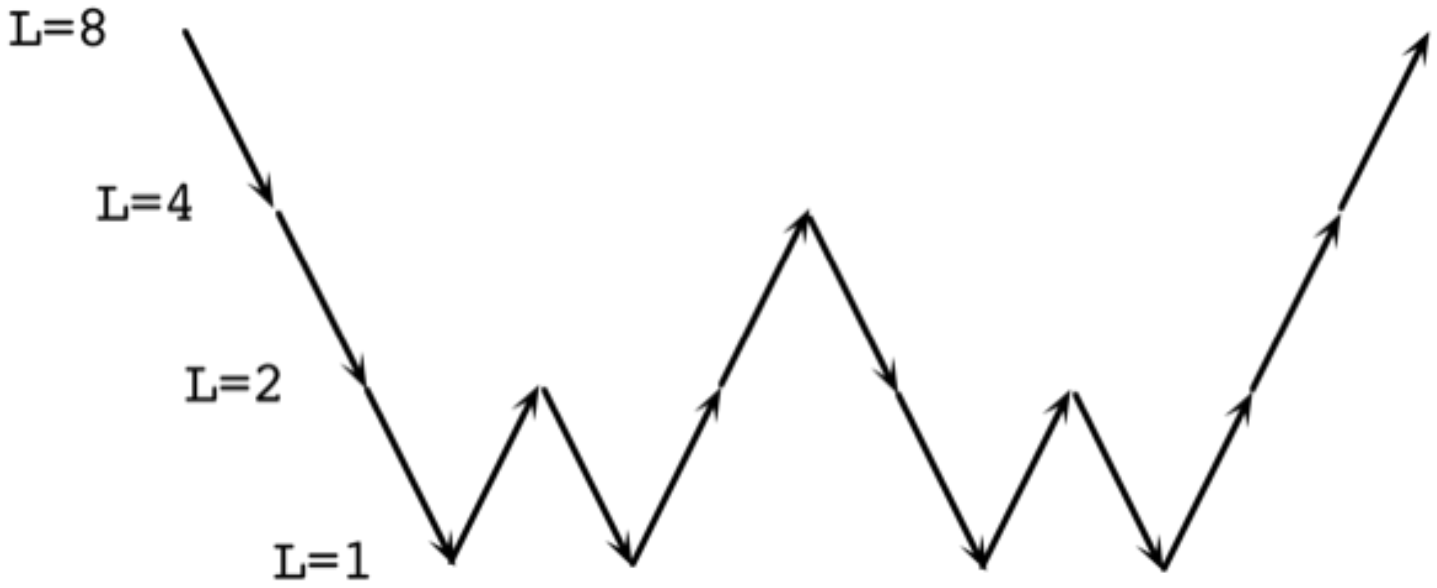




Renormalized coarse spin model

Multigrid MC

- **Uncoarsening**
  Recover the fine spins
- **Multigrid cycling**
  Do it recursively



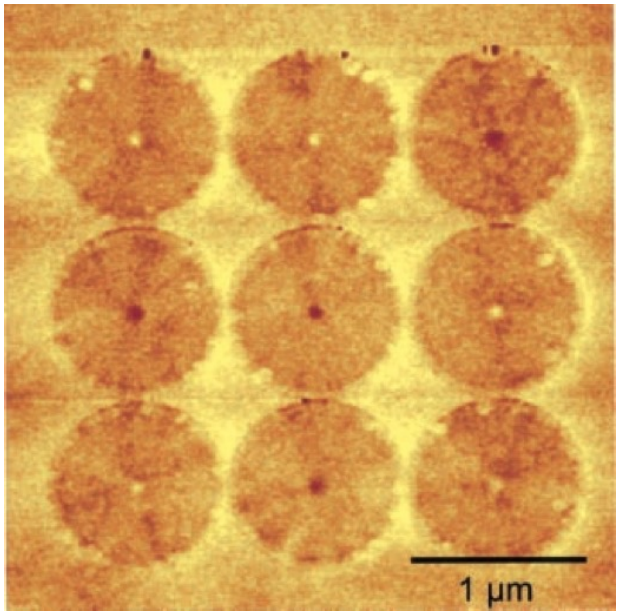
$O(N)$ MC with Long-Range Interaction?

International Journal of Modern Physics C, Vol. 6, No. 3 (1995) 359–370

$O(N\log N)$ MC algorithm

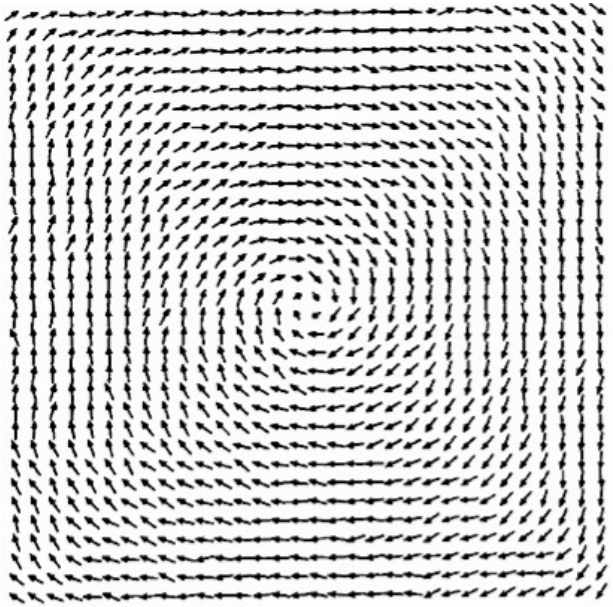
MONTE CARLO METHOD FOR SPIN MODELS WITH LONG-RANGE INTERACTIONS

ERIK LUIJTEN* and HENK W. J. BLÖTE
Faculty of Applied Physics, Delft University of Technology
P.O. Box 5046, 2600 GA Delft, The Netherlands



Magnetic vortex core

T. Shinjo *et al.*, *Science* **289**, 930 ('00)



$O(N)$ cluster MC algorithm

Journal of Computational Physics 228 (2009) 2629–2642

Order-N cluster Monte Carlo method for spin systems with long-range interactions

Kouki Fukui [a,1], Synge Todo [a,b,*]

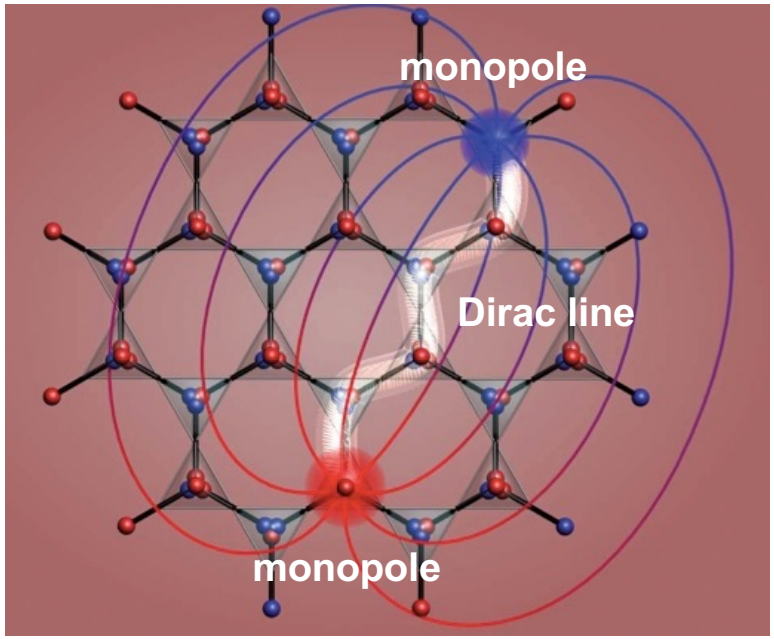
Exotic Magnets

nature Vol 451|3 January 2008|doi:10.1038/nature06433

LETTERS

Magnetic monopoles in spin ice

C. Castelnovo[1], R. Moessner[1,2] & S. L. Sondhi[3]



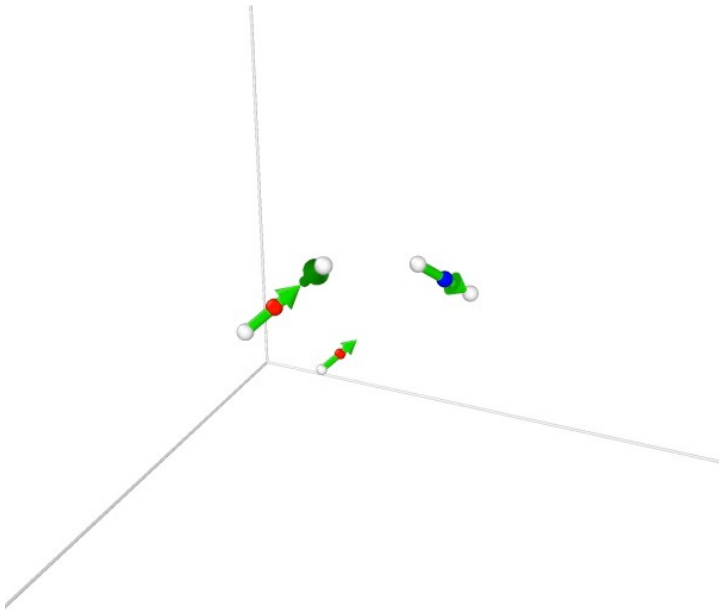
$$H = \frac{J}{3}\sum_{\langle ij\rangle} S_i S_j + Da^3 \sum_{(ij)} \left[\frac{\hat{\mathbf{e}}_i \cdot \hat{\mathbf{e}}_j}{|\mathbf{r}_{ij}|^3} - \frac{3(\hat{\mathbf{e}}_i \cdot \mathbf{r}_{ij})(\hat{\mathbf{e}}_j \cdot \mathbf{r}_{ij})}{|\mathbf{r}_{ij}|^5} \right] S_i S_j$$

MAGNETISM

Qubit spin ice

Andrew D. King[1]*, Cristiano Nisoli[2]*, Edward D. Dahl[1,3], Gabriel Poulin-Lamarre[1], Alejandro Lopez-Bezanilla[2]

Science **373**, 576–580 (2021)



Monte Carlo simulation

Cluster MC for Particles

VOLUME 92, NUMBER 3 PHYSICAL REVIEW LETTERS week ending 23 JANUARY 2004

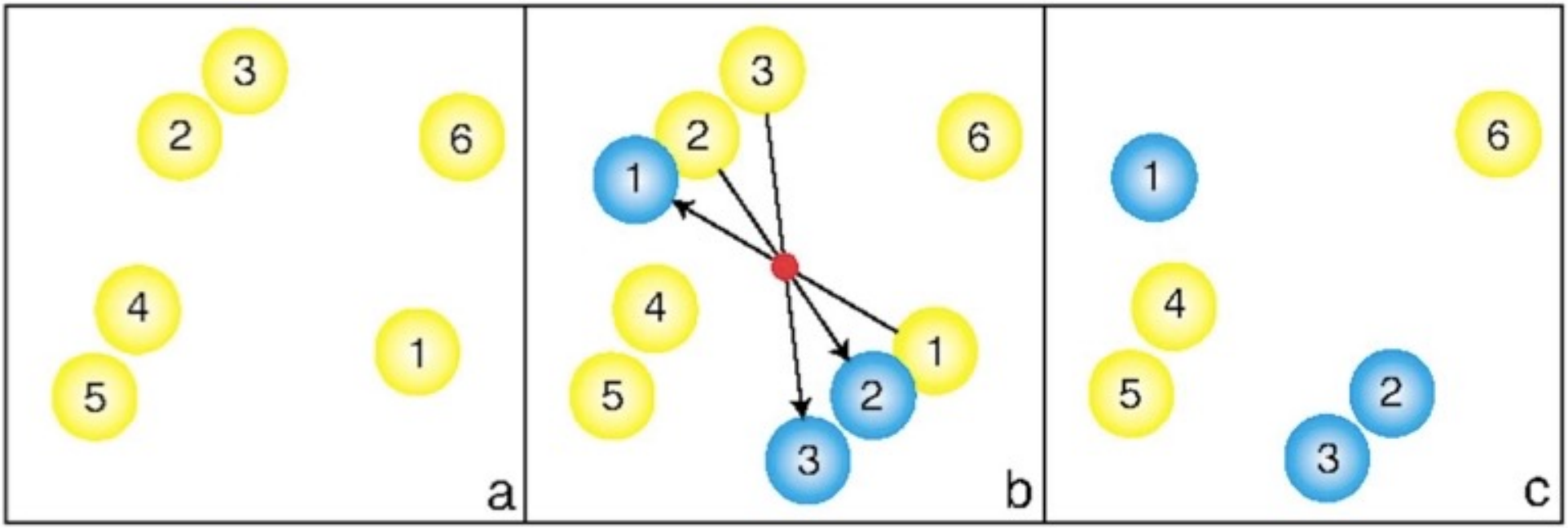
Rejection-Free Geometric Cluster Algorithm for Complex Fluids

Jiwen Liu and Erik Luijten*

Department of Materials Science and Engineering, University of Illinois at Urbana-Champaign, Urbana, Illinois 61801, USA

(Received 23 September 2003; published 23 January 2004)

We present a novel, generally applicable Monte Carlo algorithm for the simulation of fluid systems. Geometric transformations are used to identify clusters of particles in such a manner that every cluster move is accepted, irrespective of the nature of the pair interactions. The rejection-free and nonlocal nature of the algorithm make it particularly suitable for the efficient simulation of complex fluids with components of widely varying size, such as colloidal mixtures. Compared to conventional simulation algorithms, typical efficiency improvements amount to several orders of magnitude.



