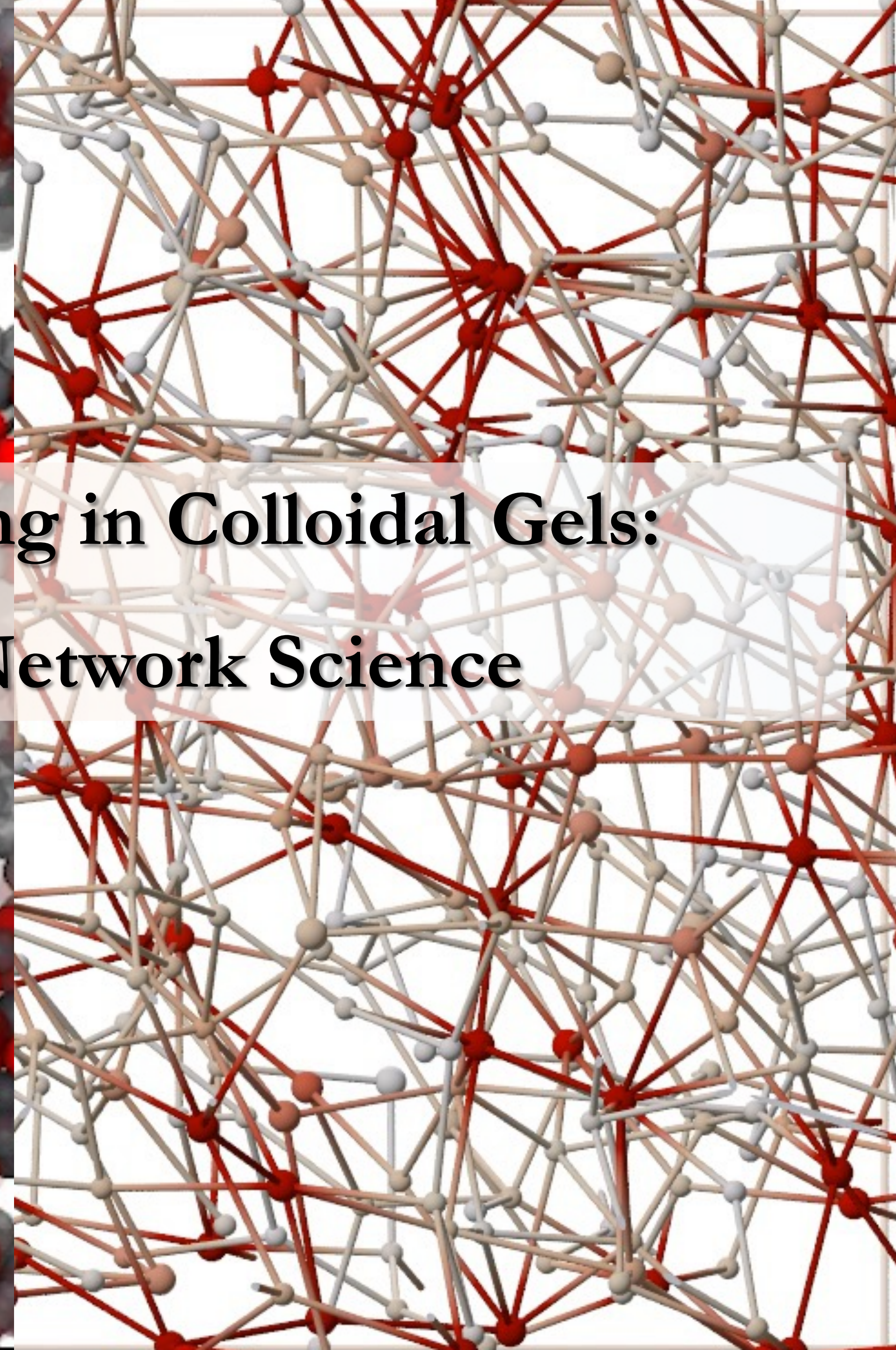
KITP Seminar, Dec 2022

Rigidity and Yielding in Colloidal Gels: Insights from Network Science



Who actually did the work…

Mohammad Nabizadeh

Babak Ravandi

Farzaneh Nasirian

DMR - DMREF

Max Bi - NEU

Lilian Hsiao - NCSU

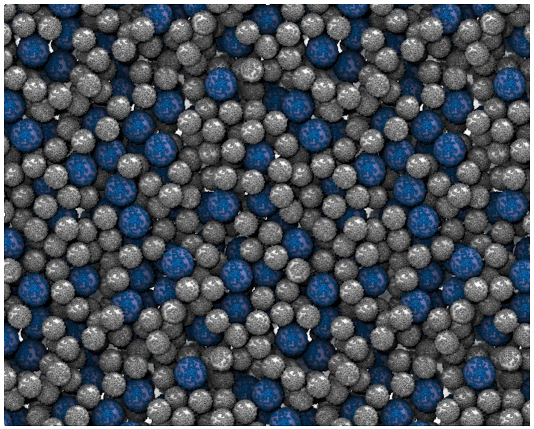
Abhinendra Singh

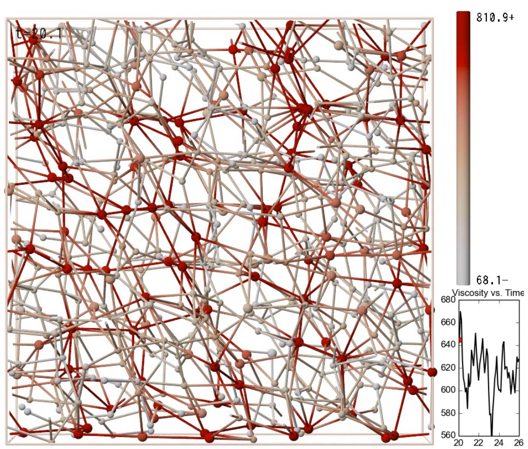
Xinzhi Li – NEU
Rony Waheibi – NCSU
Yug Sarawat – NCSU

“network” physics in colloidal systems

Bridging the microscopic structure to macroscopic rheology

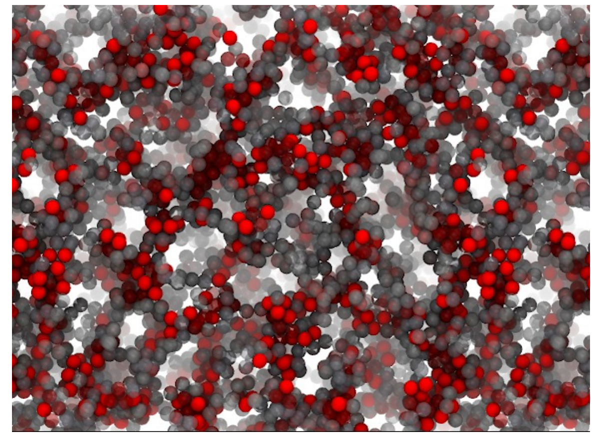
“force” or “contact” networks in dense suspensions

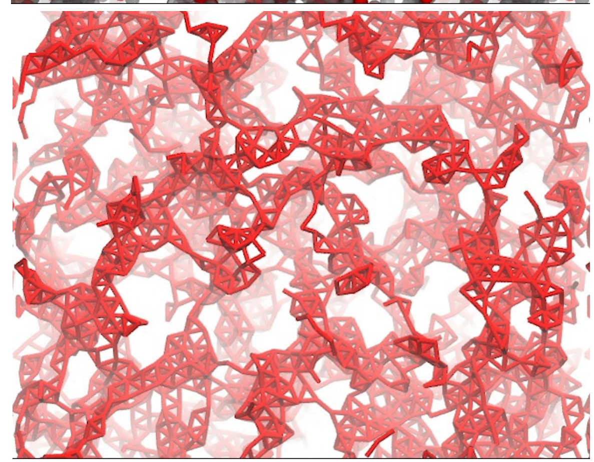




Jamali and Brady, *PRL*, 2019, *JOR*, 2020
Nabizadeh, Singh and Jamali, *PRL*, 2022

“space-spanning” colloidal bond network in gels

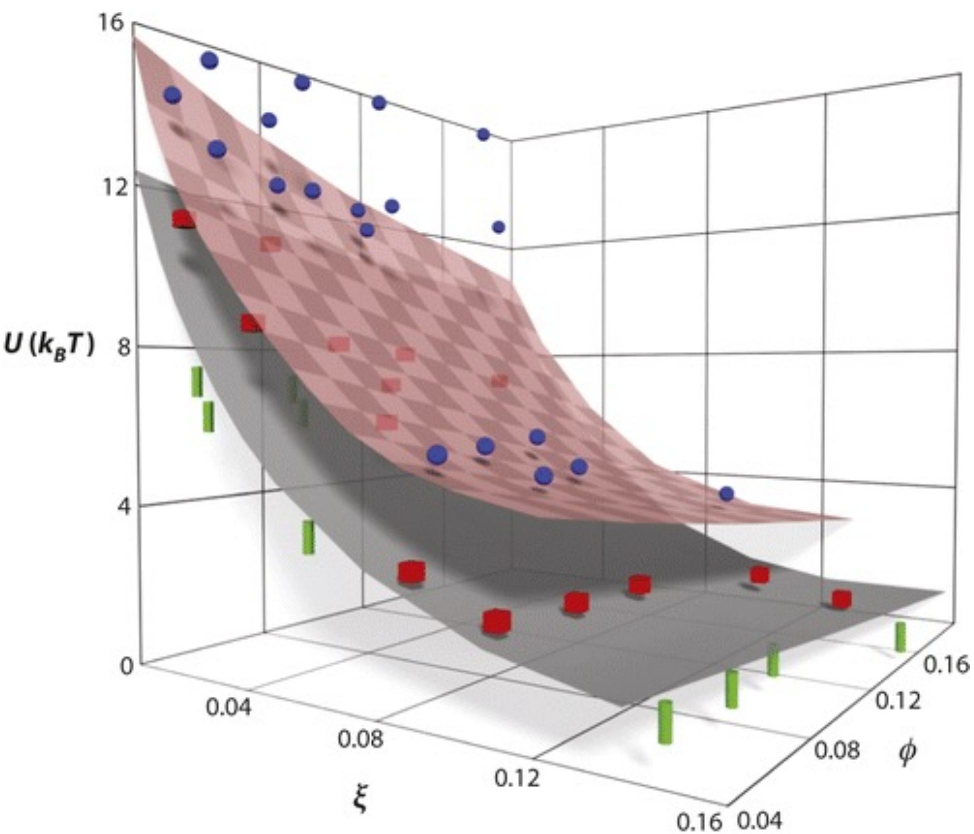


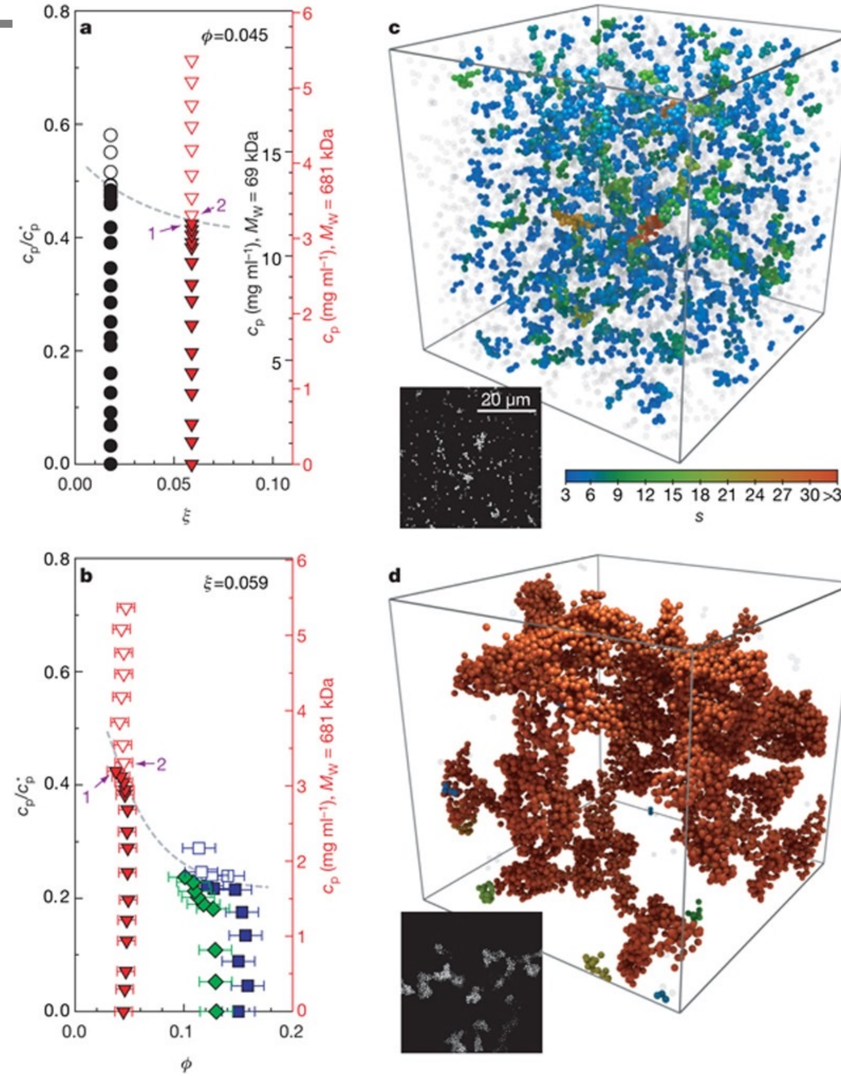


Nabizadeh and Jamali, *Nat. Comm.*, 2021

Colloidal gelation: a phase transition

Phase boundary is not as clear





Lu and Weitz, *Annu. Rev. Condens. Matter Phys.*, 2013
Lu et al., *Nature*, 2008

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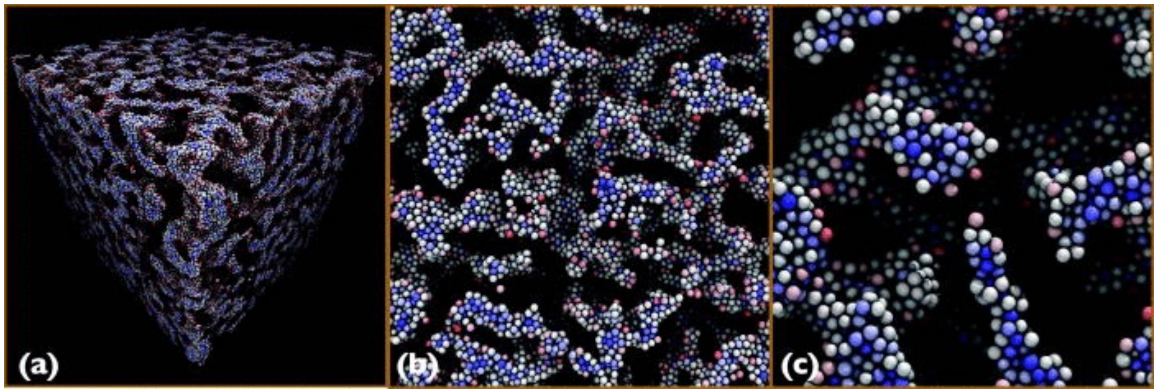
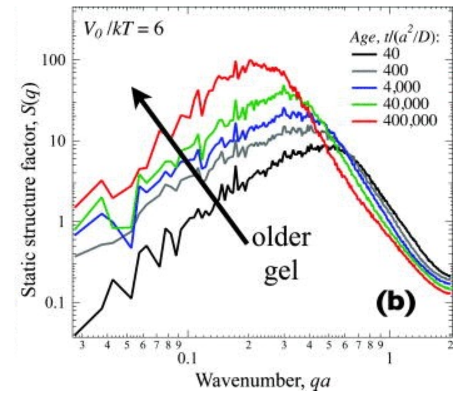
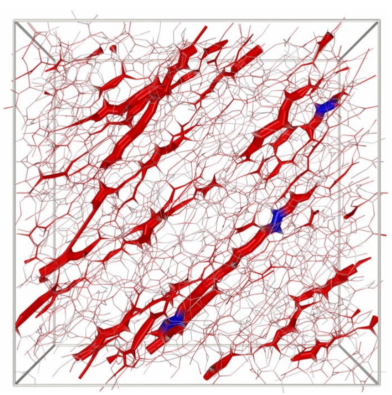
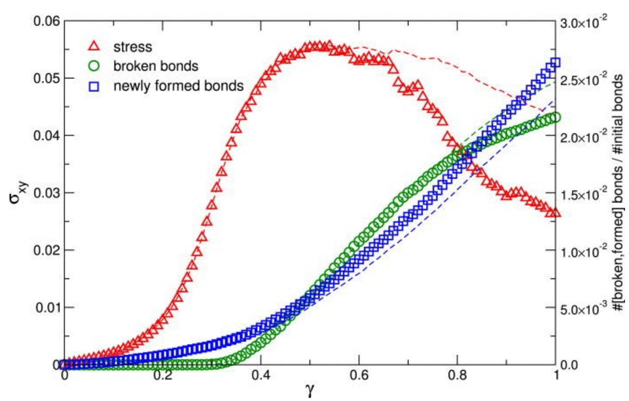
Gels: Formation and Yielding





Zia, Landrum and Russel, *Journal of Rheology*, 2014

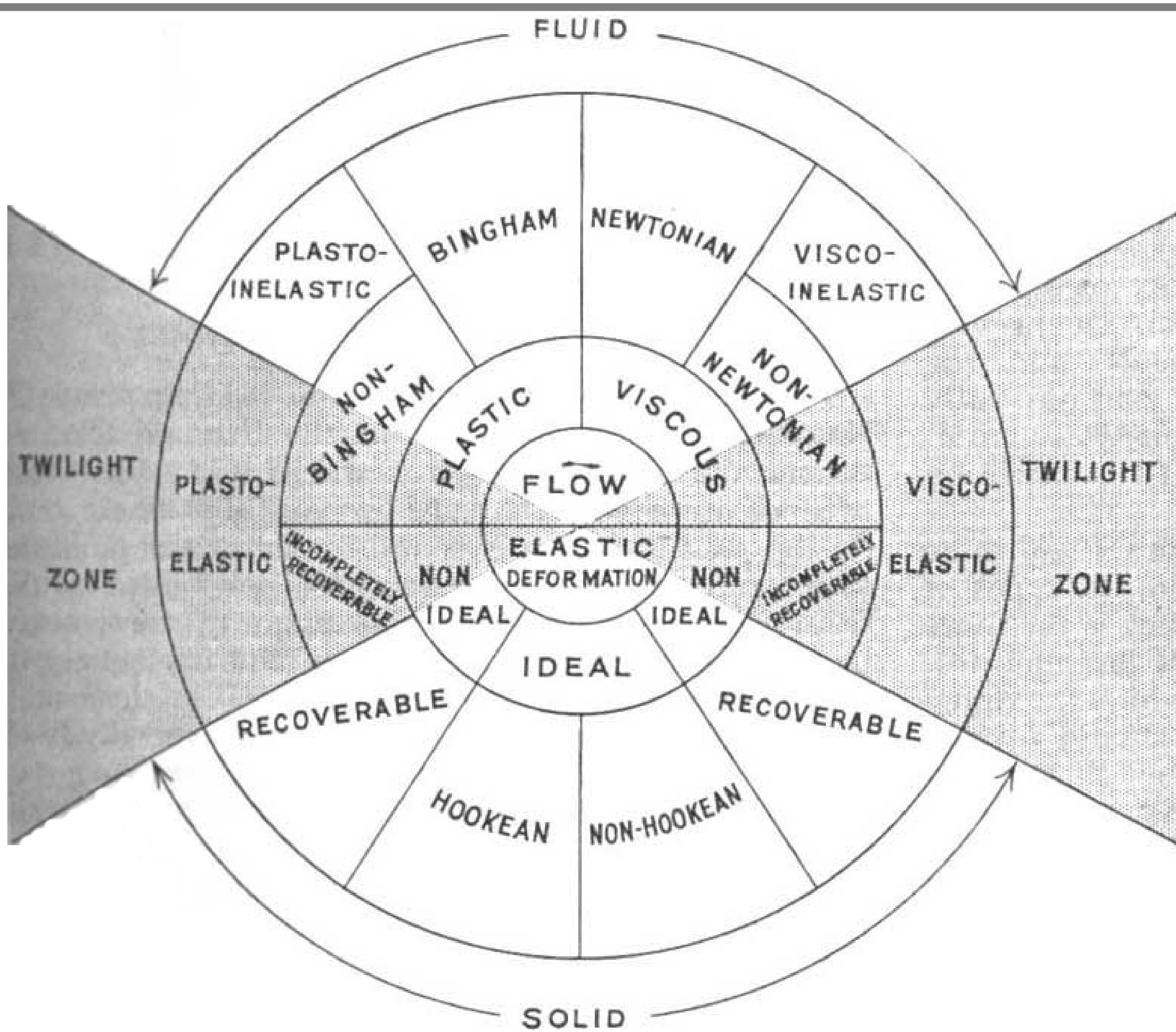




Colombo and Del Gado, *Journal of Rheology*, 2014

Others:
Poon, Petekidis, Vlassopoulos, Cipelletti, Zaccarelli, Weitz, Helgeson, Wagner, Manneville, Divoux, Fielding, Cates, Solomon…

