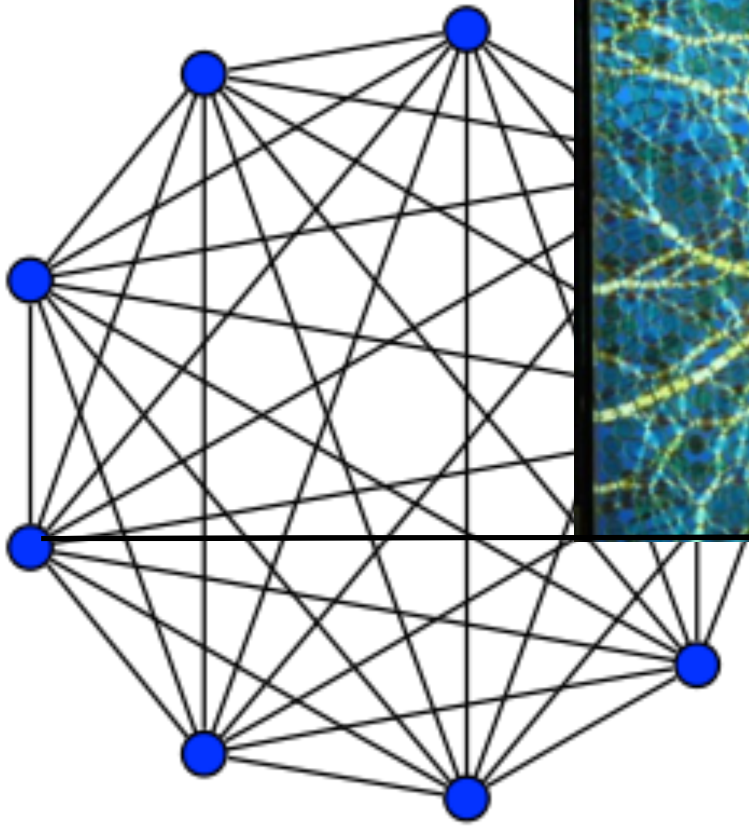
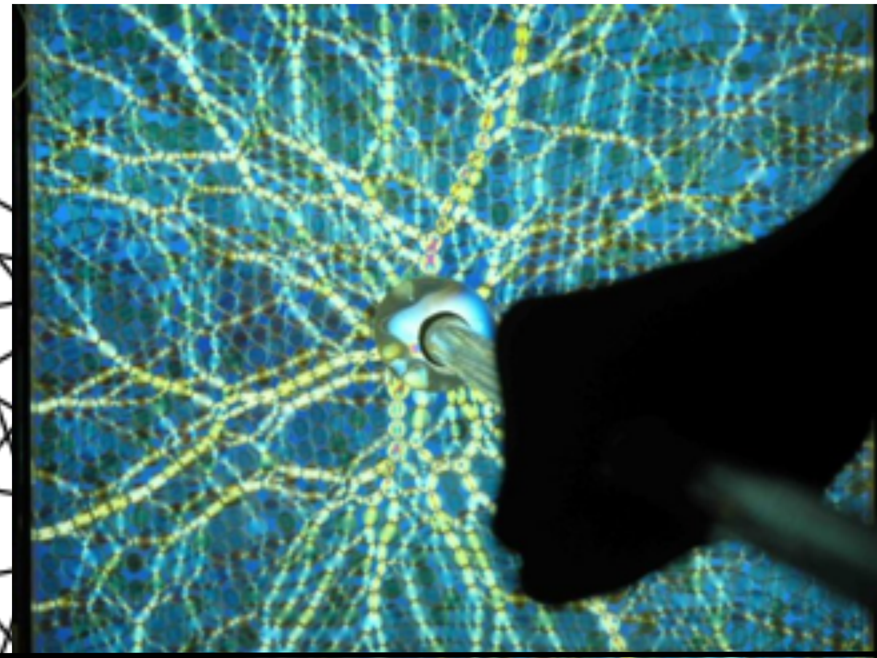




Elasticity and mixing on random graphs

Marija Vucelja
The Rockefeller University

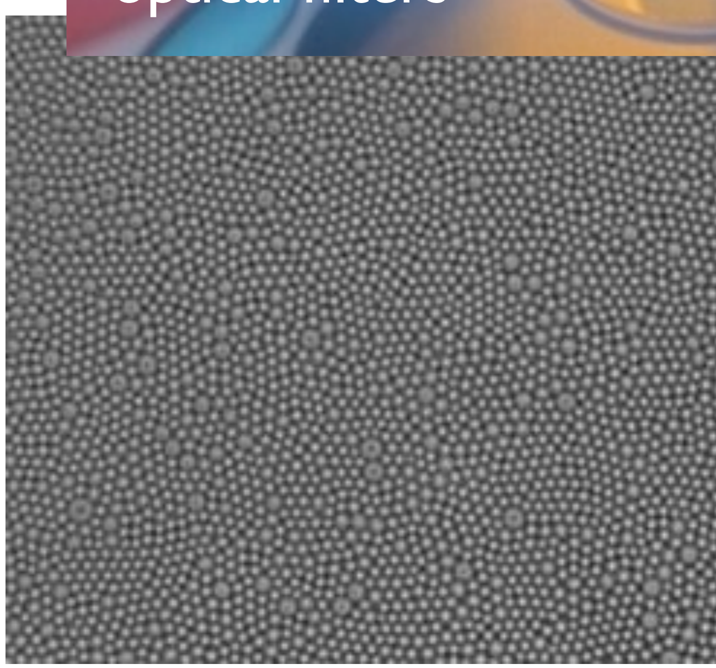
UVa Physics Condensed Matter Seminar, 2013

Amorphous solids are ubiquitous

Molecular glasses, colloids, granular matter, gels, fibrous networks, semi-flexible networks


optical filters


CDRW: AgInSbTe


DNA coated colloids


IR lens

Physical properties:

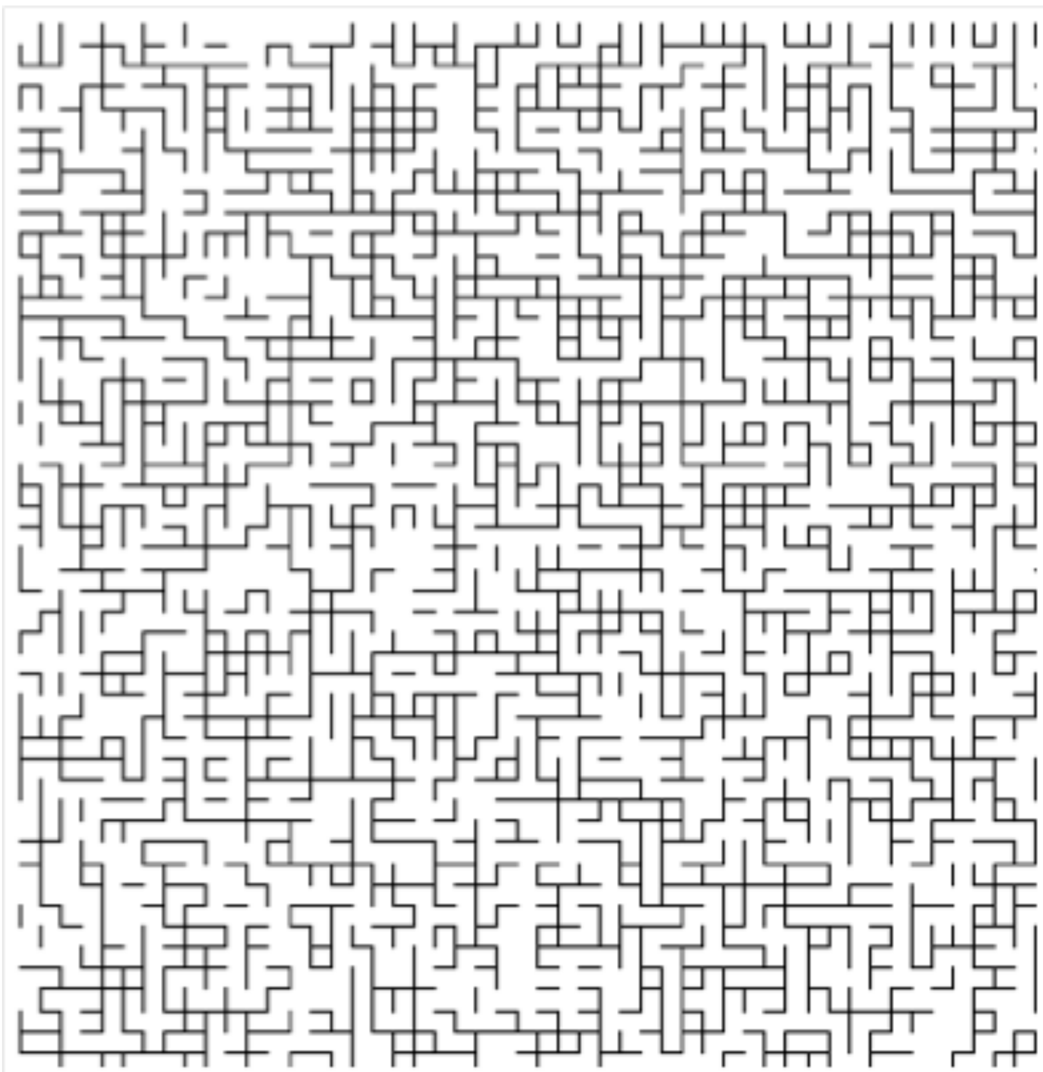
- out of equilibrium
- quenched and emergent disorder
- elastic response is typically very heterogeneous
- wide separation of scales between bending and stretching modes
- dissimilar interaction strengths

$$\frac{\text{covalent bond energy}}{\text{hydrogen bond energy}} \approx 100$$

Outline

- Elasticity of random networks:
  - vibrational modes of Laplacian Matrices, Stiffness Matrics
- Mixing on random graphs:
  - new kind of Monte Carlo algorithms