Multicanonical & Multirange MC

VOLUME 68, NUMBER 1 PHYSICAL REVIEW LETTERS 6 JANUARY 1992

Multicanonical Ensemble: A New Approach to Simulate First-Order Phase Transitions

Bernd A. Berg [1),(2),(a)] and Thomas Neuhaus [1)]
[1)] *Fakultät für Physik, Universität Bielefeld, D-4800 Bielefeld, Federal Republic of Germany*
[2)] *Supercomputer Computations Research Institute, Tallahassee, Florida 32306*
(Received 19 July 1991)

Phys. Rev. Lett. **68**, 9 ('92)

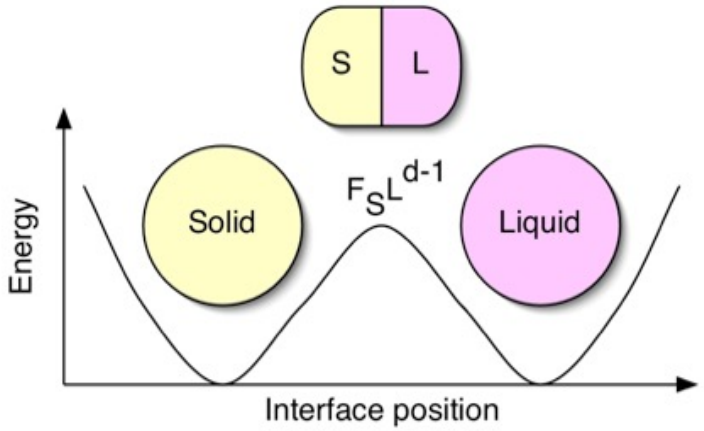
VOLUME 86, NUMBER 10 PHYSICAL REVIEW LETTERS 5 MARCH 2001

Efficient, Multiple-Range Random Walk Algorithm to Calculate the Density of States

Fugao Wang and D. P. Landau
Center for Simulational Physics, The University of Georgia, Athens, Georgia 30602
(Received 25 October 2000)

Phys. Rev. Lett. **86**, 2050 ('01)

First-order phase transition $\tau \sim \exp\left(F_S L^{d-1}\right)$



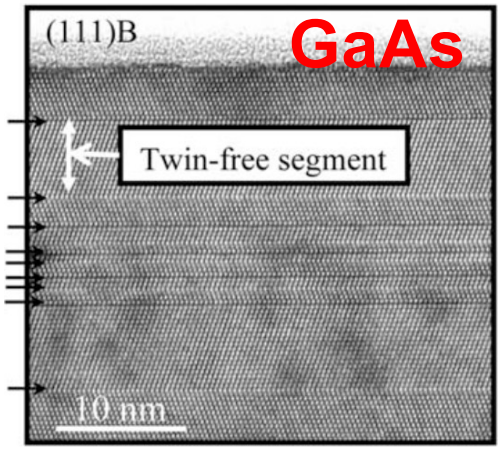
Multicanonical MC

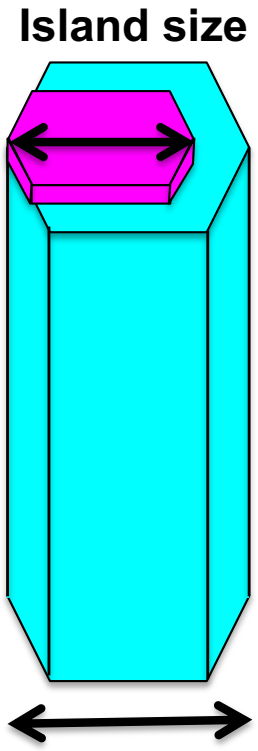
$\tau \sim L^{d\alpha}$ $\alpha \approx 1$

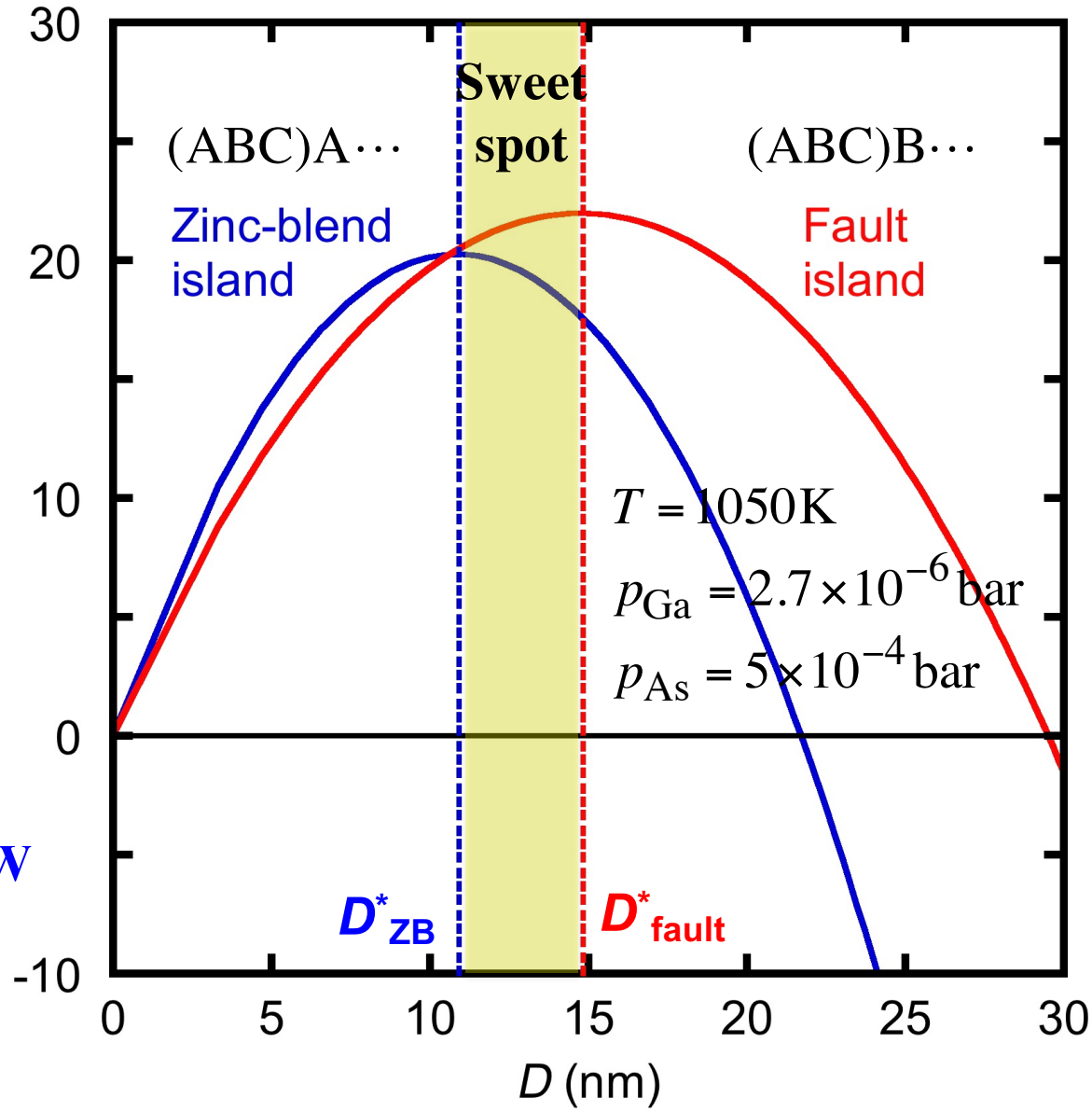
Stacking-Fault Elimination in Nanowire?

- **Gibbs free energy change for the nucleation of an island of an ad-bilayer at a corner**

$$G = E_{\text{island}} - N_{\text{Ga}}\mu_{\text{Ga}}^{\text{gas}}(p_{\text{Ga}}, T) - N_{\text{As}}\mu_{\text{As}}^{\text{gas}}(p_{\text{As}}, T)$$







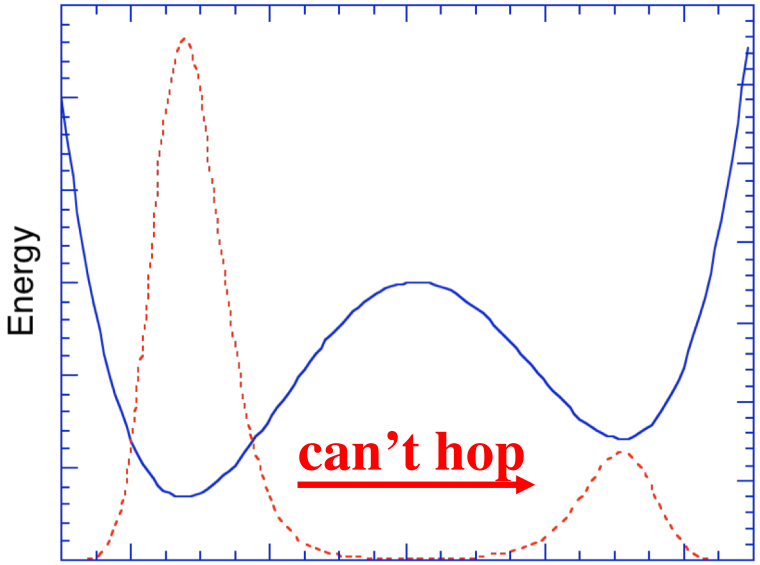
- **There is a *narrow* range of diameter in which twin-free NW is grown: $D^*_{\text{ZB}} < D_W < D^*_{\text{fault}}$**

Z. Yuan *et al.*, *Appl. Phys. Lett.* **100**, 163103 ('12); *Nano Lett.* **13**, 4925 ('13)

Multicanonical Ensemble

Metropolis walk based on Boltzmann factor: slow

$$\rho_{\mathrm{B}}(E,T) = D(E)P_{\mathrm{B}}(E,T)$$
$$P_{\mathrm{B}}(E,T) = \exp(-\mathrm{E}/k_{\mathrm{B}}T)$$



1-dimensional random walk in energy space: fast

$$\rho_{\mathrm{M}}(E) = D(E)P_{\mathrm{M}}(E) = \text{constant}$$

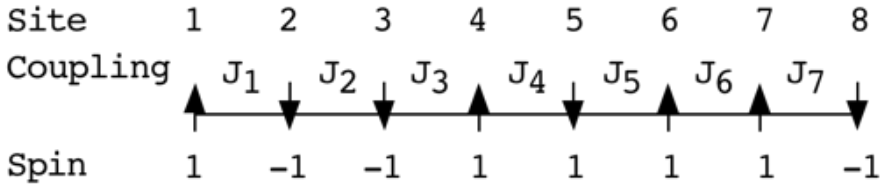
Multicanonical MC algorithm

1. **Set-up run to estimate density of states, *D*(*E*)**
2. **Metropolis run using 1/*D*(*E*) as a prob. density**
3. **Obtain Boltzmann distribution by re-weighting**

$$\rho_{\mathrm{B}}(E,T) \sim \rho_{\mathrm{M}}(E)P_{\mathrm{M}}^{-1}(E)\exp(-\mathrm{E}/k_{\mathrm{B}}T)$$