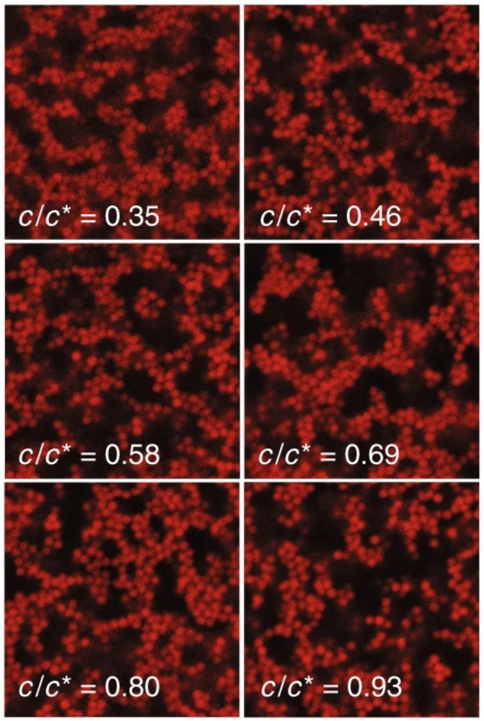
A Mechanical Perspective

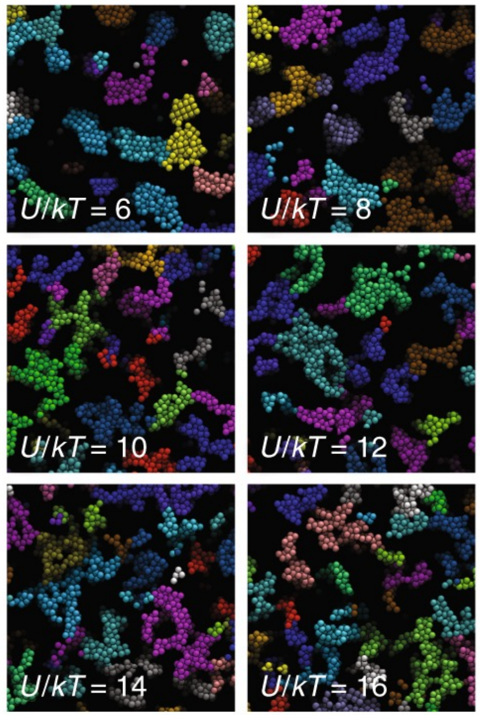


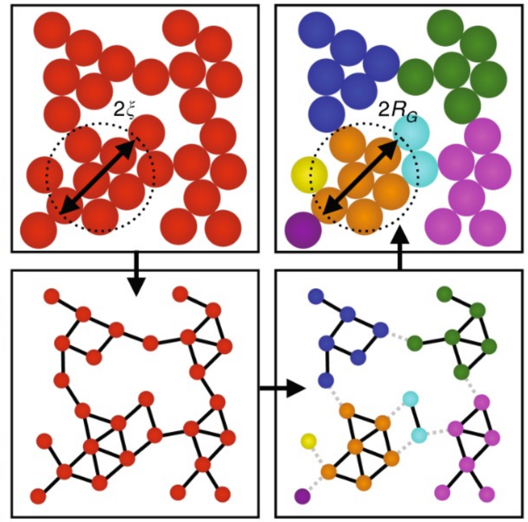
L. Bilmes, *Nature*, 150, p.432, 1942

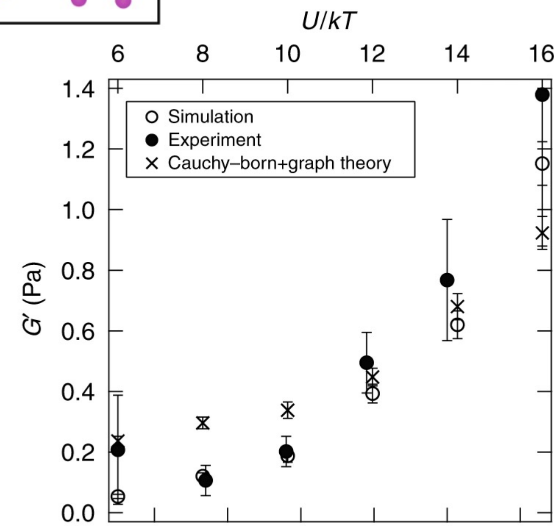
Graph theory applied to colloidal gels

Emergence of elasticity in colloidal gels







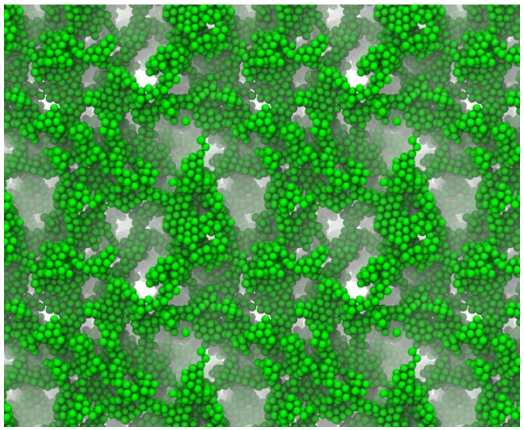


Whitaker et al., *Nat. Comm.*, 2020

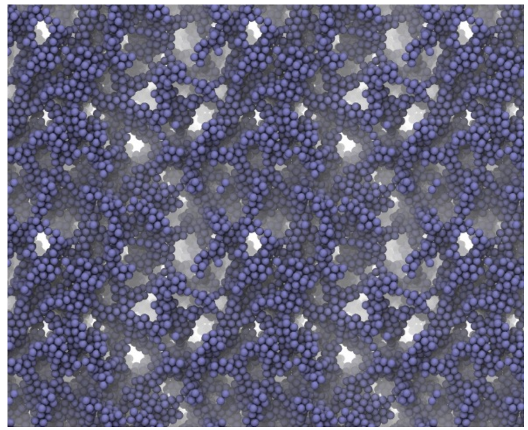
Gels with different strengths of attraction

Elastic modulus increases by increasing attraction

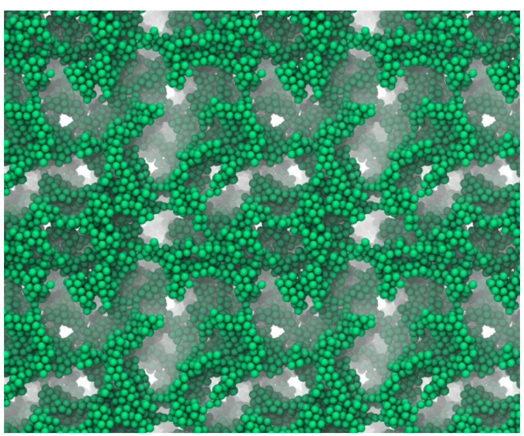
$U/kT = 6$



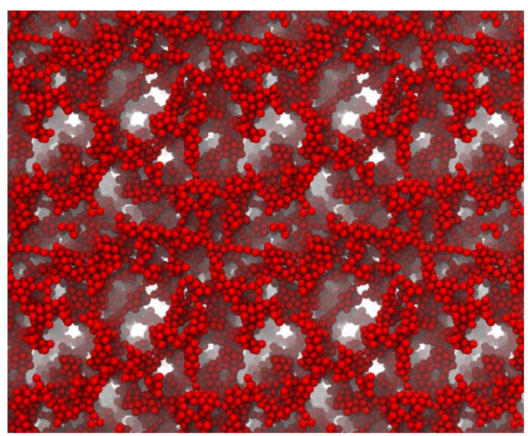
$U/kT = 12$

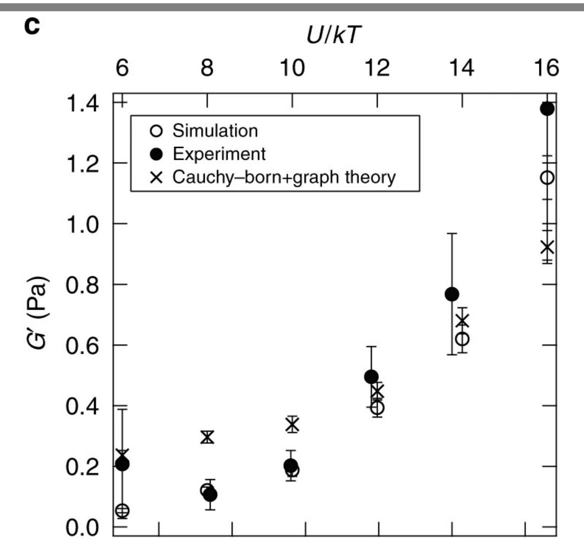


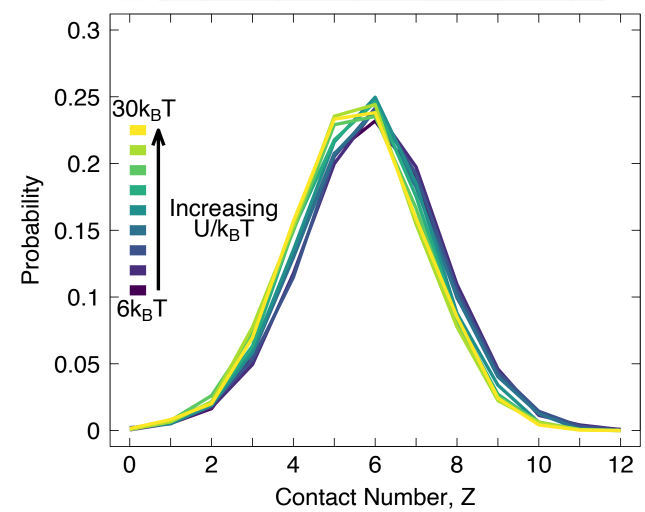
$U/kT = 18$



$U/kT = 30$



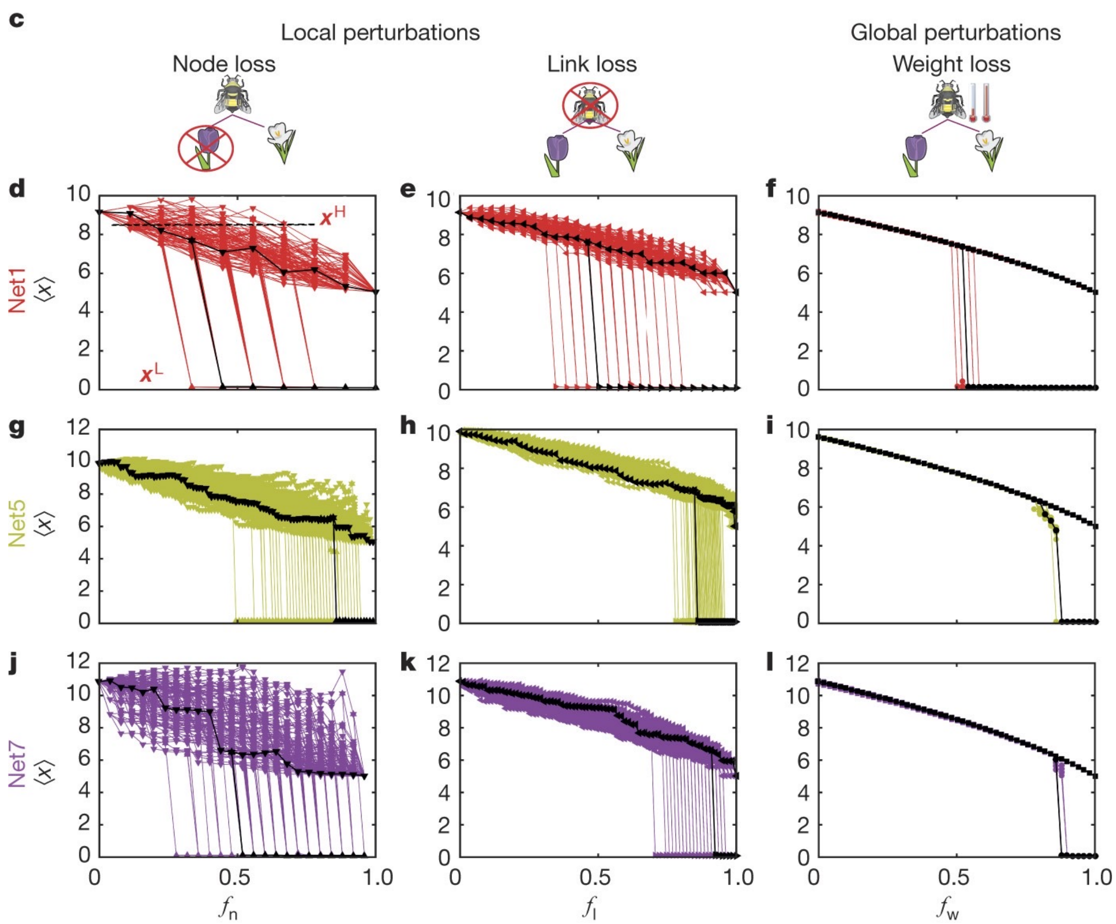




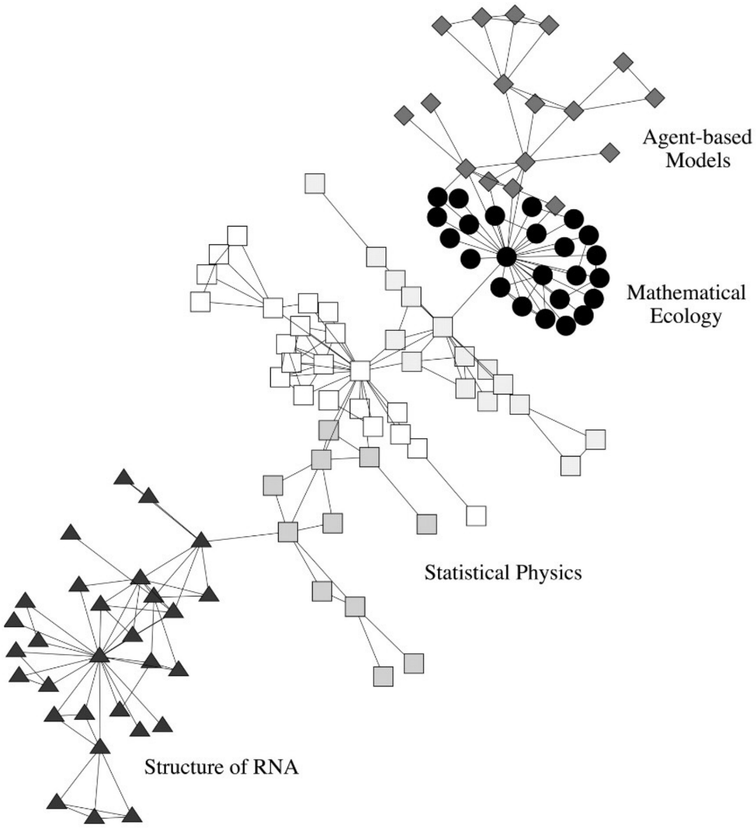
Whitaker et al., *Nat. Comm.*, 2020

Network science and resilience

Well-established science of network in complex systems



Gao, *Nature*, 2016



Girvan & Newman, *PNAS*, 2002

What about network measures?

Edge betweenness centrality as measures of importance

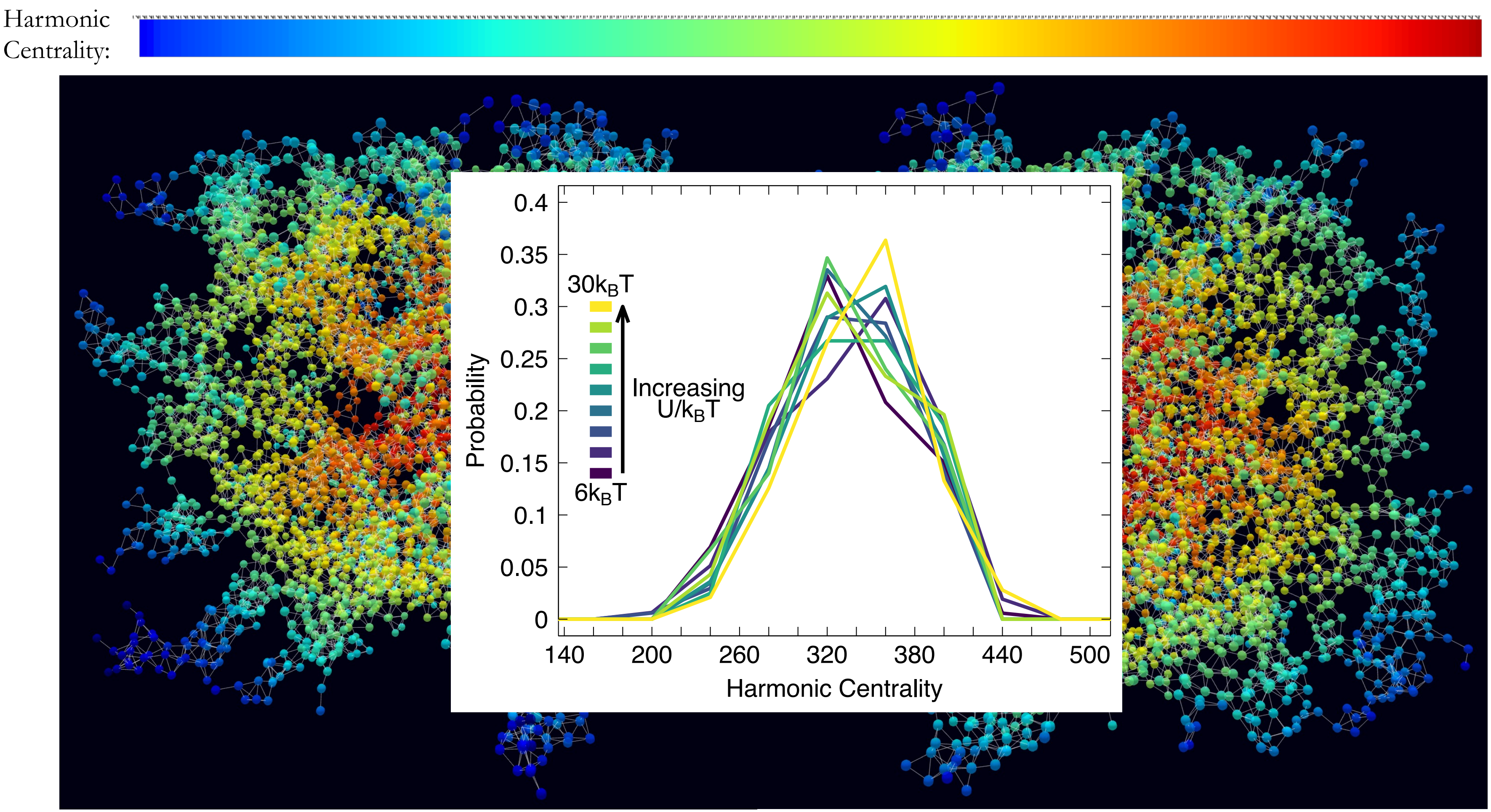
Betweenness Centrality:

$$c_B(e) = \sum_{s,t \in V} \frac{\sigma(s,t|e)}{\sigma(s,t)}$$

Edge betweenness centrality of a given edge/node shows the fraction of all shortest paths in the network passing through that edge/node. This measure of centrality indicates which nodes/edges act as central bridges connecting different parts of the network..

