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

Eric Corwin

Peter Morse

University of Oregon

Department of Physics

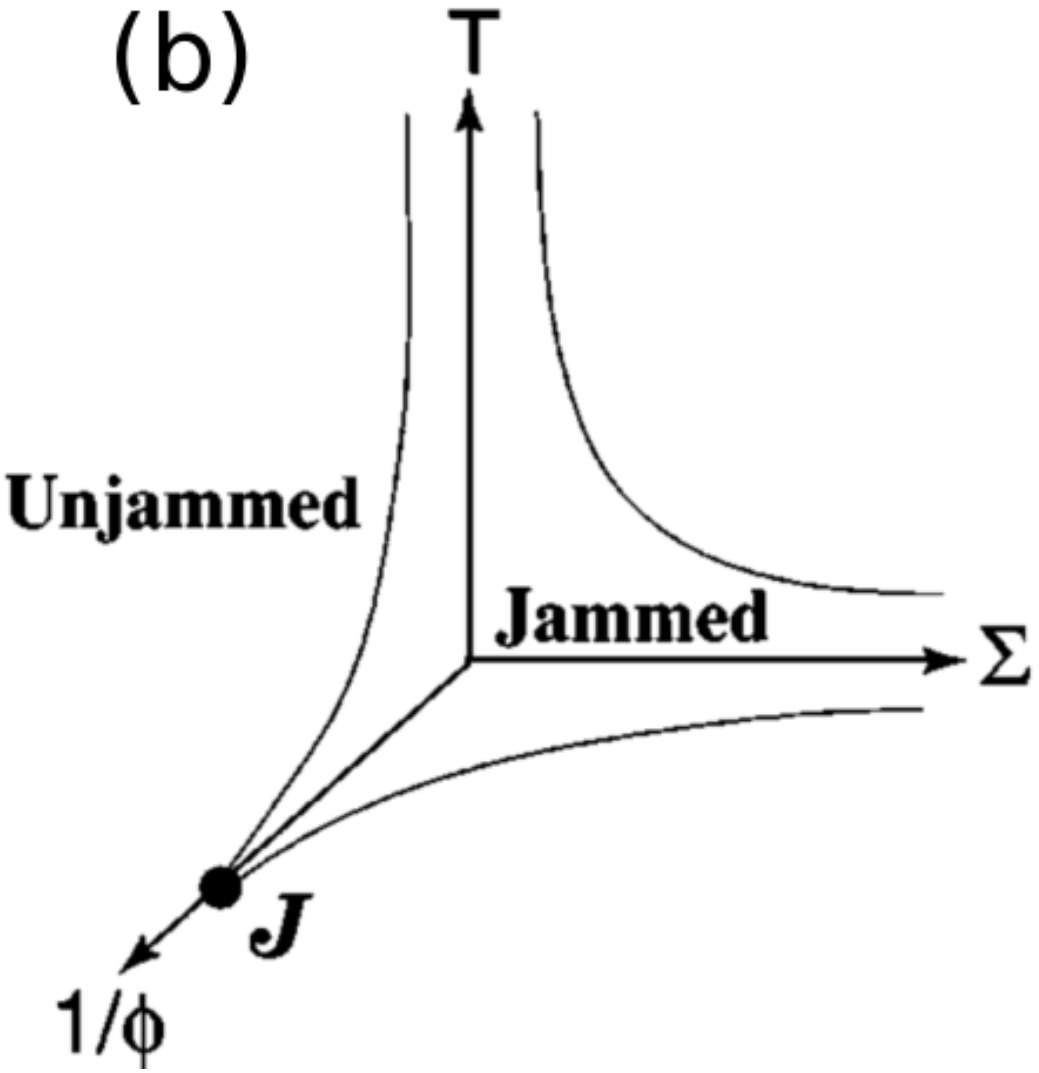
materials science institute


Peter Morse

Granular Materials: Chunks are Different

- Neither solid nor liquid nor gas
- Athermal state of matter

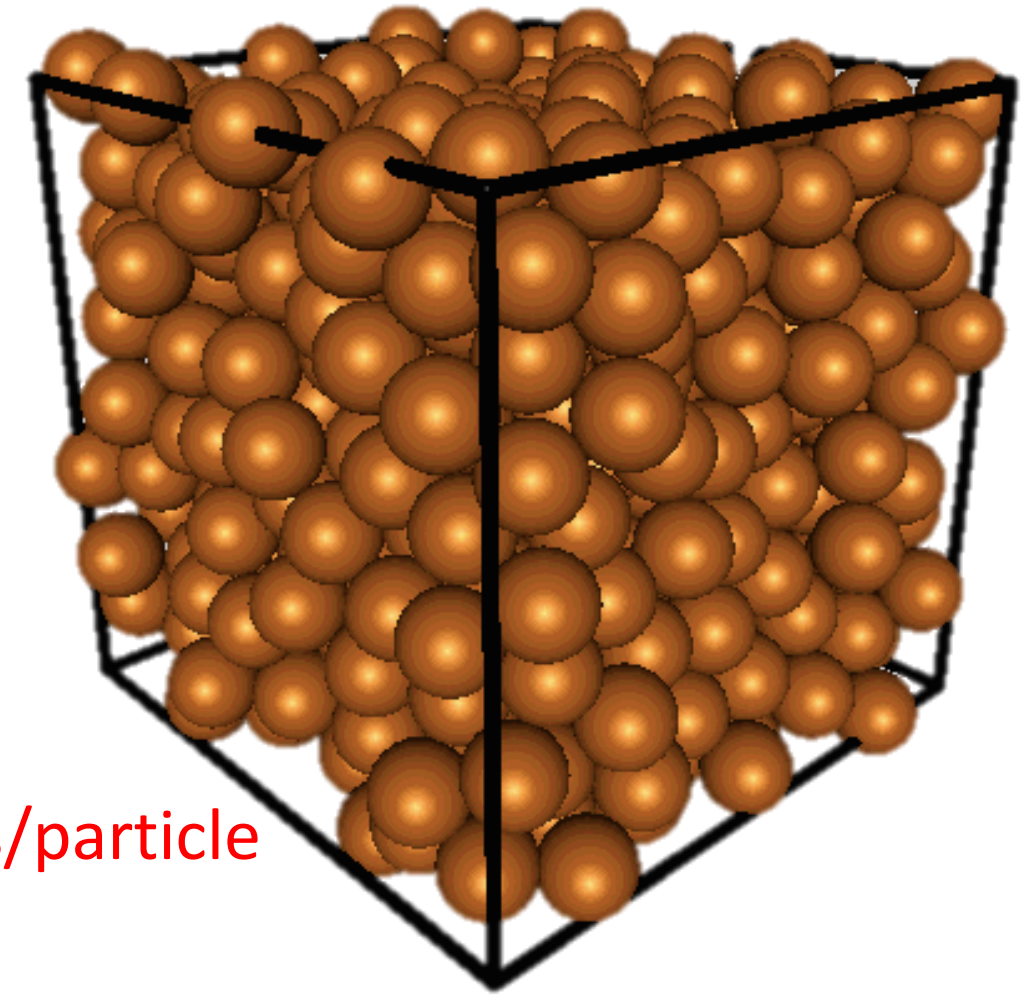
The Jamming Transition



Maxwell's Criterion!

Given: No particles can move

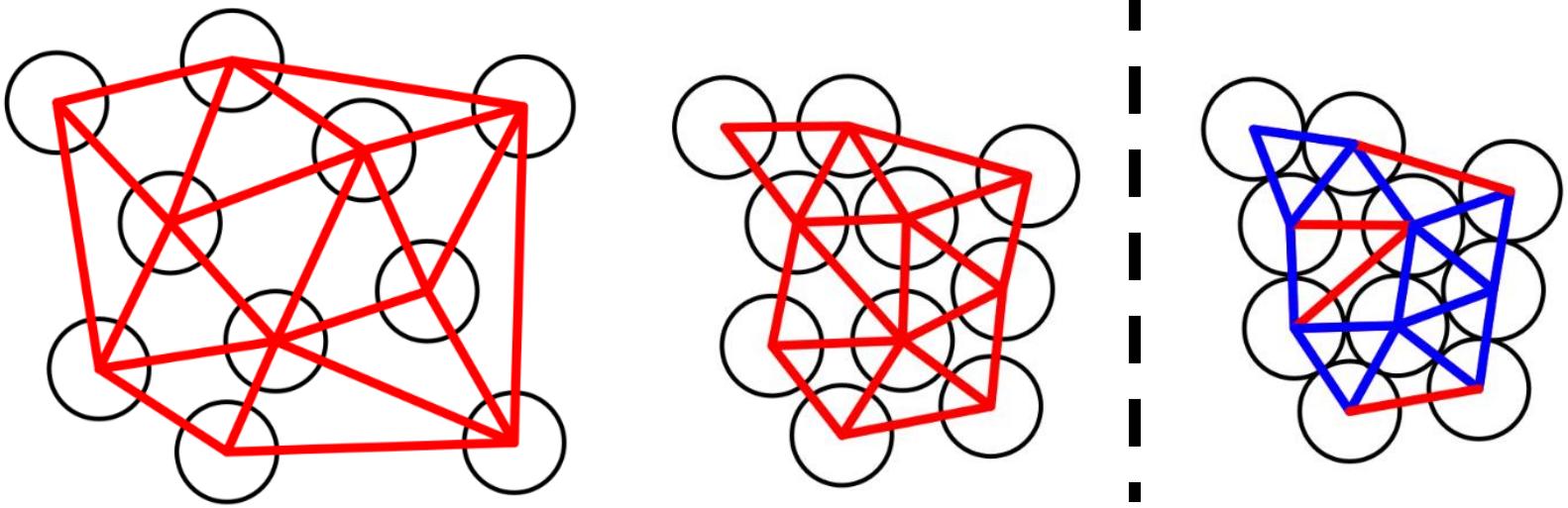
- Must constrain:
  - up/down
  - left/right
  - forward/back