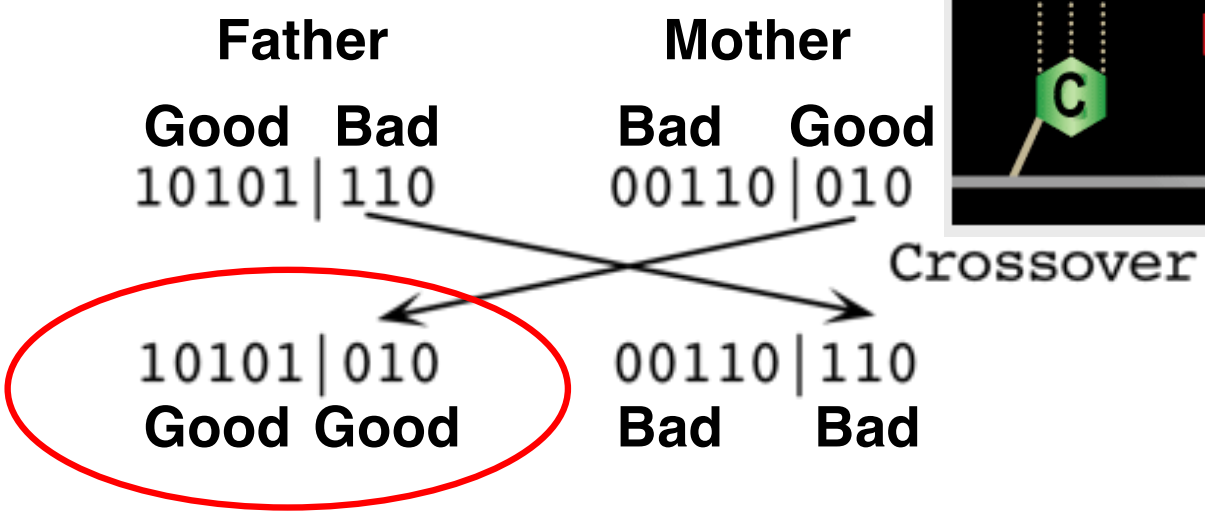
Genetic Algorithm

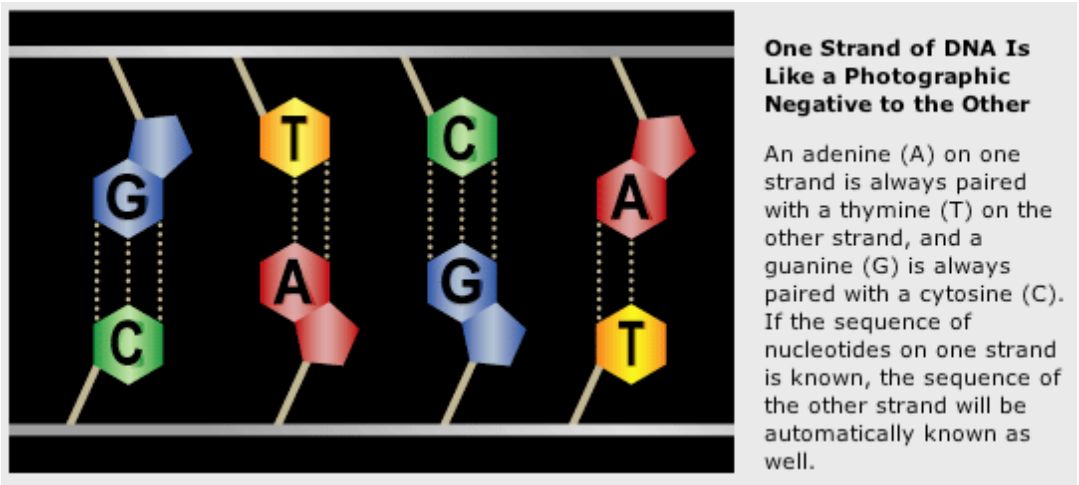
1D Ising model



Gene = bit string = (10011110)

- **Population in the solution space: Multiple chains, diversity**
- **Selection: Elitist strategy = survival of the fittest**
- **Crossover**





Statistical Mechanical Analysis of GA

PHYSICAL REVIEW
LETTERS

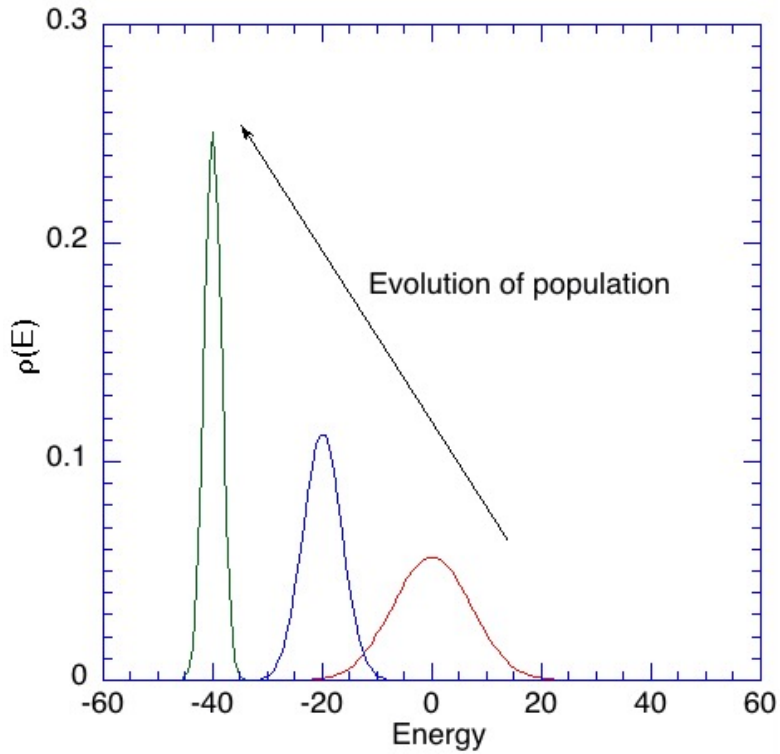
VOLUME 72 | 28 FEBRUARY 1994 | NUMBER 9

Analysis of Genetic Algorithms Using Statistical Mechanics

Adam Prügel-Bennett and Jonathan L. Shapiro
Department of Computer Science, University of Manchester, Manchester, M13 9PL, United Kingdom
(Received 11 June 1993)

A formalism is developed for studying genetic algorithms by considering the evolution of the distribution of fitness in the population. The effects of selection on the population are problem independent. The formalism predicts the optimal amount of selection. Crossover is solved for a model problem—finding low energy states of the one dimensional Ising spin glass. The theory is found to be in good agreement with simulations.

Phys. Rev. Lett. **72**, 1305 ('94)



$$\rho_t(E) \xrightarrow{\text{selection}} \rho_t^S(E) \xrightarrow{\text{crossover}} \rho_t^{SC} = \rho_{t+1}(E)$$

Replica Exchange MC

JOURNAL OF CHEMICAL PHYSICS VOLUME 118, NUMBER 14 8 APRIL 2003

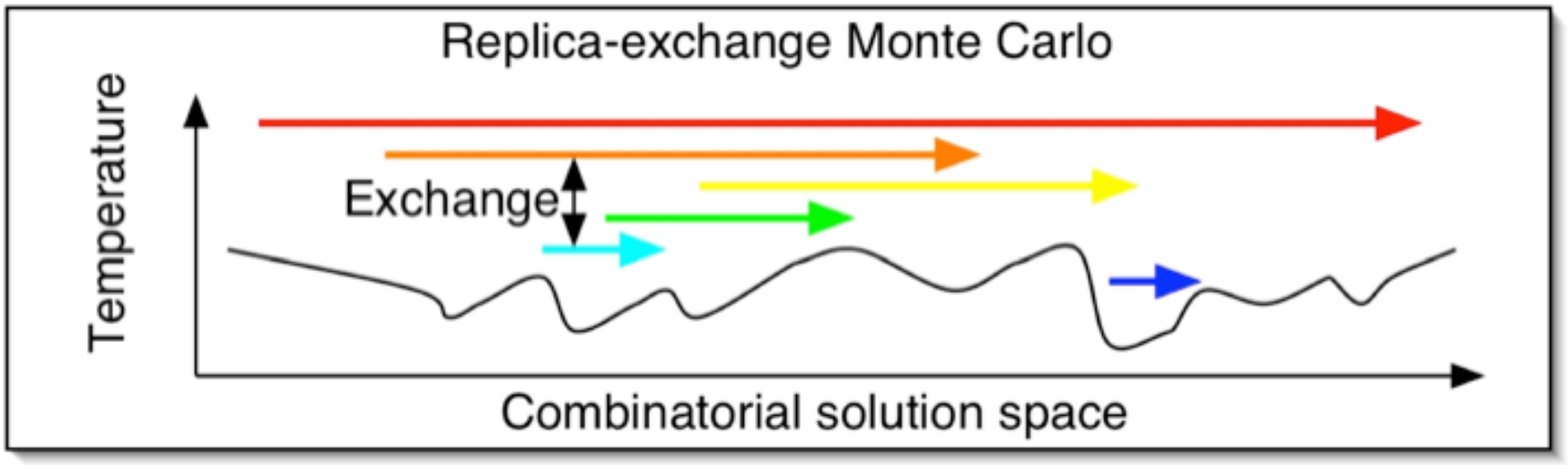
Replica-exchange multicanonical and multicanonical replica-exchange Monte Carlo simulations of peptides. I. Formulation and benchmark test

Ayori Mitsutake[a)]
Department of Physics, Faculty of Science and Technology, Keio University, Yokohama, Kanagawa 223-8522, Japan

Yuji Sugita[b)] and Yuko Okamoto[c)]
Department of Theoretical Studies, Institute for Molecular Science, Okazaki, Aichi 444-8585, Japan and Department of Functional Molecular Science, The Graduate University for Advanced Studies, Okazaki, Aichi 444-8585, Japan

J. Chem. Phys. **118**, 6664 ('03)

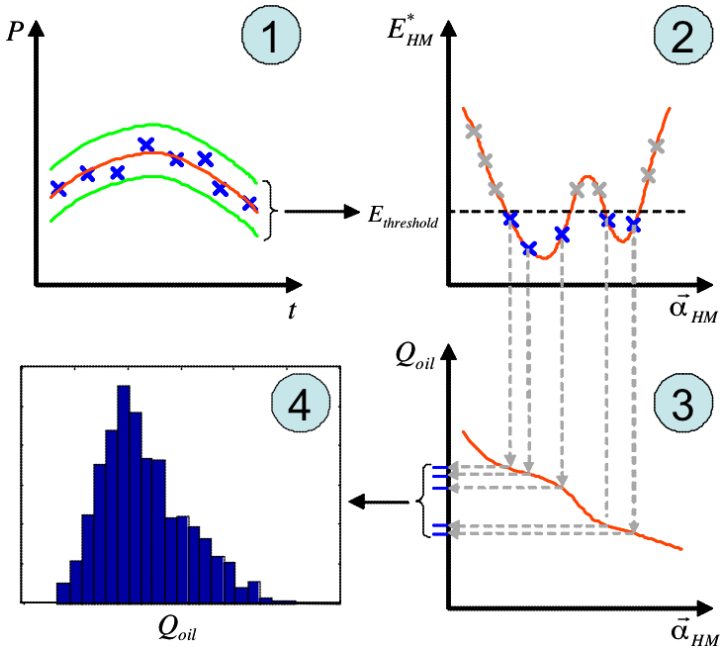
Multiple Markov chains at different temperatures

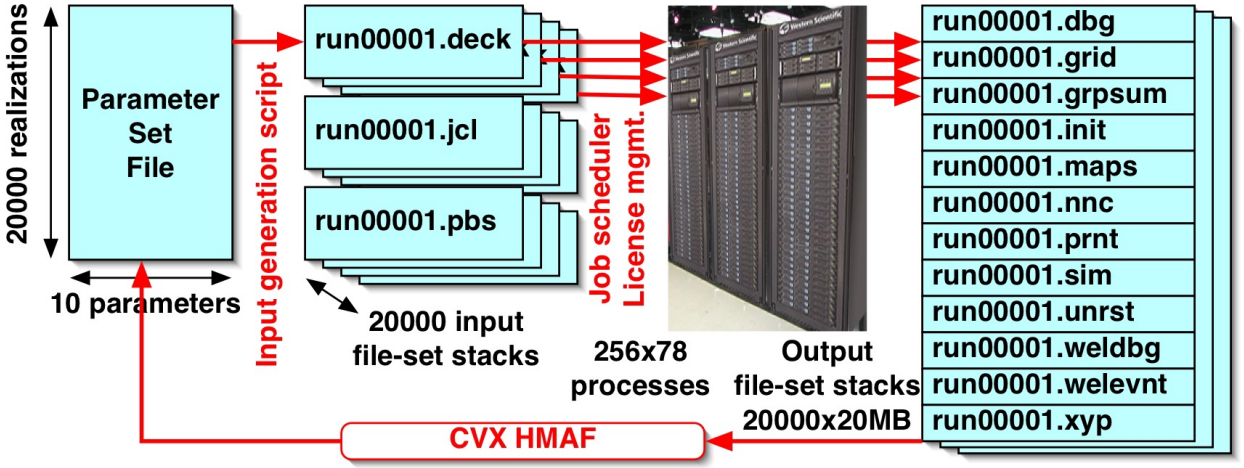


Parallel History Matching

- **Provide USC's parallel computing environment to demonstrate parallel execution of CVX's history match & associated forecast (HMAF) framework.**
- **History matching of a real field case (offshore Africa, North Sea & Gulf of Mexico) with 10,000-20,000 forward simulation runs on CACS high performance computing resources.**