What about network measures?

Harmonic and bridging centralities as measures of connectedness



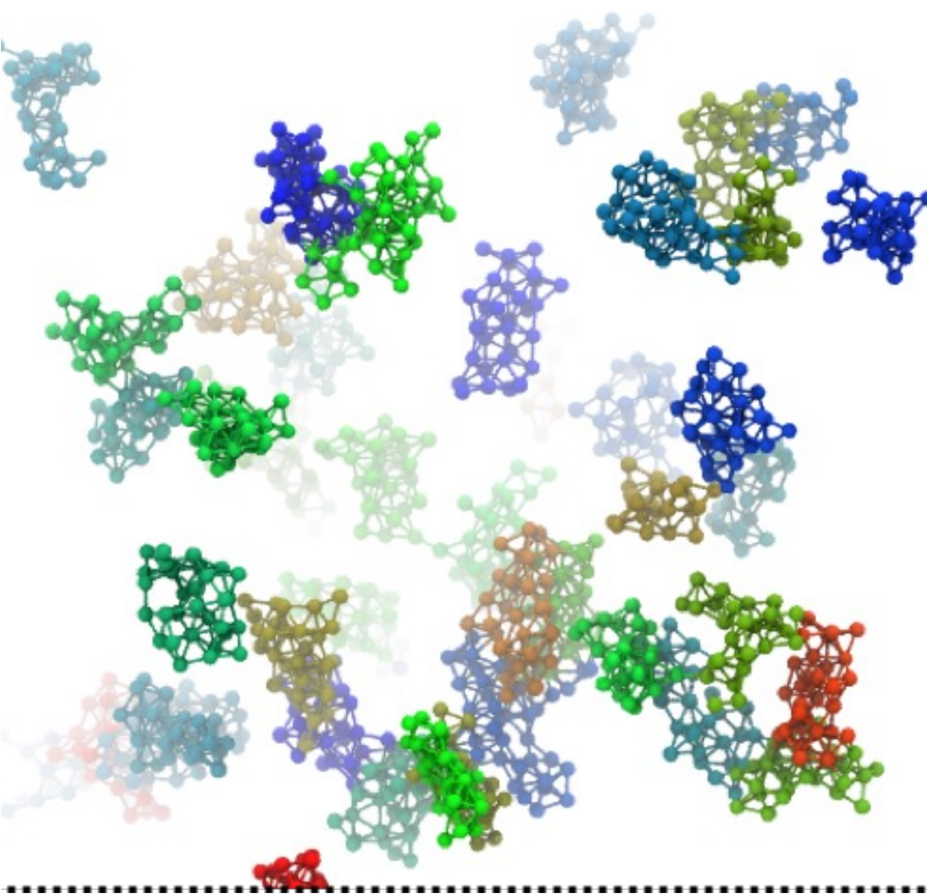
$U / kT = 6$ $U / kT = 30$

Communities: GMM for clustering

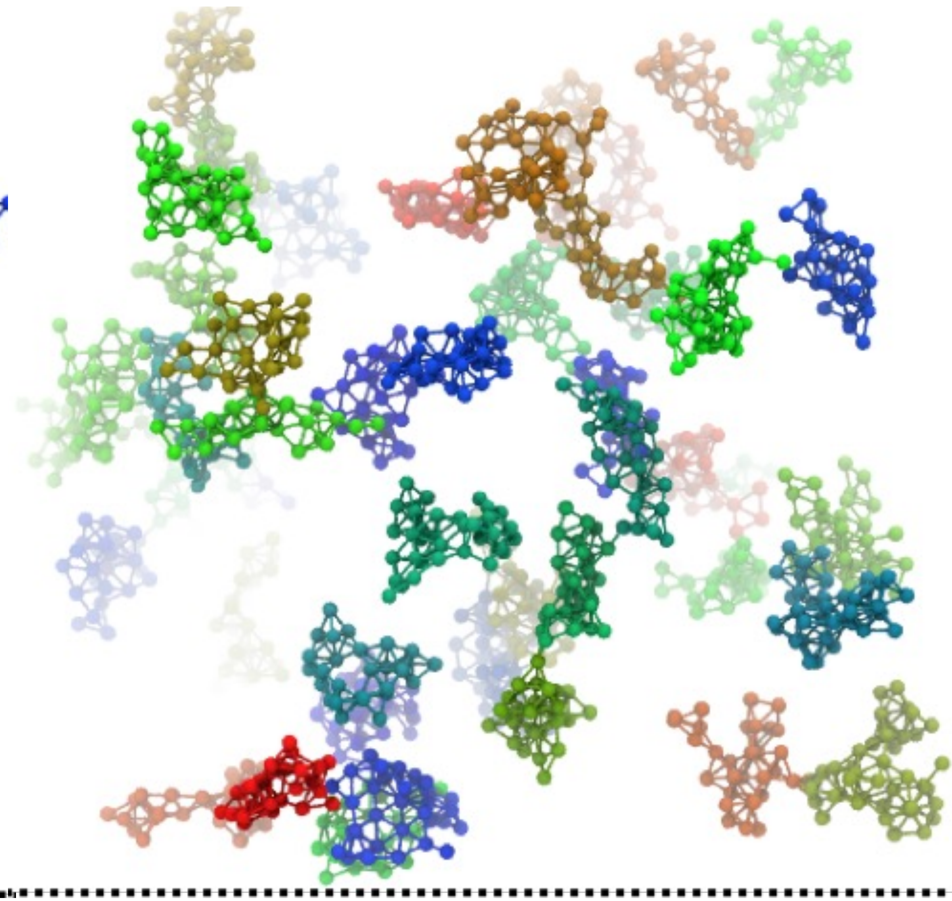
Visualizing the clusters

Only a small portion is showed for visual purposes

$U / kT = 6$



$U / kT = 30$

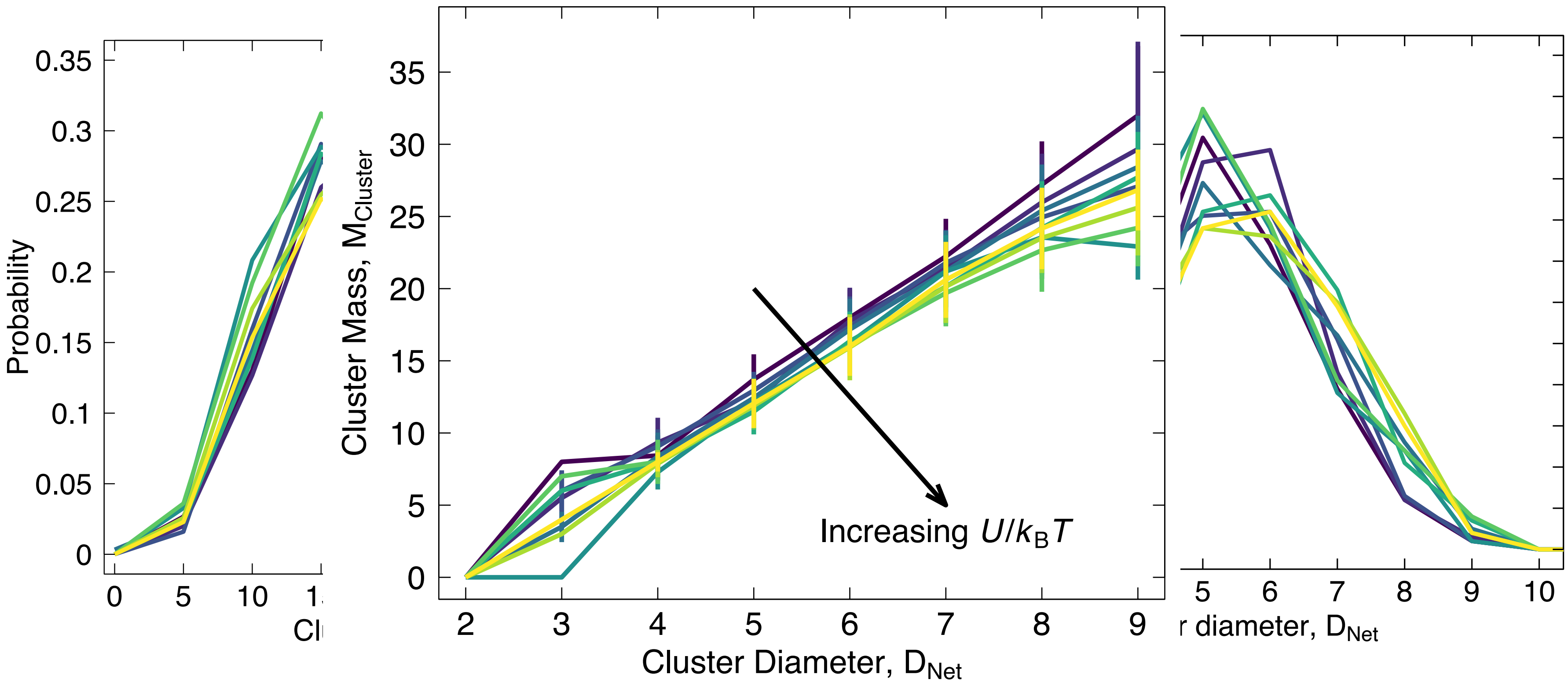


Clustering with GMM

The only condition to satisfy is correlation with physical size

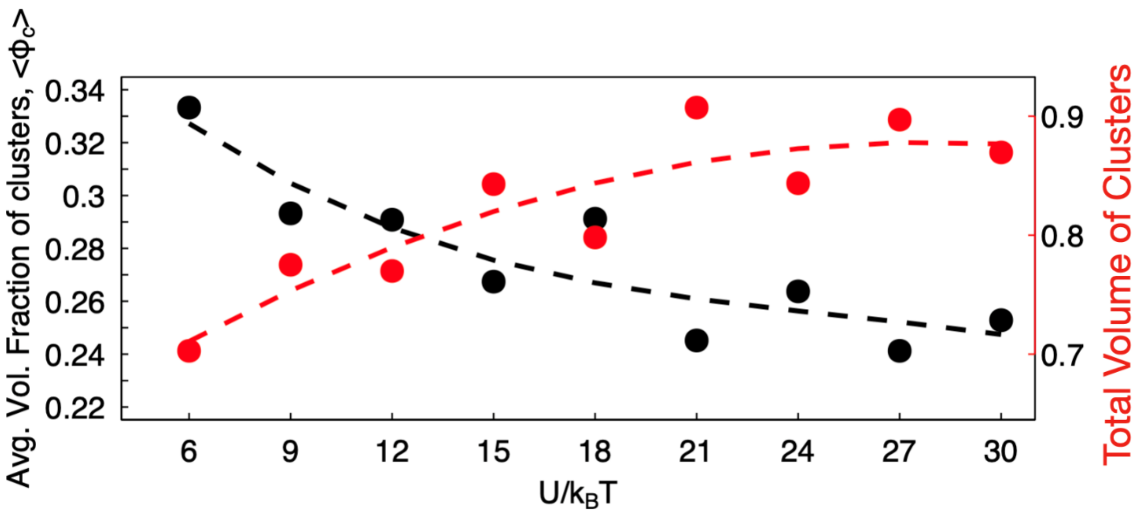
At large enough cluster sizes, at the same physical distance, it takes more "hops" for the weaker gel to walk the path between the two nodes

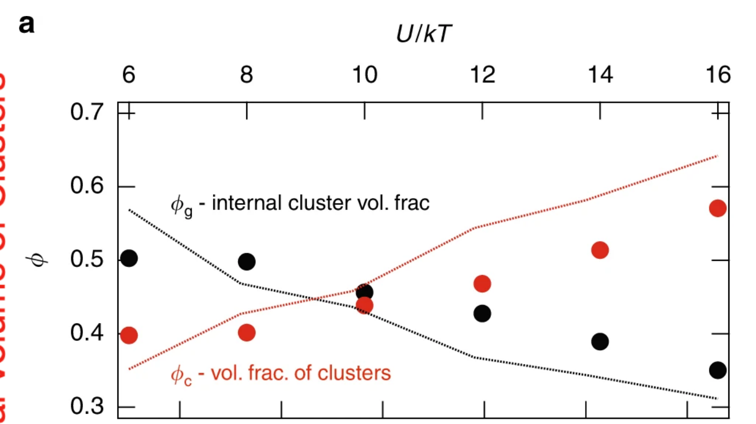
Stronger attraction → More elongated clusters



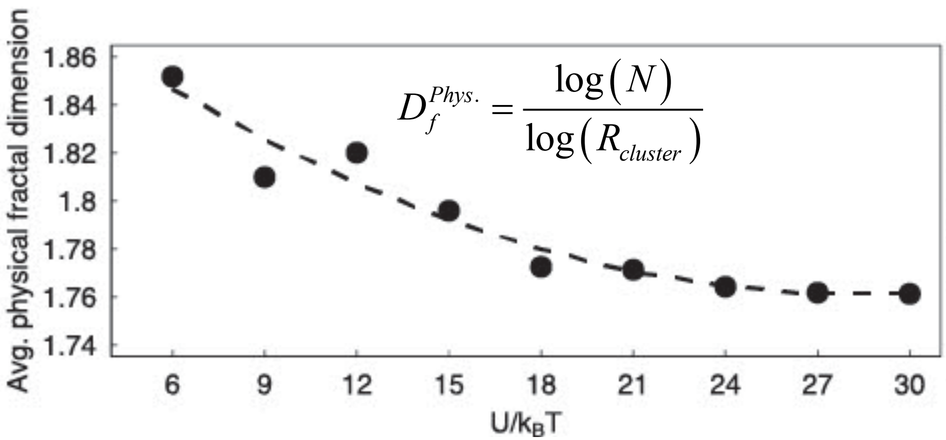
Structure of clusters

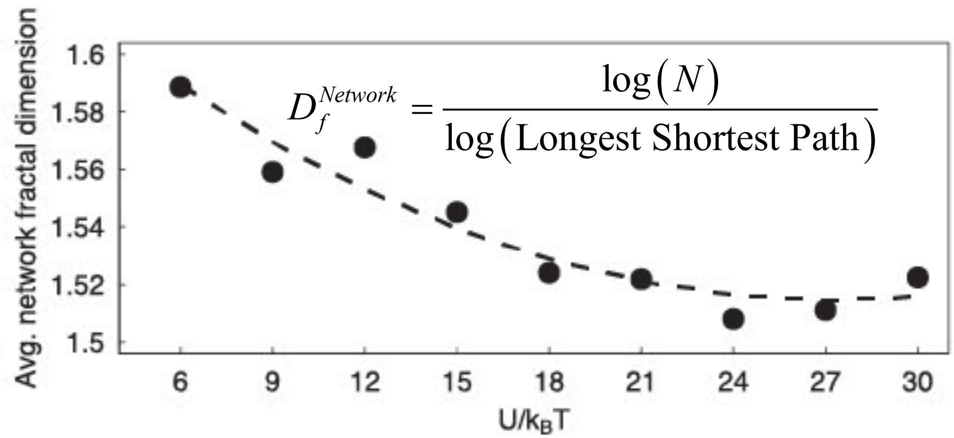
Internal vs. overall fraction of clusters





