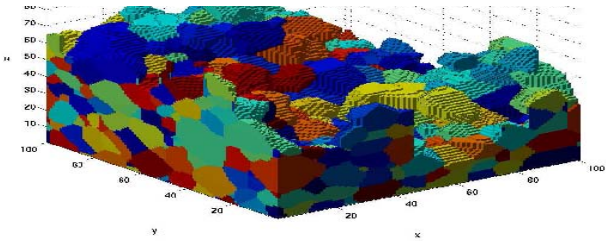
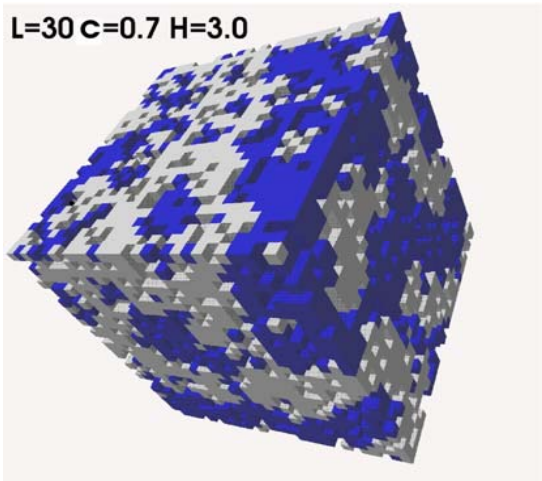
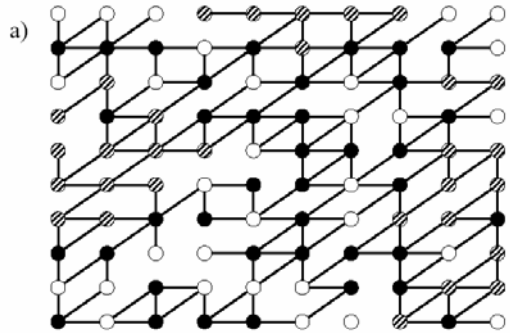
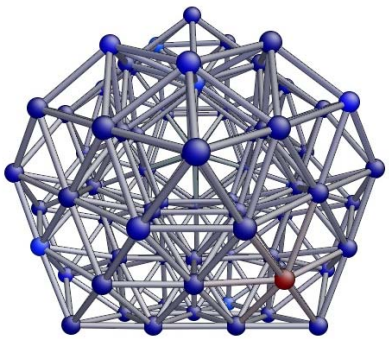
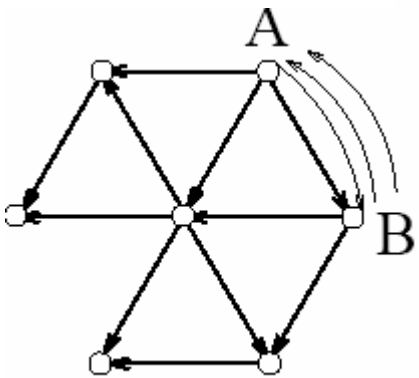
Combinatorial Optimization and Statistical Physics

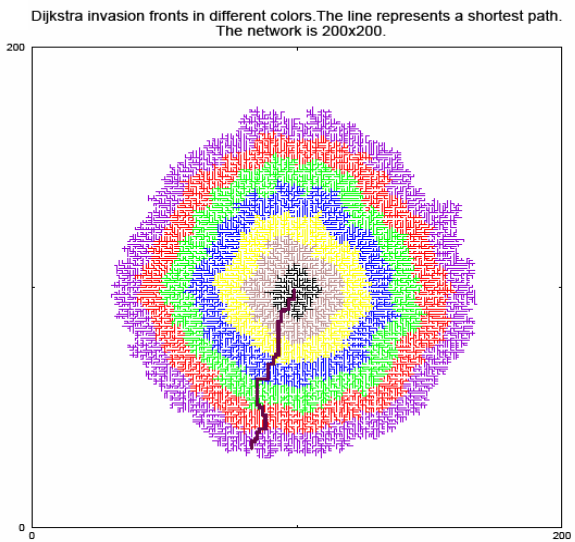












Phillip M. Duxbury, Condensed Matter Theory, MSU

Thanks to the DOE for support

Equilibrium statistical physics: Algorithmic demands

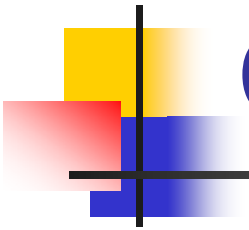
- Thermodynamic limit i.e. volume of the sample goes to infinity
- Equilibrium = Ground states or lowest free energy states
- Phase transitions : Singular behavior in the thermodynamic limit
- Complex energy landscapes, glassiness, frustration. Many competing objectives.
- Exact solutions play a key role.
- In hard problems it is relatively easy to find heuristics which get within a few percent of exact. The last few percent is really expensive due to the fact that metastable (local) minima are “far” from the true ground states – but are they statistically equivalent??
- Differences between the effect of short range and long range edges on behavior (dimensionality).

“Simple” network algorithms important in statistical physics

- Minimum spanning tree: In a network where each edge has a cost c_{ij}, a minimum spanning tree is a spanning tree which has minimum total cost. (Prim’s algorithm)
- Shortest path between two points: In a network where each edge has a cost c_{ij}, a shortest path is a path on which the sum of the edge weights Is smallest. (Dijkstra’s algorithm – positive costs)
- The maximum s-t flow in a network: In a network where each edge has flow capacity u_{ij}, the maximum s-t flow through the network is the maximum flow possible between the source s and the target t, given the capacities u_{ij}. When a maximum flow occurs through the network, there is a cut on which the network capacities are saturated. This cut a minimum cut. (Augmenting paths, push-relabel)

Other algorithms widely used in statistical physics

- Search (Breadth first, depth first)
- Matching algorithms
- Convex optimization (also integer flows)
- Genetic algorithms
- Belief propagation (Survey propagation-Zecchina)
- Branch and cut (Cologne spin glass server)
- Tournaments (Liga)



Outline

- Some History (Ising models)
- A. Percolation (Rigidity, Bootstrap...)
- B. Applications of network optimization methods
  - Paths and chains
  - Surfaces and interfaces
  - Domain structures
- C. Nanostructure determination
- D. Hard core lattice gas problems

Ising Models - Definition

- General spin half Ising model in a field. Defined on a lattice or graph where sites are indexed by i or j. The energy is given by,

$$E = -\Sigma_{ij} J_{ij} S_i S_j - \Sigma_i (h_i + H) S_i,$$

Where spins $S_i = +1$ or -1 (ie a **binary** variable), J_{ij} is the exchange coupling between spins, H is an applied field and h_i is a local field.

Brief Ising Algorithm History

- The general Ising model partition function can be written as a problem of counting dimer coverings or equivalently perfect matchings on a graph, ie it is number complete in general (Kasteleyen, Fisher, Temperley 1960's, Zecchina).
- The square lattice Ising model partition function can be written as a finite sum of determinants, so it is polynomial for general couplings and analytically solvable for some special cases.
- The ground state of the general Ising spin glass is NP-complete (Barahona 1982, Istrail STOC 2000)
- The ground state of the square lattice spin glass can be solved using a matching algorithm – solvable in polynomial time (Bieche et al. 1980).
- The ground state of the random field Ising model maps to the min-cut/max-flow problem (Ogielski 1986). This procedure can also be used to solve the diluted antiferromagnetic in an applied field which is a key experimental system.
- Domain walls in Ising ferromagnets, at zero temperature, can be found using min-cut/max-flow (Middleton 1995, Alava and Duxbury 1996)

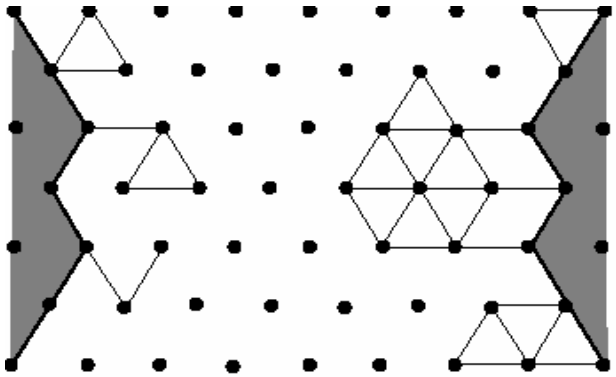
A. Three percolation problems

- Connectivity percolation: Does a connected path exist between points separated by large distances? Does an extensive giant cluster exist? Breadth first search, biconnected components (burning algorithm).
- Rigidity percolation: Can a truss network support an applied stress. In 2-d maps to bipartite matching in (Hendrickson 1992).
- Bootstrap percolation: The same as k-core percolation. i.e. sites which have k neighbors are stable, all other sites are culled (recursively)

Rigidity percolation: How many edges are required to make a graph rigid?

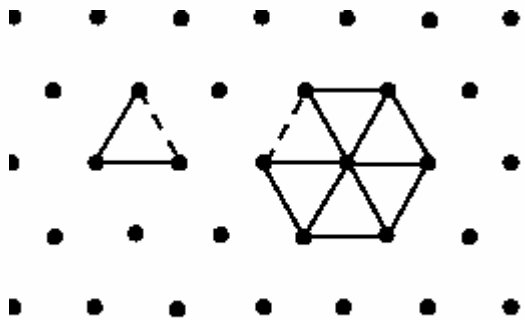
- Consider a graph consisting of nodes and edges where the edges are replaced by stiff Hookian springs. The Hookian springs yield stiff central force constraints, but they are freely rotatable.
- **The graph rigidity problem seeks to identify the combinatorial conditions for subgraphs to be overconstrained, isostatic or underconstrained. i.e. use counting to find rigid clusters**

Comparison of connectivity and rigidity percolation on triangular lattices



Left: Connected to the substrate

Right: Rigidly connected to the substrate



Redundant edges (dashed)

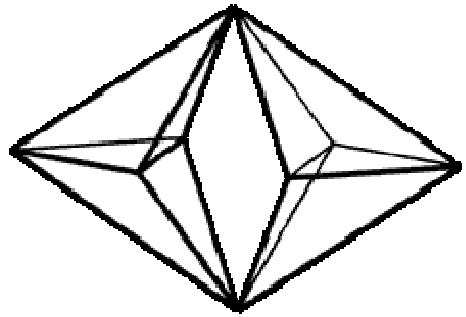
Left: Connectivity

Right: Rigidity

Combinatorial rigidity: e.g. counting constraints in a 2d bar-joint network

- James Clerk Maxwell analyzed the rigidity of truss networks by comparing the number of degrees of freedom in the network with the number of constraints. For example for a planar network each node has two degrees of freedom. If there are B edges then, if all edges are independent, the number of internal floppy modes is $F = 2N - 3 - B$. However some edges are redundant (dependent), so a more complete formula is
- $F = 2N - 3 - B + R$
- If we have a fast algorithm to find R, then some important problems are solved.
- Two books: Combinatorial Rigidity, Graver, Servatius, Servatius, AMS; Rigidity theory and applications, Thorpe and Duxbury eds, Plenum.

Two theorems and a conjecture



Laman's theorem (1970): A graph (V,E) is rigid for dimension 2 if And only if:

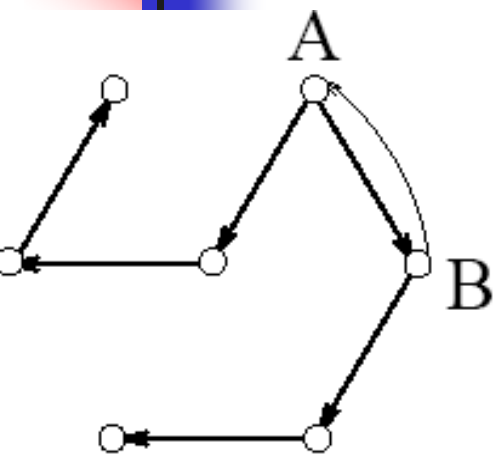
1. $|E| = 2|V|-3$
2. There a no redundant bonds

Tay-Whiteley theorem (1980's): Generalized Laman's theorem to body-bar networks in arbitrary dimensions (body-bar networks don't have bananas! – see figure)

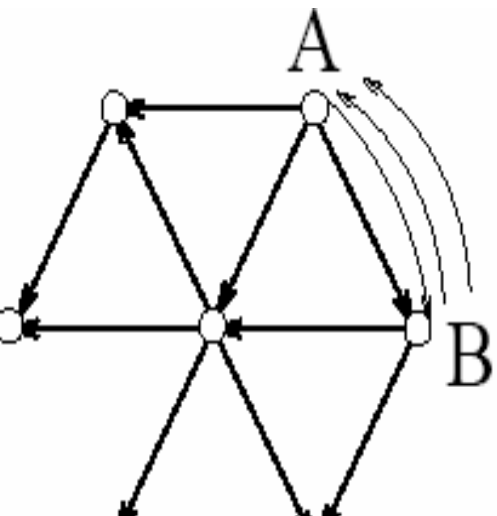
Molecular Framework conjecture(1980's Tay-Whiteley) : Molecular networks with strong bonding bending forces but freely rotatable dihedral degrees of freedom are solved by an extension of Laman's theorem: Applications to molecular glasses and proteins (See Thorpe Talk)

Matching algorithm

Hendrickson (1992): If matching fails, edge is redundant. Number of redundant edges acts like a free energy for rigidity percolation