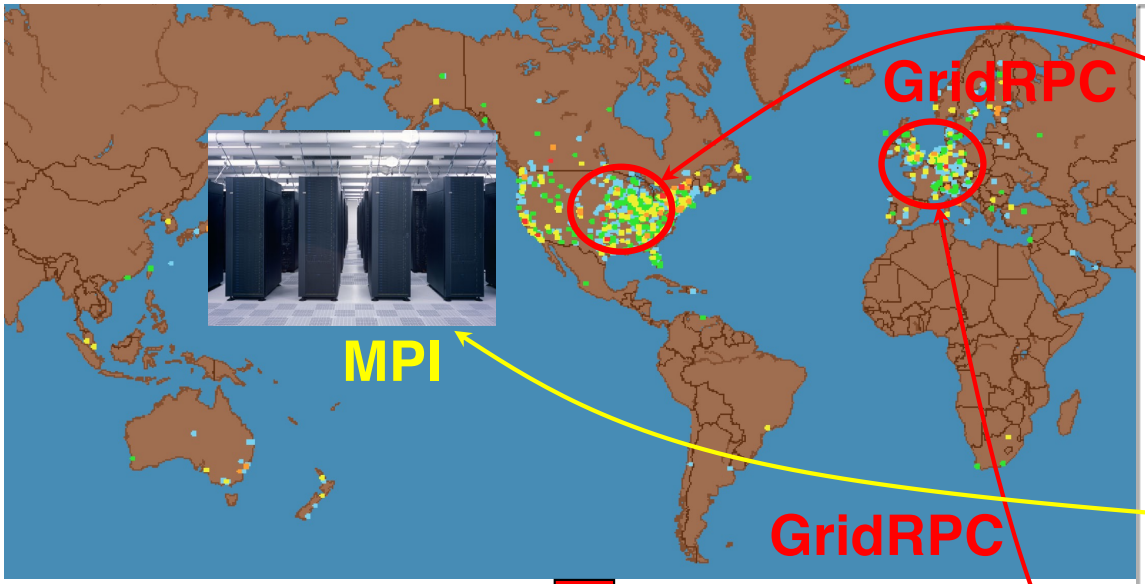
http://cisoft.usc.edu

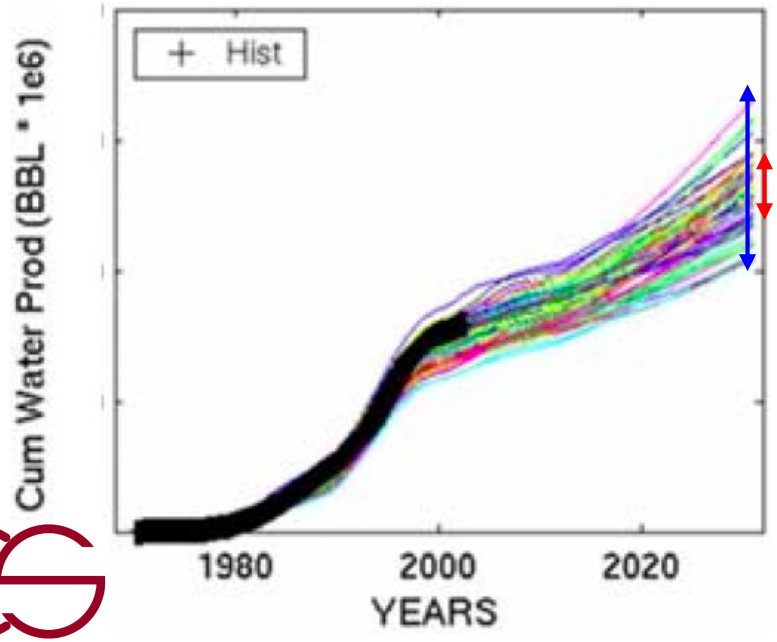


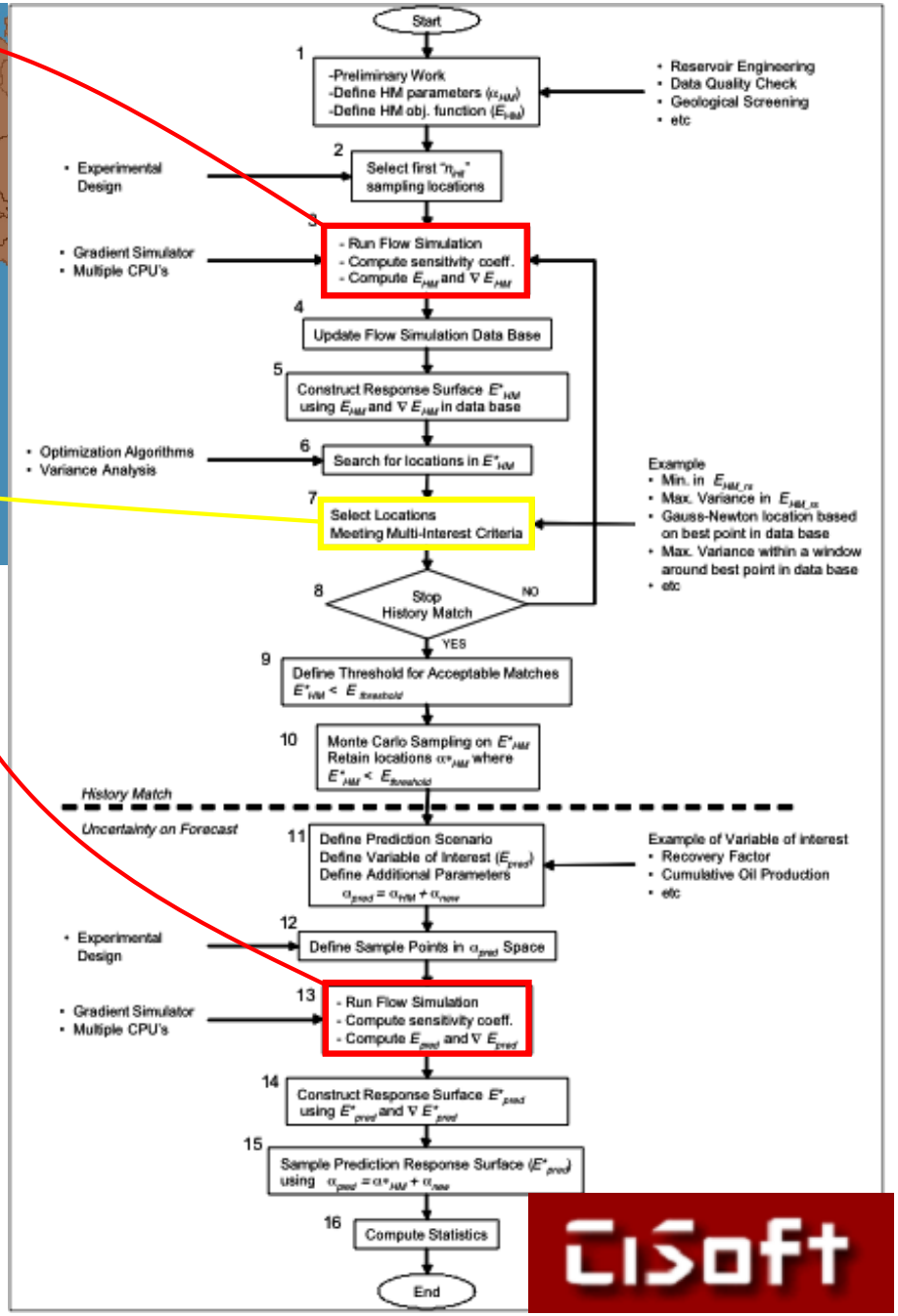


K. Nomura et al., *J. Supercomputing* **41**, 109 ('07)

Opportunity: Overnight HMAF on a Grid







Final Project at the Frontier of Science?

The Nobel Prize in Physics 1977

"for their fundamental theoretical investigations of the electronic structure of magnetic and disordered systems"

Philip Warren Anderson

1/3 of the prize

USA

Bell Telephone Laboratories
Murray Hill, NJ, USA

b. 1923

Sir Nevill Francis Mott

1/3 of the prize

United Kingdom

University of Cambridge
Cambridge, United Kingdom

b. 1905
d. 1996

John Hasbrouck van Vleck

1/3 of the prize

USA

Harvard University
Cambridge, MA, USA

b. 1899
d. 1980

The Nobel Prize in Physics 1973

"for their experimental discoveries regarding tunneling phenomena in semiconductors and superconductors, respectively"

"for his theoretical predictions of the properties of a supercurrent through a tunnel barrier, in particular those phenomena which are generally known as the Josephson effects"

Leo Esaki

1/4 of the prize

Japan

IBM Thomas J. Watson Research Center
Yorktown Heights, NY, USA

b. 1925

Ivar Giaever

1/4 of the prize

USA

General Electric Company
Schenectady, NY, USA

b. 1929
(in Bergen, Norway)

Brian David Josephson

1/2 of the prize

United Kingdom

University of Cambridge
Cambridge, United Kingdom

b. 1940

3D Ising Problem is NP-Complete

Statistical Mechanics, Three-Dimensionality and NP-completeness *

I. Universality of Intractability for the Partition Function of the Ising Model Across Non-Planar Lattices

[Extended Abstract]

Sorin Istrail
Sandia National Laboratories
Applied Mathematics Department, MS 1110
Albuquerque, NM 87185-1110
scistra@cs.sandia.gov

STOC 2000 Portland Oregon USA
1-58113-184-4/00/5

Nobel laureate Richard Feynman wrote in 1972 of the three-dimensional Ising model that "the exact solution for three dimensions has not yet been found."

Other researchers who have tried read like a roll call of famous names in science and mathematics: Onsager, Kac, Feynman, Fisher, Kasteleyn, Temperley, Green, Hurst, and more recently Barahona.

Says Istrail, "What these brilliant mathematicians and physicists failed to do, indeed cannot be done."

Lattice Model of Protein Folding

- **Levinthal's paradox: How the nature solves the NP-complete problem in polynomial (linear?) time?**

Predicting Protein Tertiary Structures from the First Principles*

Yuko Okamoto(okamotoy@ims.ac.jp)

Department of Theoretical Studies, Institute for Molecular Science
Department of Functional Molecular Science, Graduate University for Advanced Studies

Okazaki, Aichi 444-8585, JAPAN

The designability of protein structures

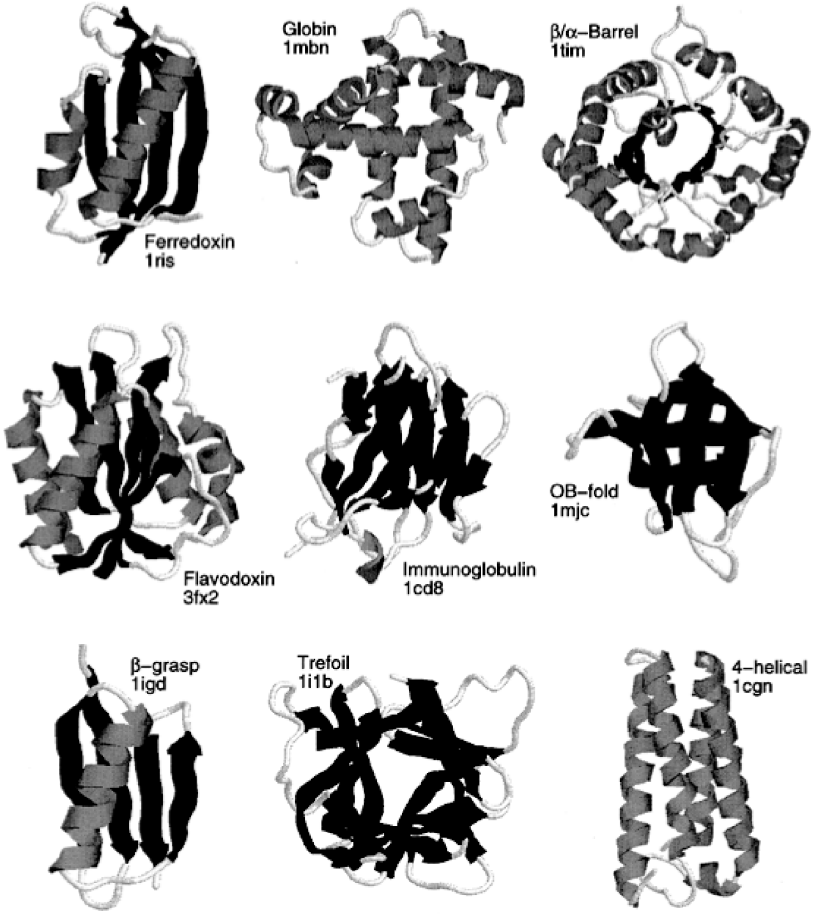
Robert Helling,[1] Hao Li,[2] Régis Mélin,[3] Jonathan Miller, Ned Wingreen, Chen Zeng,[4] and Chao Tang

