Mechanical Transitions in Cells and Tissues: Day 2

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Boulder School 2001: Nonequilibrium Statistical Physics: Glasses, transport & friction, biological systems, and turbulence

July 2-27, 2001

Scientific Coordinators:

E. Bodenschatz (Cornell)
M. C. Marchetti (Syracuse)
A. A. Middleton (Syracuse)

Boulder School 2024: Self-Organizing Matter: From Inanimate to the Animate

July 1-26, 2024

Scientific Coordinators

Shiladitya Banerjee (Carnegie Mellon)
Andela Saric (IST Austria)
Eric R. Dufresne (Cornell)
Margaret L. Gardel (Chicago)

Trajectory

Recap: Rigidity Percolation in Spring Networks: Maxwell criterion

J. C. Maxwell, Philos. Mag., 1864

Consider a lattice of N nodes in d dimensions, z coordination number, and bond occupation probability p

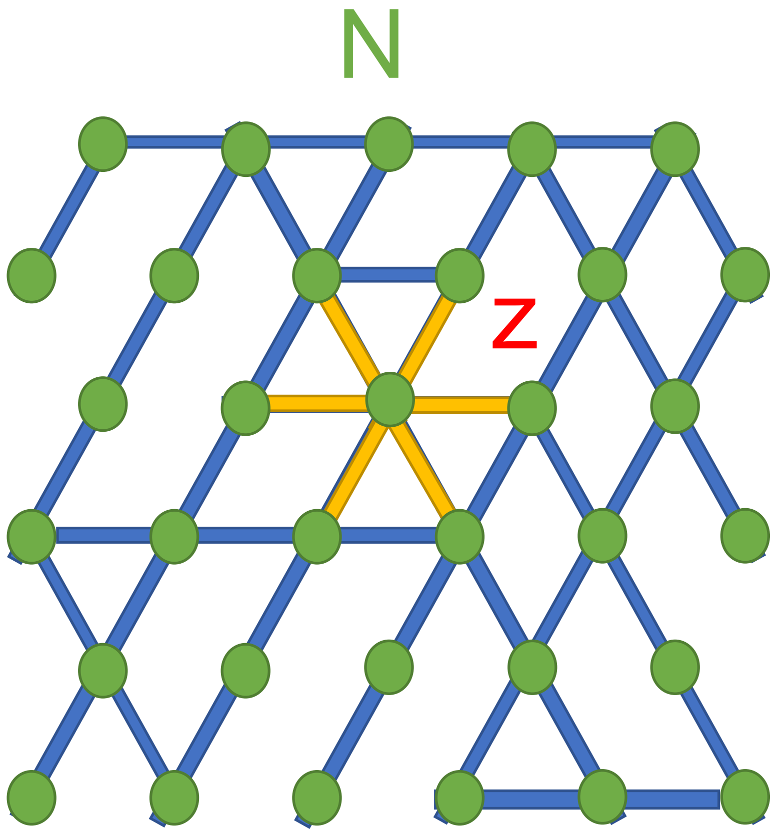
# of degrees of freedom $= Nd$

constraints $= \frac{N}{2} z p$

Maxwell criterion: Balance # constraints and # degrees of freedom

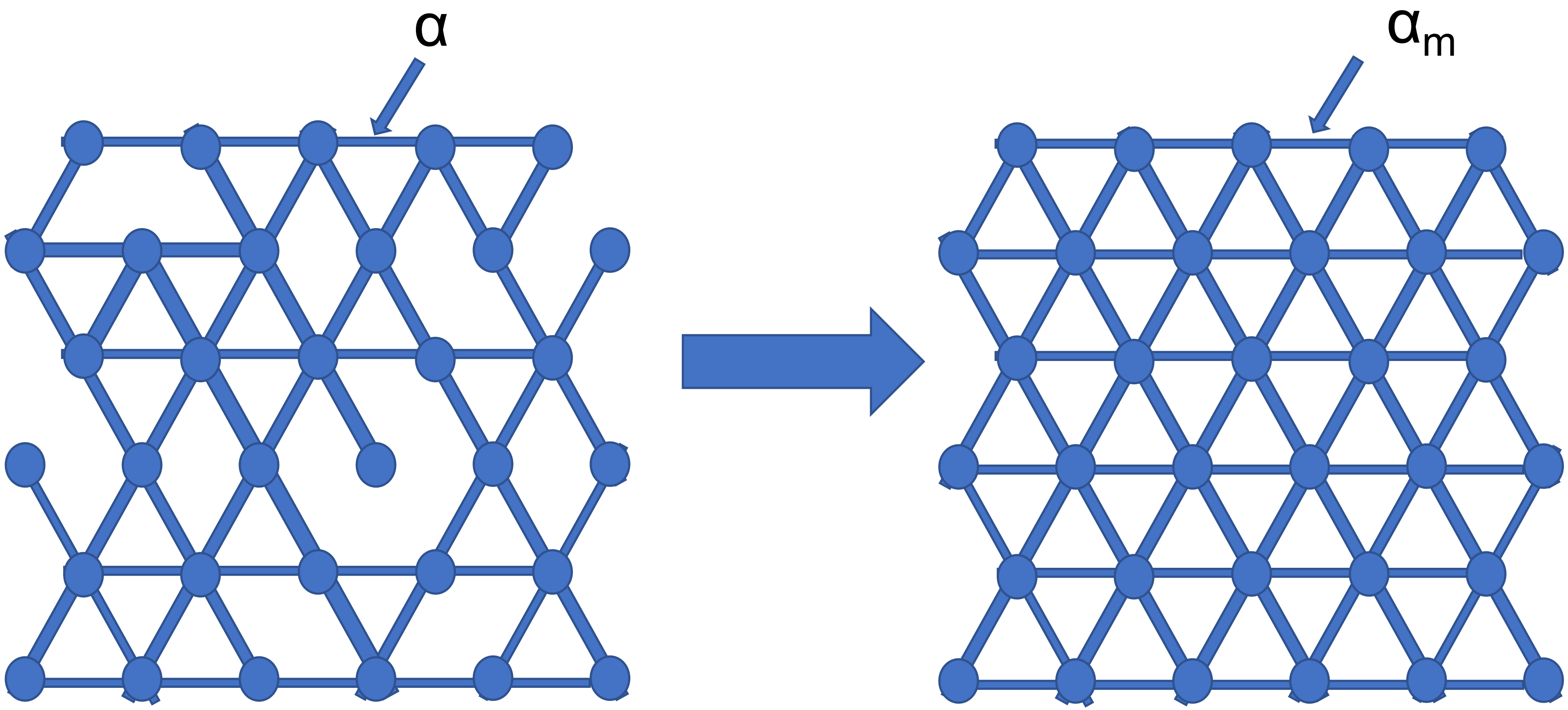
$p_c = 2d/z, \quad z_c = 2d$ Isostatic coordination