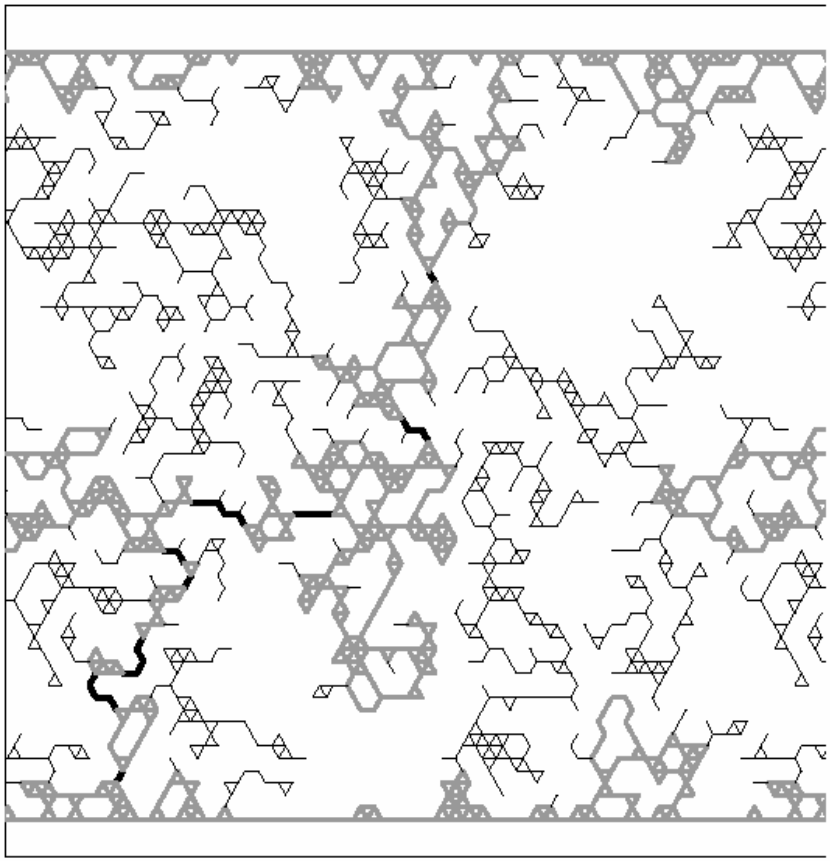
Connectivity: Each node has at most one arrow (edge) pointing to it.



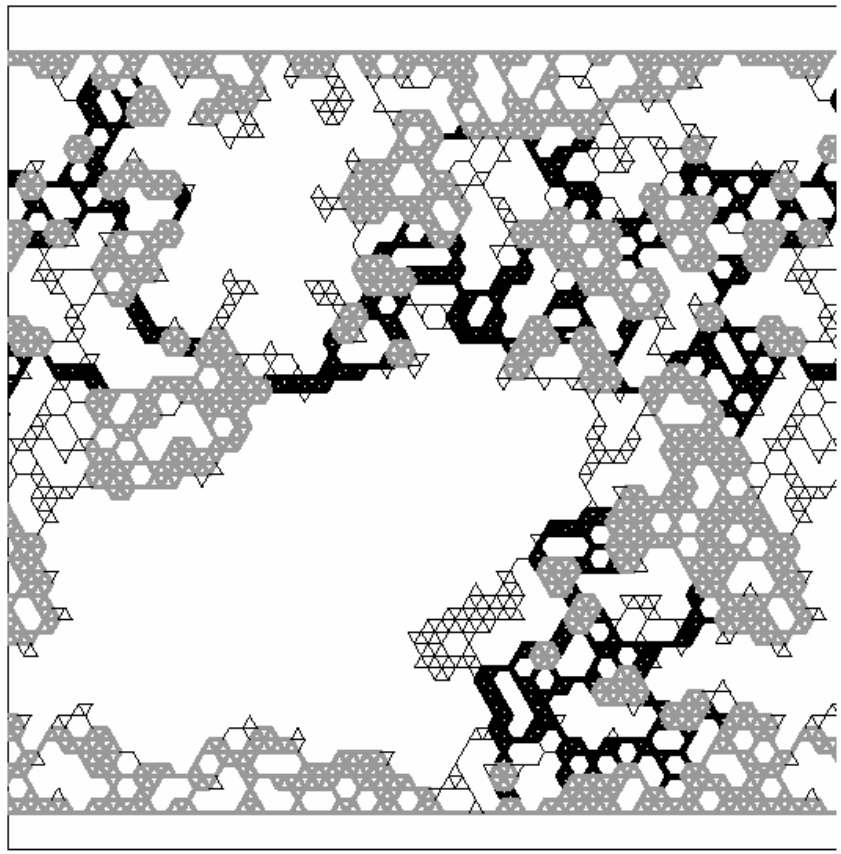
Rigidity: Each node has at most two arrows (edges) pointing to it.

Percolating geometries: Triangular lattices: 10^7 nodes on a pc

Connectivity



Rigidity



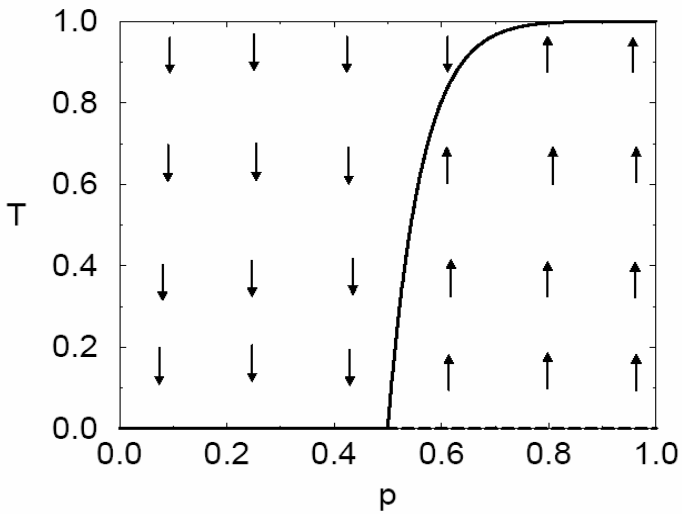
Moukarzel and Duxbury Phys. Rev. Letts. 1995,

Jacobs and Thorpe Phys. Rev. Letts. 1995.

Phase transitions: Random graphs with fixed maximum co-ordination(z)

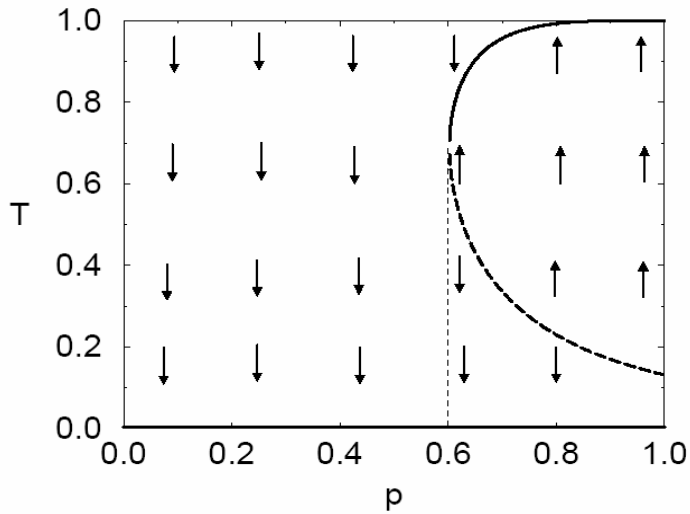
Connectivity:

Z=3, g=1



Rigidity

Z=6, g=2



Rigidity percolation is first order on random graphs;

g = number of degrees of freedom per node

Duxbury et al. Phys. Rev. E, 1997, 1999

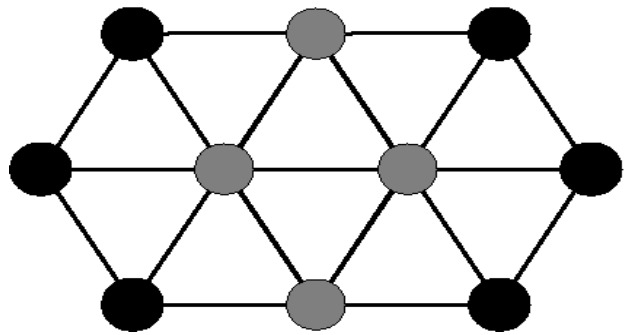
m-Bootstrap percolation =k-core percolation: e.g. Triangular lattice

Nodes are stable provided they are k co-ordinated.

Nodes which have co-ordination less than k are culled recursively

Elementary avalanches:

Start with a fully bonded triangular lattice then:

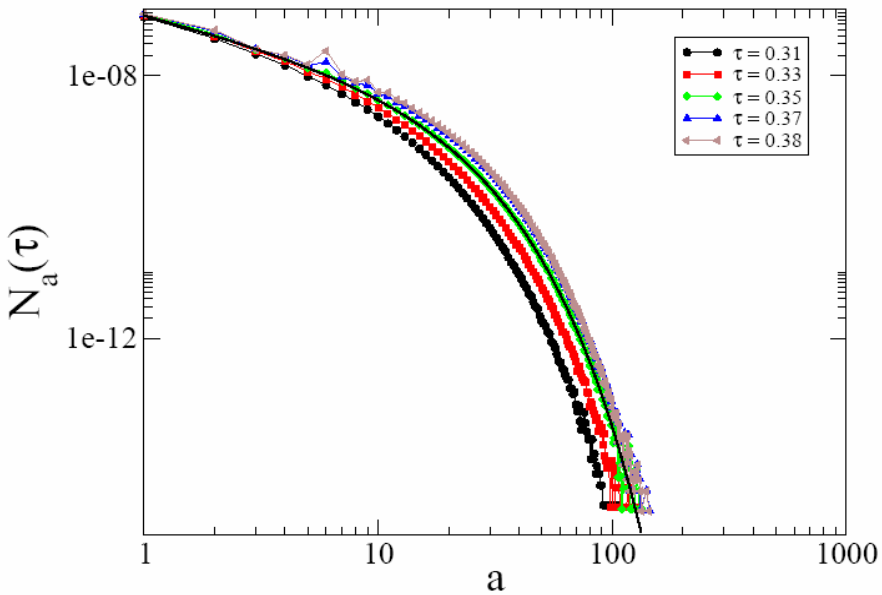


Remove a node randomly and recursively cull all unstable sites. The number of sites culled is an elementary avalanche

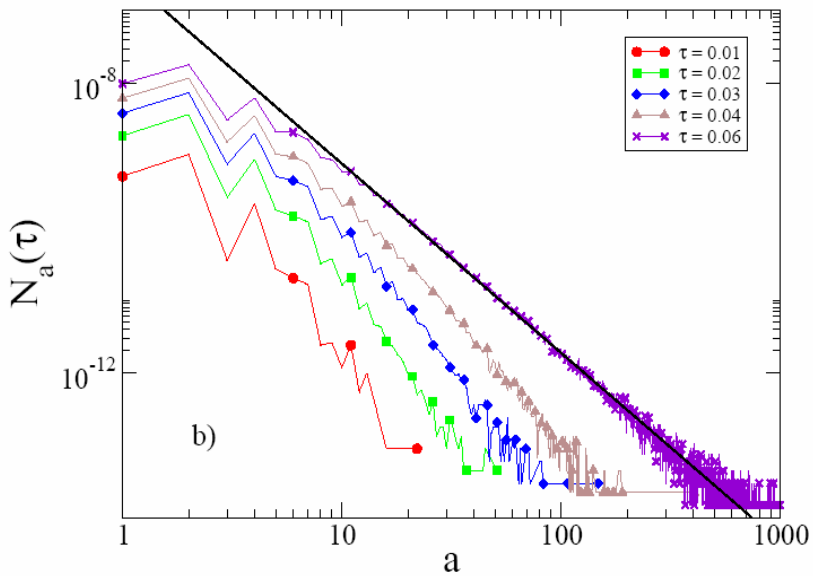
Farrow and Duxbury Phys. Rev. E. 2006

Cumulative avalanche distributions: Triangular lattices

k=3



k=4



Farrow and Duxbury

Phys. Rev. E. 2006

Results for regular lattices and random graphs

- On regular lattices of co-ordination z, bootstrap (k-core) percolation is second order for $2<k<z/2+1$, with a finite threshold. k-core percolation is first order for $k>z/2$ and in this case the threshold, p_c goes to one though for $k=z/2$ with slow finite size effects (metastability)
- On random graphs k-core is first order for $k>2$ and has a finite threshold for all $k<z$.
- In second order cases elementary avalanches are small and the cumulative avalanche distribution is weaker than power law.
- In first order cases the elementary avalanches are large and the cummulative avalanche distribution is a power law with an exponent close to 5/2, numerically.