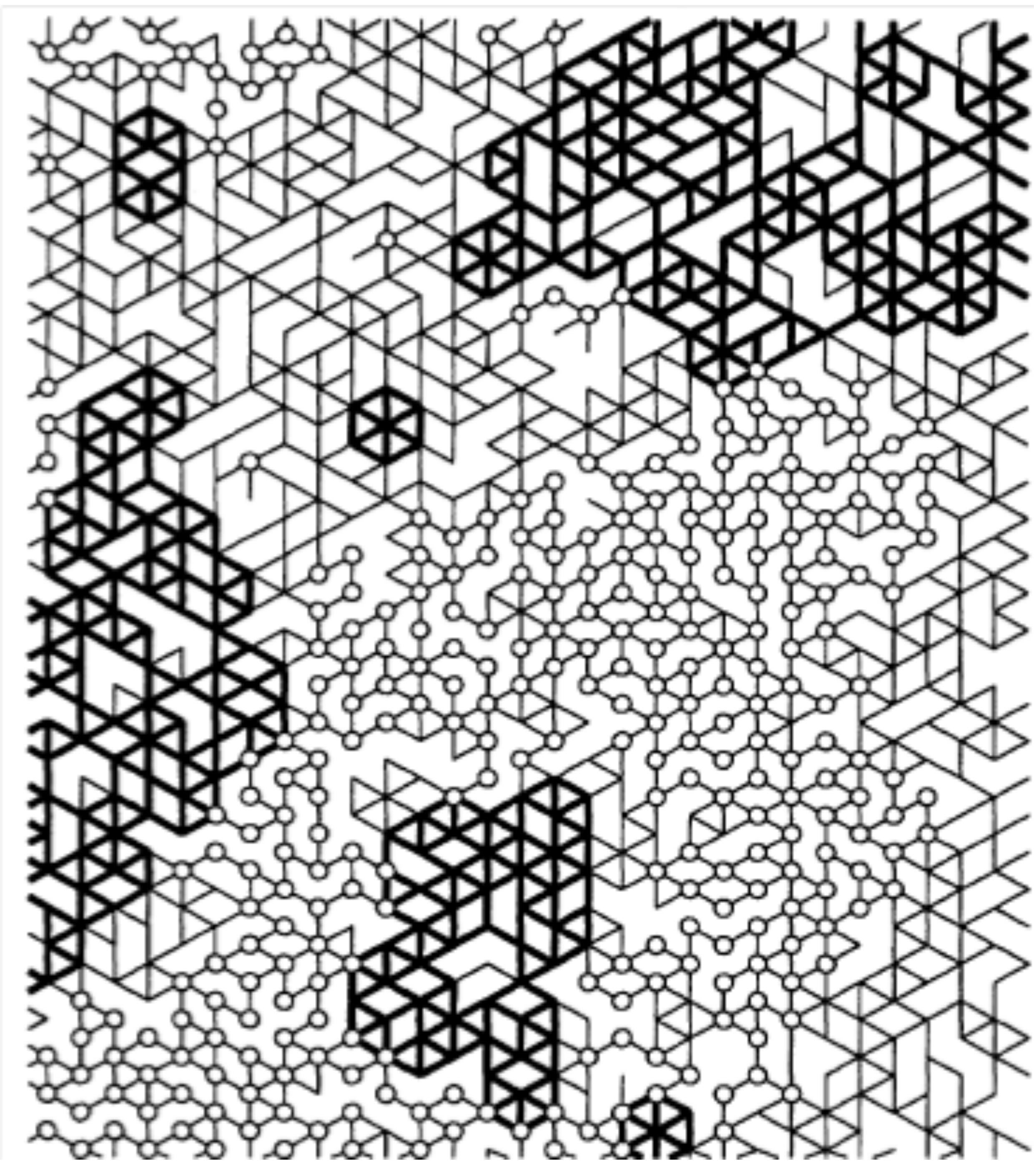
Percolation



- electrical conductivity, diffusion in random media ...
- bonds deposited with probability p
- $p > p_c$ finite conductivity
- $p = p_c$ fractal percolating cluster

Rigidity Percolation

Phillips, Thorpe, 1985
Guyon, Crapo et al, 1990



- probability p of a spring

force balance at each node i

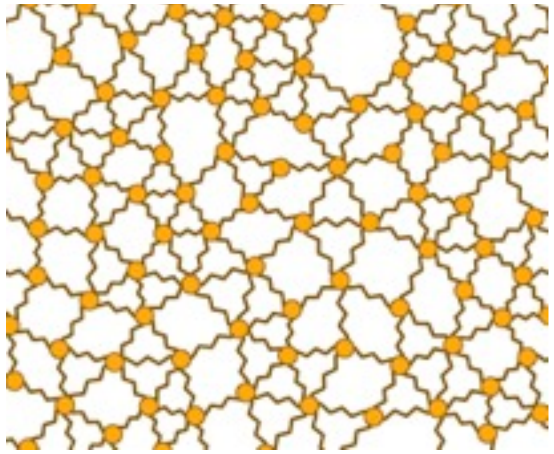
$$\sum_{\langle ij\rangle}[(\delta\boldsymbol{R}_i - \delta\boldsymbol{R}_j)\cdot\boldsymbol{n}_{ij}]\boldsymbol{n}_{ij} = \boldsymbol{F}_i$$

$\boldsymbol{n}_{ij}$ unit vector from *i* to *j*

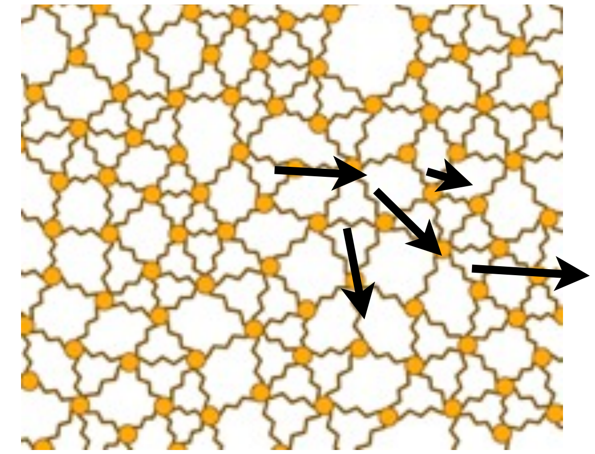
$\mathcal{M}$ stiffness matrix - random and sparse

$$\mathcal{M}|\delta\boldsymbol{R}\rangle = |\boldsymbol{F}\rangle$$

Floppy network has soft modes (low energy excitations)

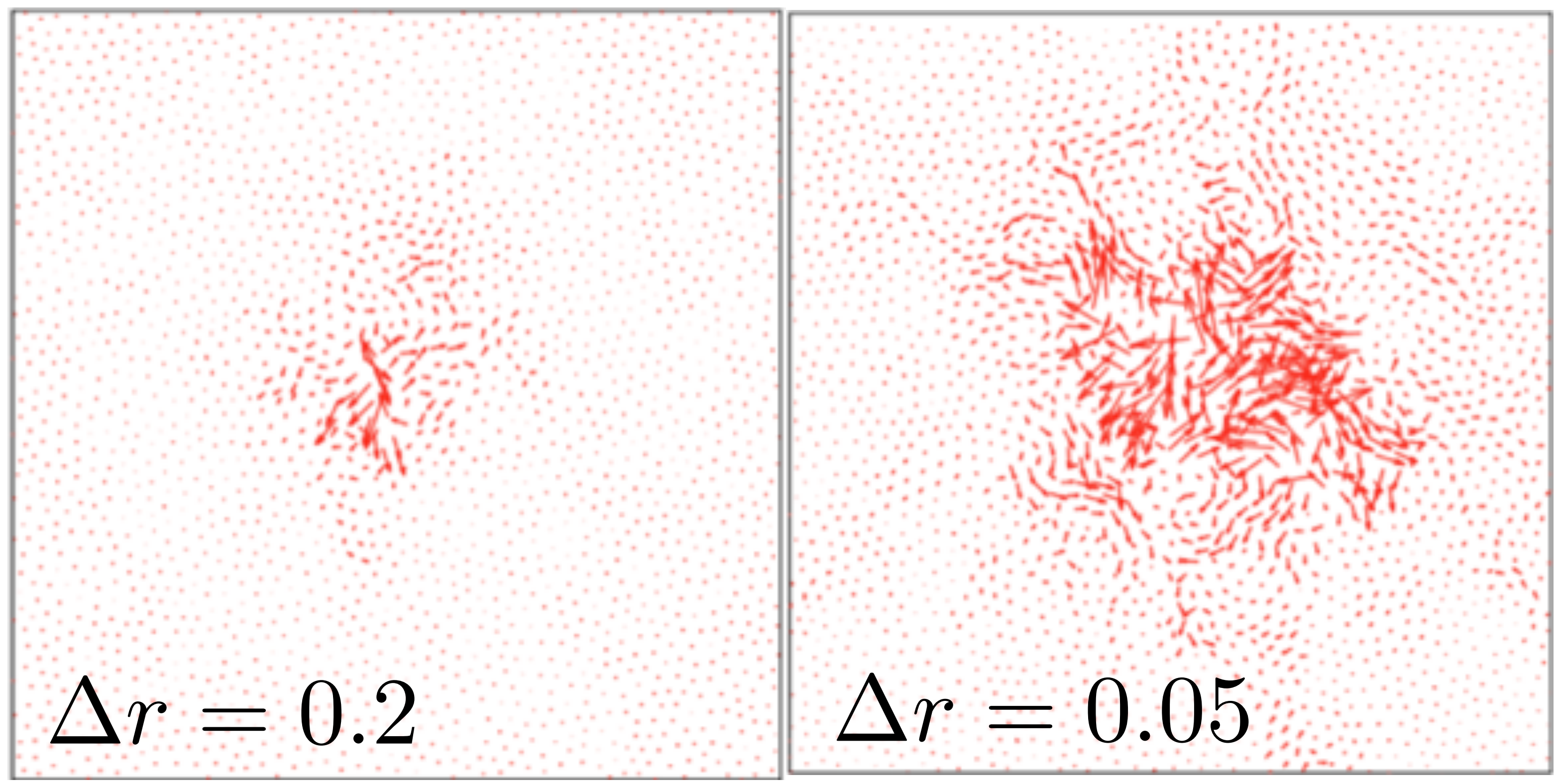


elongate a spring & measure response



over-damped rearrangements at different *r*:

$$\Delta r \equiv r_c - r$$

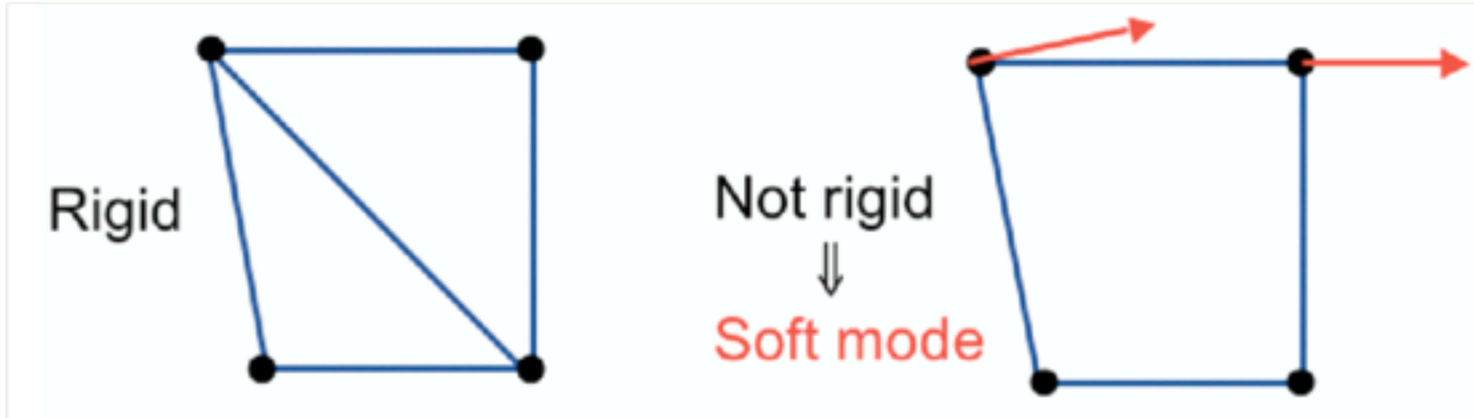


local nature

extended

Soft modes are typically extended!

