Jamming Meets Experiments (Day 2: Theoretical Frameworks)

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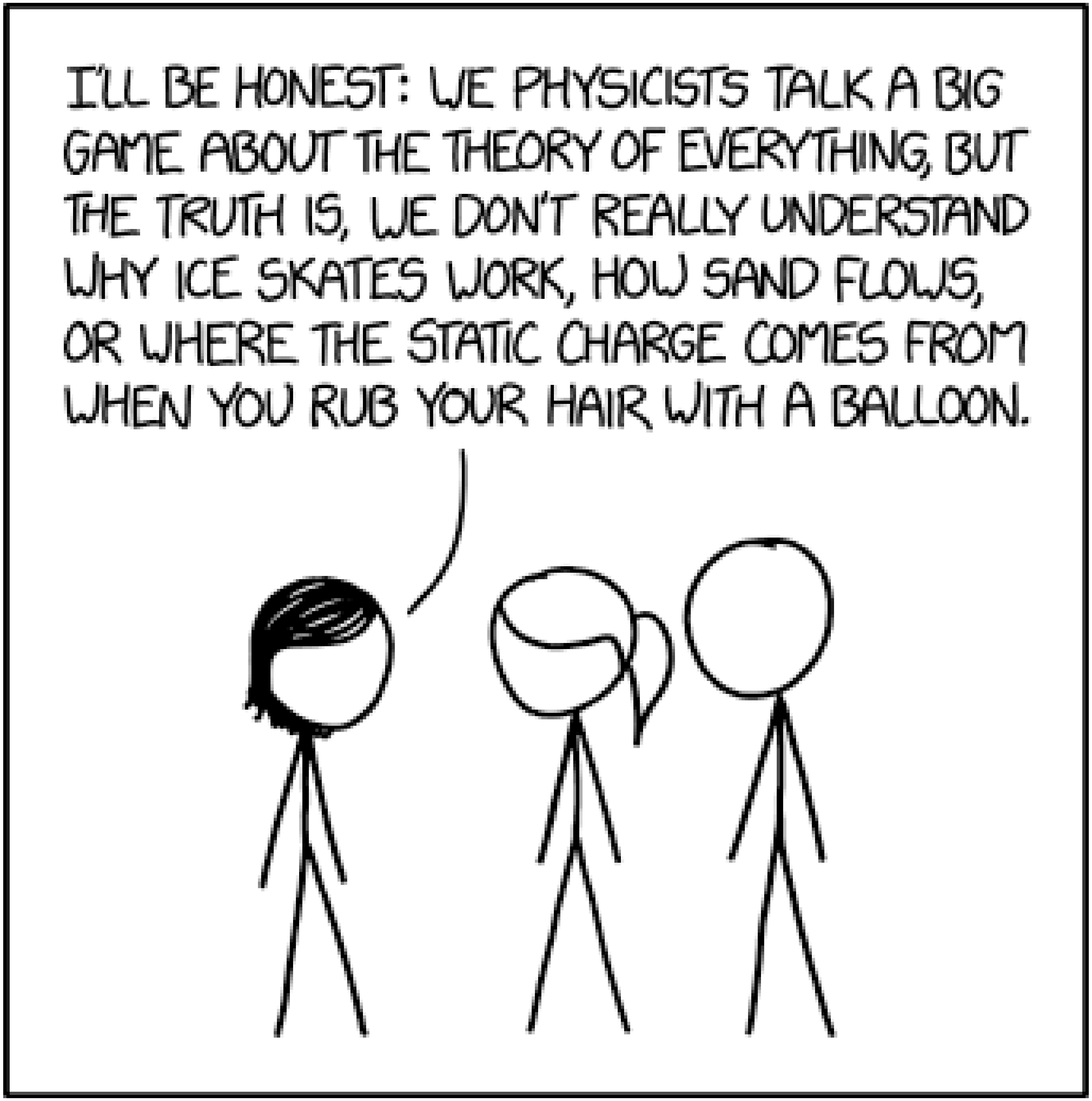
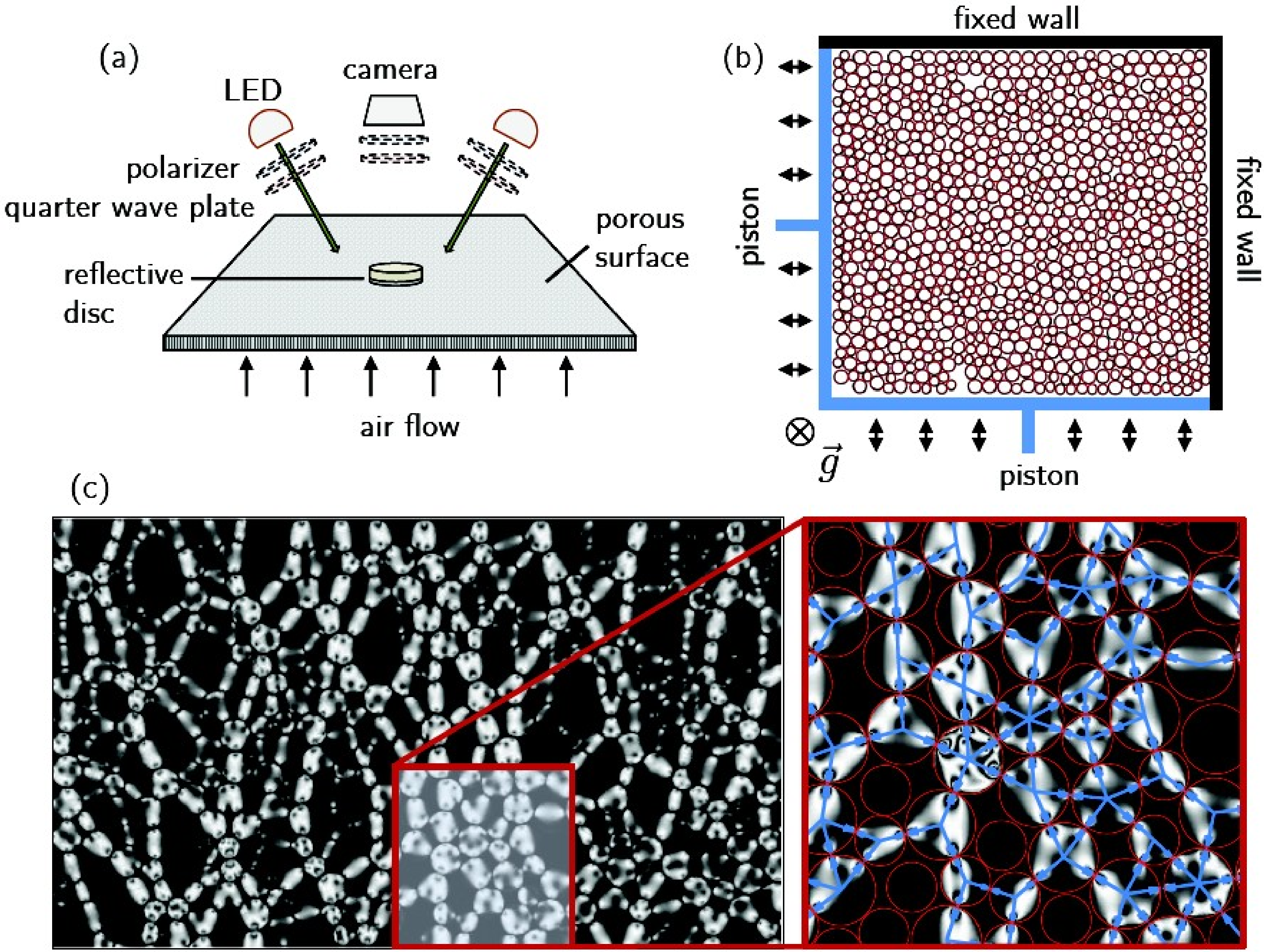
NSF JSMF IFPRI International Fine Particle Research Institute

Boulder School 2017: Frustrated and Disordered Systems

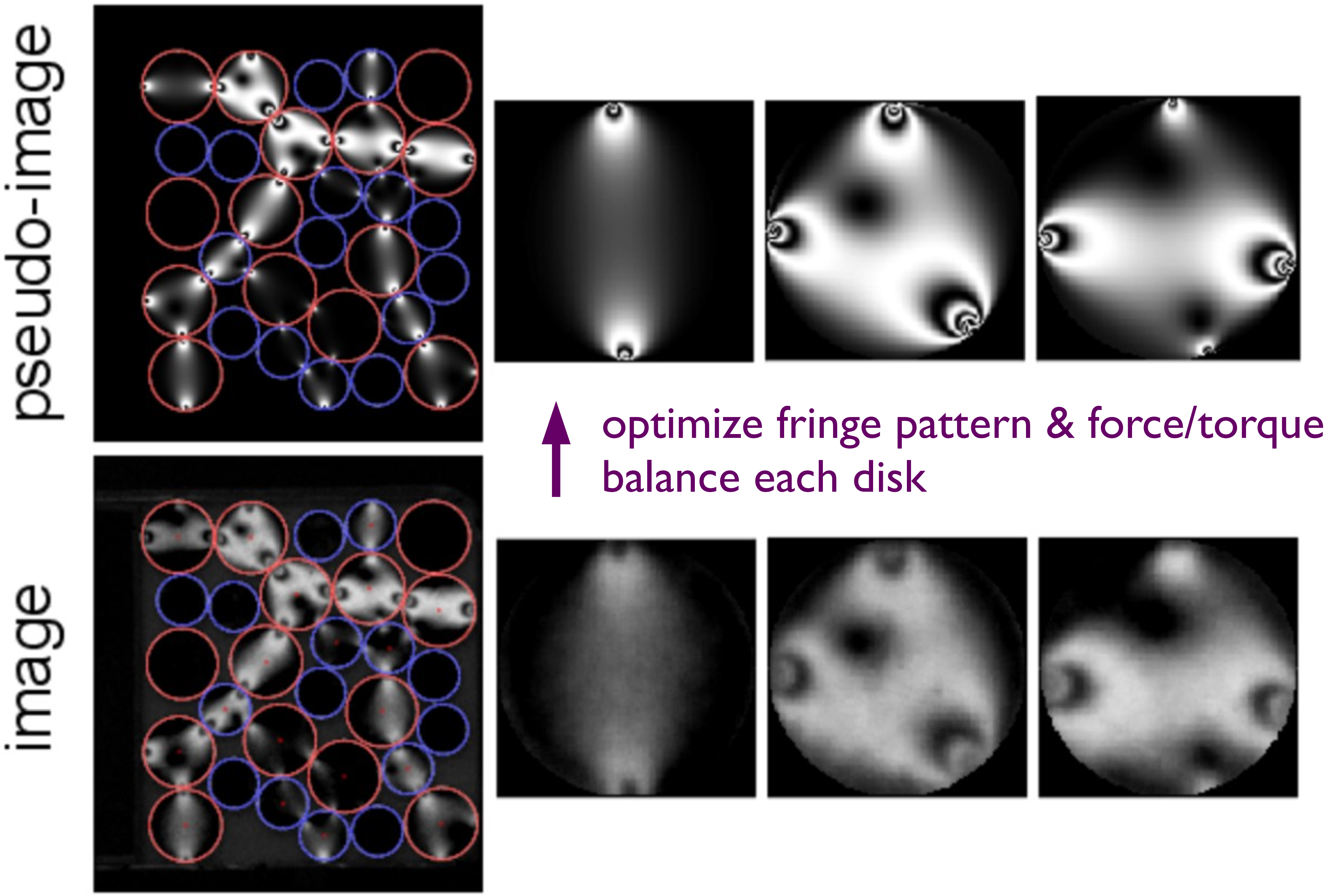


https://xkcd.com/1867/

quasi-2D experiments



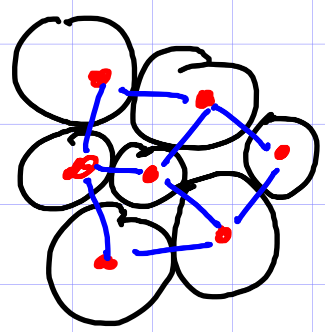
Photoelastic Inversion



Daniels, Kollmer, Puckett. *Rev. Sci. Inst. (2017)*

Network Science

Representing Packings as networks



centers = nodes (vertices)

contacts = edges (bonds)

↳ can be weighted by force

magnitude or normal or tangential force ?

write adjacency matrix

$$A_{ij} = \begin{cases} 0 & \text{non-contact} \\ 1 & \text{contact} \end{cases}$$

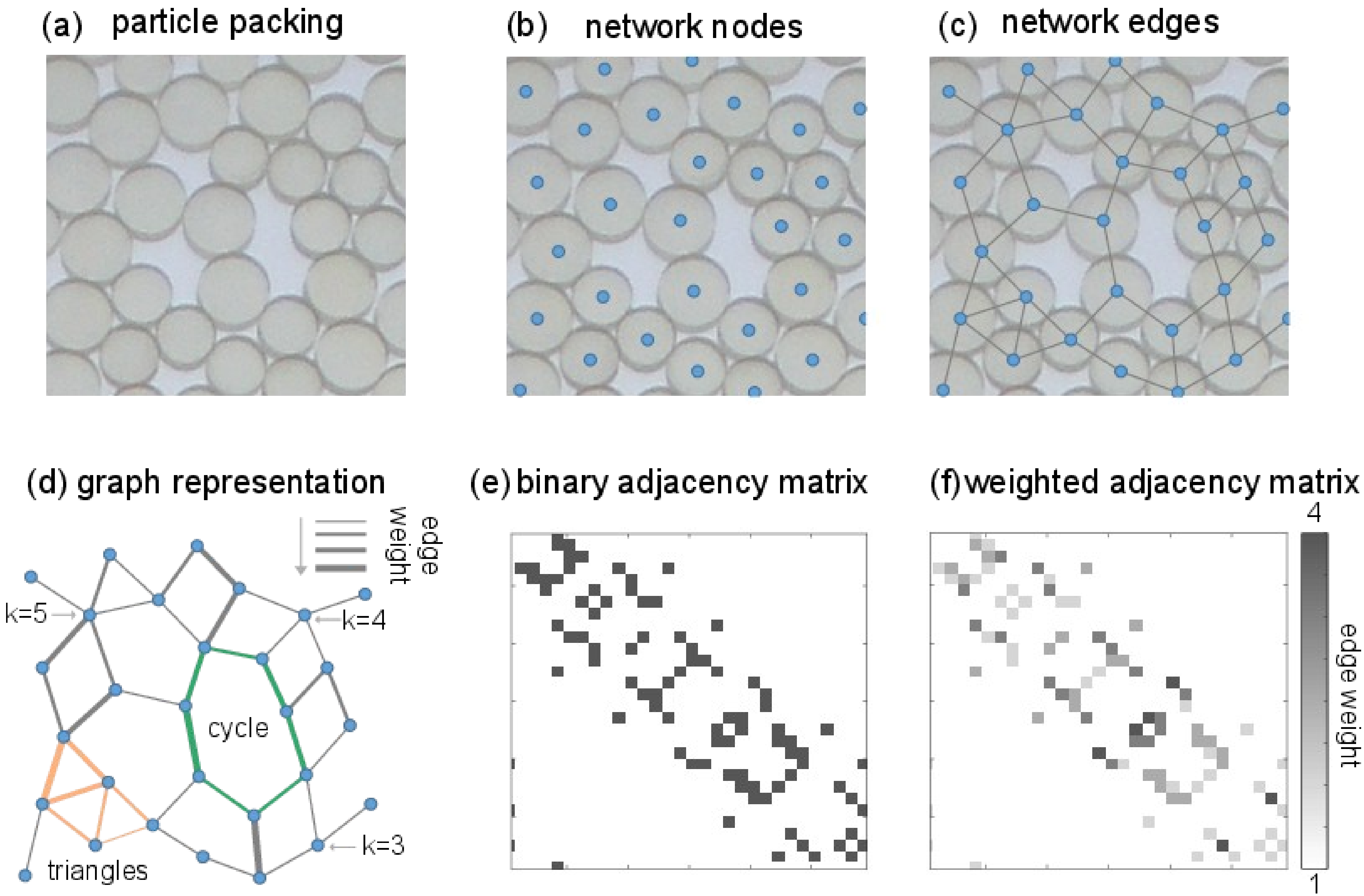
or weighted adjacency matrix

$$W_{ij} = \begin{cases} 0 & \text{non-contact} \\ w_{ij} & \text{force @ contact} \end{cases}$$

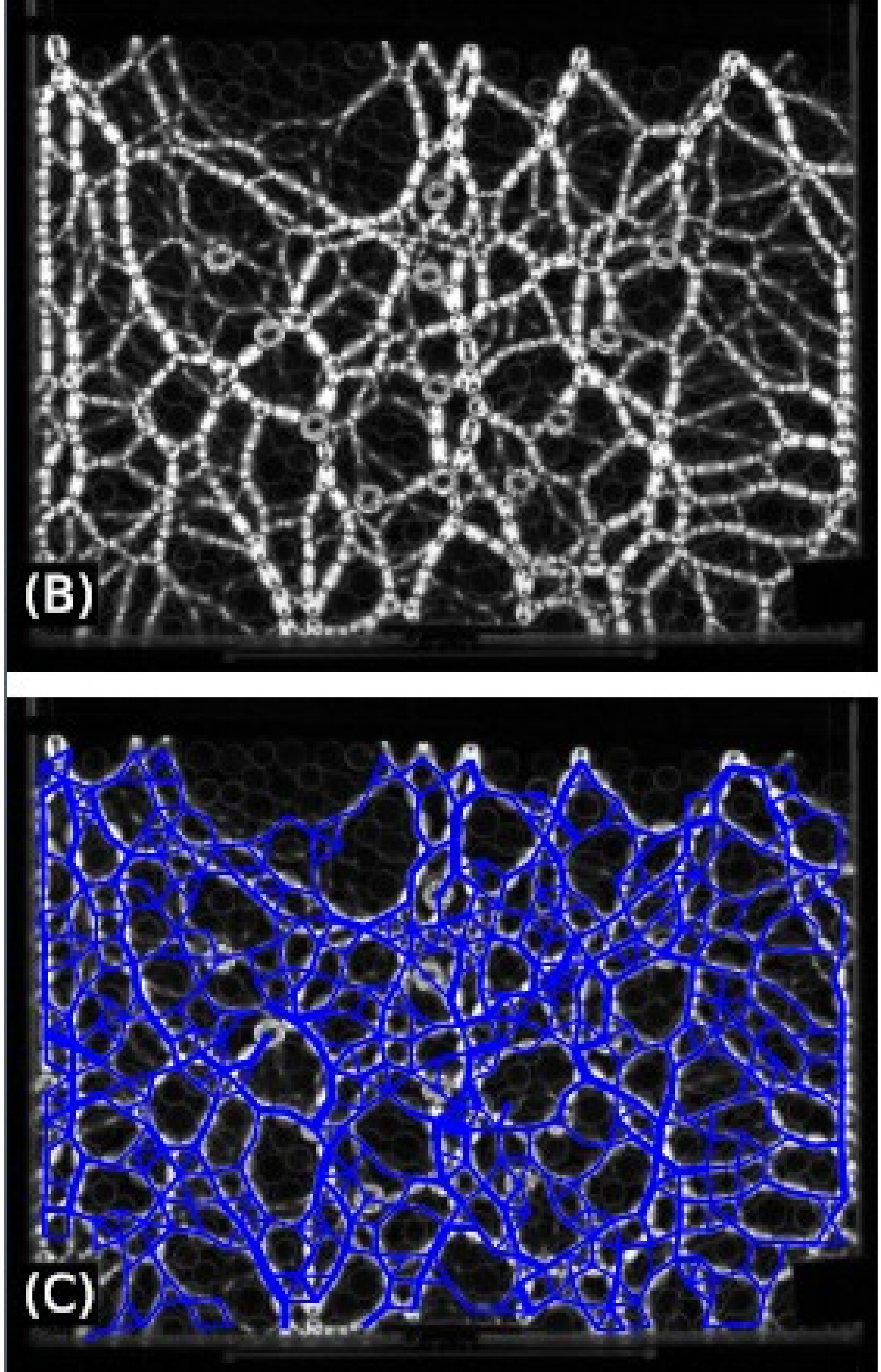
matrix should be symmetric by Newton's 2nd Law

show image of adjacency matrices

Writing Data as an Adjacency Matrix



Papadopoulos, Daniels, Porter, Bassett (on arXiv soon!)