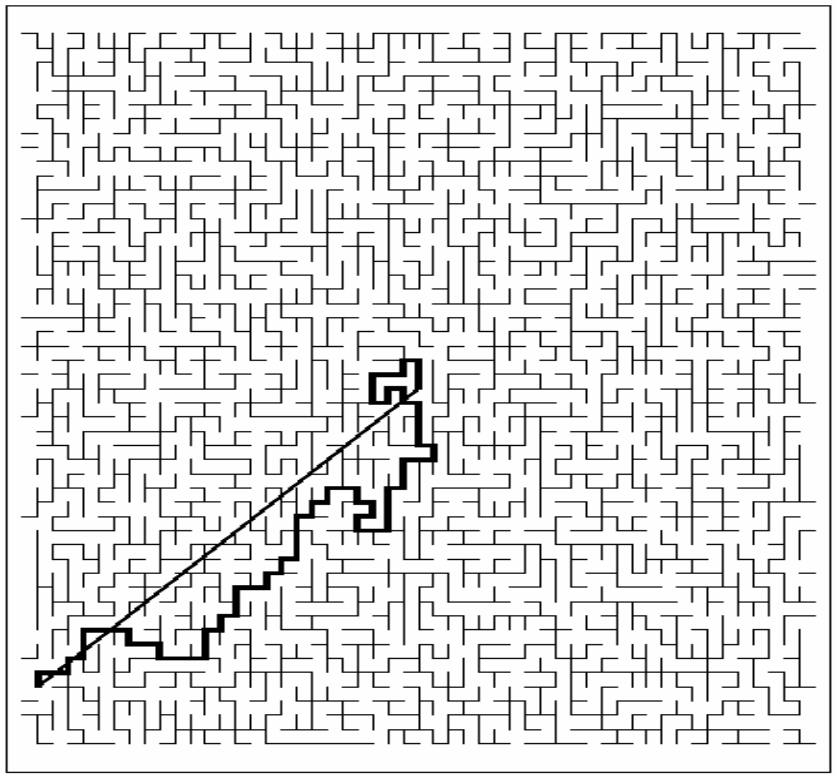
B. Network optimization problems and their applications

- Minimum spanning tree
- Shortest path
- Min-cut/Max-flow
- Convex optimization

  continuous flows

  integer flows

Minimum spanning tree: Square lattice with random edge weights



Paths on minimum spanning trees have the lowest barriers

Paths are fractal

$N \sim R^y$

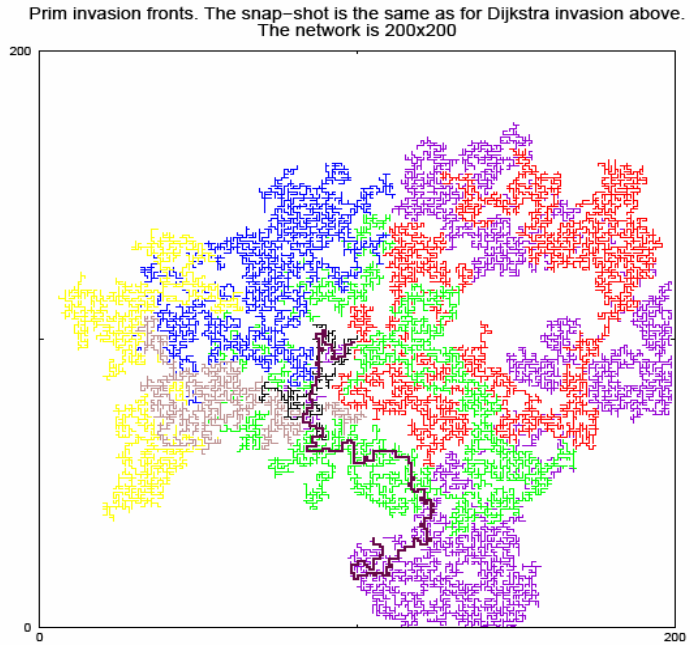
y=1.22 (1) (square)

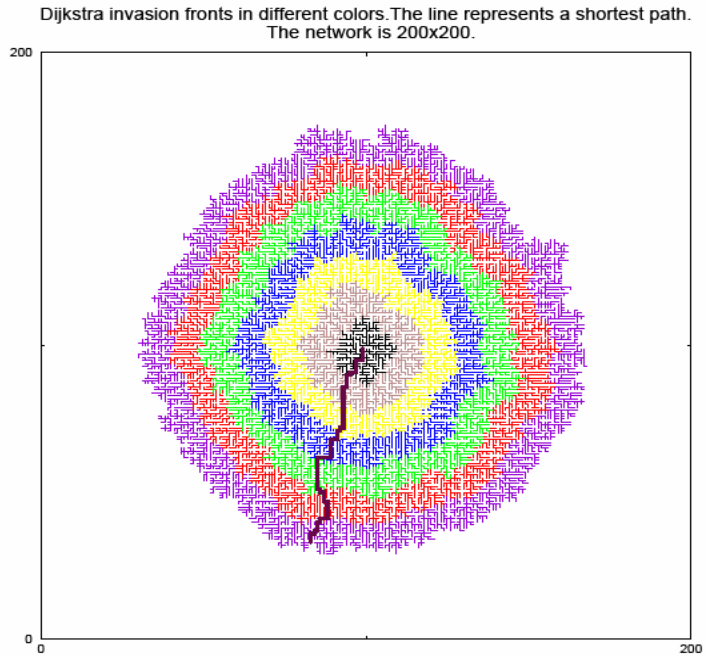
y= 1.41 (2) (Cubic)

Dobrin, Duxbury, Phys. Rev. Letts. 2001

Path exponent is independent of disorder distribution

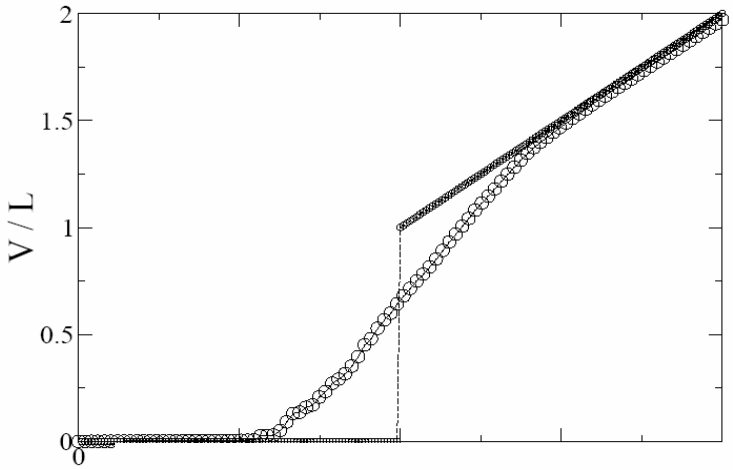
Growth of paths, Prim and Dijkstra on a square lattice with random positive edge weights





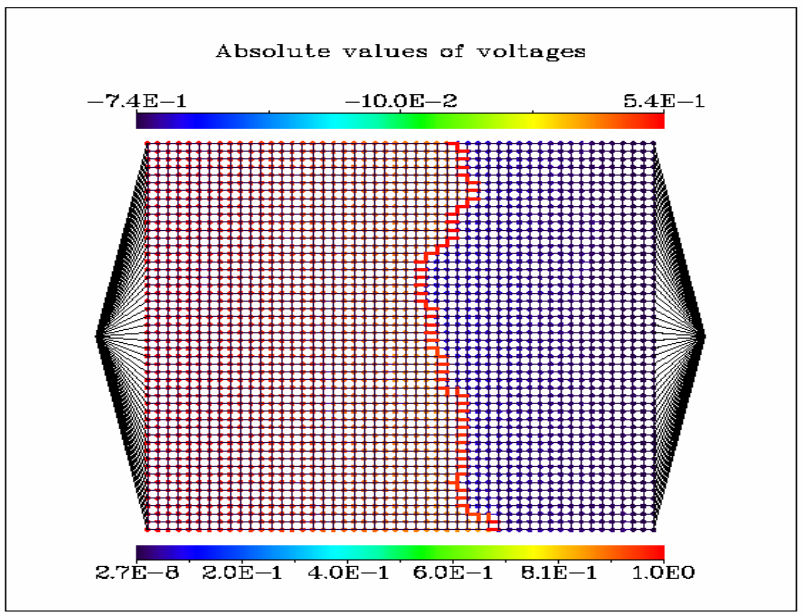
PRIM is the same as invasion percolation, Dijkstra paths for weak disorder have roughness; $w \sim R^{2/3}$

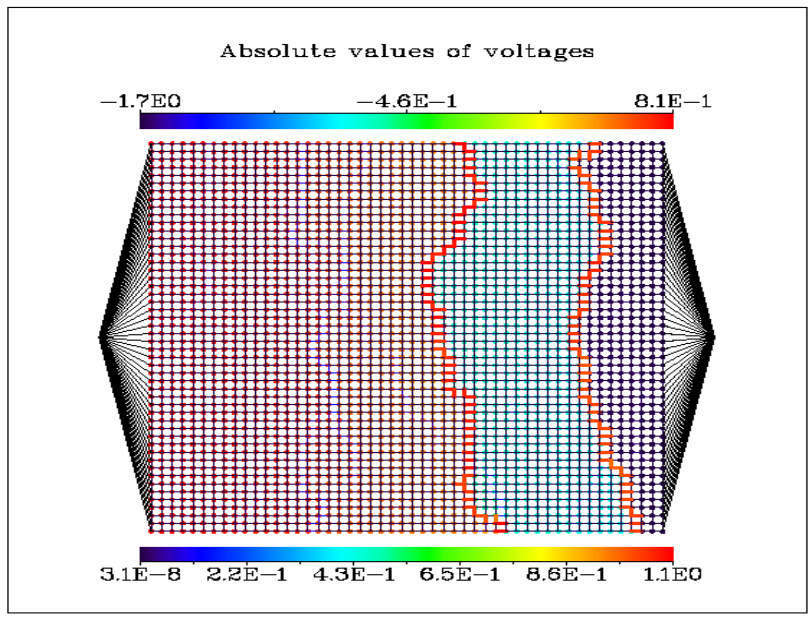
Alava, Duxbury, Moukarzel, Rieger, Domb and Lebowitz Vol 18.

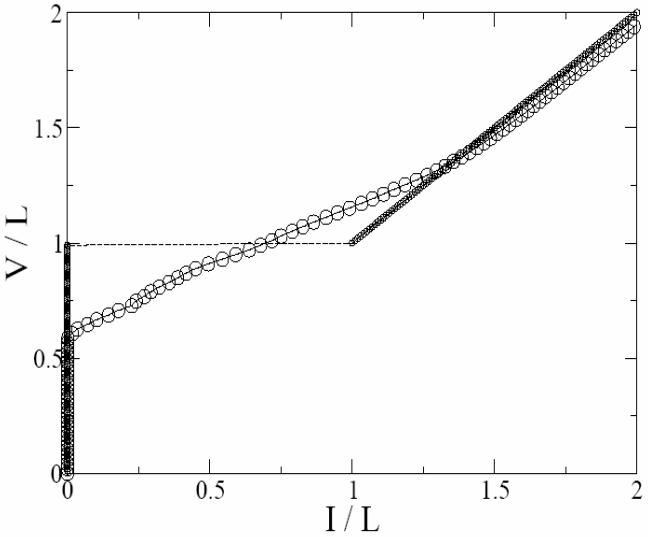


Voltage localization in Superconductor nets: Random critical current on each edge

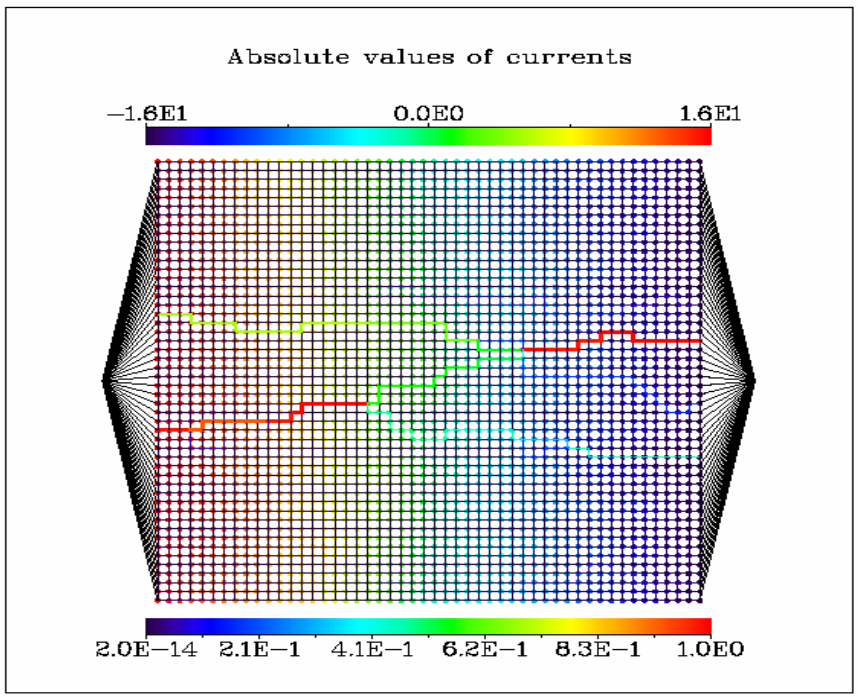
Donev, Musolff, Duxbury, J. Phys. A 2001, Duxbury et al, Mechanics of Materials 2006.

