

Jamming shapes up: geometry and energy landscape near the jamming transition

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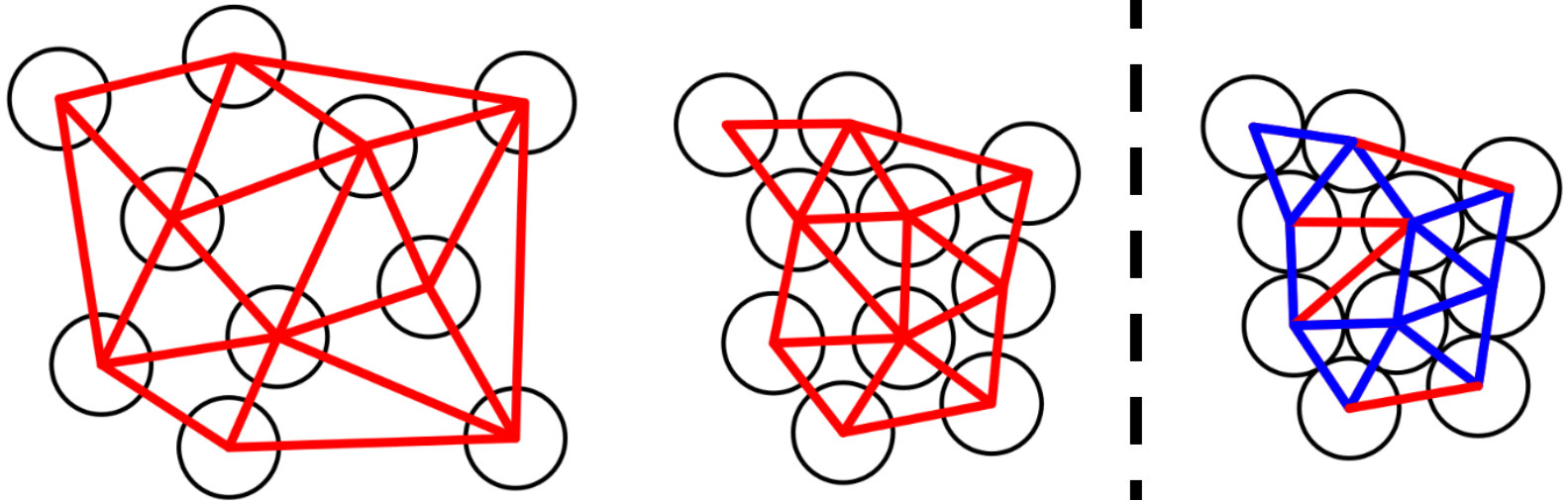
Peter Morse

Outline

- Focus on athermal soft spheres
- New order parameters defined over **all** phase space
- New geometric phase transition
- Do empirical renormalization (reverse engineering)
- Explore energy landscape

Geometry über alles: order parameters defined for all ϕ

Increasing ϕ \longrightarrow ϕ_j



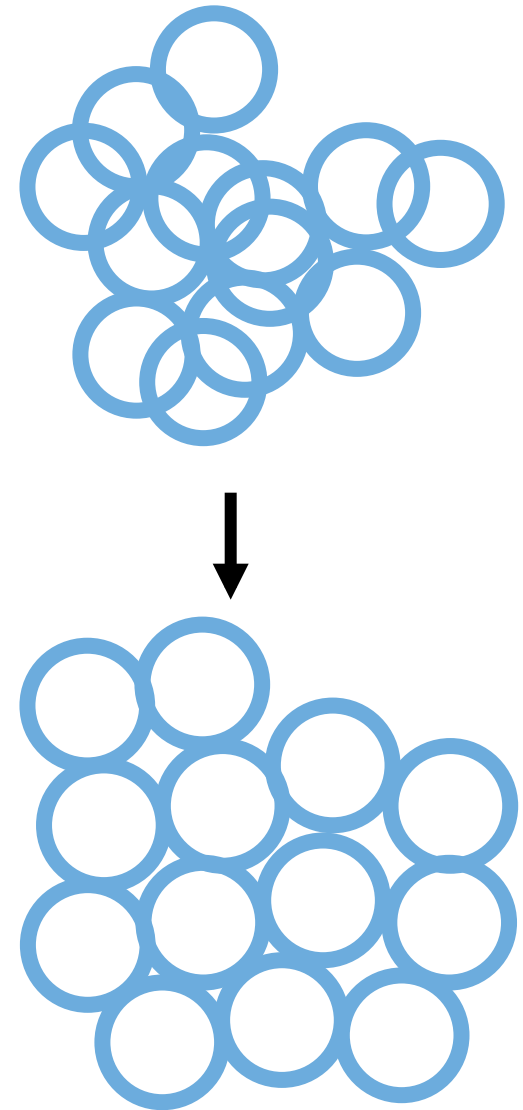
Red lines = Neighbor Link

Blue lines = Contact (and Neighbor) Link

Mechanical order parameters defined only above ϕ_j

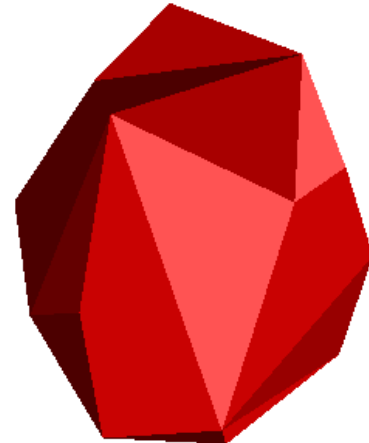
Simulated Frictionless Spheres

- Vary **dimension**
- Vary **packing fraction ϕ**
- Periodic boundary conditions
- Infinite temperature quench down to $T = 0$
- Find local energy minimum (inherent structure) using Conjugate Gradient Minimization or FIRE on GPU cluster
- BIG (up to 2^{17} particles)

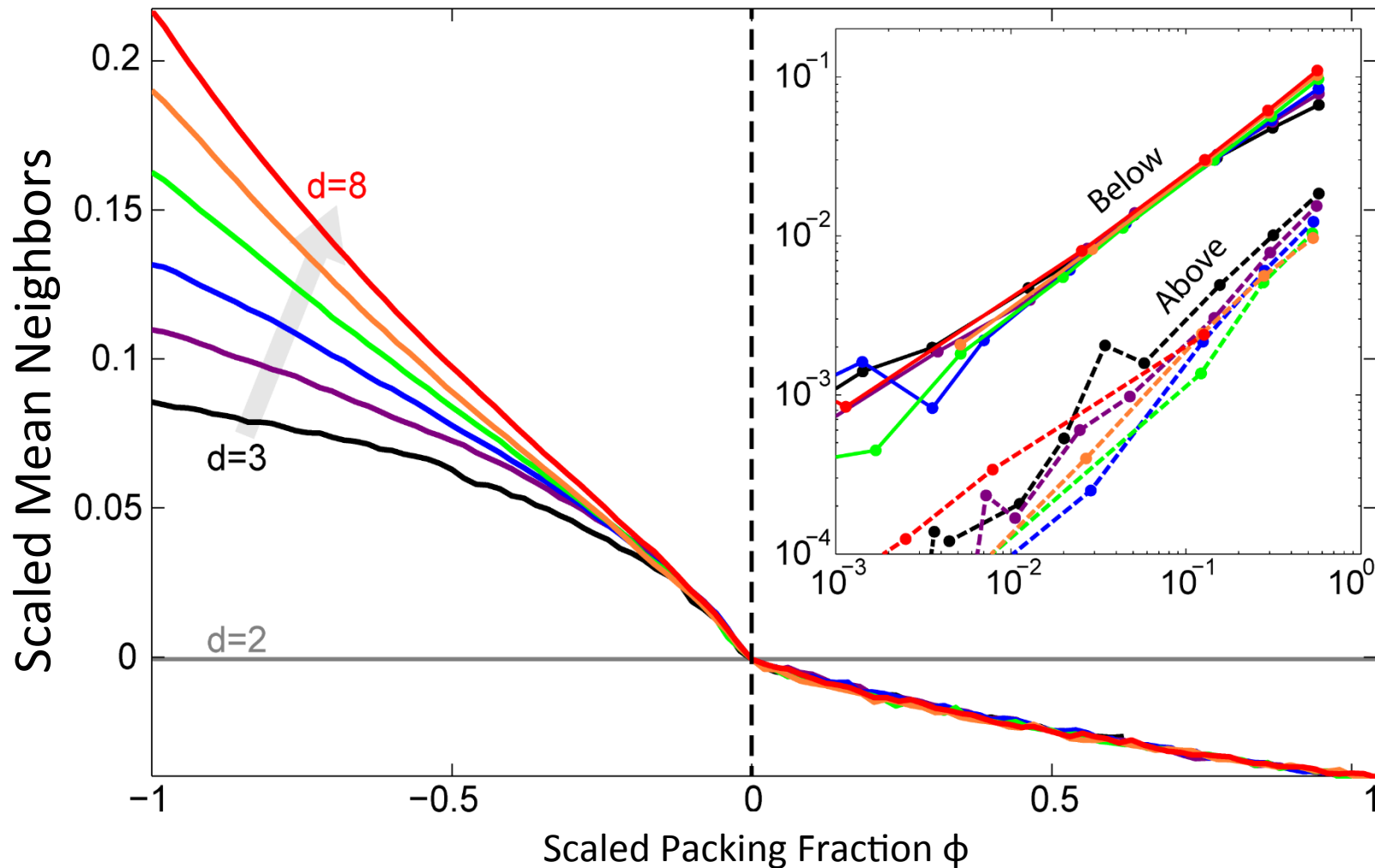


Voronoi Cell

- Defined by all space closest to a given sphere
- Look at any geometric quantity
 - Number of Sides
 - Maximum Inscribed Sphere
 - Surface Area
 - Volume
 - Aspect Ratio
 - Moment of Inertia
- Look at how these change as function of ϕ