$p > p_c, z > z_c$ Condition for rigidity



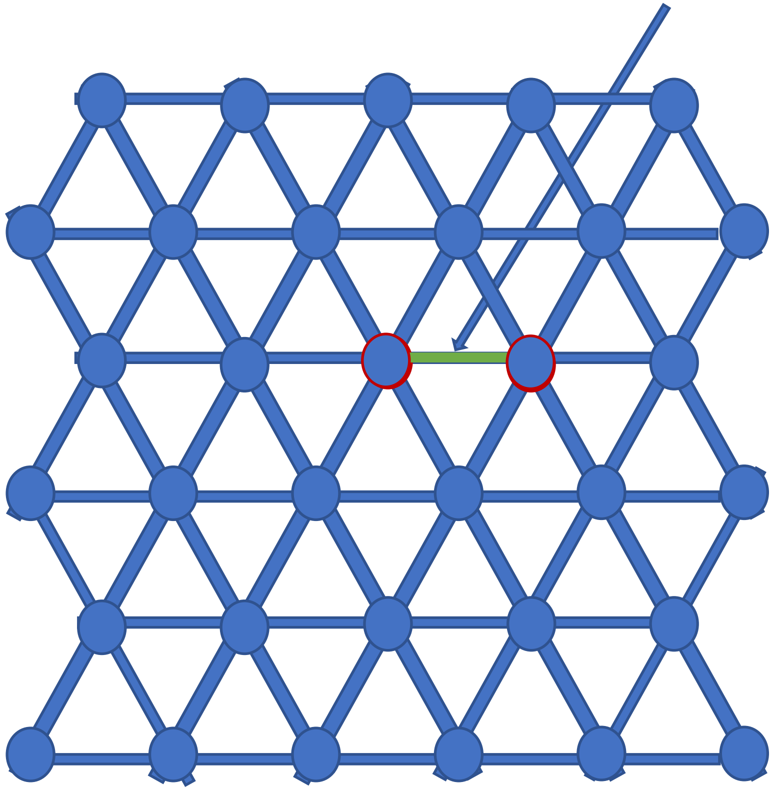
Recap: EMT for central force (spring) networks

Feng, Thorpe, Garboczi, PRB 1985



Recap: EMT for central force (spring) networks

$$\alpha_{eff} = \frac{\alpha_m}{\alpha^*} - \alpha_m + \alpha$$



Extra displacement due to replaced bond

$$\delta_u = \frac{f}{\frac{\alpha_m}{\alpha^*} - \alpha_m + \alpha}$$

$$f = \delta_{um}(\alpha_m - \alpha)$$

$$\boxed{\delta_u = \frac{\delta_{um}(\alpha_m - \alpha)}{\frac{\alpha_m}{\alpha^*} - \alpha_m + \alpha}}$$

Recap: EMT for central force (spring) networks

Replace bonds with spring constant α_m by α (probability p) and by 0 (probability (1-p)).

When averaged over the entire system, the fluctuations δ_u should go to 0.

$$\int \frac{\alpha_m - \alpha'}{\frac{\alpha_m}{a^*} - \alpha_m + \alpha'} * P(\alpha')\, d\alpha' = 0$$

Where $P(\alpha') = p\delta(\alpha' - \alpha) + (1-p)\delta(\alpha')$

$$\frac{\alpha_m}{\alpha} = \frac{p - a^*}{1 - a^*}$$

Recap: EMT for central force (spring) networks

What is a^*?

