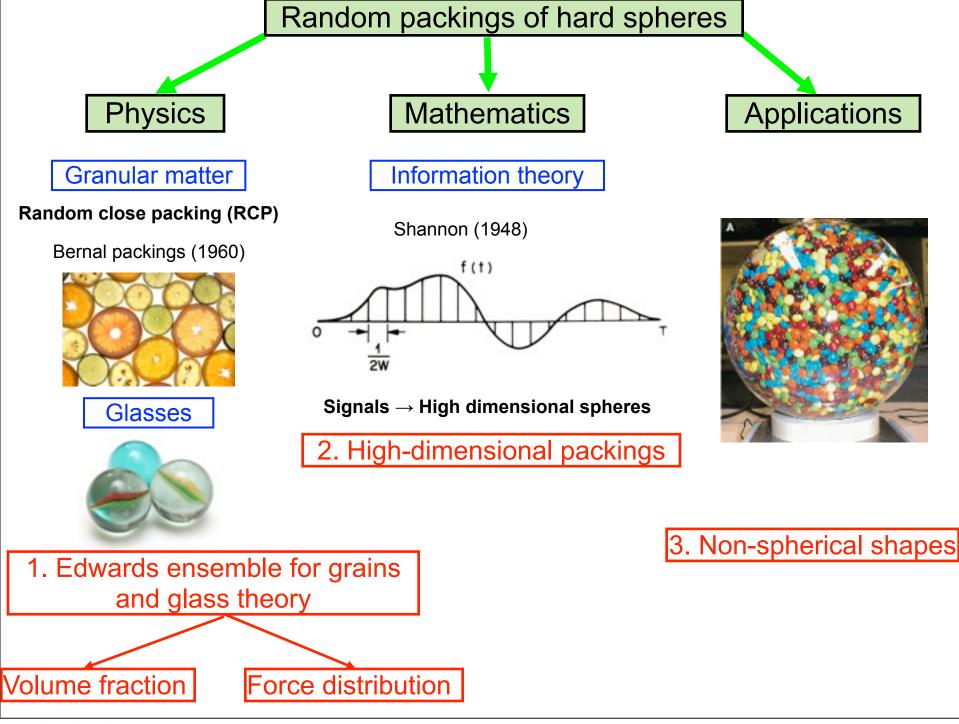
Commonalities between Edwards ensemble and glasses

Hernan Makse City College of New York Adrian Baule Lin Bo Max Danisch Yuliang Jin Romain Mari Louis Portal Chaoming Song

jamlab.org

Workshop: Physics of glassy and granular materials July 16-19, Kyoto



Theoretical approach I: Statistical mechanics (Edwards' ensemble)

Edwards and Oakeshott, Physica A (1989)

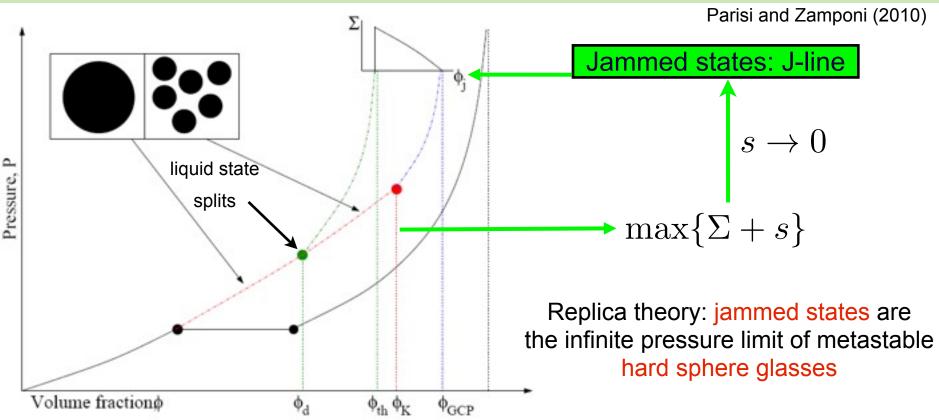
Constraint optimization problem

$$\mathcal{Z}(X,T) = \int \exp[-\mathcal{W}(\vec{x})/X] \exp[-\mathcal{H}(\vec{x},\vec{f})/T] \mathcal{D}\vec{x}\mathcal{D}\vec{f}$$

Minimize volume (X=0) with constraint of force balance (T=0) and non-overlaping.

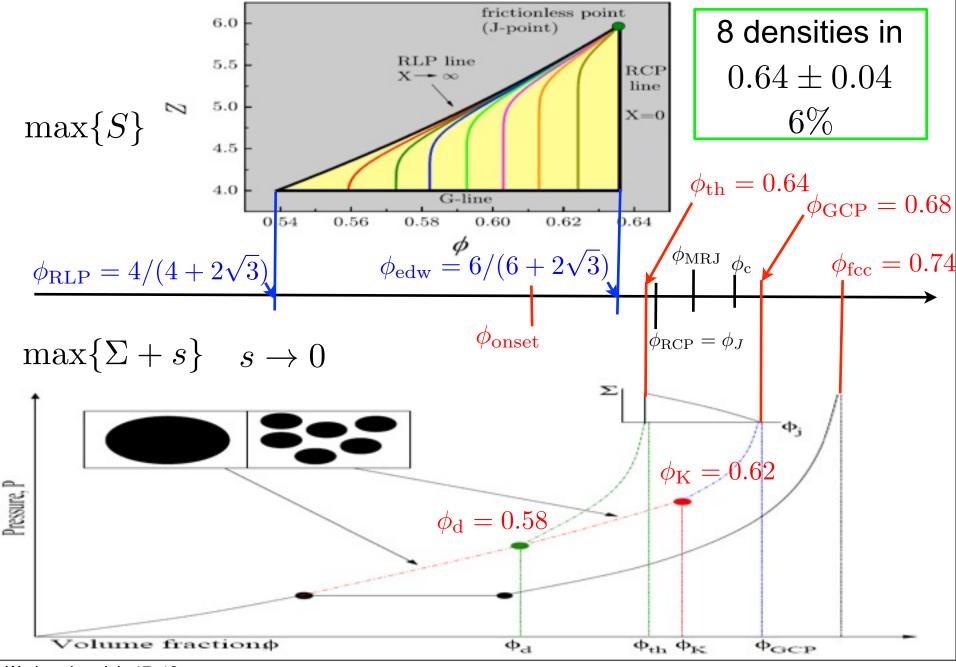
OPTIMIZATION	STATISTICAL PHYS	EDWARDS
instance	sample	packing
cost function	energy	volume
optimal configuration	ground state	RCP at X=0
minimal cost	ground state energy	minimal volume

Theoretical approach II: Mean field theory of jammed hard-sphere (remnant of RSB solution from replica theory)



- Approach jamming from the liquid phase.
- Predict a range of RCP densities $[\phi_{\rm th}, \phi_{\rm GCP}] \approx [0.64, 0.68]$
- Mean field theory based on RSB solution in the glass phase.

(un)Commonalities between Edwards ensemble and RT: 3d



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Very difficult in practice: very small range for 3d equal-size spheres