(B)
(C)

Some useful network-science metrics

(see e.g. Mark Newman Intro to Networks (efficient!)
netwiki.amath.unc.edu
arXiv soon: Papadopoulos, Porter, Daniels, Bassett

measures exist at the particle or chain or network scale

open question: which are useful?

nodes:

node degree: $k_i = \sum_{j=1}^{N} A_{ij}$ local

($= z$ in jamming terms)

(global) $\langle k \rangle = \frac{1}{N} \sum_i k_i = \langle z \rangle$

node strength: $\sigma_i = \sum_{j=1}^{N} W_{ij}$

clustering: $\frac{\#\text{ of closed triangles}}{\#\text{ of connected triplets of vertices}}$ = 3 nodes + 2 edges

paths: d_{ij} = shortest # of hops between two nodes
(also can be weighted: least total)

network efficiency

$$E = \frac{1}{N(N-1)} \sum_{i \neq j} \frac{1}{d_{ij}}$$

Centrality: how many paths go through a particular node?

(ie a major intersection in transport)

Closeness centrality: $H_i = \frac{N-1}{\sum_{i \neq j} d_{ij}}$

betweenness centrality:

$$B_i = \sum_{j \neq m} \frac{\psi_{jm}(i)}{\psi_{jm}} \qquad i \neq j \neq m$$

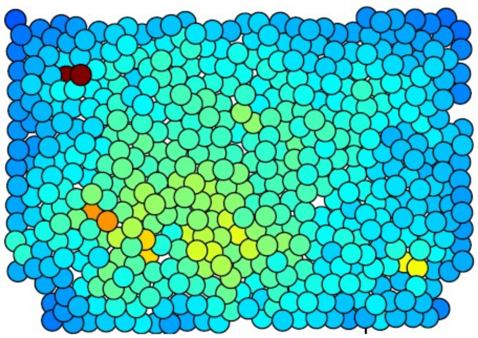
numerator: # of paths that go through i

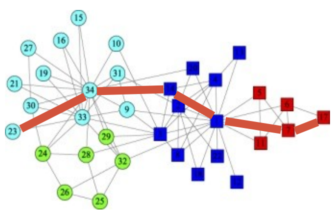
denominator: # of paths that don't

Network science metrics for different scales

http://netwiki.amath.unc.edu/

System

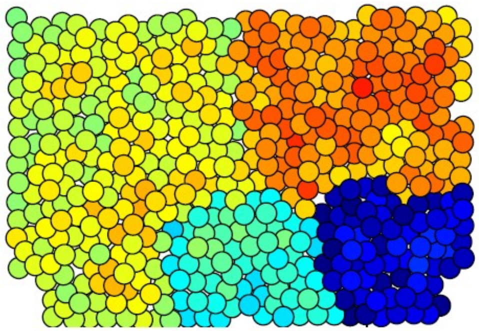


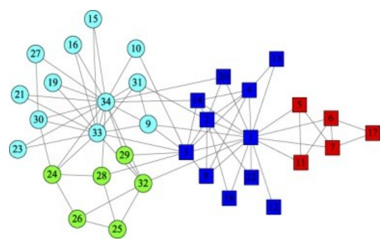


Global Efficiency

- Efficiency of global signal transmission

2D Domain

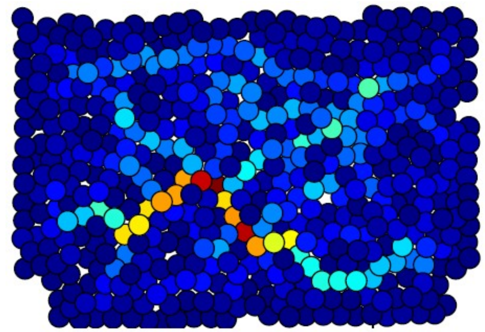


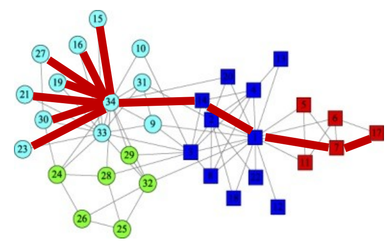


Modularity

- Local geographic domains

1D Curves

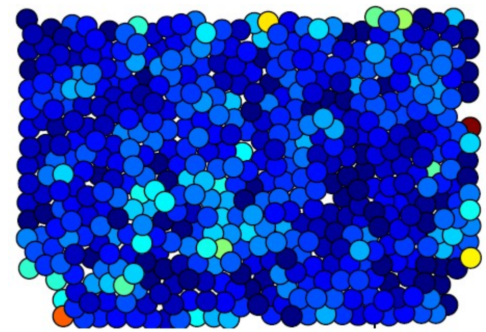


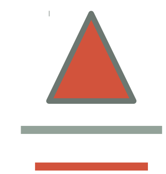


Geodesic Node Betweenness

- Bottlenecks or centrality

0D Particles





Clustering Coefficient

- Local loop structures

Bassett, Owens, Daniels, Porter. *PRE* (2012)

Force Network Ensemble

for any given packing (network of nodes + edges)

↓

many possible valid solutions for forces (edge weights)

friction: ① provides history-dependence
② changes the counting of valid states

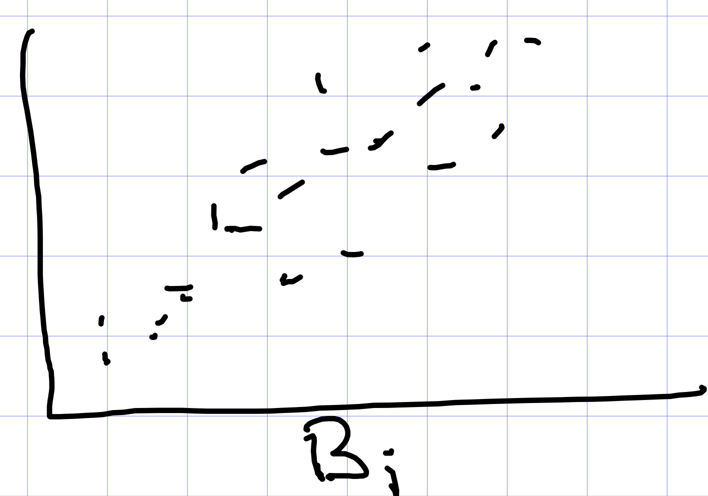
revisit ensemble of valid networks movie

→ why is the graph in the lower right "popular"?

betweenness centrality!

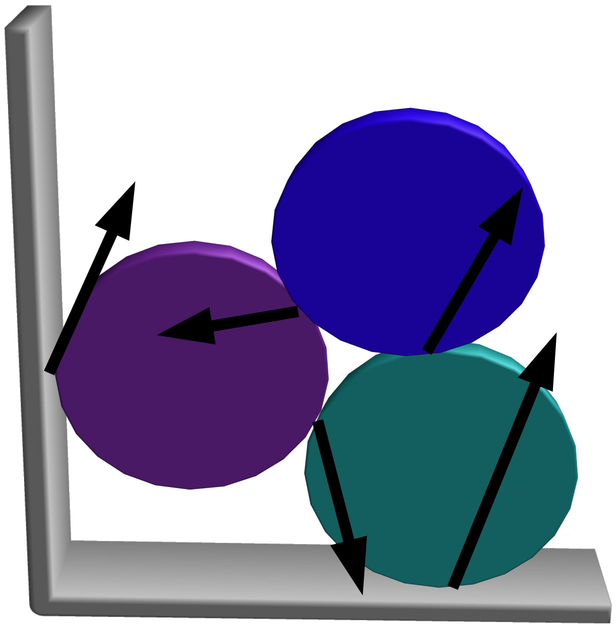
importance

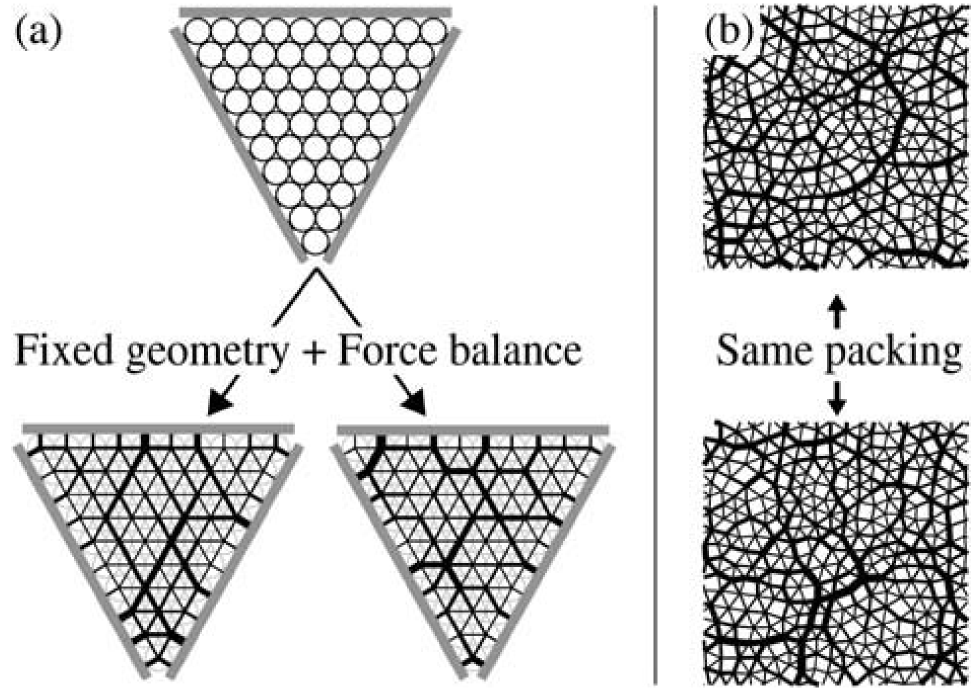
$\sigma_i (1 - std(\sigma_i))$



lots of paths = important

Force Network Ensemble



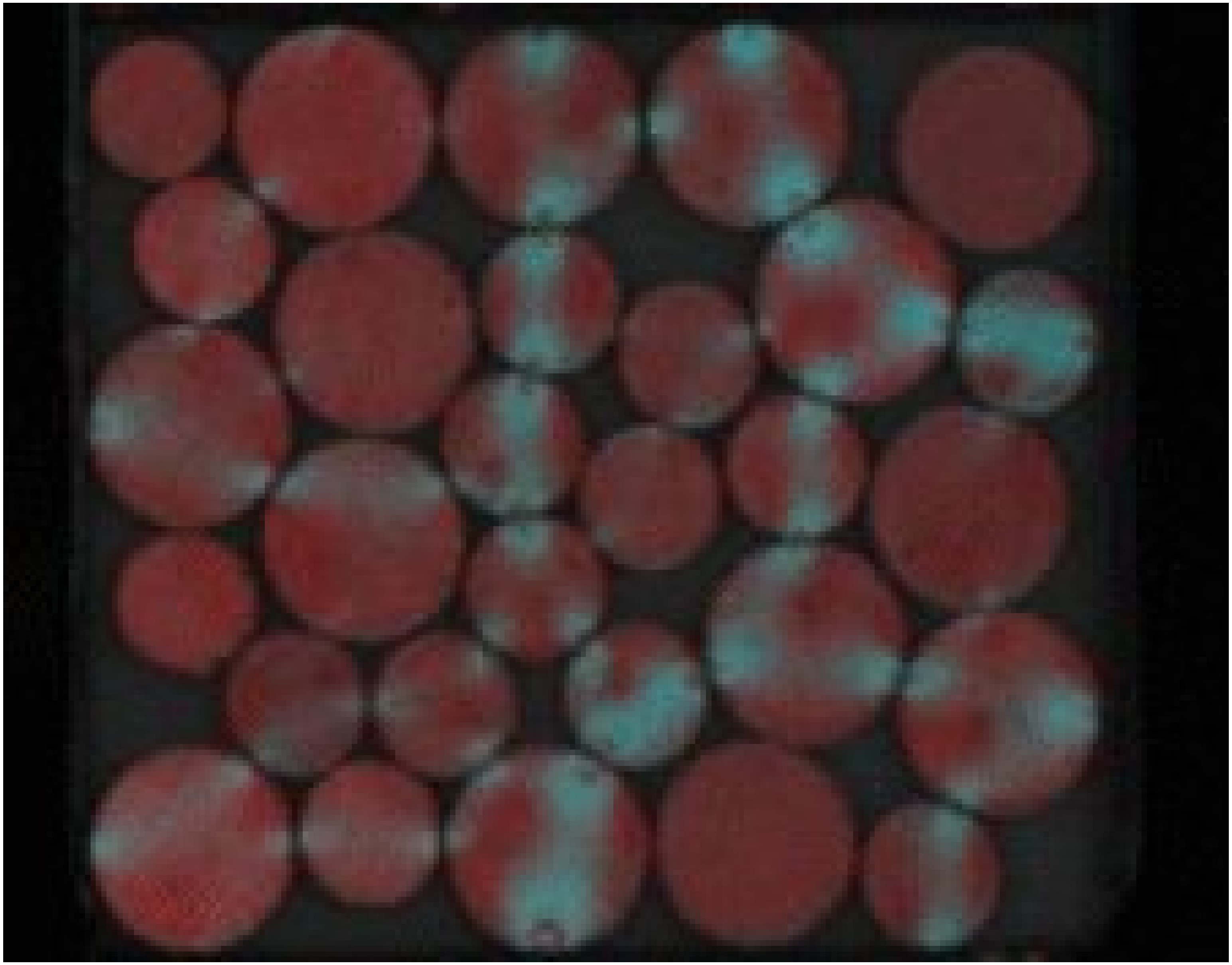


Tighe, Snoeijer, Vlugt, van Hecke.
Soft Matter (2010)

- count equations & constraints → # of degrees of freedom
- friction – provides history-dependence

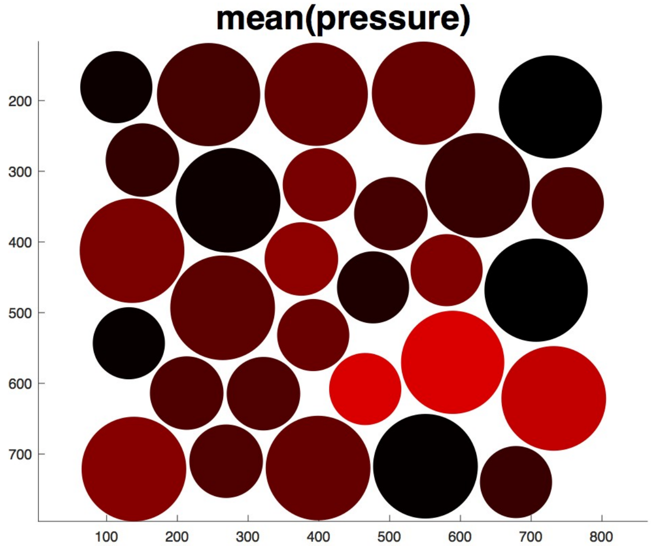
  – changes the counting of valid states