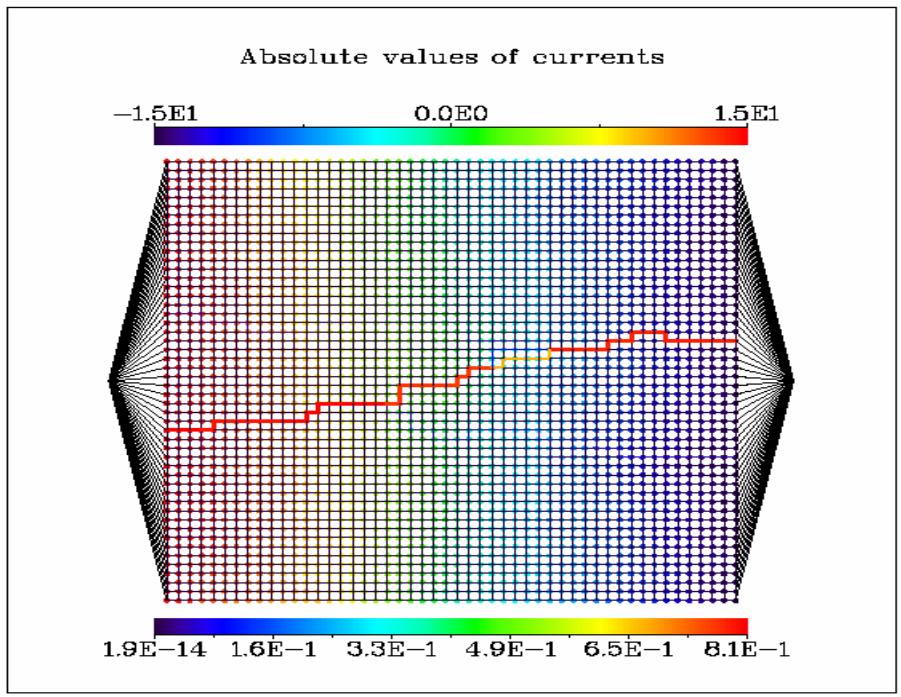






Current localization in varistor networks: Random voltage onset on each edge





Relations to shortest path and minimum cut.

- In a net where each edge has a threshold current, the surface on which the sum of edge currents is smallest is the minimum cut and its capacity is the maximum flow = Critical current. ie capacity $u_{ij} = I_{ij}$

  $I_{\text{minimum cut}} = \Sigma_{(ij) \text{ on minimum cut}} \; I_{ij}$

- In a net where each edge has a threshold voltage v_{ij} for onset of current flow, the path on which current first flows is the shortest path on which the threshold for flow is: ie cost $c_{ij} = v_{ij}$

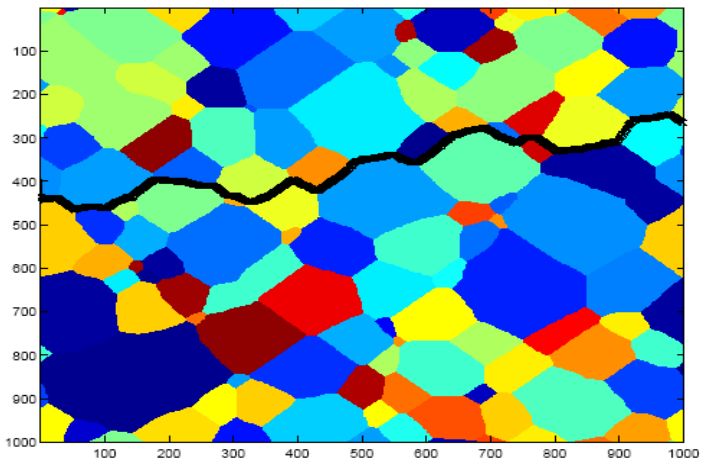
  $V_{\text{shortest path}} = \Sigma_{(ij) \text{ on shortest path}} \; v_{ij}$

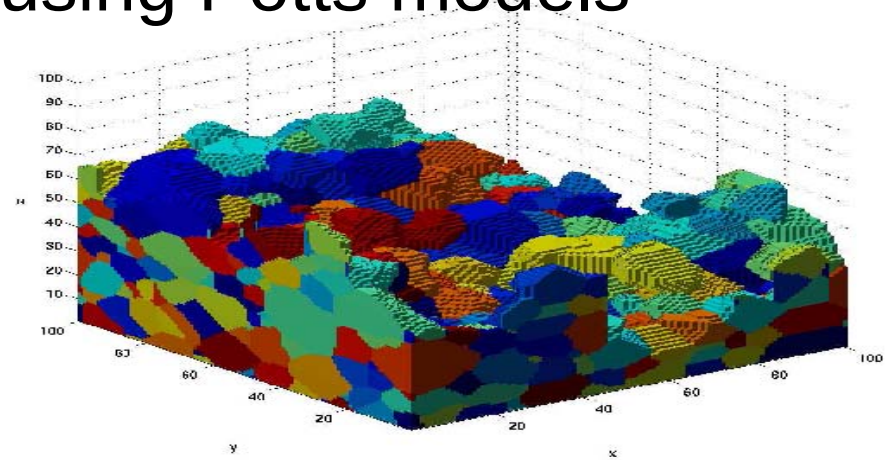
Another interpretation of min-cut and shortest path - Energy

- Low energy paths are very important in pinning of linear structures, such as polymers, flux lines and dislocations. Moreover many lines can be treated, with contact repulsion, using integer flows.
- The capacity of links in a network can also be mapped to energy, for example in the case of domain walls in magnets, or if we want the lowest energy surface of separation in a graph. In that case the capacity maps to the cohesive energy of the edge or bond (ij).

Decohesion surfaces in network models of polycrystals

Decohesion surface -> minimum cut
Edge capacity -> edge energy of grain boundary
Polycrystals grown using Potts models

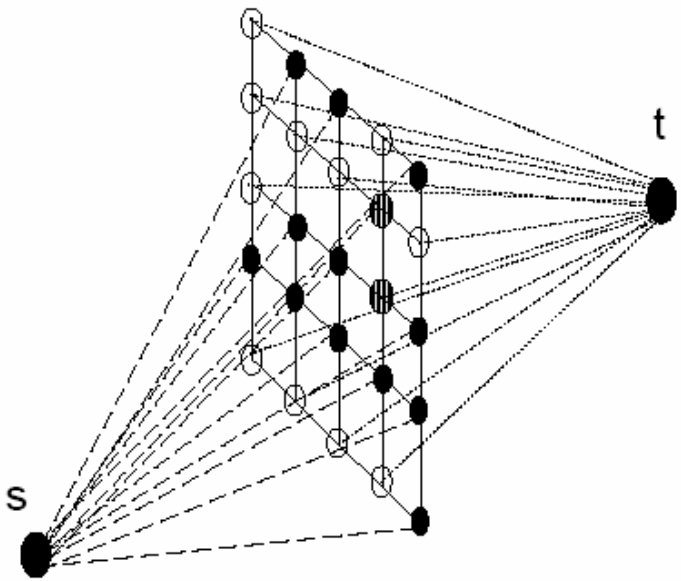




E.S. McGarrity, P.M. Duxbury, E.A. Holm, Phys. Rev. E (2005)
E.S. McGarrity, K.S. McGarrity, P.M. Duxbury, B. Reed, E.A. Holm, MSMSE (2007) in press

Random field magnets (RFIM) and diluted antiferromagnets in a field

- $E = -\Sigma_{ij} J S_i S_j - \Sigma_i h_i S_i$ $\quad J>0$, h_i are random
- $E = E_{exchange} + E_{field} + E_{cut}$
- E.g. see example for a square lattice. Positive random fields are connected to s, while negative random fields are connected to t. The capacities of edges in the square are J, while the capacities of edges connected to s or t are $|h_i|$. E_{cut} is the capacity of the minimum cut. The cut defines a domain structure

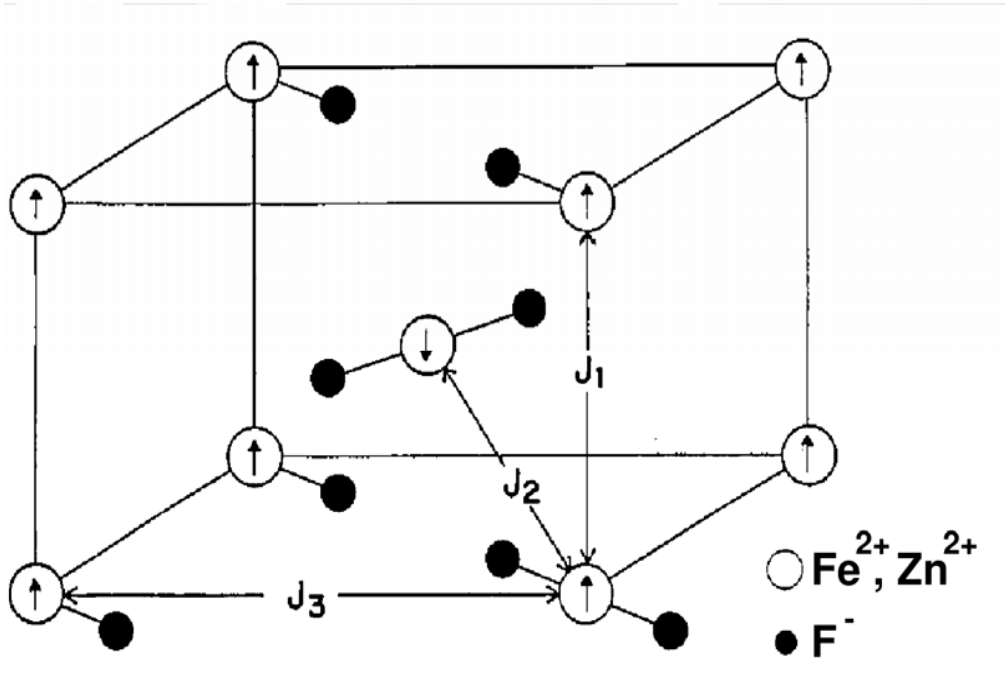


Most Studied DAFF Materials: $Fe_xZn_{1-x}F_2$: Ising-like

$E = \Sigma_{ij} J e_i e_j S_i S_j - \Sigma_i H S_i$

$e_i = 1$ with probability x

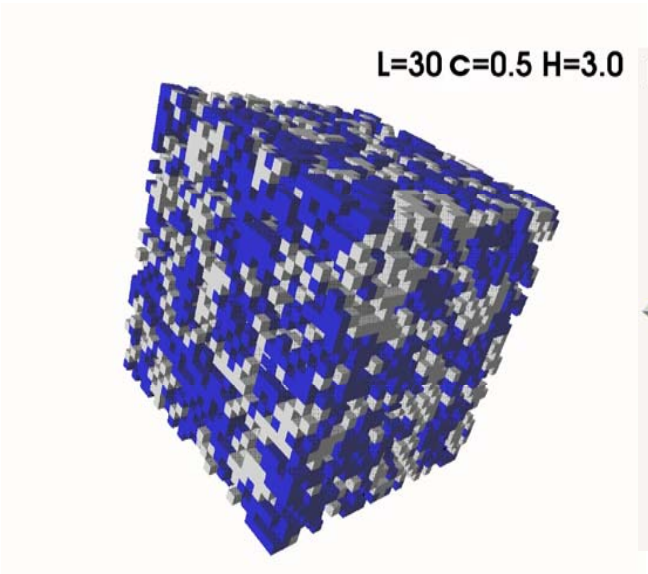
$e_i = 0$ with probability1- x

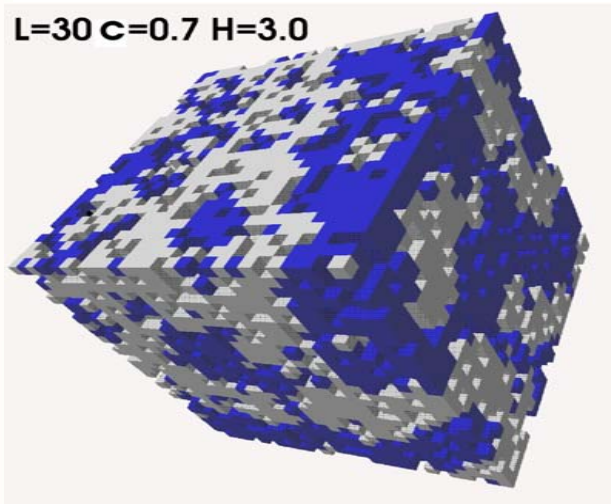


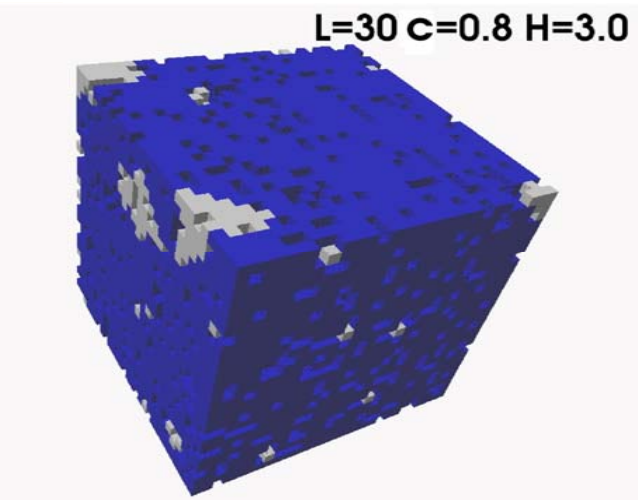
DAFF – Cubic Lattice ground state

Exact ground states can be found using network optimization methods (Ogielski 1986 PRL, Alava et al, Domb and Lebowitz vol. 18 - 2001, Hartmann and Rieger book)