Must be 2d=6 constraints/particle

Geometry über alles: order parameters defined for all ϕ

Increasing ϕ → ϕ_J



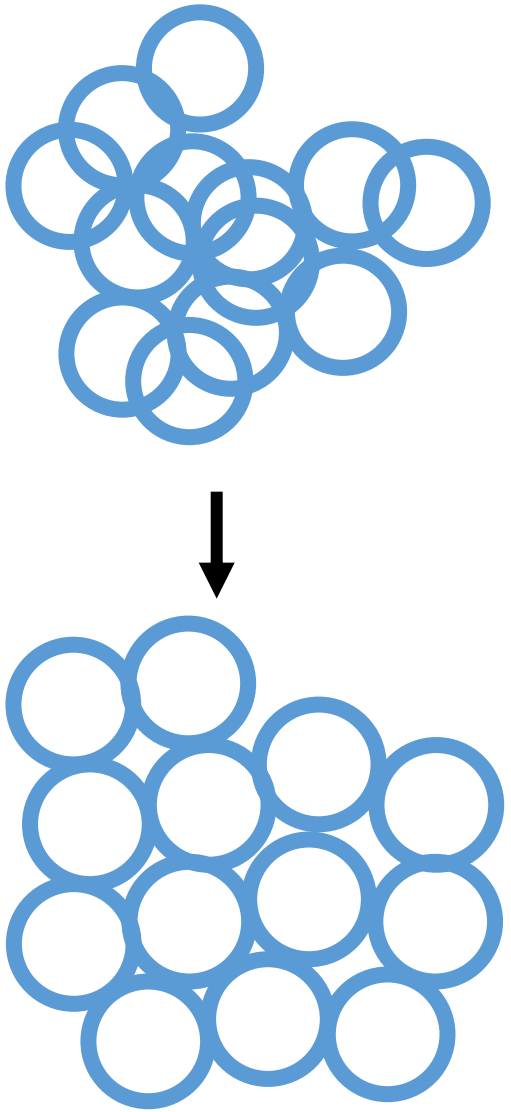
Red lines = Neighbor Link

Blue lines = Contact (and Neighbor) Link

Mechanical order parameters defined only above ϕ_J

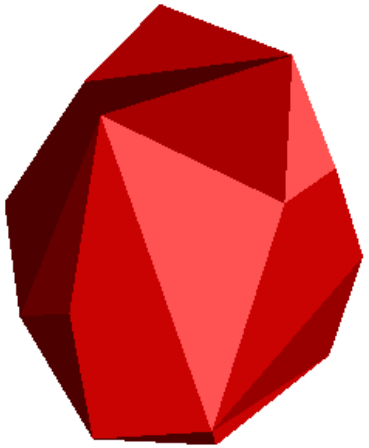
Simulated Frictionless Spheres

- 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)

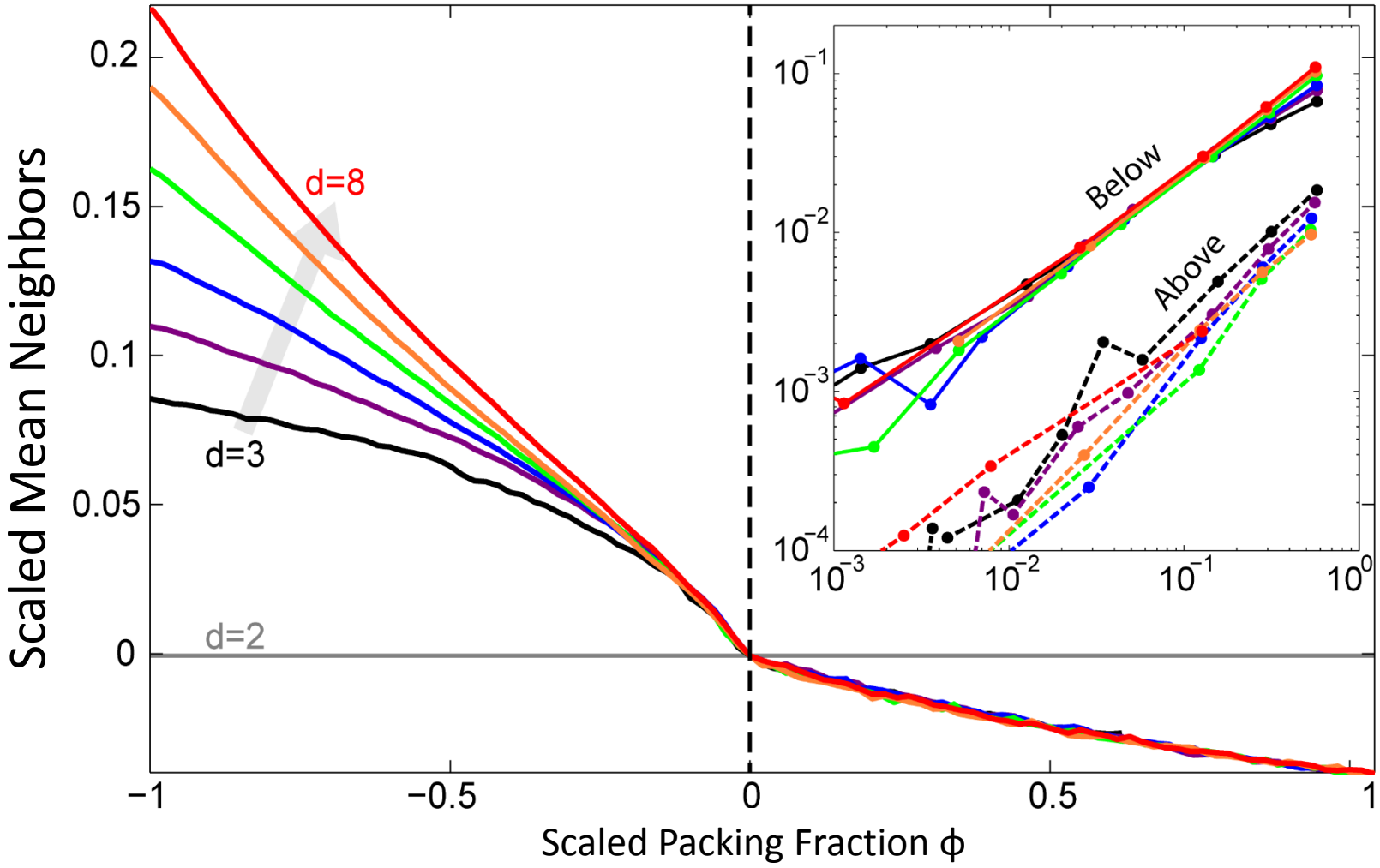


Voronoi Cell

- 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



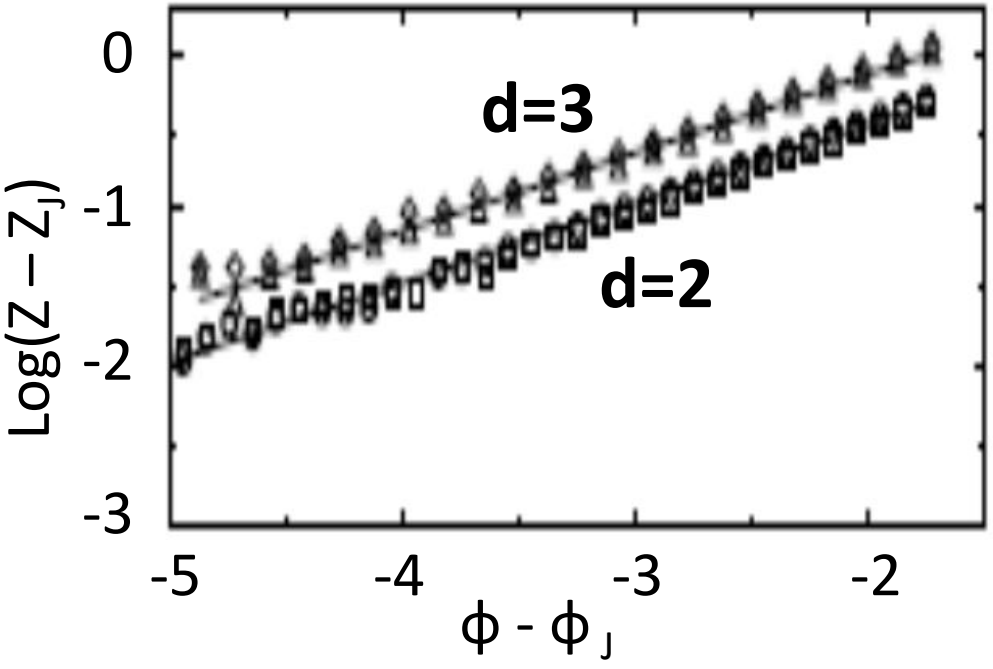
Number of Neighbors: $d_{UCD} \geq 3$



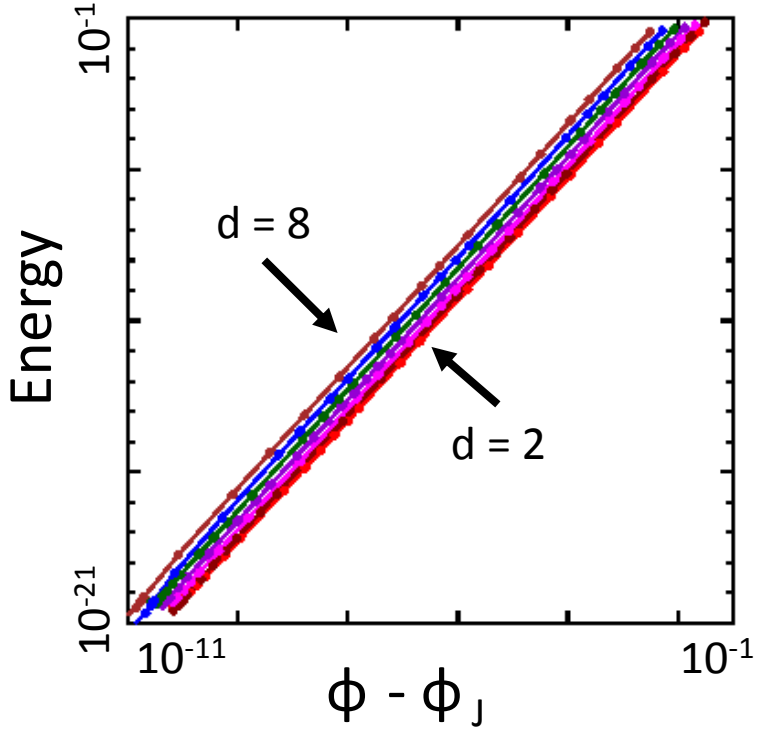
P. K. Morse, E. I. Corwin, Geometric Signatures of Jamming in the Mechanical Vacuum, PRL (2014)

But What About Mechanics?