Experiment Version of FNE

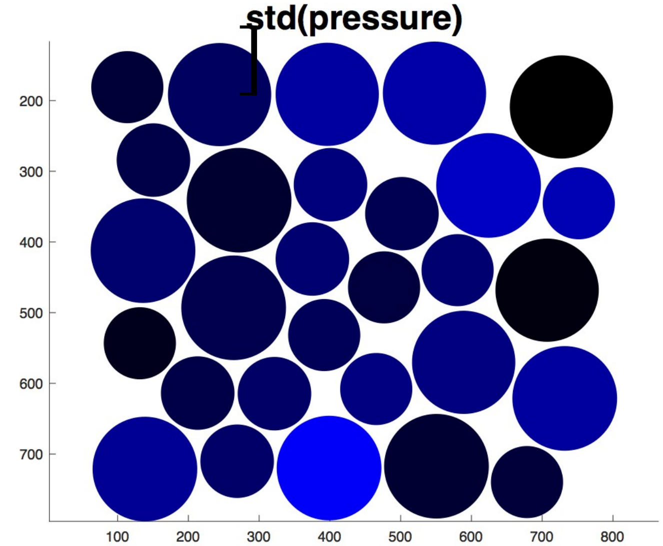


Kollmer & Daniels, *Powders & Grains 2017*

σ_i

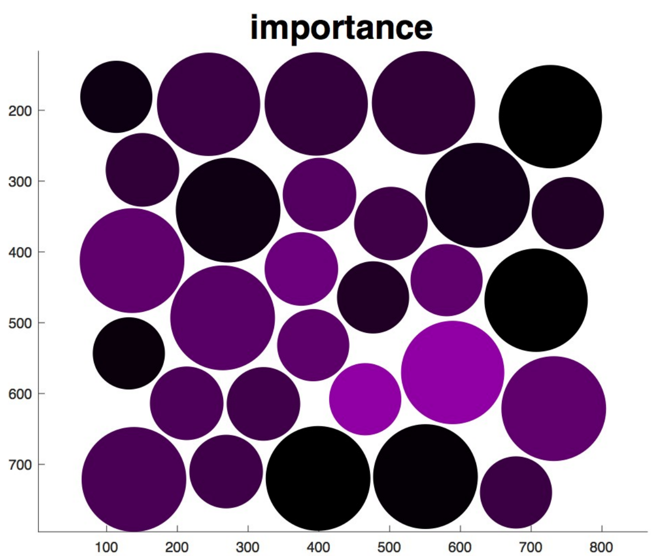


$\text{std}[\sigma_i]$

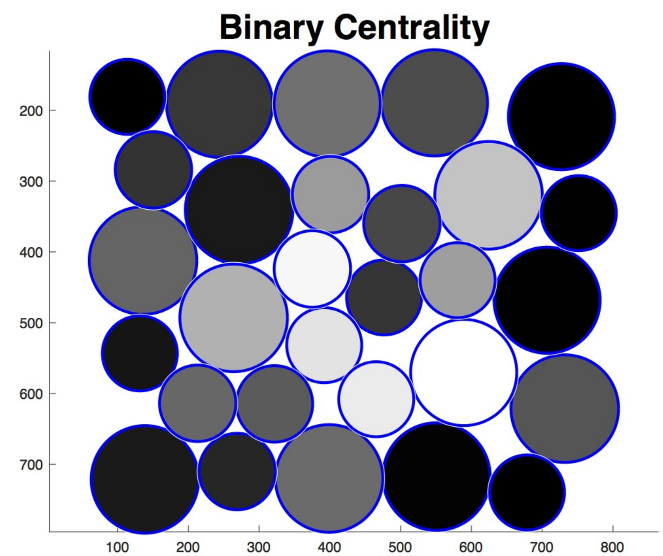


Jonathan Kollmer

$\sigma_i\,(1-\text{std}[\sigma_i])$



B_i



Communities: particles that are more strongly connected to others in their community than to those outside

many highly-weighted edges within communities vs. weaker edges between communities

optimize assignment to communities by maximizing Q (quality) = modularity

$$Q = \sum_{i,j} (w_{ij} - \gamma P_{ij}) \, \delta(g_i, g_j)$$

- w_{ij} ↑ weighted adjacency
- γ ↑ resolution parameter (knob for more/less communities)
- P_{ij} ↑ null model
- δ ↑ (Dirac) if i & j are in same community

(Louvain)

heuristic algorithm to optimize assignments
- agglomerate nodes that would increase Q
- need to run multiple times

our early work: Newman-Girvan null model (any particle can be connected to any other particle)

"overly null"

looses the character of the packing (show choice of null model matters: compare to all contacts having average force

$$P_{ij} = \langle s_i \rangle A_{ij} \qquad \text{(show)}$$

show examples

need to choose the resolution parameter

$\gamma = 1$ = divide ≈ at mean force

<u>not</u> an absolute thresholding at the mean value

larger γ → smaller communities

smaller γ → larger communities

our choice of γ has been guided by either

$$\text{gap factor} = \frac{\text{hop distance}}{\text{physical distance}}$$

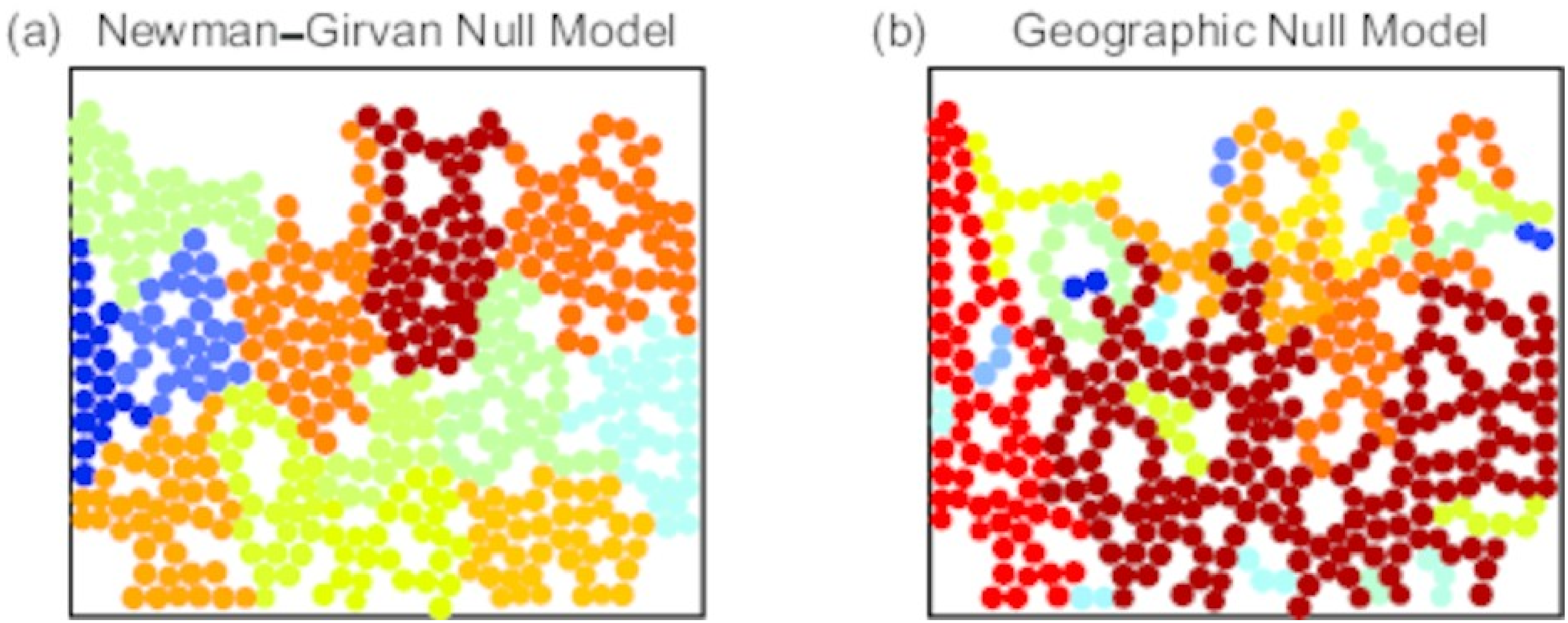
bigger = more branched-chain-like

$$\text{hull ratio} = \frac{\text{volume of particles}}{\text{volume of convex hull}}$$

smaller → more branched-chain-like

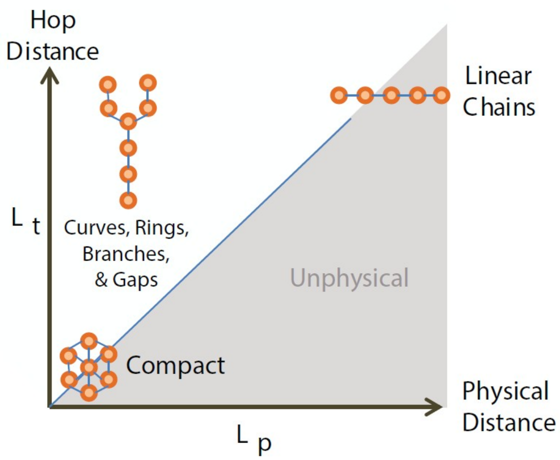
either one gives a value $\gamma \sim 1$

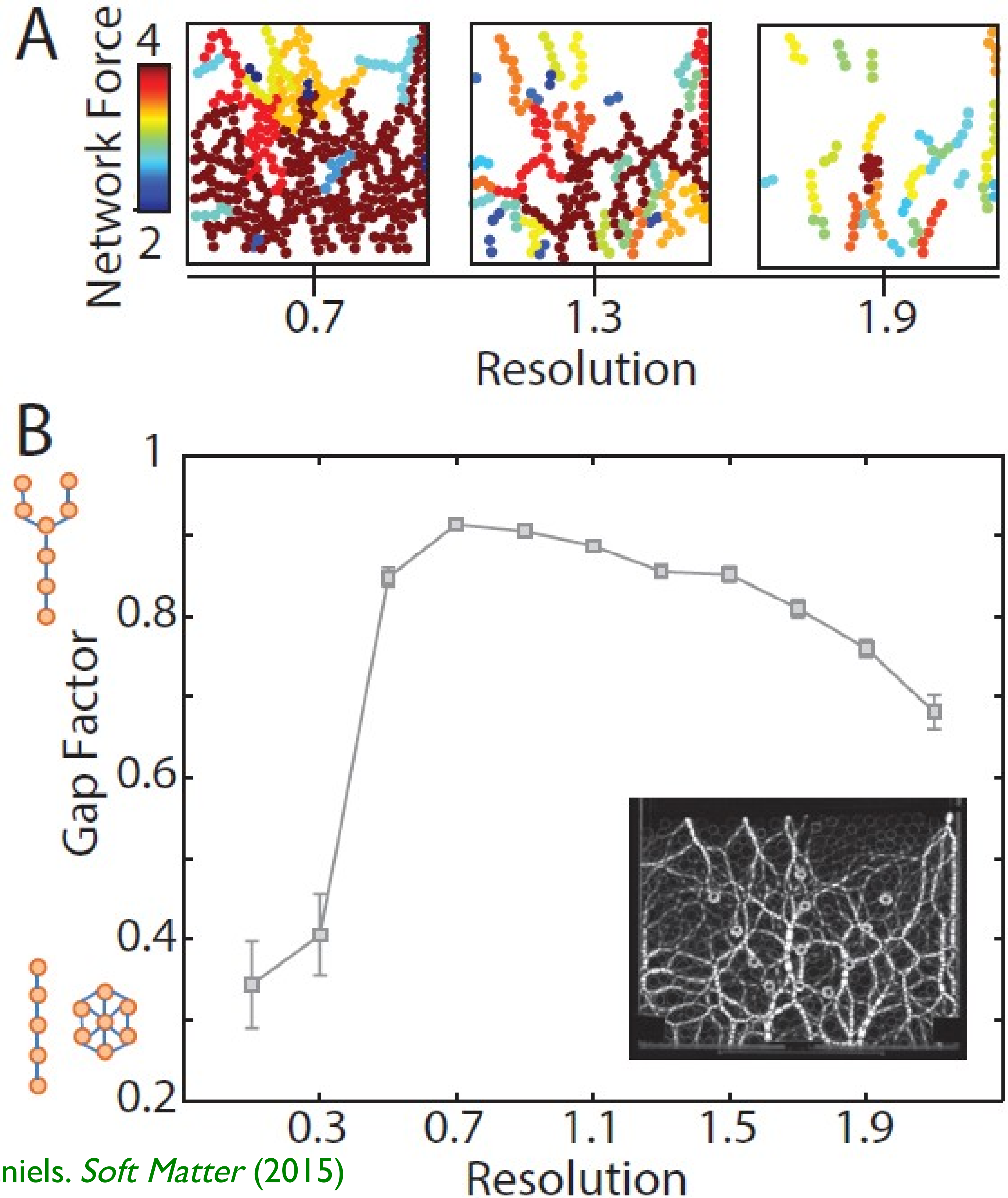
Null Model Matters



Bassett, Owens, Porter, Manning, Daniels. *Soft Matter* (2015)

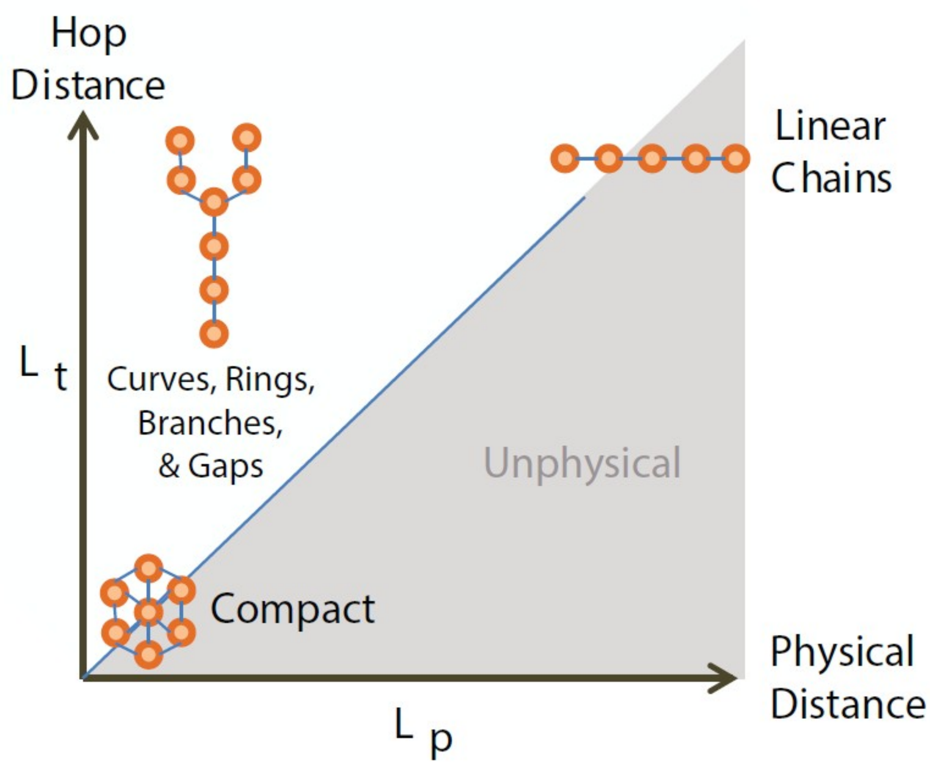
Effect of Resolution Parameter γ





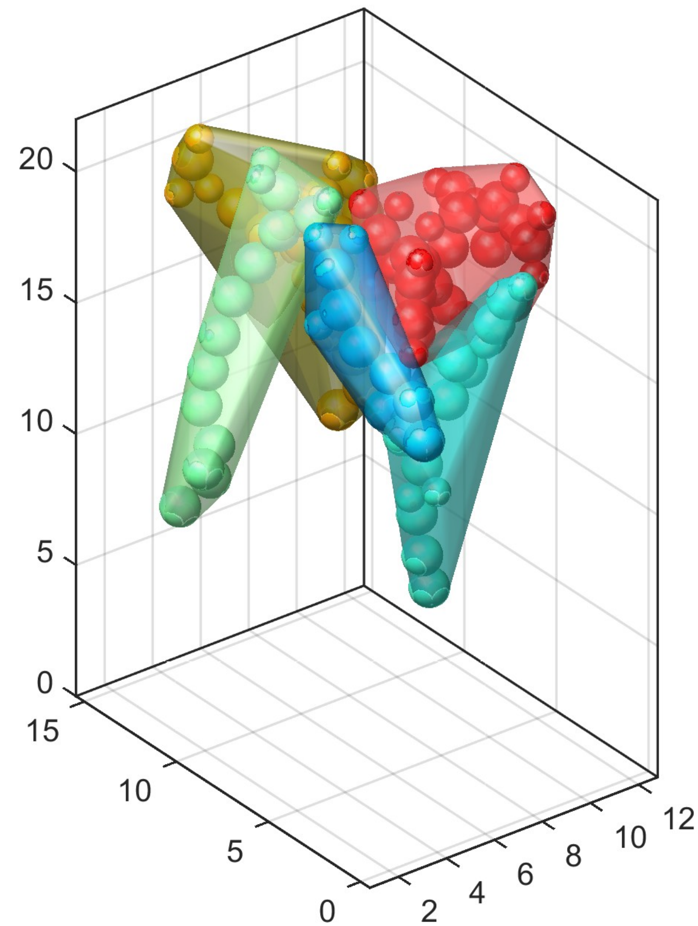
Bassett, Owens, Porter, Manning, Daniels. *Soft Matter* (2015)

Gap Factor



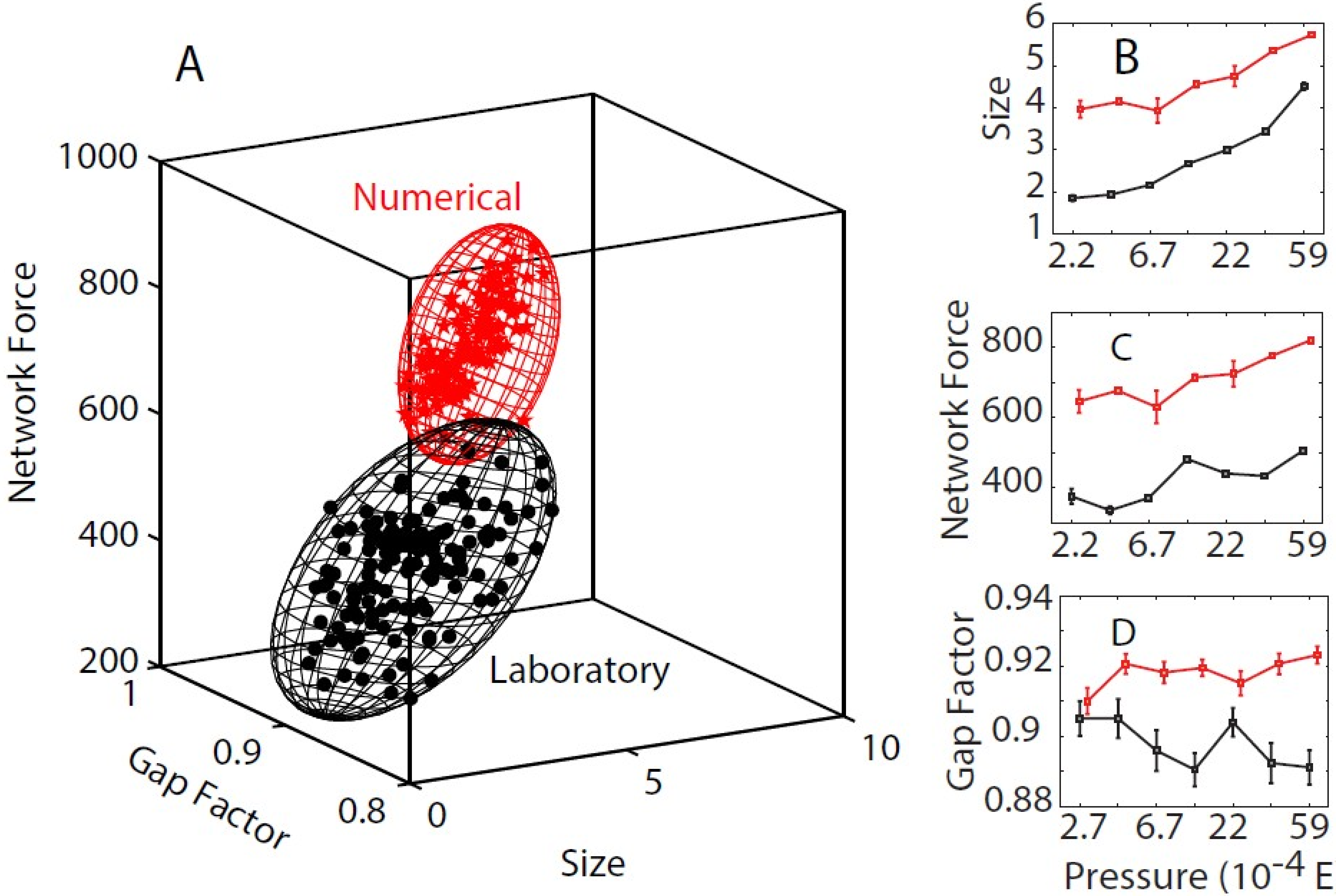
Bassett, Owens, Porter, Manning, Daniels. *Soft Matter* (2015)