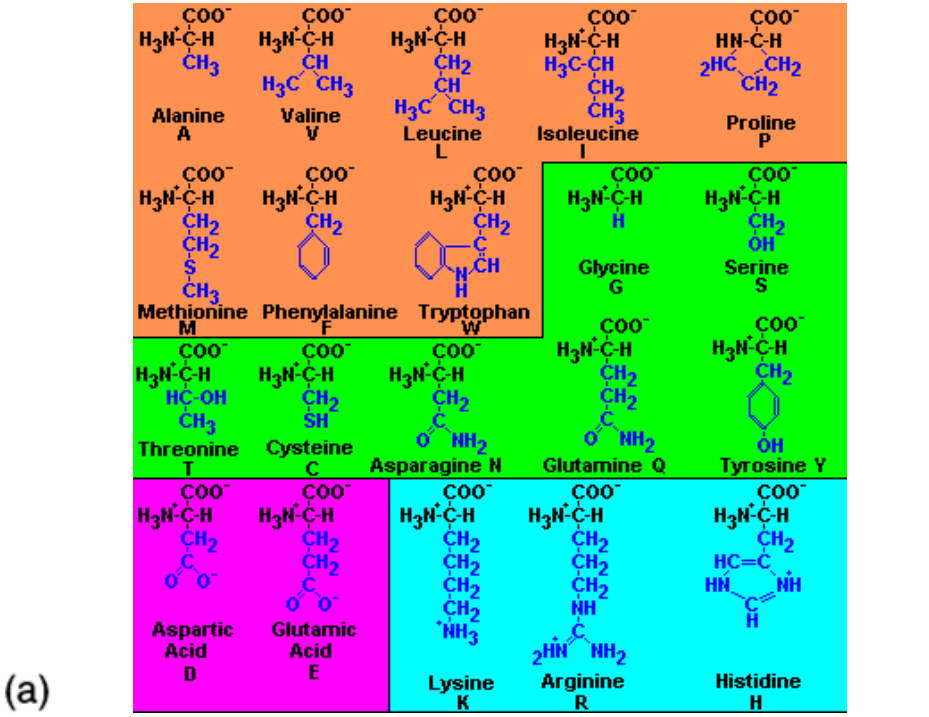
NEC Research Institute, Princeton, NJ, USA

Lattice Model of Protein Folding

Protein code = sentence with a 20-letter alphabet of amino acids = {alanine, glutamine, ...}

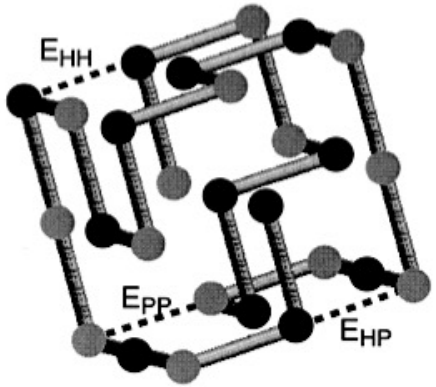
To be discovered: Principle of rapid folding codes





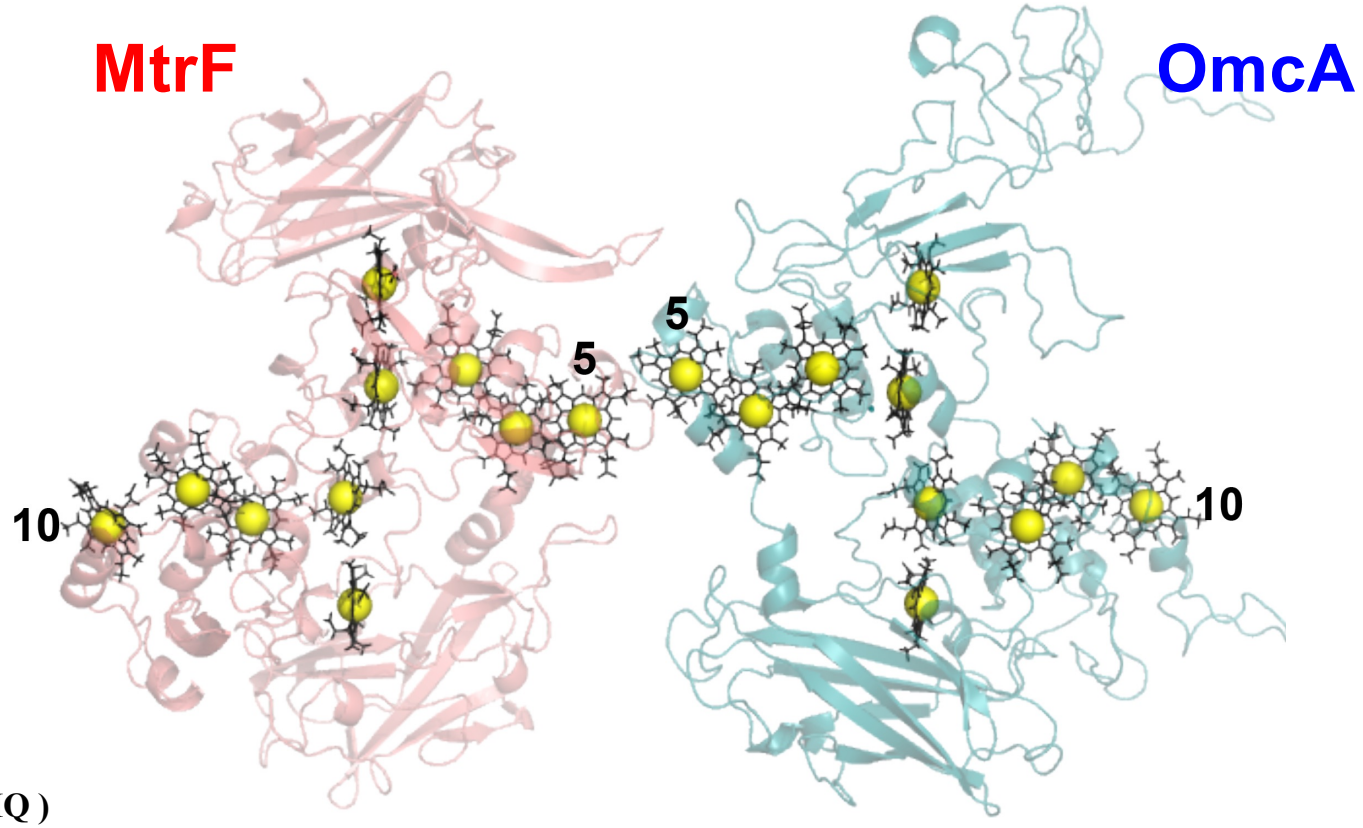
(a)

(b)



e 4. A 3D lattice HP model. A sequence of H (dark disc) and P (light disc) (a) is folded into a 3D structure (b).

MtrF-OmcA Example



MtrF (PDB file 3PMQ)

CGGSDGDDGSPGEPGKPPAMTISSLNISVDKVAISDGIAQVDYQVSNQENQAVVGIPSATFIAAQLLPQGATGAGNSSEWQHFTSETCAASCPGTFVDHKNGHYSYRFSATFNG
MNGVTFLSDATQRLVIKIGGDALADGTVLPITNQHYDWQSSGNMLAYTRNLVSIDTCNSCHSNLAFHGGRYNQVETCVTCHNSKKVSNAADIFPQMIHSKHLTGFPQSISNCQ
TCHADNPDLADRQNWYRVPTMEACGACHTQINFPAGQGHPAQTDNSNCVACHNADWTANVHSNAAQTSALAQFNASISSASMDANGTITVAVSLTNPTTGTAYADSADKL
KFISDLRIYANWGTSFDYSSRSARSIRLPESTPIAGSNGTYSYNISGLTVPAGTESDRGGLAIQGRVCAKDSVLVDCSTELAEVLVIKSSHSYFNMSALTTTGRREVISNAKCASC
HGDQQLNIHGARNDLAGQCQLCHNPNMLADATATNPSMTSFDFKQLIHGLHSSQFAGFEDLNYPGNIGNCAQCHINDSTGISTVALPLNAAVQPLALNNGTFTSPIAAVCSNC
HSSDATQNHMRQQGAVFAGTKADATAGTETCAFCHGQGTVADVLKVHPIN

OmcA (PDB file 4LMH)

CGGSDGKDGEDGKPGVVGVNINSTSTLKAKFTNATVDAGKVTVNFTLENANGVAVLGLTKDHDLRFGIAQLTPVKEKVGETEADRGYQWQAAYINAKKEPGTVPSGVDNLN
PSTQFQANVESANKCDTCLVDHGDGSYSYTYQVNVANVTEPVKVTYSADATQRATMELELPQLAANAHFDWQPSTGKTEGIQTRNVVSIQACYTCHQPESLALHGGRRIDIE
NCASCHTATSGDPESGNSIEFTYMIHAIHKGGERHTFDATGAQVPAPYKIIGYGGKVIDYGKVHYPQKPAADCAACHVEGAGAPANADLFKADLSNQACIGCHTEKPSAHHSS
TDCMACHNATKPYGGTGSAAKRHGDVMKAYNDSLGYKAKFSNIGIKNNALTFDVQILDNKDQPIGKEFISDPSAYTKSSIYFSWGIDKDYPAYTAGSRYSDRGFALSNSKVST
YNEATKTFTIDSTNSNLKLPADLTGMNVELYAGVATCFNKGGYGVEDVVATPCSTDTRYAYIQDQPFRFKWNGTDTNSAAEKRRAIIDTAKCSGCHNKEIVHYDNGVNCQA
CHTPDKGLKTDNTYPGTKVPTSFAWKAHESEGHYLKYAGVQSGTVLKTDCATCHTADKSNVVTGIALGRSPERAWLYGDIKNNGAVIWVSSDAGACLSCHQKYLSDAAKS
HIETNGGILNGTSAADVQTRASESCATCHTPSQLMEAHGN

Recursive Algorithm of Folding?

Optimal structure for 2D lattice model

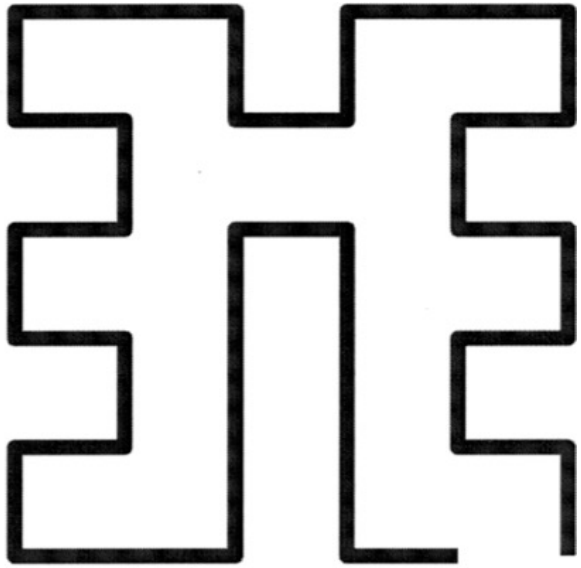
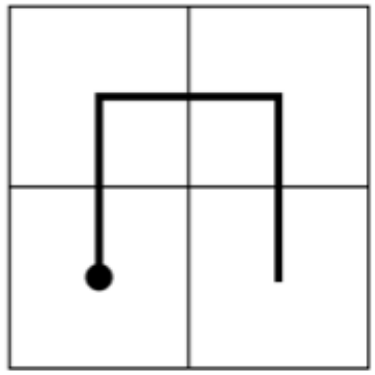
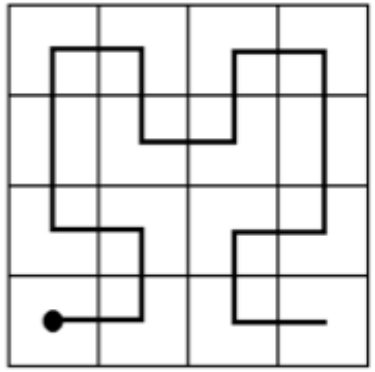


Figure 8. The top structure for the 2D 6 × 6 system.