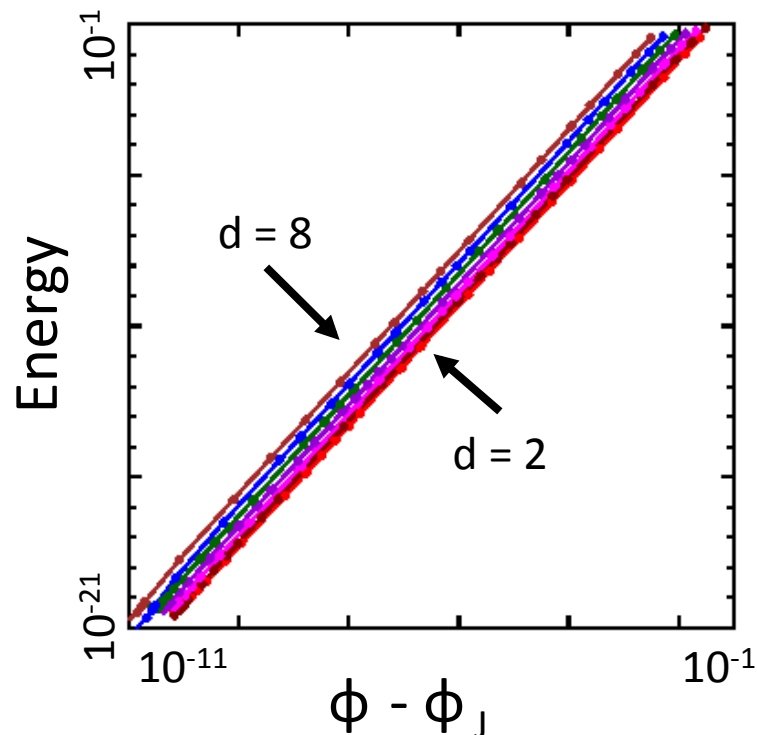
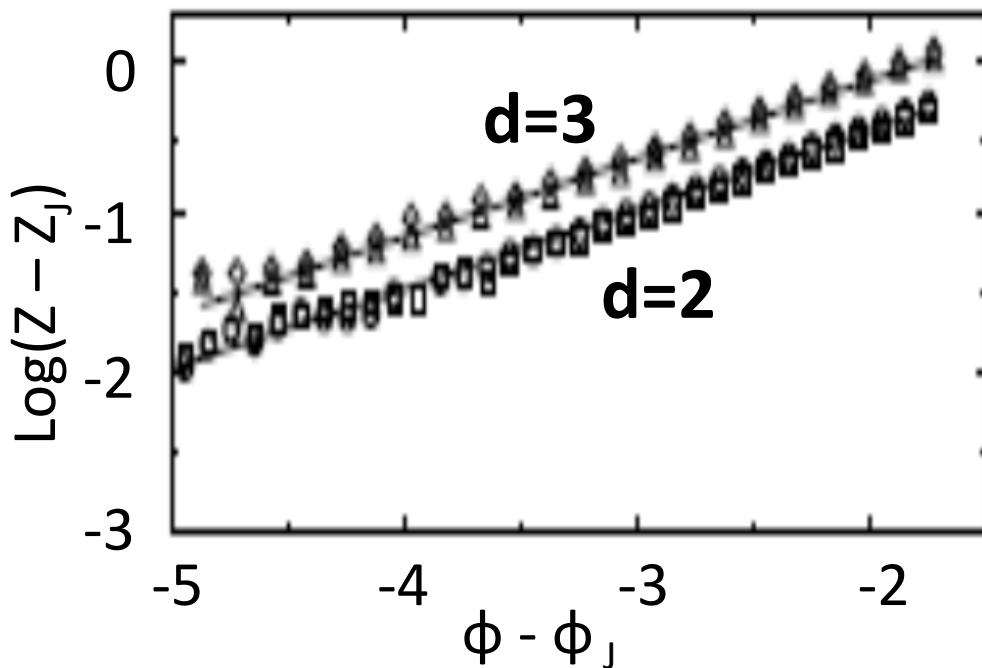


Number of Neighbors: $d_{UCD} \geq 3$

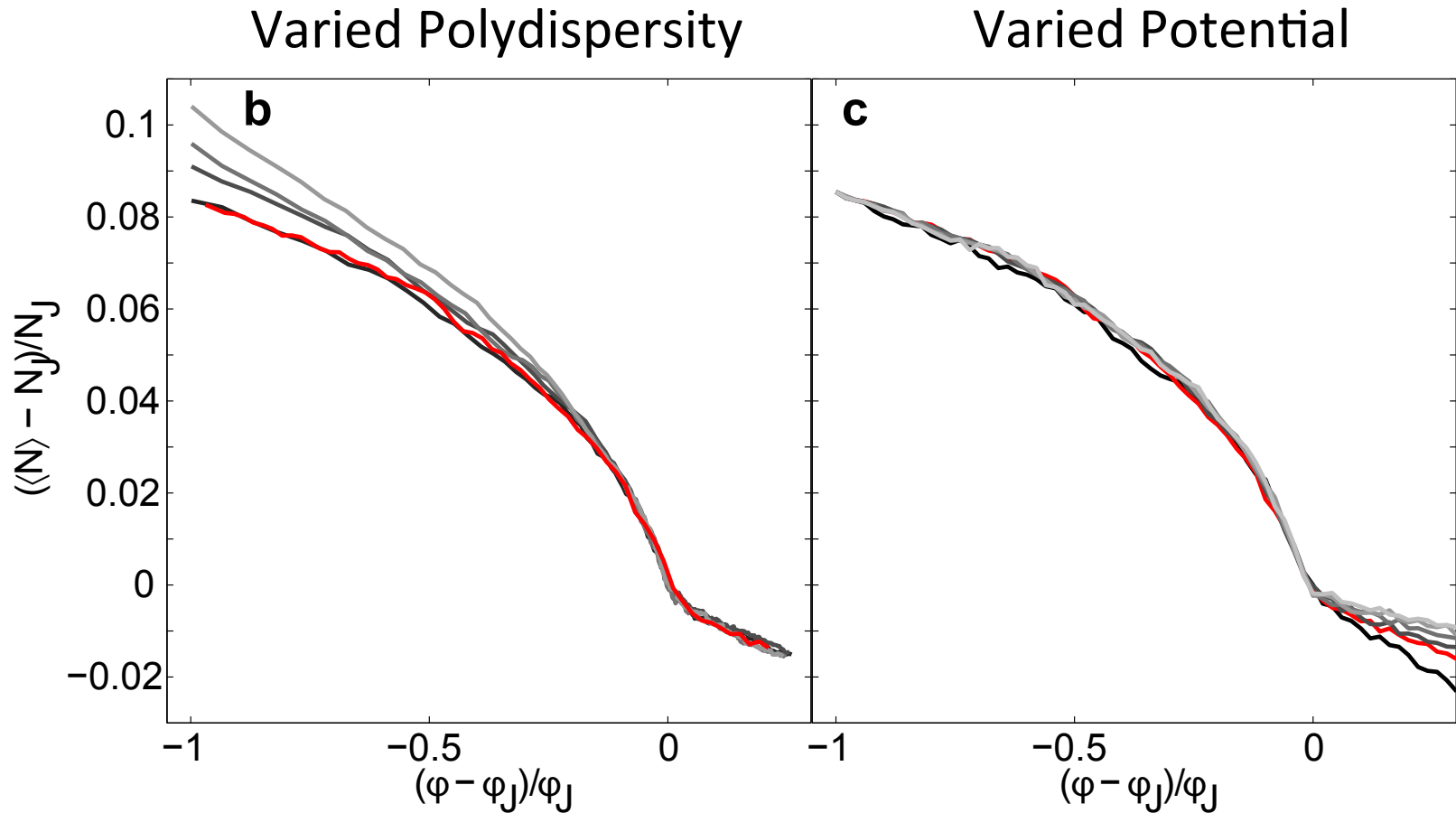


But What About Mechanics?

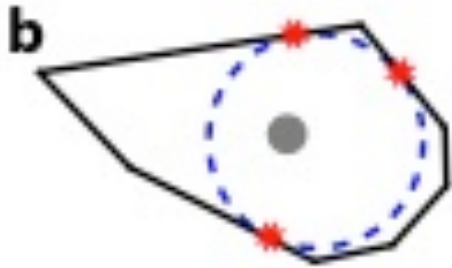
- Mechanical jamming has $d_{\text{UCD}} \leq 2$
- Either **same underlying physics** or two different phase transitions at same point