Blue: One AF phase; Grey: the other AF phase



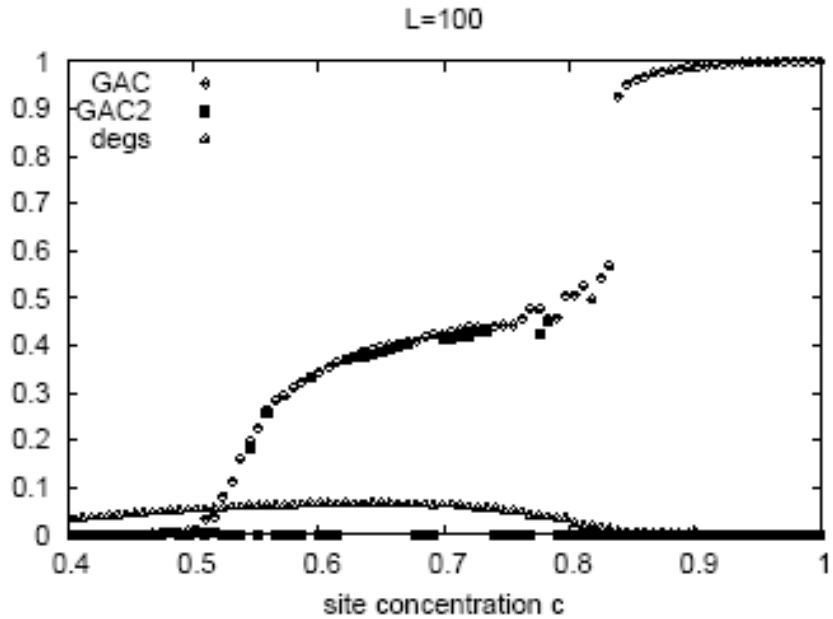


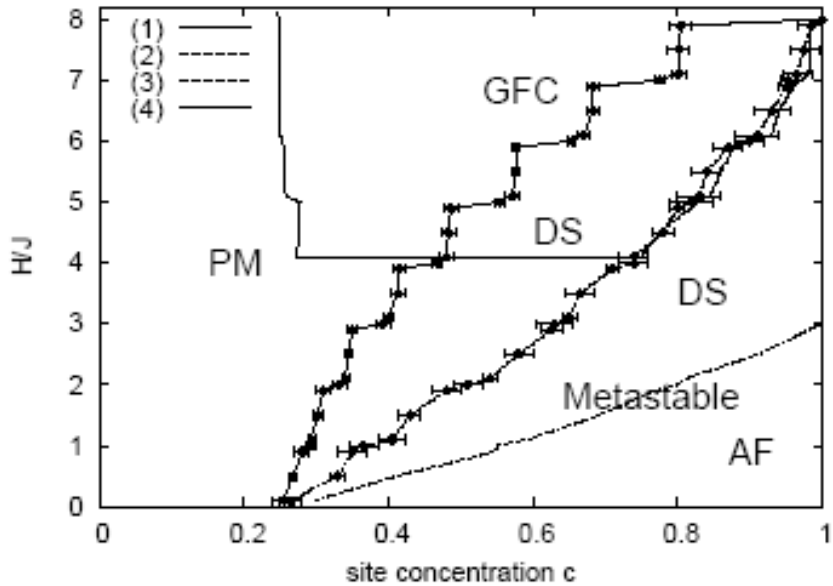


Percolating Phases : Diluted Ising Antiferromagnet in a Field

- Site diluted, nearest neighbor, spin ½ Ising antiferromagnet in a uniform Applied field (H). Constant exchange ($J=J_2$). Concentration of magnetic sites (c) – randomly placed. Body Centered Cubic Lattice.
- Probability of being on the Largest Ferro Cluster (GFC)
- Probability of being on the Largest AF cluster (GAC)
- Probability of being on the second largest AF cluster (GAC2)

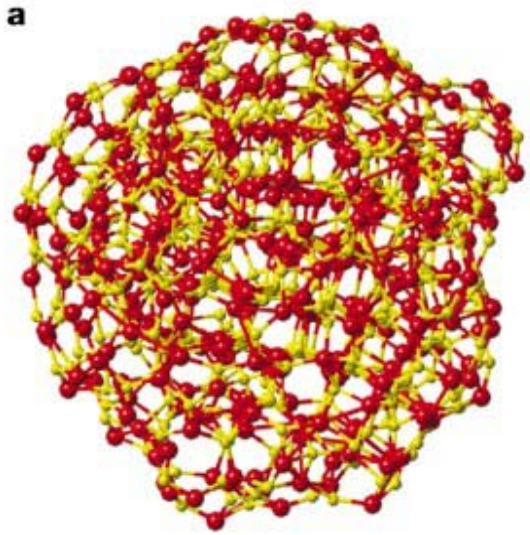
DAFF phase diagram (T=0)
Glaser, Jones, Duxbury PRB 2005

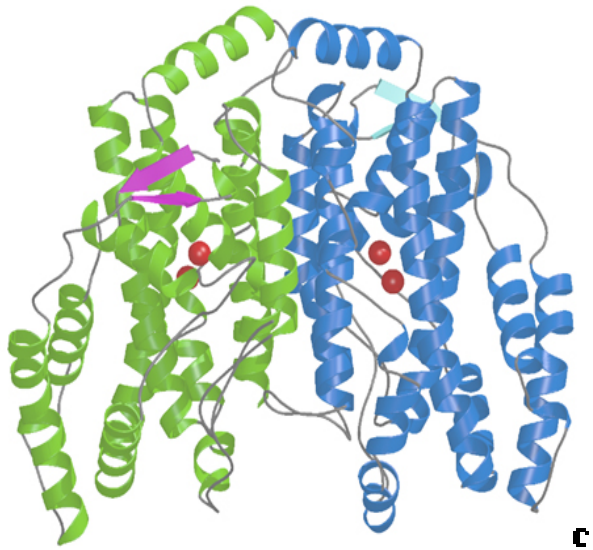




C. Ab-initio determination of local atomic structure of non-crystalline materials

Nanoparticles e.g. ZnS.

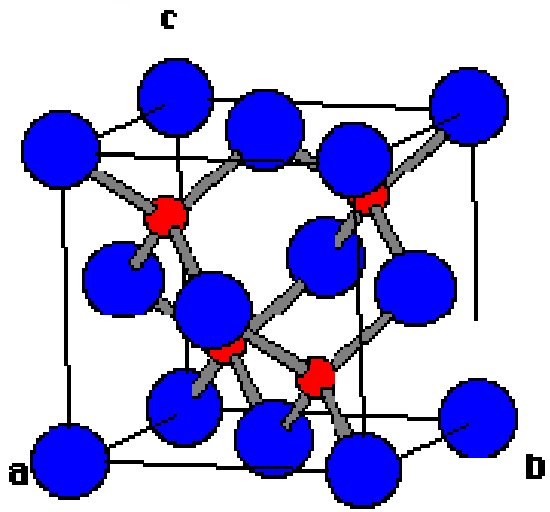




Proteins

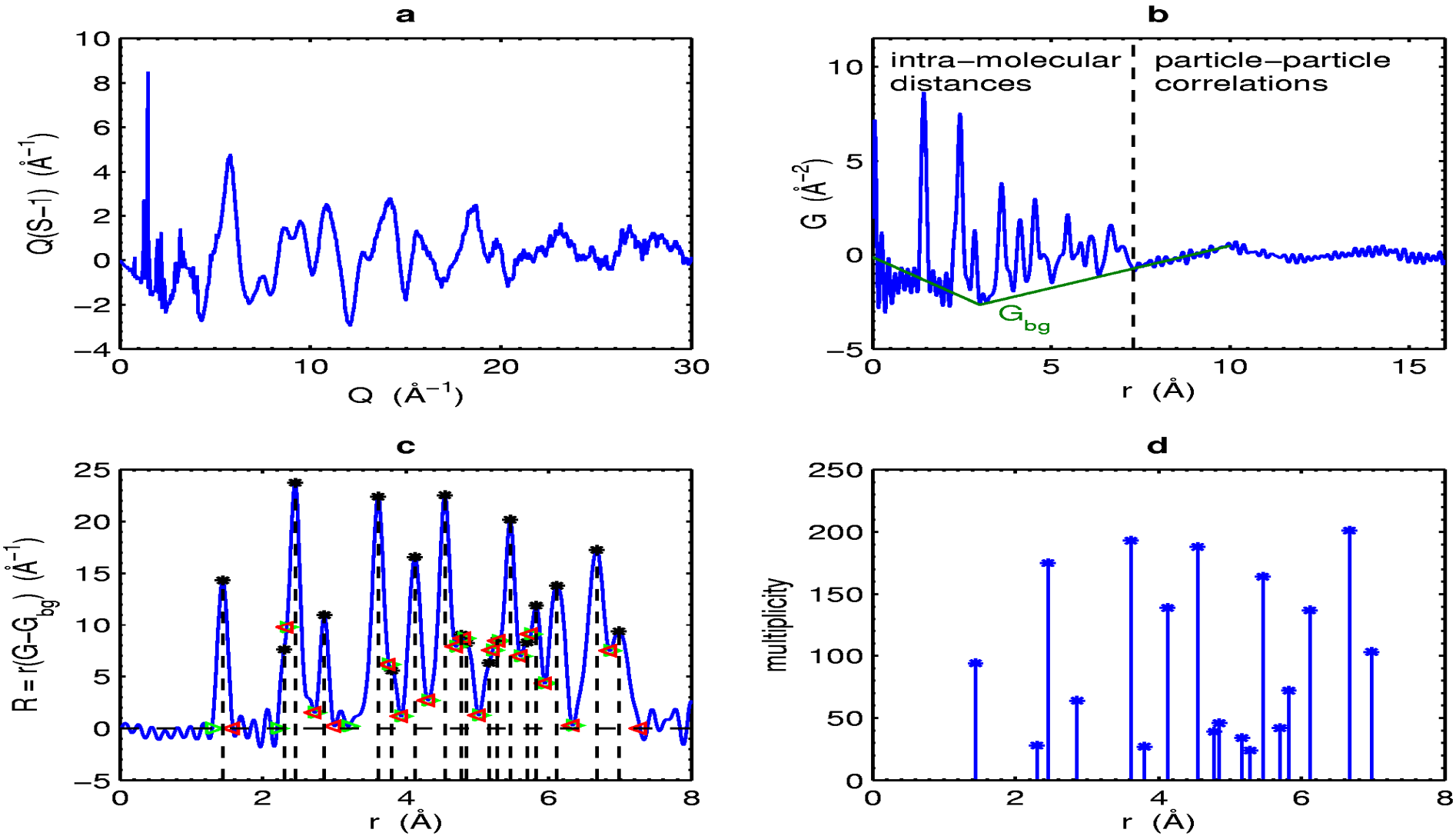
Methods:

1. ***Solution from Single Crystals***
   (Not always possible or complete)
2. ***TEM, Imaging***
3. ***EXAFS, PDF, NMR***
   (Is there enough information)



Locally distorted materials e.g InGaAs

PDF Data gives a set of interatomic distances – Can we find atomic structure from them???



How many inter-atomic distances do we need?

- In the generic case all distances are unique, ie. Random structures. A molecule with N atoms has 3N degrees of freedom. We need at least 3N-6 constraints (distances). If we have less than this number the problem is underconstrained and not solvable. Finding unique structures from > 3N-6 distances seems combinatorially hard.
- BUT. Many nanostructures have special symmetries and have distances which have high multiplicity. This is the non generic case – there are no general theorems.
- We have taken a practical approach.

  - Given a set of distances can we find structure?

Algorithms for reconstruction

N Atoms, N(N-1)/2 target interatomic distances, $d_i^{target.}$ Given the distances find the atom positions R_k.

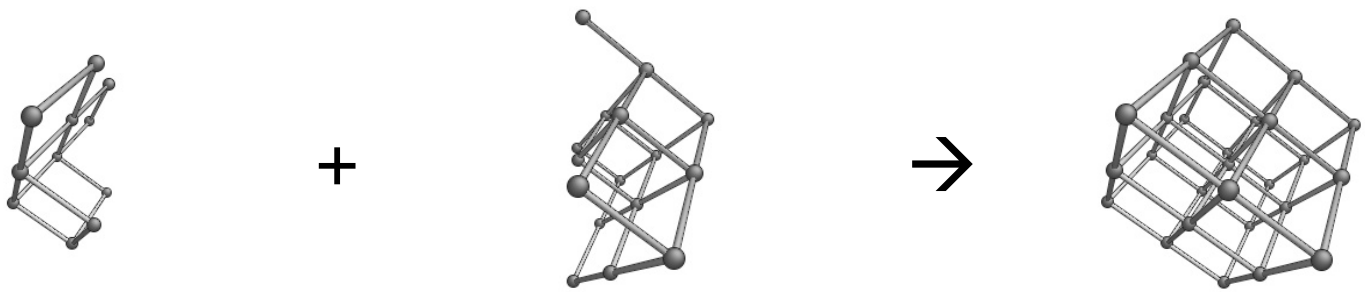
$d_i = |R_j - R_k|$. Energy = $\Sigma (d_i - d_i^{target})^2$

Simulated annealing

- Slow, unsuccessful for larger clusters (N>20)

Genetic algorithm

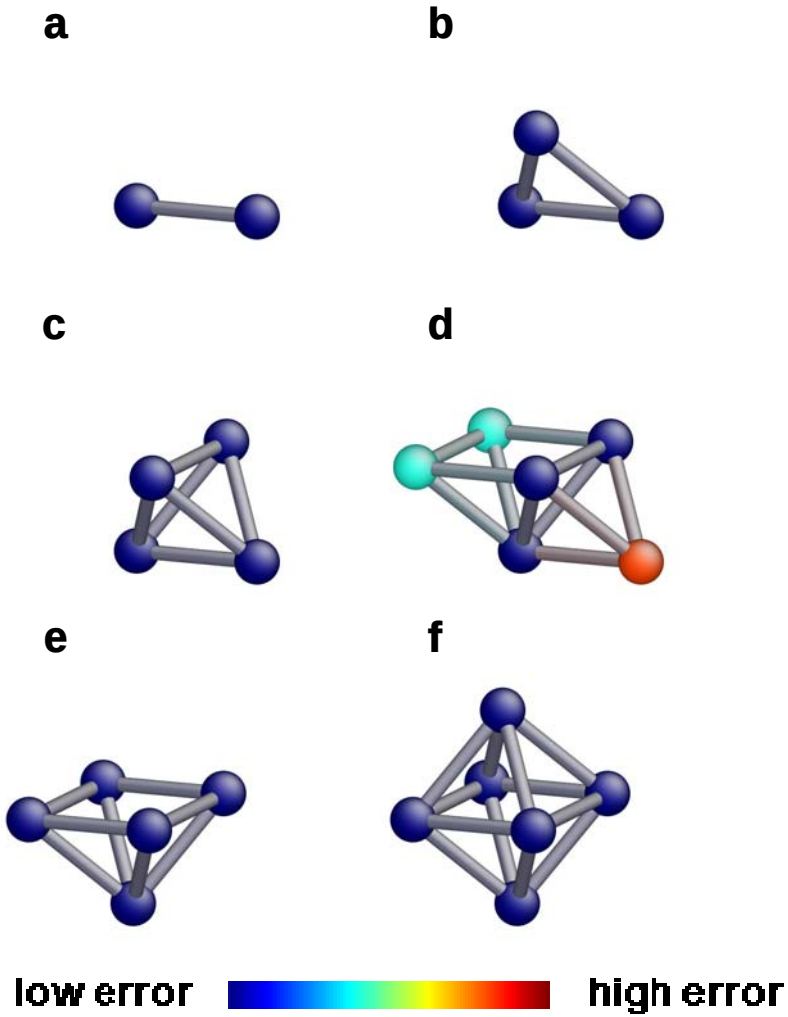
- Based on [Deaven, D. M. and Ho, K. M. PRL 75, 288-291 (1995)]
- Starts with population of random clusters
- Cut and paste good structures to produce better ones, refine using gradient descent e.g.