Hull Ratio



Huang & Daniels. *Granular Matter.* (2015)

Network Measures Distinguish Exp/Sim



Bassett, Owens, Porter, Manning, Daniels. *Soft Matter* (2015)

multilayer communities - link across time or strain

coupling parameter ω (similar to γ)
temporal resolution parameter

$\omega = 0$ completely decoupled layers
↓
increase to couple the layers
↓ "diagonal edges" to distinguish the ones inside each layer

need to start from particle-tracked data in order to know the diagonal edges

$$Q_{multi} = \sum_{ijlm} \left[(W_{ijl} - \gamma P_{ijl}) \delta_{lm} + \omega \, \delta_{ij} \right] \delta(g_{il}, g_{jm})$$

$ijlm$ — edge layers

δ_{lm} ↑ same layer

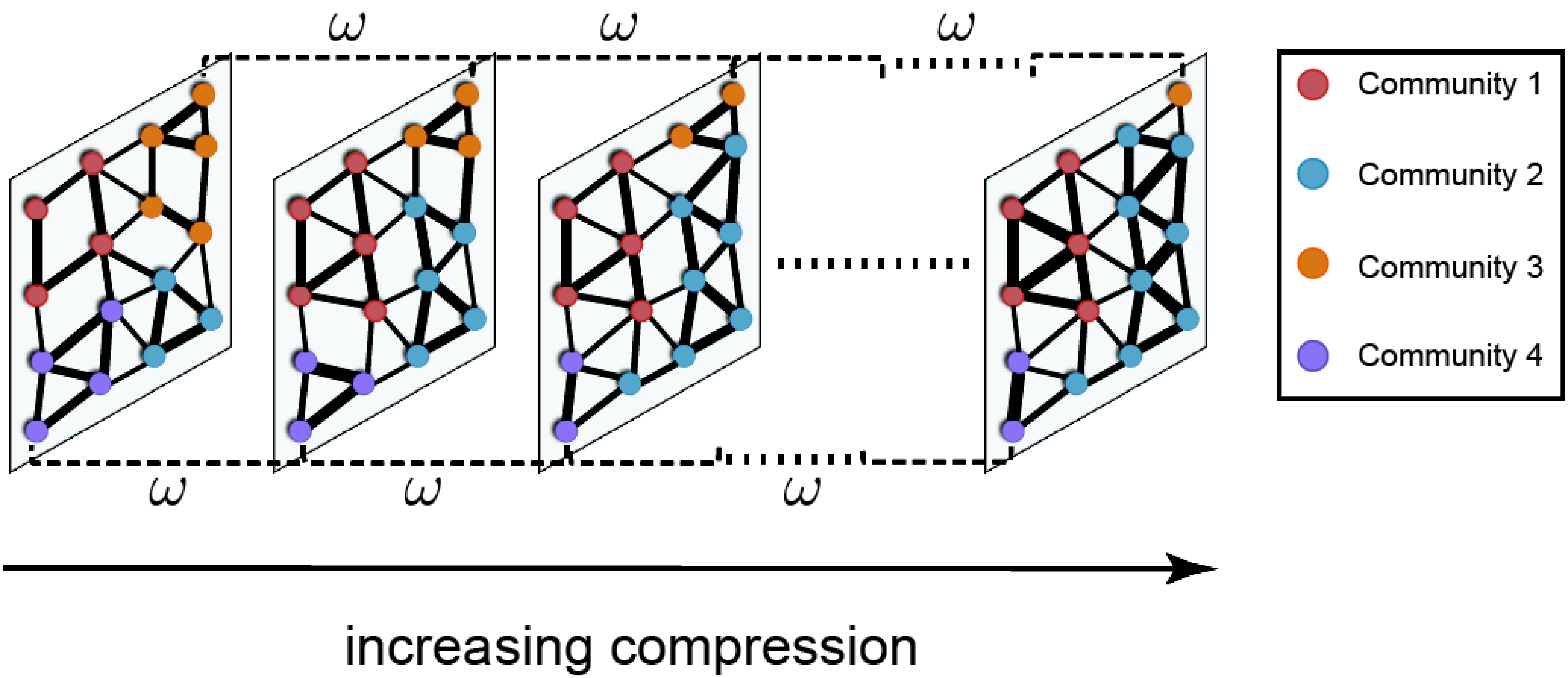
δ_{ij} ↑ same particle

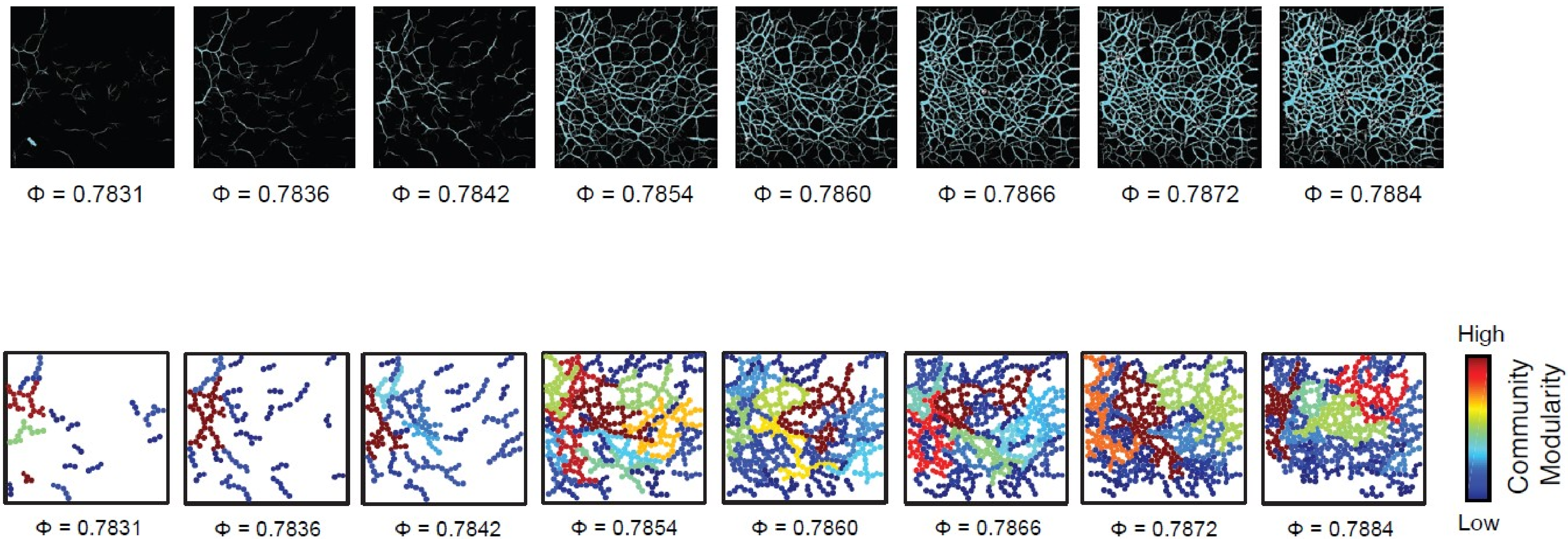
$\delta(g_{il}, g_{jm})$ — community assignments

γ can be layer-dependent

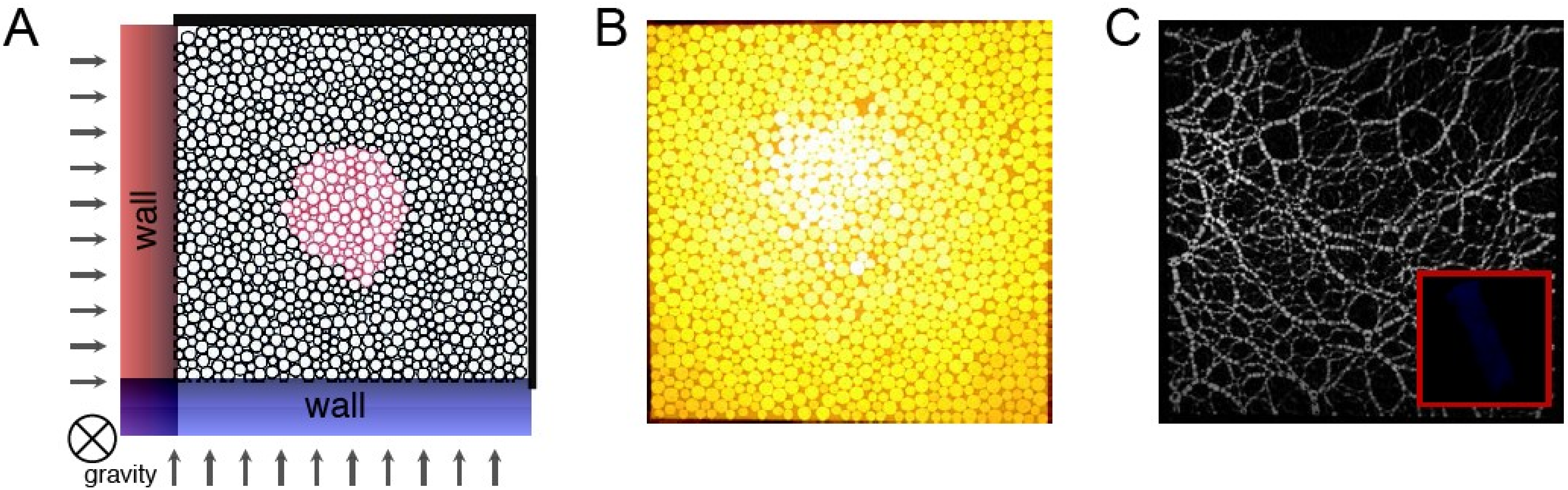
ω can be particle (node)-dependent

Multilayer Networks

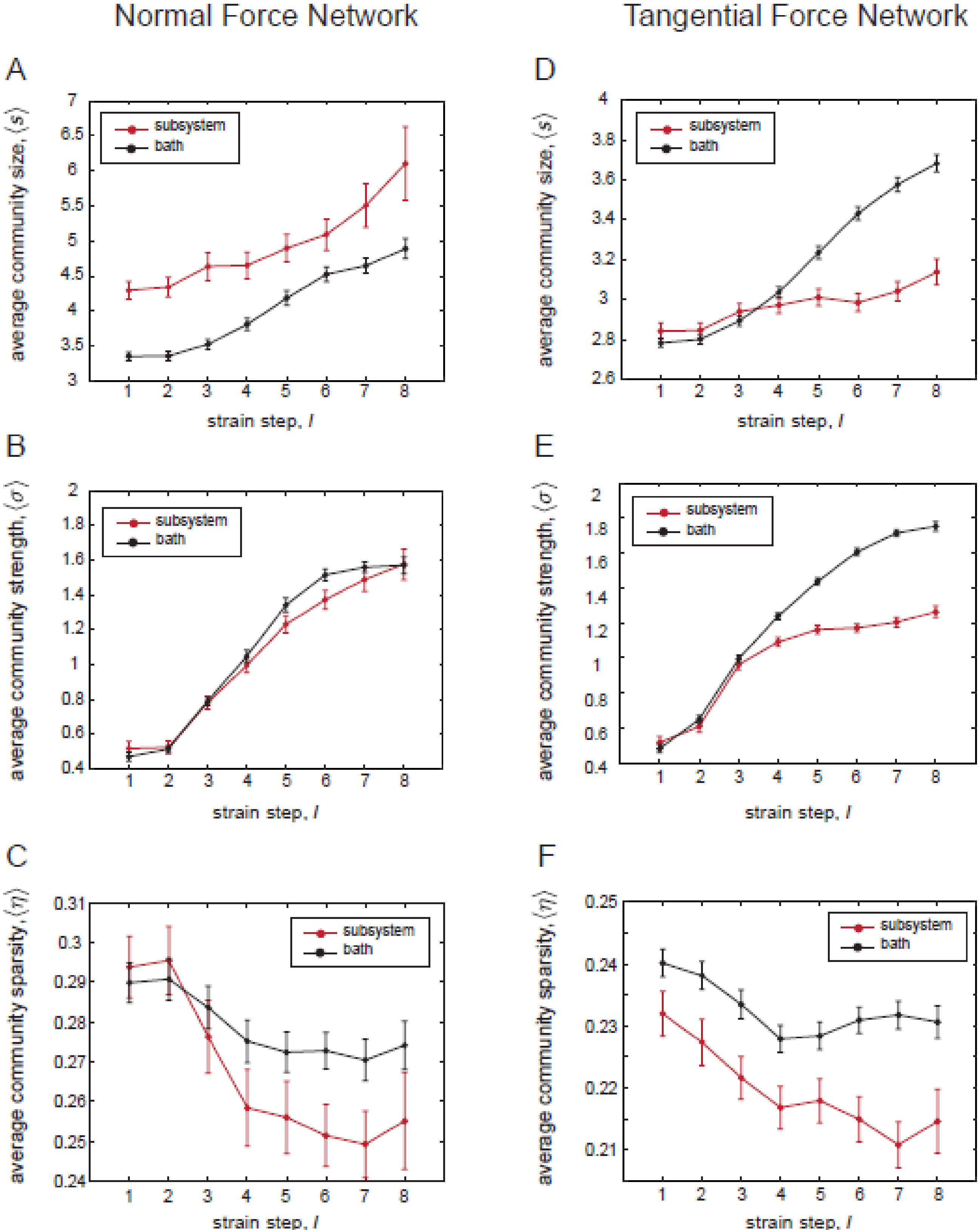



Φ = 0.7831
Φ = 0.7836
Φ = 0.7842
Φ = 0.7854
Φ = 0.7860
Φ = 0.7866
Φ = 0.7872
Φ = 0.7884
Φ = 0.7831
Φ = 0.7836
Φ = 0.7842
Φ = 0.7854
Φ = 0.7860
Φ = 0.7866
Φ = 0.7872
Φ = 0.7884
High
Community Modularity
Low

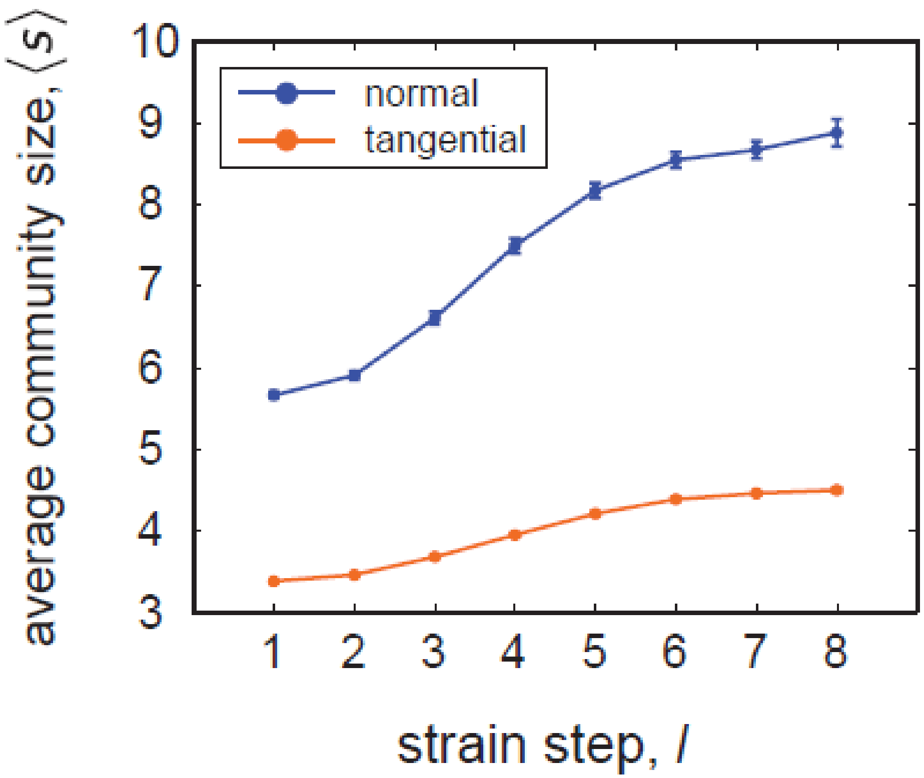
Black = Higher Friction Bath
Red = Lower Friction Subsystem

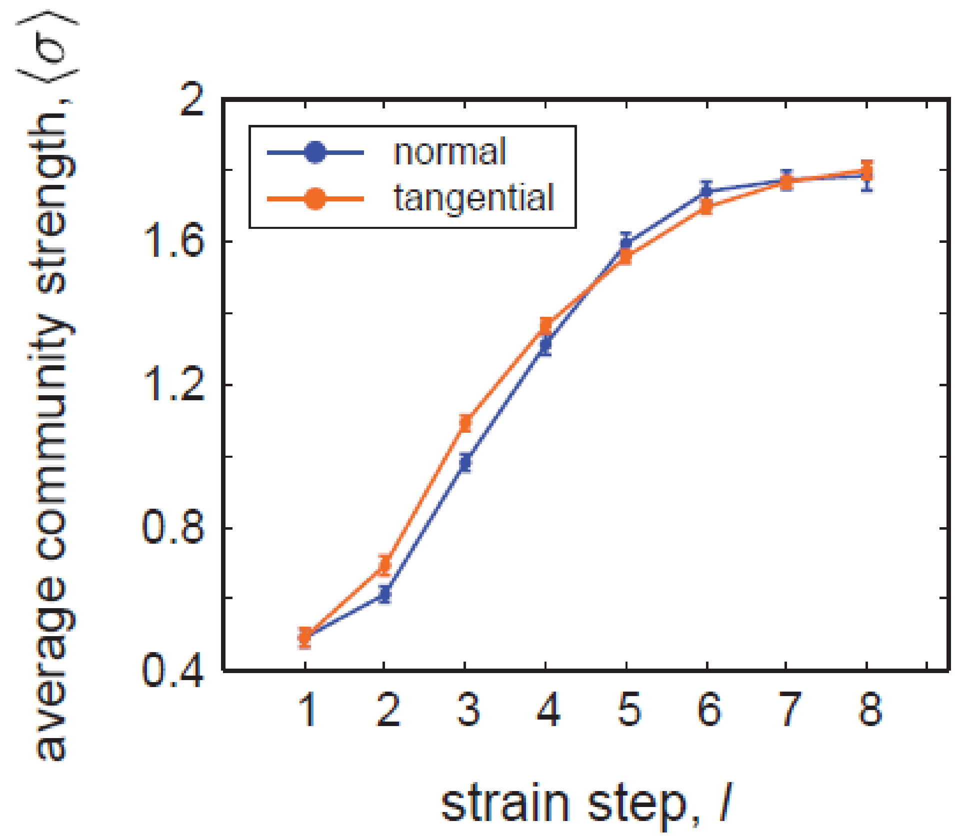


Puckett & Daniels PRL (2013)
Papadoploulos, Puckett, Daniels, Bassett. *PRE* (2016)



Papadopoulos, Puckett, Daniels, Bassett. *PRE* (2016)





Papadoploulos, Puckett, Daniels, Bassett. *PRE* (2016)

Configurational Entropy & Statistical Ensembles

Physica A 157 (1989) 1080–1090
North-Holland, Amsterdam

Sam Edwards

THEORY OF POWDERS

S.F. EDWARDS and R.B.S. OAKESHOTT
Cavendish Laboratory, Madingley Road, Cambridge CB3 0HE, UK

Received 20 February 1989

“If a powder consists for example of uniform cubes of salt, and is poured into a container, falling at low density uniformly from a great height, one expects a salt powder of a certain density. Repeating the preparation reproduces the same density. A treatment such as shaking the powder by a definite routine produces a new density and the identical routine applied to another sample of the initial powder will result in the same final density. Clearly a Maxwell demon could arrange the little cubes of NaCl to make a material of different properties to that of our experiment, but if such demonics are ignored, and we restrict ourselves to extensive operations such as stirring, shaking, compressing – all actions which do not act on grains individually – then well defined states of the powder result.”