Maxwell rigidity criterium: mechanical stability



d dimension, N nodes, N_c constrains

$$Nd - N_c - \frac{d(d+1)}{2} \simeq Nd - N_c$$ vibrational number of degrees of freedom

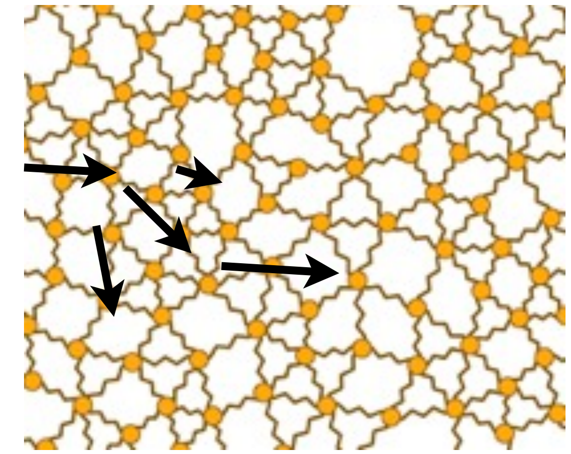
$r = 2N_c/N$ average connectivity

Isostatic network: $Nd = N_c \Rightarrow r_c = 2d$

Maxwell criterium		
	rigid	$r > r_c$
	isostatic	$r = r_c$
	floppy	$r < r_c$

Stiffness matrix $\mathcal{M}$

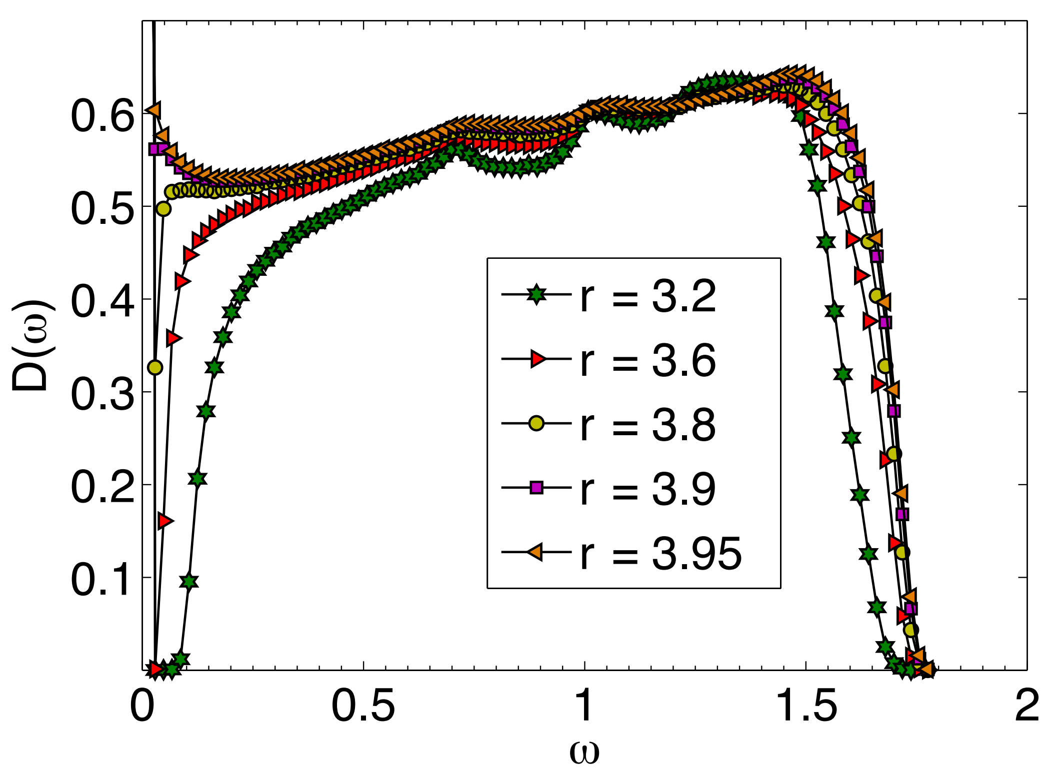
A small change in the displacement of the modes

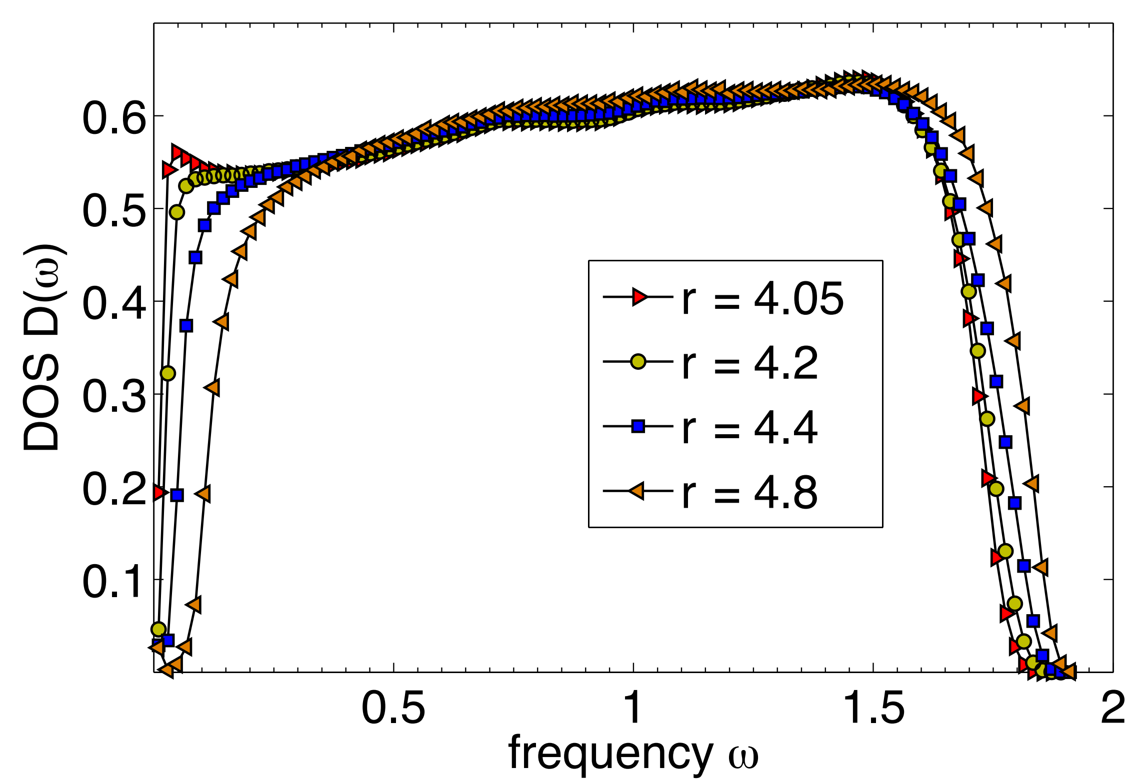


$$\delta E \simeq \frac{1}{2}\sum_{\langle ij\rangle}\left((\delta \boldsymbol{R}_j - \delta \boldsymbol{R}_i)\cdot \boldsymbol{n}_{ij}\right)^2 = \langle \delta \boldsymbol{R}|\mathcal{M}|\delta \boldsymbol{R}\rangle$$

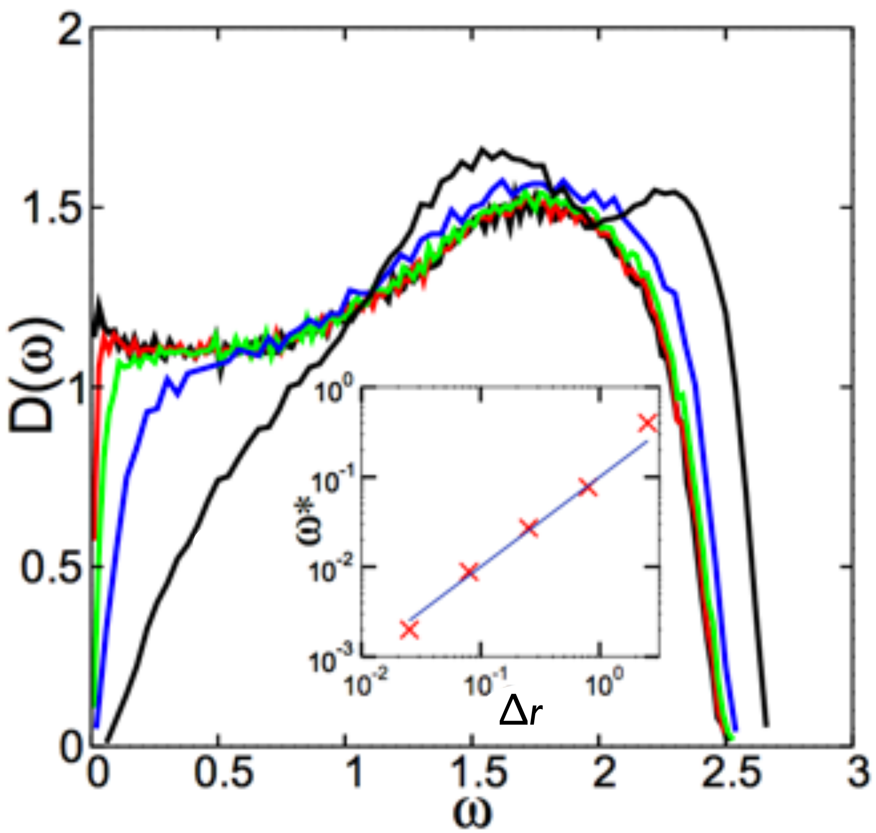
$$\mathcal{M}_{ij} = -\frac{1}{2}\delta_{\langle ij\rangle}\boldsymbol{n}_{ij}\otimes \boldsymbol{n}_{ij} + \frac{1}{2}\delta_{ij}\sum_{l=1}^{N}\delta_{\langle il\rangle}\boldsymbol{n}_{il}\otimes \boldsymbol{n}_{il}$$

numerics



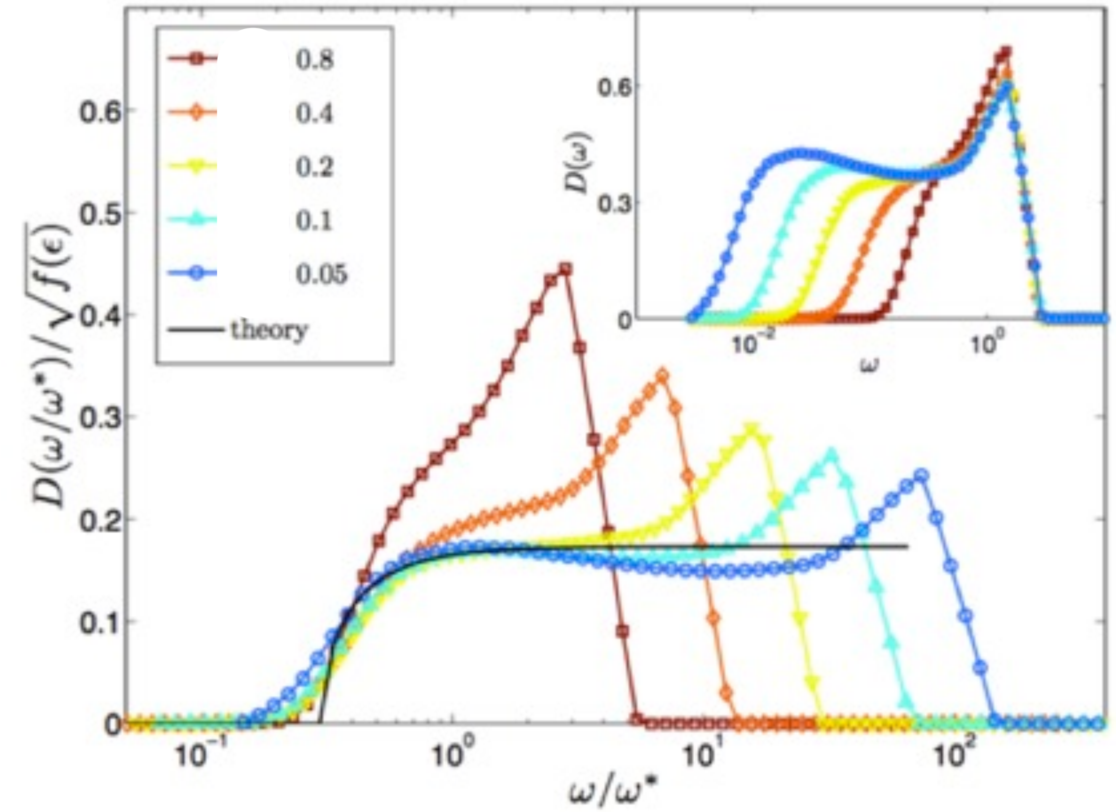


Density of states of vibrational modes



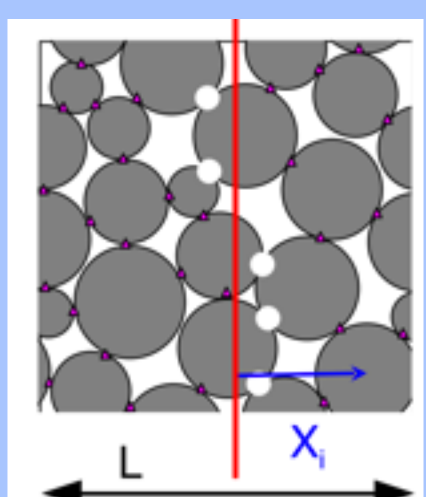
Wyart, et al 2005

1024 spheres interacting repulsive harmonic potential, above jamming threshold.