- Geometric constant relating geometry of lattice to rigidity
- Evaluated in terms of Dynamical Matrix

$$a^* = \frac{1}{3} \sum_q Tr\left[\boldsymbol{D}\ (q) \cdot \boldsymbol{D}^{-1}(q)\right]$$

Dynamical Matrix

Expand the total energy about structural equilibrium coordinates

$$E = E_0 + \frac{\partial E}{\partial u}.u + \frac{1}{2!}\frac{\partial^2 E}{\partial u^2}.u^2 + \frac{1}{3!}\frac{\partial^3 E}{\partial u^3}u^3 + ...$$

At equilibrium the O(1) term is 0.

$$E = E_0 + \frac{1}{2}\sum \boldsymbol{u}_{\alpha,\kappa,a}.\Phi^{\kappa,\kappa'}_{\alpha,\alpha'}.\boldsymbol{u}_{\kappa',\alpha',a} + ...$$

where $\boldsymbol{u}_{\alpha,\kappa,a}$ is the displacement of atom κ in unit cell *a* in Cartesian direction α

Dynamical Matrix

Expand the total energy about structural equilibrium coordinates

$$E = E_0 + \frac{\partial E}{\partial u}.u + \frac{1}{2!}\frac{\partial^2 E}{\partial u^2}.u^2 + \frac{1}{3!}\frac{\partial^3 E}{\partial u^3}u^3 + ...$$

At equilibrium the O(1) term is 0.

$$E = E_0 + \frac{1}{2}\sum \boldsymbol{u}_{\alpha,\kappa,a}.\Phi^{\kappa,\kappa'}_{\alpha,\alpha'}.\boldsymbol{u}_{\kappa',\alpha',a} + ...$$

In the Harmonic Approximation *O(3)* and higher order terms are negligible

Dynamical Matrix

$$E = E_0 + \frac{1}{2}\sum \boldsymbol{u}_{\alpha,\kappa,a}.\Phi^{\kappa,\kappa'}_{\alpha,\alpha'}.\boldsymbol{u}_{\kappa',\alpha',a}$$

The matrix of *force constants*

$$\boxed{\begin{aligned}\Phi^{\kappa,\kappa'}_{\alpha,\alpha'}(a) &= \frac{\partial^2 E}{\partial \boldsymbol{u}_{\alpha,\kappa}\partial \boldsymbol{u}_{\kappa',\alpha'}} \\ &= -\frac{\partial F_{\boldsymbol{u}_{\alpha,\kappa,a}}}{\partial \boldsymbol{u}_{\kappa',\alpha',a}}\end{aligned}}$$

The dynamical matrix is the Fourier transform of this force constant matrix

Dynamical Matrix

$$E = E_0 + \frac{1}{2} \sum \boldsymbol{u}_{\alpha,\kappa,a} . \Phi^{\kappa,\kappa'}_{\alpha,\alpha'} . \boldsymbol{u}_{\kappa',\alpha',a}$$

The matrix of *force constants*

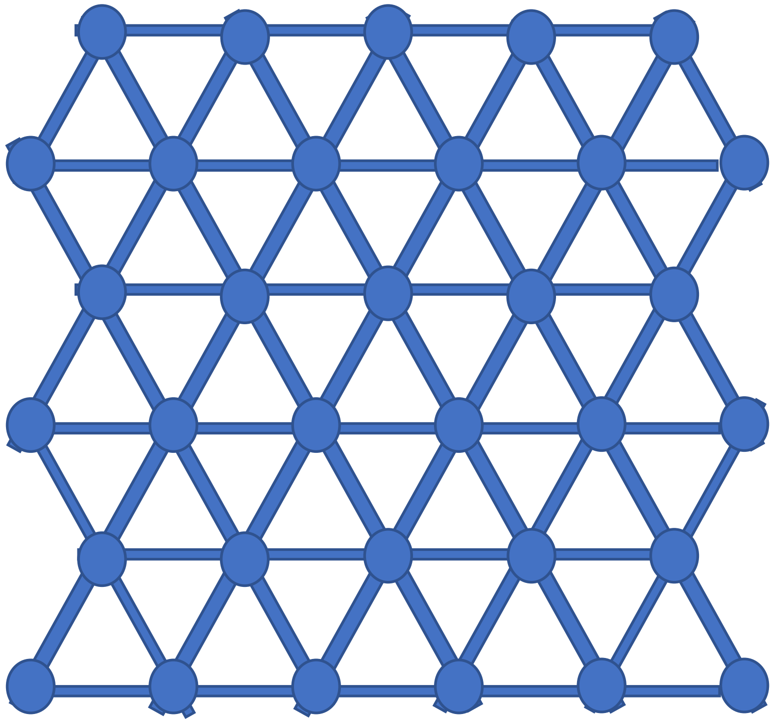
$$\boxed{\begin{aligned} \Phi^{\kappa,\kappa'}_{\alpha,\alpha'}(a) &= \frac{\partial^2 E}{\partial \boldsymbol{u}_{\alpha,\kappa} \partial \boldsymbol{u}_{\kappa',\alpha'}} \\ &= -\frac{\partial F_{\boldsymbol{u}_{\alpha,\kappa,a}}}{\partial \boldsymbol{u}_{\kappa',\alpha',a}} \end{aligned}}$$