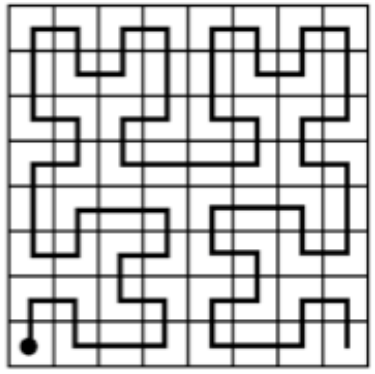
level 1



level 2



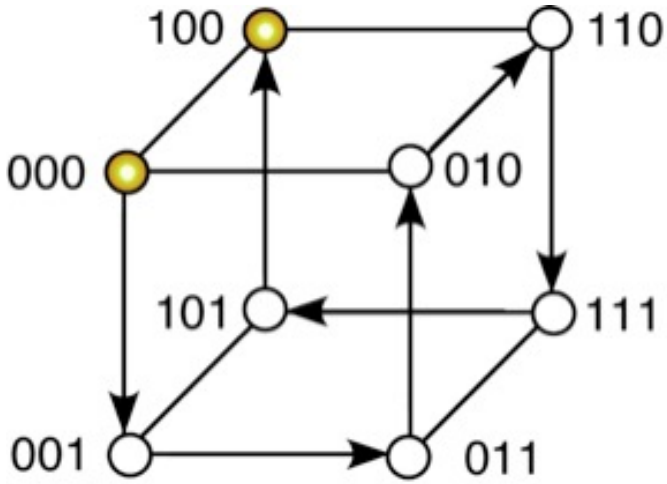
level 3



2D Hilbert (spacefilling) curve

Hilbert Curve

- **Recursive algorithm for k-bit Gray code**
  (1) G(1) is a sequence: 0 1.
  (2) G(k+1) is constructed from G(k) as follows.
    a. Construct a new sequence by appending a 0 to the left of all members of G(k).
    b. Construct a new sequence by reversing G(k) and then appending a 1 to the left of all members of the sequence.
    c. G(k+1) is the concatenation of the sequences defined in steps a and b.
- **Gray code keeps Hamming distance 1 for successive elements**
- **Used for embedding 1D list in *n*-D space, preserving spatial proximity of consecutive list elements**



Spacefilling Curve for Data Compression

Computer Physics Communications 131 (2000) 78–85

Computer Physics Communications

www.elsevier.nl/locate/cpc

Scalable I/O of large-scale molecular dynamics simulations: A data-compression algorithm

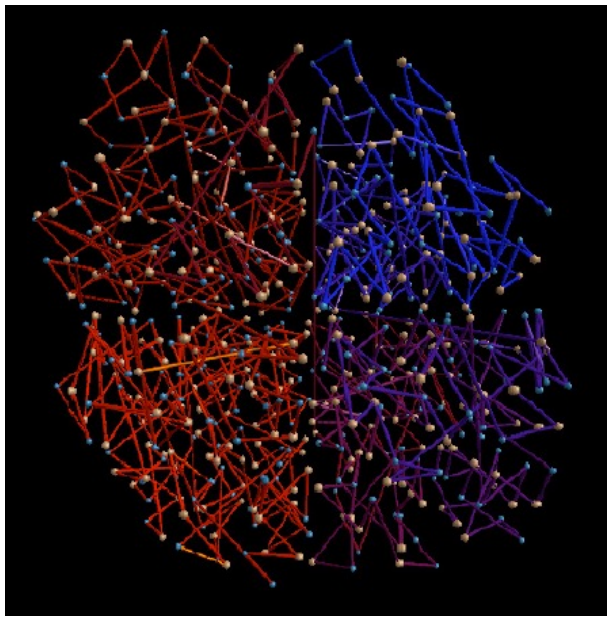
Andrey Omeltchenko, Timothy J. Campbell, Rajiv K. Kalia, Xinlian Liu, Aiichiro Nakano *, Priya Vashishta

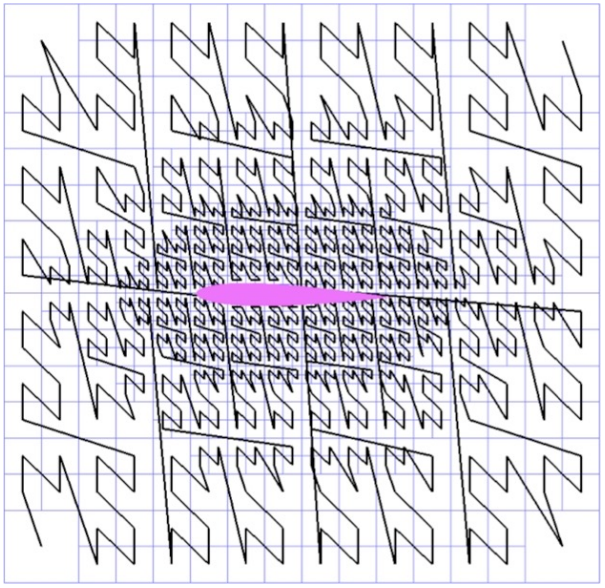
Concurrent Computing Laboratory for Materials Simulations, Department of Computer Science, Department of Physics and Astronomy, Louisiana State University, Baton Rouge, LA 70803-4020, USA

Received 28 December 1999

Abstract

Disk space, input/output (I/O) speed, and data-transfer bandwidth present a major bottleneck in large-scale molecular dynamics simulations, which require storing positions and velocities of multimillion atoms. A data compression algorithm is designed for scalable I/O of molecular dynamics data. The algorithm uses octree indexing and sorts atoms accordingly on the resulting space-filling curve. By storing differences of successive atomic coordinates and using an adaptive, variable-length encoding to handle exceptional values, the I/O size is reduced by an order-of-magnitude with user-controlled error bound.





Also used for load balancing in parallel computing, compiler optimization, *etc*.

Hilbert Curve for NP-Complete Problem

PHYSICAL REVIEW
LETTERS

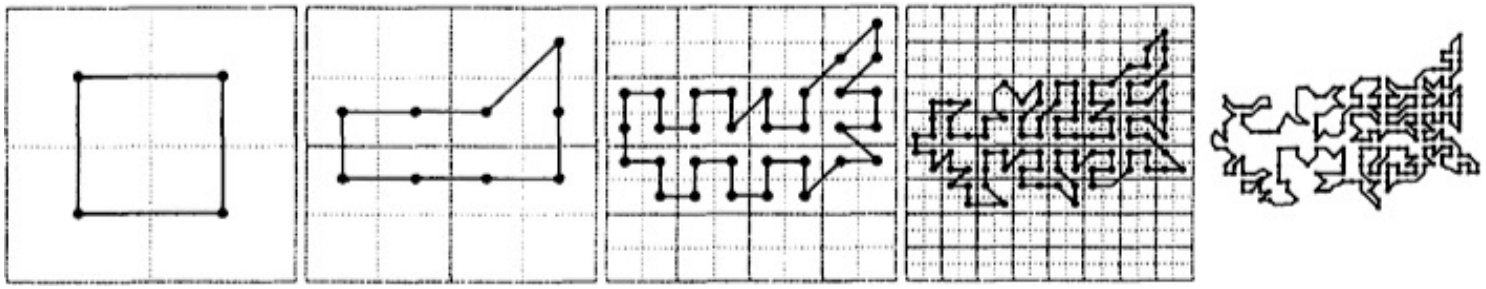
VOLUME 75 | 28 AUGUST 1995 | NUMBER 9

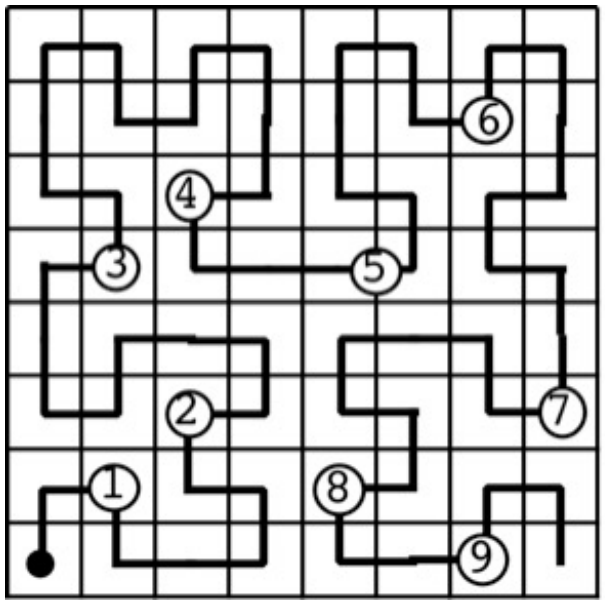
New Method of Solving the Traveling Salesman Problem Based on Real Space Renormalization Theory

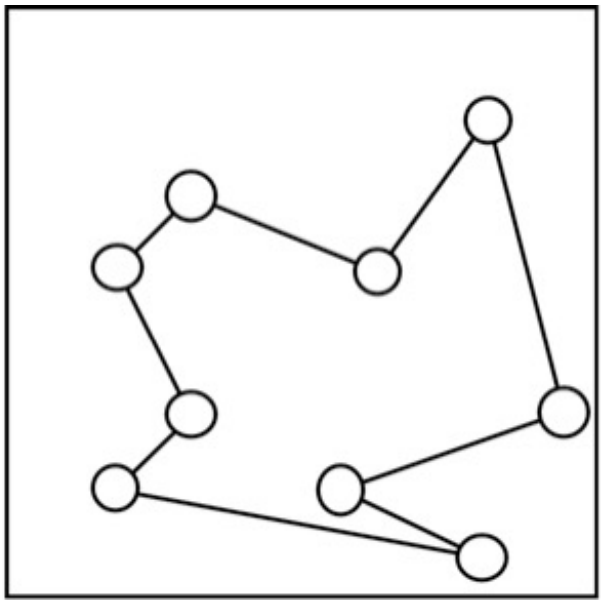
Usami Yoshiyuki[1,*] and Kano Yoshiki[2]

[1]*Institute of Physics, Kanagawa University, Rokkakubashi 3-27-1, Kanagawa-ku, Yokohama 221, Japan*
[2]*Department of Electrical Engineering, Kanagawa University, Rokkakubashi 3-27-1, Kanagawa-ku, Yokohama 221, Japan*

Phys. Rev. Lett. **75**, 1683 ('95)





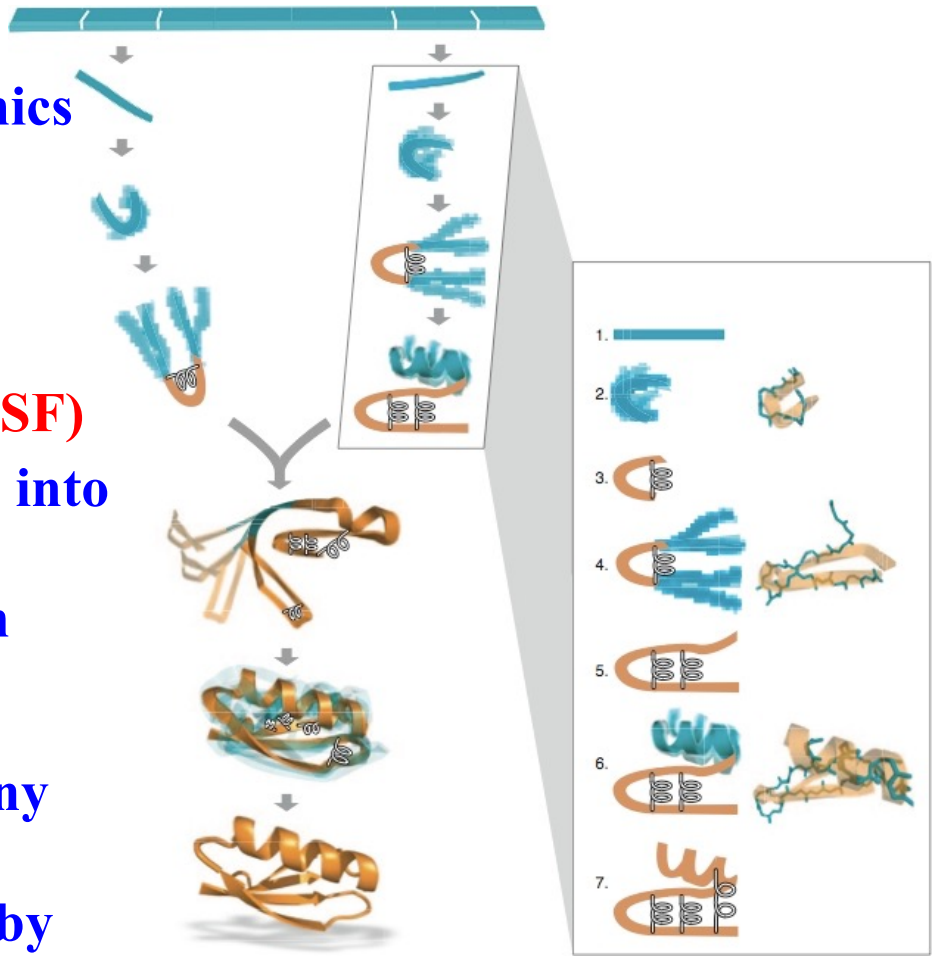


Divide-&-Conquer Protein Folding

- **Levinthal paradox (1968): How the Nature folds an amino-acid sequence into a global energy minimum 3D structure (which is known to be NP complete) within microseconds (~ billion molecular-dynamics steps).**
- **Sequential kinetic Monte Carlo not good enough.**

Zip-&-assembly algorithm (Ken Dill at UCSF)

1. **(Divide) Chop the amino-acid sequence into ~10 residue fragments.**
2. **(Conquer) For each fragment, perform replica-exchange (~ temperature accelerated) molecular dynamics simulation & detect the formation of any stable hydrophobic contacts.**
3. **(Combine) Grow the stable fragments by adding surrounding residues while freezing (~ constraint) the found stable contacts.**