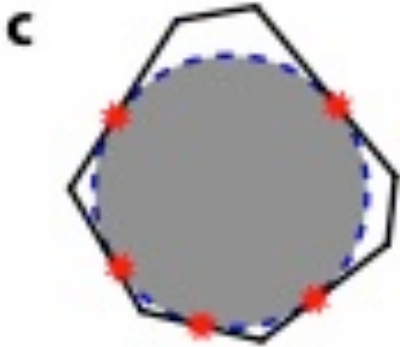
Universal Behavior Below Jamming



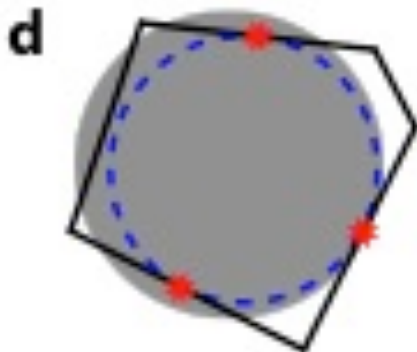
Maximum Inscribed Sphere



- Below Jamming: Insphere larger than physical sphere, $M = d+1$

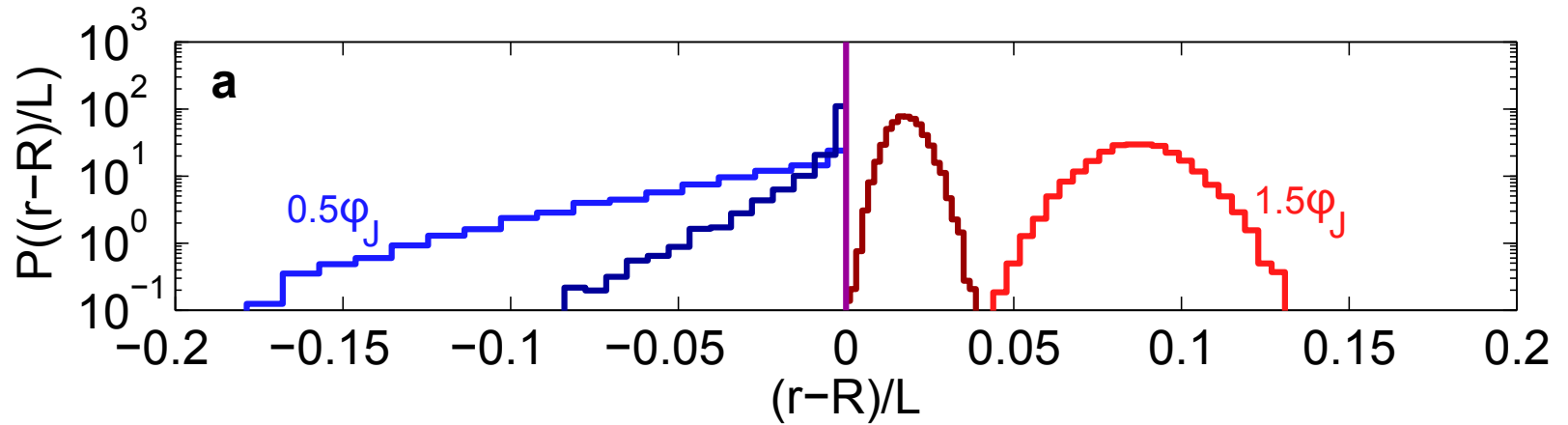


- At Jamming: Insphere exactly equal to physical sphere $\langle M \rangle = 2d$

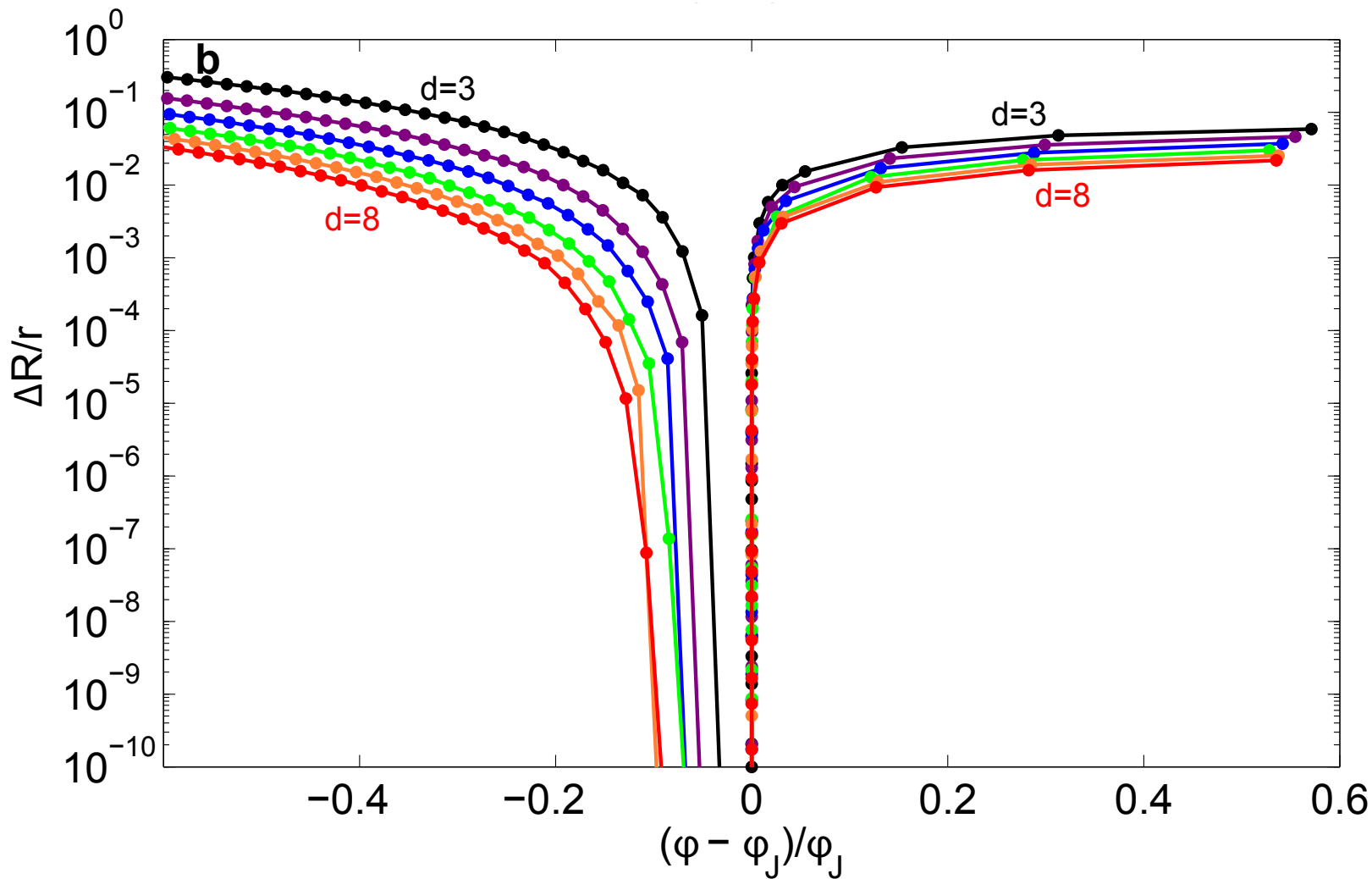


- Above Jamming: Insphere smaller than physical sphere $M = d+1$

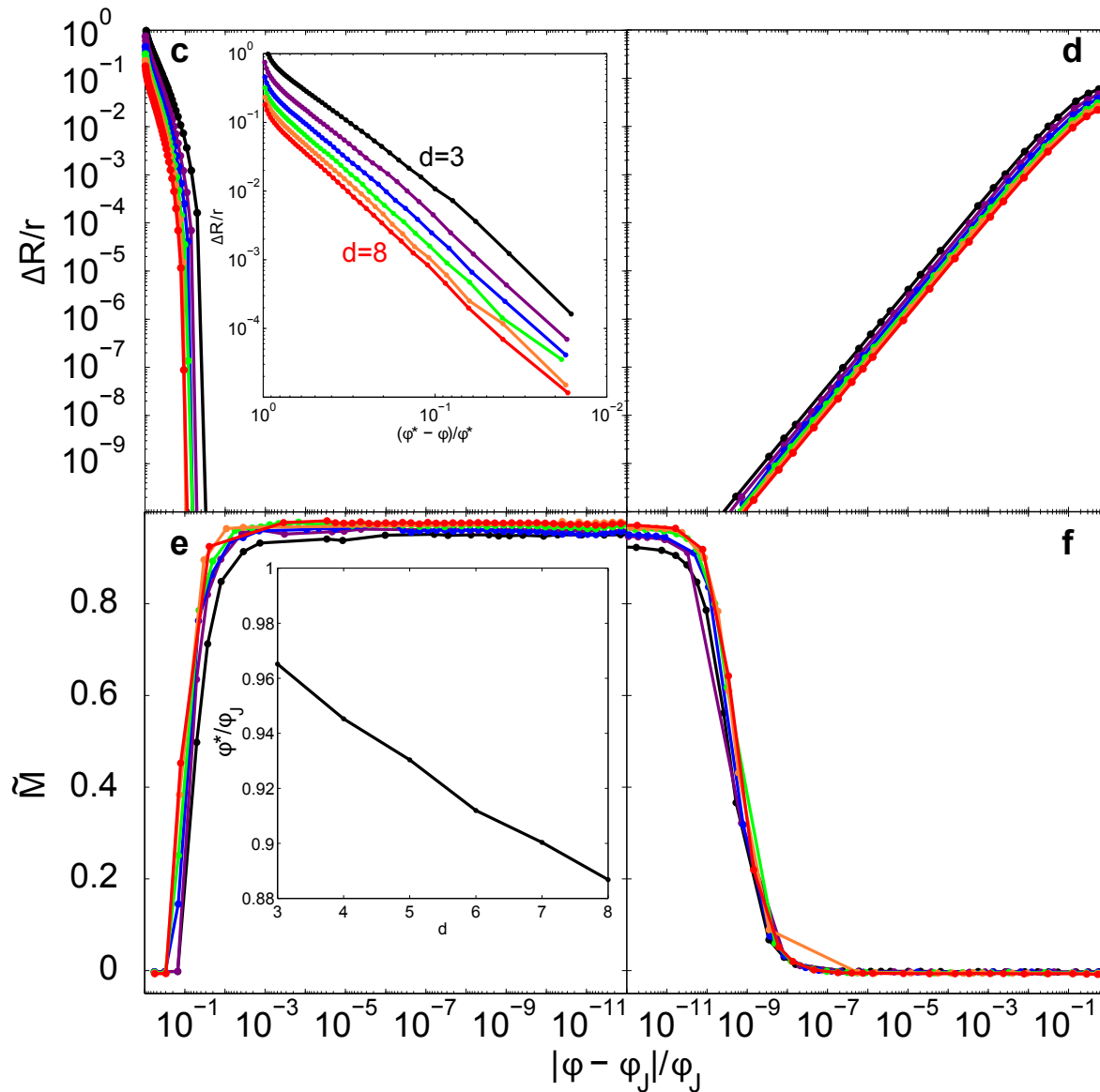
Insphere Distribution



Insphere Distribution II

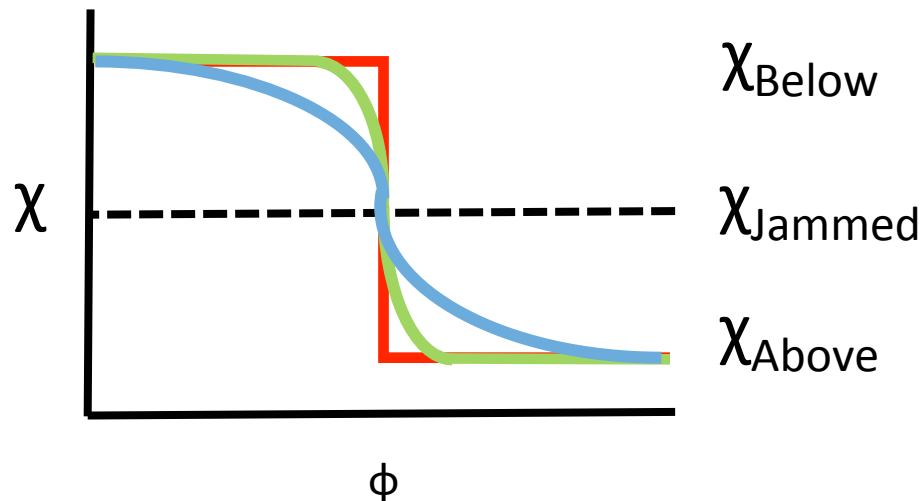


Insphere Distribution III



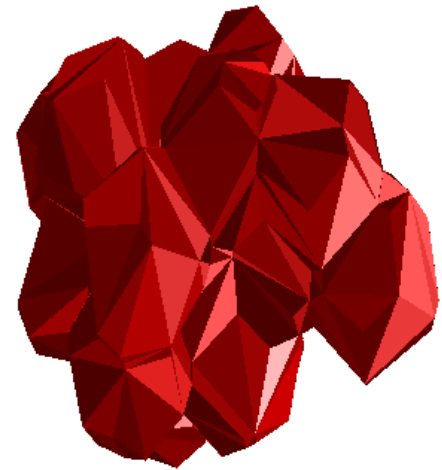
Toward Renormalization

- We don't have a field theory: reverse engineer one!
- On high renormalization step, order parameter χ (any of the previous metrics) should (?) become a step