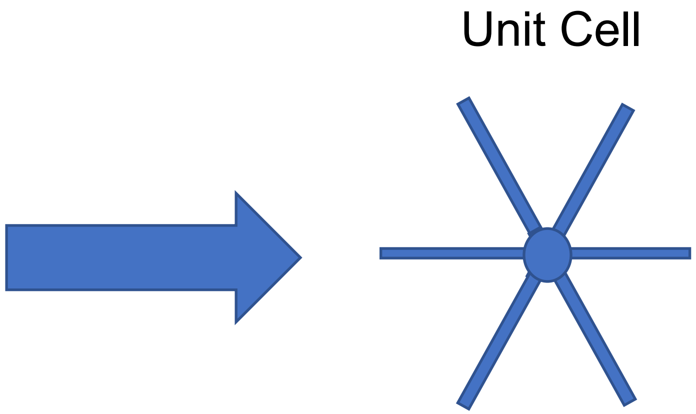
The dynamical matrix is the Fourier transform of this force constant matrix

To obtain vibrational modes, solve $D^{\kappa,\kappa'}_{\alpha,\alpha'}(\boldsymbol{q}) \boldsymbol{\varepsilon}_{m\alpha,\kappa\boldsymbol{q}} = \omega^2_{m,\boldsymbol{q}} \boldsymbol{\varepsilon}_{m\alpha,\kappa\boldsymbol{q}}$

where $\boldsymbol{u}_{\alpha,\kappa} = \boldsymbol{\varepsilon}_{m\alpha,\kappa\boldsymbol{q}} e^{i\boldsymbol{q}.\boldsymbol{R}_{\alpha,\kappa} - \omega t}$

Dynamical Matrix for a Triangular Lattice





$$E_{spring} = \frac{\alpha_m}{2} \sum_{\langle ij \rangle} p_{ij} (\vec{u}_{ij} . \hat{r}_{ij})^2$$

$$\boldsymbol{D}_s(q) \;=\; \alpha_m \sum_{\langle ij \rangle} \left[1 - e^{-i\boldsymbol{q}.\hat{\boldsymbol{r}}_{ij}} \right] \hat{\boldsymbol{r}}_{ij} \hat{\boldsymbol{r}}_{ij}$$

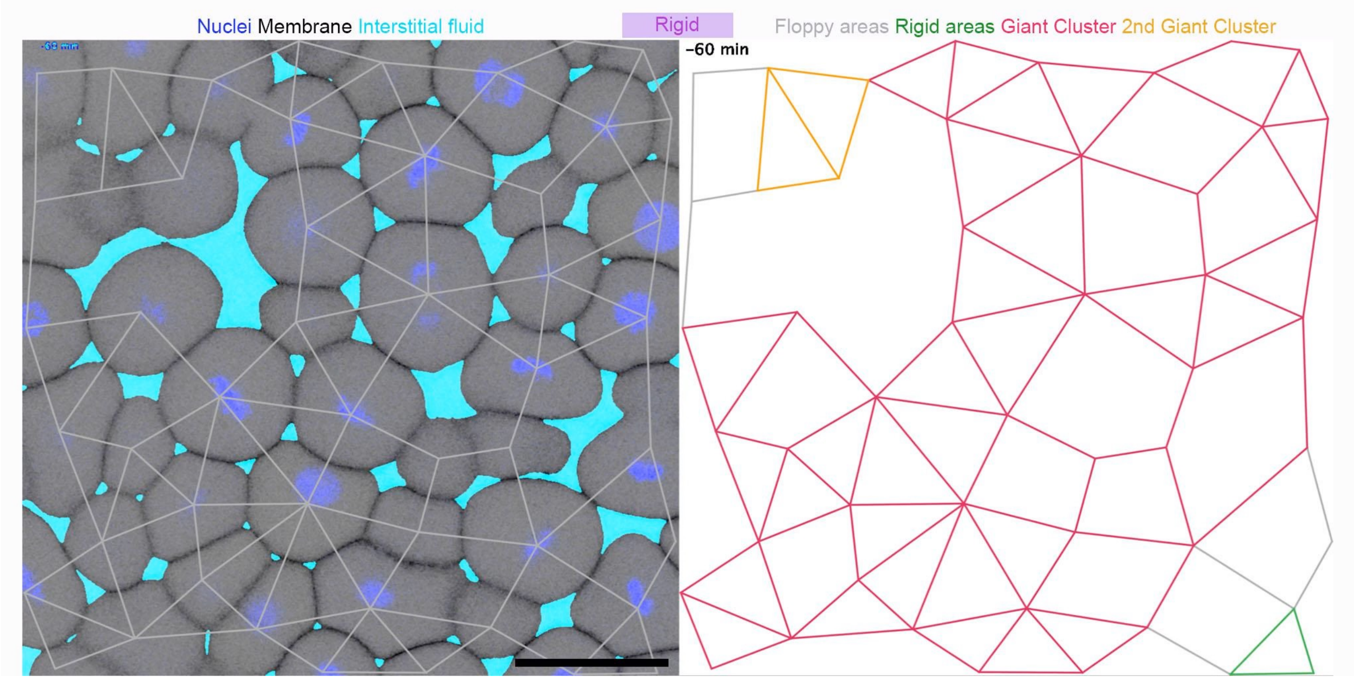
For a spring network on a triangular lattice