10000 spheres interacting repulsive harmonic potential, above jamming threshold.

Lerner,During and Wyart, 2013



18 particles confined in a periodic box

Plato in the density of states

cut gives: L^{d-1} modes

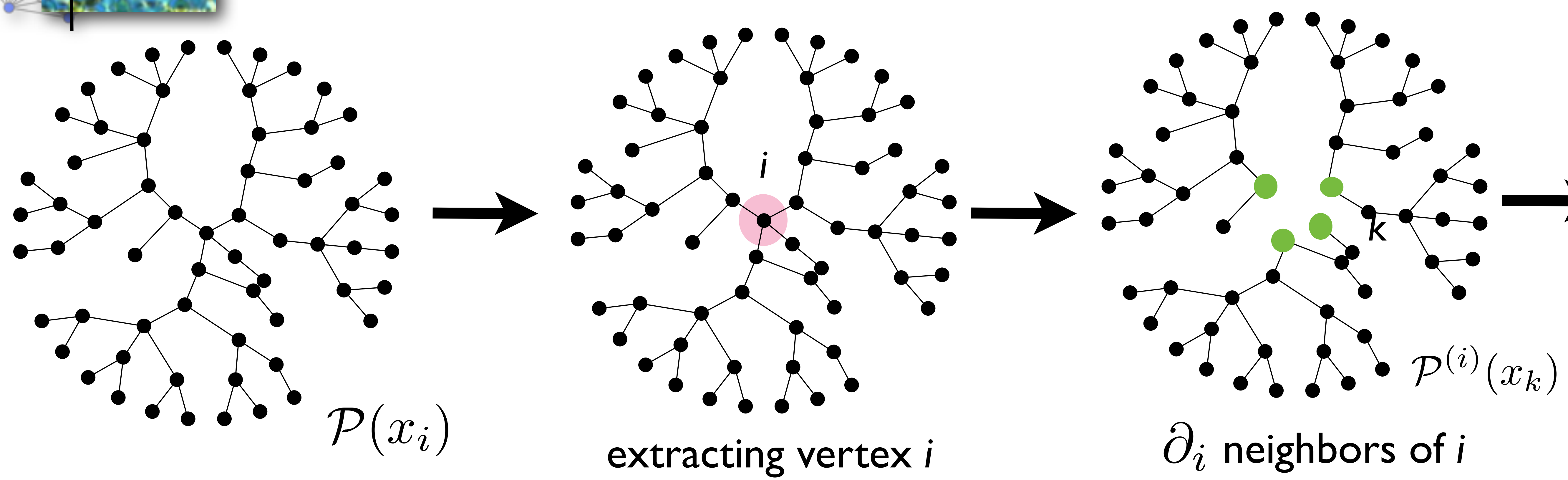
extended modes - approximated by sine waves with frequencies L^{-1}

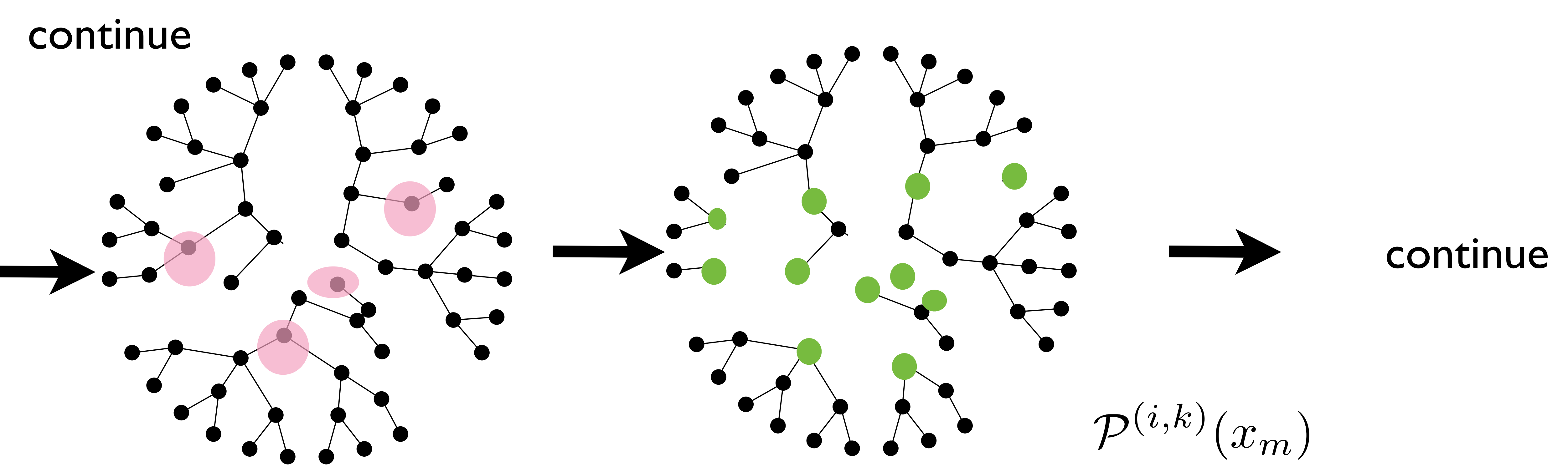
density of states

$$D(\omega) \propto \frac{L^{d-1}}{L^{-1}L^{d}} = \text{const}$$

Cavity method

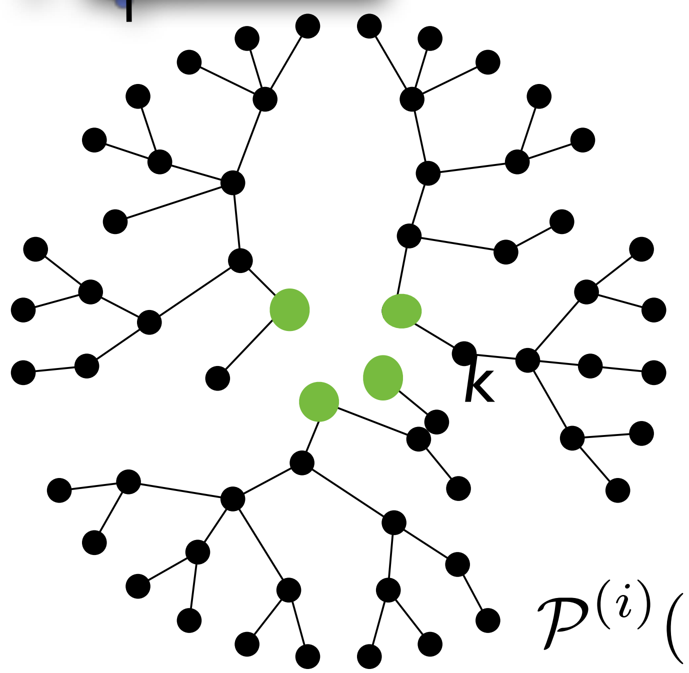
Mezard, Parisi, Virasoro, 1985





Cavity method

Mezard, Parisi, Virasoro, 1985



∂_i neighbors of *i*

assumptions

- subgraphs factorize (are independent)

$$\mathcal{P}^{(k)}(\boldsymbol{x}) = \prod_{j \in \partial_k} \mathcal{P}^{(k)}(x_j)$$

$$\mathcal{P}^{(k,m)}(\boldsymbol{x}) = \prod_{j \in \partial_m \setminus k} \mathcal{P}^{(k,m)}(x_j)$$

- closure

$$\mathcal{P}^{(k)}(x_j) = \mathcal{P}^{(k,m)}(x_j)$$

Gaussian ansatz

$$\mathcal{P}^{(k)}(x_m) \sim \exp[-ix_m^2/2G_{mm}^{(k)}]$$

- exact on a tree
- notice that subtrees independent
- generally uncontrolled approximation due to loops
- works well for large loops ~log*N*

Diffusion on random graph

diffusion on a line

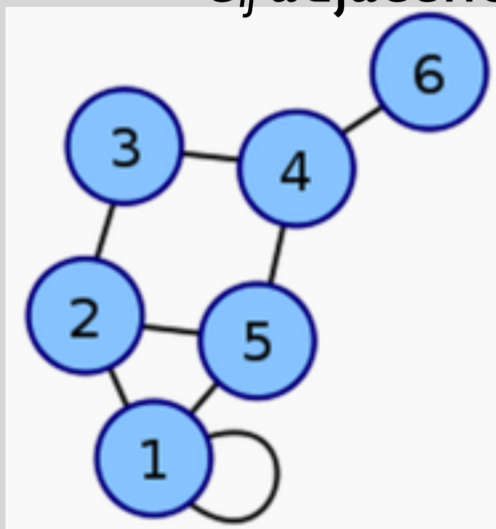
$$\partial_t c(x,t) = \kappa \nabla^2 c(x,t) \quad \to \quad \partial_t c(x_i,t) \simeq \kappa \frac{1}{(\Delta x)^2} \sum_j J_{ij} c(x_j,t)$$

J_{ij} diffusion between *i* and *j* nodes on the graph

r coordination number

$$J_{ij} \equiv -\frac{1}{r} C_{ij} + \delta_{ij} \frac{1}{r} \sum_{k=1}^{N} C_{ik}$$

C_{ij} adjacency matrix



$$\begin{pmatrix} 1 & 1 & 0 & 0 & 1 & 0 \\ 1 & 0 & 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 1 & 1 \\ 1 & 1 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \end{pmatrix}$$

density of states of *J*

Edwards, Jones, 1976

$$\rho_J(\lambda) = \frac{1}{N\pi} \mathrm{Im} \left(\frac{\partial}{\partial z} \ln\left(\det\left(zI - J\right)\right) \right) = \frac{-2}{N\pi} \mathrm{Im} \left(\frac{\partial}{\partial z} \ln \mathcal{Z} \right) = \frac{1}{\pi N} \mathrm{Im}\left(\mathrm{Tr}\, G(z)\right)$$

Hamiltonian $\mathcal{H}(\boldsymbol{x}) = \frac{i}{2} \boldsymbol{x}^T (zI - J) \boldsymbol{x}$ $\qquad \mathcal{P}(\boldsymbol{x}) = \mathcal{Z}^{-1} \exp[-\mathcal{H}(\boldsymbol{x})]$

diagonalizing a matrix "substituted" graph dynamics of fields ***x*** or finding the Green's function *G*

Cavity Equations

$$G_{ii} = \left[z - \sum_{j \in \partial_i} \left(\frac{J_{ij}^2 G_{jj}^{(i)}}{1 + J_{ij} G_{jj}^{(i)}} - J_{ij} \right) \right]^{-1},$$

$$G_{ii}^{(k)} = \left[z - \sum_{j \in \partial_i \setminus k} \left(\frac{J_{ij}^2 G_{jj}^{(i)}}{1 + J_{im} G_{jj}^{(i)}} - J_{ij} \right) \right]^{-1}$$