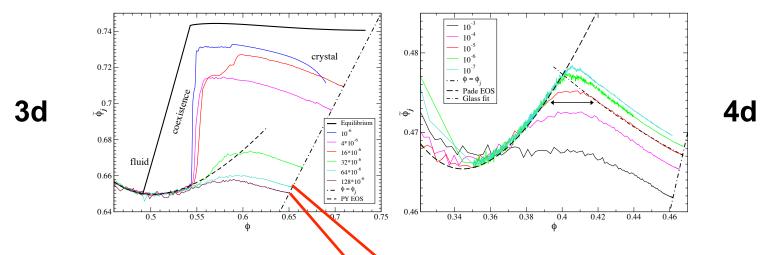
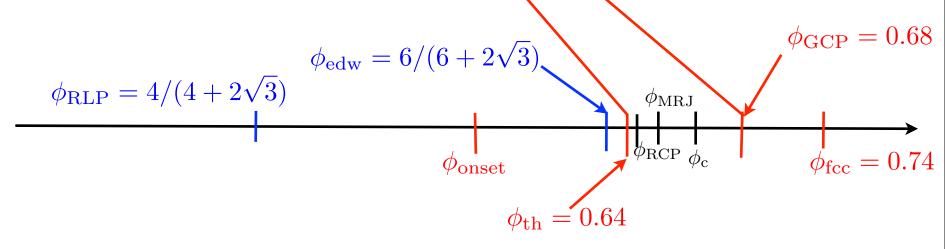
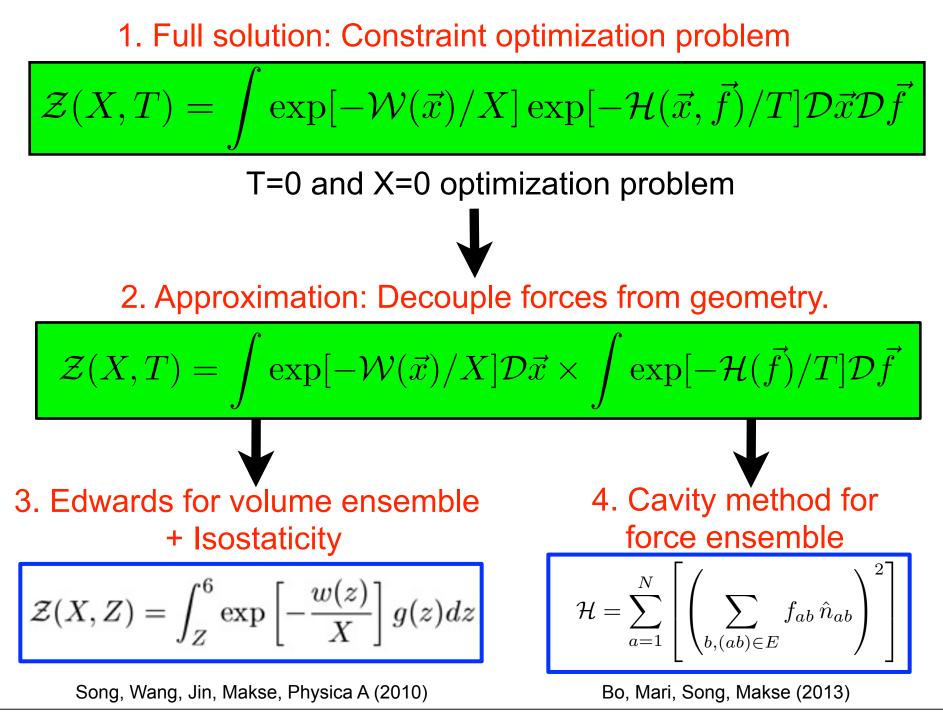
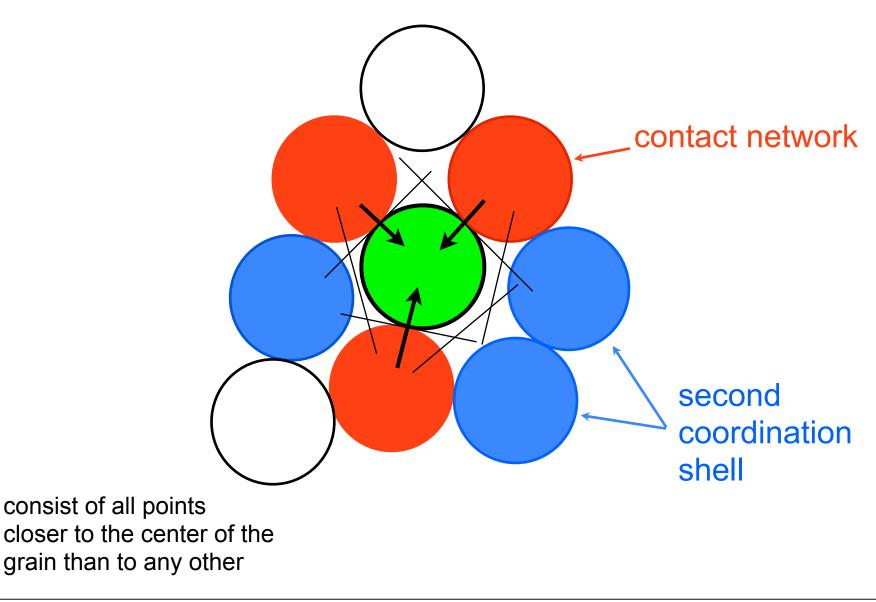


FIG. 1 (From (Skoge *et al.*, 2006)) Evolution of the pressure during compression at rate γ in d = 3 (left) and d = 4 (right). The density φ is increased at rate γ and the reduced pressure $p(\varphi) = \beta P/\rho$ is measured during the process. See (Skoge *et al.*, 2006) for details. The quantity $\tilde{\varphi}_j(\varphi) = \frac{p(\varphi)\varphi}{p(\varphi)-d}$ is plotted as a function of φ . If the system jams at density φ_j , $p \to \infty$ and $\tilde{\varphi}_j \to \varphi_j$. Thus the final jamming density is the point where $\tilde{\varphi}_j(\varphi)$ intersects the dot-dashed line $\tilde{\varphi}_j = \varphi$. (Left) The dotted line is the liquid (Percus-Yevick) equation of state. The curves at high γ follow the liquid branch at low density; when they leave it, the pressure increases faster and diverges at φ_j . The curves for lower γ show first a drop in the pressure, which signals crystallization. (Right) All the curves follow the liquid equation of state (obtained from Eq.(9) of (Bishop and Whitlock, 2005)) and leave it at a density that depends on γ . In this case no crystallization is observed. For $\gamma = 10^{-5}$ the dot-dashed line is a fit to the high-density part of the pressure (glass branch). The arrow marks the region where the pressure crosses over from the liquid to the glass branch.



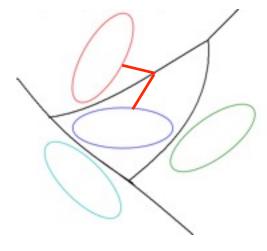


The Volume function is the Voronoi volume



"Easily" generalizable to other systems

equal size spheres



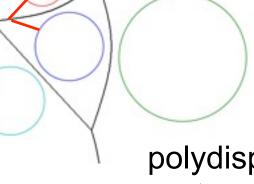
polydisperse system

ellipsoids, spherocylinders, non-convex particles, rods, sphere/ellipsoids mixtures, etc.

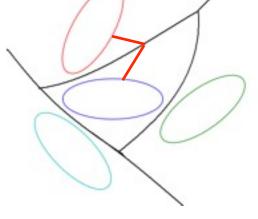
any dimension

"Easily" generalizable to other systems

equal size spheres

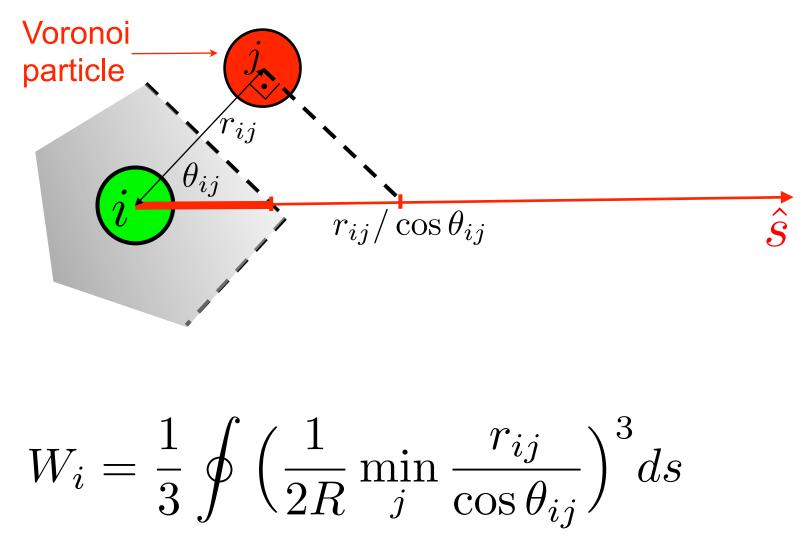


polydisperse system

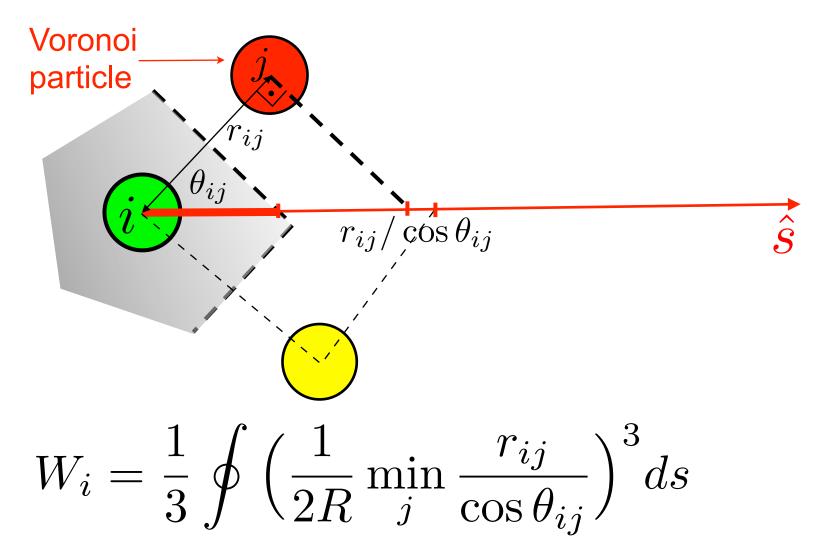


ellipsoids, spherocylinders, non-convex particles, rods, sphere/ellipsoids mixtures, etc.