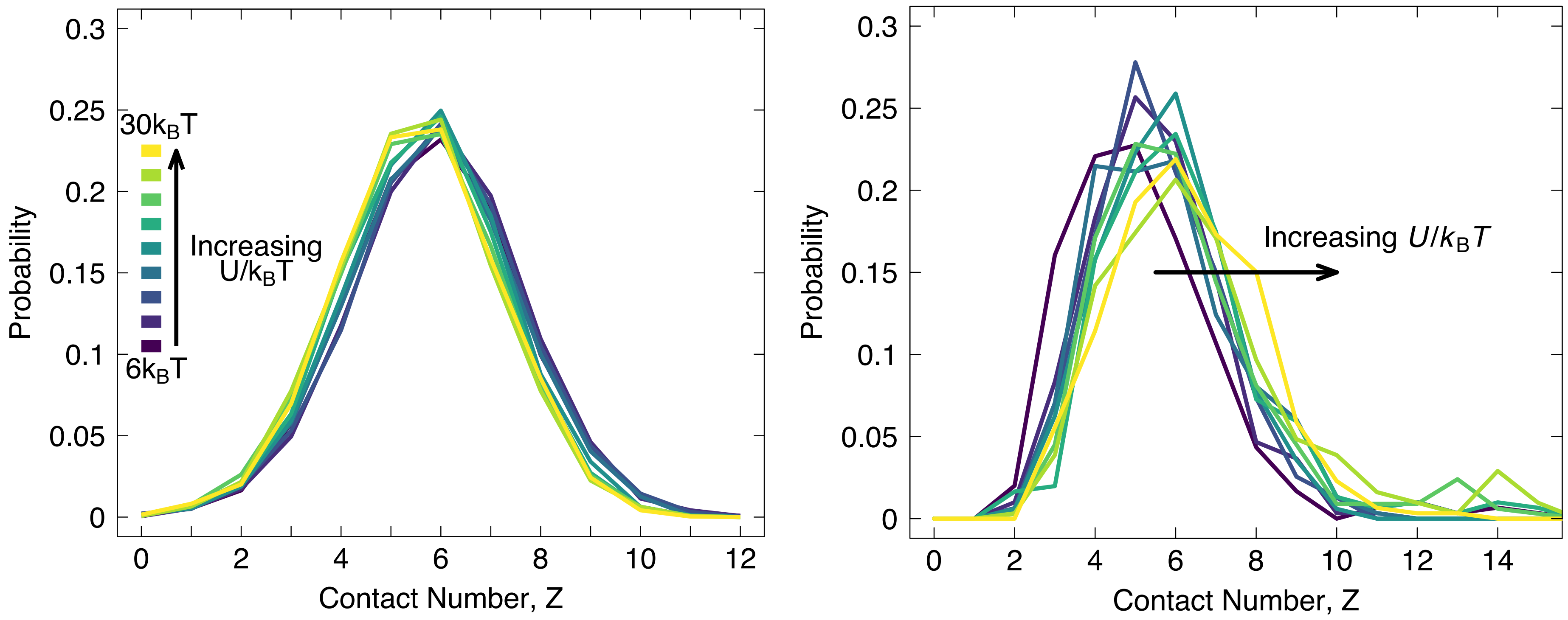
Whitaker et al., *Nat. Comm.*, 2020





Cluster coordination number

Degree distribution is now distinctly different



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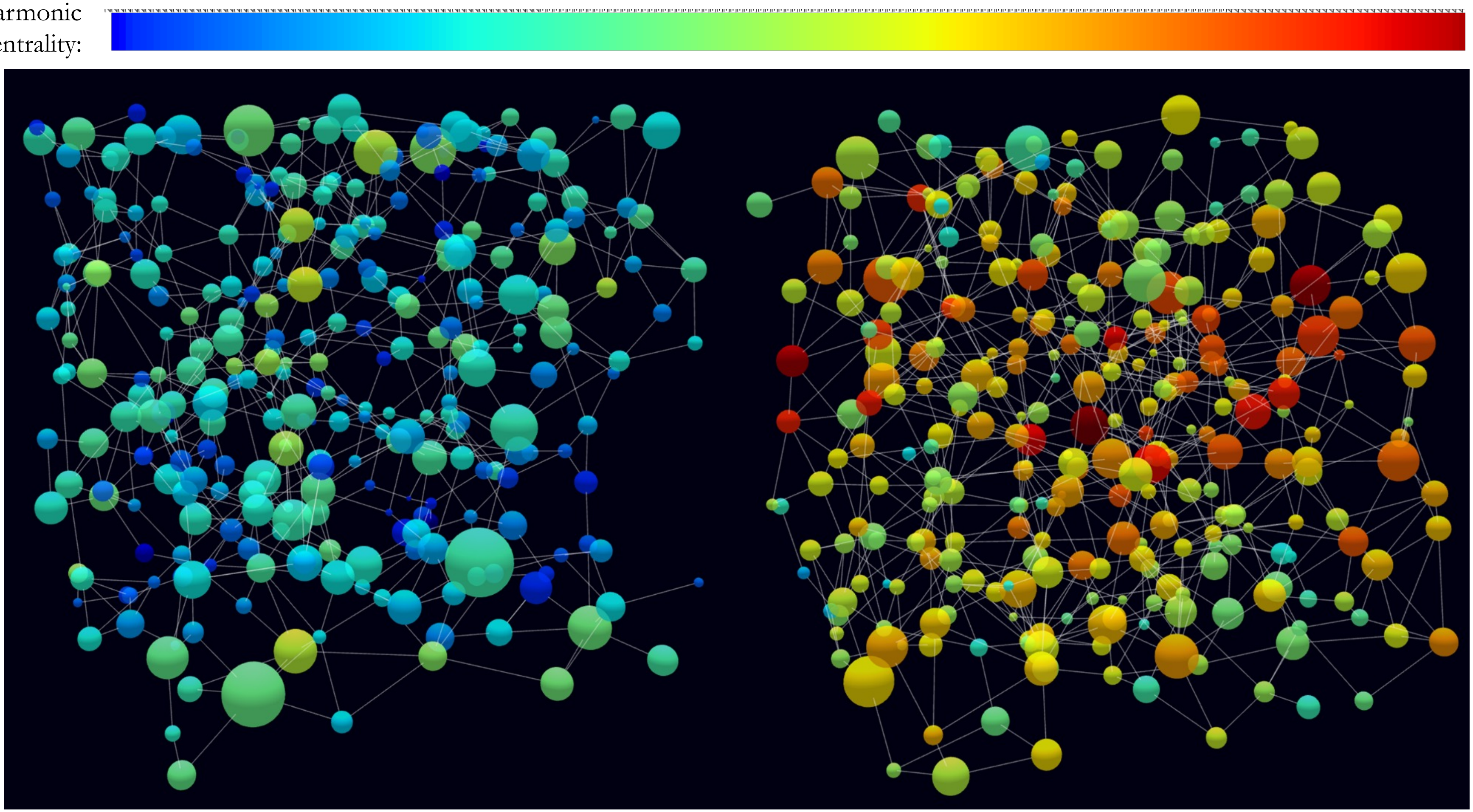
Harmonic centrality for clusters?

Harmonic and bridging centralities as measures of connectedness

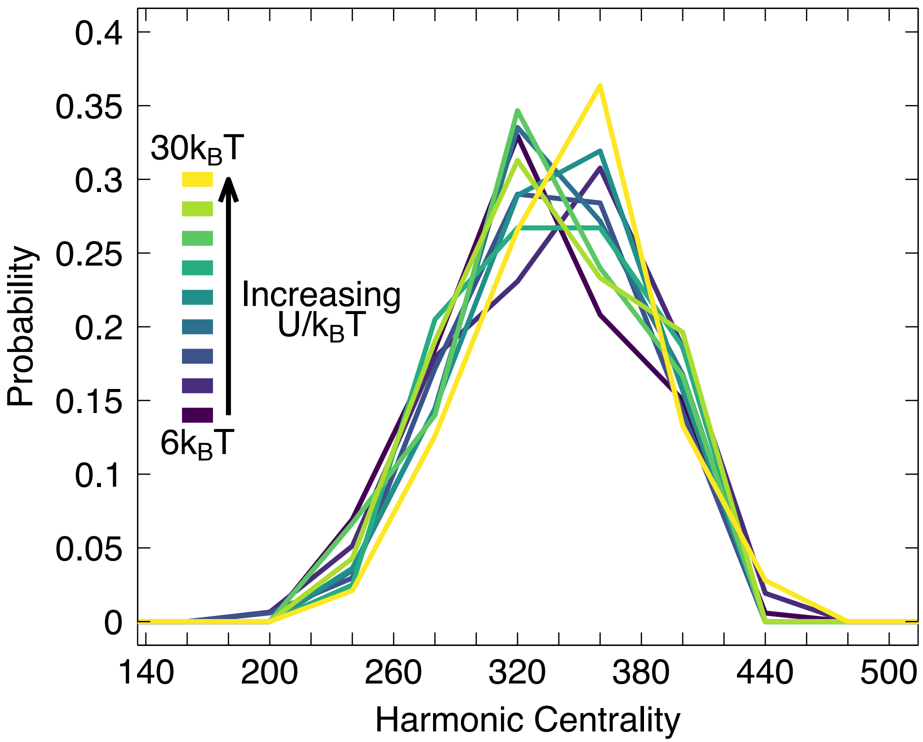
Harmonic Centrality:

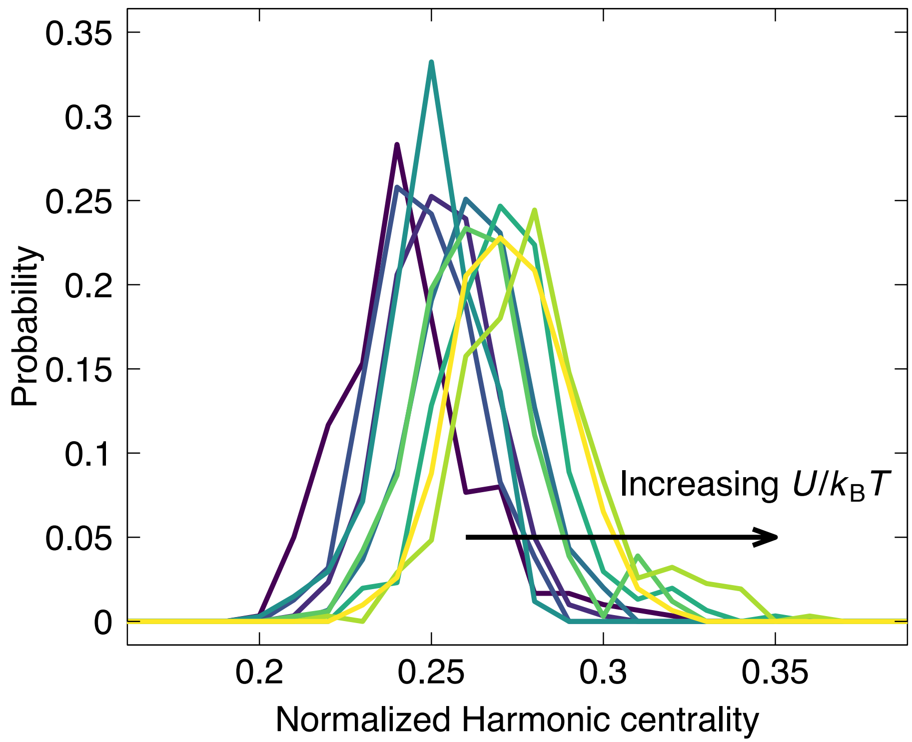


$U\,/\,kT = 6$ $\qquad$ $U\,/\,kT = 30$

Harmonic centrality for nodes/clusters

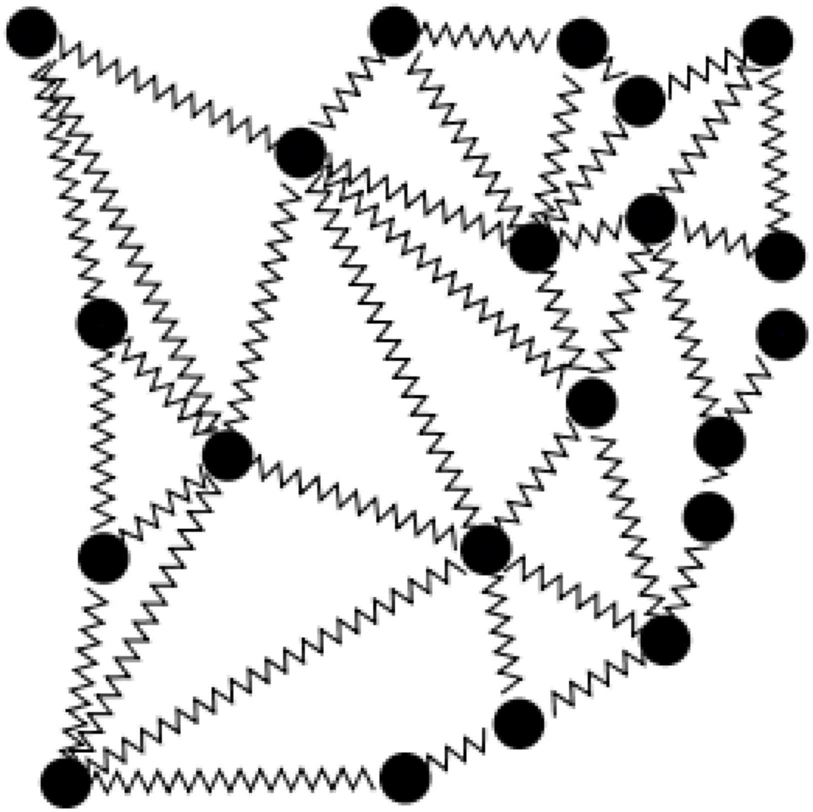
The coarse-grained harmonic centrality shows distinct features

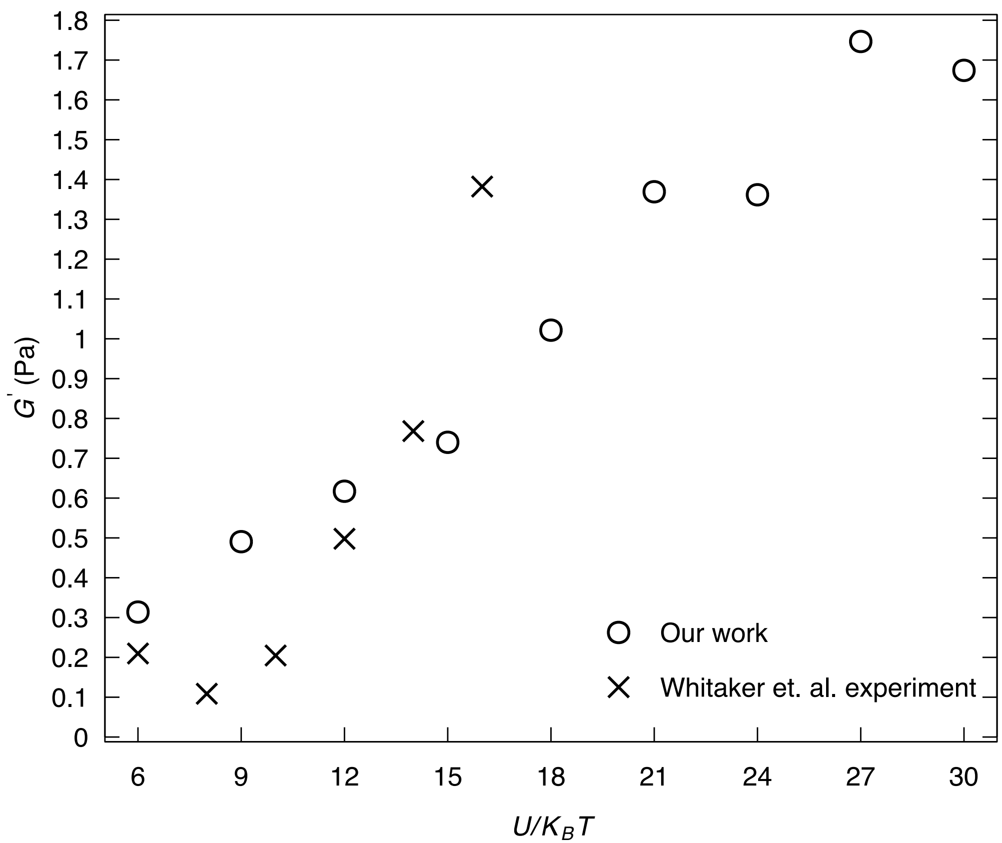




Modulus of the "cluster network"

We use a simple mass-spring model for calculations

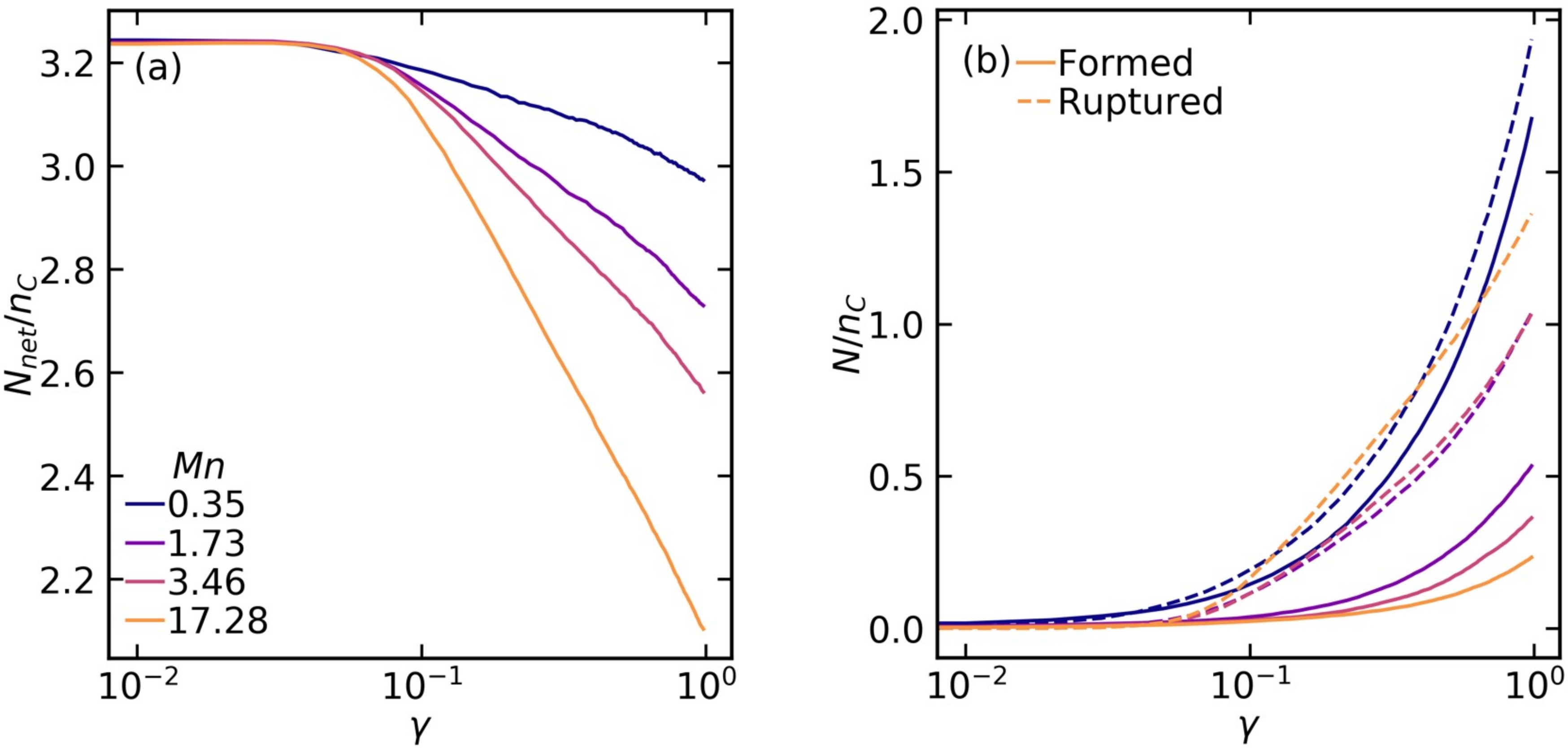




Resilience of the cluster network

First, we need to decide on which edges to remove

Which bonds' loss will result in yielding of the gel?



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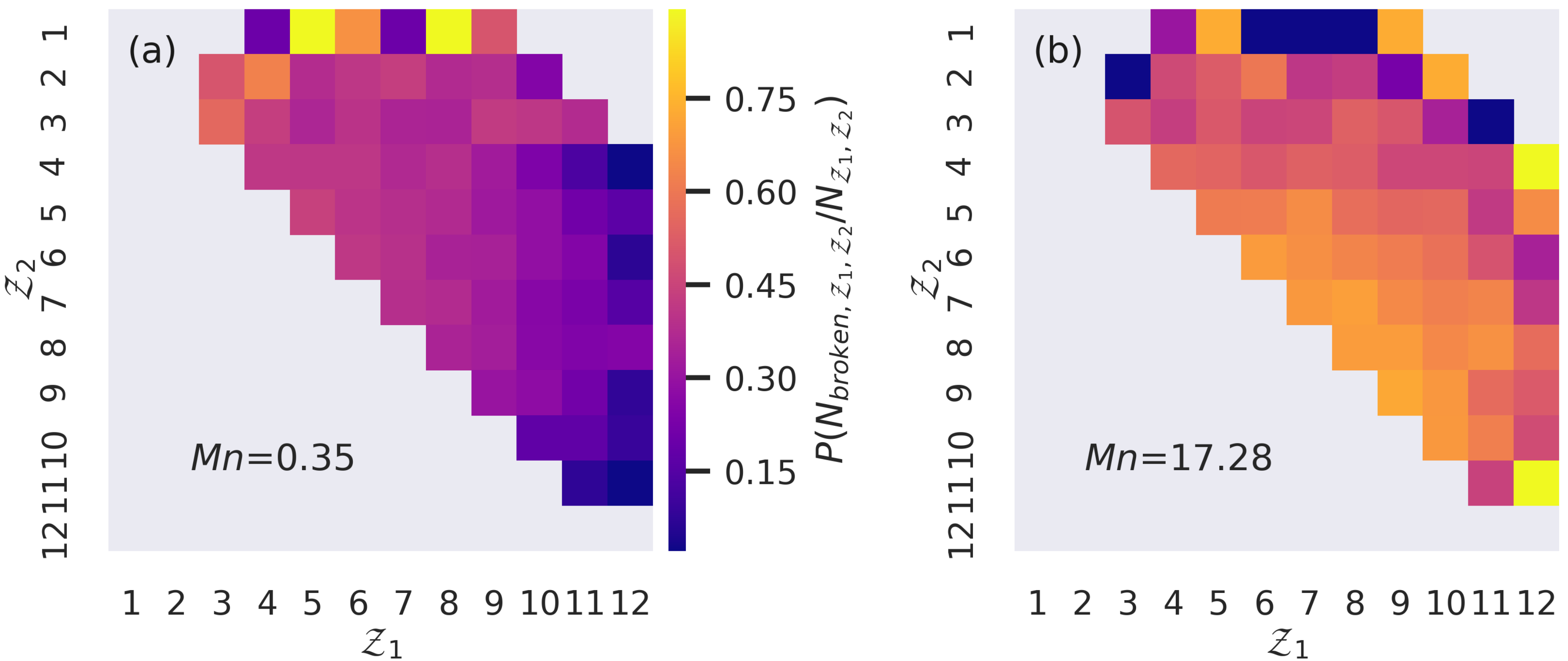

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Resilience of the cluster network