- Finite Size Effects will smooth out the step function



Renormalization Scheme

- Goal: Build larger structures that preserve underlying relationships to collapse phase space
- Scheme:
 - Pair Voronoi cells with neighbors that share highest surface area
 - Calculate quantities for new cell
 - Repeat

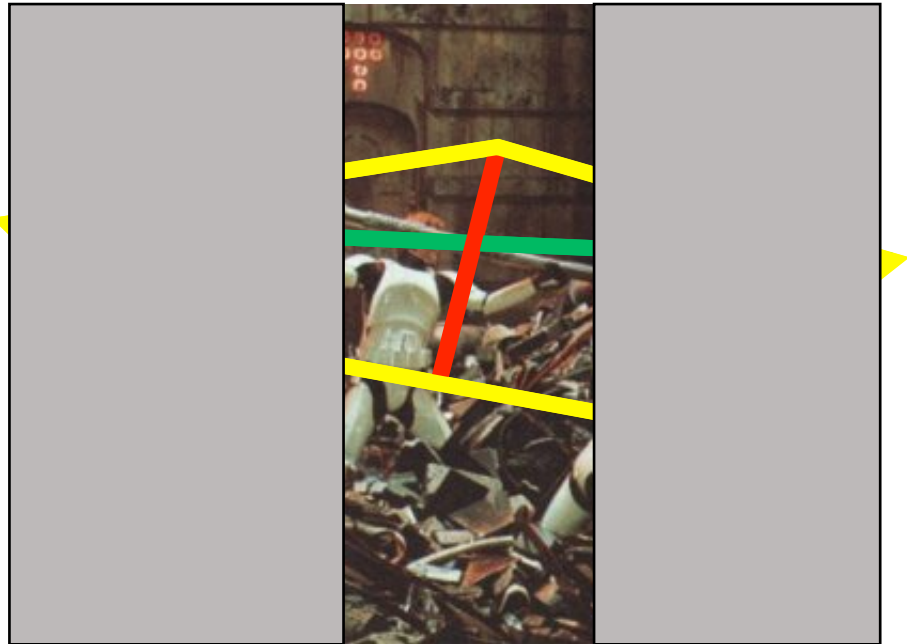


Aspect Ratio / Eccentricity Definition

- “Trash compactor” aspect ratio

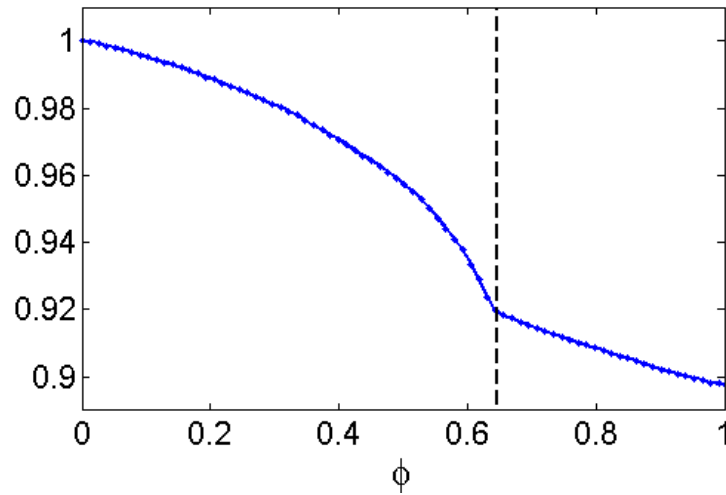
- Define:
$$k = \frac{d_{\text{long}}}{d_{\text{short}}} - 1$$

- If concave, take the convex hull first
- $k = 0$ when spherical

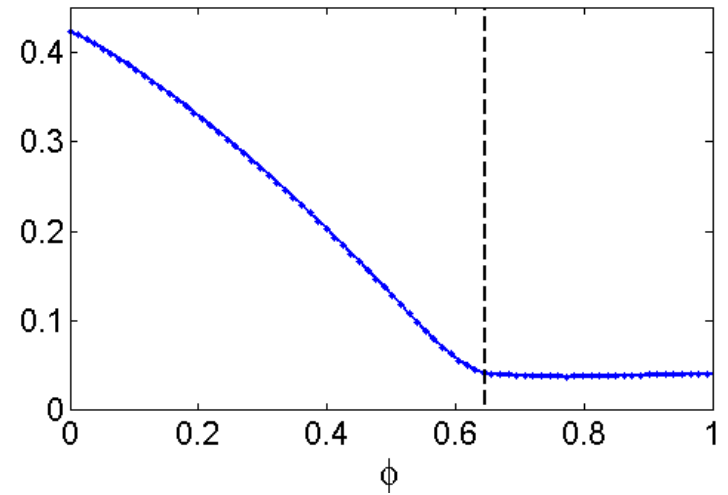


All show signatures of jamming!

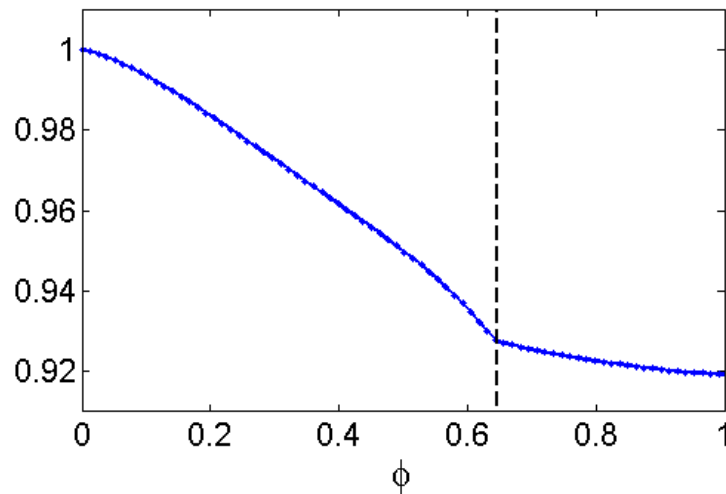
Scaled Mean Neighbors



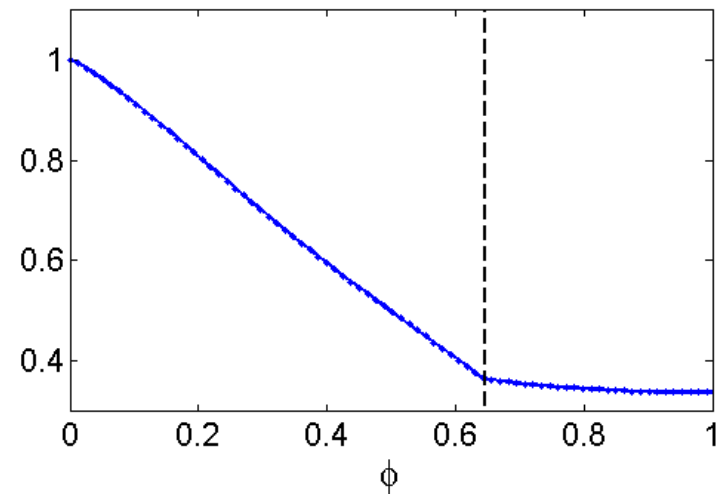
Std(Volume)