Why consider ensembles?

granular materials exhibit particle-scale property distributions that depend on only a few quantities (volume, stress)

ensemble of microstates → macroscopic variables

↓

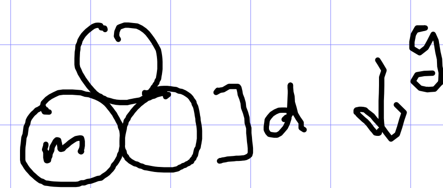
equation of state?

possible problems:

- generating ensembles ✓

  no temperature: need new methods

  $k_B T \sim 10^{-12}\, mgd$



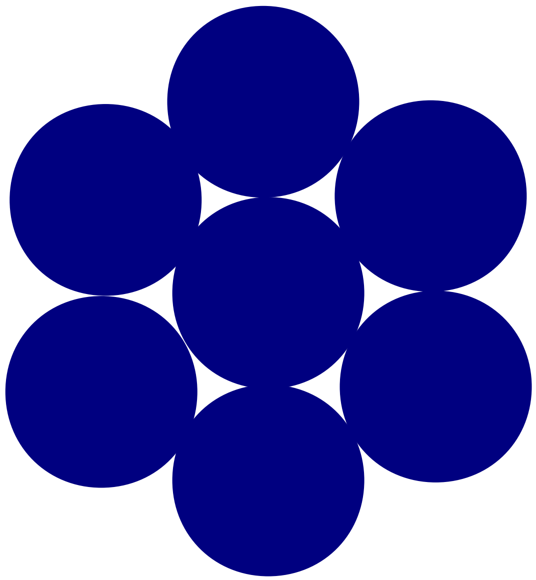
- identifying correct macroscopic variables
- dissipative, history-dependent
- poor separation of micro/macro scales (force chains = meso)

Edwards-like ensembles (show quote)

extension by analogy (show fig)

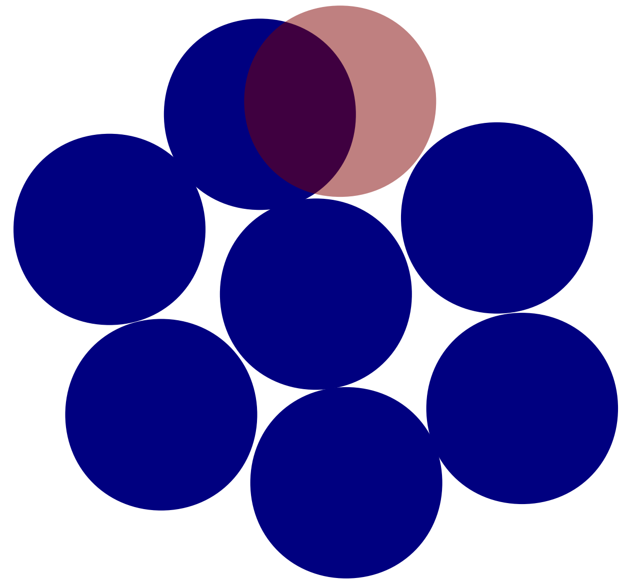
count valid configs:	$\Omega(E)$ subject to cons. of energy	$\Omega(V)$ jammed configs	$\Omega(\Sigma)$ jammed configs
entropy:	$S = k \ln \Omega$	$S = \ln \Omega$ configurational	$S = \ln \Omega$ configurational
equilibrates:	temperature $\frac{1}{T} = \frac{\partial S}{\partial E}$	compactivity $\frac{1}{X} = \frac{\partial S}{\partial V}$	angoricity $\alpha_{ij} = \frac{\partial S}{\partial \Sigma_{ij}}$ (tensor!)
	$T=0$ abs. zero	$X=0$ at ϕ_{RCP}	$\alpha_{ij}=0$ @ jamming
	low T: can't take out more E	low X: can't remove more volume	high α: can't relieve stress
	assumption: all valid configs equally likely	✓ confirmed by Frankel + Chakraborty (2017), but <u>only</u> at ϕ_J	??
	$e^{-E/kT}$	$e^{-V/X}$	$e^{-\alpha_{ij}\sigma_{ij}}$

Edwards' Central Idea



smallest system volume

only one valid configuration



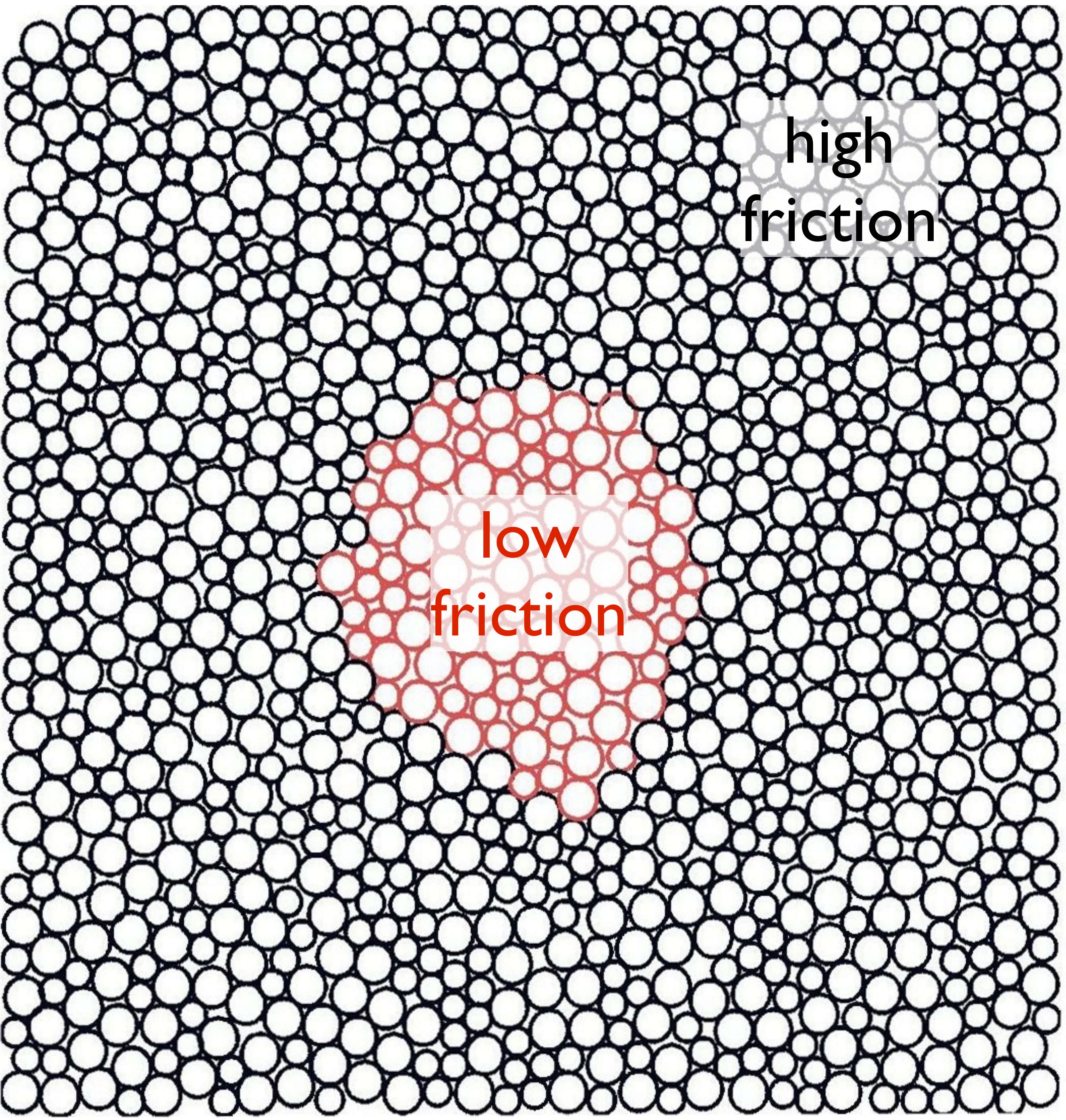
larger volume

more valid configurations

$$S = \ln \Omega(V)$$

$$\frac{1}{X} = \frac{\partial S}{\partial V}$$

Test the "Zeroth Law"



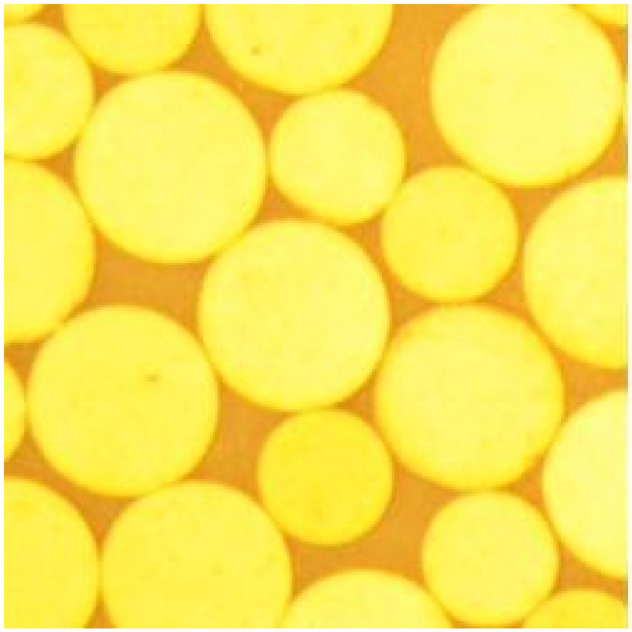
Zeroth law requires temperature equilibration

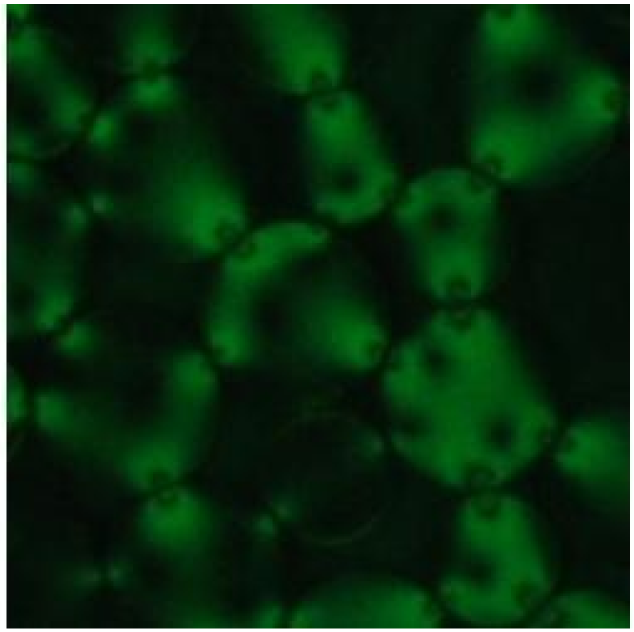
Does $X_{bath} = X_{subsys}$?

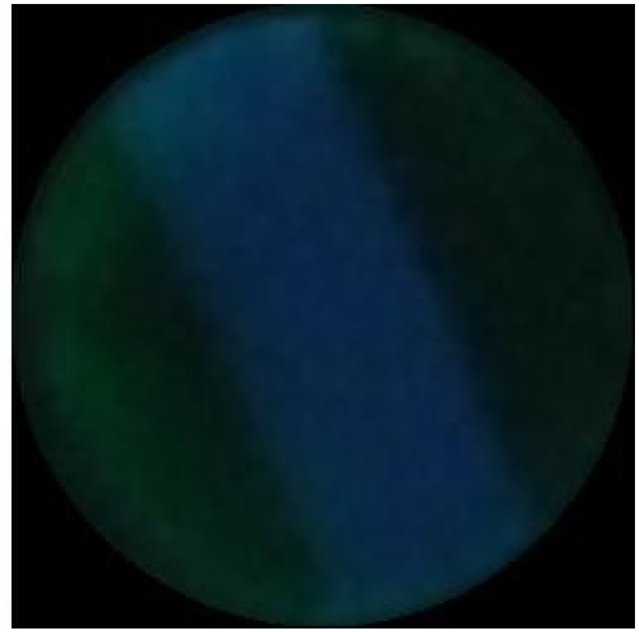
James Puckett

Puckett & Daniels. *PRL* (2013)

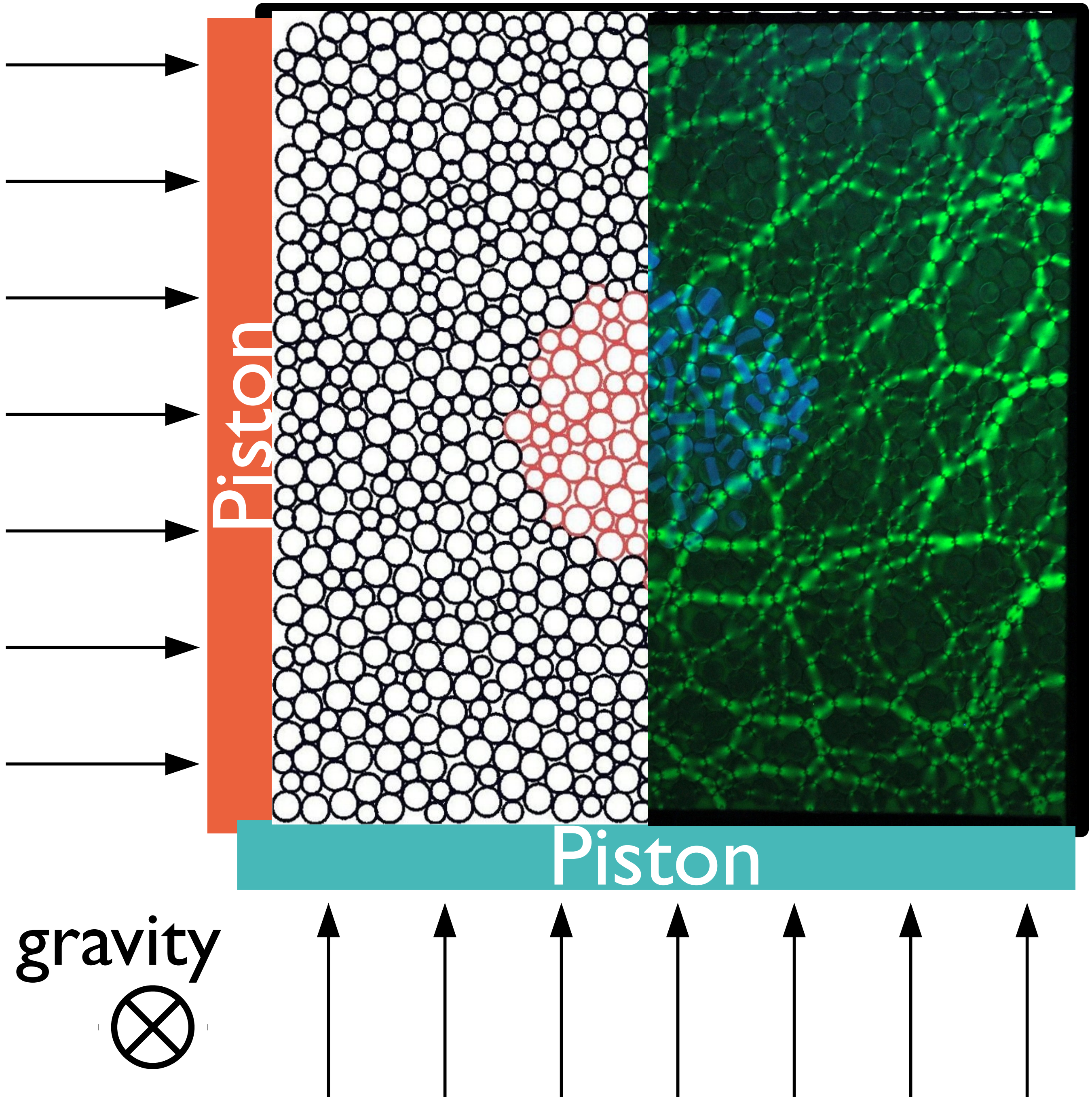
3 lighting schemes







white light	polarized light	fluorescence
$\Downarrow$	$\Downarrow$	$\Downarrow$
particle positions	contact forces	identify low-friction


Piston
Piston
gravity

Histograms are "thermometers"

(Dean + Lefevre 2003
McNamara et al PRE 2004)

Probability of observing a macroscopic volume V:

$$P(V) = \frac{\Omega(V)}{Z(X)} e^{-V/X}$$

$\Omega(V)$ ← multiplicity (not known, but independent of X)