LIGA ALGORITHM

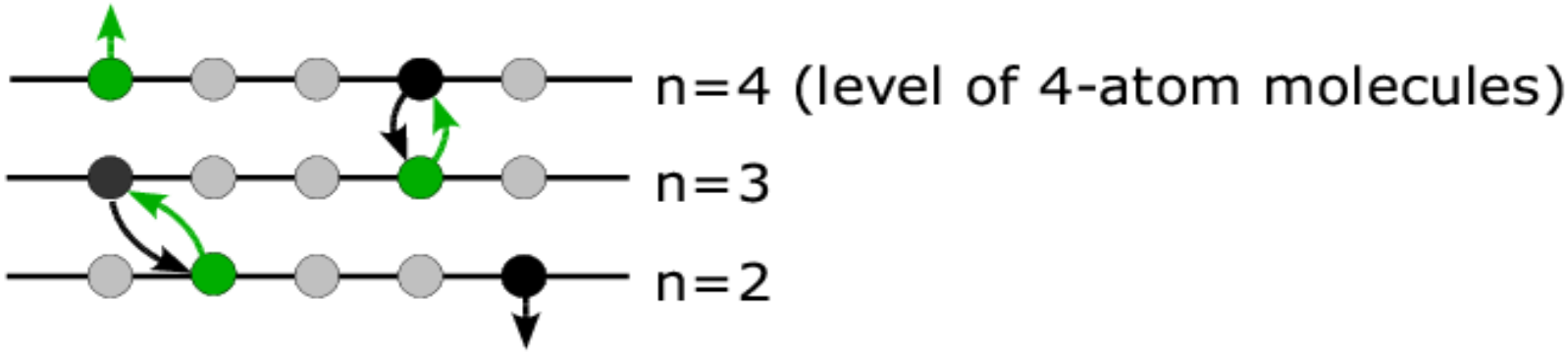
- Starts with an empty box
- Gradual build-up and repair of partial clusters
  - Uses distance list to choose atoms to add
  - Best triangle/tetrahedron method
- Selection of improved clusters using soccer league like competition
  - Promotion and relegation based on performance
  - Performance is measured through deviations of distances from distance list
- Best performance in speed and success rate for reconstruction of non-generic structures

Illustration of cluster buildup-Octahedron



- octahedron has 15 lengths: d^e = [12×1, 3×√2]
- **a-c** atoms are by constructing triangles or pyramids using available lengths
- because tetrahedron **c** is not part of an octahedron, addition of more atoms induces errors **d**
- **e** the worst atom is removed allowing convergence to the correct solution **f**
- when should the atoms be added and when removed?

Liga algorithm



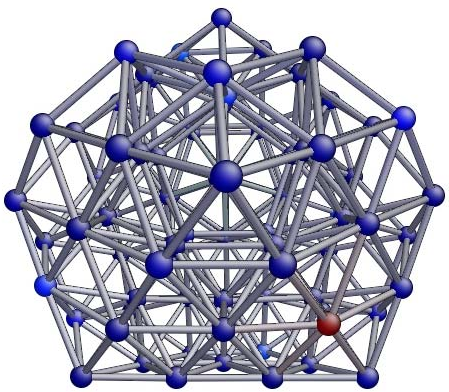
- relative cluster quality is obtained by comparison with peer clusters
- promotion-relegation system inspired by soccer league
- keeps arrays of different clusters at every possible size, n = 1,2,3,...,N
- partial sub-clusters of the same size form a league “division”
- “winners” and “losers” are selected using random weighted procedure
- “winner” clusters grow and are promoted to higher divisions
- “loser” clusters descend to lower levels by firing “bad” atoms
- “losers” may copy the structure of winning opponents

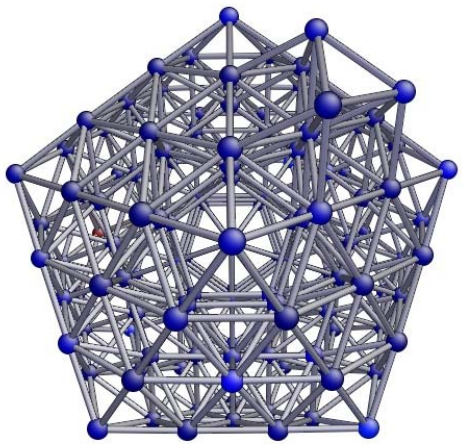
Shape reconstruction from ideal distance lists – Ground state structures found from theory

- Lennard-Jones clusters

gllj88t3cbar-fps12.mpg

- $N = 88$ $N = 150$



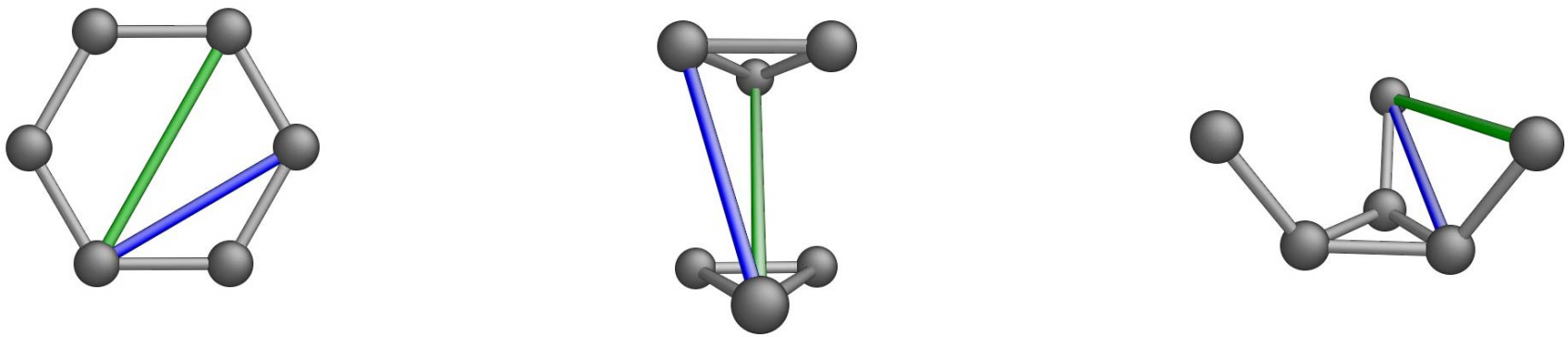


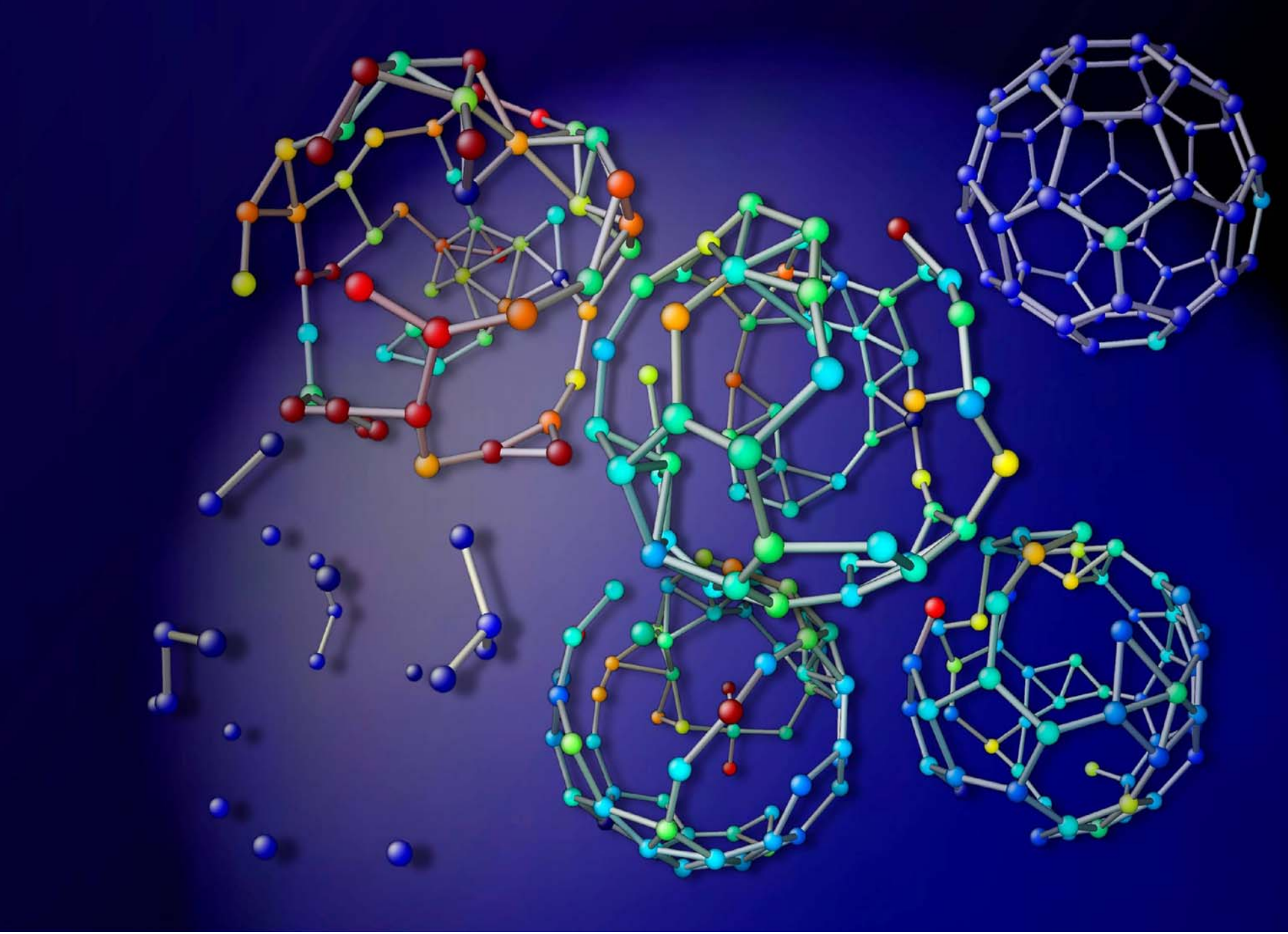
Uniqueness of shape reconstruction

- tested on variety of clusters with up to 150 atoms
- repeated runs using ideal distance lists
- vast majority of simulations converged to the original cluster
- few high-symmetric clusters (e.g., square or hexagon) have non-unique solution

example: hexagon distance-morphs

- hexagon has 15 lengths: d^e = [6×1, 6×√3, 3×2]
- these lengths are exactly reproduced in 3 different objects