Surface Area

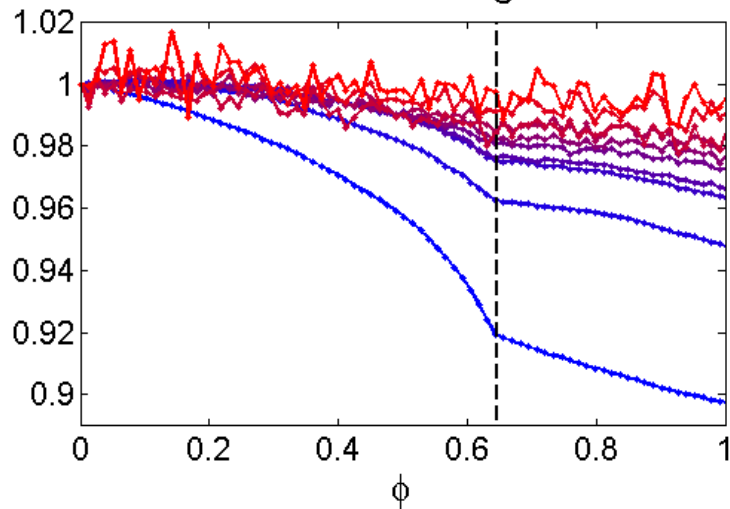


Scaled Eccentricity

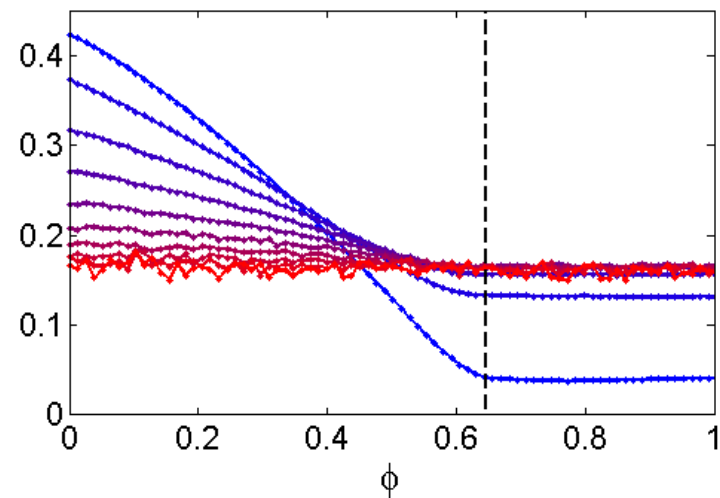


Renormalization

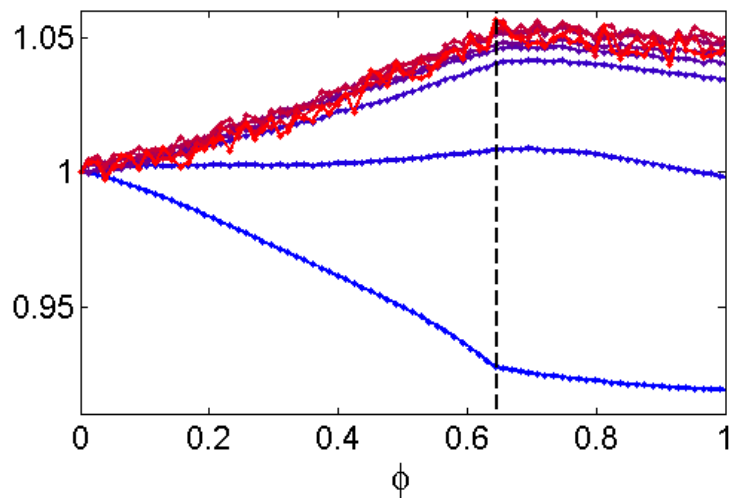
Scaled Mean Neighbors



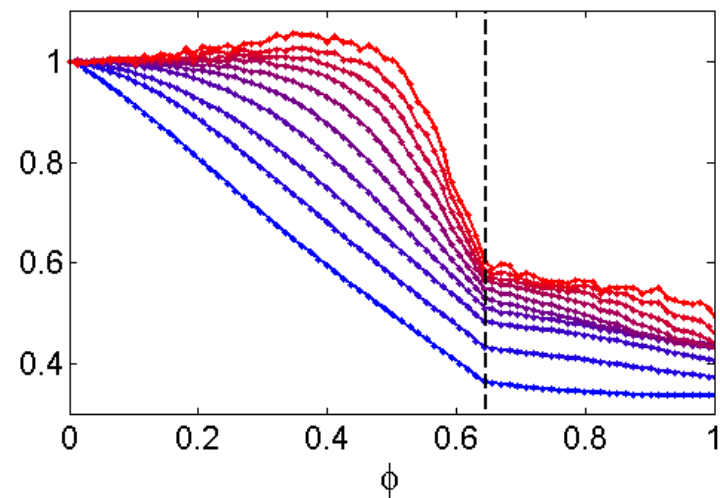
Std(Volume)