X ← compactivity

$Z(X)$ ← partition function (not known)

ratio of two $P(V)$ gives relative compactivity

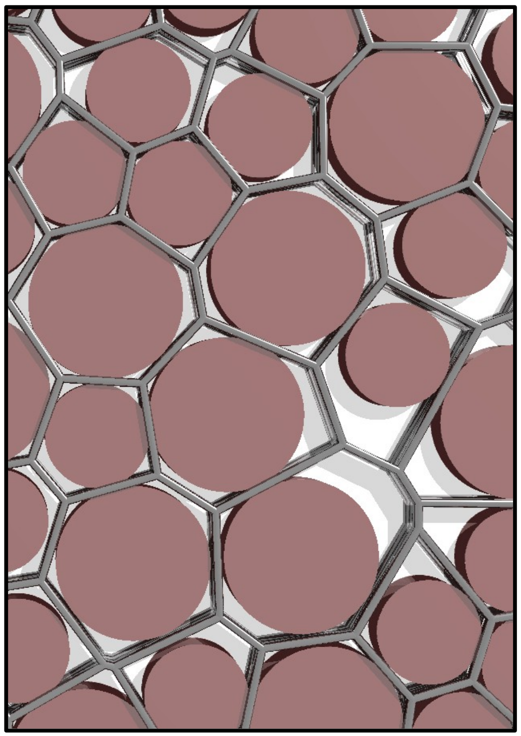
$$\mathcal{R} = \frac{P(V, \phi_1)}{P(V, \Phi_2)} = \frac{Z(X_2)}{Z(X_1)} e^{V\left(\frac{1}{X_2} - \frac{1}{X_1}\right)}$$

↑ experiments at two different Φ (global)

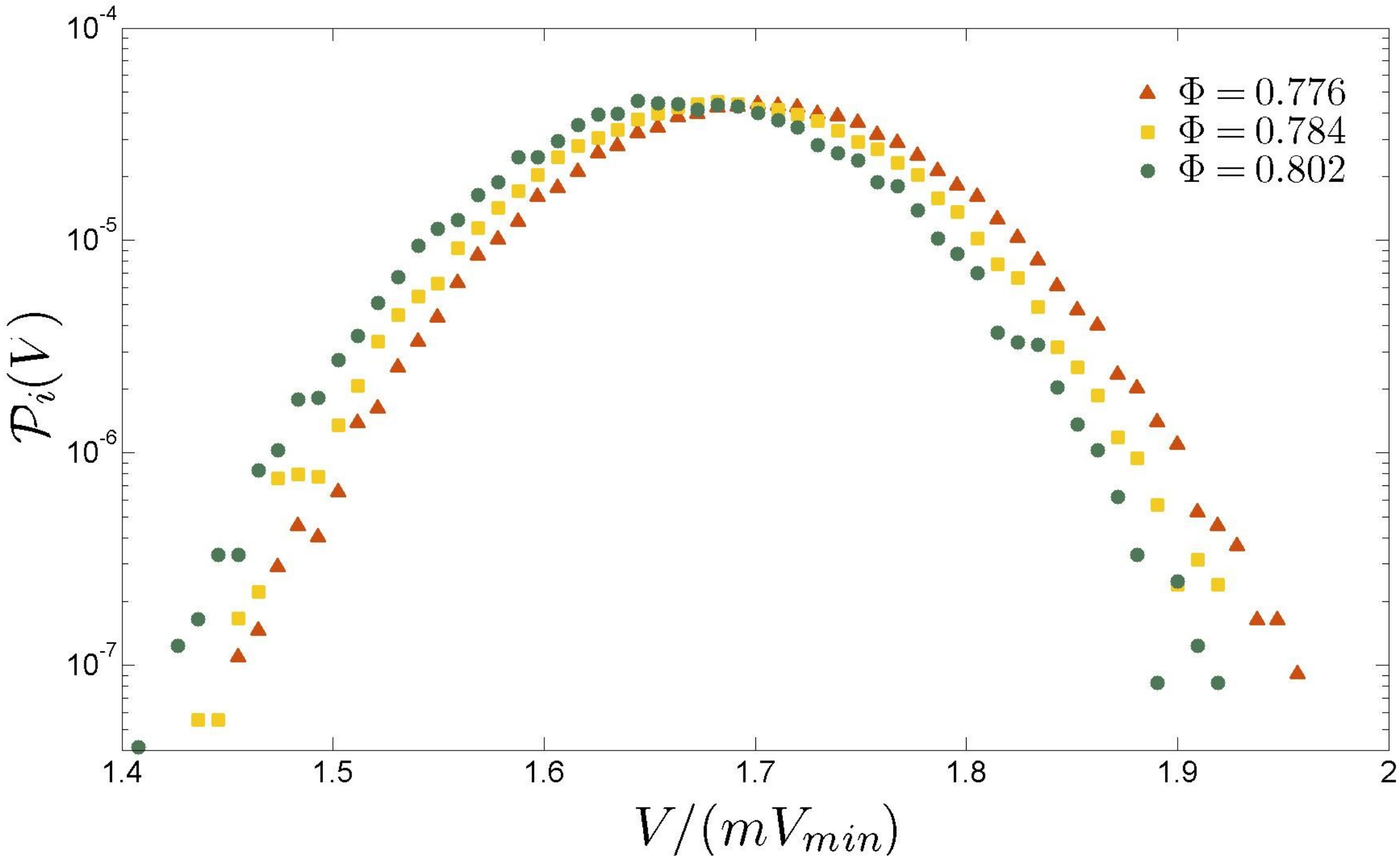
↑ relative

Local Voronoï Volumes

sample Voronoï tessellation



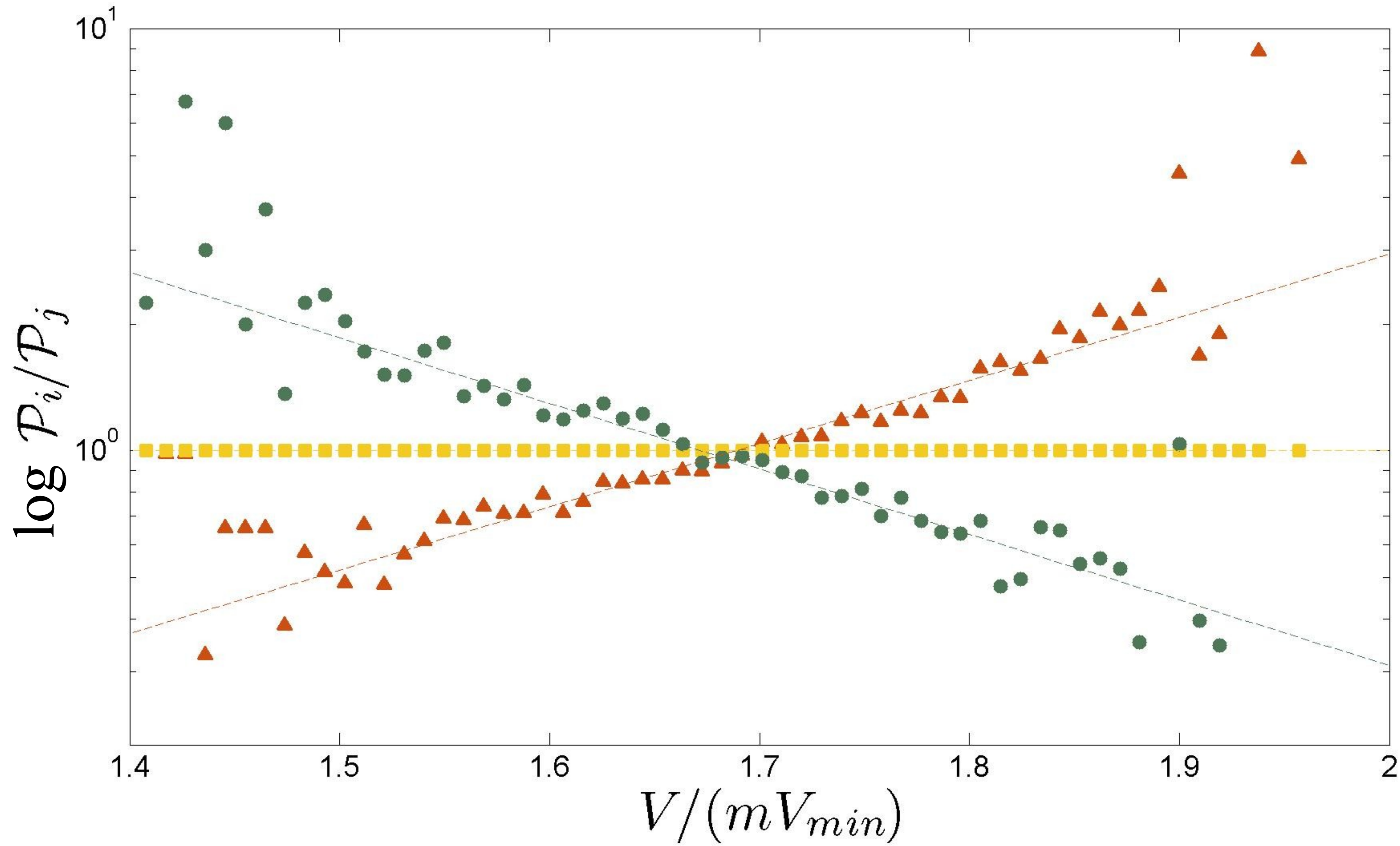
3 example histograms (for subsystem only)



Puckett & Daniels. *PRL* (2013)

Plot the Overlapping Histograms

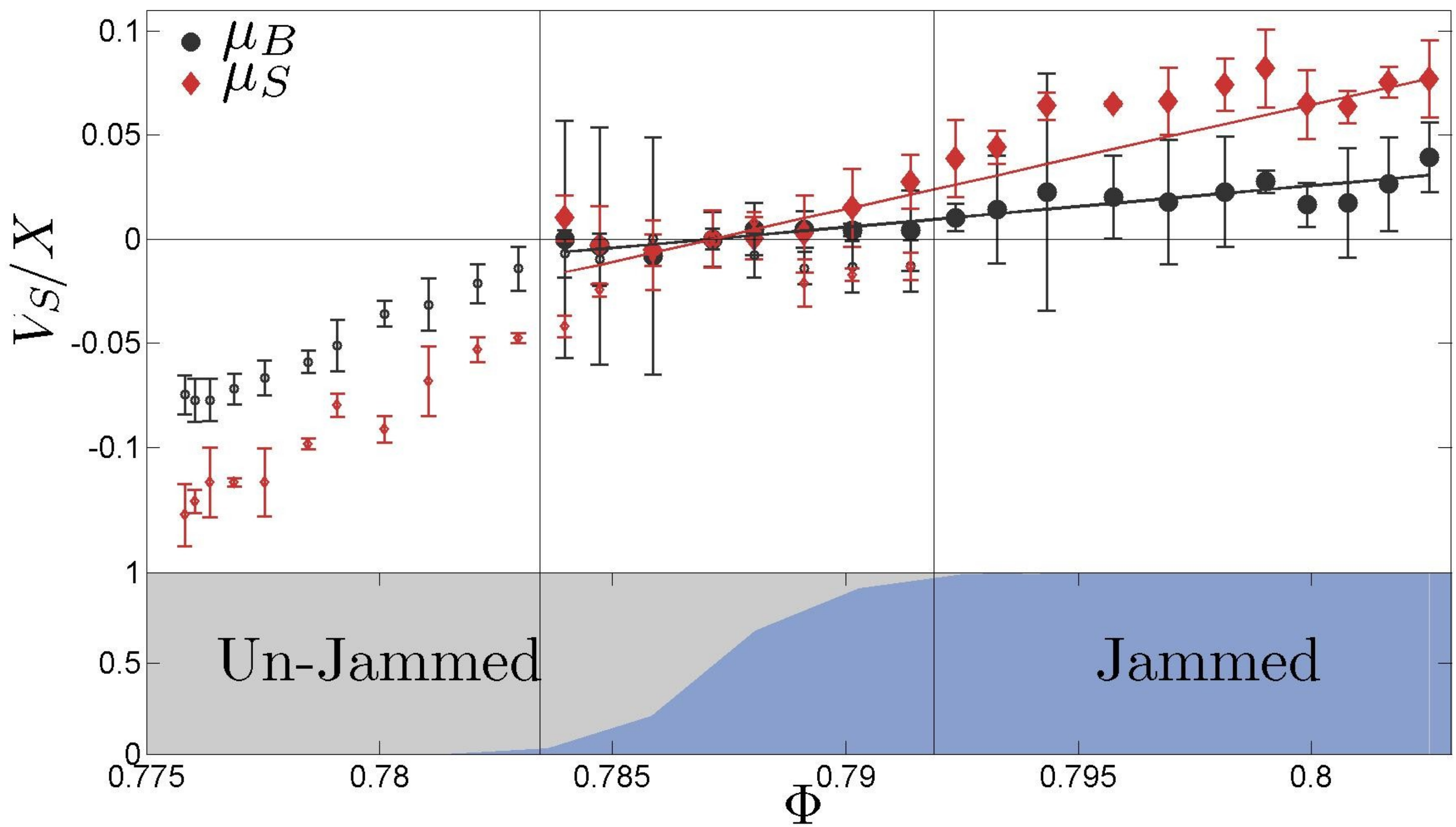
slope → difference in compactivity



Puckett & Daniels. *PRL* (2013)

Compactivity Fails to Equilibrate

red (low-friction system) and black (high-friction bath) do not have the same compactivity



Puckett & Daniels PRL 2013

Compactivity Fails to Equilibrate

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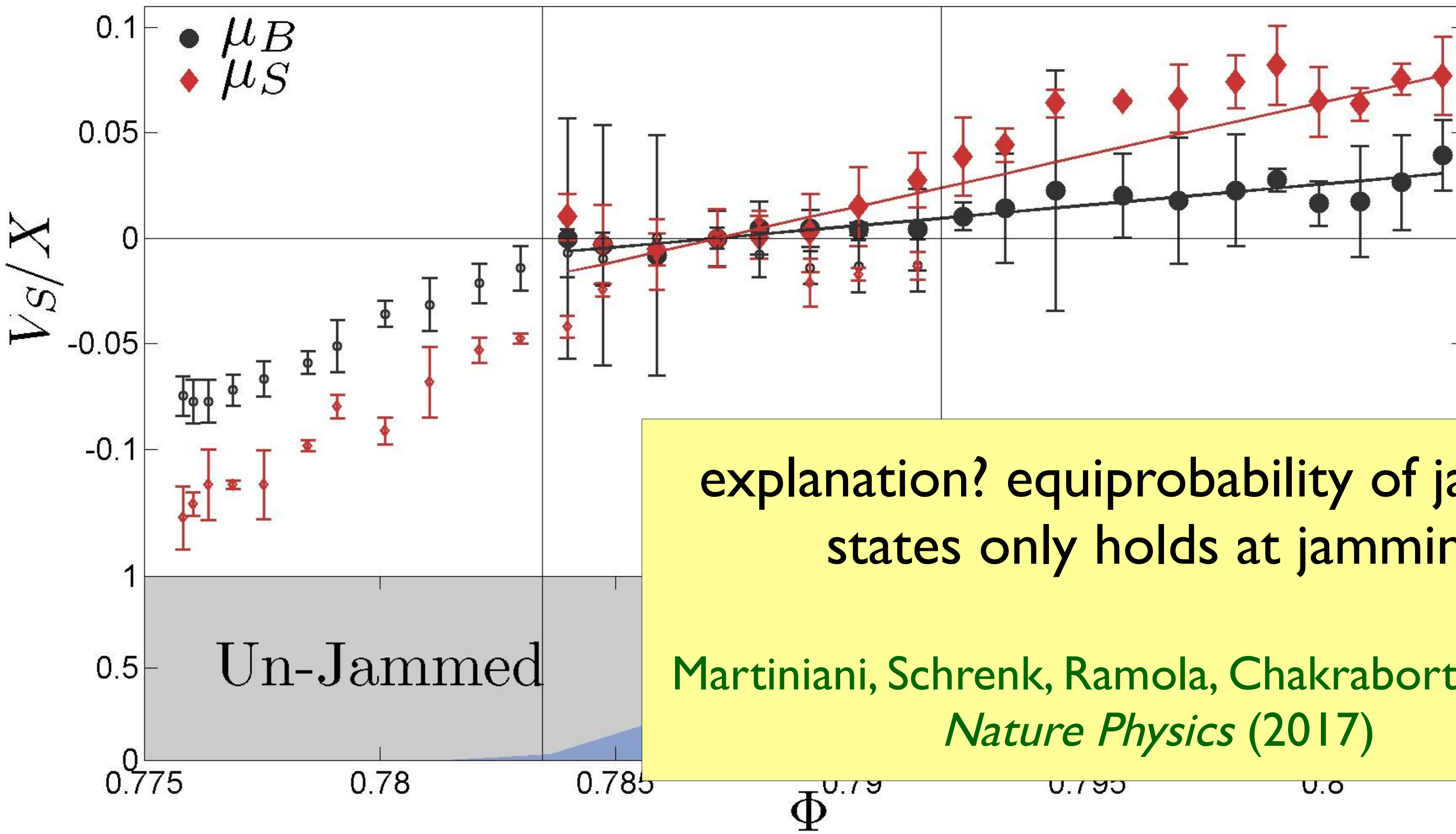


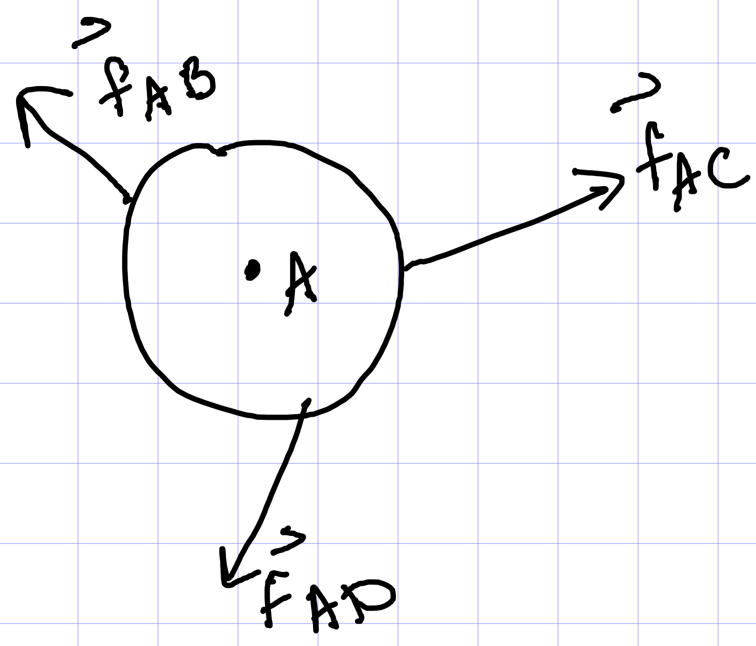
explanation? equiprobability of jammed states only holds at jamming