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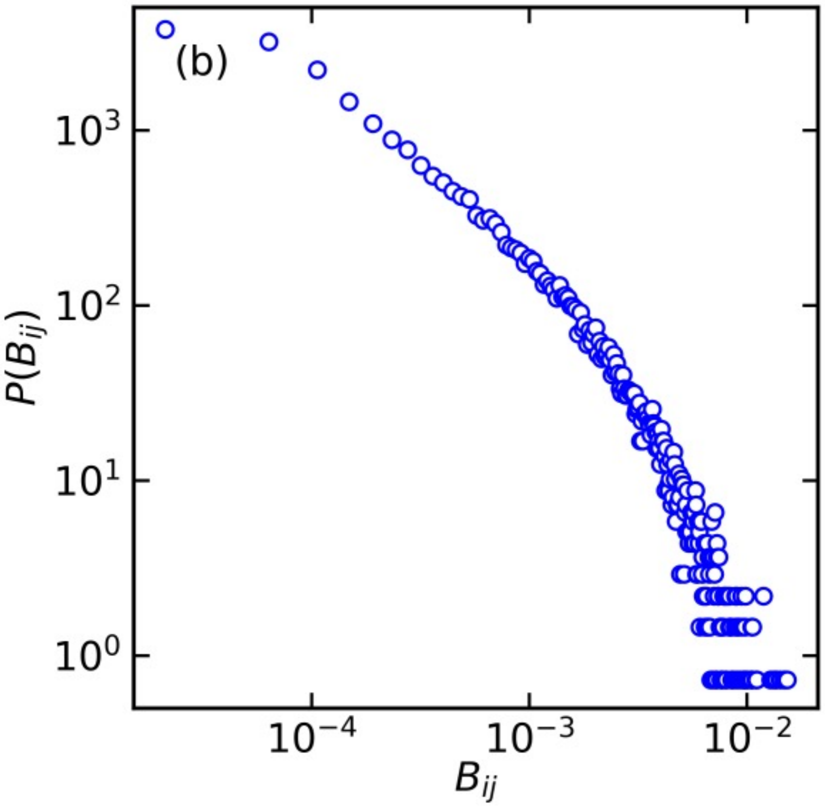

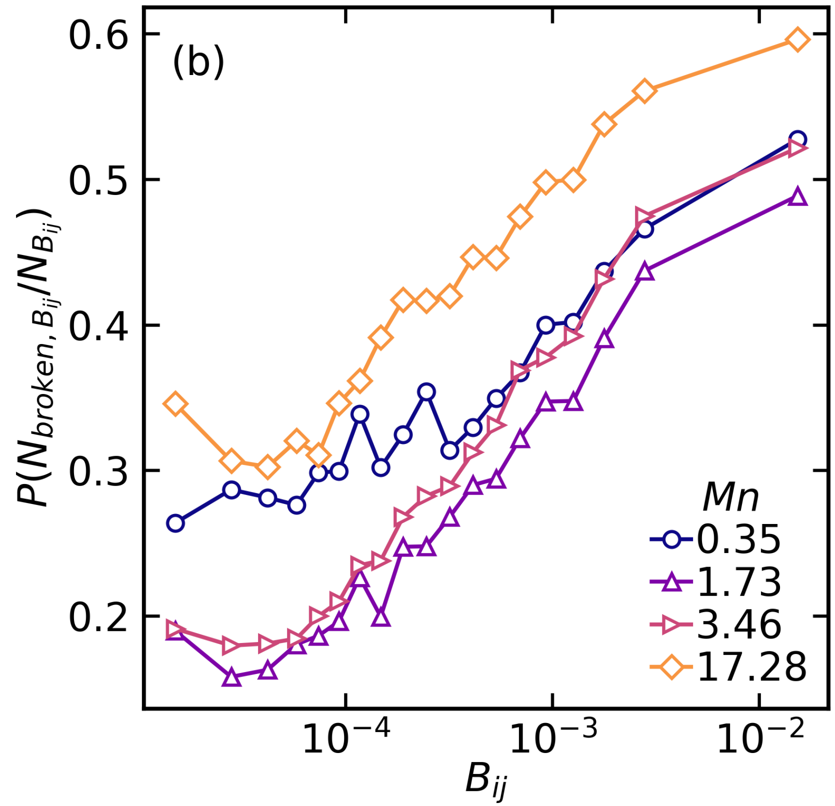

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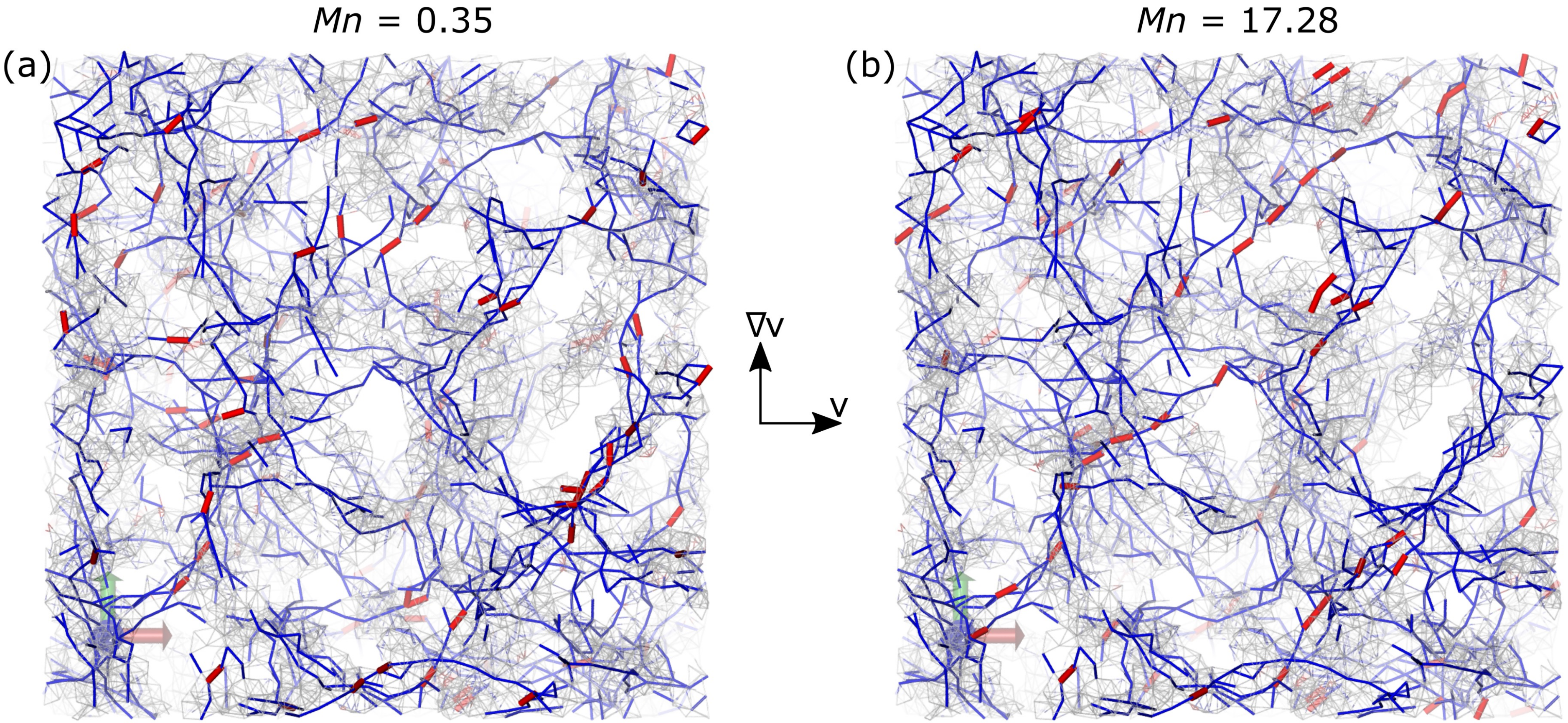
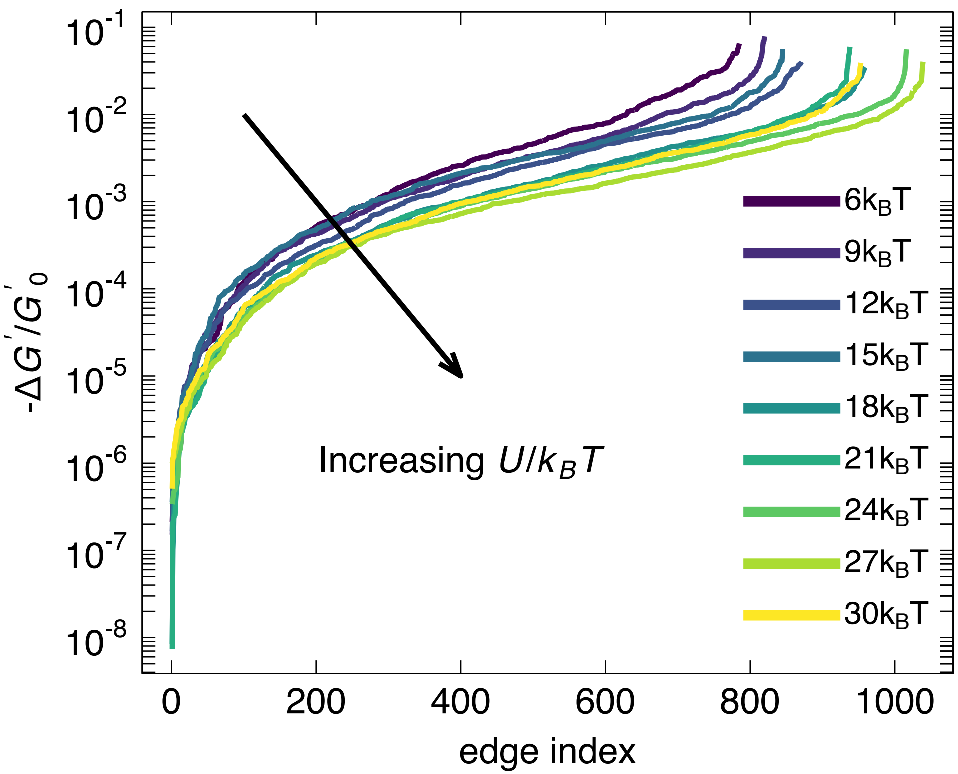
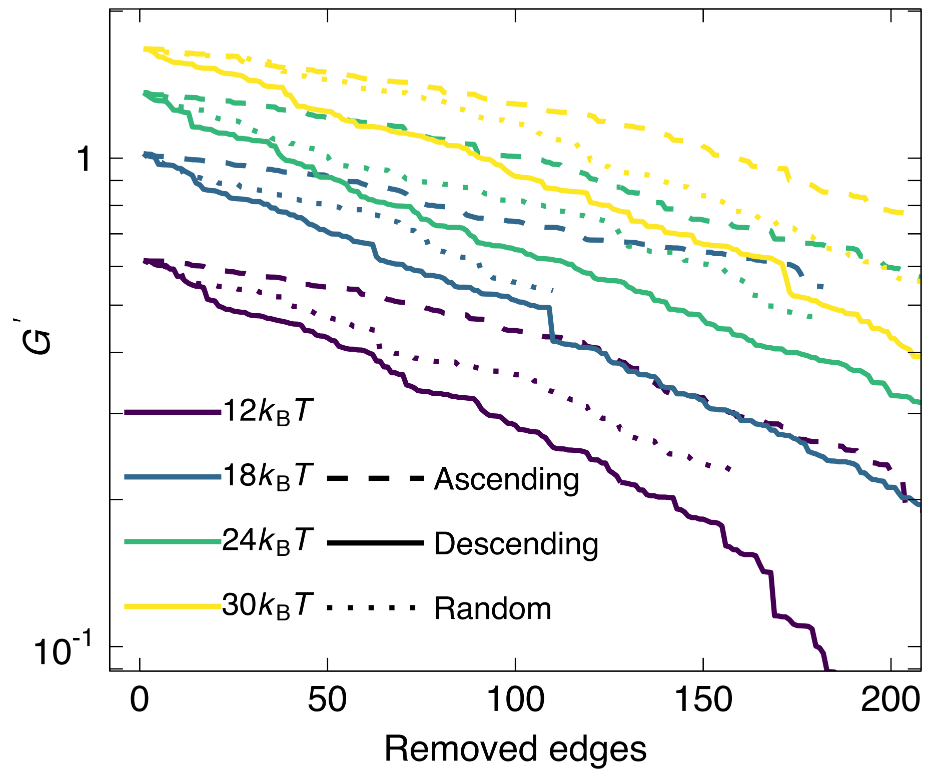


Resilience of the cluster network

First, we need to decide on which edges to remove

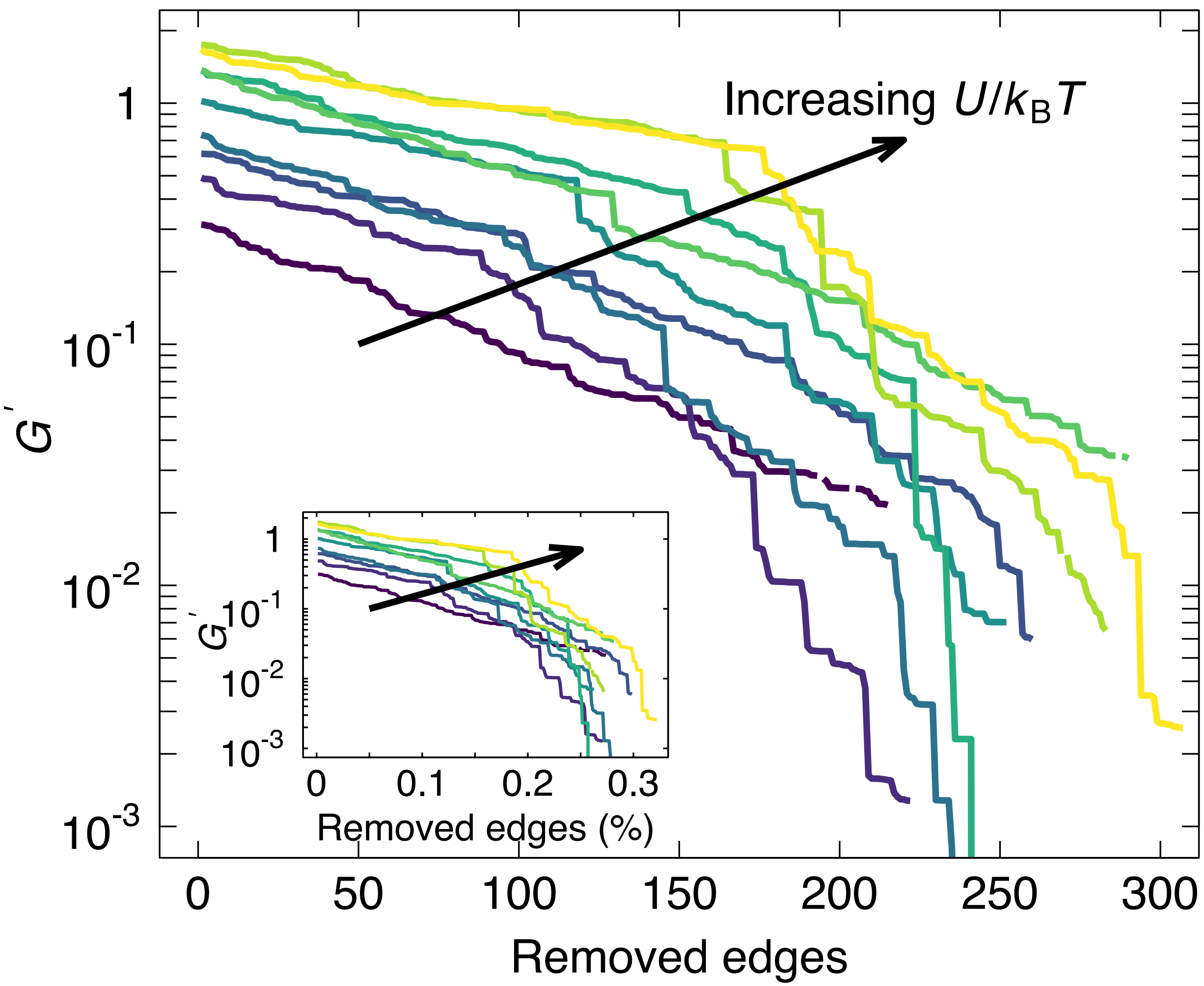
Loss of bonds with higher betweenness centrality is more detrimental to the network's elasticity, so we attack the network of clusters based from the highest BC to its lowest value