F. L. Metz, I. Neri, and D. Bollè, 2010

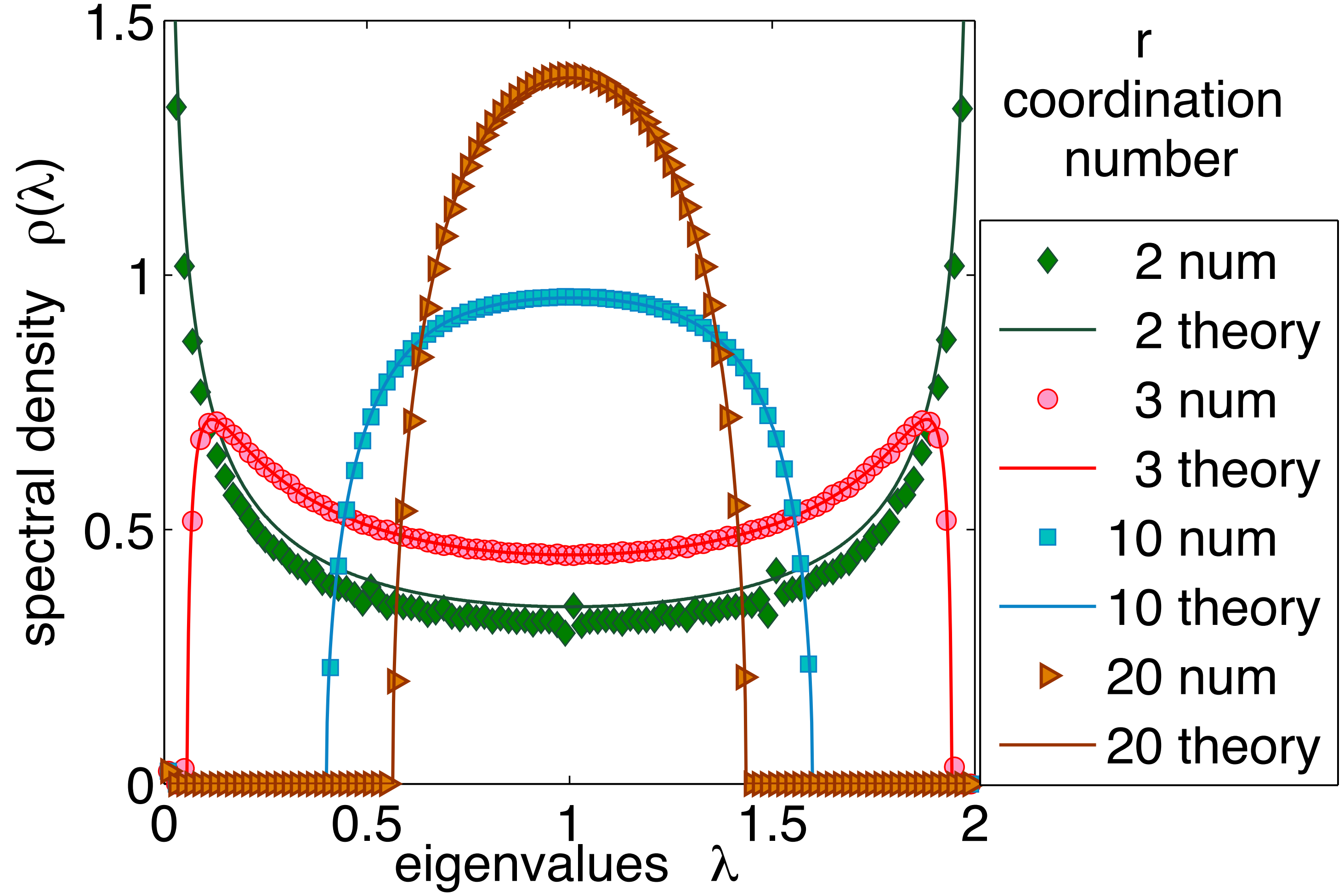
$$G = \left[z - \frac{r}{r - G^{()}} \right]^{-1}$$

$$G^{()} = \left[z - \frac{r-1}{r - G^{()}} \right]^{-1}$$

$$\rho(\lambda) = \frac{\delta(\lambda)(2-r) I_{[0,2]}(r)}{2} + \frac{\sqrt{r^2 \lambda (2-\lambda) - (r-2)^2}}{2\lambda(\lambda - 2)}$$

Markov Chain Monte Carlo

excellent agreement - theory and numerics



$$\rho(\lambda) = \frac{\delta(\lambda)(2-r)I_{[0,2]}(r)}{2} + \frac{\sqrt{r^2\lambda(2-\lambda)-(r-2)^2}}{2\lambda(\lambda-2)}$$

Cavity equations solution - small heterogeneity

Cavity Equations

$$\left(G^{-1}\right)_{ii} = \omega^2 I - \sum_{j\in\partial_i} \mathcal{M}_{ij} \left[\left(\left(G^{-1}\right)^{(i)}_{jj} + \mathcal{M}_{ij} \right)^{-1} \mathcal{M}_{ij} - I \right]$$

$$\left(G^{-1}\right)^{(k)}_{ii} = \omega^2 I - \sum_{j\in\partial_i \setminus k} \mathcal{M}_{ij} \left[\left(\left(G^{-1}\right)^{(i)}_{jj} + \mathcal{M}_{ij} \right)^{-1} \mathcal{M}_{ij} - I \right]$$

components

$$\left(G^{-1}\right)_{ii} = \begin{pmatrix} A_{ii} & B_{ii} \\ B^*_{ii} & D_{ii} \end{pmatrix}, \; \left(G^{-1}\right)^{(k)}_{ii} = \begin{pmatrix} a^{(k)}_{ii} & b^{(k)}_{ii} \\ b^{(k)*}_{ii} & d^{(k)}_{ii} \end{pmatrix}$$

isotropy, simplifies:

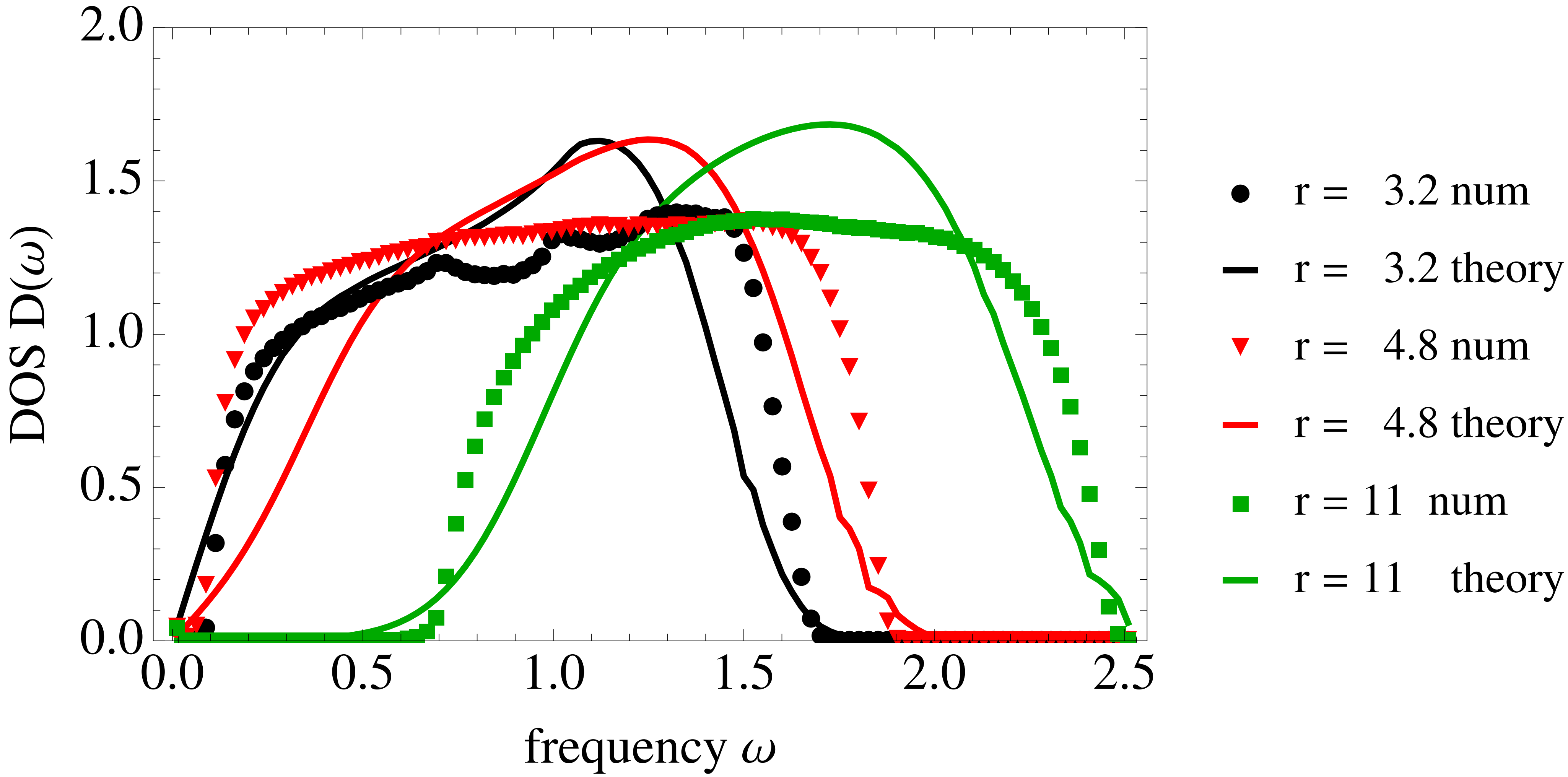
$$a = d, A = d, b = 0, B = 0$$

$$a = \omega^2 + \frac{r-1}{2} \left(1 + \xi_{r-1}\right) \frac{a}{1-2a},$$

$$A = \omega^2 + \frac{r}{2} \left(1 + \xi_r\right) \frac{a}{1-2a}$$

$$\xi_s = s^{-1} \sum_{i=1}^{s} \cos\phi_s$$

Vibrational modes $D(\omega)$



$$D(\omega) = \int_{-\infty}^{\infty} \mathrm{d}\xi \sqrt{\frac{r-1}{\pi}} e^{-(r-1)\xi^2} 2(r+(r-1)\xi) \frac{\sqrt{32\omega^2 - (3-r-(r-1)\xi+4\omega^2)^2}}{\pi\omega(3(r+(r-1)\xi)-4\omega^2)}$$