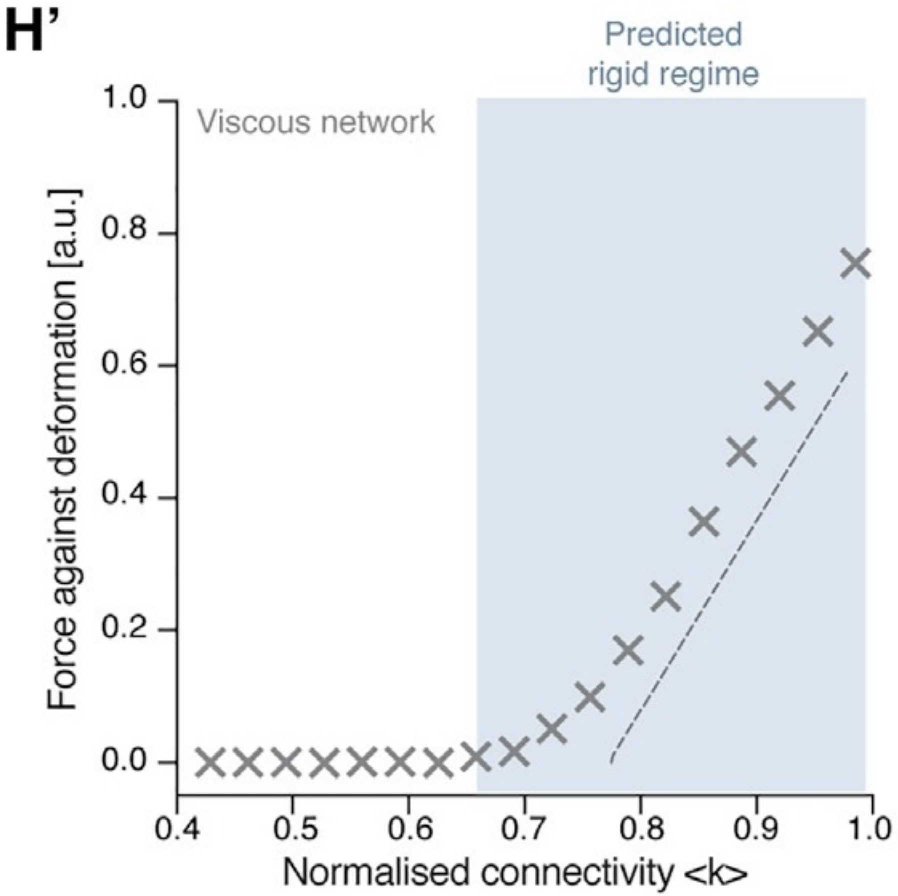
$$a^* = \frac{1}{3}\sum_q Tr\left[\boldsymbol{D}_s(q)\cdot\boldsymbol{D}^{-1}(q)\right] = \frac{2}{3}$$

$$\frac{\alpha_m}{\alpha} = \begin{cases} \frac{p-a^*}{1-a^*} & \text{if } p > a^* \\ 0 & \text{if } p \le a^* \end{cases}$$

$p_c = \frac{2}{3}$ is our rigidity percolation threshold!

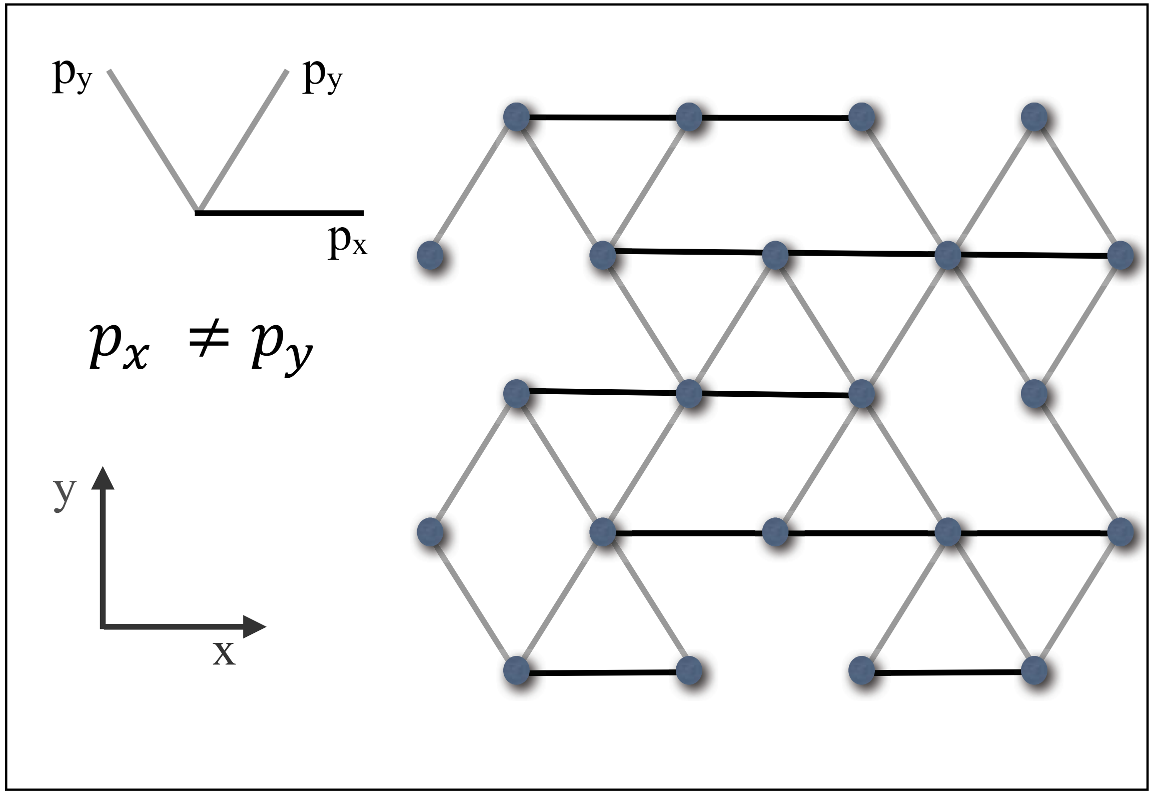
Phase Transition in Tissue Mechanics during Morphogenesis