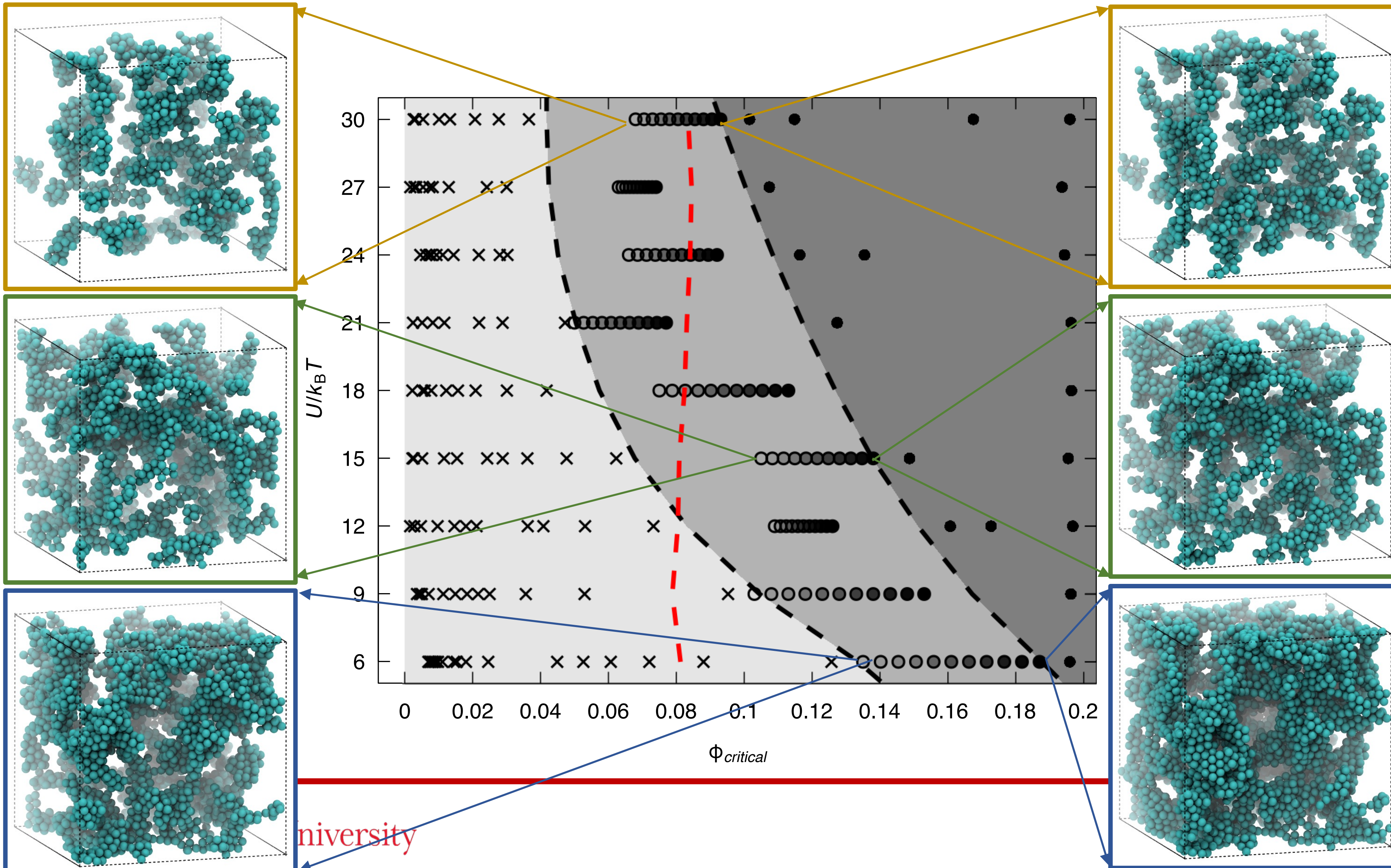
Elasticity-Resilience correlation

The networks with higher elasticity prove to be more resilient



Recovering the *phase diagram*

Back-tracking where the elasticity emerges from resilience



Recovering the *phase diagram*

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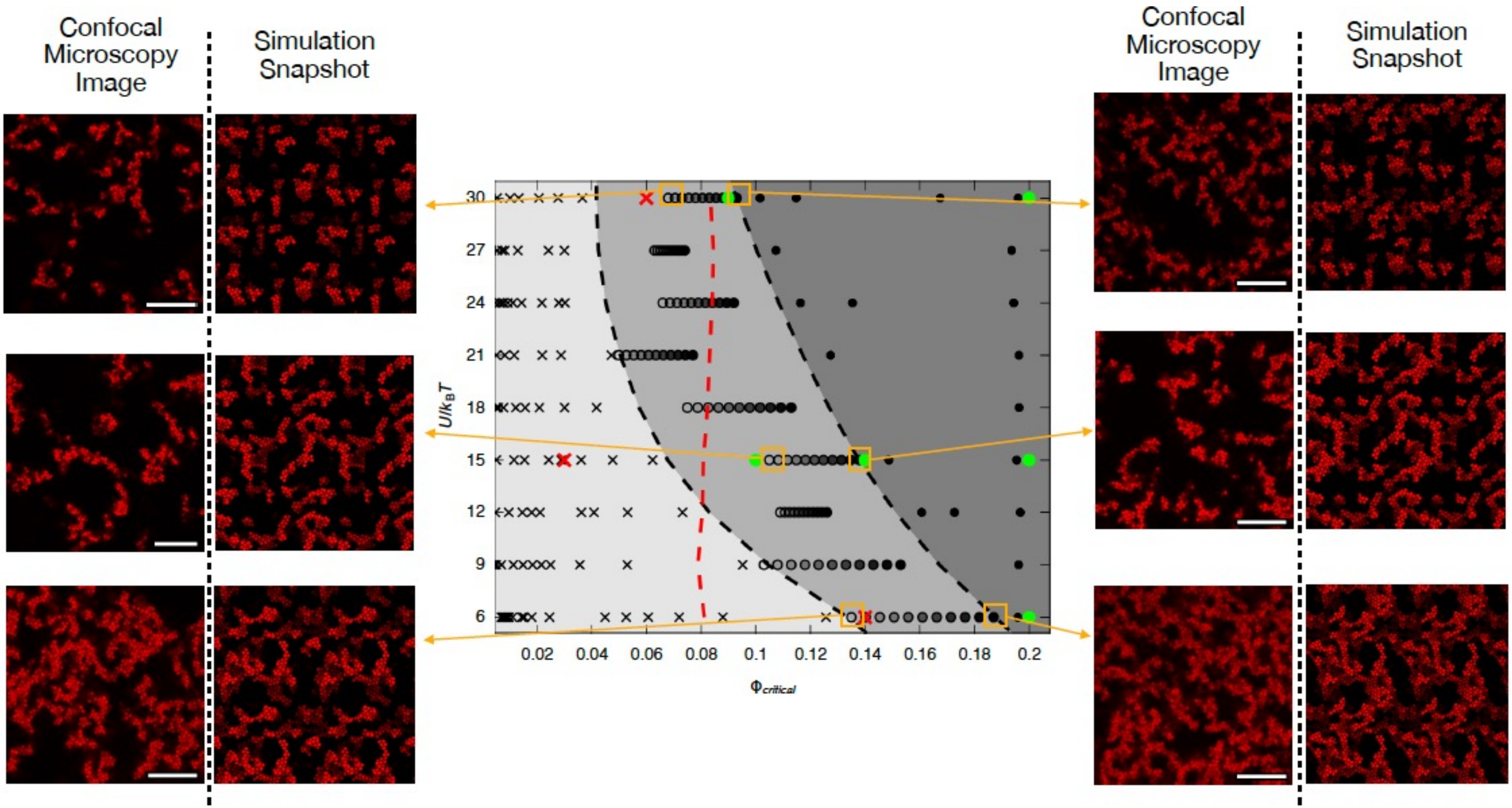
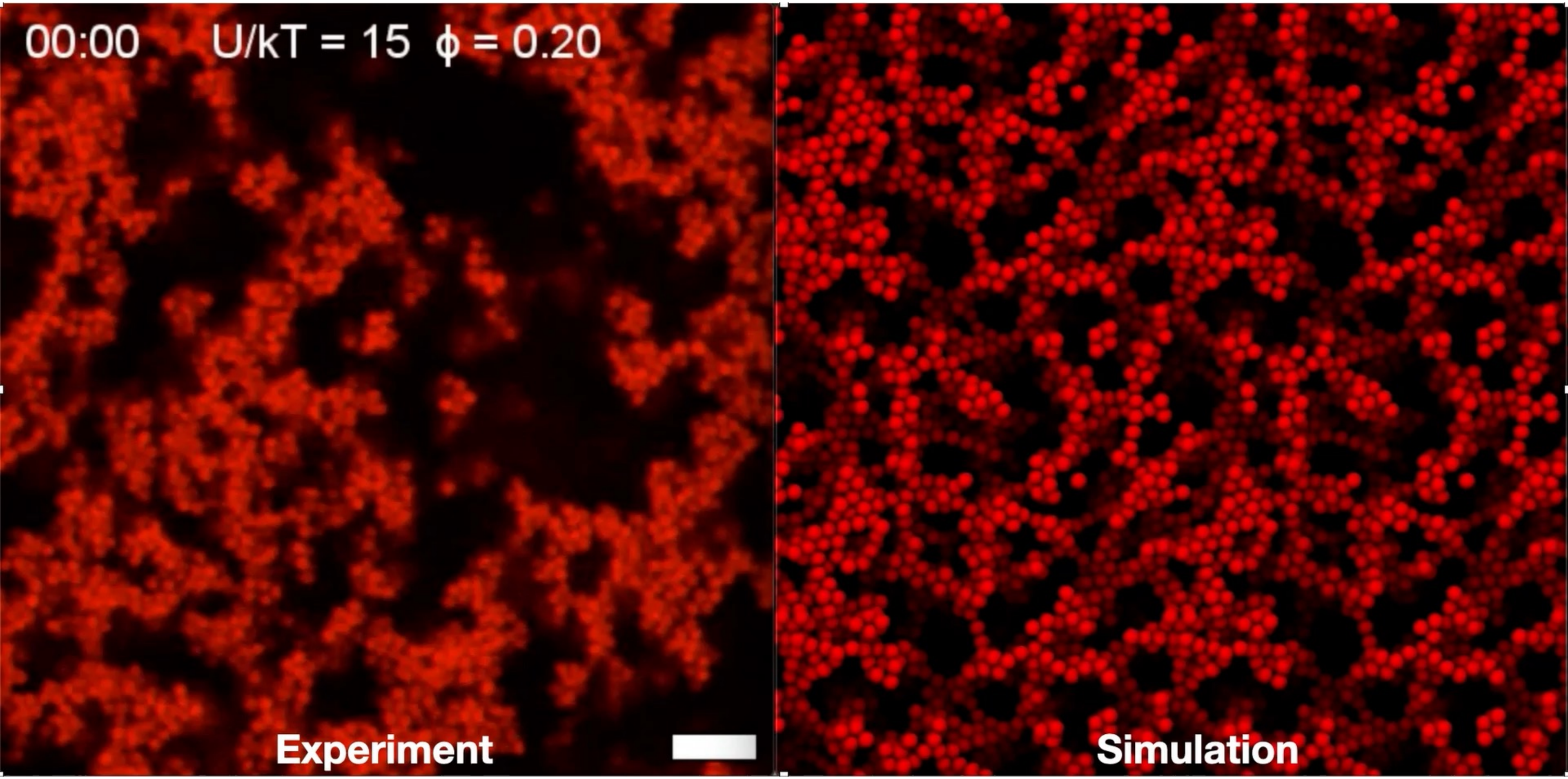


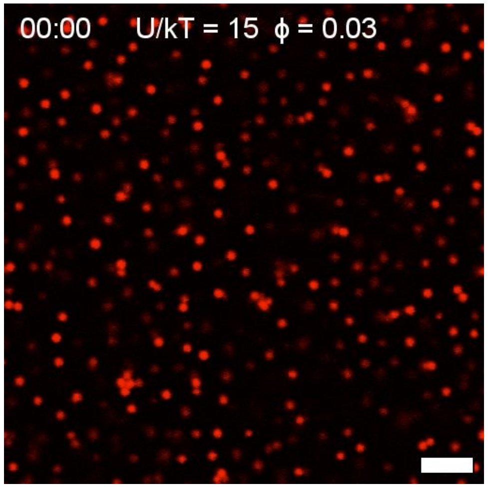
Visualizing the *phase diagram*

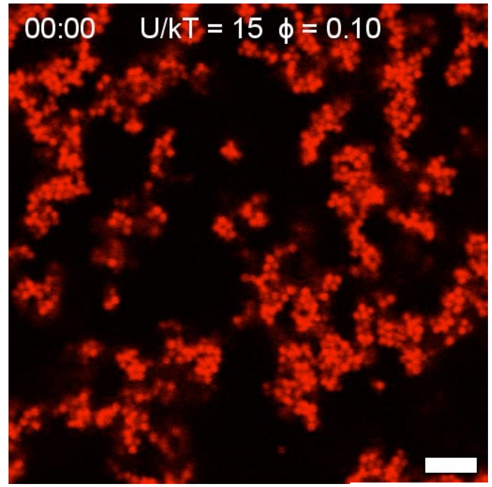
Simulation and experiments indeed recover same dynamics

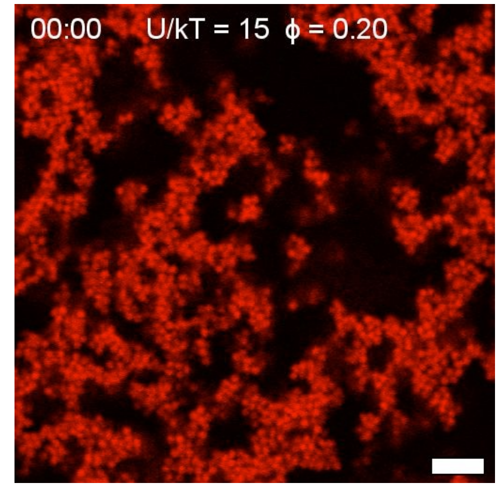


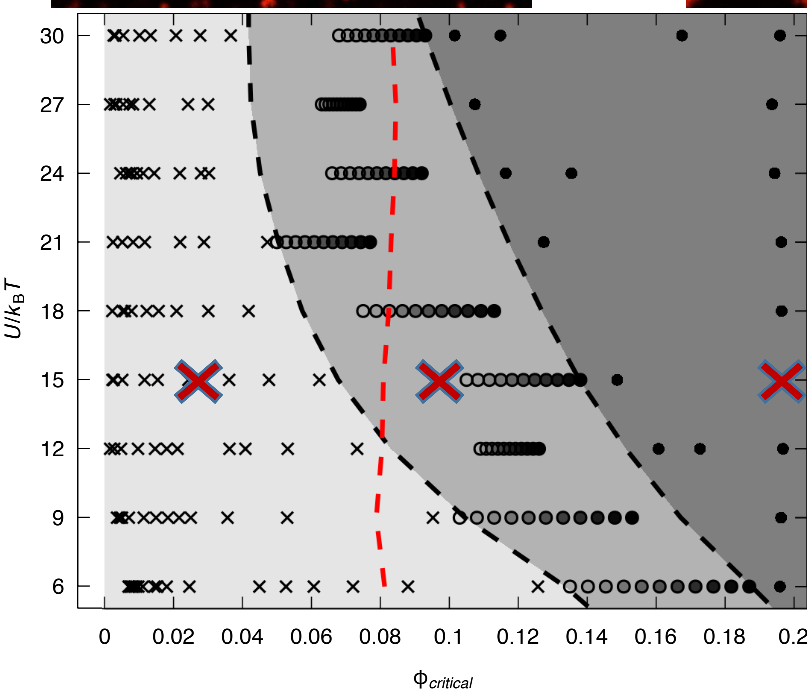
Visualizing the *phase diagram*

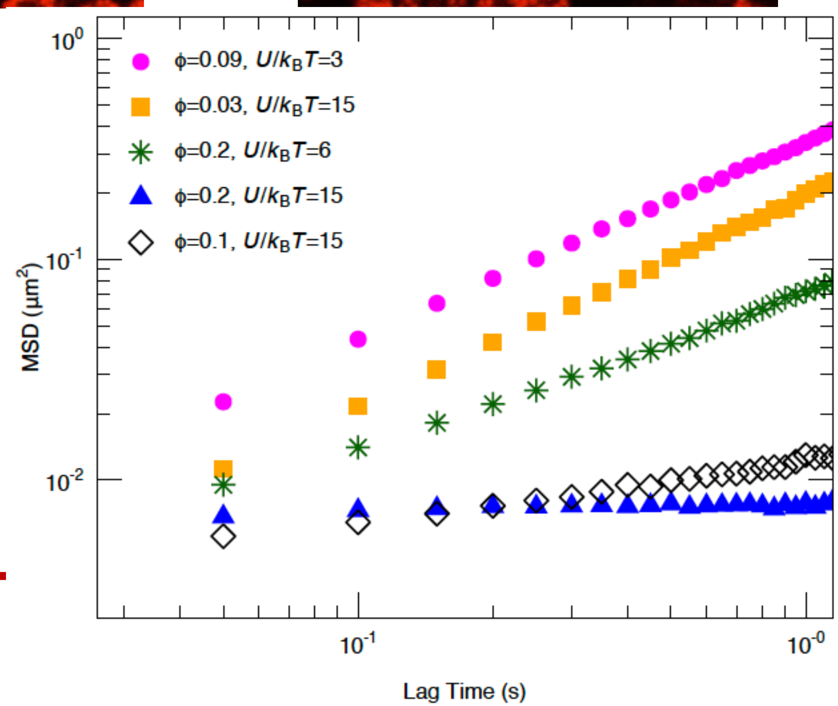
How do we know these are solid/fluid or gel/suspension?