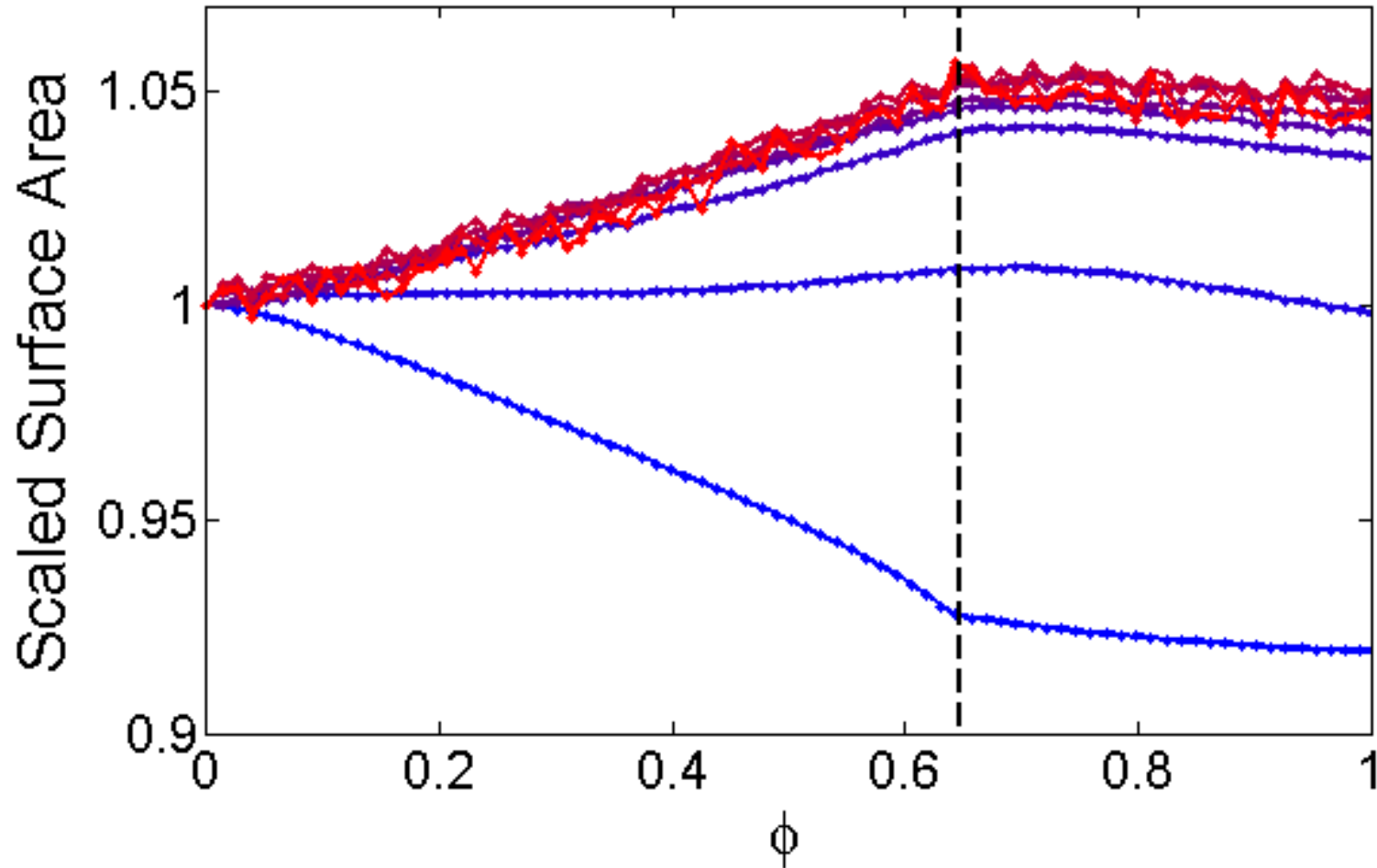
Surface Area



Scaled Eccentricity

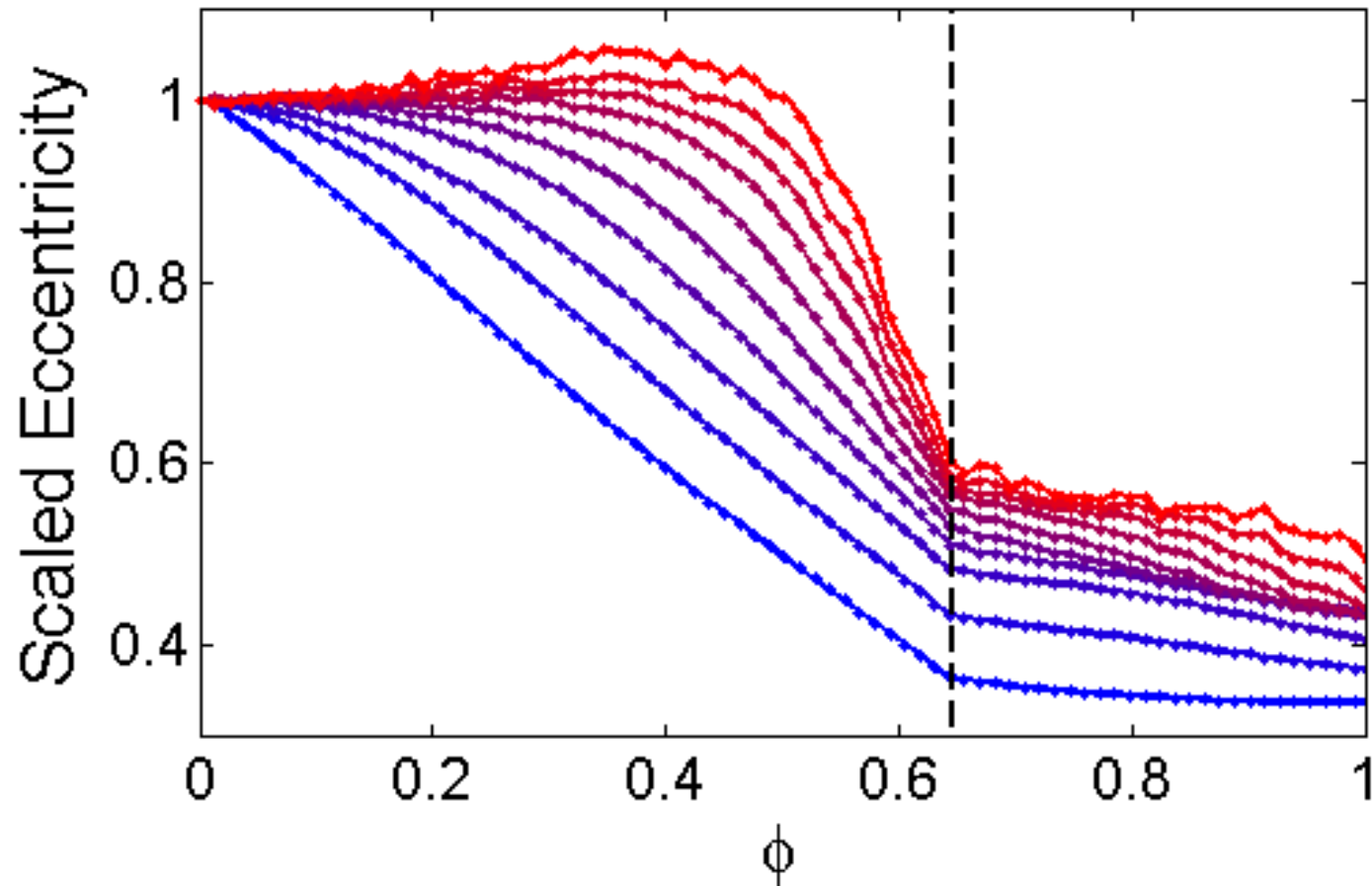


Surface Area (renorm)



- Master curve has perfect memory
- Still contains signature of jamming at high steps

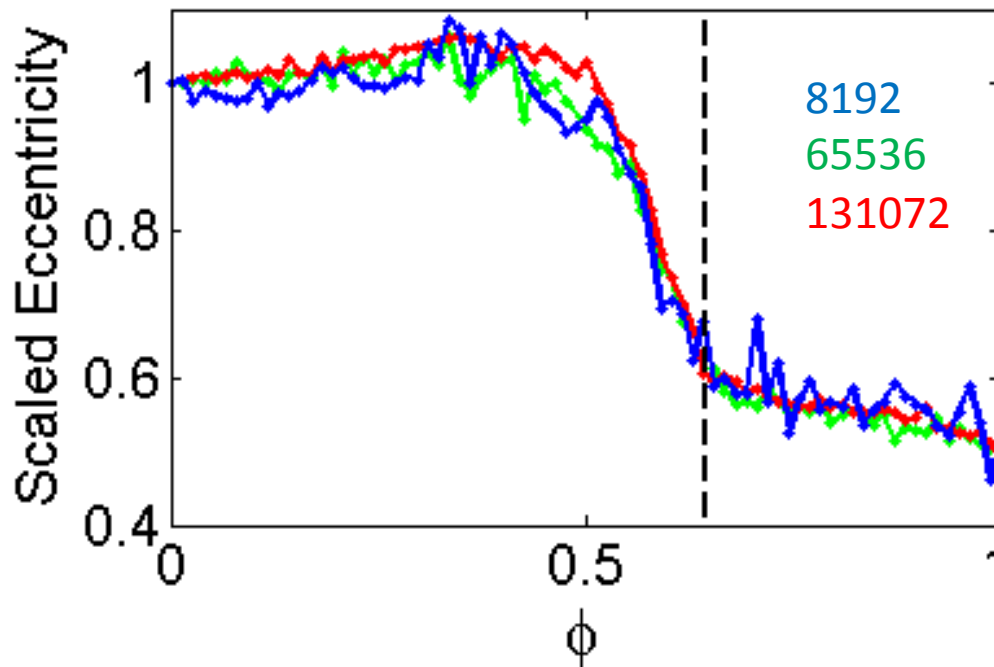
Aspect Ratio (renorm)



- Asymptotically approaching a step function
- Gives a base line for determining scaling near the transition

Aspect Ratio: Finite Size

- Finite size effects round out corners
- Increase size, doesn't become more step-like
- Look at high iteration (9th step) of renormalization:



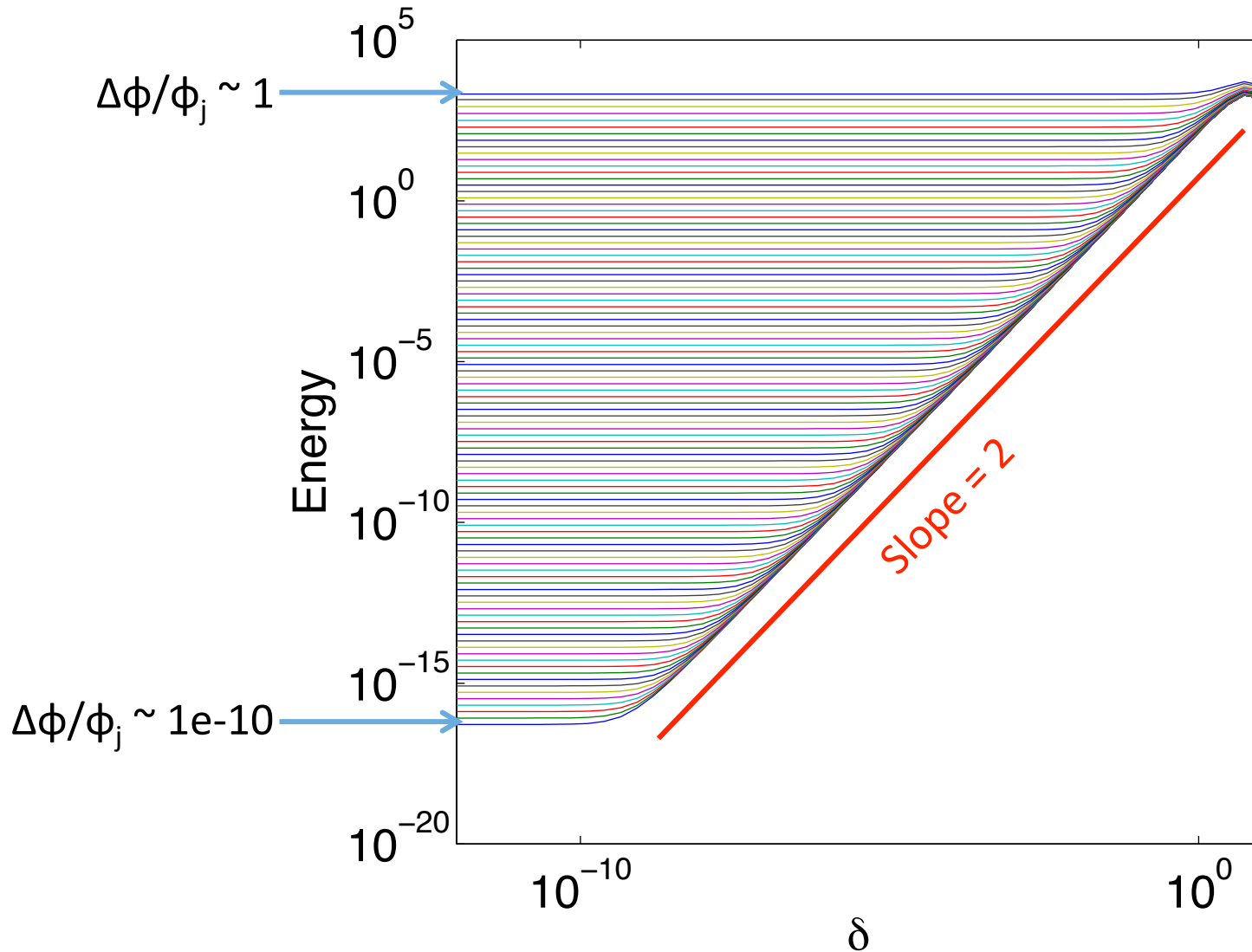
Energy Landscape

- Problem: Can't map ultra-high dimensional phase space
- Solution: **Random transects**
- Minimize system at fixed ϕ then
 - Pick random direction
 - Calc Energy as a function of distance δ
 - Repeat and average over many directions (~ 100)
- Results independent of system dimension!