Petridou, Corominas-Murtra, Heisenberg, Hannezo Cell 2021

An Example of Anisotropic Spring Network

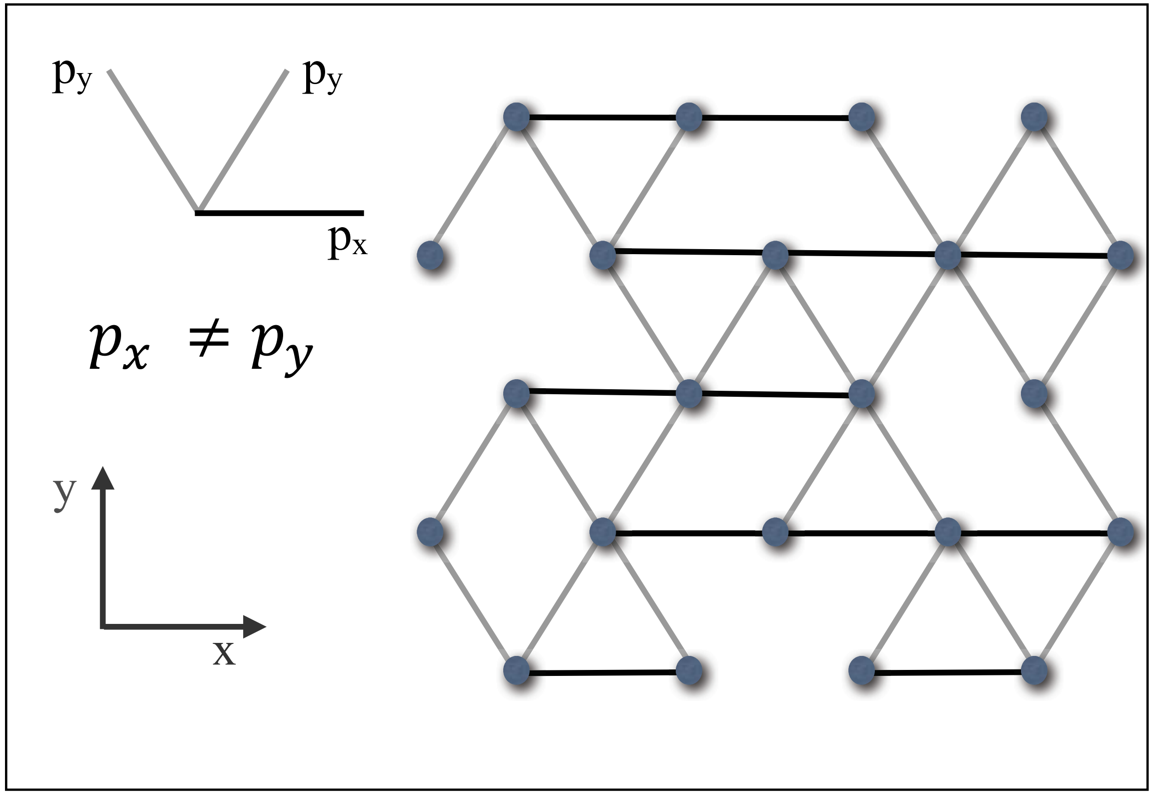


\# of degrees of freedom $= Nd$

\# of constraints = (1/2) (z_x N p_x + z_y N p_y)

See: T. Zhang, J.M. Schwarz, MD, PRE 2014

An Example of Anisotropic Spring Network



\# of degrees of freedom $= Nd$

\# of constraints = (1/2) (z_x N p_x + z_y N p_y)