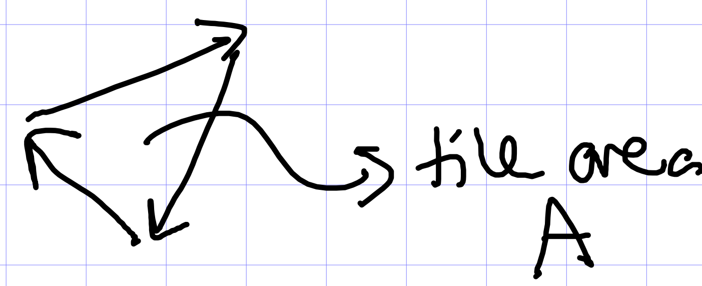
Martiniani, Schrenk, Ramola, Chakraborty, Frenkel. *Nature Physics* (2017)

Puckett & Daniels PRL 2013

Force-Moment Ensemble

(Bi, Daniels, Henkes, Chakraborty 2015)





$$\vec{r}_{AB} = \vec{r}_A - \vec{r}_B$$

3 constraints on possible values of $\{\vec{r}\}, \{\vec{f}\}$

① $\displaystyle\sum_{i=1}^{z} \vec{f}_{Ai} = 0$ force balance

② $\displaystyle\sum_{i=1}^{z} \vec{r}_{iA} \times \vec{f}_{iA} = 0$ torque balance

③ area of tiles conserved (Maxwell-Cremona)

Direct Product: $\vec{A}\,\vec{B} = \begin{pmatrix} A_x \\ A_y \\ A_z \end{pmatrix} \begin{pmatrix} B_x & B_y & B_z \end{pmatrix}$

$$= \begin{pmatrix} A_x B_x & A_x B_y & A_x B_z \\ A_y B_x & A_y B_y & A_y B_z \\ A_z B_x & A_z B_y & A_z B_z \end{pmatrix}$$

Force-Moment tensor.

$$\hat{\Sigma} = \sum_{m,n} \vec{r}_{mn} \vec{f}_{mn}$$

$$\hat{\sigma} = \sum_{cluster} \hat{\Sigma} \quad \text{(we'll use 8 grains)}$$

eigenvalues σ_1 + σ_2

Pressure: $\Gamma = Tr\ \hat{\sigma}$

Normal Stress = $\frac{1}{2}(\sigma_1 + \sigma_2)$

Deviatoric Stress = $\frac{1}{2}(\sigma_1 - \sigma_2)$

Histograms are "thermometers" (same as before)

Probability of observing a macroscopic stress state σ:

multiplicity (not known, but independent of α)

$$P(\sigma) = \frac{\Omega(\sigma)}{Z(\sigma)} e^{-\alpha \sigma}$$

angoricity (α)

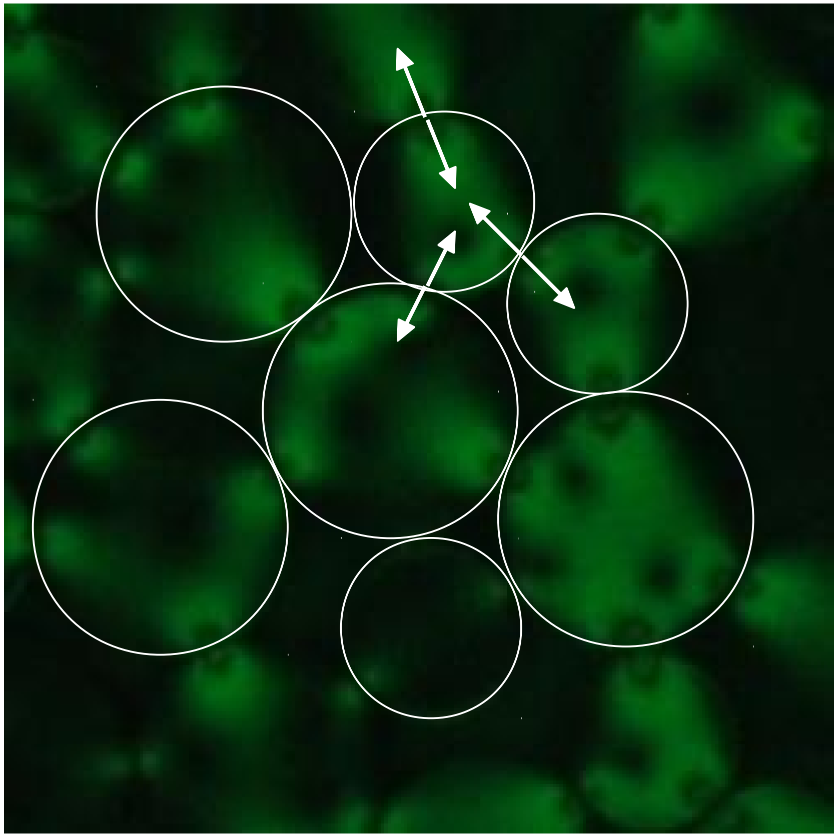
partition function (not known) (Z)

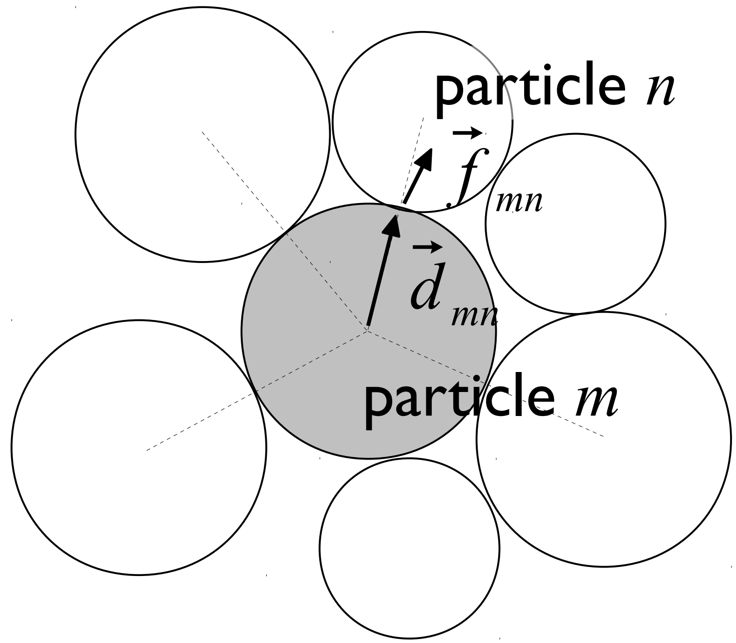
$\sigma = p$ or τ $\qquad$ α = associated angoricity

ratio of two $P(\sigma)$ gives relative angoricity

$$R = \frac{P(\sigma | \Gamma_i)}{P(\sigma | \Gamma_j)} = \frac{Z(\alpha_j)}{Z(\alpha_i)} e^{\sigma(\alpha_j - \alpha_i)}$$

Quantifying Interparticle Forces





Bi, Henkes, Daniels, Chakraborty.
Ann. Rev. Cond. Matt. (2015)

force-moment tensor

$$\hat{\Sigma} = \sum_{m,n} \vec{d}_{mn} \vec{f}_{mn}$$

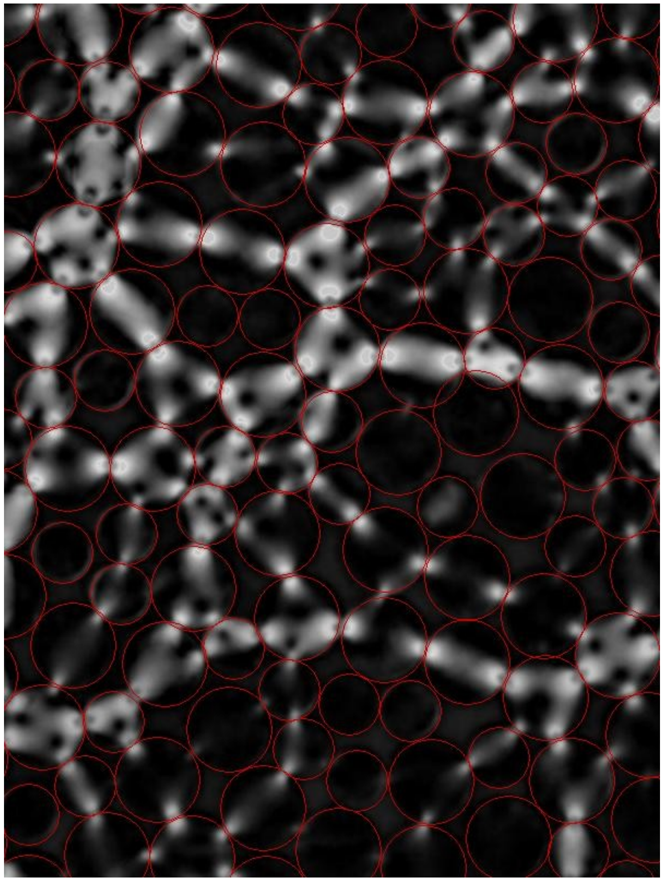
stress tensor

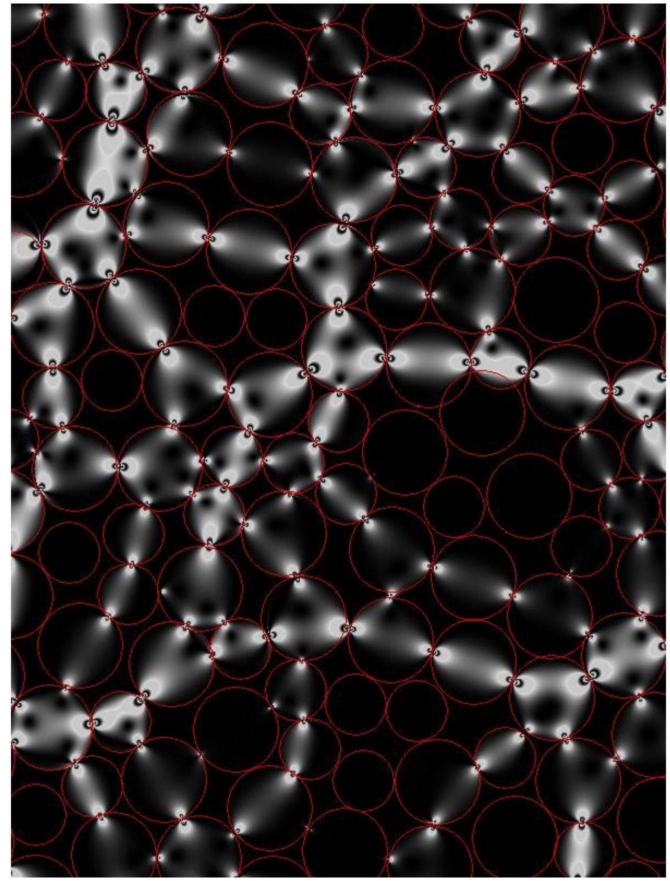
$$\hat{\Sigma} = V\,\hat{\sigma}$$

pressure

$$\Gamma = Tr\,\hat{\Sigma}$$

Photo → Vector Forces → Pseudo-photo





Daniels, Puckett, Kollmer. *Rev. Sci. Inst* (2017)   http://github.com/jekollmer/PEGS

grain scale force-moment tensor:

$$\hat{\Sigma} = \sum_{m,n} \vec{d}_{mn} \vec{f}_{mn}$$

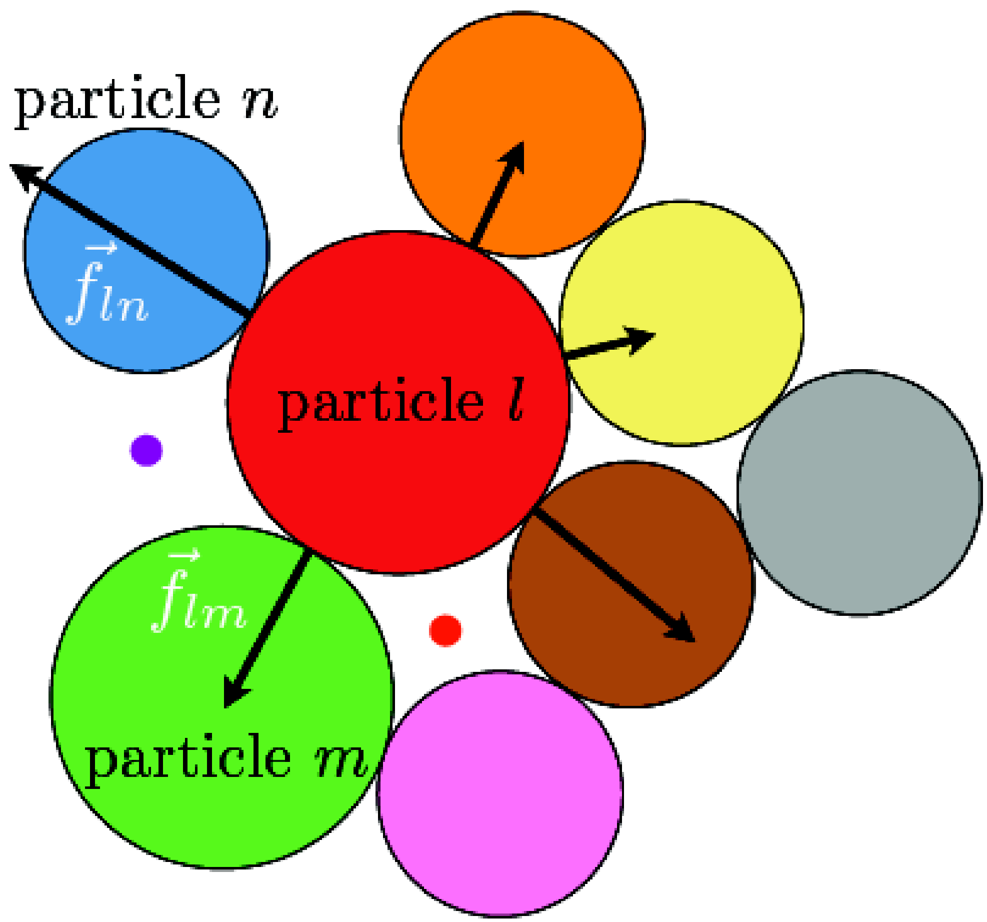
$$\hat{\sigma} = \sum_{cluster} \hat{\Sigma}$$

decompose into normal, deviatoric:

$$p = \frac{1}{2}(\sigma_1 + \sigma_2)$$

$$\tau = \frac{1}{2}(\sigma_1 - \sigma_2)$$

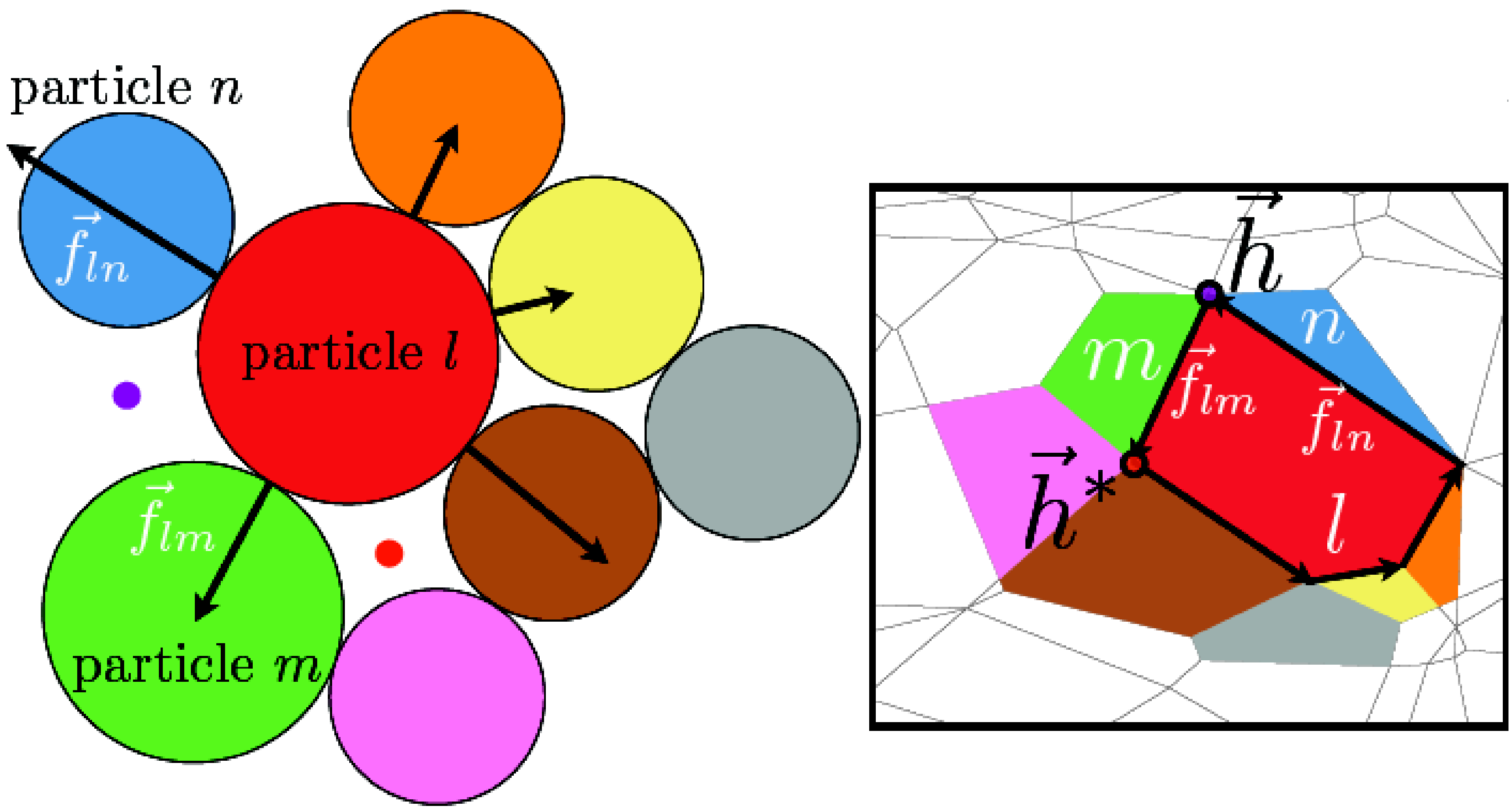
Constraints on Interparticle Forces



What do you know about the 5 black arrows?