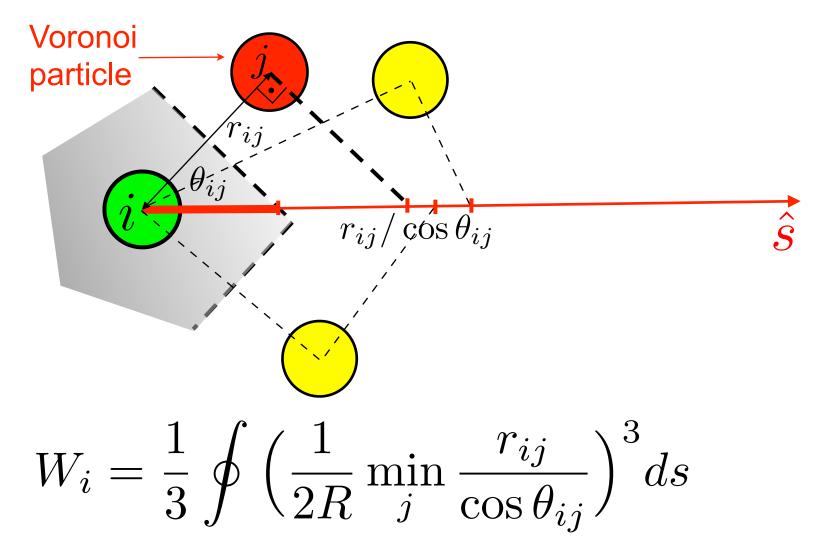
any dimension



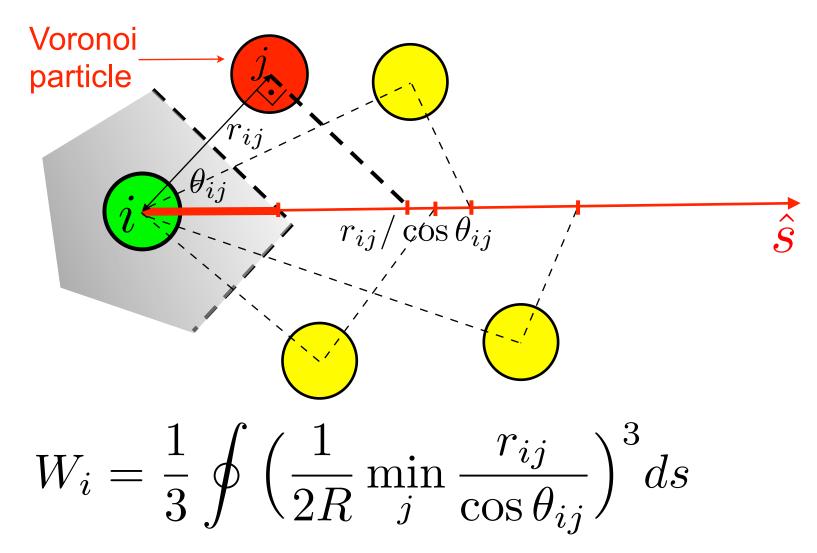
Important: global minimization. Reduce to one-dimension



Important: global minimization. Reduce to one-dimension



Important: global minimization. Reduce to one-dimension



Important: global minimization. Reduce to one-dimension

Average free-volume per particle

-

$$w = \int_{1}^{\infty} (c^{3} - 1)p(c)dc = \int_{0}^{1} (c^{3} - 1)dP_{>}(c)$$
Voronoi
boundary
$$V^{*}(c)$$

$$F^{*}(c)$$

$$C = r/\cos\theta$$

$$P_{>}(c)$$

$$-\frac{\partial P_{>}(c)}{\partial c} = p(c)$$
Probability to find all
particles outside excluded
volume and surface:

$$V^{*}(c)$$

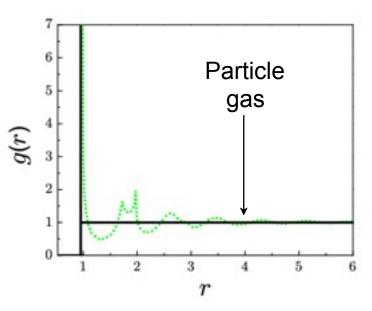
$$S^{*}(c)$$

Mean-field approximation analogous to decorrelation principle

particles belong to bulk or in contact:

$$P_{>}(c) = P_{B}(c) \times P_{c}(c)$$

$$g_2(r) \simeq \frac{z}{\rho S_{d-1}} \delta(r-1) + \Theta(r-1)$$



Similar to car parking problem (Renyi, 1960). Probability to find a spot with $V^*(c)$ in a volume V

- *

Particle gas

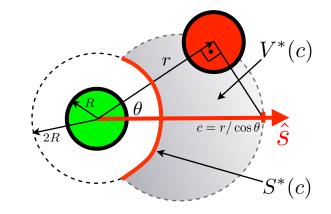
^e
$$P(V^*) = (1 - V^*/V)^N \to e^{-\rho V}$$

C)

Calculation of P>(c)

Particles are in contact and in the bulk:

$$P_{>}(c) = P_{B}(c) \times P_{c}(c)$$



Bulk term:

$$P_B(c) = e^{-\rho V^*(c)} \quad \rho(w) = \frac{1}{w}$$

mean free volume density

Contact term:

$$P_C(c) = e^{-\rho_s S^*(c)}$$

$$\rho_s(z) = \frac{1}{\langle S^* \rangle} = \frac{\sqrt{3}}{4\pi} z$$

Z = geometrical coordination number

mean free surface density

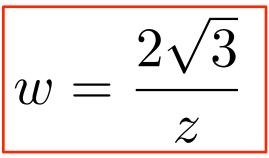
Average Voronoi volume

$$P_{>}(c) = P_{B}(c) \times P_{c}(c)$$

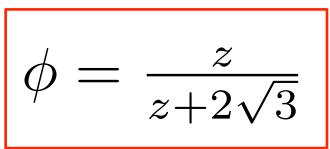
$$P_{>}(c) = \exp\left[-\frac{1}{w}\left((c^{3}-1)-3(1-\frac{1}{c})\right) - \frac{\sqrt{3}}{2}z(1-\frac{1}{c})\right]$$
Self-consistent equation:
$$w = \int_{0}^{1}(c^{3}-1) \ d \exp\left[-\frac{1}{w}\left((c^{3}-1)-3(1-\frac{1}{c})\right) - \frac{\sqrt{3}}{2}z(1-\frac{1}{c})\right]$$
equal to zero
$$w = \frac{2\sqrt{3}}{z}$$
represent the average free-volume of a single particle