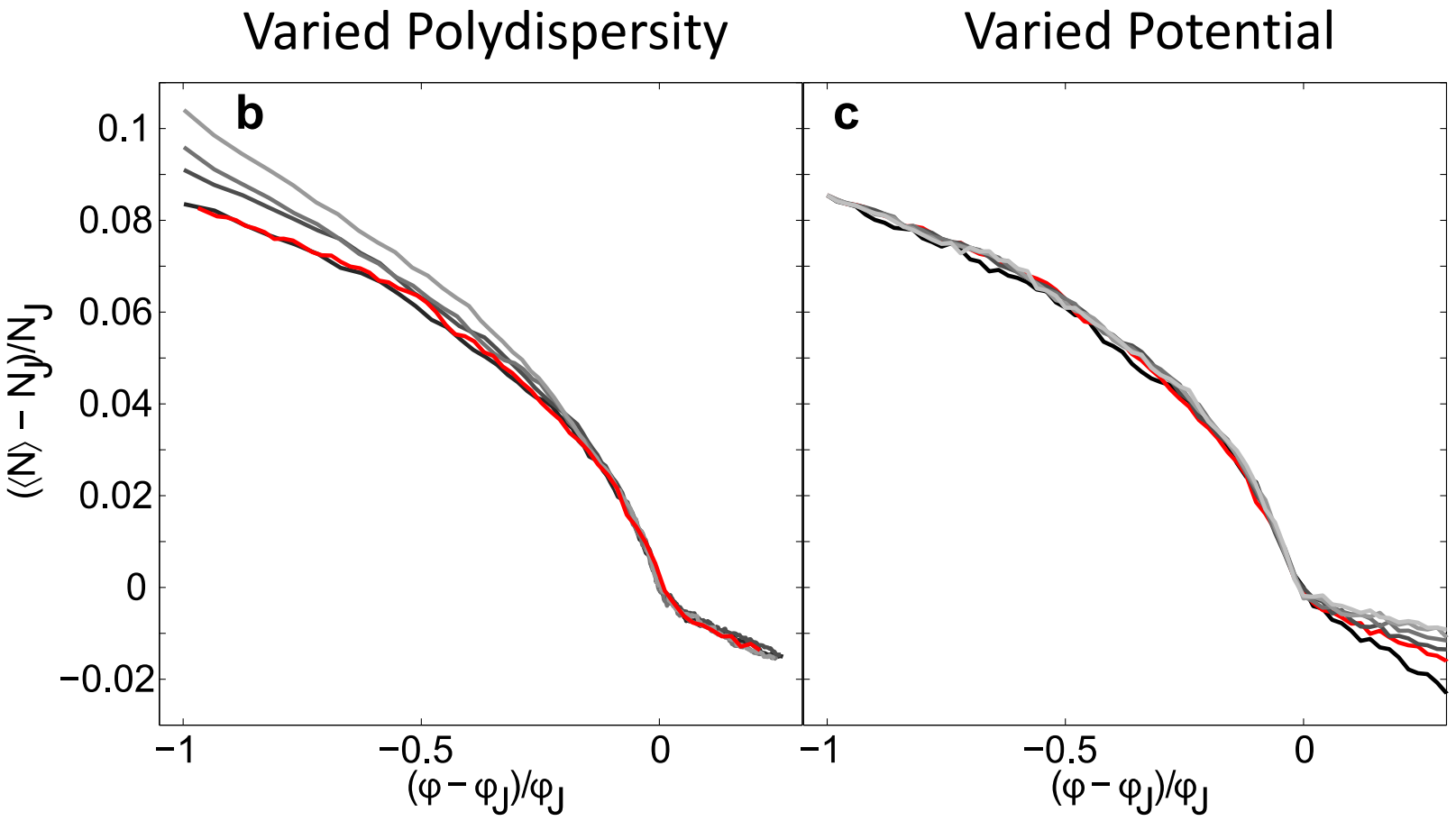
- Mechanical jamming has $d_{UCD} \leq 2$
- Either same underlying physics or two different phase transitions at same point