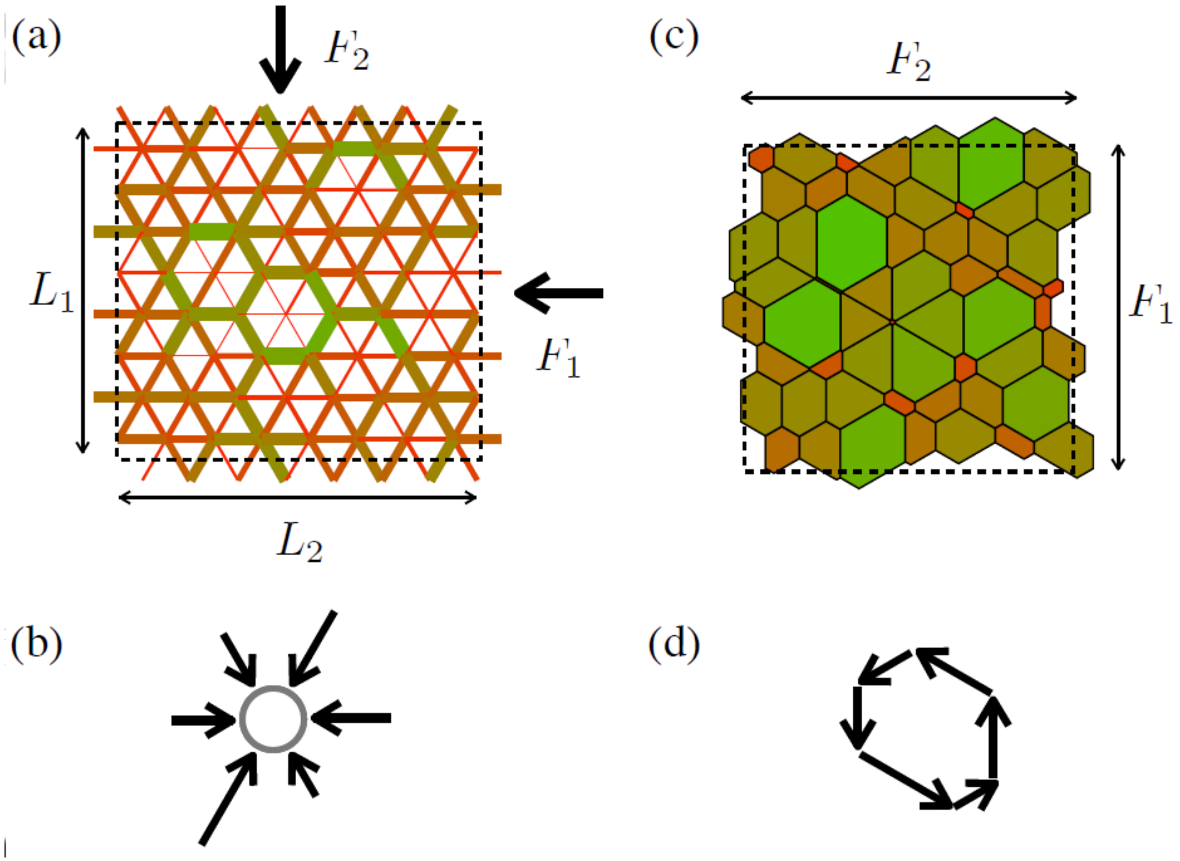
Bi, Henkes, Daniels, Chakraborty. *Ann. Rev. Cond. Matt.* (2015).

Force Balance → Tiles



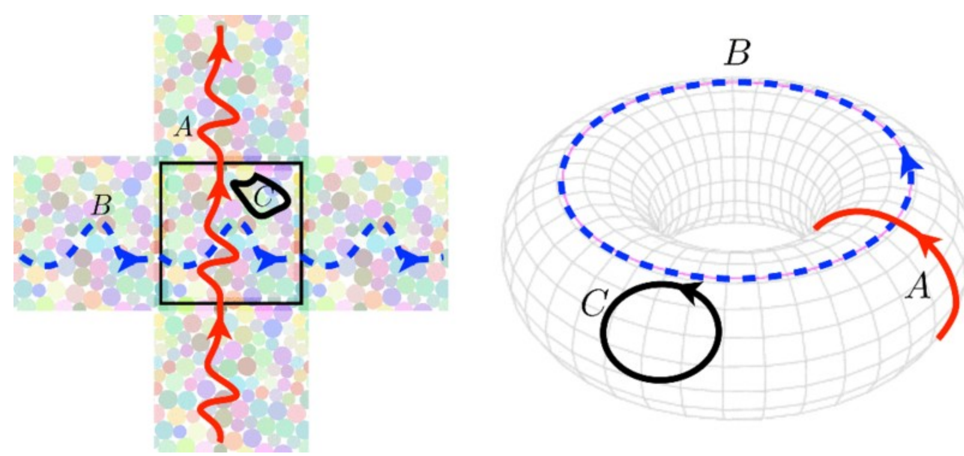
Bi, Henkes, Daniels, Chakraborty. *Ann. Rev. Cond. Matt.* (2015).

Conservation: Maxwell-Cremona tile area

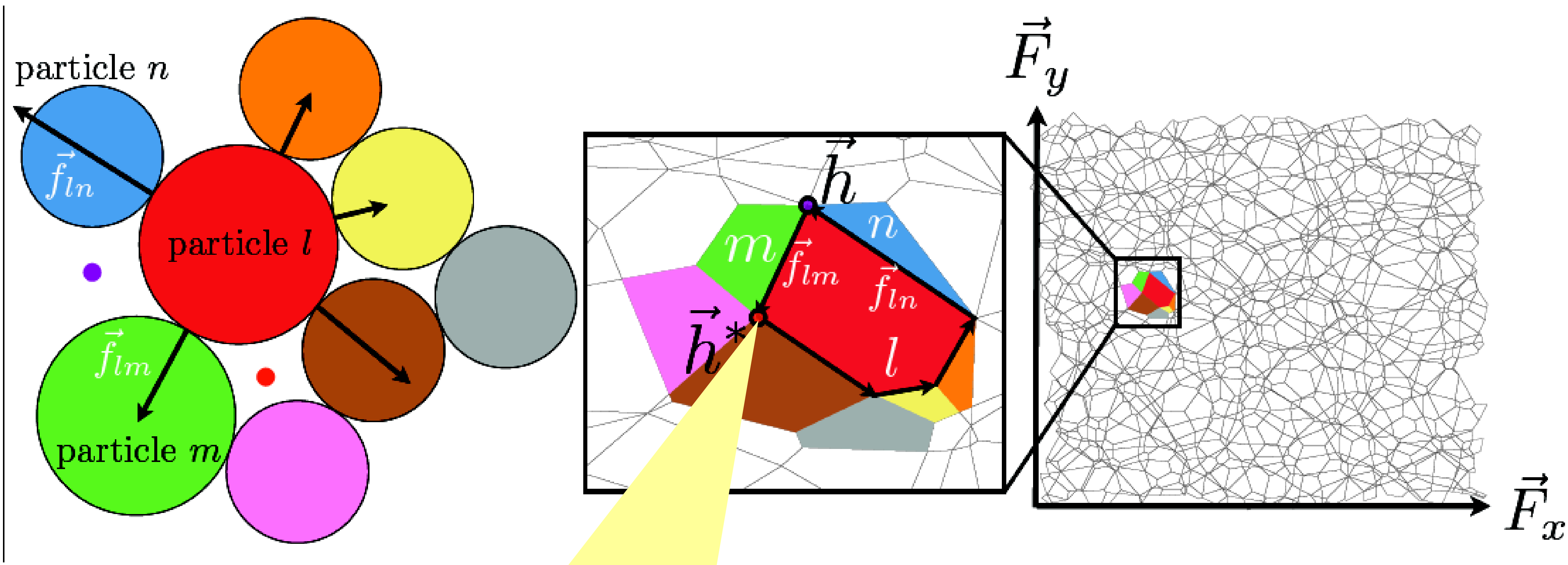


Tighe & Vlugt JSTAT 2010.

Sarkar, Bi, Zhang, Ren, Behringer, Chakraborty. PRE 2016

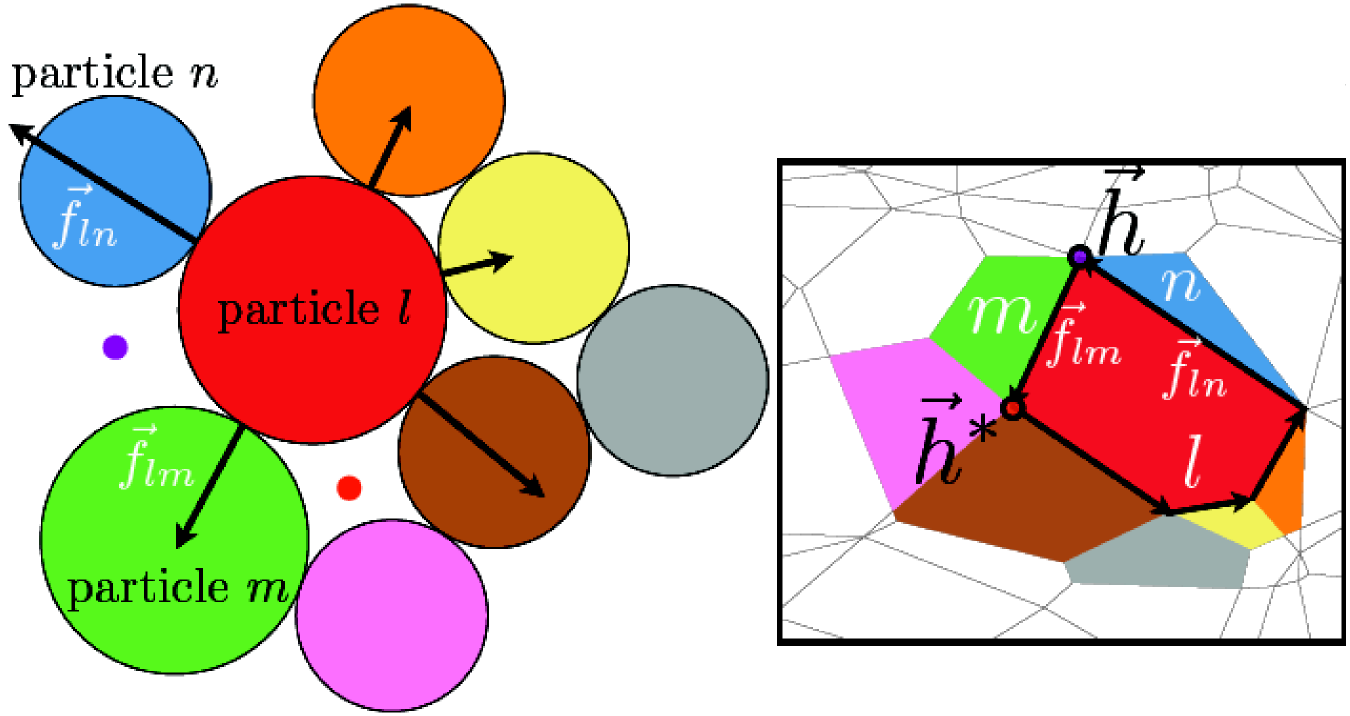


Represent Whole Packing in Force Space



moving this point corresponds
to adjusting the contact forces
in a way that preserves force balance

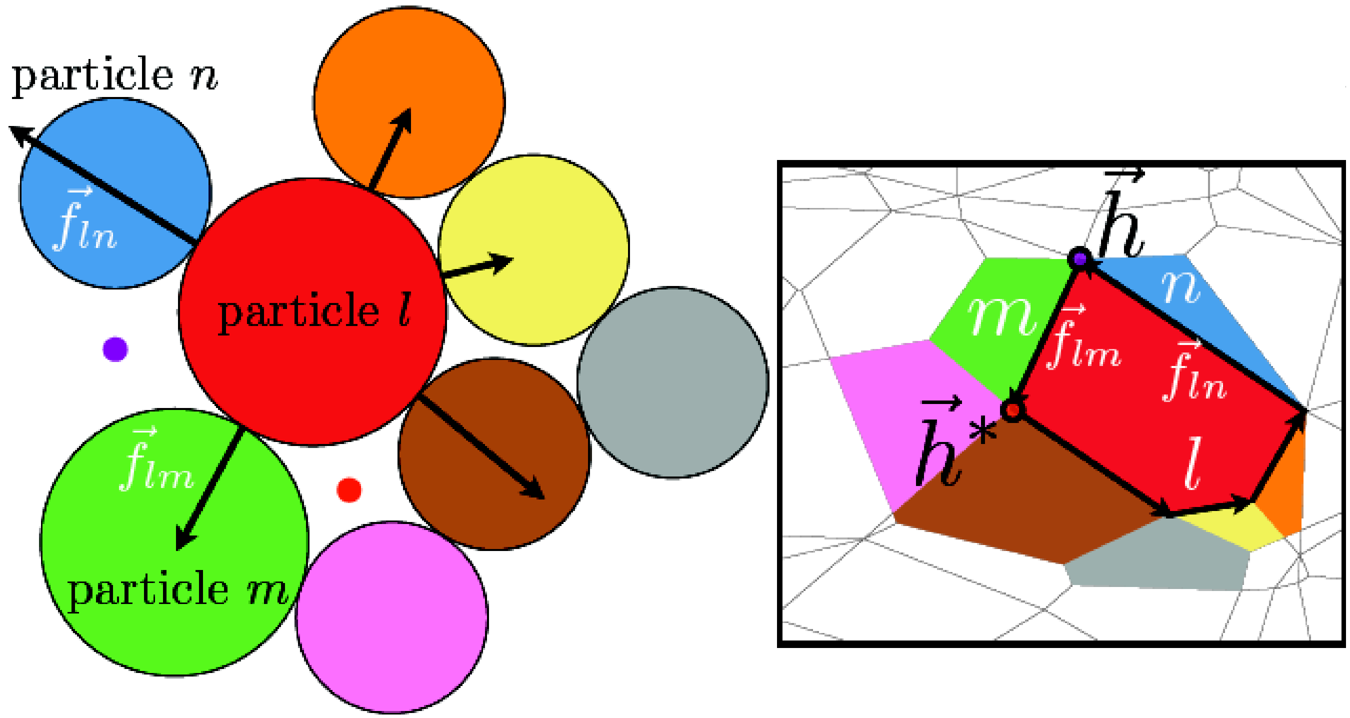
Forces → Field Theory



- define a vector gauge field *h(x, y)* on the dual space of voids (●, ●)
- going counterclockwise around a grain, increment the height field by the contact force between the two voids: $\vec{h}^* = \vec{h} + \vec{f}_{lm}$

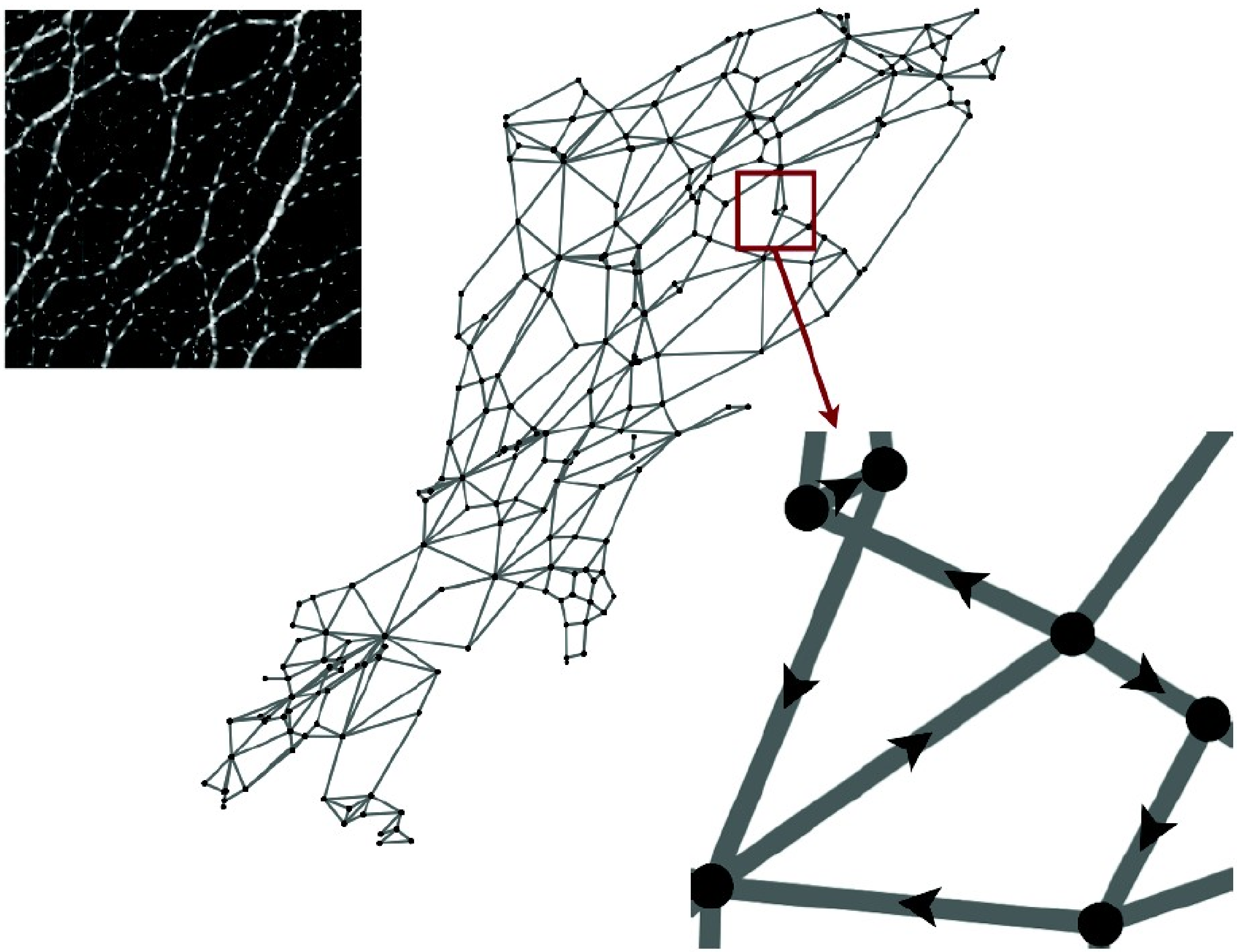
Ball & Blumenfeld *PRL* (2002) DeGiuli & McElwaine *PRE* (2011)
Henkes & Chakraborty *PRL* (2005) *PRE* (2009)

Relationship to Continuum Mechanics



- forces are locally balanced → $\hat{\Sigma} = V\,\hat{\sigma}$ is conserved
- Cauchy stress tensor can be calculated from the height field: $\hat{\sigma} = \vec{\nabla} \times \vec{h}$

Caveat: friction can cause non-convexity



Sarkar, Bi, Zhang, Behringer, Chakraborty. *PRL* (2013)