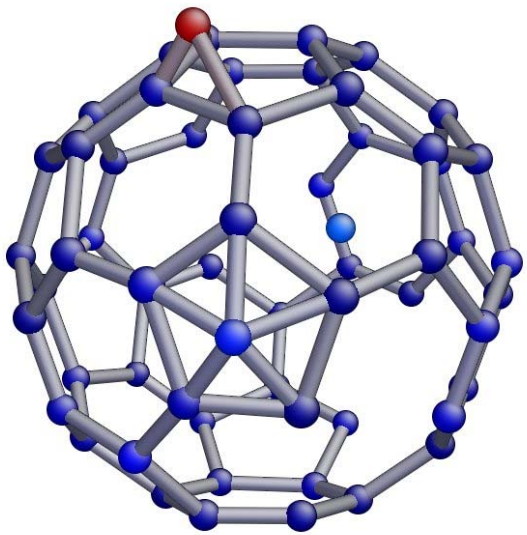




C60gld-t1-wbg.mpg

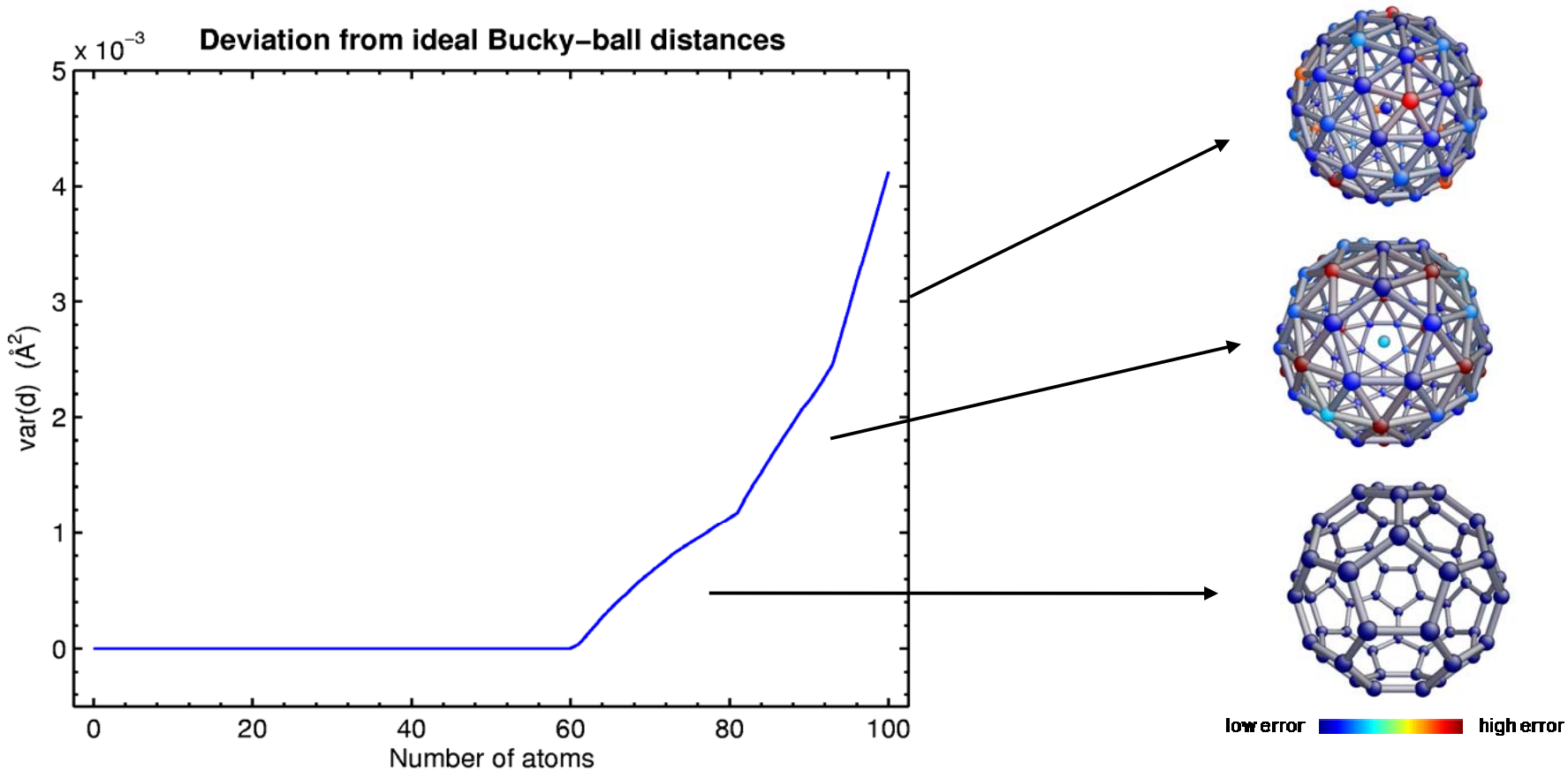
Structure solution of C_{60} from experimental PDF Distance data

- Distance list extracted from data:
  - “tight” with (60*59/2) = 1770 distances
  - Only 18 different ones ie. Lots of distance degeneracy
  - Note Ideal buckyball has 21 unique distances

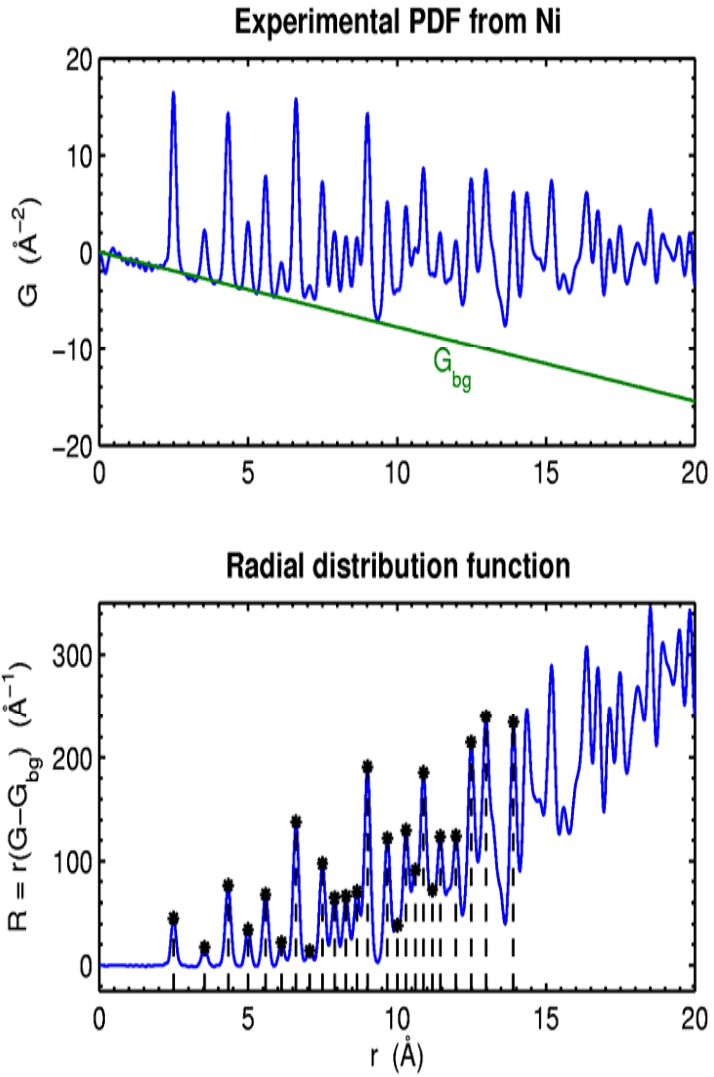


Structure solution from “free” distance list

- Clusters can be uniquely reconstructed even when distance multiplicities are infinite
- Tetrahedron is the largest object with a single pair distance value
- C_{60} is the largest object built from infinite pool of ideal Bucky ball distances

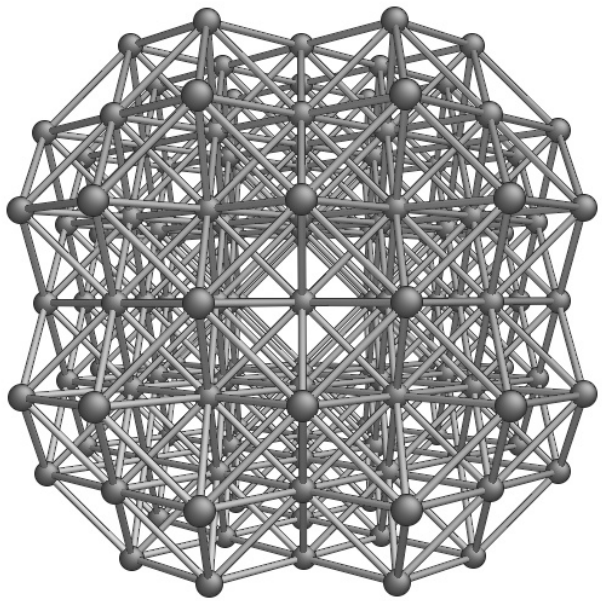


Structure solution of Ni from free distance list



- Synchrotron XRD from Ni was measured at 6ID-D beamline, APS, Argonne lab
- Fitting of free distance list gives spherical cut-off from f.c.c. lattice

  (no periodic boundary conditions)



Algorithm performance

Table 1 | Performance comparison of distance geometry algorithms.

Genetic algorithm		CPU time (s)			
Shape	Success rate	Average	Standard deviation	Minimum	Maximum
C_{60}	35/62 (56%)	6,330	8,200	1,100	35,150
LJ-20	100/100 (100%)	39	75	7.3	620
LJ-38	103/113 (91%)	880	2,500	76	14,300
LJ-60	23/58 (40%)	10,080	12,500	1,200	48,100
LJ-88	35/43 (81%)	36,800	25,800	14,600	122,000
Liga algorithm		CPU time (s)			
Shape	Success rate	Average	Standard deviation	Minimum	Maximum
C_{60}	100/100 (100%)	1.1	0.74	0.17	3.7
LJ-20	100/100 (100%)	16	9.3	2.7	56
LJ-38	100/100 (100%)	3.0	2.8	0.1	14
LJ-60	100/100 (100%)	690	290	180	1,460
LJ-88	100/100 (100%)	2,650	1,800	937	15,200

All shapes were solved using unassigned ideal distances. The convergence criterion was $\mathrm{var}(d) < 10^{-4}$ Å^2. CPU times were measured on an Intel Pentium 4, 2.66 GHz Linux PC.

Future developments

- Increase efficiency – Structures with thousands of atoms?
- Develop algorithm for multi-element compounds (Saurabh Guraji – Some progress with divide and conquer)
- Develop algorithm for drug molecules (problems with rings)
- Add constraints, e.g. chemical constraints, co-ordination constraints.
- Add information from other methods eg. Both neutron and x-ray PDF, EXAFS, NMR. We need good distance lists.

Support

- Department of Energy, account DE-FG02-97ER45651

Publication

P. Juhas, D. Cherba, P.M.D, W. Punch, SJB, Nature 440 (2006)

D. Maximum independent set (MIS) = Hard core lattice gas

MIS Definition: Given a graph G consisting of a set of nodes and edges, find a largest cardinality subset of nodes with the property that no two nodes in this subset share an edge.

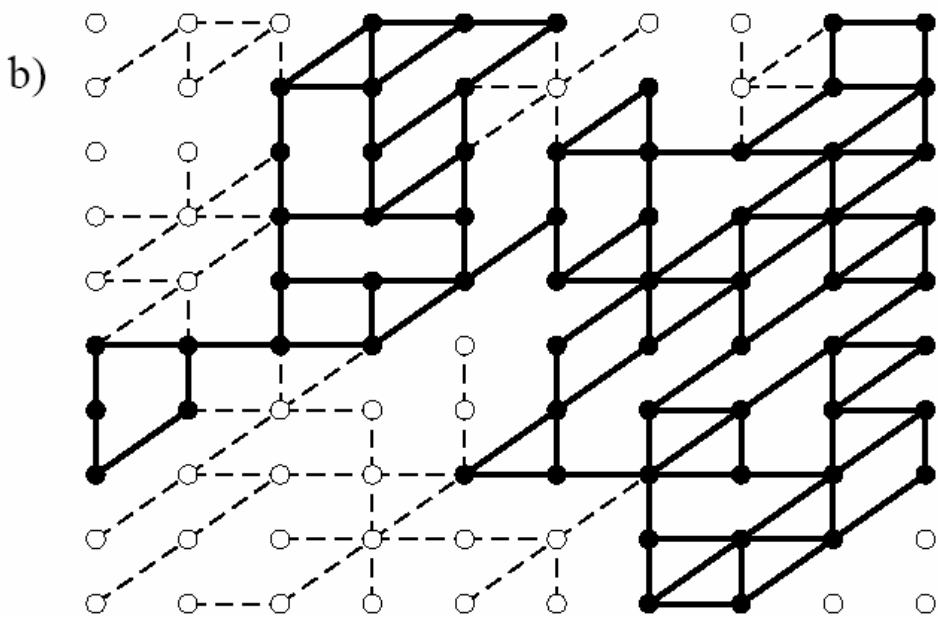
Physics interpretation: Consider a lattice gas with hard core nearest neighbor repulsion. Find the maximum packing density of this hard core gas.