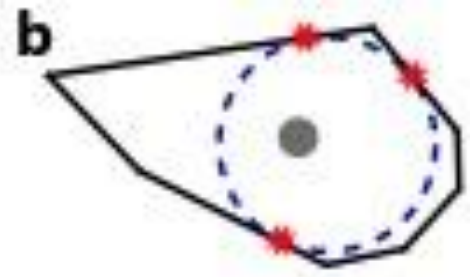
C. O'Hern *Phys. Rev. Lett.* 2002



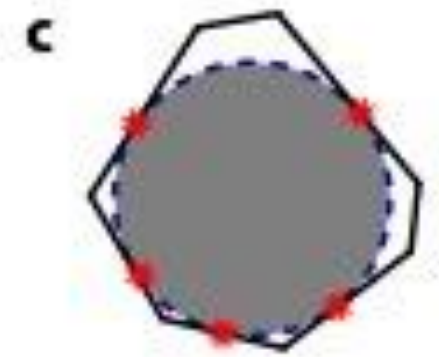
Universal Behavior Below Jamming



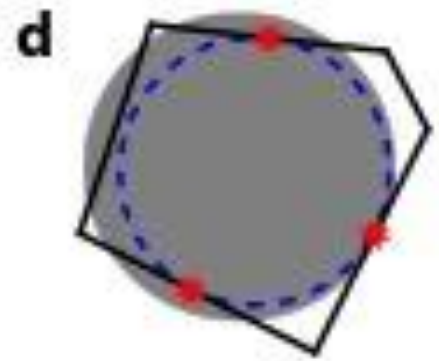
Maximum Inscribed Sphere



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

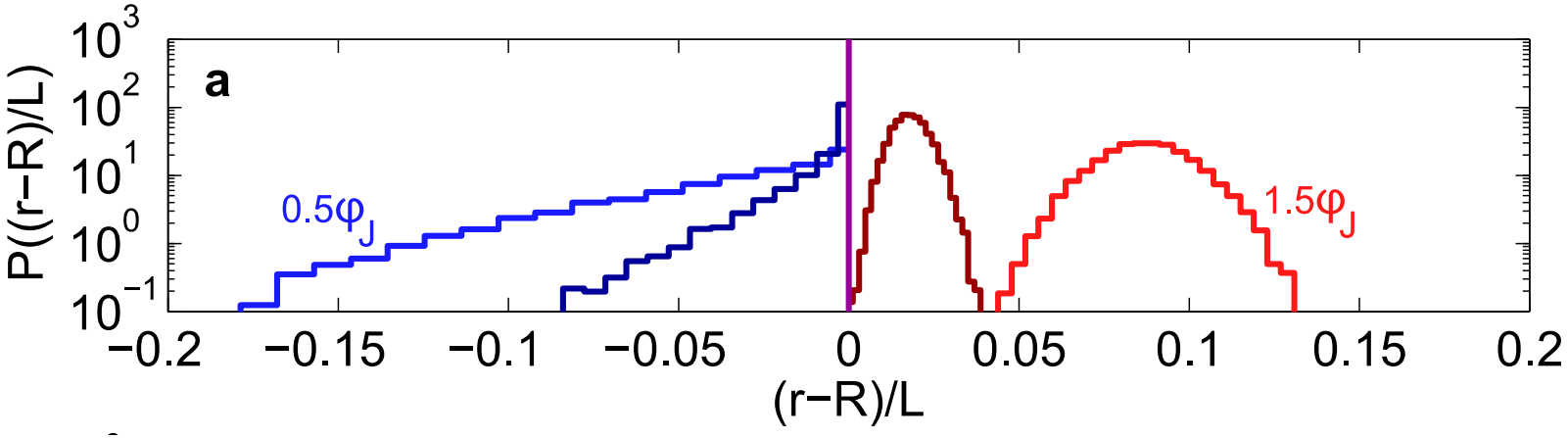


- At Jamming: Insphere exactly equal to physical sphere $\langle M \rangle = 2d$

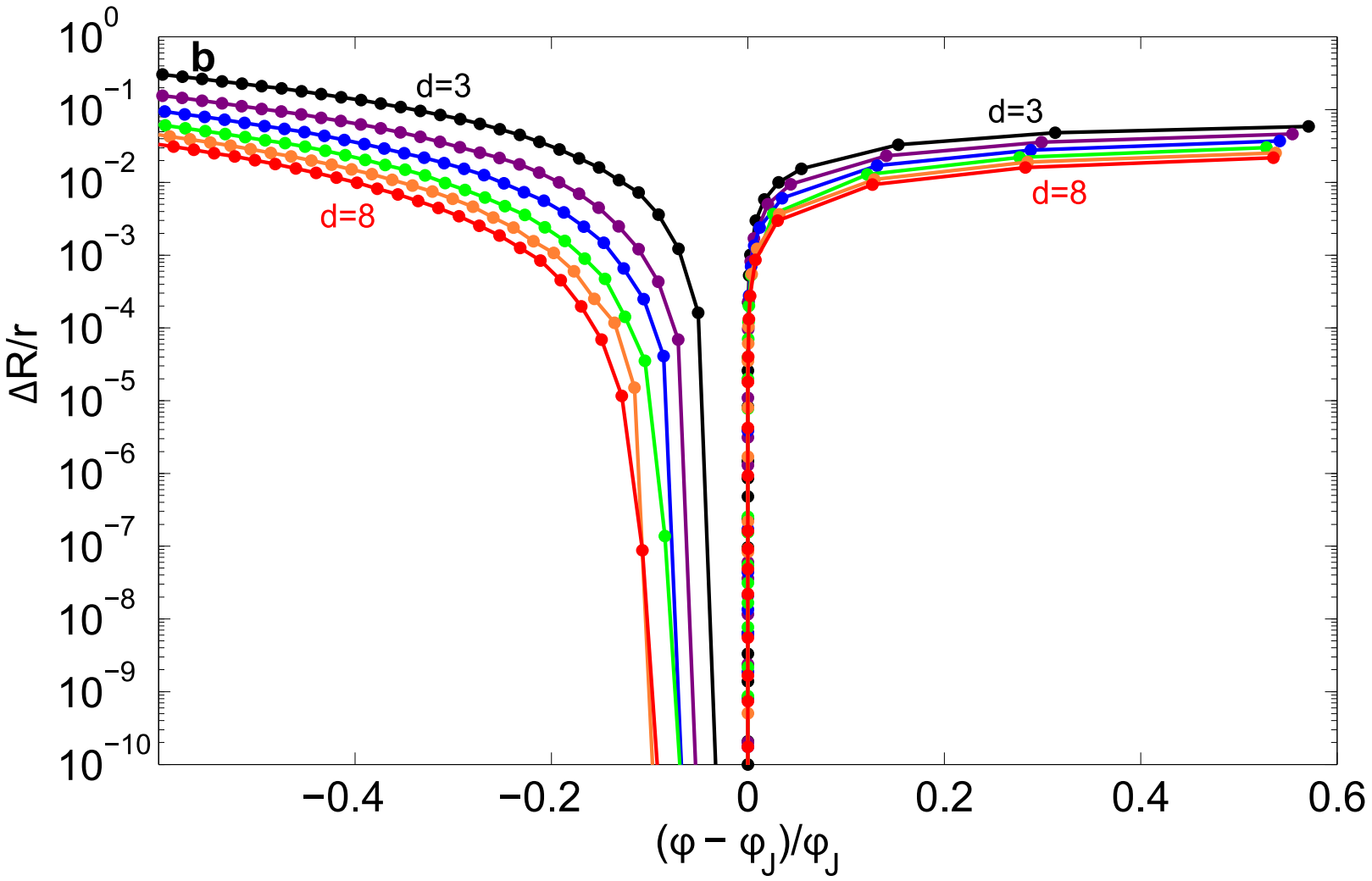


- Above Jamming: Insphere smaller than physical sphere $M = d+1$

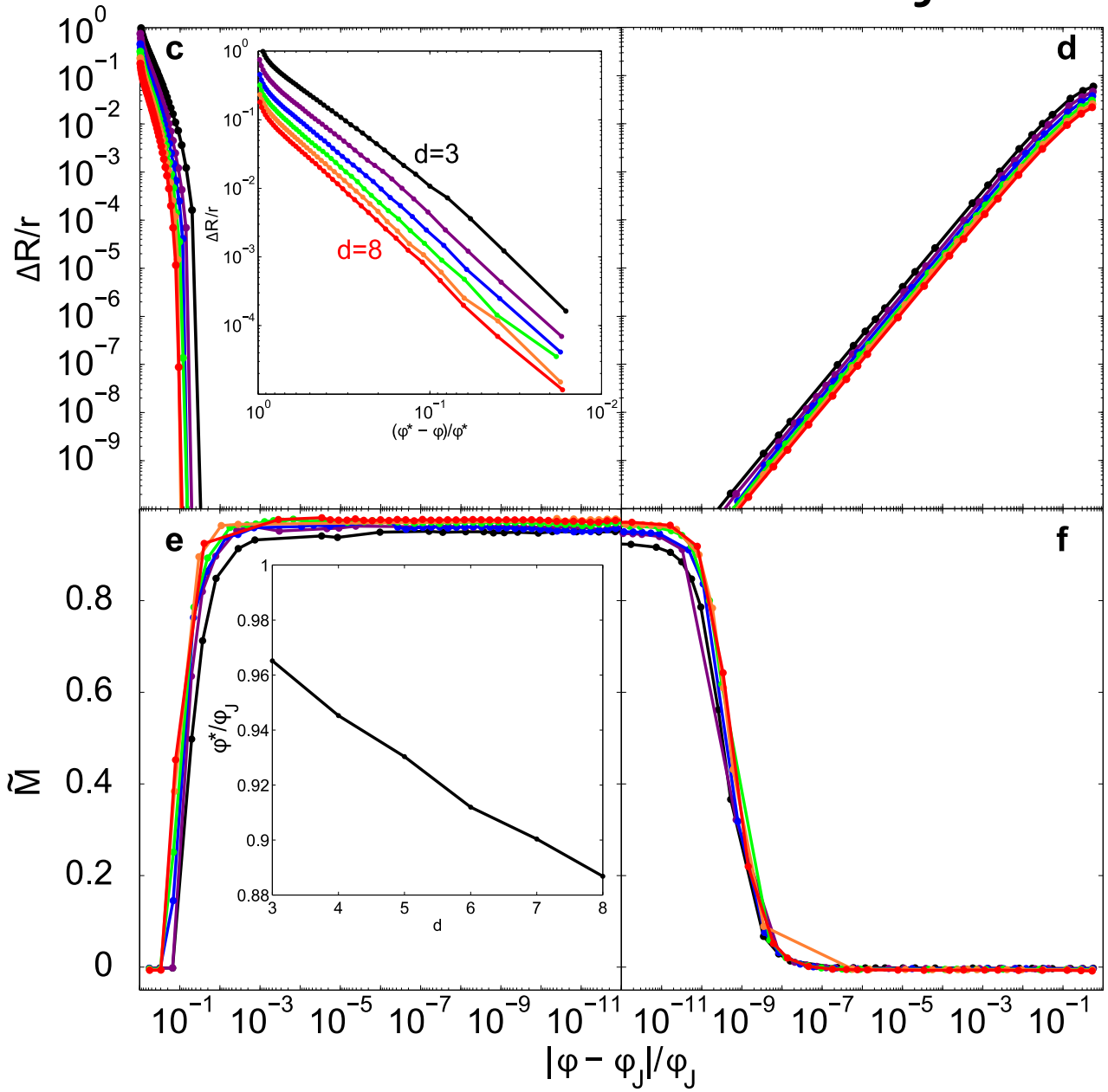
Insphere Distribution



Width of Insphere Distribution

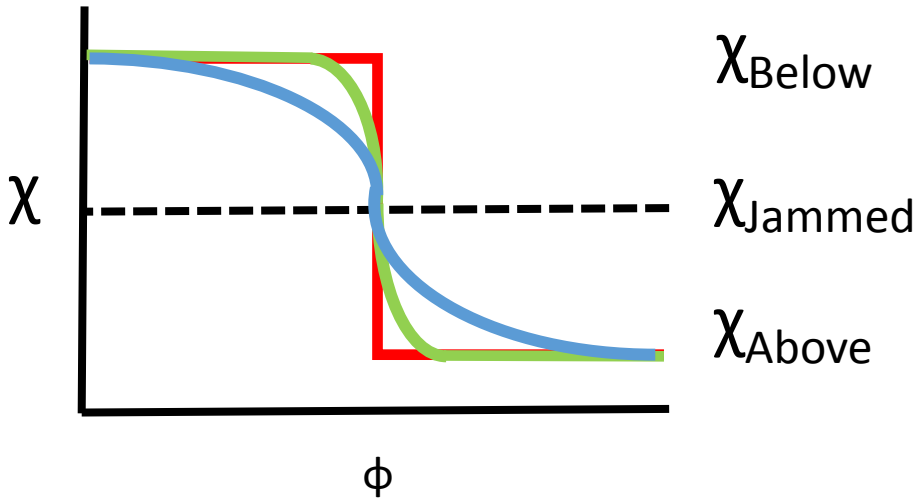


Another transition below jamming?



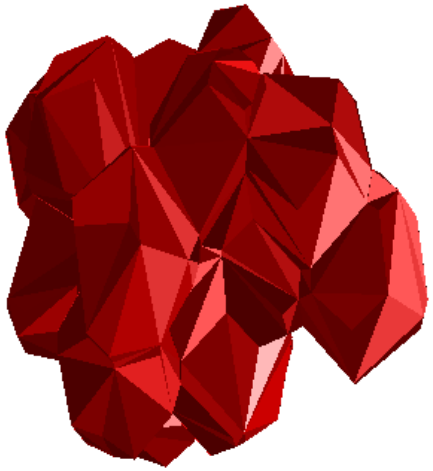
Toward Renormalization

- 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

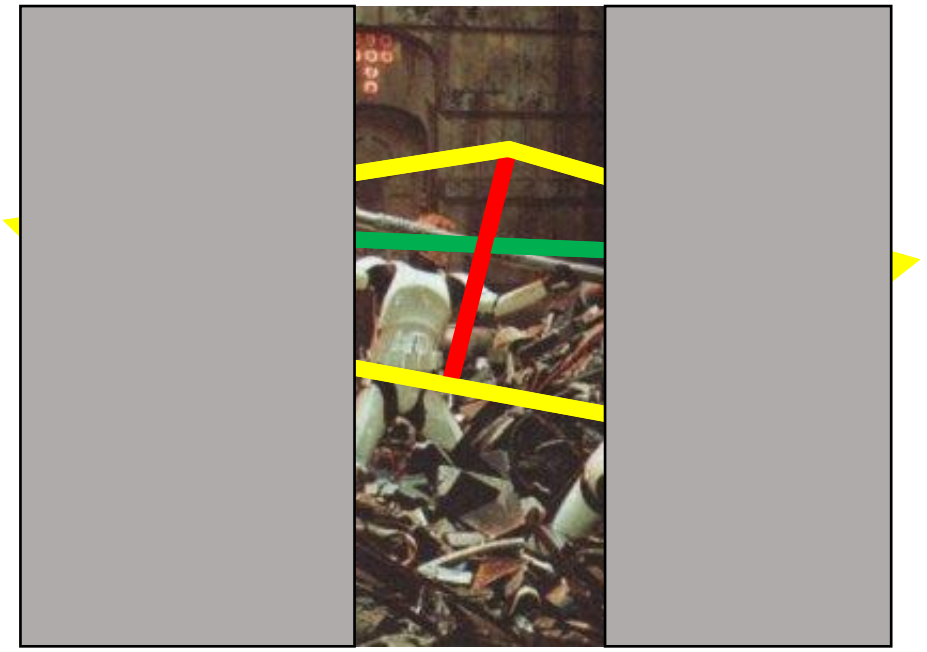


Aspect Ratio / Eccentricity Definition

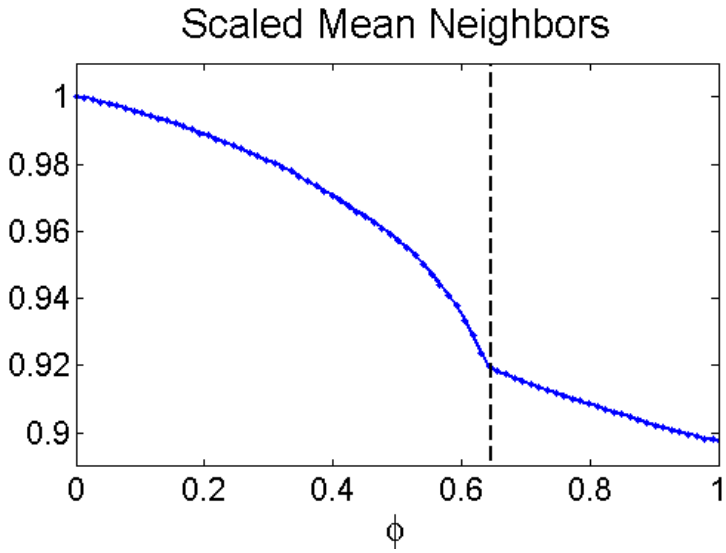
- “Trash compactor” aspect ratio
- Define:

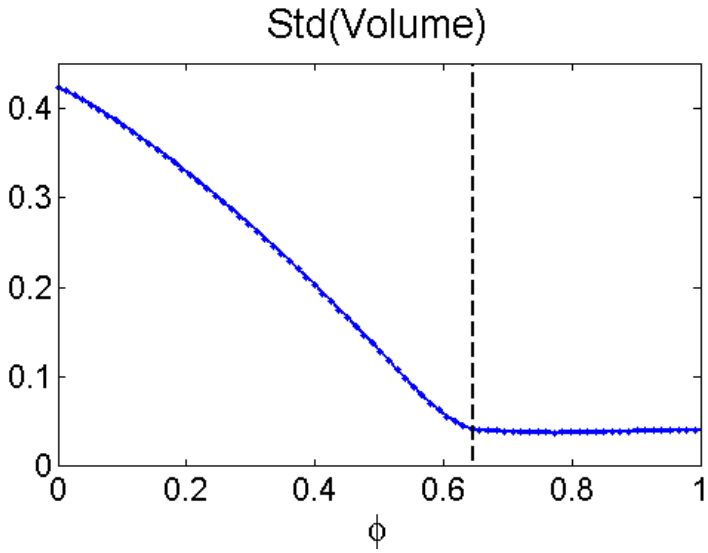
$$k = \frac{d_{\text{long}}}{d_{\text{short}}} - 1$$

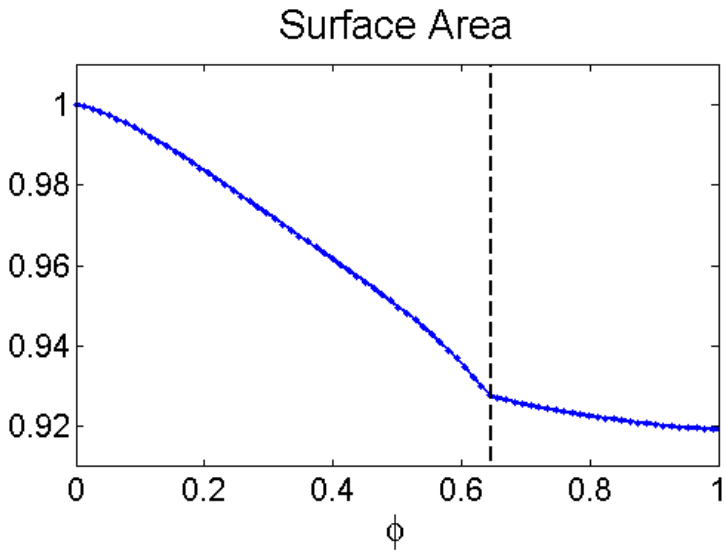
- If concave, take the convex hull first
- k = 0 when spherical