Prediction: volume fraction vs z

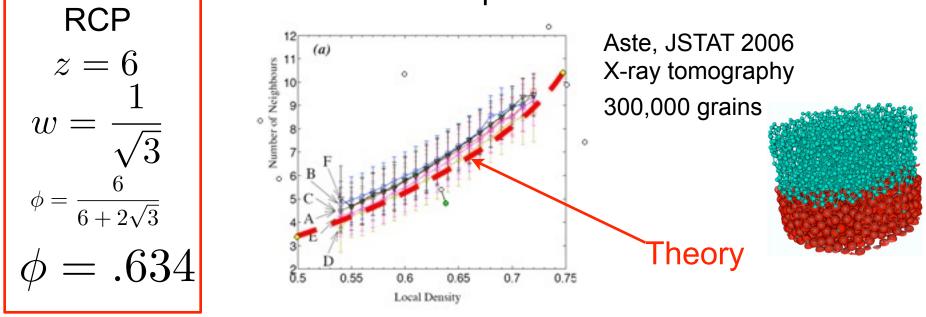
free volume



volume function



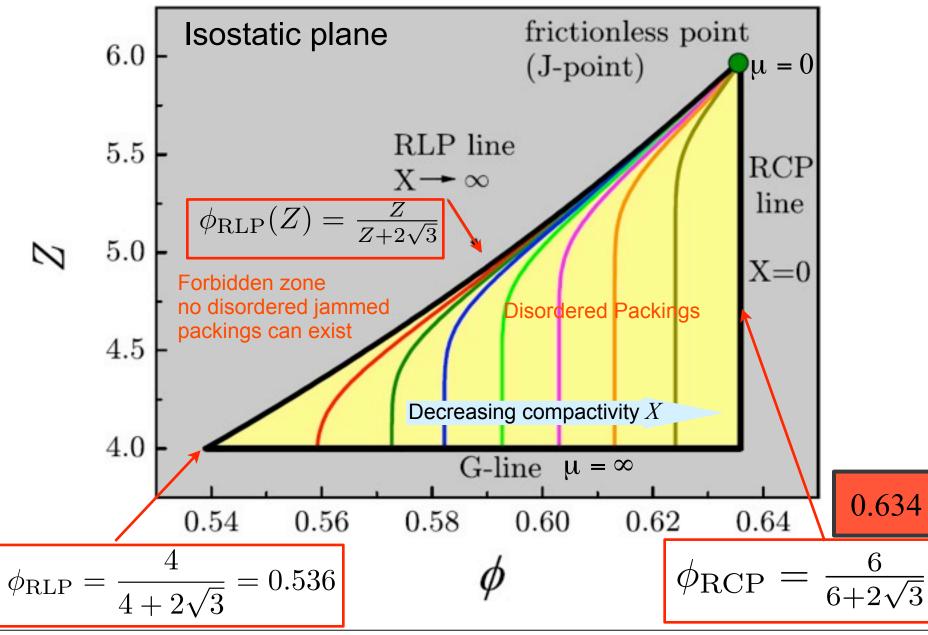
Equation of state agrees well with simulations and experiments



Definition of jammed state: geometric coordination z bounded by mechanical coordination Z

 $4 = d + 1 \le Z \le 2d = 6$ $\mu = \infty$ $Z \leq z \leq 2d = 6$ Z=3Ndpositions zN/2 geometrical constraints $z \leq 2d$ $|r_i - r_j| = 2R$ effectively excludes the ordered states

Edwards phase diagram for hard spheres



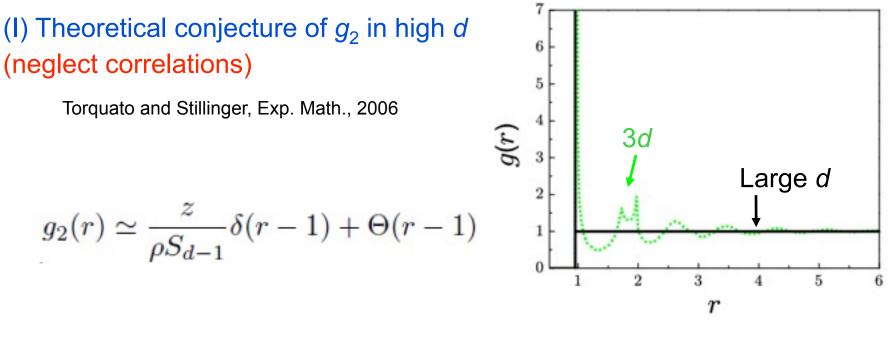
Jammed packings in high dimensions

Rigorous bounds

Minkowsky lower bound: $\phi \sim 2^{-d}$ Kabatiansky-Levenshtein upper bound: $\phi \sim 2^{-0.5990...d}$

Question: what's the density of RCP in high dimensions? Conjecture: are disordered packings more optimal than ordered ones?

Conjecture: $P_>(c)$ becomes valid in the high-dimensional limit



(II) Factorization of $P_>(c)$

$$P_{>}(c) = P_B(c)P_C(c)$$

Comparison with other theories

Edwards' theory

$$\phi \sim \frac{4d}{3} 2^{-d}$$

Isostatic packings (z = 2d) with unique volume fraction

Jin, *Charbonneau, Meyer, Song, Zamponi*, PRE (2010)

Agree with Minkowski lower bound

Glass transition RT

$$\phi \in [6.26 \, d \, 2^{-d}, d \, \ln(d) \, 2^{-d}]$$

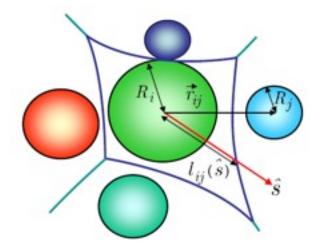
Parisi and Zamponi, Rev. Mod. Phys. (2010)

Isostatic packings (z = 2d) ranging volume fraction increases with dimensions

No unified conclusion at the mean-field level (infinite *d*). Neither dynamics nor jamming. Does RCP in large *d* have higher-order correlations missed by theory?: Test of replica th. Edwards solution seems to corresponds to ϕ_{th} . Higher entropy state.

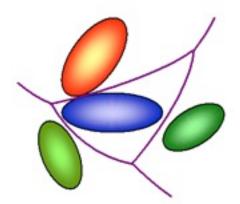
Generalizing the theory of monodisperse sphere packings

Polydisperse spheres



Non-spherical objects

(dimers, triangles, tetrahedra, spherocylinders, ellipsoids ...)



Distribution of radius P(r)

Distribution of angles $P(\hat{s})$

Extra degree of freedom

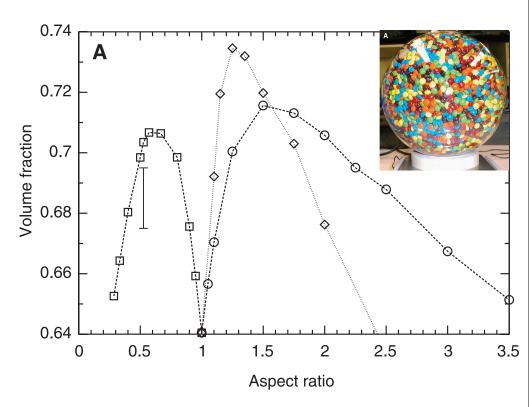
treated as in Onsager 1949

Optimizing random packings in the space of object shapes

- Simulation results on packings of *ellipsoids*:
- Ellipsoids pack *denser* than spheres
- > Peak at aspect ratio

 $\alpha \approx 1.4$

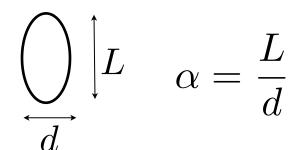
Spheres appear as a singular limit



Donev et al, Science 2004

Edwards prediction

• Non-spherical objects:



 $\phi(\alpha) = \phi(Z(\alpha), \alpha)$

 $z < 2d_f$

Edwards prediction

• Non-spherical objects:

$$\bigcup_{\substack{\leftarrow \\ d}} \int L \quad \alpha = \frac{L}{d}$$

$$\phi(\alpha) = \phi(Z(\alpha), \alpha)$$

 $\phi(Z, \alpha)$

Statistical theory of Voronoi volume

 $z < 2d_f$

Edwards prediction

 $\phi(\alpha) = \phi(Z(\alpha), \alpha)$

• Non-spherical objects:

 $\phi(Z,\alpha)$

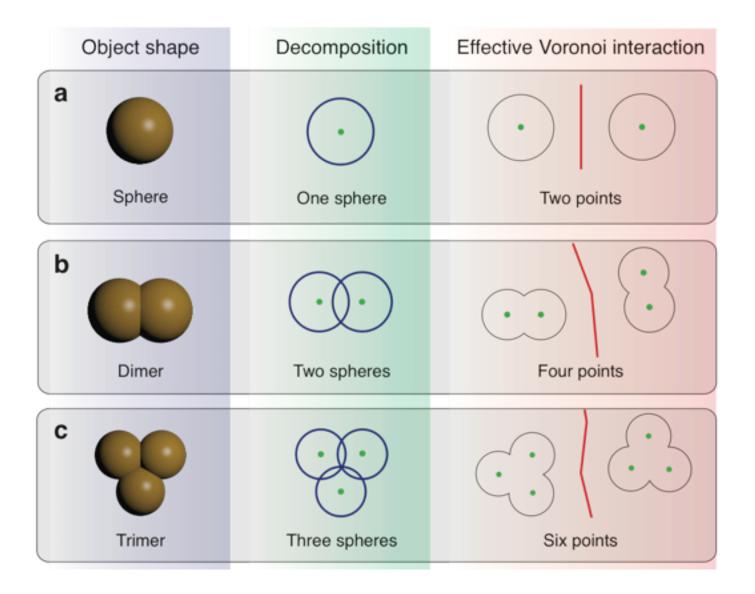
Statistical theory of Voronoi volume Evaluating the probability of degenerate configurations: ellipsoids are hypoconstrained