Summary - elasticity

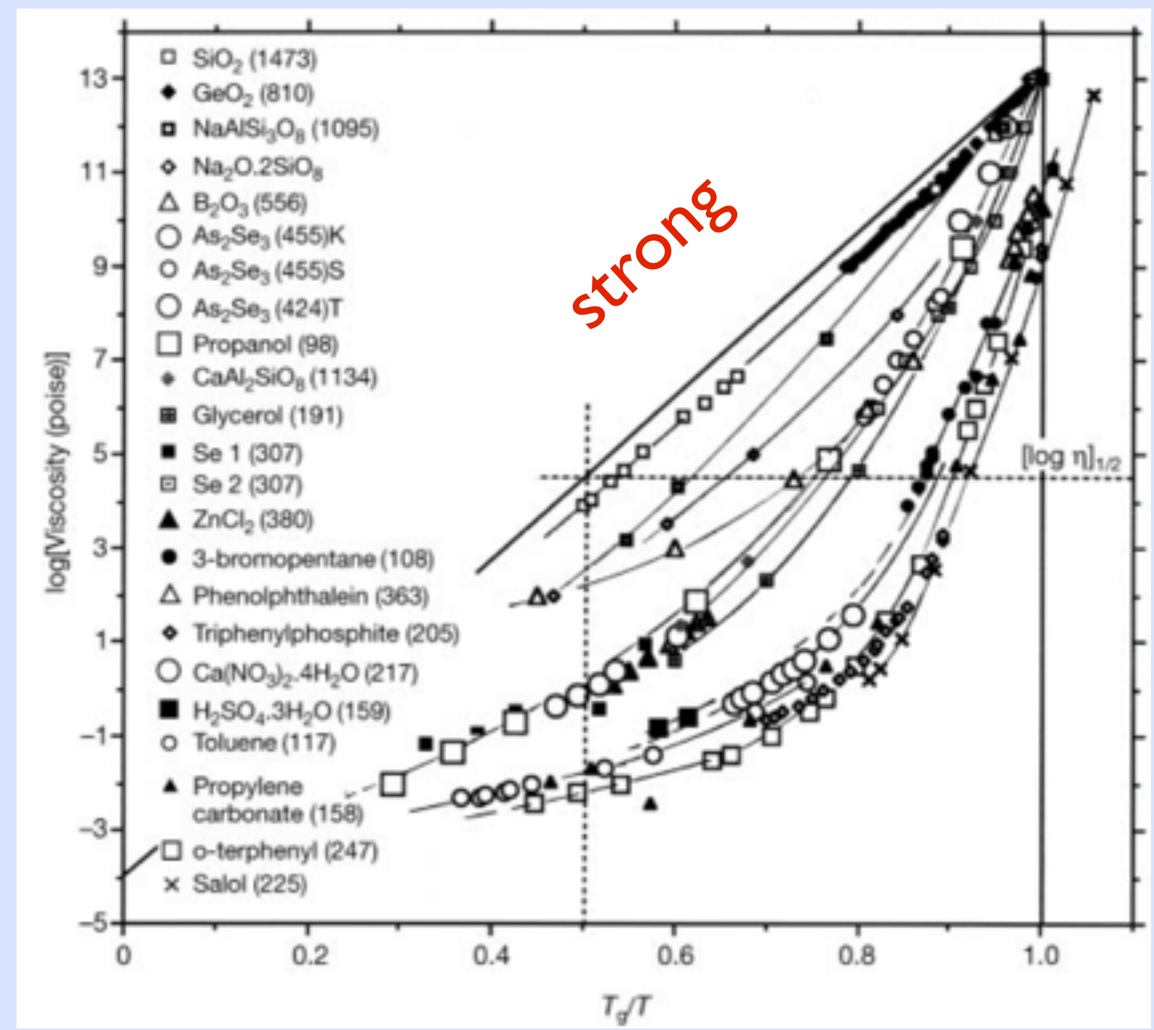
•**thermodynamics:** What is the role of the coordination number in thermodynamics?

•What distinguishes fragile from strong glasses?

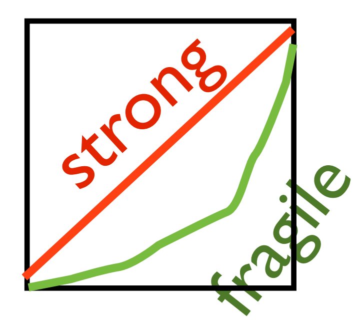
•compressed random networks.

•cases with stronger spatial inhomogeneities

Angell plot - strong and fragile glasses



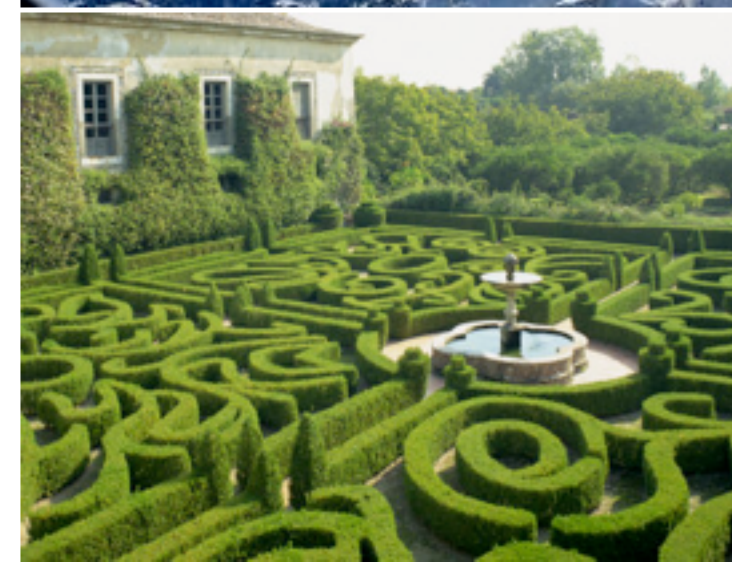
Angell, 1997



Mixing on random graphs

Slow relaxation to a equilibrium, due to:

- **energy barriers** glassy landscapes



- **entropy barriers** regions of high probability are separated by narrow paths (small entropy)

- **high entropy** a large phase space, that is flat in energy

Detailed balance

Ω set of states

$T(x,y)$ transition matrix

$$\pi^{t+1}(y) = \sum_{x\in\Omega} \pi^t(x) T(x,y)$$

stochastic matrix

$$\sum_{y\in\Omega} T(x,y) = 1 \quad \forall x \in \Omega$$

If $T(x,y)$ is irreducible the a steady state exists and it is unique $\pi_s(y) = \sum_{x\in\Omega} \pi_s(x) T(x,y)$

Balance condition $\sum_{x\in\Omega} [\pi_s(x)T(x,y) - \pi_s(y)T(y,x)] = 0$

Detailed balance (reversibility): $\pi_s(x)T(x,y) = \pi_s(y)T(y,x)$

Detailed balance is sufficient, but not necessary!

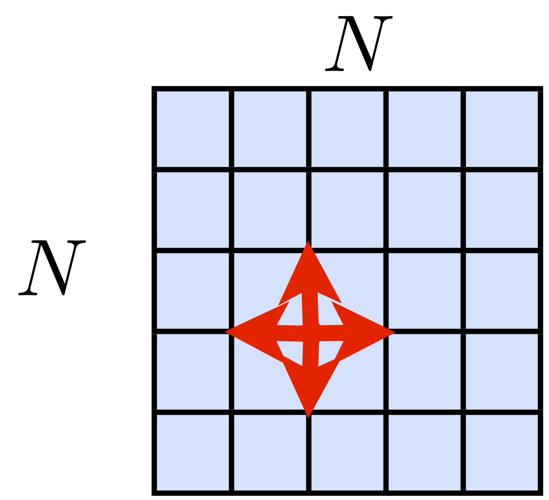
- How about breaking Detailed balance?

After all if you want your coffee sweet,
it is better to stir the sugar,
than to wait for it diffuse around the cup.