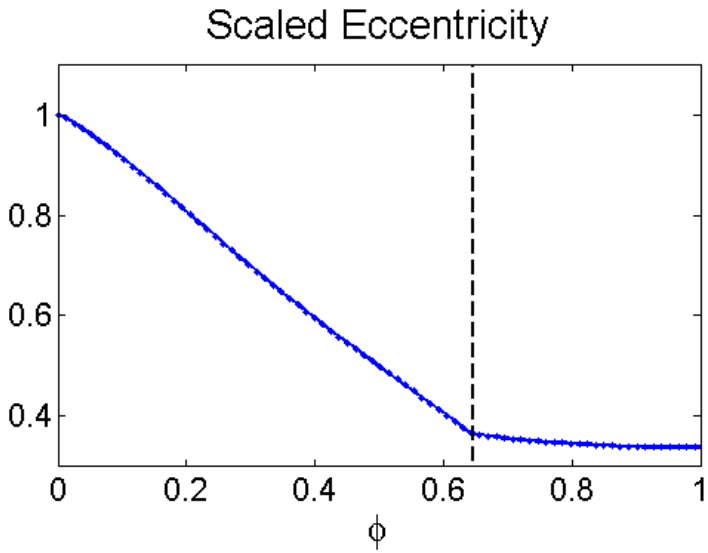


All show signatures of jamming!