 $Z(\alpha)$

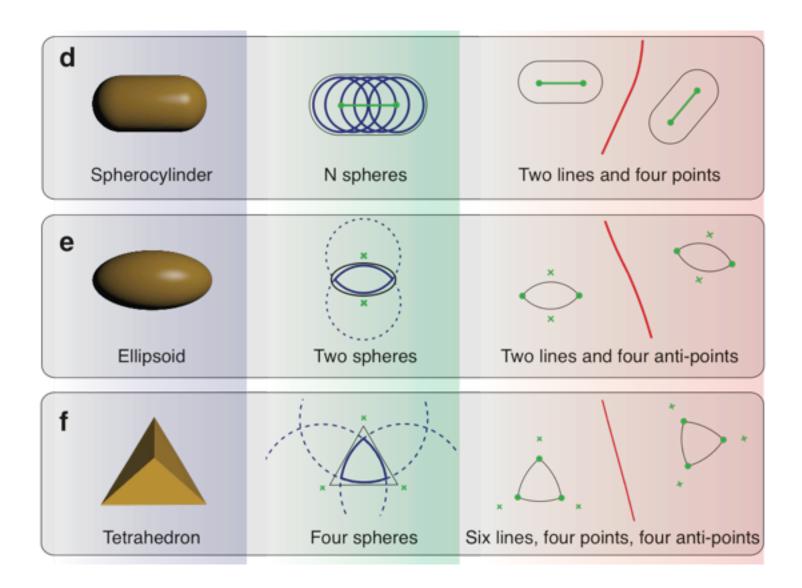
L

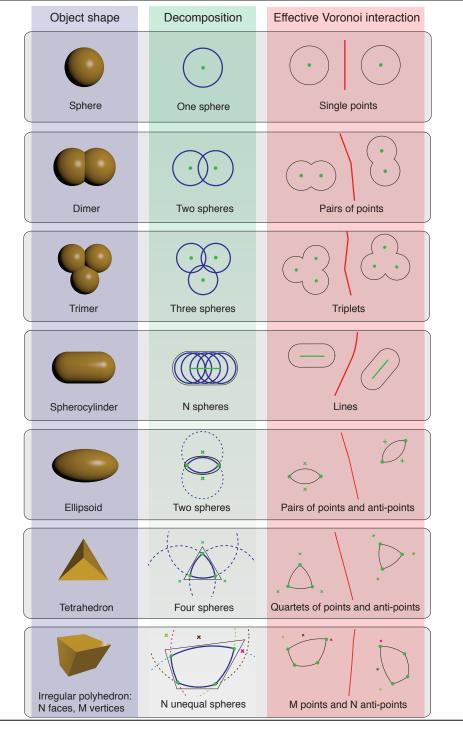
$$z < 2d_f$$

Voronoi for non-spherical shapes



General non-spherical shapes

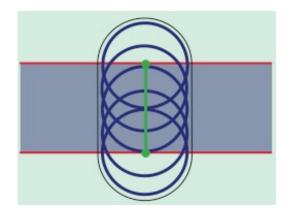




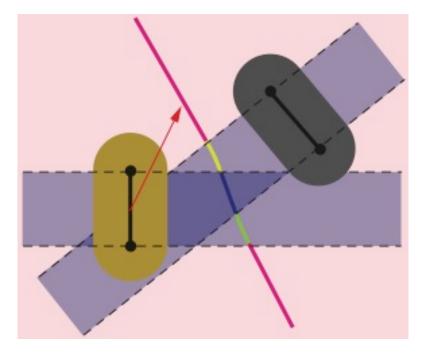
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Spherocylinders

• Separation lines:



- Four different interactions:
 - Line Line
 - Line Point
 - Point Line
 - Point Point



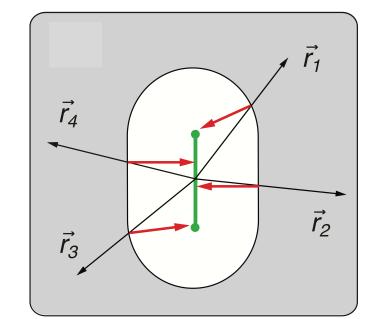
Exact equation for each case analytic expressions for VB

Calculation of coordination number: Degenerate configurations

- Mechanical equilibrium:
 - 3 force equations
 - 2 torque equations (torque along symmetry axis vanishes)

Linearly independent?

$$Z_c = 2d_f = 10$$

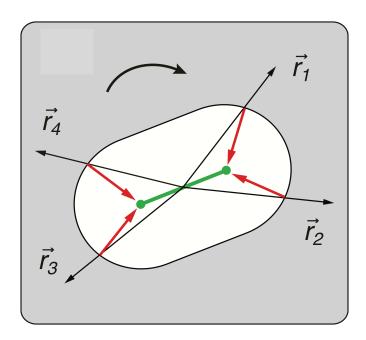


→ Effective number of degrees of freedom can be reduced!

Degenerate configurations

- Mechanical equilibrium:
 - 3 force equations
 - 2 torque equations (torque along symmetry axis vanishes)

Linearly independent?

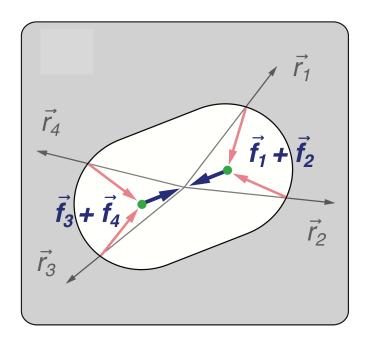


→ Effective number of degrees of freedom can be reduced!

Degenerate configurations

- Mechanical equilibrium:
 - 3 force equations
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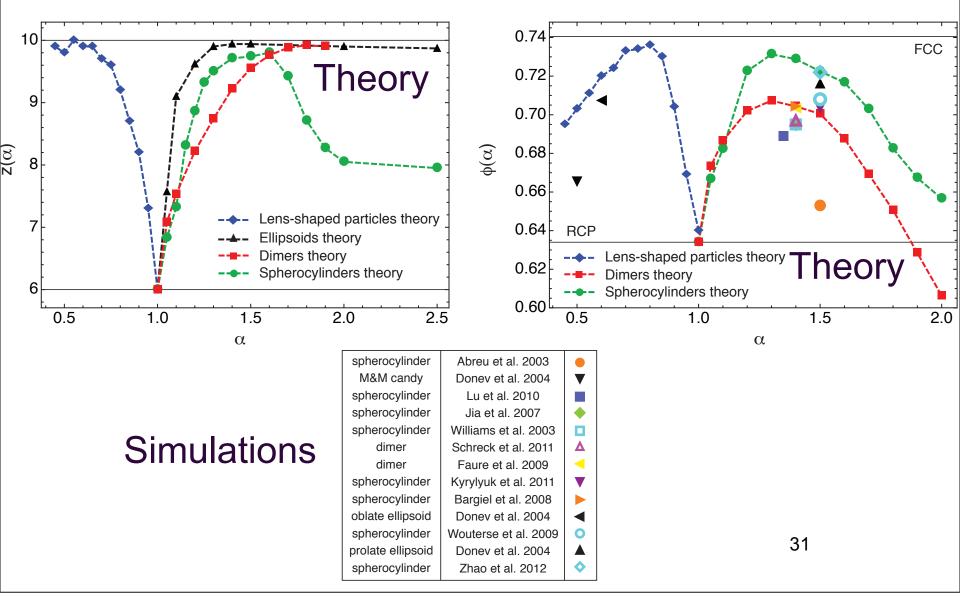
Linearly independent?



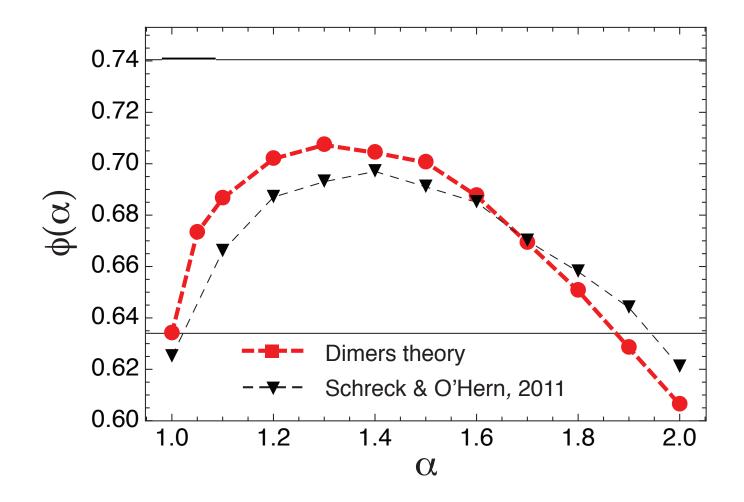
Maximal degenerate configuration: Condition of force balance automatically implies torque balance!