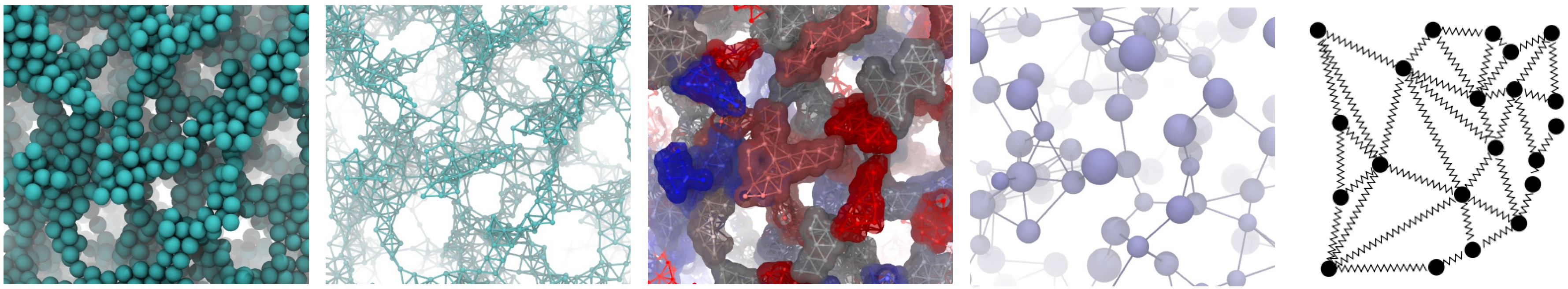




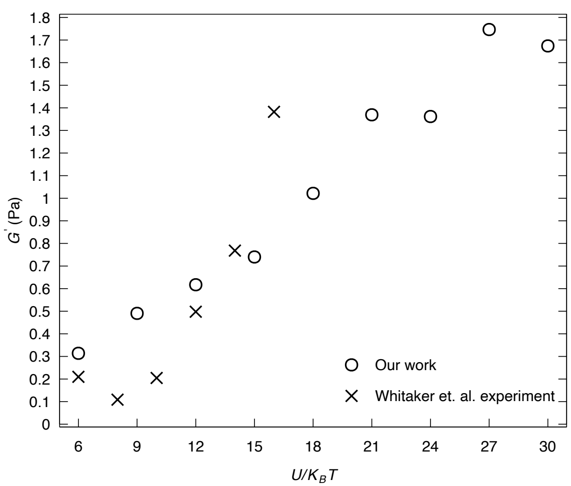


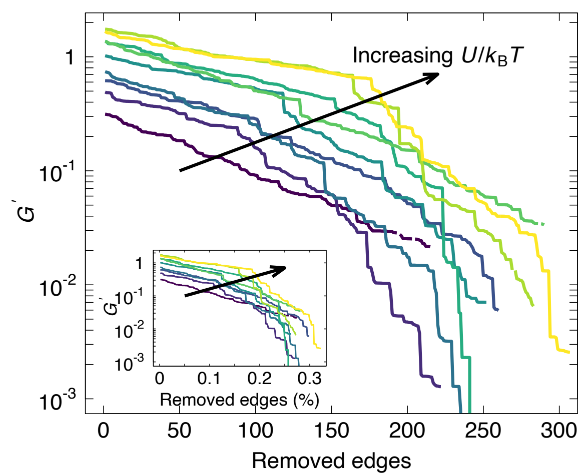
Summary 1

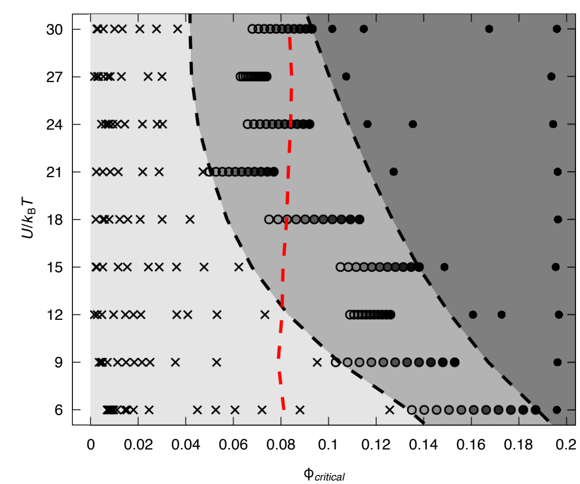
Coarse-Graining the gel network



Resilience-Elasticity correlation

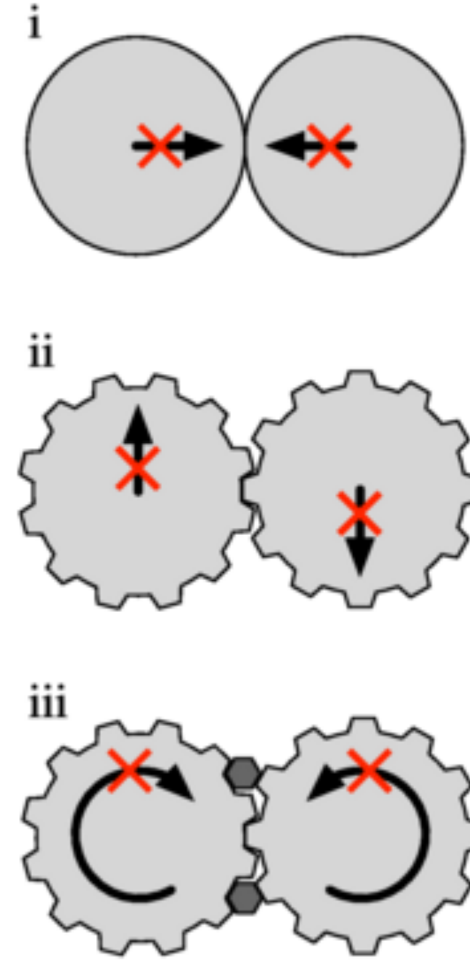






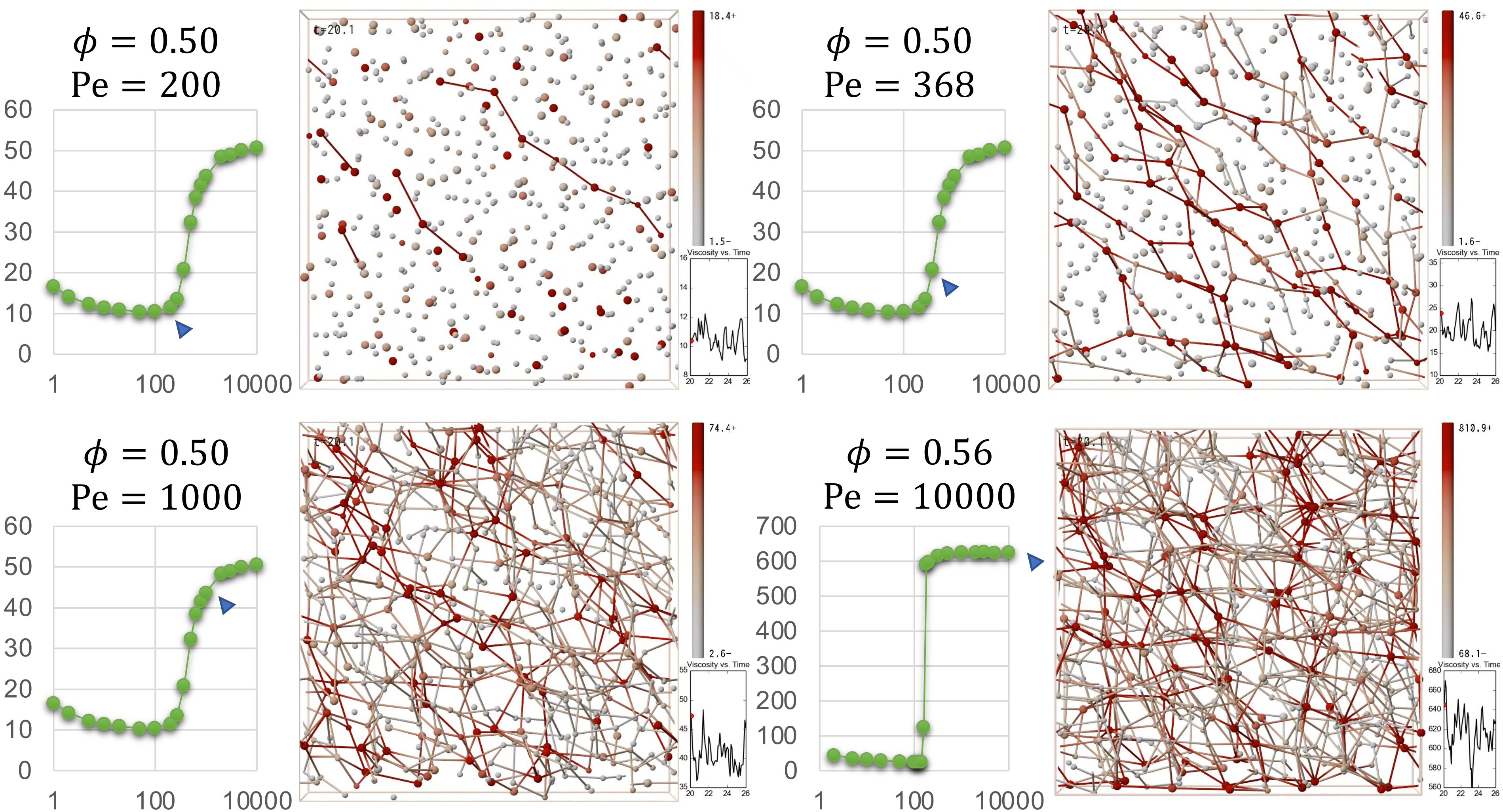
Shear Thickening: A constraint-based view