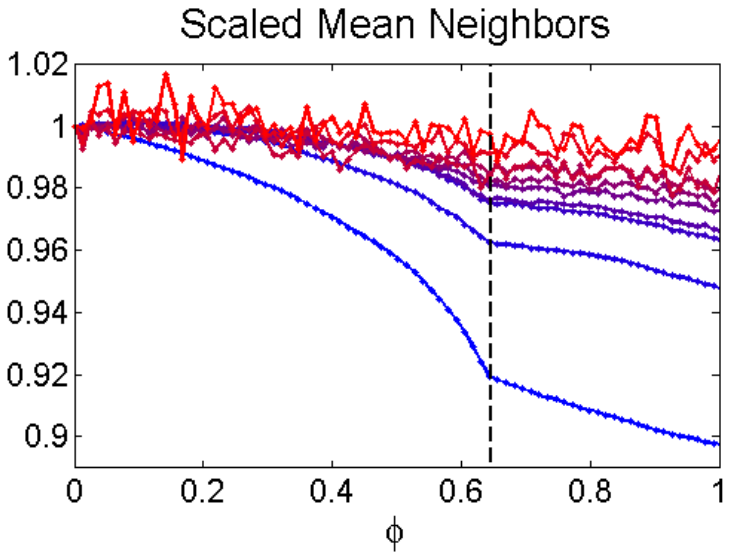


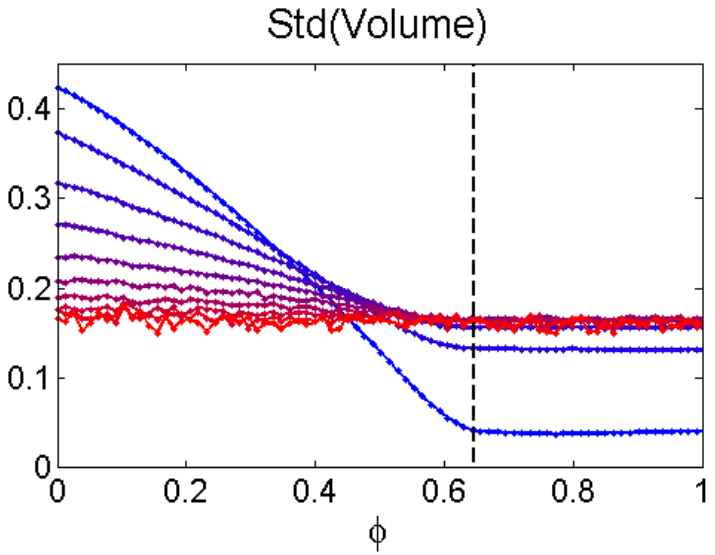


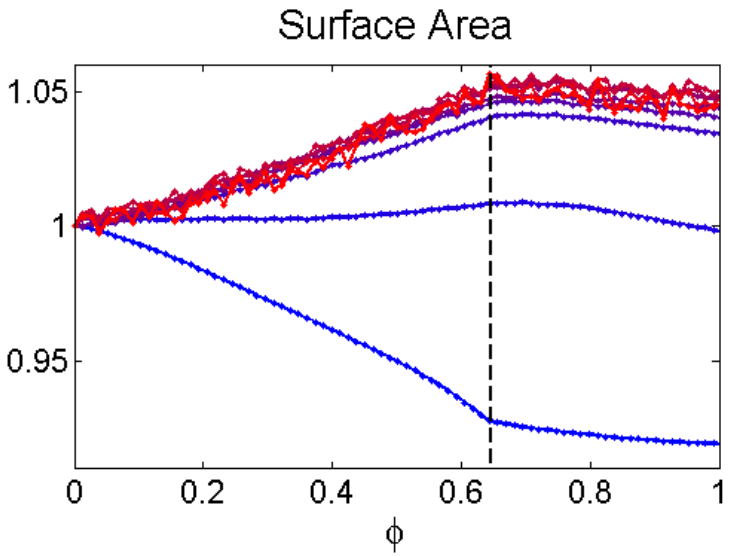


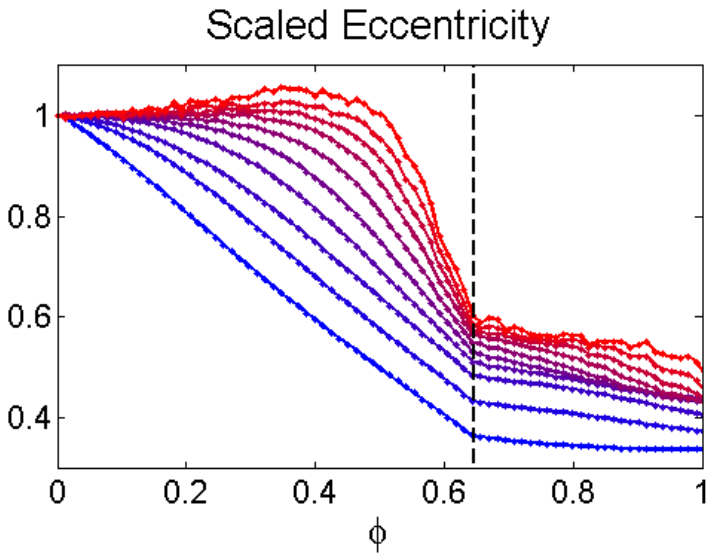


Renormalization

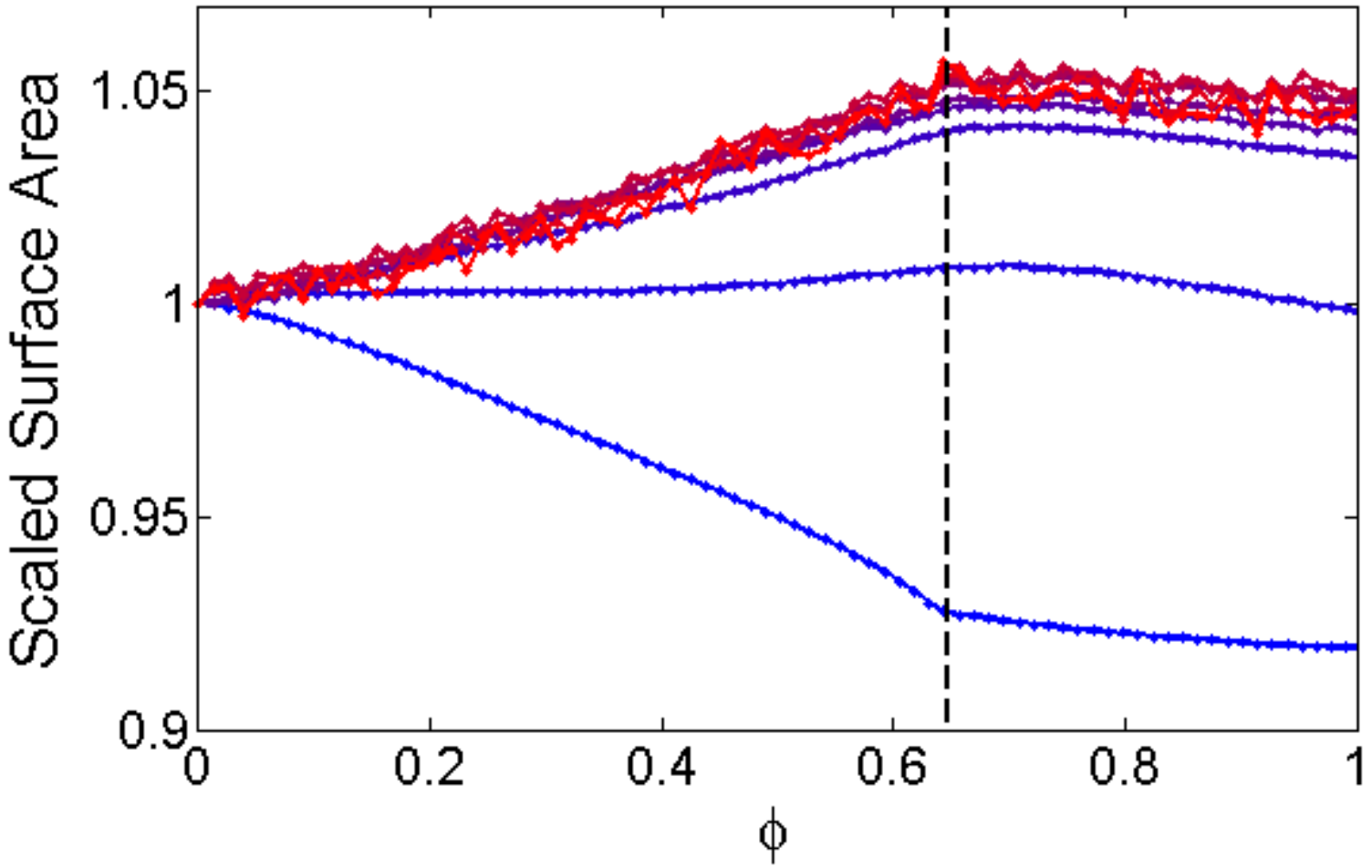






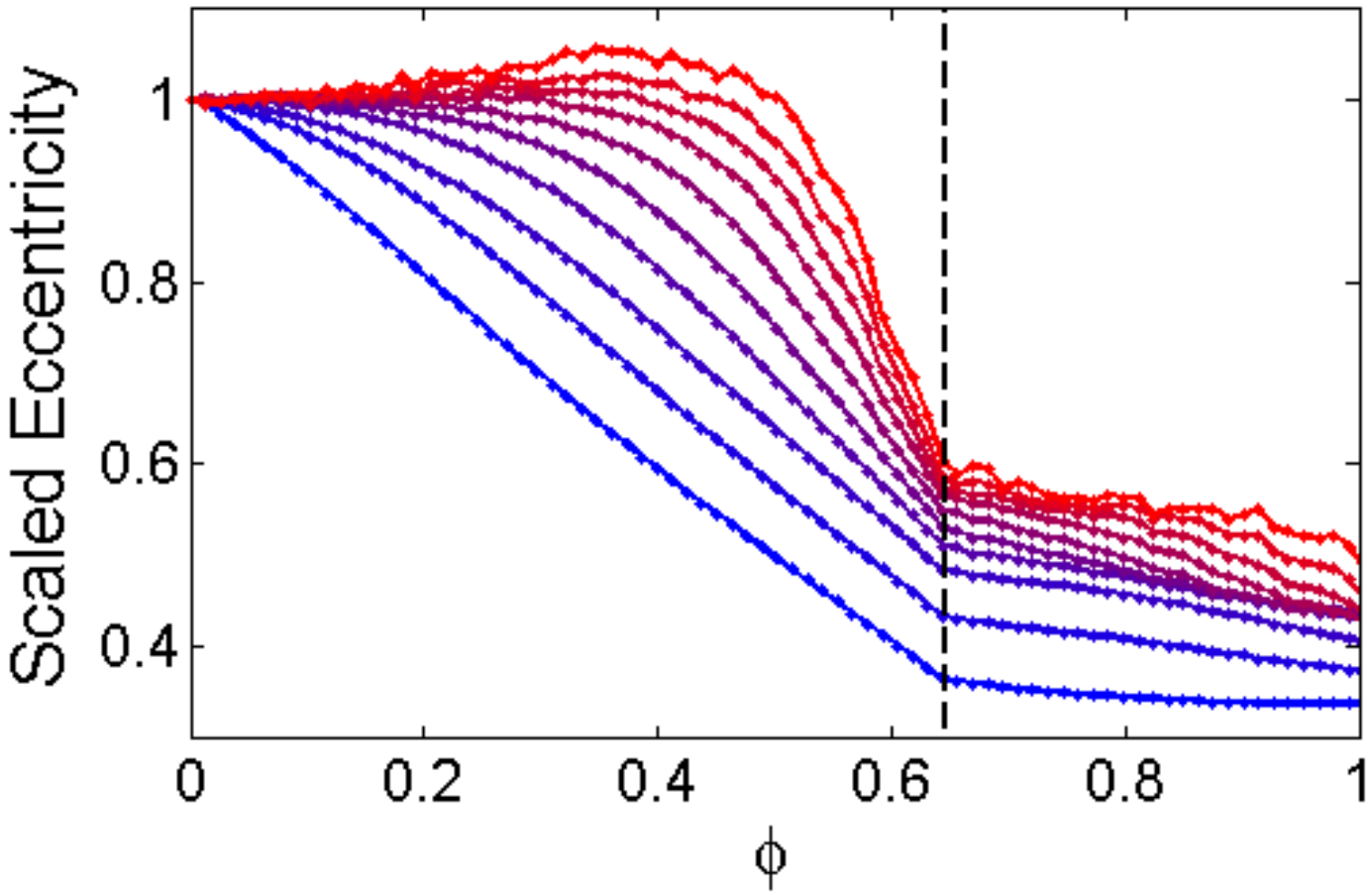


Surface Area (renorm)



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

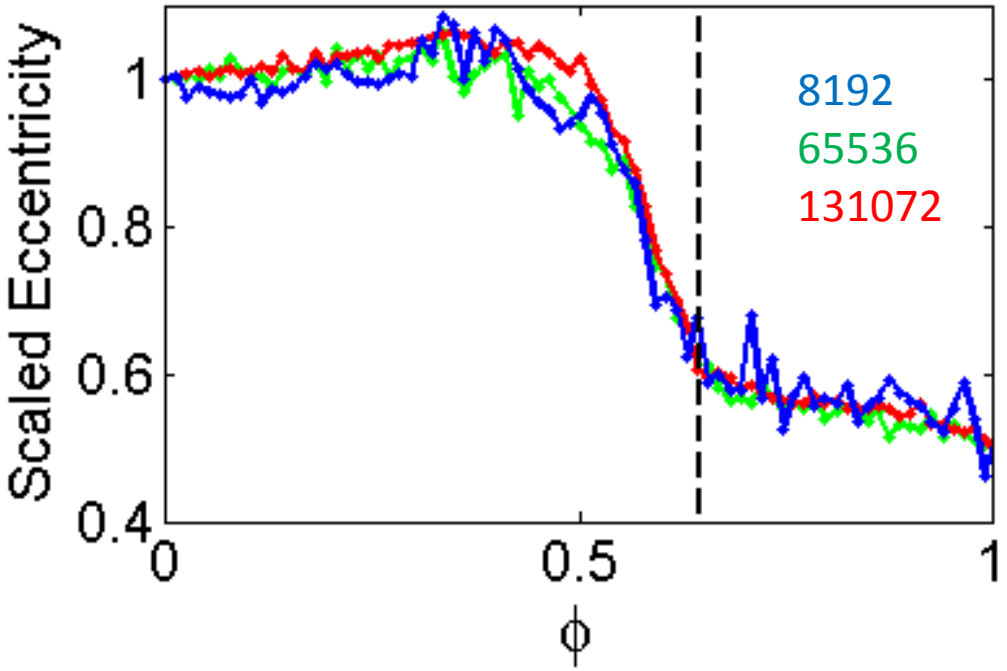
Aspect Ratio (renorm)