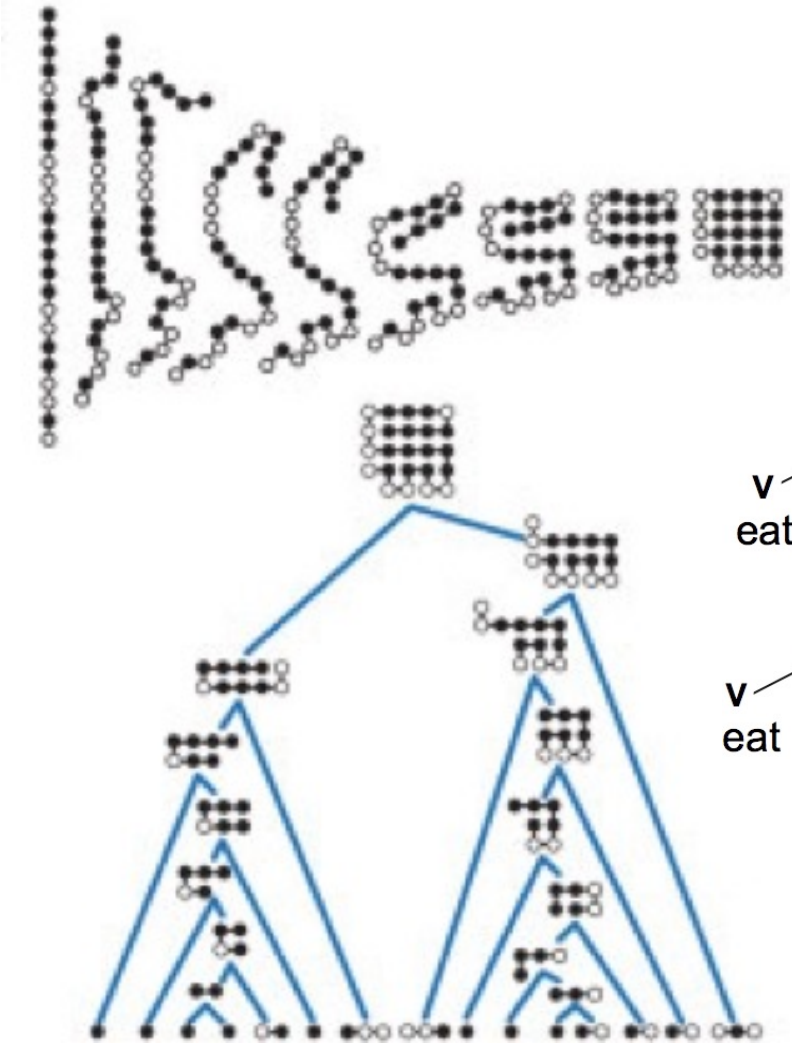
S.B. Ozkan *et al.*, *PNAS* **104**, 11987 ('07)

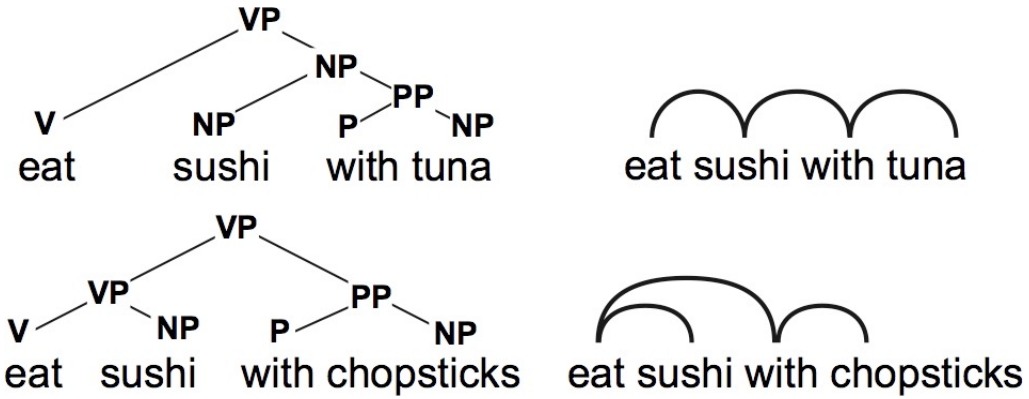
Parsing Protein-Folding Routes

Computational linguistics

(1) Formal grammar to describe protein-folding routes

(2) Dynamic programming for an efficient algorithm for the folding routes





K. A. Dill *et al.*, *Polymer* **48**, 4289 ('07)

Disconnectivity Graph

The topology of multidimensional potential energy surfaces: Theory and application to peptide structure and kinetics

Oren M. Becker
School of Chemistry, Tel Aviv University, Ramat Aviv, Tel Aviv 69978, Israel and Department of Chemistry, Harvard University, Cambridge, Massachusetts 02138

Martin Karplus
Department of Chemistry, Harvard University, Cambridge, Massachusetts 02138 and Laboratoire de Chimie Biophysique, Institut Le Bel, Université Louis Pasteur, 67000 Strasbourg, France

J. Chem. Phys. **106** (4), 22 January 1997 0021-9606/97/106(4)/1495/23/$10.00

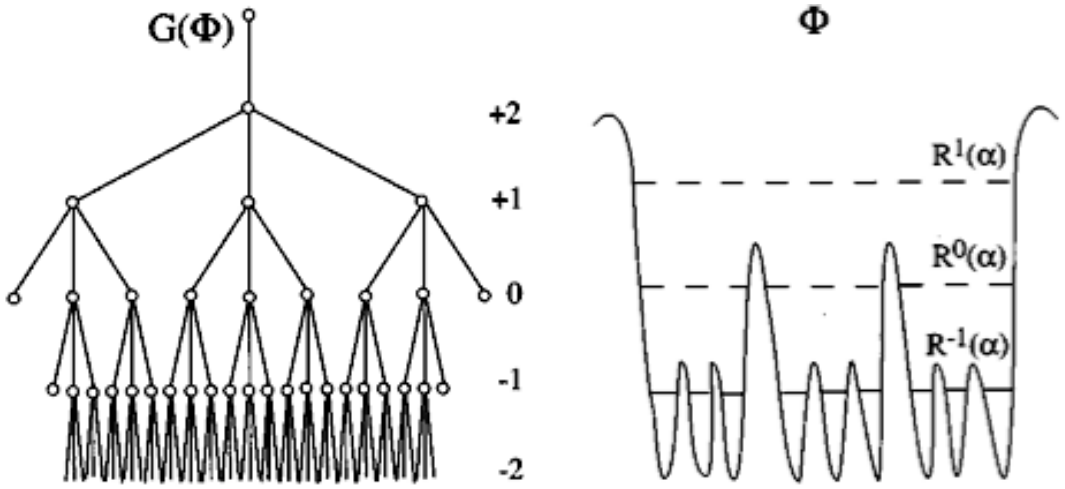
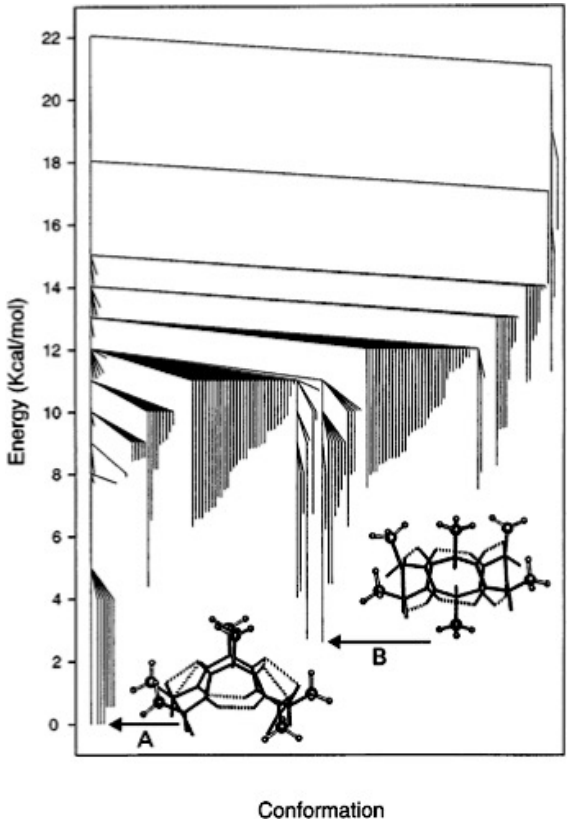


FIG. 2. A schematic one-dimensional partial cross section through a rough $3N$-dimensional potential energy hypersurface Φ (triadic Koch curve). The horizontal lines on the PES Φ correspond to the energies used by the map $M^a(\mathbf{r};E)$ to define the $R(\alpha)$ basins. These energies determine the corresponding levels on the disconnectivity graph $G^E(\Phi)$.



Ultrametricity

Ultrametricity for physicists

R. Rammal

Centre de Recherches sur les Très Basses Températures, Centre National de la Recherche Scientifique, BP 166 X, 38042 Grenoble-Cédex, France

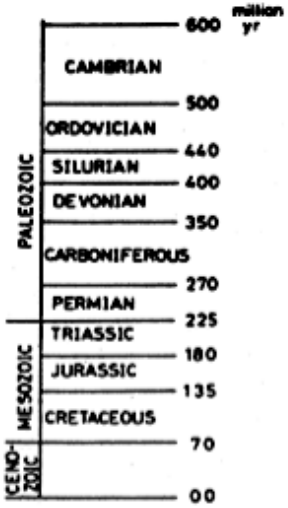
G. Toulouse

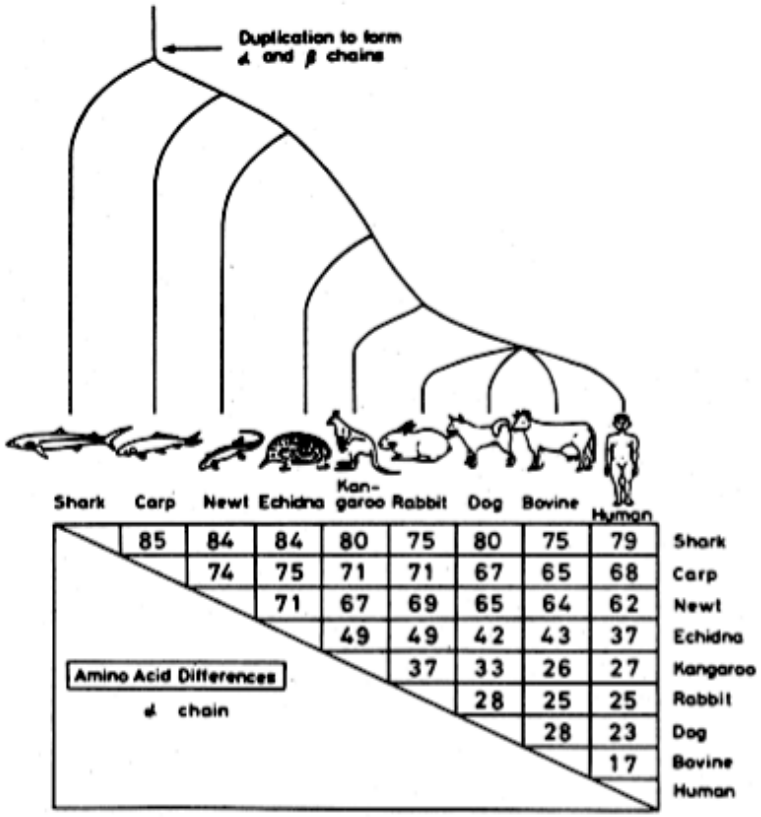
Ecole Supérieure de Physique et Chimie Industrielles, 10 rue Vauquelin, 75231 Paris, France

M. A. Virasoro

Dipartimento di Fisica, Universita di Roma I, I-00185 Roma, Italy

Ultrametricity is a simple topological concept, but its appearance in the languag
This review provides all the elementary background (from mathematics, taxonom
and surveys the main fields of development (spin glasses, optimization theory). St
are covered. From present knowledge, one can already draw some tentative cor
causes for the occurrence of ultrametric structures in nature. Some perspectives c
physics and biology are also presented.