$$\rightarrow \quad Z(\alpha) = 2\langle \tilde{d}_f(\alpha) \rangle$$

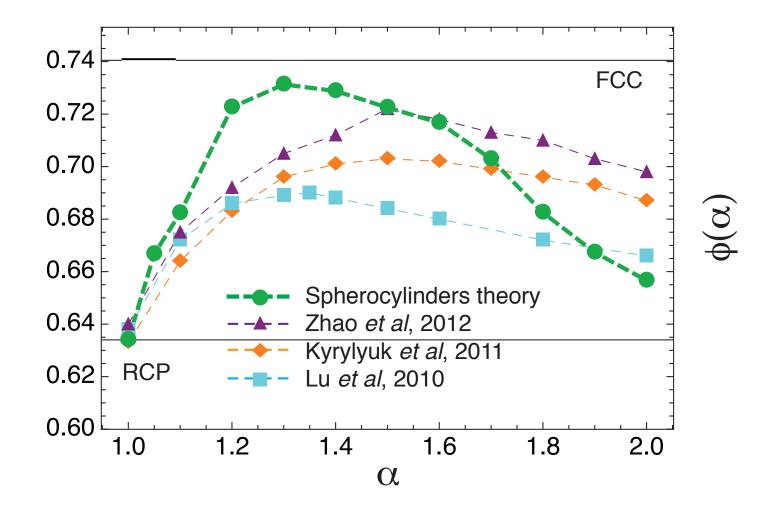
Theoretical predictions



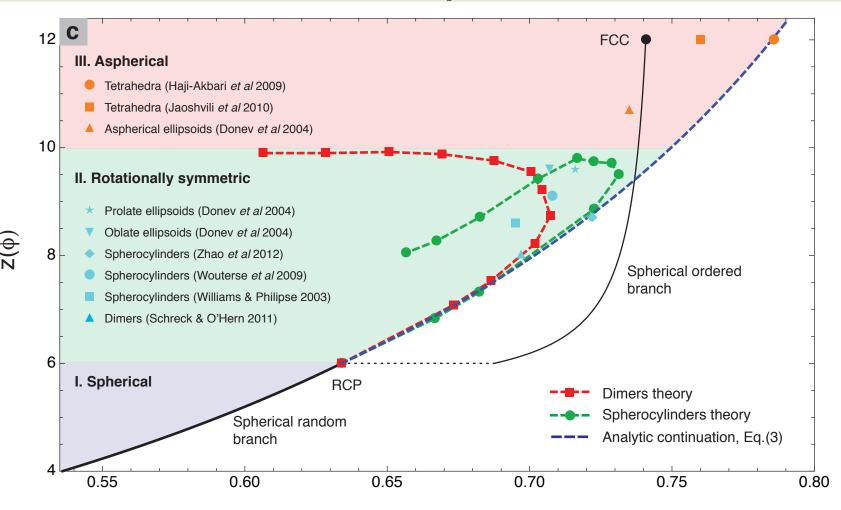
Results for packing fraction: dimers



Results for packing fraction: spherocylinders



Edwards phase diagram for many shapes



RCP is not singular: analytical continuation of spheres

Summary

Ode to Edwards!

- 1. Edwards ensemble to predict RCP for spheres.
- 2. Edwards ensemble for non-spherical particles.
- Edwards ensemble for packings in large dimensions to compare with replica theory of hard sphere glasses.
- 4. Edwards replica trick or cavity method for proper average over quenched disorder for force distribution for any system: spheres, non-spheres, friction and frictionless, any dimension.
- 5. Extending Maxwell argument: Cavity method at RS level for solution-no solution transition to calculate Z_c from frictionless isostatic grains to frictional grains.
- 6. Edwards CAVEAT: 1 5 done at expense of drastic (yet controlled) approximations.

Cavity Method for Force Transmission

$$\mathcal{Z}(X,T) = \int \exp[-\mathcal{W}(\vec{x})/X] \mathcal{D}\vec{x} \times \int \exp[-\mathcal{H}(\vec{f})/T] \mathcal{D}\vec{f}$$

Edwards volume ensemble predicts: $\phi(Z)$

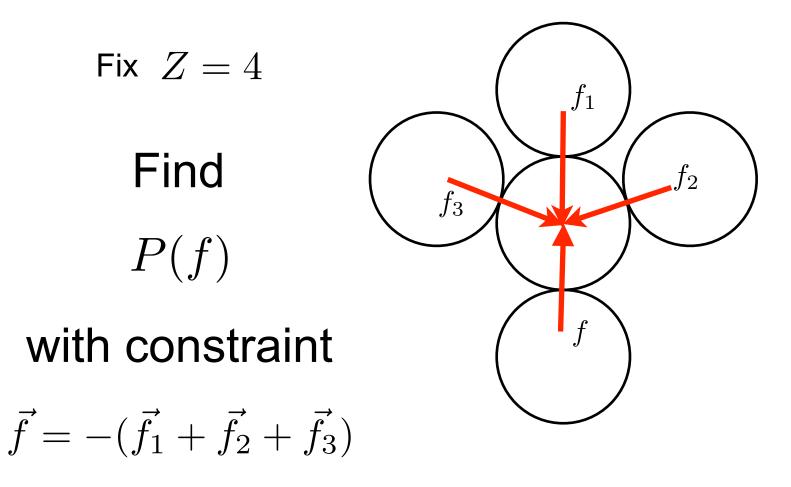
Cavity method predicts Z:

 $Z(\alpha)$

and Force Distribution:

Force transmission problem: back to Edwards (simplest model)

Edwards model = q-model = annealed disorder average



Boltzmann equation for *P(f)*



quenched disorder

Boltzmann equation:

assuming uncorrelated forces (MF)

$$P(f) = \int P(f_1, \lambda_1) P(f_2, \lambda_2) \tau(\lambda_1, \lambda_2) \delta(f - \lambda_1 f_1 - \lambda_2 f_2) d\lambda_1 d\lambda_2 df_1 df_2$$

Edwards: "Tiresomely complicated function well modelled by integrating between 0 and 1"

Fourier transform:

annealed disorder —

 f_1

$$P(f) = \frac{f}{p}e^{-\frac{f}{p}}$$

Annealed versus quenched disorder

Experimentally: first find the distribution for a fixed (quenched) packing, then average over the ensemble of packings

Average must be carried over a physical observable: free energy, not the partition function.