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

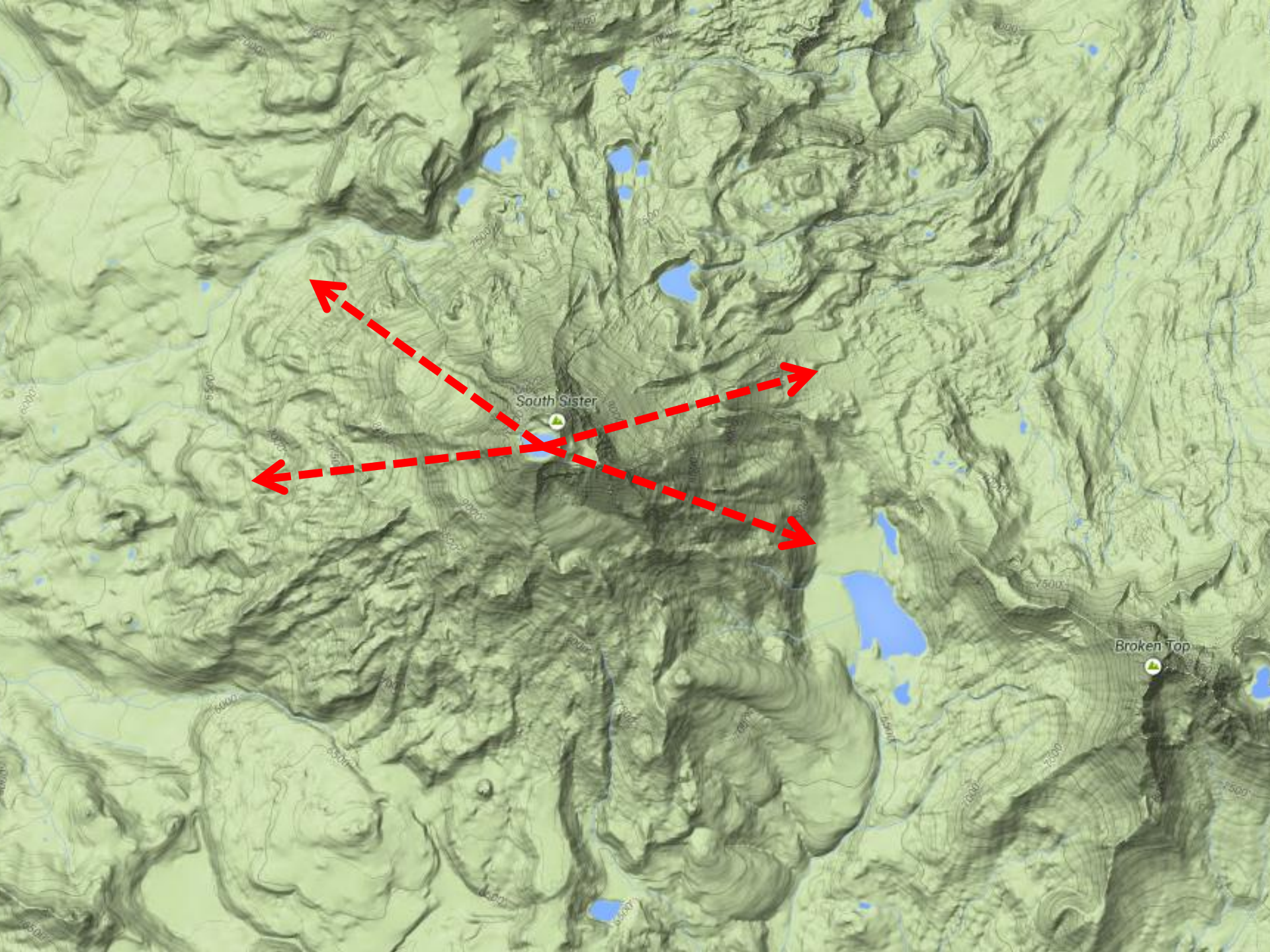
Aspect Ratio: Finite Size

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

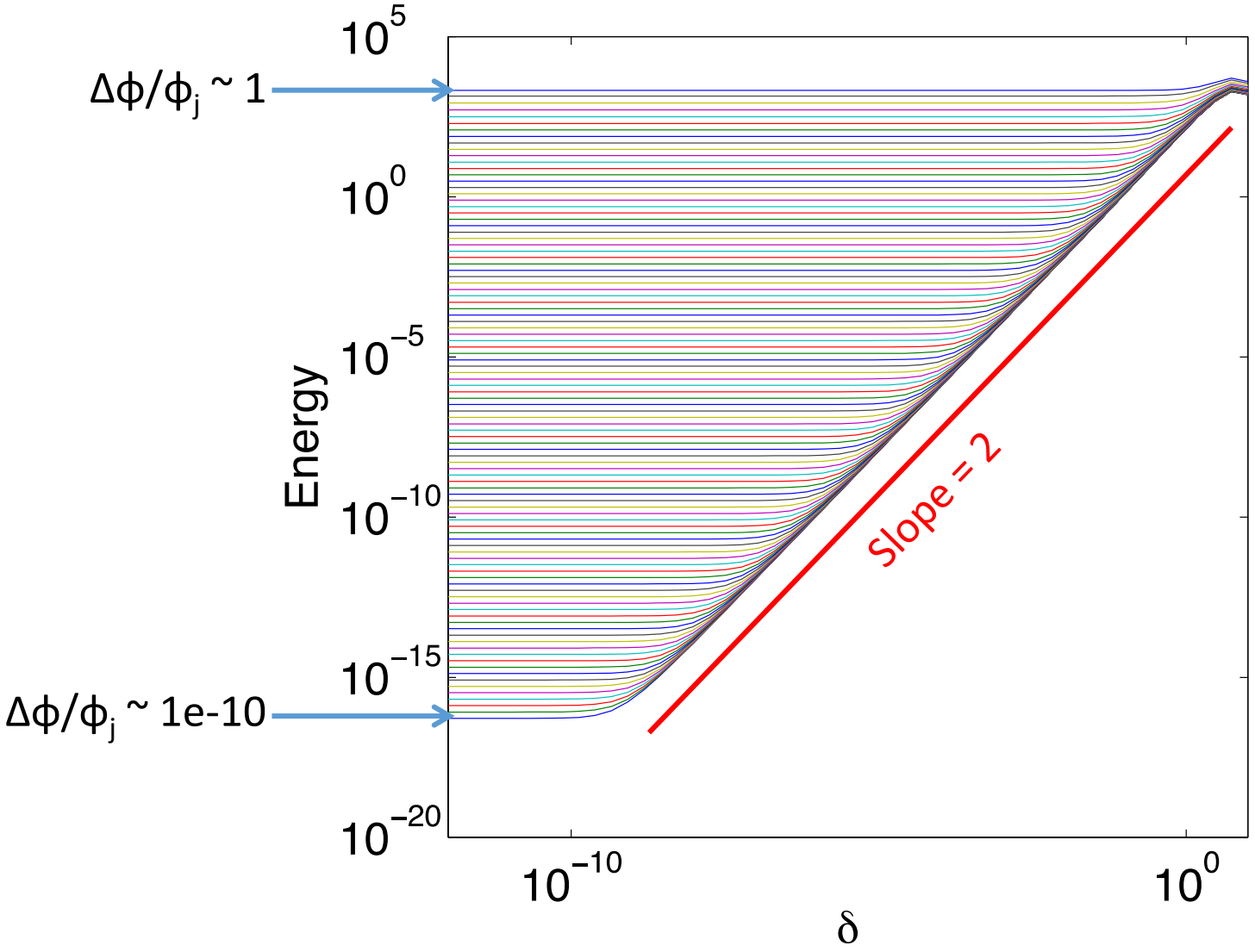


Energy Landscape

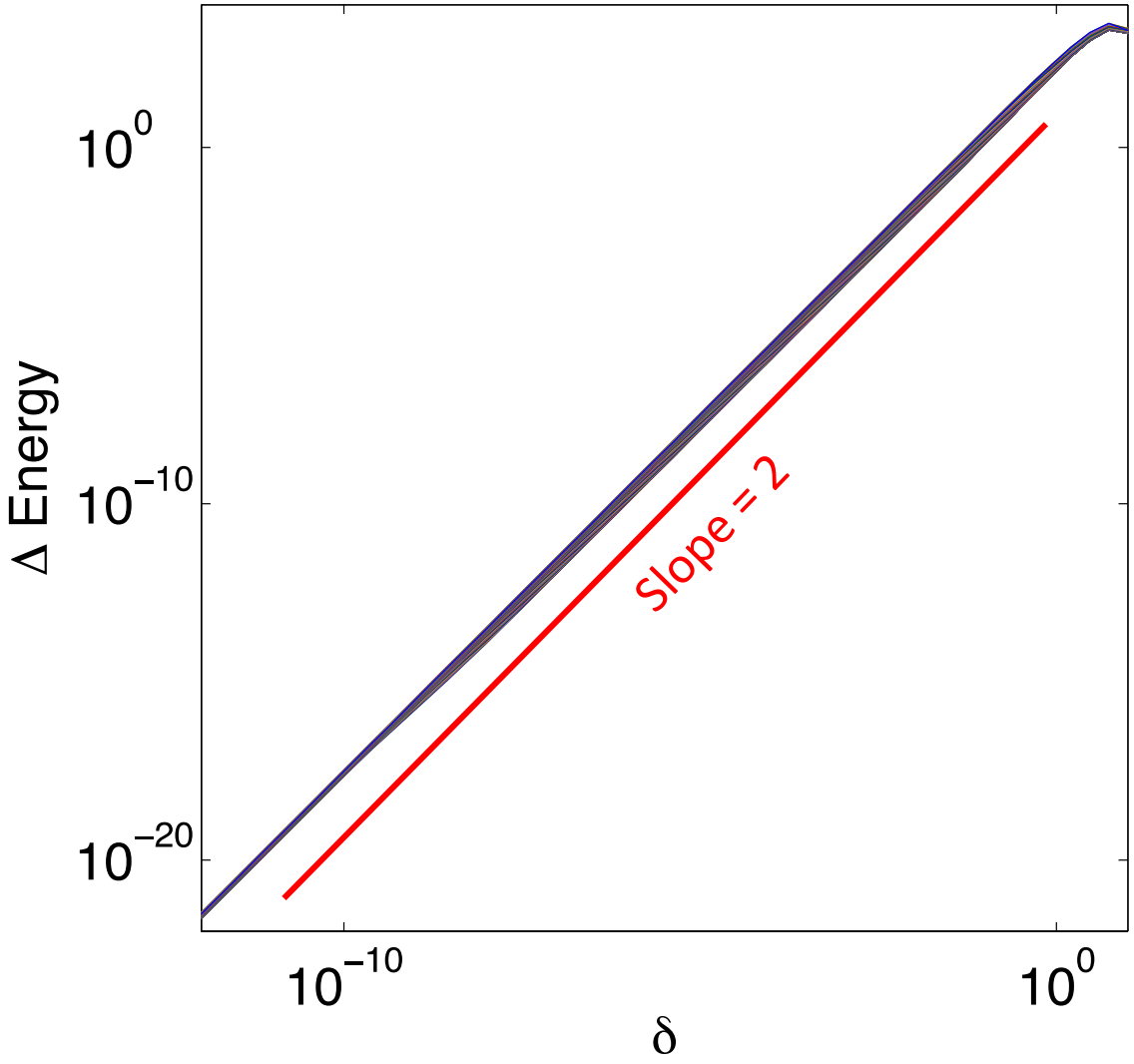
- Problem: Can't map ultra-high dimensional phase space
- Solution: Random transects
- Minimize system at fixed ϕ then
  - Pick random direction
  - Calc Energy as a function of distance δ
  - Repeat and average over many directions (~100)
- Results independent of system dimension!