Geometry of phylogenetic tree

Exploring Energy Landscapes

Available online at www.sciencedirect.com
ScienceDirect
Computer Physics Communications 176 (2007) 292–299
Computer Physics Communications
www.elsevier.com/locate/cpc
ELSEVIER

Pathfinder: A parallel search algorithm for concerted atomistic events

Aiichiro Nakano

Available online at www.sciencedirect.com
ScienceDirect
Computer Physics Communications 178 (2008) 280–289
Computer Physics Communications
www.elsevier.com/locate/cpc
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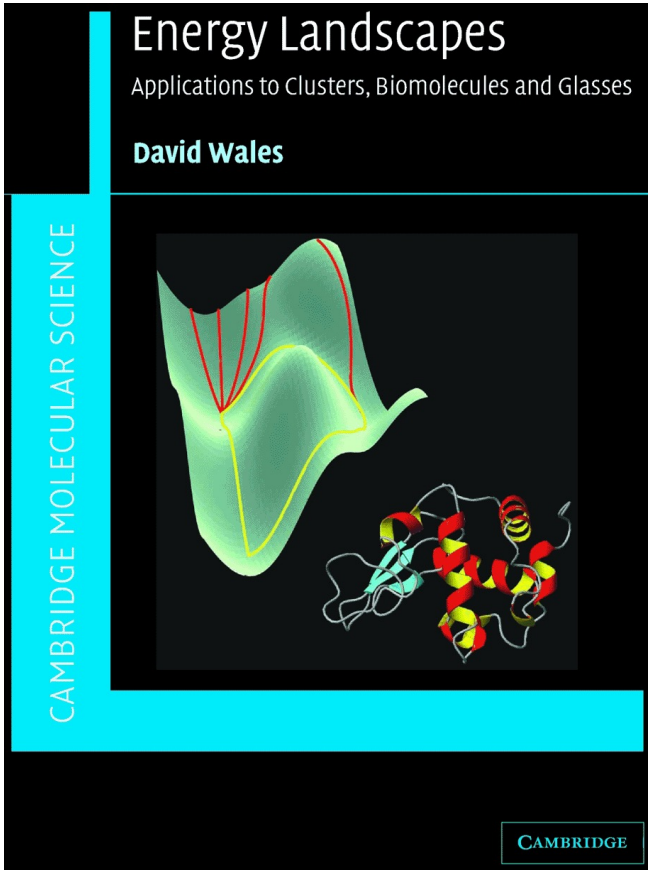
A space–time-ensemble parallel nudged elastic band algorithm for molecular kinetics simulation

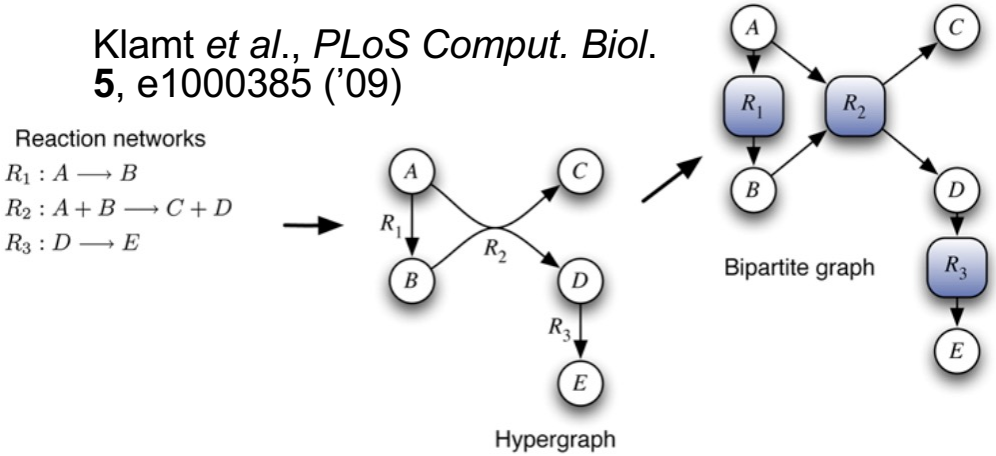
Aiichiro Nakano

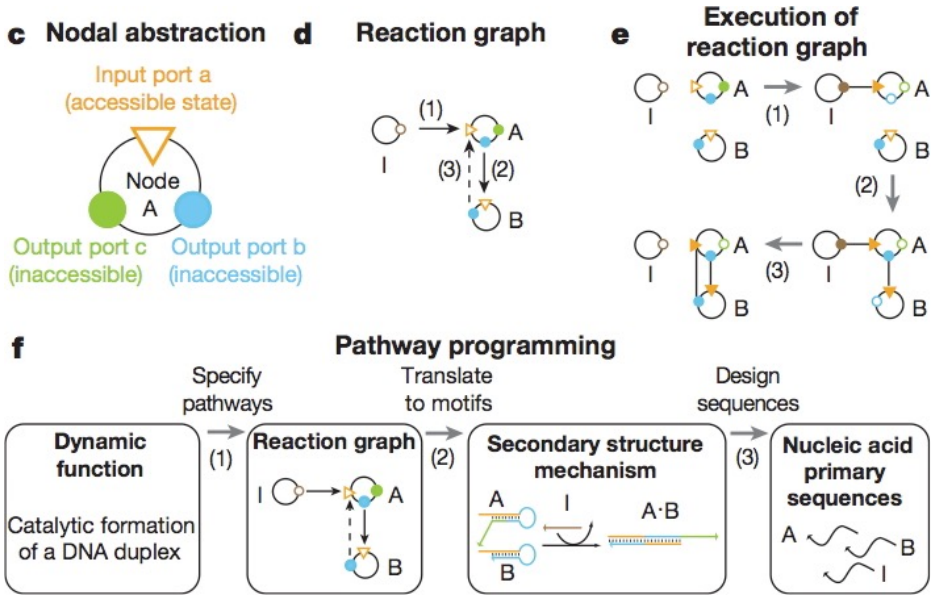


Elitist mechanics
= transition-state theory
+ discrete abstraction/combinatorial search
+ evolutionary population control

Chemical Reaction Network

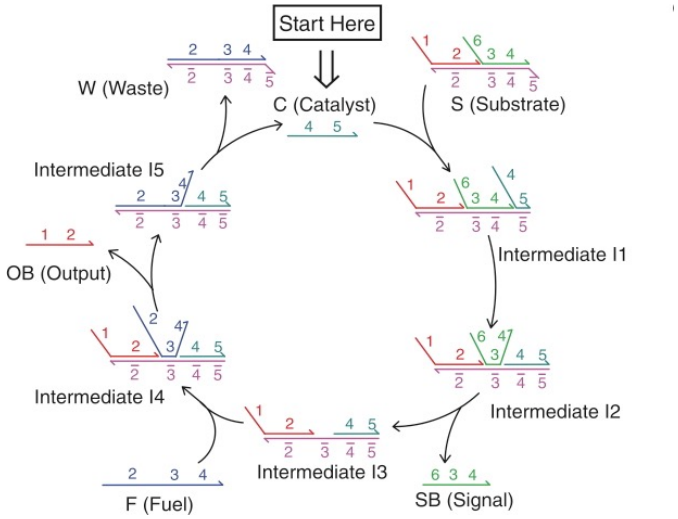
Klamt *et al*., *PLoS Comput. Biol.* **5**, e1000385 ('09)

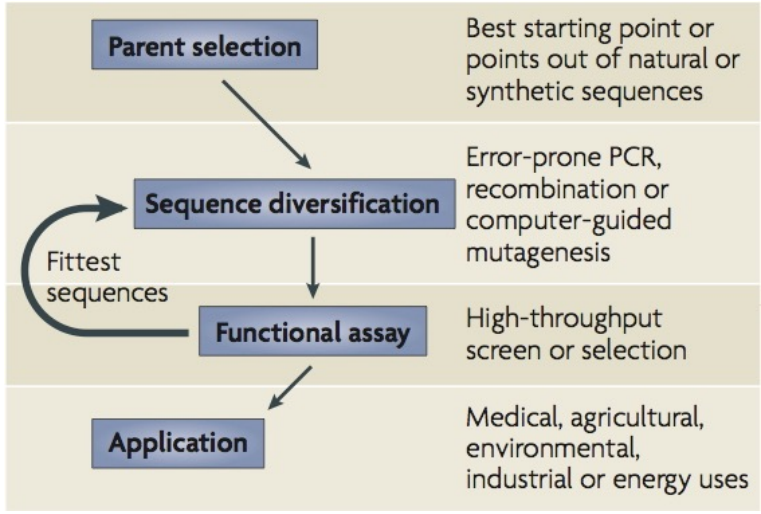


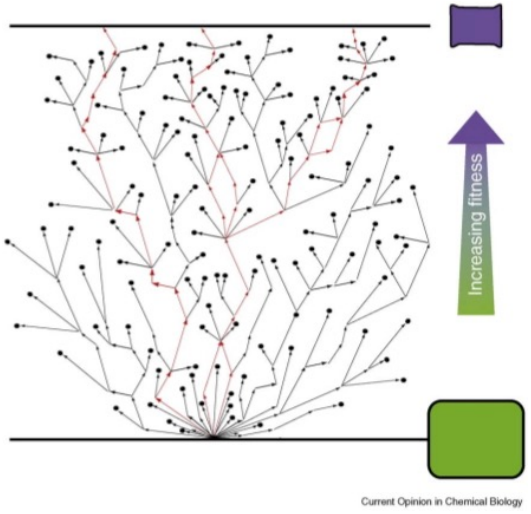


Yin et al., *Nature* **451**, 318 ('08)

Zhang *et al*., *Science* **318**, 1121 ('07)







Arnold group, *Nature Rev. MCB* **10**, 867('09); *COCB* **13**, 3 ('09)

Reaction graph = language for self-assembly & catalytic cycle design

Directed & accelerated evolution

Statistical Mechanics & Graph Theory

Mean-field approximation (heuristic from statistical mechanics) to count the number of Hamilton cycles of a graph

J. Bascle, T. Garel, and H. Orland, "mean-field theory of polymer melting," *J. Phys. A* **25**, L1323 ('92)

PHYSICAL REVIEW E VOLUME 58, NUMBER 1 JULY 1998

Field theoretic approach to the counting problem of Hamiltonian cycles of graphs

Saburo Higuchi*
Department of Pure and Applied Sciences, The University of Tokyo, Komaba, Meguro, Tokyo 153-8902, Japan
(Received 14 November 1997; revised manuscript received 3 February 1998)

A field theoretic representation of the number of Hamiltonian cycles of graphs is studied. By integrating out quadratic fluctuations around the saddle point, one obtains an estimate of a number which reflects characteristics of graphs well. The accuracy of the estimate is verified by applying it to two-dimensional square lattices with various boundary conditions. This is an example of how to extract meaningful information from the quadratic approximation of the field theory representation. [S1063-651X(98)14306-4]

Phase Transition in Computer Science

ELSEVIER

Artificial Intelligence 81 (1996) 1–15

Artificial Intelligence

Editorial

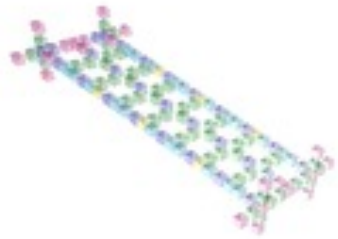
Phase transitions and the search problem

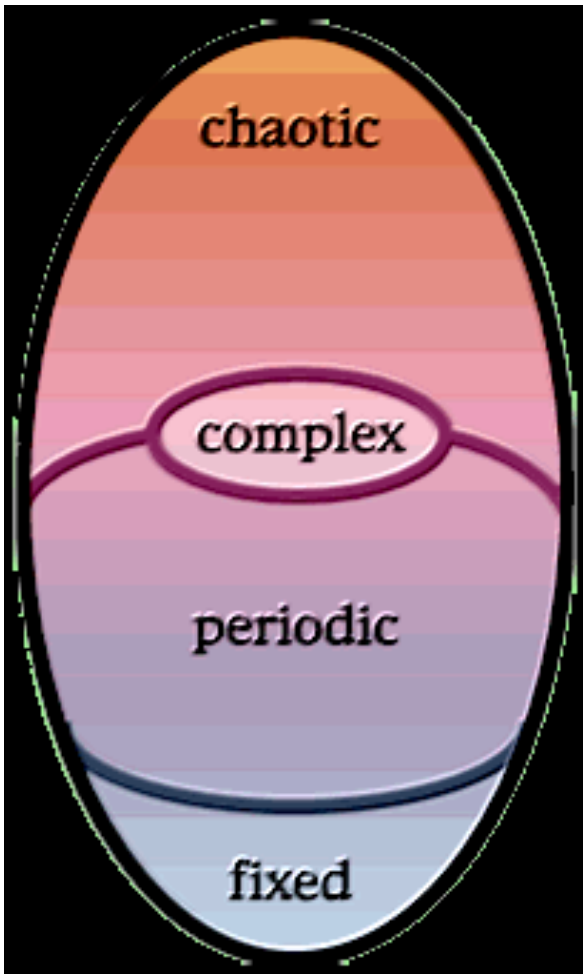
Tad Hogg [a,*], Bernardo A. Huberman [a,1], Colin P. Williams [b,2]

[a] *Dynamics of Computation Group, Xerox Palo Alto Research Center, Palo Alto, CA 94304, USA*

[b] *Knowledge Systems Lab, Stanford University, Stanford, CA 94305, USA*

"Life at the edge of chaos",
***Complexity* by M. M. Waldrop**





Artificial Life
(self-reproducing cellular automaton)