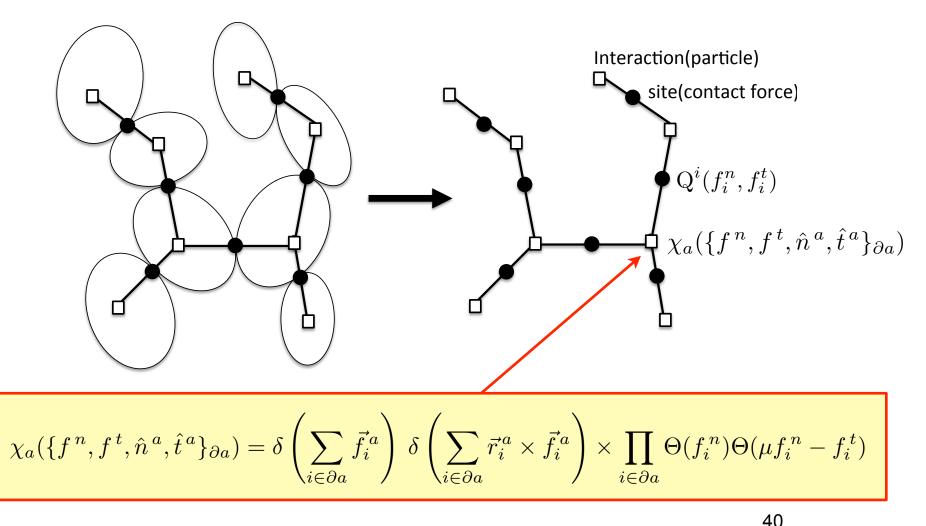
 $F = -kT \, \ln Z$

annealed disorder

$$F = -kT \ \ln \overline{Z}$$

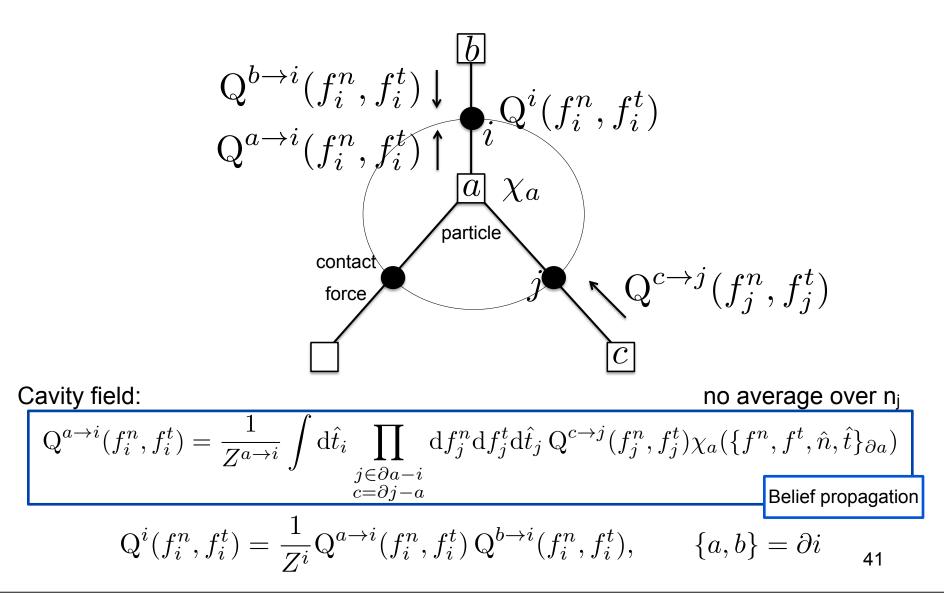
Replica trick(Edwards-Anderson) $\ln Z = \lim_{n \to 0} (Z^n - 1)/n$ Granular matter: Cavity Method \longrightarrow Performed average over forces then over contact network

Building the factor graph of contacts from a packing

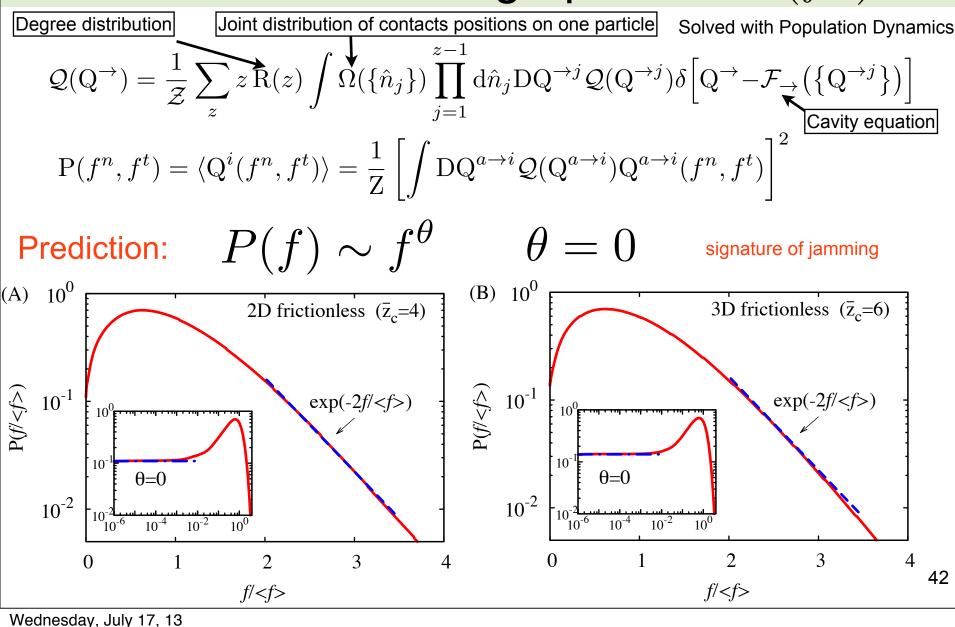


Constraint: force balance + torque balance + repulsive + Coulomb

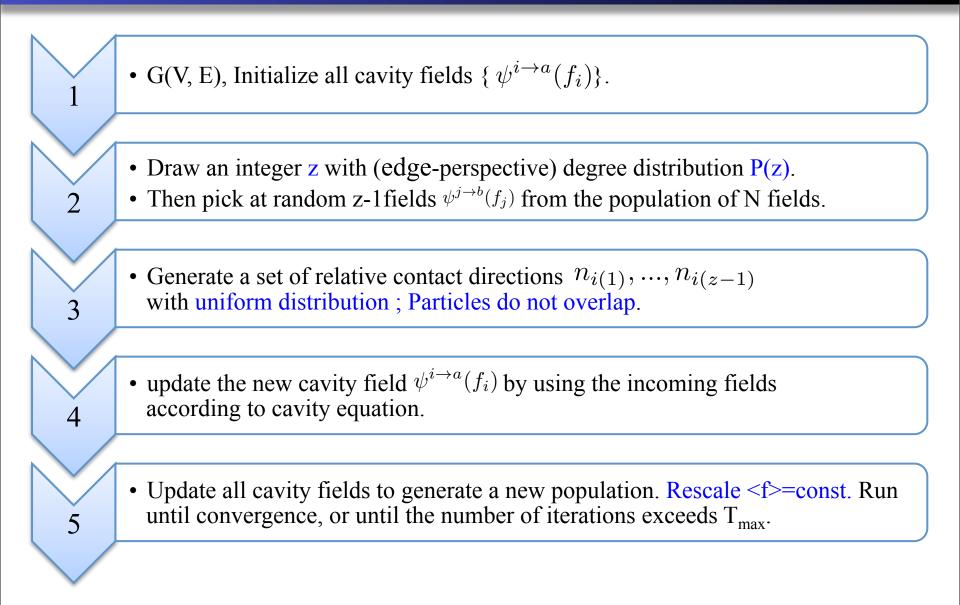
Compute marginal belief for a fix contact network $Q^i(f_i^n, f_i^t)$



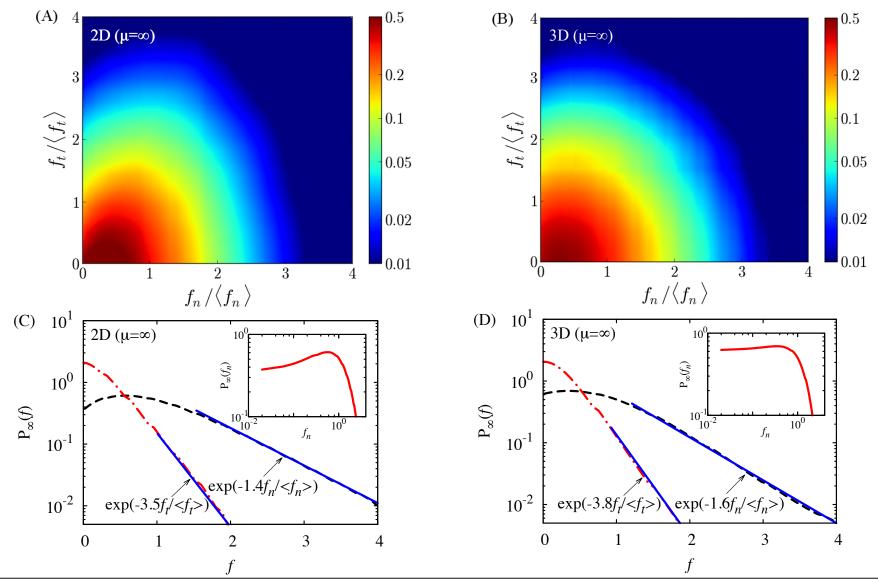
Force probability over an ensemble of random graphs $P(f^n)$



The Population Dynamics Algorithm



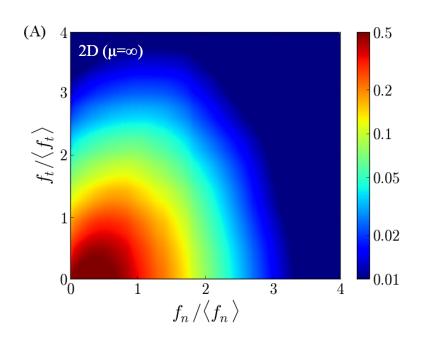
Force probability over an ensemble of random graphs $P_{\mu}(f^n, f^t)$



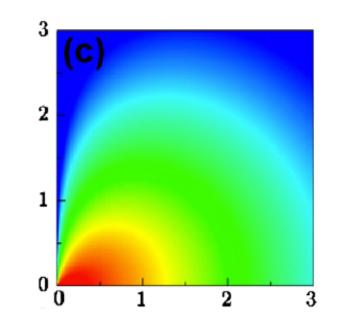
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Comparison with simulations