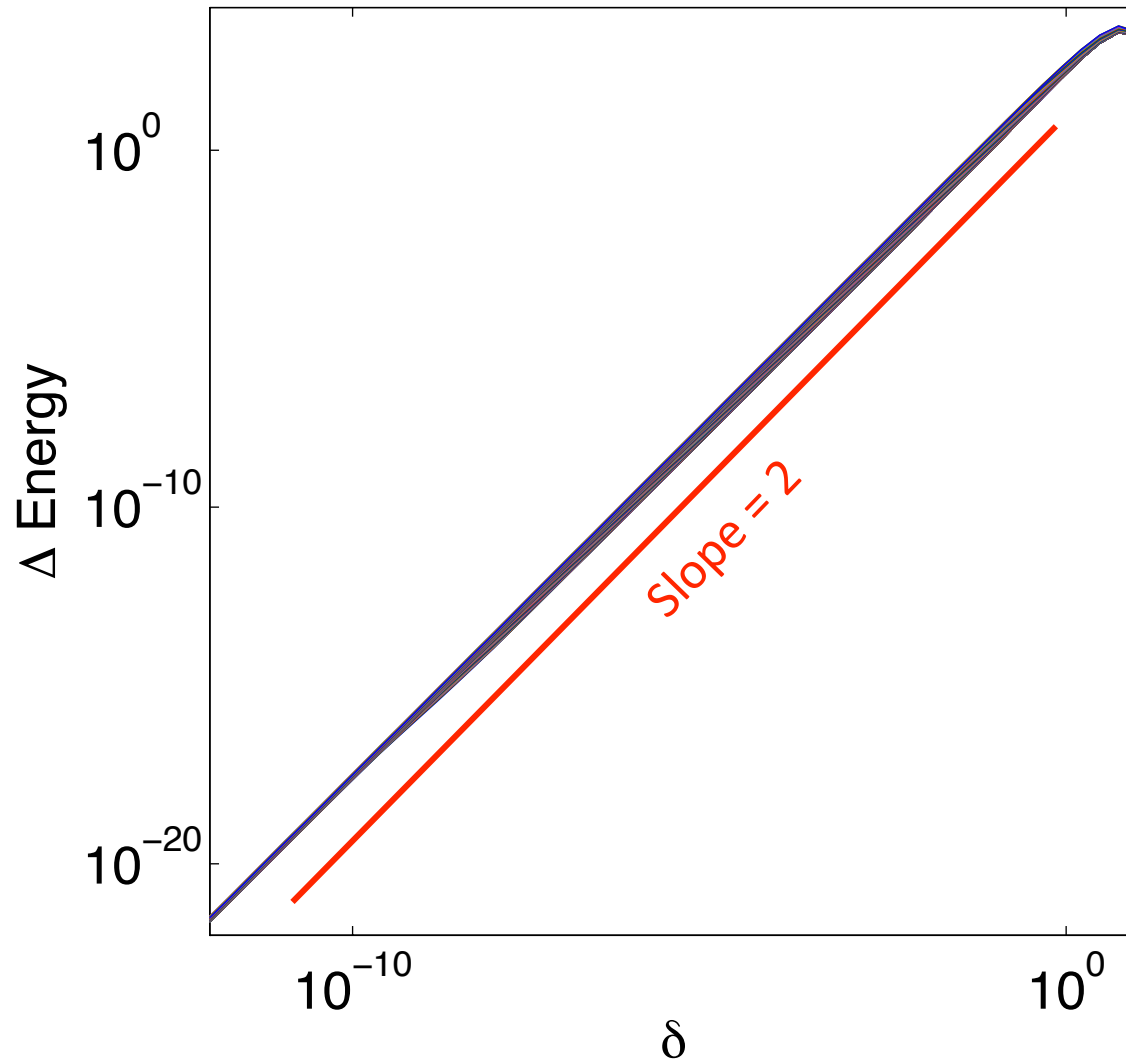


Capri - A

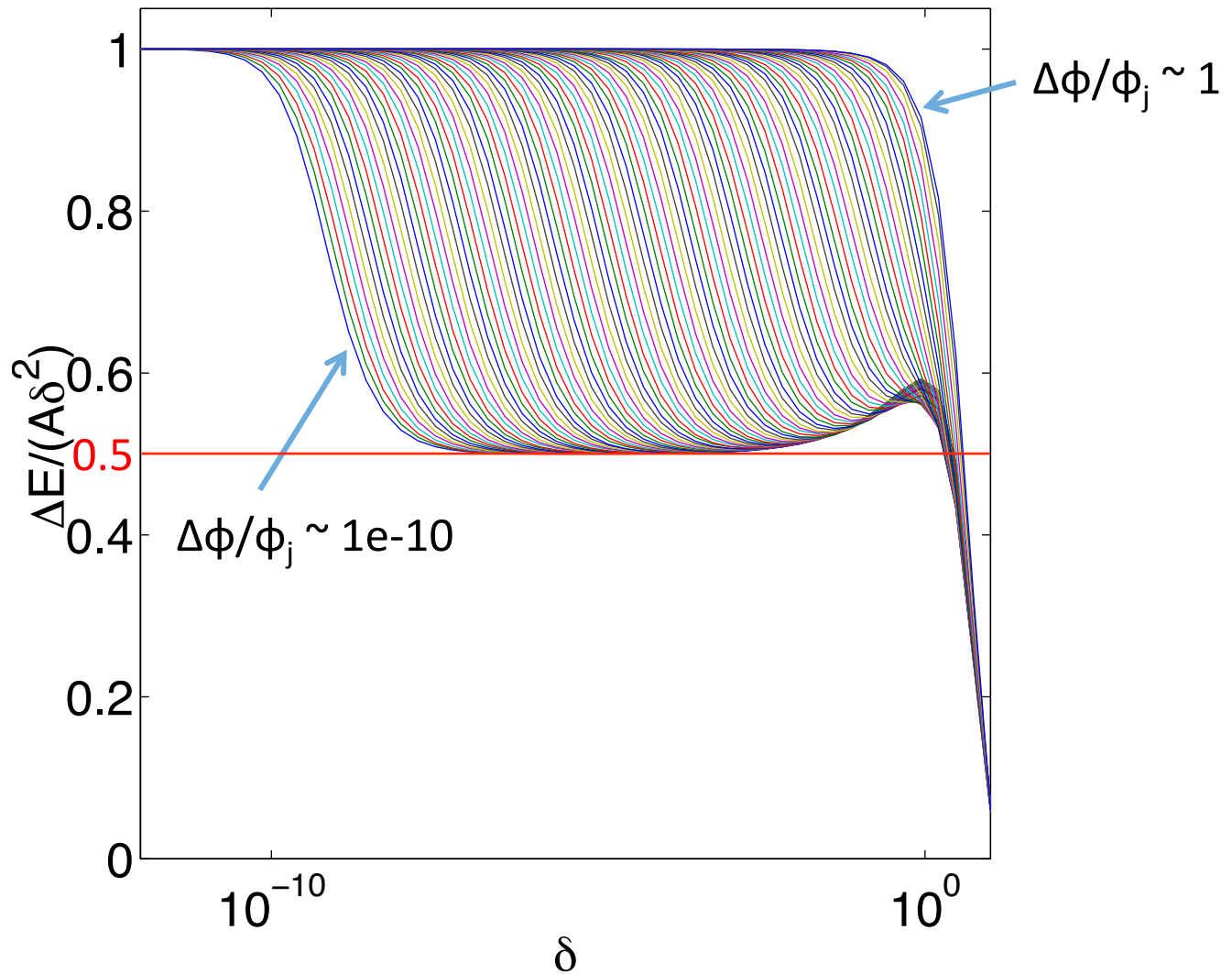
Harmonic Contact Pot, $D=4$, $N=8192$



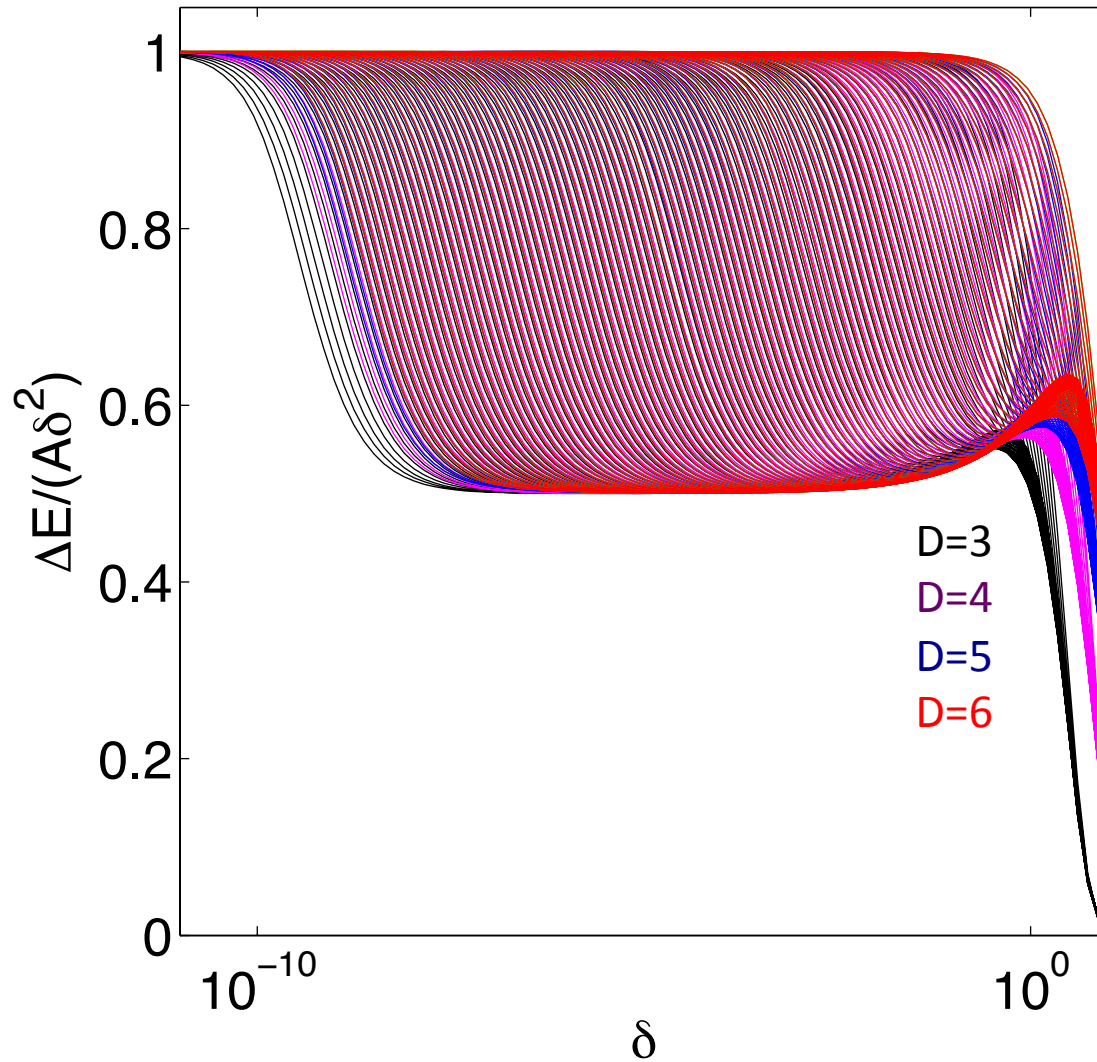
Subtract Starting Energy



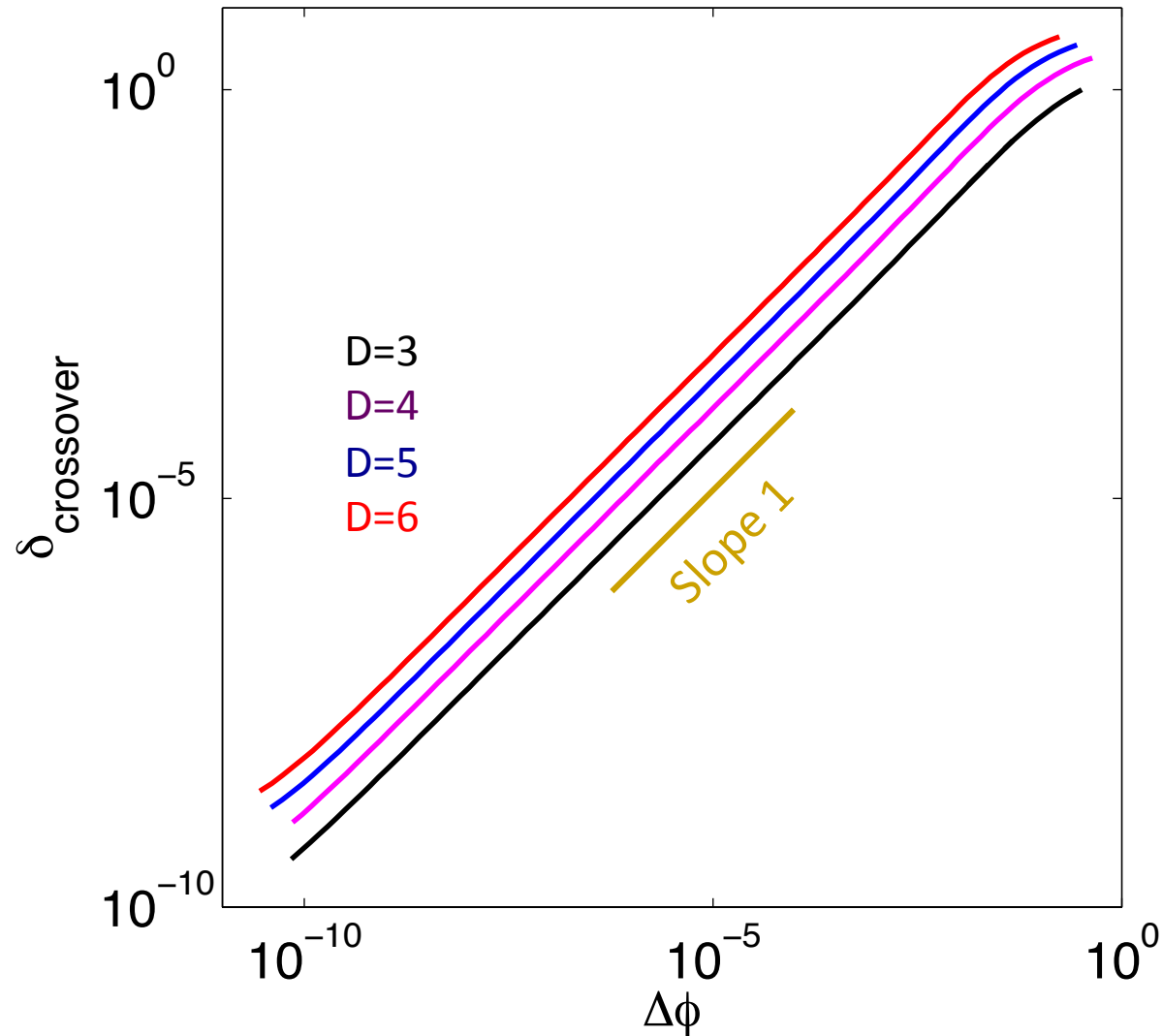
Two Different Harmonic Regimes!



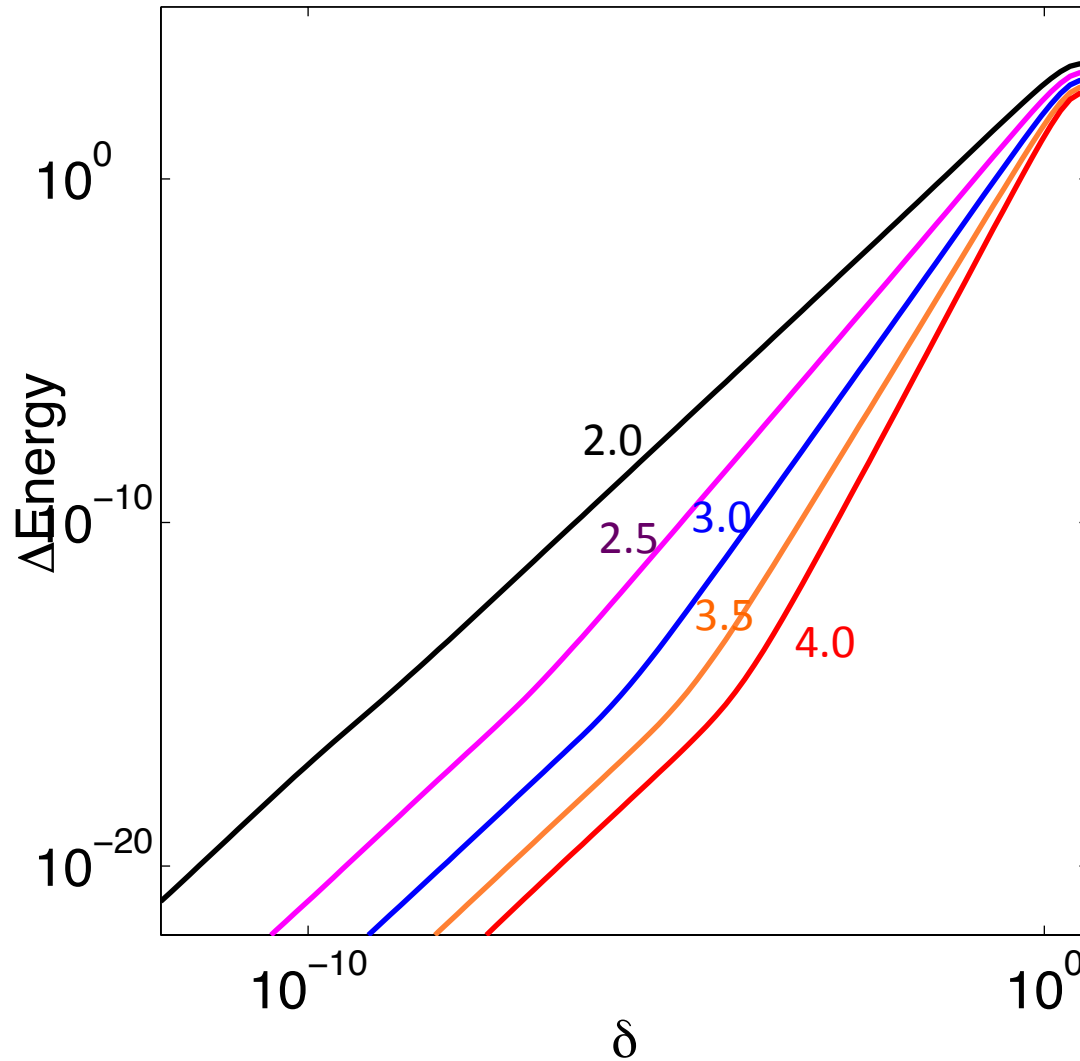
Dimension Independent



Crossover distance Linear in $\Delta\phi$



Two Regimes: Linear, Pot. Dependent



Conclusions

- All geometric signatures we've shown contain the phase transition
- Surface Area keeps a memory of underlying packing upon renormalization
- Aspect Ratio is a good renormalizable order parameter, can look at scaling and finite size effects
- Universal behavior in energy landscape
- Transition from linear to potential-dependent

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