$H = \Sigma_{ij} J n_i n_j - \mu \Sigma_i n_i$ J,μ large, μ/J ->0

The first sum is over edges in the graph

Diluted graphs – leaf removal (Tarjan, 1970's)

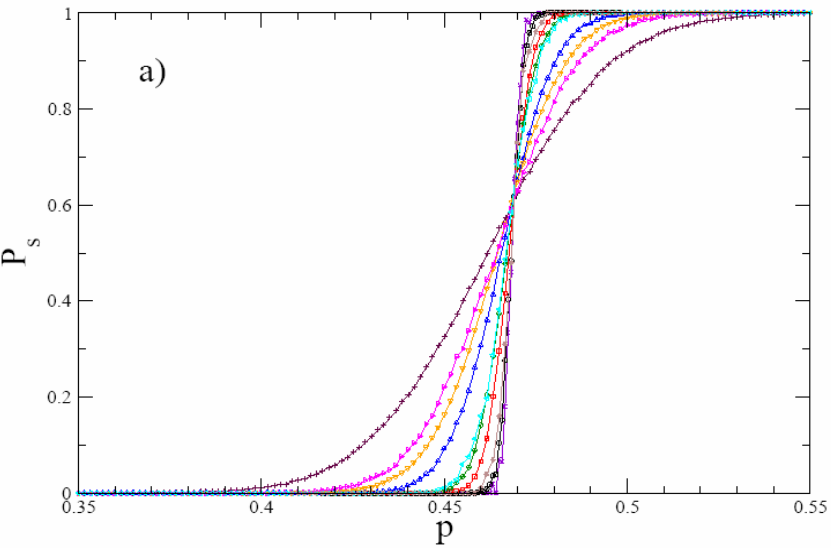
Fay, Liu Duxbury, Phys. Rev. E. 2006

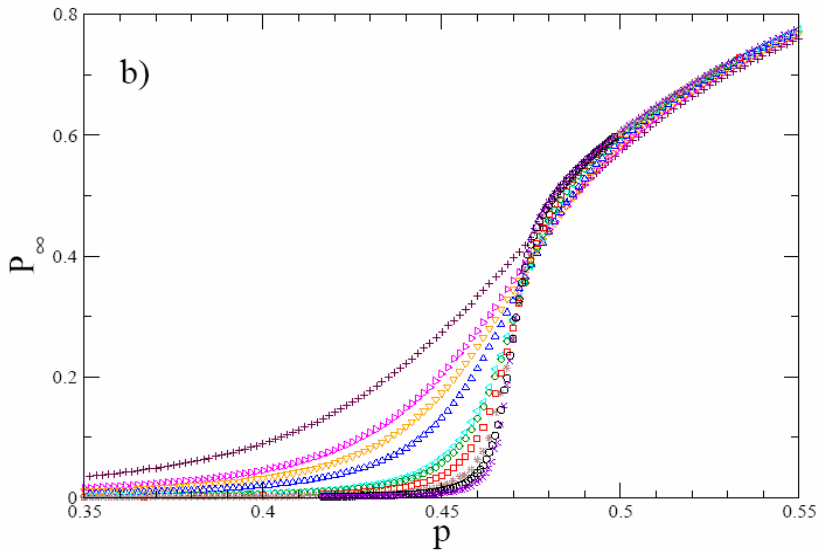


Algorithm: Recursively remove leaves, the nodes connected to both ends of the leaves and all edges connected to both of these nodes.

For initial bond concentrations less than a threshold value, the irreducible core is not extensive. Below this core percolation threshold the problem is in P

Core percolation threshold c*
For c<c*, MIS is in P





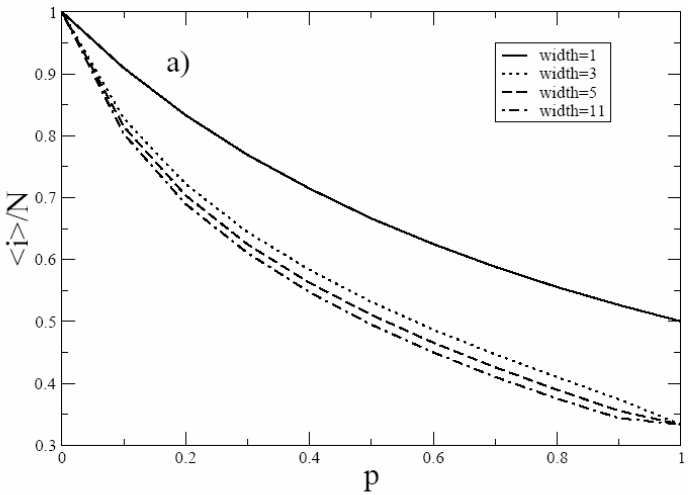
a) Spanning probability for the core

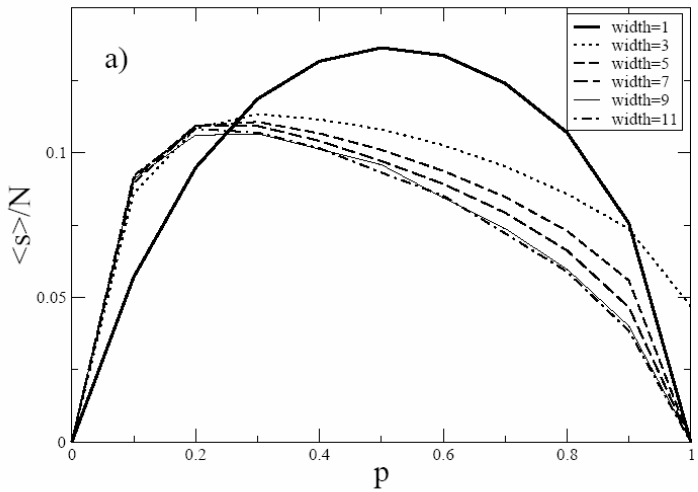
b) Probability of a node being on the giant cluster

Random graphs: Core threshold is at c*=2.718...

Karp and Sipser, Bauer and Golinelli (2001)

Tranfer matrix: Numerical method to find exact cardinality and degeneracy of lattices





Slabs of finite width and length 1000.

Local probability recursion algorithms: Belief propagation,survey propagation... Pearl 1988, Mezard, Parisi, Zecchina Science 2001

MIS vertex algorithm

Define I_i = probability that site i is part of MIS.

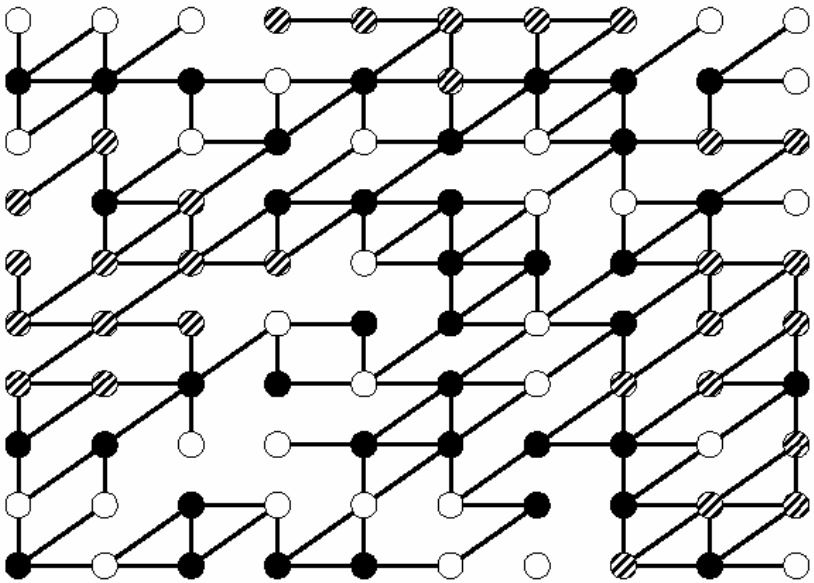
Then asynchronously carry out recursion of:

$I_i = \Pi_{\text{(j a neighbor of i)}} (1-I_j)$

Fay, Liu, Duxbury, Phys. Rev. E 2006

Vertex and Bond LoPR on a triangular lattice

a)



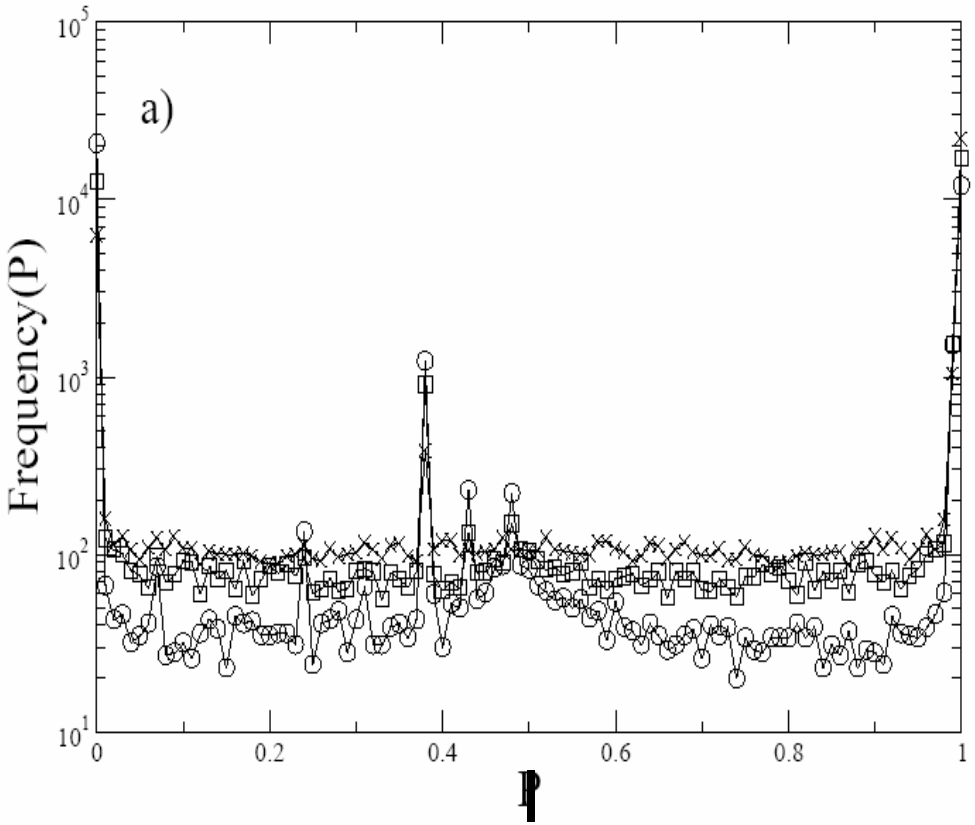
Open circles: I->1

Solid circles: I->0

Hatched 0<I<1

i.e. degenerate.

Frequency distribution P(I): Non-trivial distribution



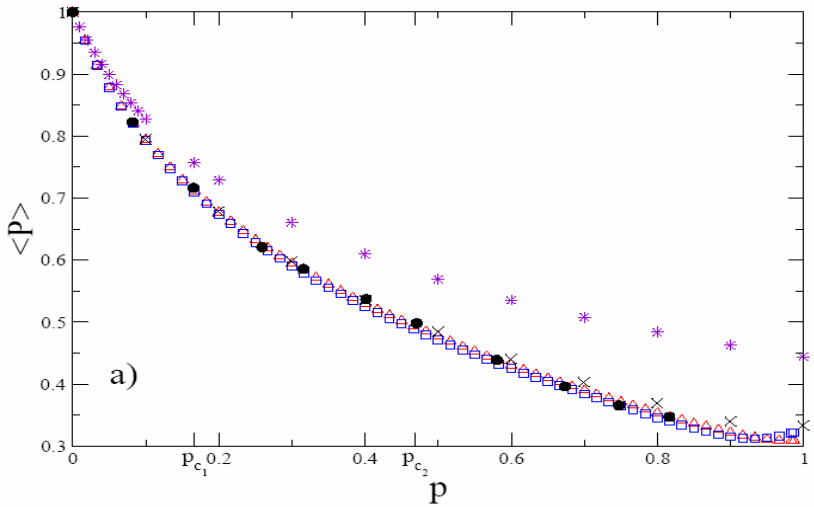
Three values of c

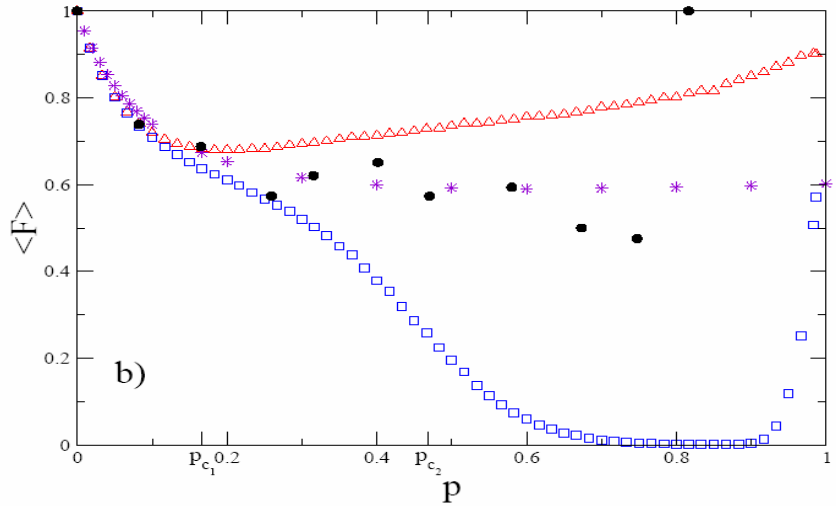
C=1 (crosses)

C=2 (boxes)

C=4 (circles)

Averaged results: Cardinality of MIS is easy, structure is harder.





Comparison of two local probability recursion methods

Vertex LoPR: Red Triangles

Bond LoPR: Blue Boxes

Closing remarks

The overlap between statistical physics and combinatorial problems is very rich, both in terms of algorithms and concepts.

Some recent successes

1. Rigidity percolation, protein structure, matching
2. Paths in disordered media, MST, shortest path
3. Random field magnets, Maximum flow
4. Minimum energy surfaces, Maximum flow
5. Recursive methods for hard ground state problems

Many opportunities, but the dialogue is time consuming. It is a gamble, but the gains can be very significant .

Acknowledgements
Support from DOE

- Rigidity: Cristian Mourkarzel, Paul Leath, Mike Thorpe, Don Jacobs. Bruce Hendrickson
- Domain walls: Mikko Alava, Eira Seppala
- RFIM and DAFF: Sorin Bastea, Andreas Glaser, Andy Jones
- Non-linear flow: Alexander Donev
- Polycrystalline materials: Liz Holm, Jan Meinke, Erin McGarrity, Bryan Reed
- Bootstrap: Chris Farrow
- MIS: Chip Fay, Jiwu Liu
- Structure determination: Simon Billinge, Pavol Juhas, Bill Punch, Dave Cherba
- Paths (MST, shortest path): Radu Dobrin