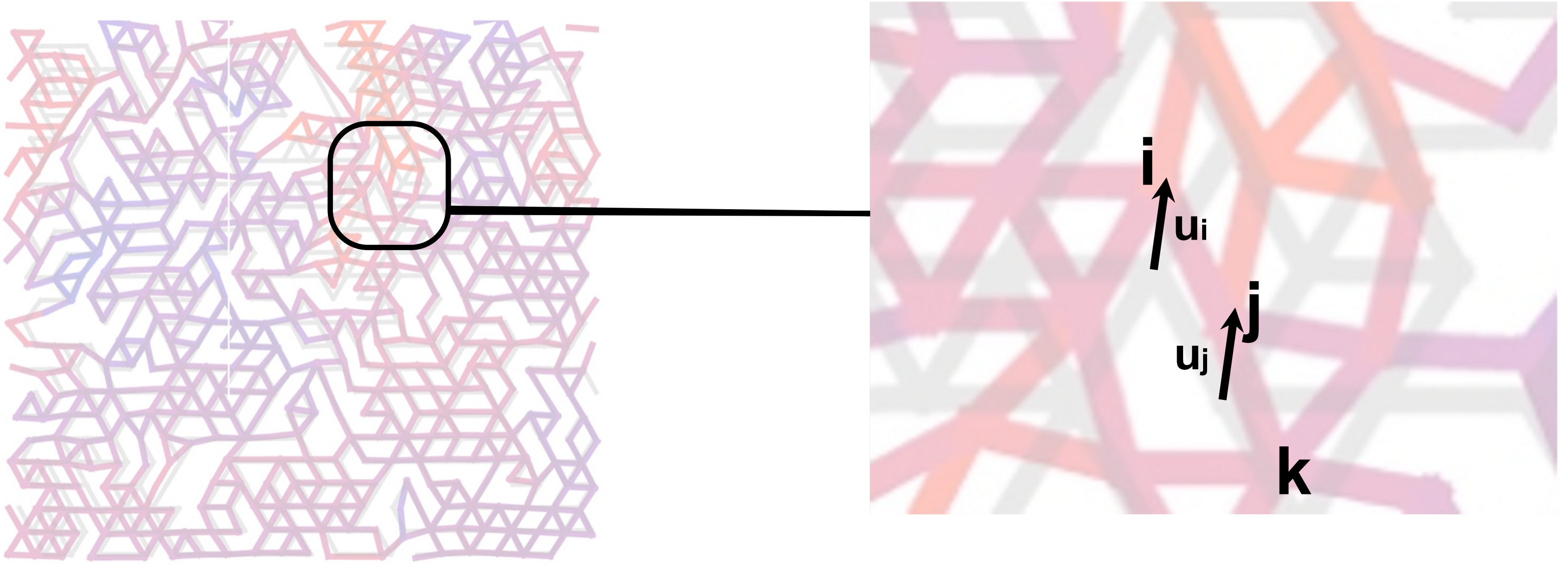
d=2, z_x = 2, z_y =4

$$\boxed{\frac{p_x}{2} + p_y = 1}$$

Check EMT gives you the same relationship

See: T. Zhang, J.M. Schwarz, MD, PRE 2014

Rigidity Percolation in Semiflexible Networks



$$E_{spring} = \frac{\alpha}{2} \sum_{\langle ij \rangle} p_{ij} (\vec{u}_{ij} . \hat{r}_{ij})^2$$

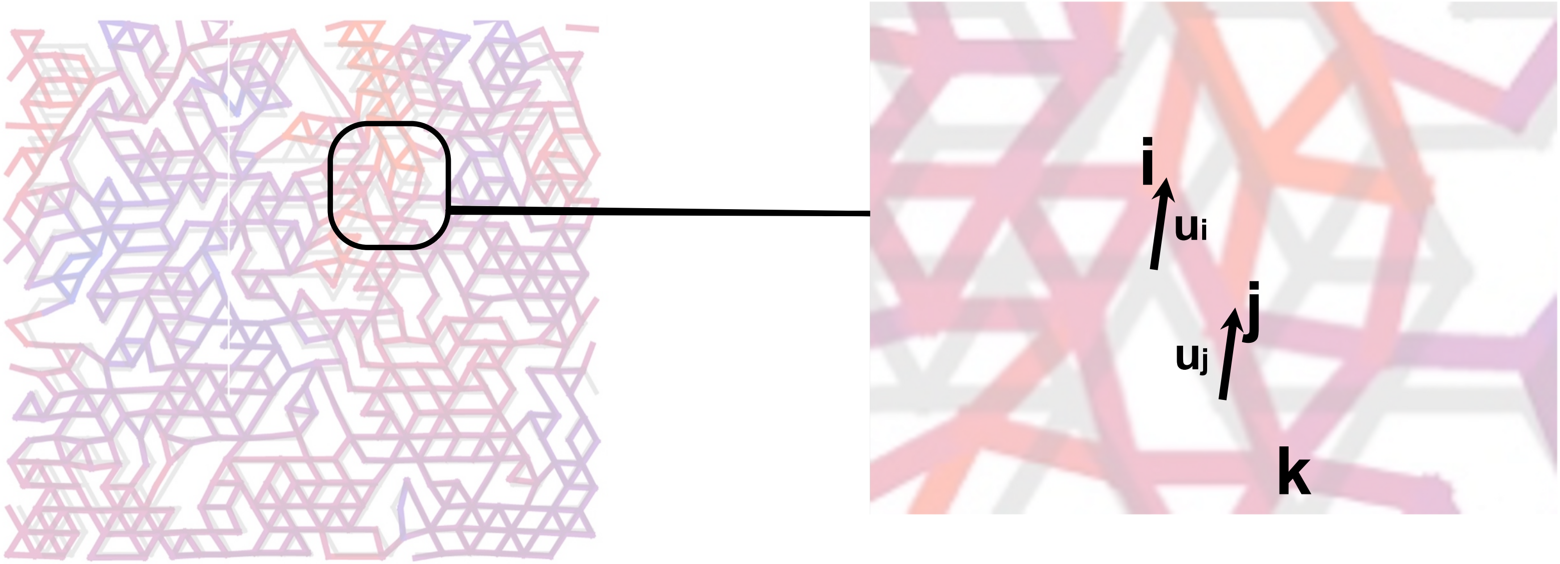
$$E_{filament\ bending} = \frac{\kappa}{2} \sum_{\langle jik \rangle} p_{ji} p_{ik} (\theta_{jik})^2$$