- We won't consider the source of constraint here



Singh et al., **PRL**, 2020

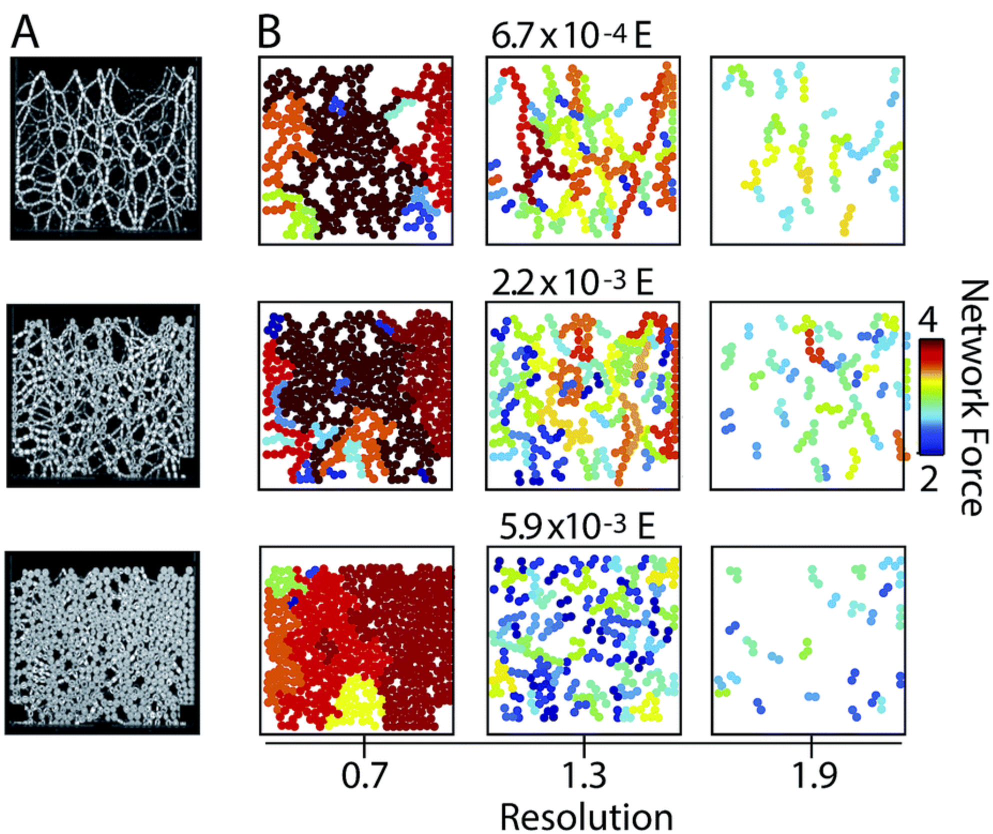
Force/contact network in ST suspensions



Wang, Jamali and Brady, *JOR*, 2020

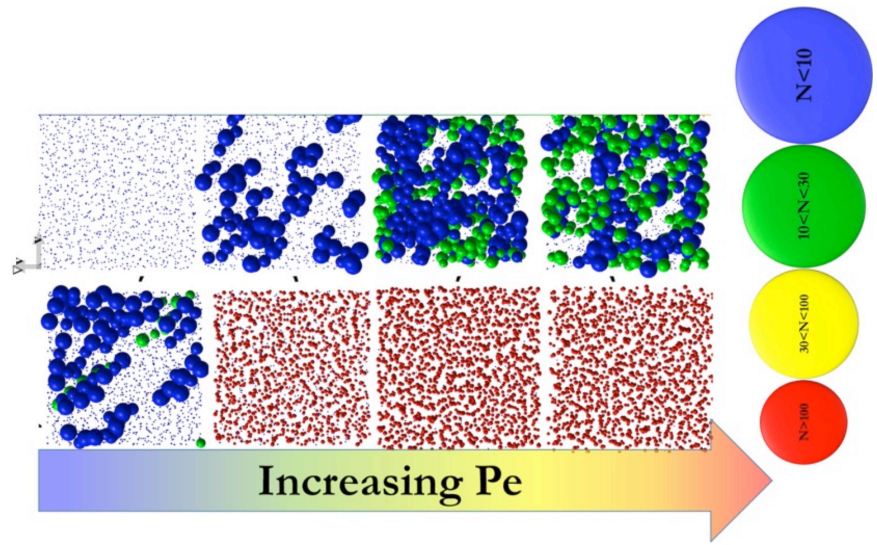
Network physics of particulate systems

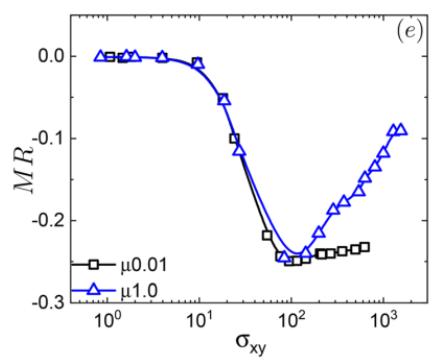
Force chains in granular systems

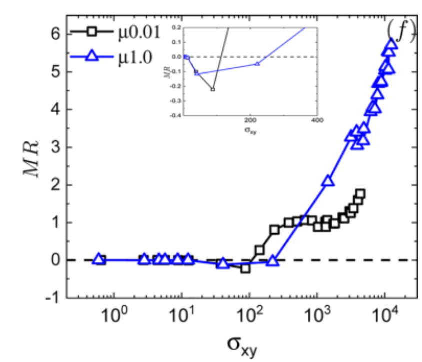


Bassett/Daniels, *Soft Matter*, 2015

Bassett/Daniels, *PRE*, 2016

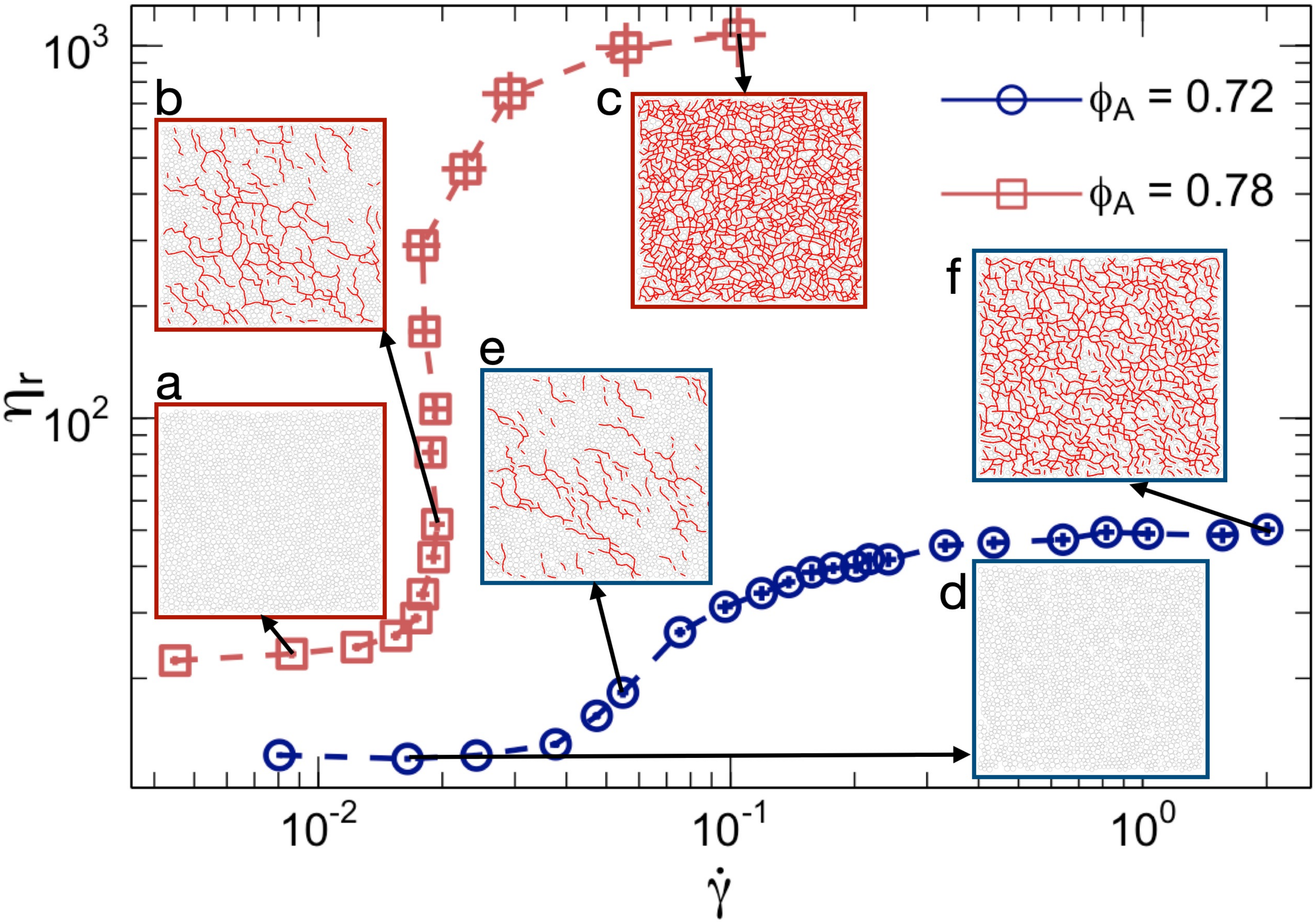




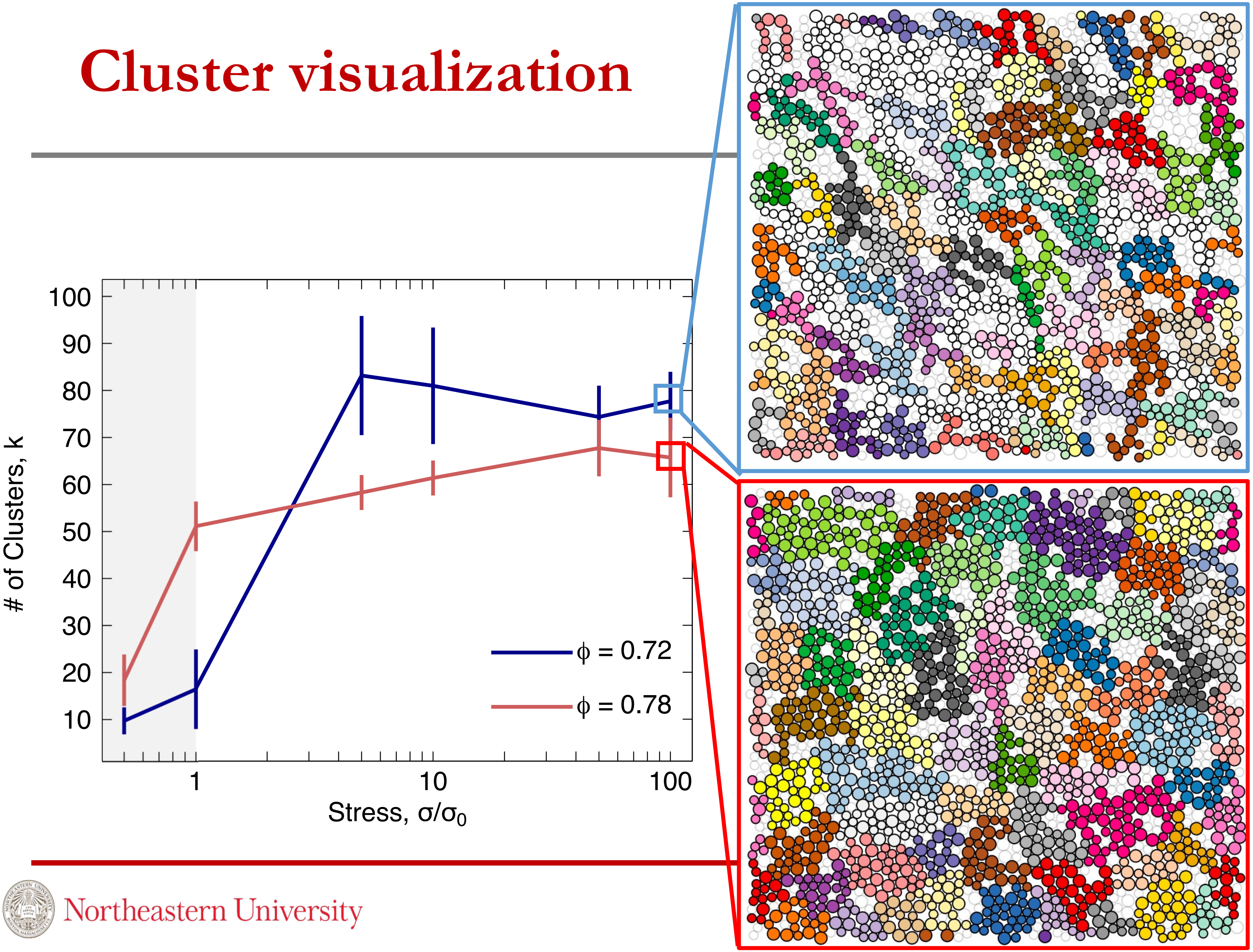


Boromand et al., *JOR*, 2017

Emergence of the network in CST/DST

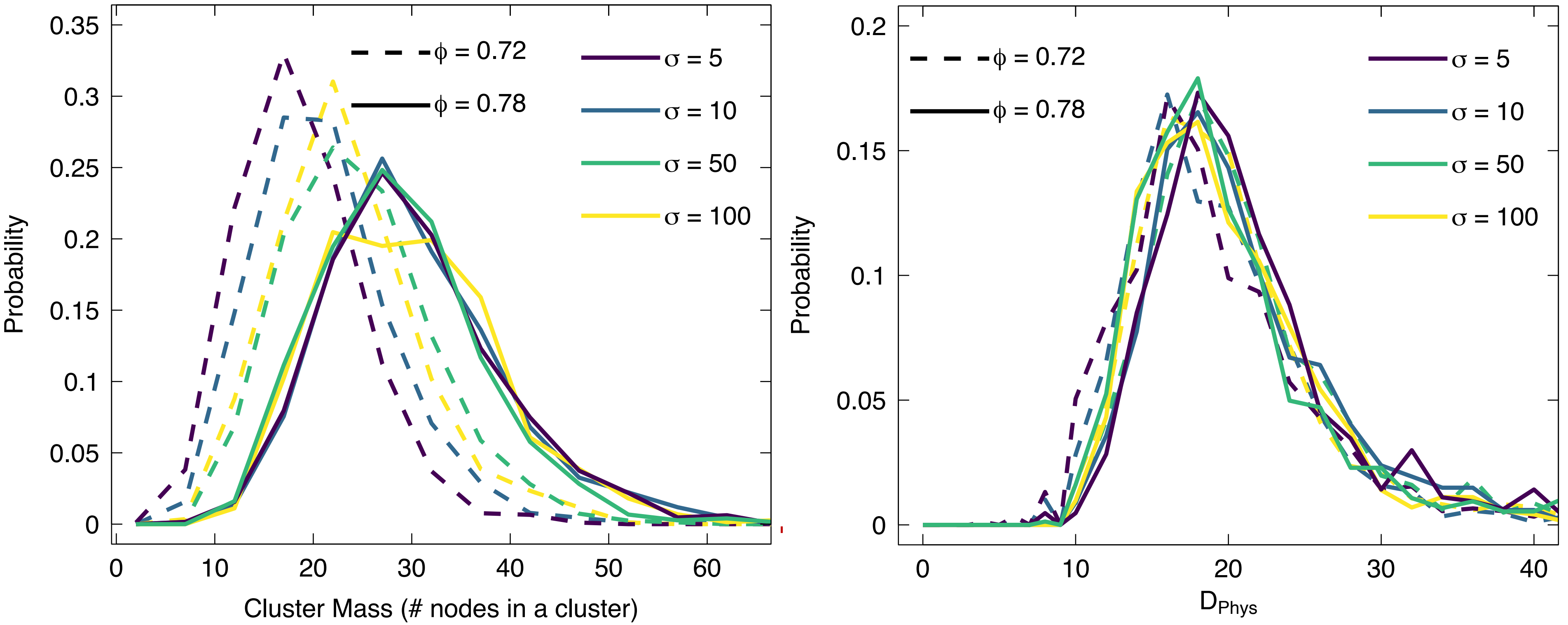


Cluster visualization



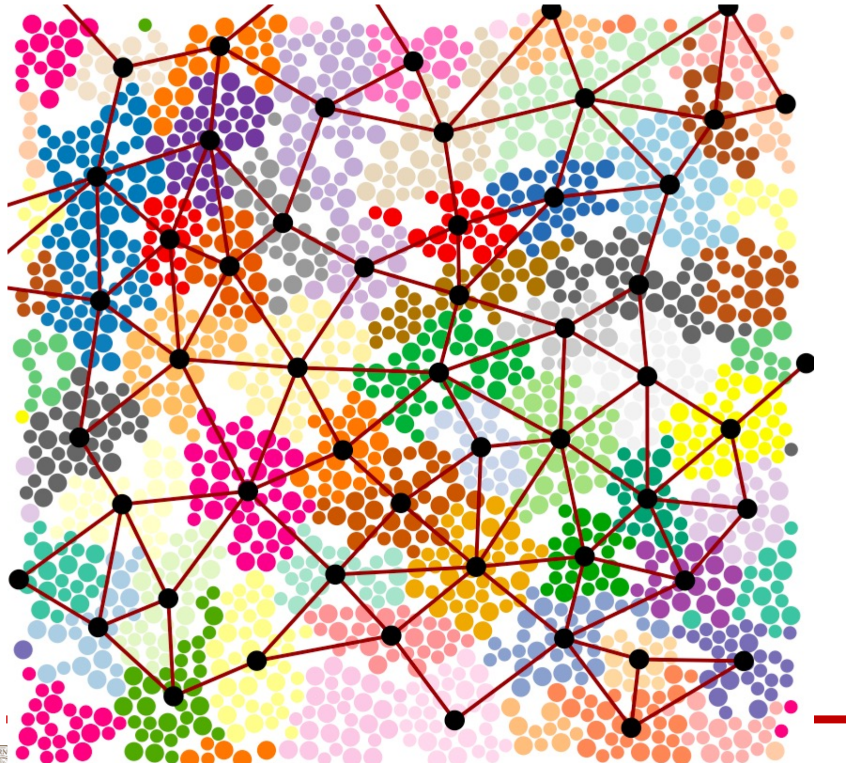
Cluster characteristics

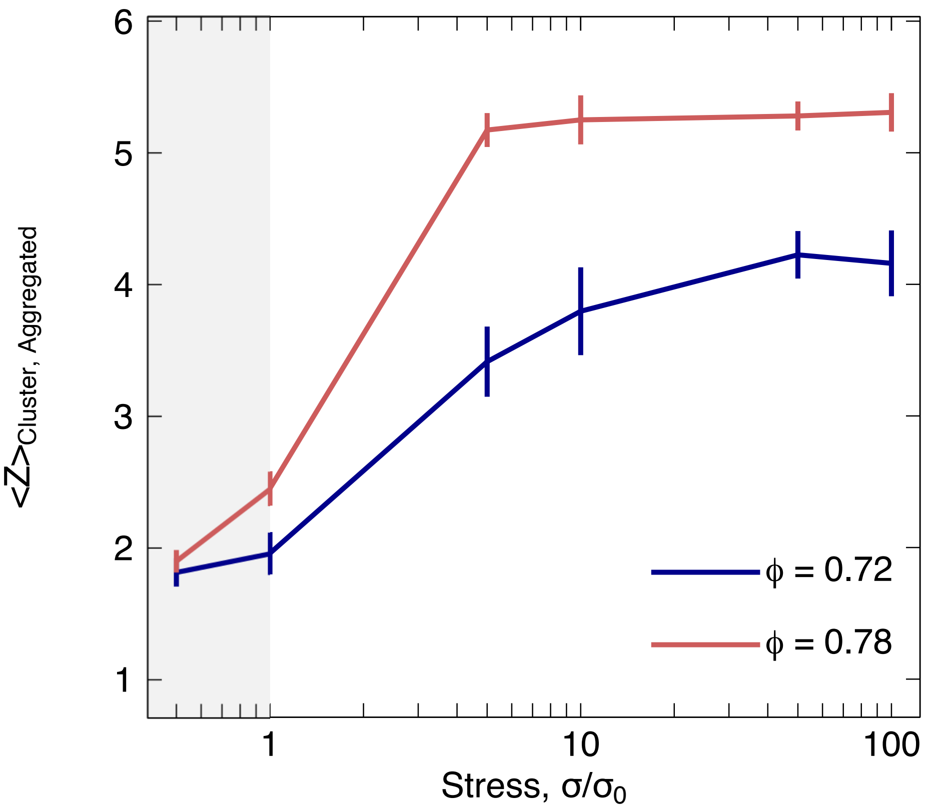
- DST clusters have many more particles in them
- DST cluster masses are rather rate-independent
- CST and DST cluster sizes are very stable



Coarse-graining the network

- Each DST cluster has an extra neighbor compared to each CST cluster in STS
    - But so did the individual particles in CST and DST

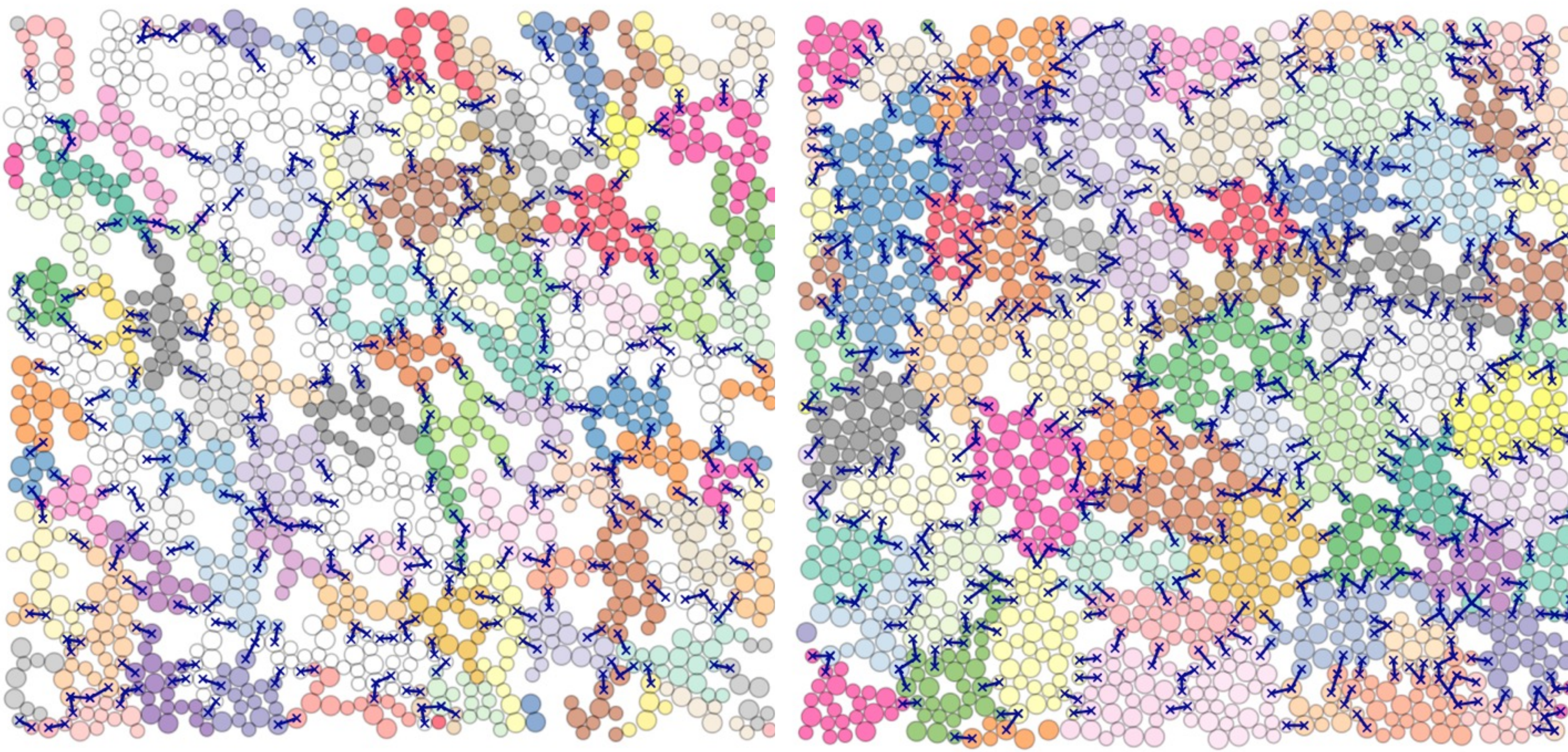




But how many cluster-cluster connections?

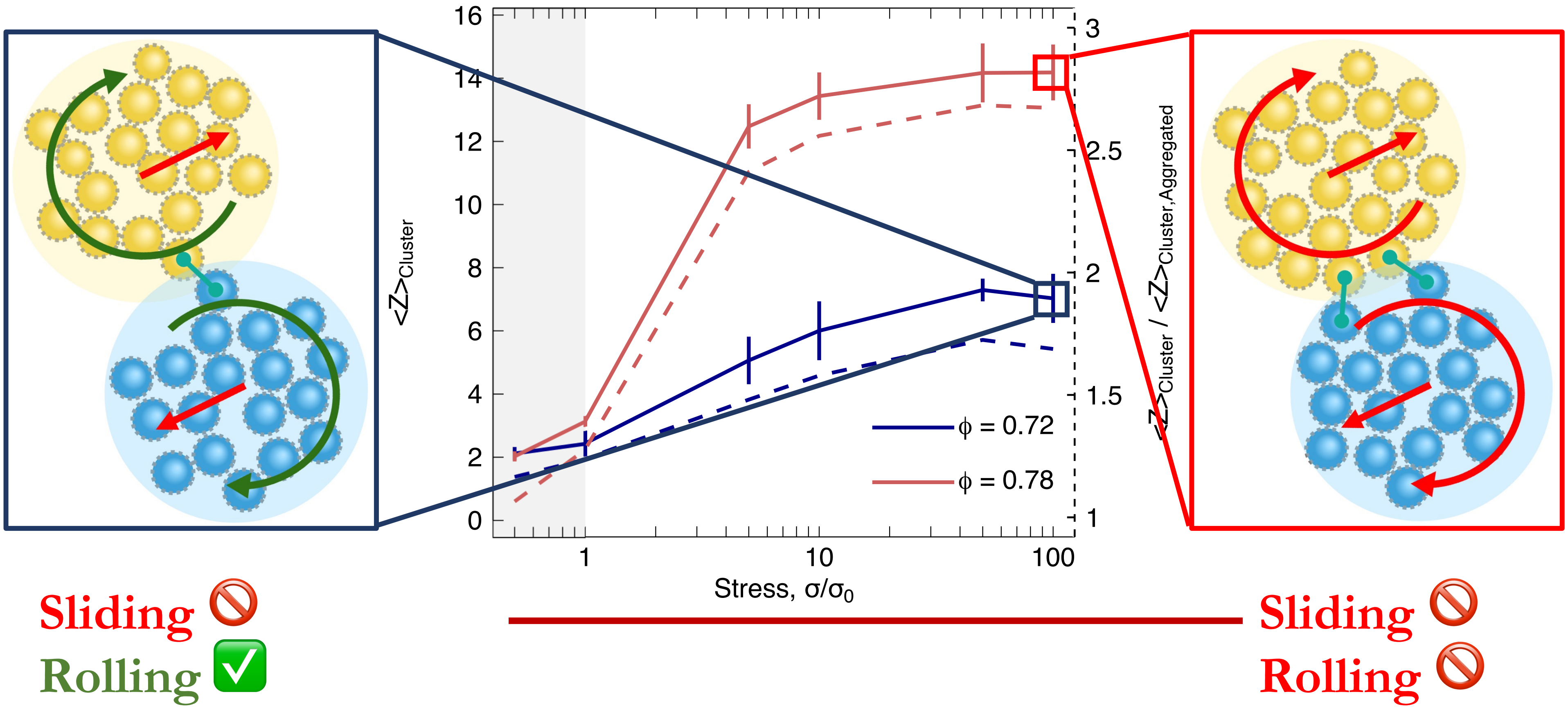
CST

DST

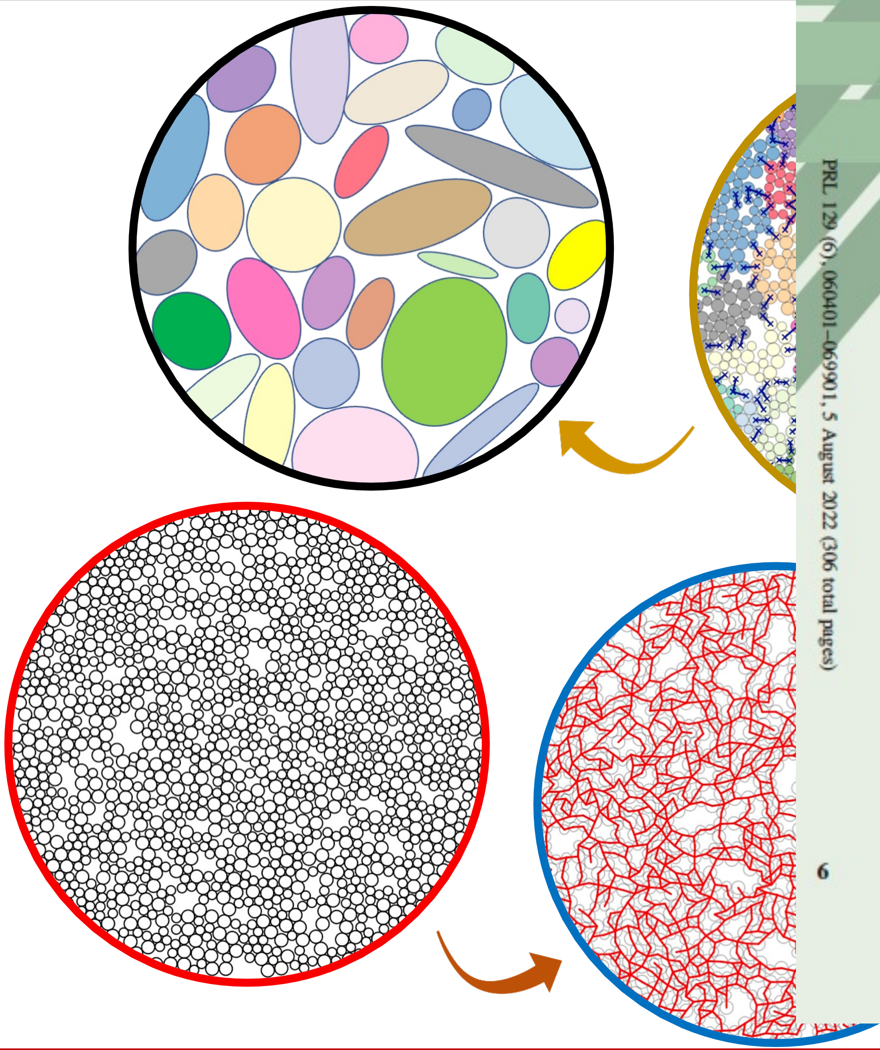


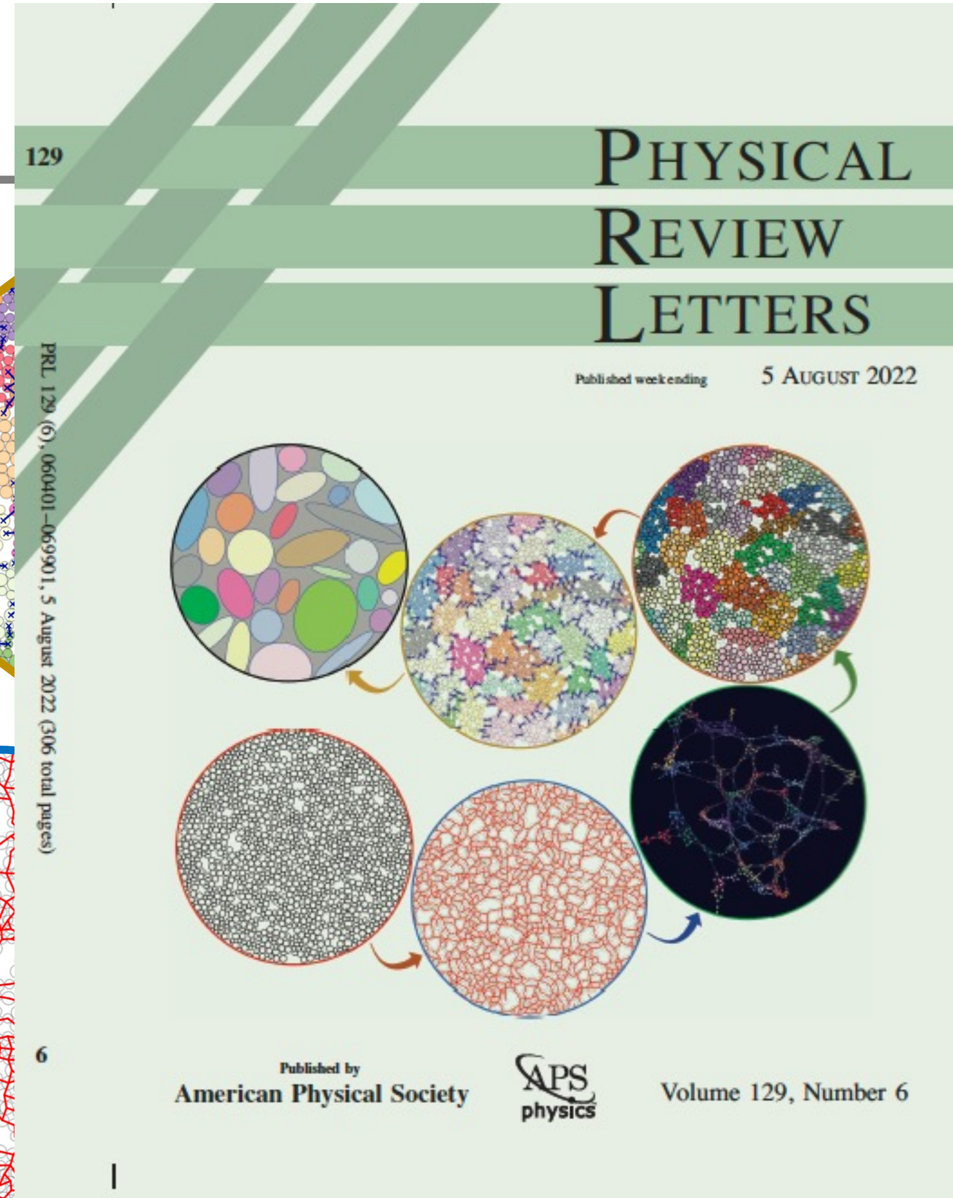
Cluster dynamics in CST vs. DST

- Each cluster-cluster connection in:
  - DST suspension represents multiple particle-level contact (2-3)
  - CST suspension represents single particle-level contact (1-2)



Summary 2

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