Lifting on a torus *Chen, Lovasz, Pak 1999*

goal: sample with uniform probability from a torus $N \times N$

Diffusion

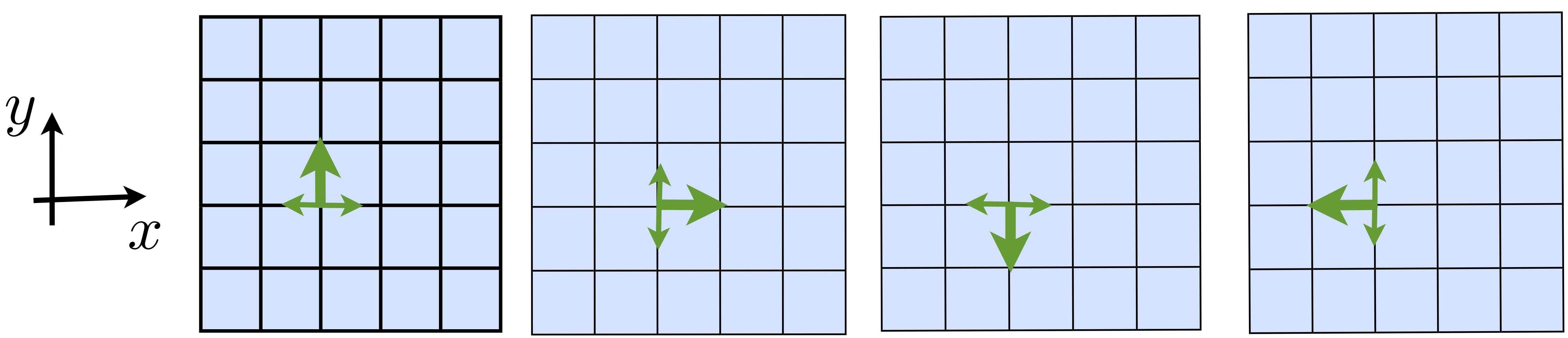


random walker on a torus
$p_N = p_W = p_E = p_S = 1/4$

mixing time on a torus $\mathcal{O}(N^2)$

Lifting

added advection



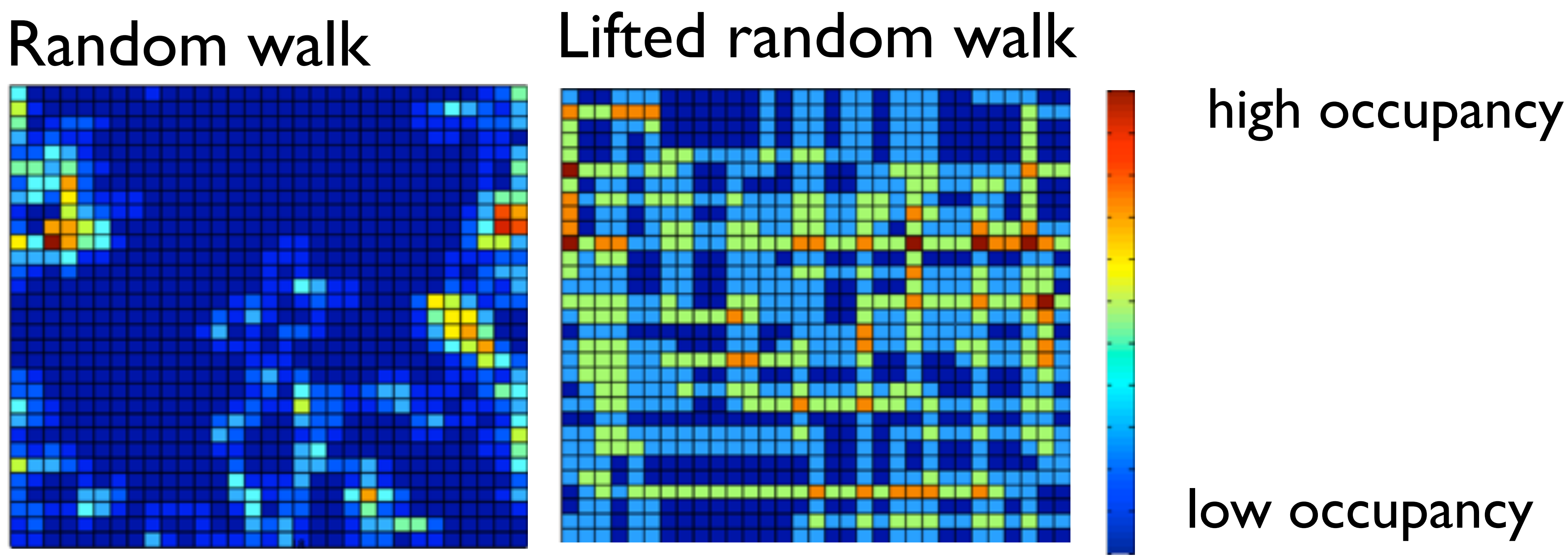
north east south west

$p_N = 1 - N^{-1}$
$p_E = p_W = (2N)^{-1}$
$p_S = 0$

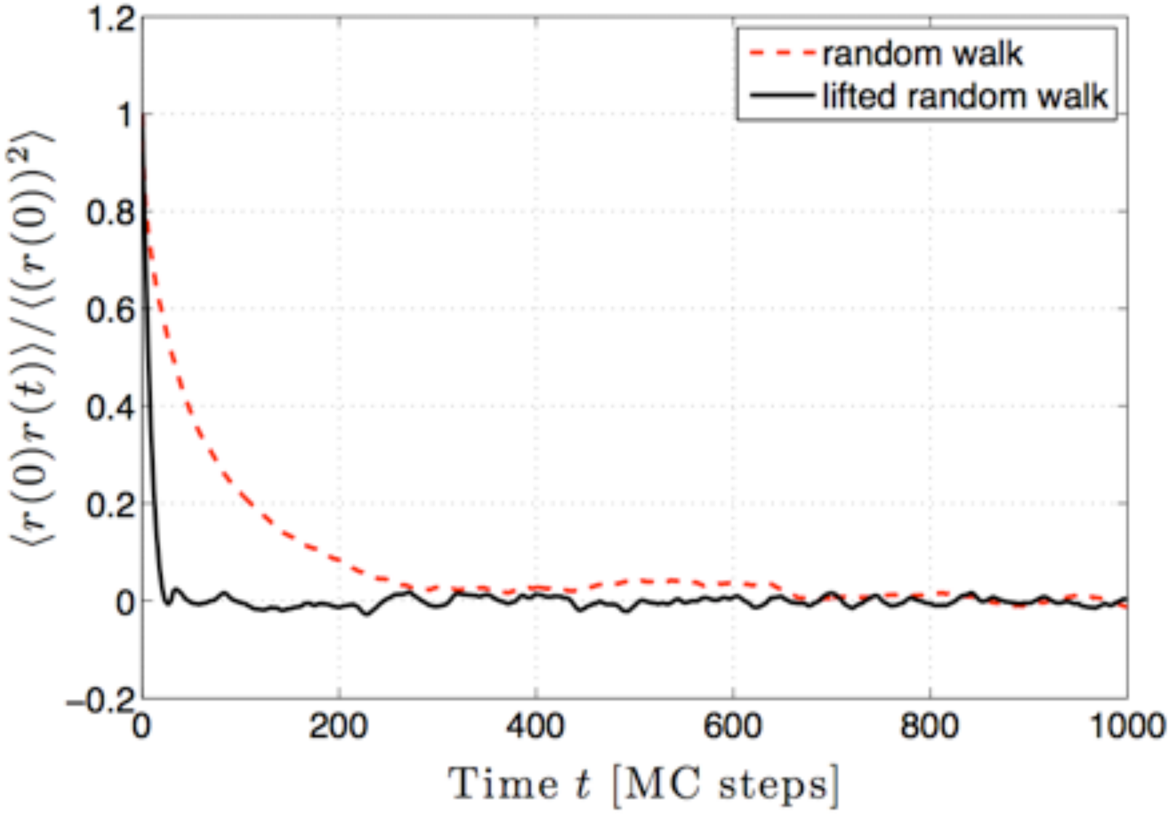
mixing time on a torus $\mathcal{O}(N)$

$\mathcal{O}(N)$ randomize along y-axis
$\mathcal{O}(N)$ randomize along x-axis

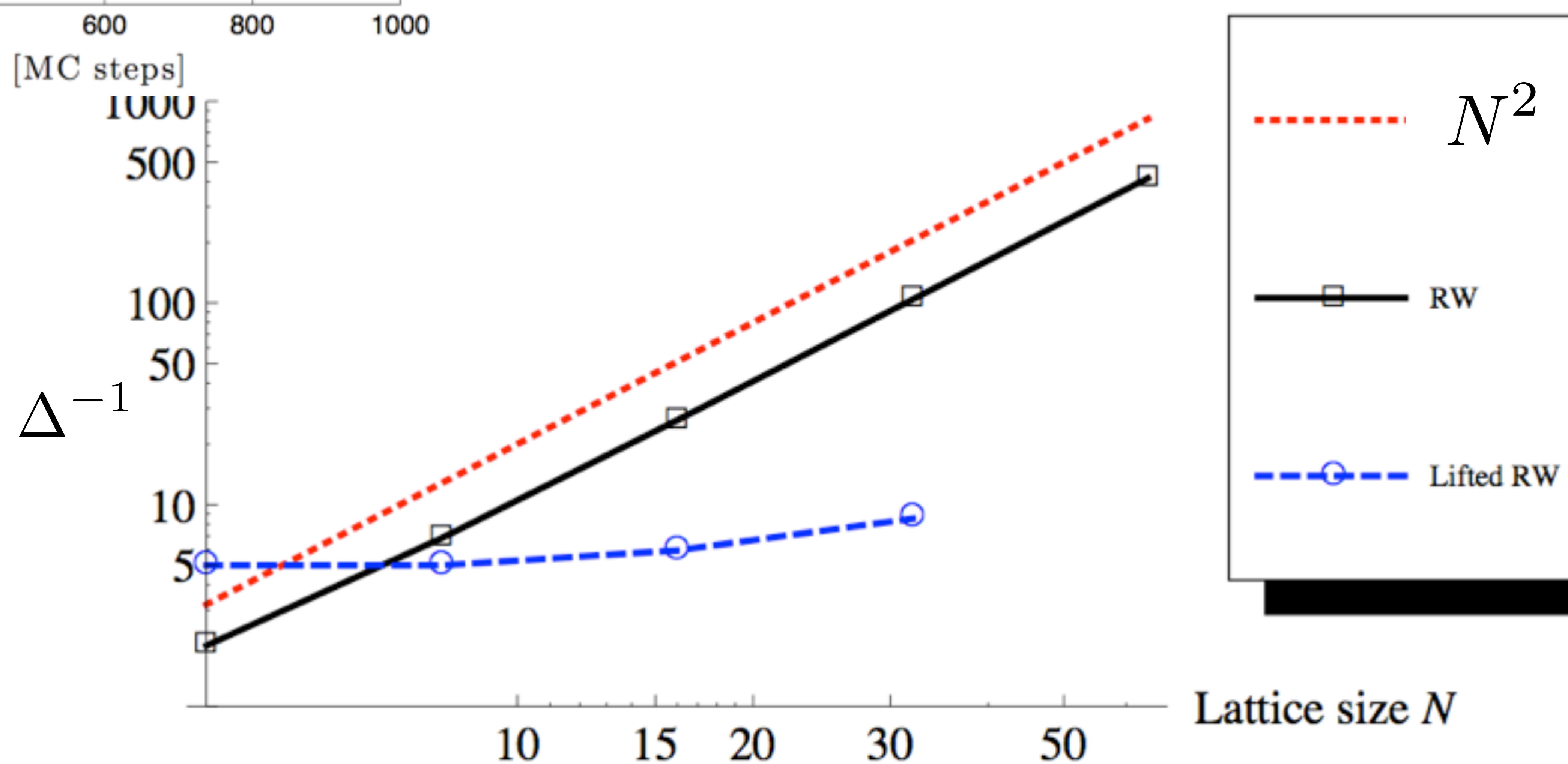
Density of visited sites on a torus of 1024 sites, after 1024 steps



Autocorrelation of distance from origin $\boldsymbol{r}(t)$



Inverse spectral gap



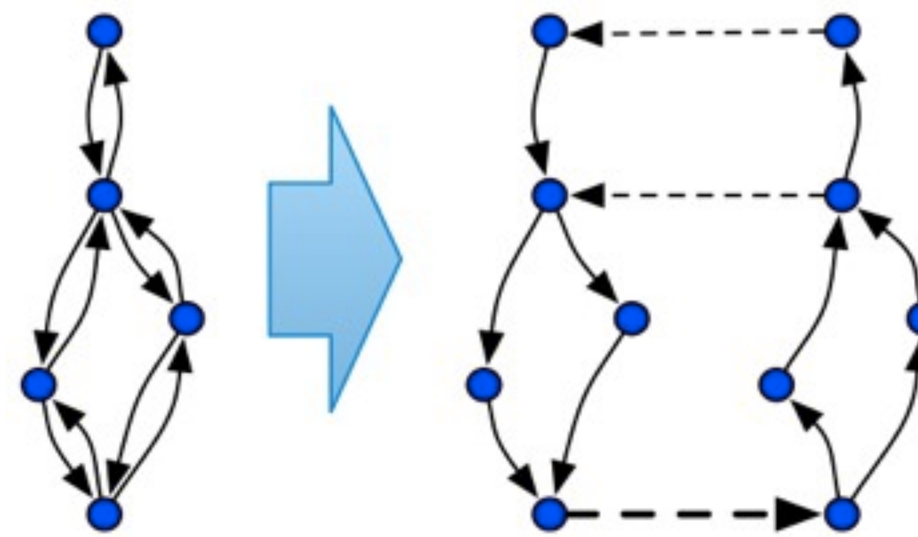
Skewed detailed balance

K. S. Turitsyn, M. Chertkov, MV (2008)

- Create two copies of the system ('+' and '-')
- Decompose transition probabilities as

$$T = T^{(+)} + T^{(-)}$$

$$\pi(x)T^{(+)}(x,y) = \pi(y)T^{(-)}(y,x)$$



- Compensate the compressibility by introducing transition between copies

$$\Lambda^{(\pm,\mp)}(x,x) = \max\left\{\sum_{y\in\Omega}\Big(T^{(\mp)}(x,y) - T^{(\pm)}(x,y)\Big), 0\right\}$$

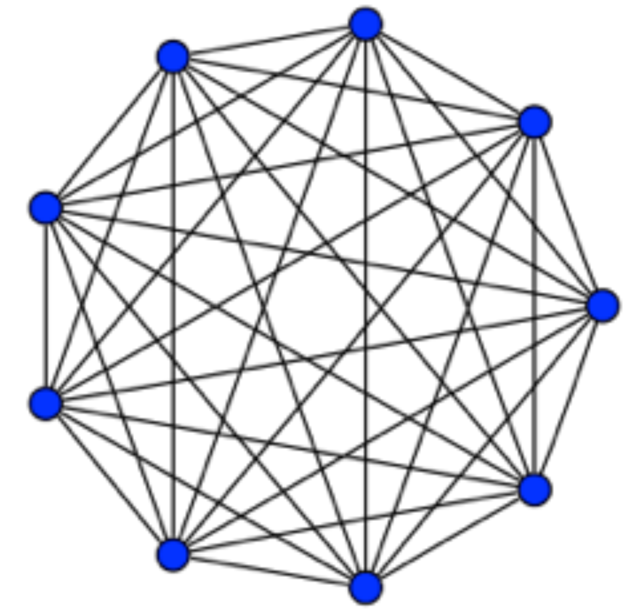
Skewed detailed balance continued

- Extended matrix satisfies balance condition and corresponds to irreversible process:

$$\mathcal{T} = \begin{pmatrix} T^{(+)} & \Lambda^{(+,-)} \\ \Lambda^{(-,+)} & T^{(-)} \end{pmatrix}$$

- Random walk becomes non-Markovian in the original space.
- System copy index is analogous to momentum in physics: diffusive motion turns into ballistic/ super-diffusive.
- No complexity overhead for Glauber and other dynamics.

Curie-Weiss Ising model



N-spins ferromagnetic cluster

Ising model on a complete graph

Stationary distribution

$$J > 0 \qquad \pi_{s_1,\ldots,s_N} = Z^{-1} \exp\left[-\frac{J}{N}\sum_{k,k'} s_k s_{k'}\right]$$

A state of the system is completely characterized by its global spin (magnetization)

$$S = \sum_k s_k$$

probability distribution of global spin

$$P(S) \sim \frac{N!}{N_+! N_-!} \exp\left(-\frac{JS^2}{2N}\right)$$

$$N_\pm = \frac{N \pm S}{2}$$

Physics of the spin-cluster continued

In the thermodynamic limit $N \to \infty$

the system undergoes a phase transition at $J = 1$

Away from the transition in the paramagnetic phase $J < 1$

$P(S)$ is centered around $S = 0$

and the width of the distribution is estimated by $\delta S \sim \sqrt{N/J}$

At the critical point (J=1) the width is $\delta S \sim N^{3/4}$

One important consequence of the distribution broadening is a slowdown observed at the critical point for reversible MH–Glauber sampling.