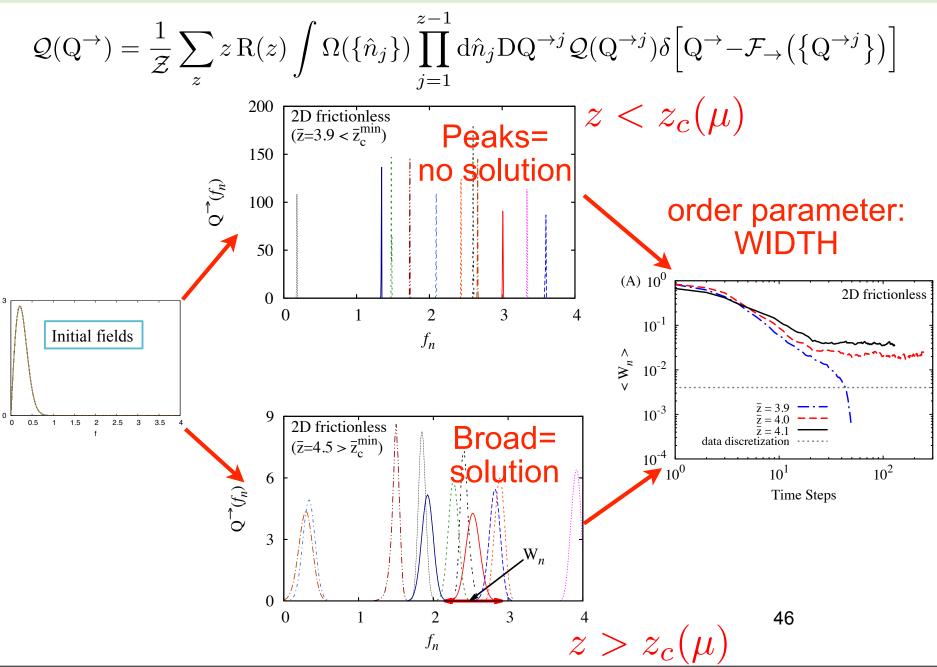
Cavity method



P. Wang et al. Physica A (2010)



Solution-no solution transition at Z_c



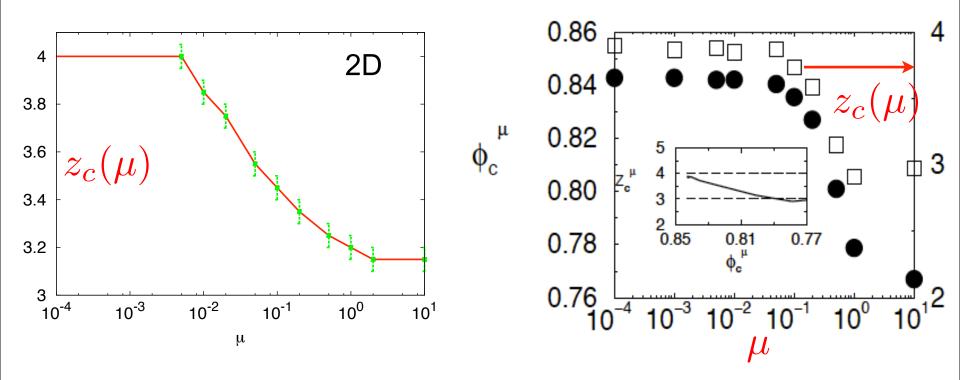
Wednesday, July 17, 13

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Comparison with simulations

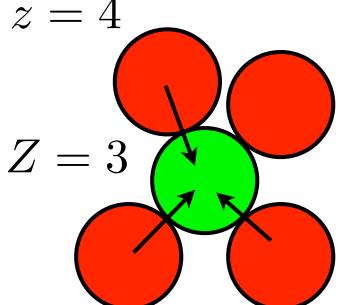
Cavity method

Silbert et al. PRE (2002)



Consistent with interpretation of $z_c(\mu)$ as a lower bound

Definition of jammed state: isostatic condition on Z



z = geometrical coordination number.
 Determined by the geometry of the packing.

Z < z < 2d = 6

Z = mechanical coordination number.

Determined by force/torque balance.

$$4 = d + 1 \le Z \le 2d = 6$$
$$\mu = 0$$

Generalizing the theory of monodisperse sphere packings

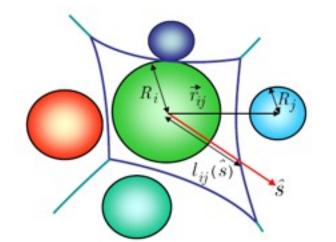
Theory of monodisperse spheres



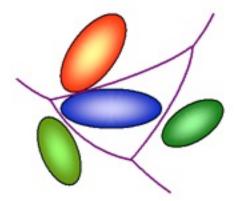
Polydisperse (binary) spheres



Non-spherical objects



(dimers, triangles, tetrahedrons, spherocylinders, ellipses, ellipsoids ...)



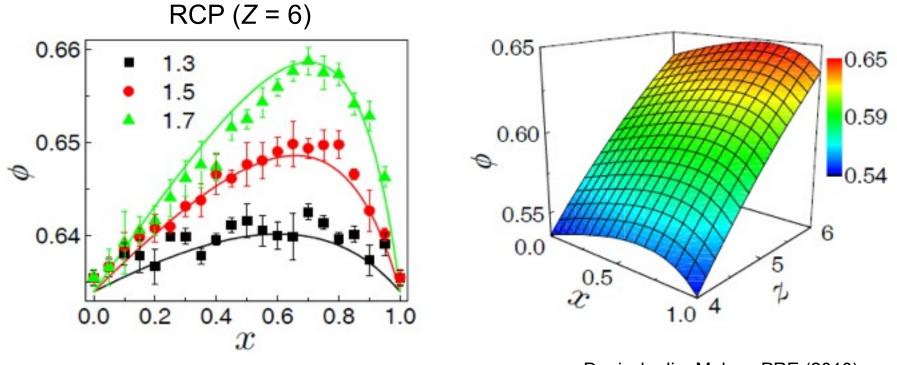
Distribution of radius P(r) Extra degree of freedom

Onsager 1949

Result of binary packings

Binary packings

$$W = \frac{\pi}{2} \sum_{i=1}^{2} x_i \int_0^\infty c^2 \exp\left\{\sum_j \left[-\rho_{ij}^s(z, x) S_{ij}^*(c) - \rho_j(W) V_{ij}^*(c)\right]\right\} dc$$



Danisch, Jin, Makse, PRE (2010)

The partition function for hard spheres

 $\mathcal{Z}(X) = \int \exp\left[-\frac{W(\vec{x})}{X}\right] \Theta_{\text{jam}}\left(\vec{x}, \vec{f}\right) \mathcal{D}\vec{x} \ \mathcal{D}\vec{f}$

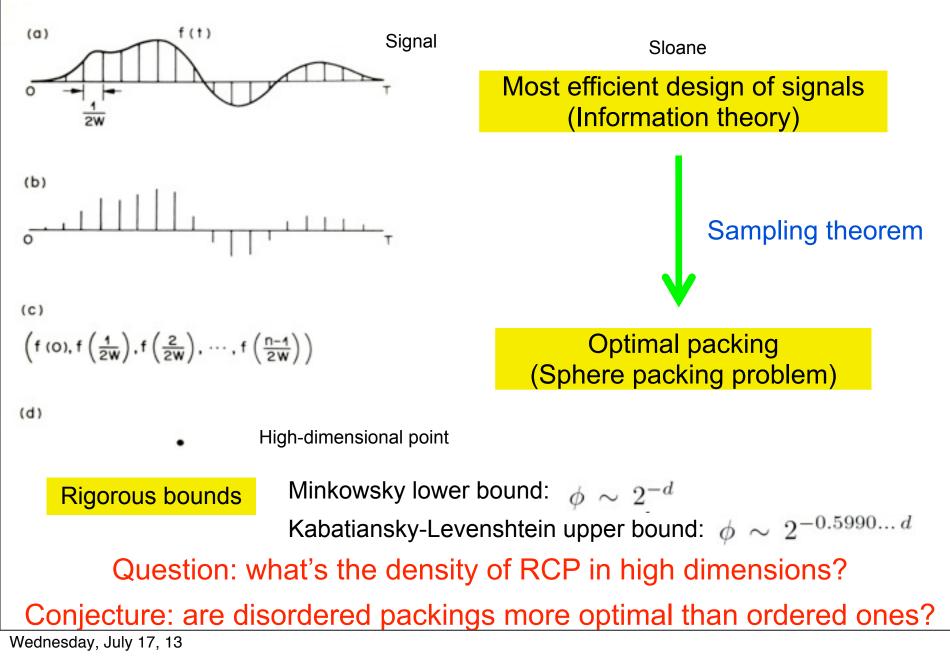
Volume Ensemble + Force Ensemble

1. The Volume Function: W (geometry)

2. Definition of jammed state: force and torque balance

Solution under different degrees of approximations

Jammed packings in infinite dimensions



Sphere packings in high dimensions