South Sister
Broken Top

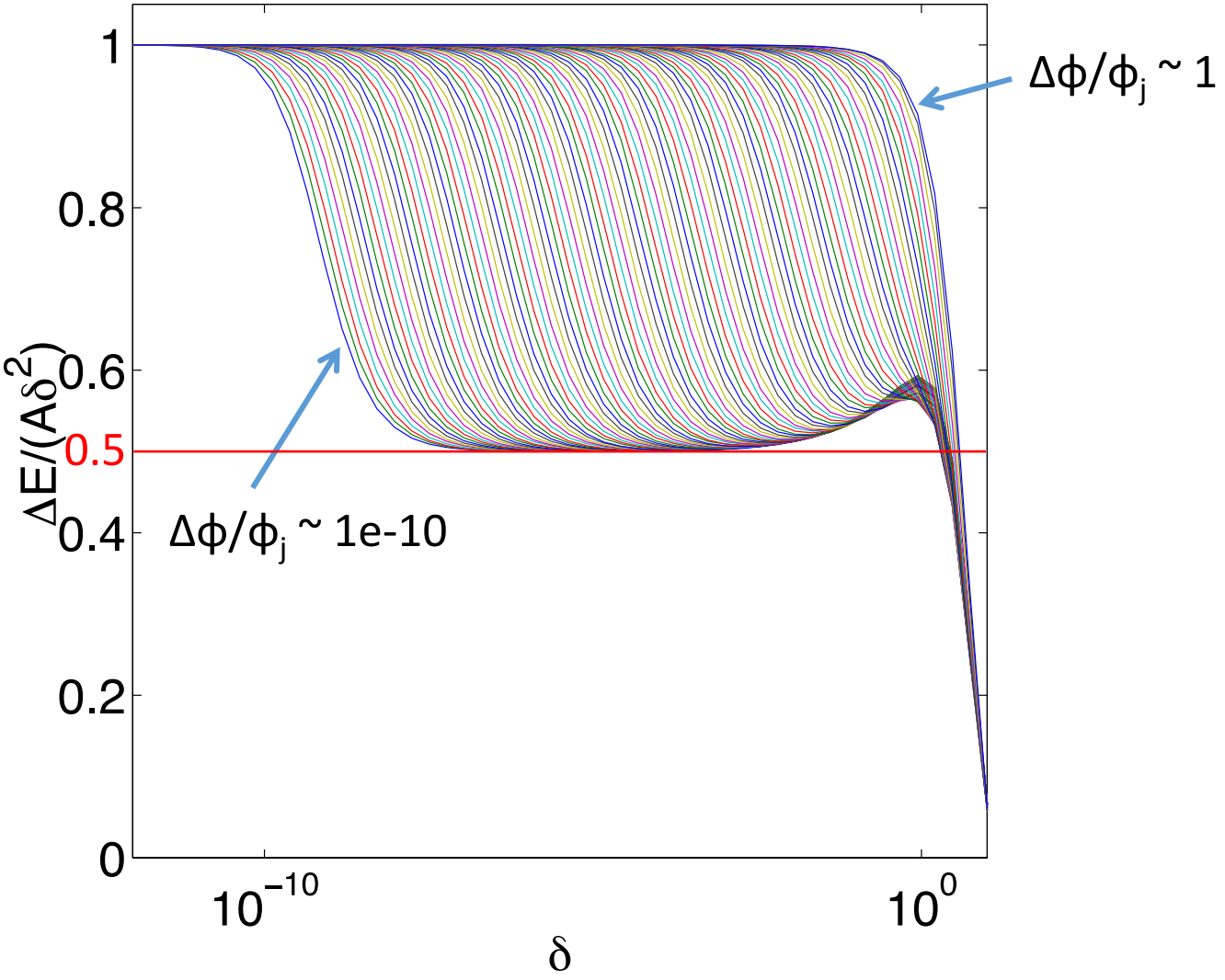
Harmonic Contact Pot, D=4, N=8192



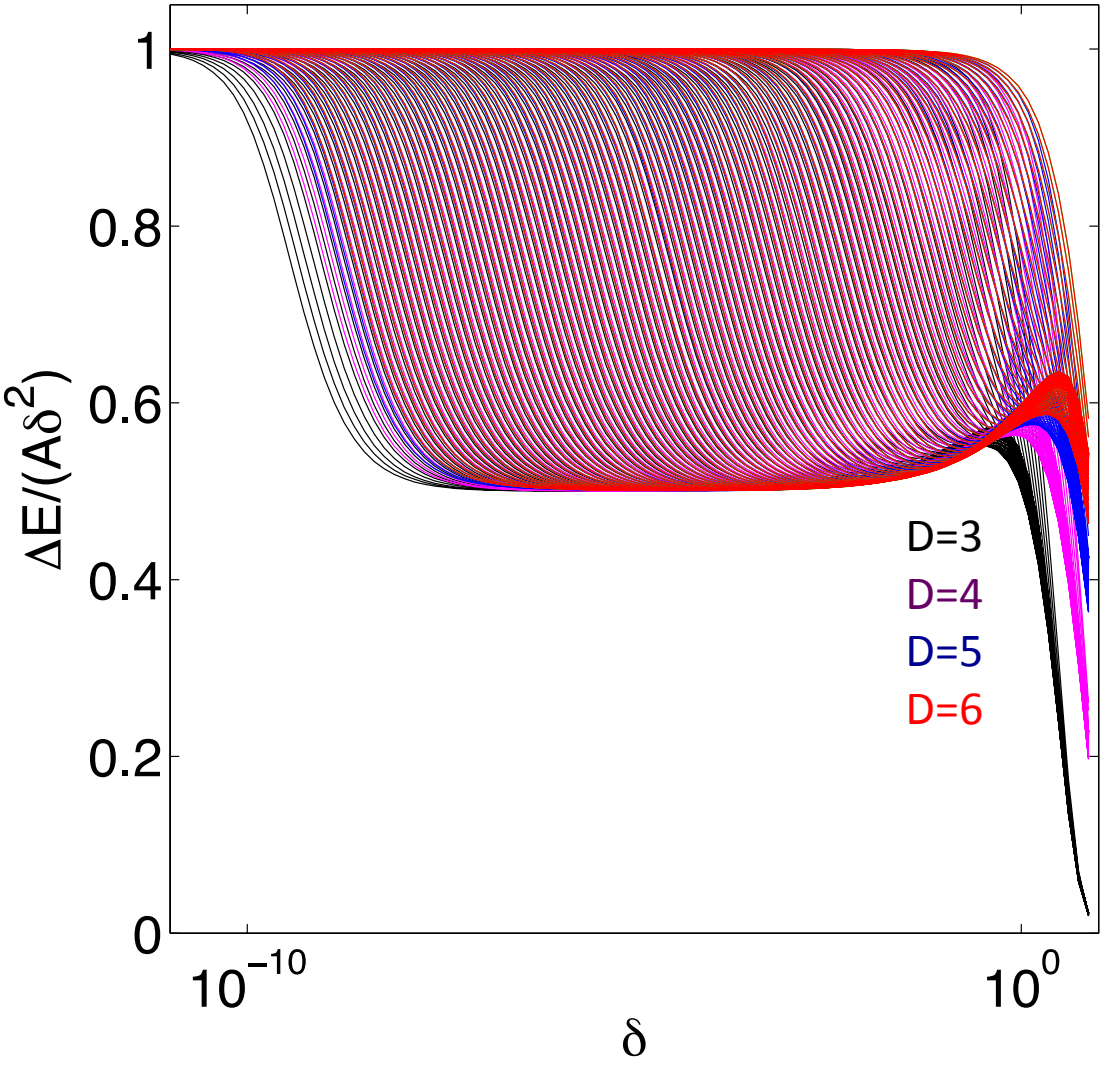
Subtract Starting Energy



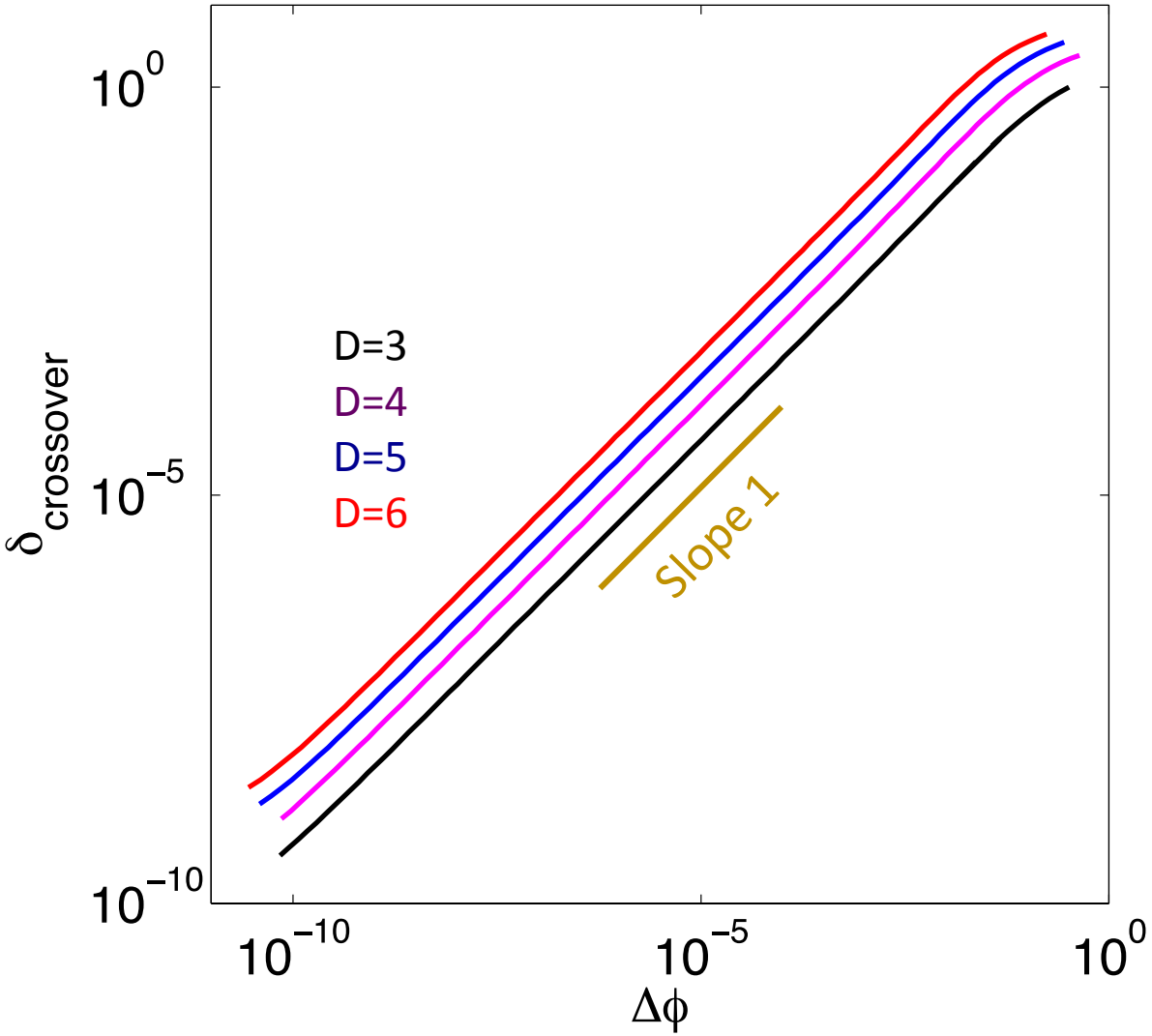
Two Different Harmonic Regimes!



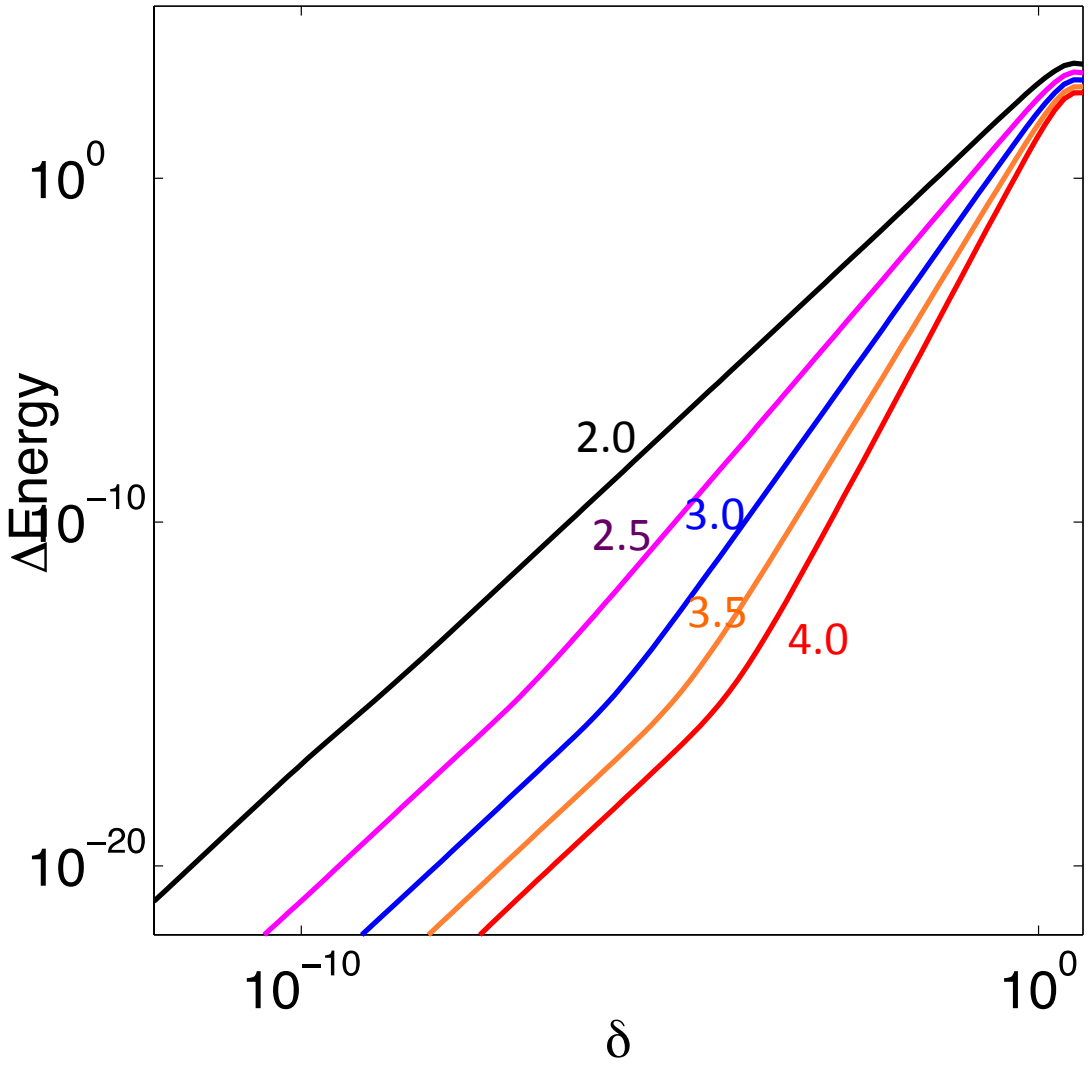
Dimension Independent



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

Funding from NSF GK-12
and NSF CAREER award
DMR-1255730