Correlation time of S reversible case

characteristic correlation time of S (measured in the number of Markov chain steps) is estimated as

$$T_{rev} \propto (\delta S)^2$$

the computational overhead associated with the critical slowdown is

$$\sim \sqrt{N}$$

Advantage of using irreversibility

The irreversible modification of the MH–Glauber algorithm applied to the spin cluster problem achieves complete removal of the critical slowdown.

Correlation time of S irreversible case

switching from one replica to another the system always go through the S = 0 state, since

$$\Lambda_{ii}^{(+,-)} = 0 \quad \text{if} \quad S > 0$$ (+) to (-) switching + spins in (+) replica

$$\Lambda_{ii}^{(-,+)} = 0 \quad \text{if} \quad S < 0$$ (-) to (+) switching - spins in (-) replica

The Markovian nature of the algorithm implies that all the trajectories connecting two consequent S = 0 swipes are statistically independent, therefore the correlation time roughly the number of steps in each of these trajectories.

Recalling that inside a replica (i.e. in between two consecutive swipes) dynamics of S is strictly monotonous, one estimates

$$T_{irr} \sim \delta S$$

$$T_{irr} \sim \sqrt{T_{rev}} \ll T_{rev}$$

Numerical verification

Analyzed decay of the pair correlation function, <S(0)S(t)>, with time.

Correlation time was reconstructed by fitting the large time asymptotics with exponential function

$$T \sim \exp(-t/T_{rev})$$
$$T \sim \exp(-t/T_{irr}) \cos(\omega t - \phi)$$

for both MH and IMH algorithms we constructed transition matrix corresponding to the random walk in S, calculated spectral gap, Δ, related to the correlation time as,

$$T = 1/Re\Delta$$

In both tests we analyzed critical point J = 1 and used different values of N ranging from 16 to 4096.

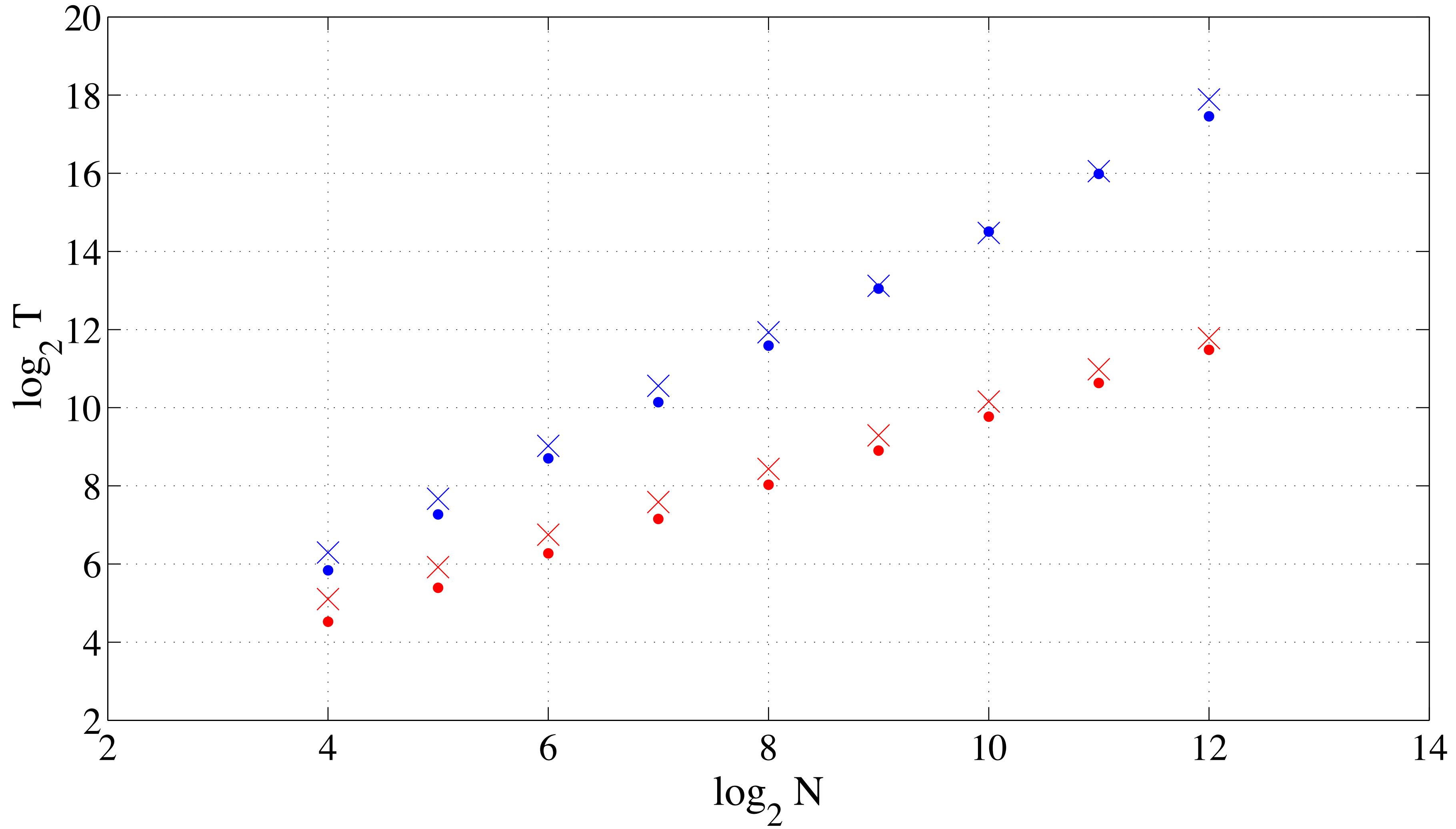
Correlation time of $\langle S(0)S(t)\rangle$ *(dots)*
Inverse spectral gap *(crosses)*

Reversible

$T \sim N^{1.43}$

Irreversible

$T \sim N^{0.85}$



A square root improvement: $T \sim N^{3/2} \to T \sim N^{3/4}$

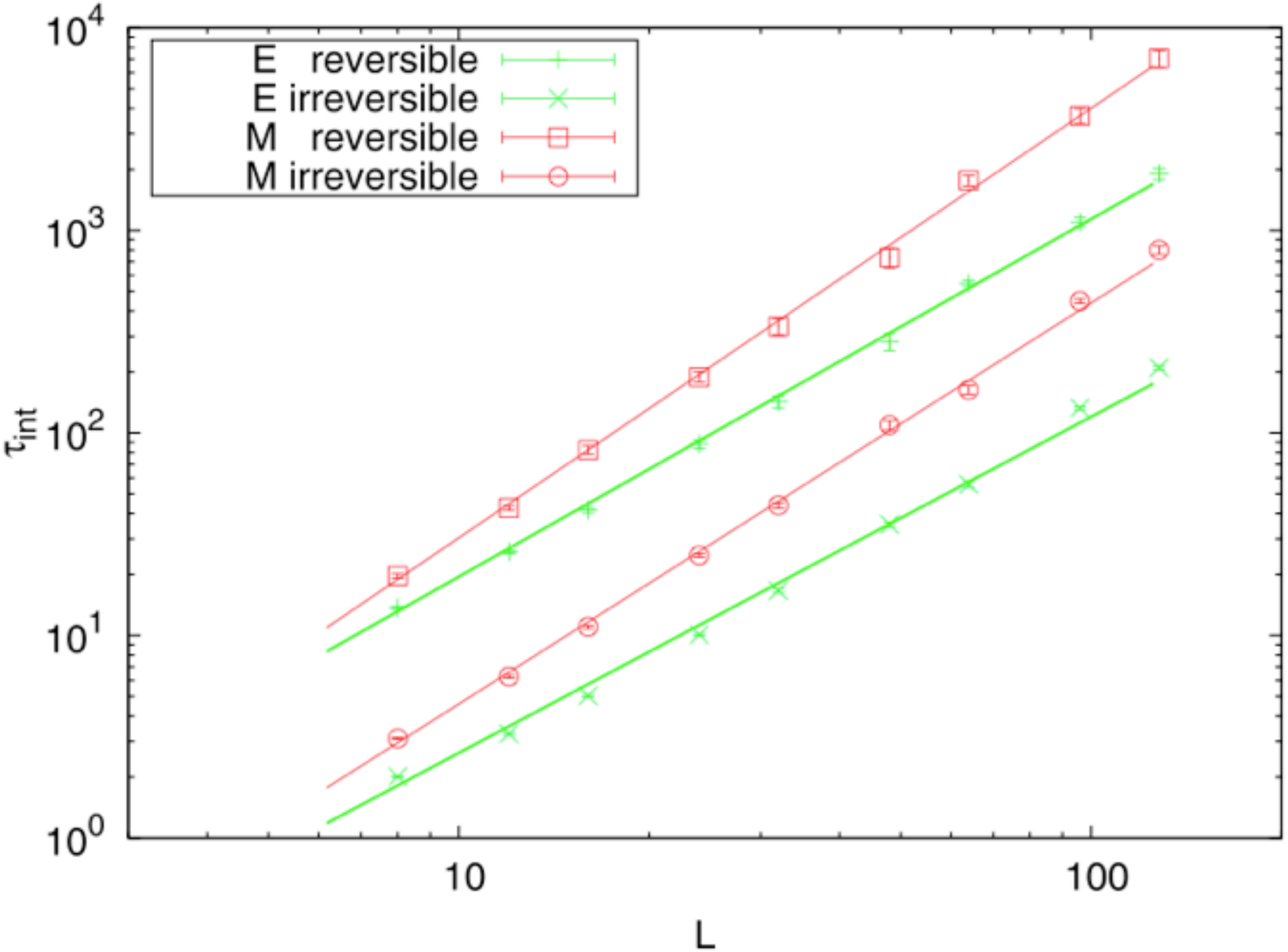
Best case scenario: square root improvement *Chen, Lovasz, Pak etc.*

(a) reversibly update $(E, y) \mapsto (E + y|\Delta E|, -y)$ with the Metropolis acceptance probability,

$$p_{\mathrm{acc}} = \min\left[1, \frac{N_{\Delta E = y|\Delta E|}}{N'_{\Delta E = -y|\Delta E|}} e^{-\beta \Delta E}\right], \tag{10}$$

(b) unconditionally negate $y \mapsto -y$,

(c) with probability θ, randomly choose a new step size $|\Delta E|$.



2d Ising

Collaborators

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MIT

Misha Chertkov
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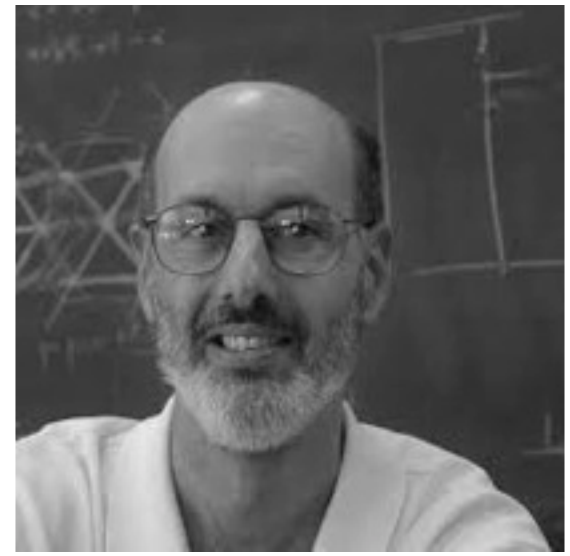

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