Deformation energy $$E = E_{spring} + E_{filament\ bending}$$

Study using effective medium theory or energy minimization

MD, MacKintosh, Levine, PRL 2007, MD, D Quint, JM Schwarz, PloS One 2012, Broedersz et al Nature Ohys 0211

Rigidity Percolation in Semiflexible Networks



Distribution of stretching and bending constants

- $P(\alpha') = p\delta(\alpha' - \alpha) + (1 - p)\delta(\alpha')$
- $P(\kappa') = p^2\delta(\kappa' - \kappa) + (1 - p^2)\delta(\kappa')$

MD, MacKintosh, Levine, PRL 2007, MD, D Quint, JM Schwarz, PloS One 2012, Broedersz et al Nature Ohys 0211

Rigidity Percolation in a semiflexible networks on triangular lattice: Dynamical Matrix

$$\boldsymbol{D}_s(q) \;=\; \alpha_m \sum_{\langle ij \rangle} \left[1 - e^{-i\boldsymbol{q}.\hat{\boldsymbol{r}}_{ij}}\right] \hat{\boldsymbol{r}}_{ij}\hat{\boldsymbol{r}}_{ij}$$

$$\boldsymbol{D}_b(q) \;=\; \kappa_m R^{-2} \sum_{\langle ij \rangle} \left[4(1-\cos(\boldsymbol{q}.\hat{\boldsymbol{r}}_{ij}))-(1-\cos(2\boldsymbol{q}.\hat{\boldsymbol{r}}_{ij}))\right] (\boldsymbol{I} - \hat{\boldsymbol{r}}_{ij}\hat{\boldsymbol{r}}_{ij})$$

$$\boldsymbol{D}(q) = \boldsymbol{D}_s(q) + \boldsymbol{D}_b(q)$$

MD, MacKintosh, Levine, PRL 2007, MD, D Quint, JM Schwarz, PloS One 2012, Broedersz et al Nature Ohys 0211

Rigidity Percolation in a semiflexible networks on triangular lattice: Effective Medium stretching and bending constants from EMT

$$\frac{\alpha_m}{\alpha} = \begin{cases} \frac{p-a^*}{1-a^*} & \text{if } p > a^* \\ 0 & \text{if } p \le a^* \end{cases}$$

$$a^* = \frac{1}{3}\sum_q Tr\left[\boldsymbol{D}_s(q)\cdot\boldsymbol{D}^{-1}(q)\right]$$

$$\frac{\kappa_m}{\kappa} = \begin{cases} \frac{p^2-b^*}{1-b^*} & \text{if } p > \sqrt{b^*}, \\ 0 & \text{if } p \le \sqrt{b^*} \end{cases}$$

$$b^* = \frac{1}{3}\sum_q Tr\left[\boldsymbol{D}_b(q)\boldsymbol{D}^{-1}(q)\right]$$

Solve self-consistently

MD, MacKintosh, Levine, PRL 2007, MD, D Quint, JM Schwarz, PloS One 2012, Broedersz et al Nature Ohys 0211

Rigidity Percolation in a semiflexible networks on triangular lattice: Effective Medium stretching and bending constants from EMT

$$\frac{\alpha_m}{\alpha} = \begin{cases} \frac{p-a^*}{1-a^*} & \text{if } p > a^* \\ 0 & \text{if } p \leq a^* \end{cases} \qquad a^* = \frac{1}{3}\sum_q Tr\left[\boldsymbol{D}_s(q)\cdot\boldsymbol{D}^{-1}(q)\right]$$

$$\frac{\kappa_m}{\kappa} = \begin{cases} \frac{p^2-b^*}{1-b^*} & \text{if } p > \sqrt{b^*}, \\ 0 & \text{if } p \leq \sqrt{b^*} \end{cases} \qquad b^* = \frac{1}{3}\sum_q Tr\left[\boldsymbol{D}_b(q)\boldsymbol{D}^{-1}(q)\right]$$

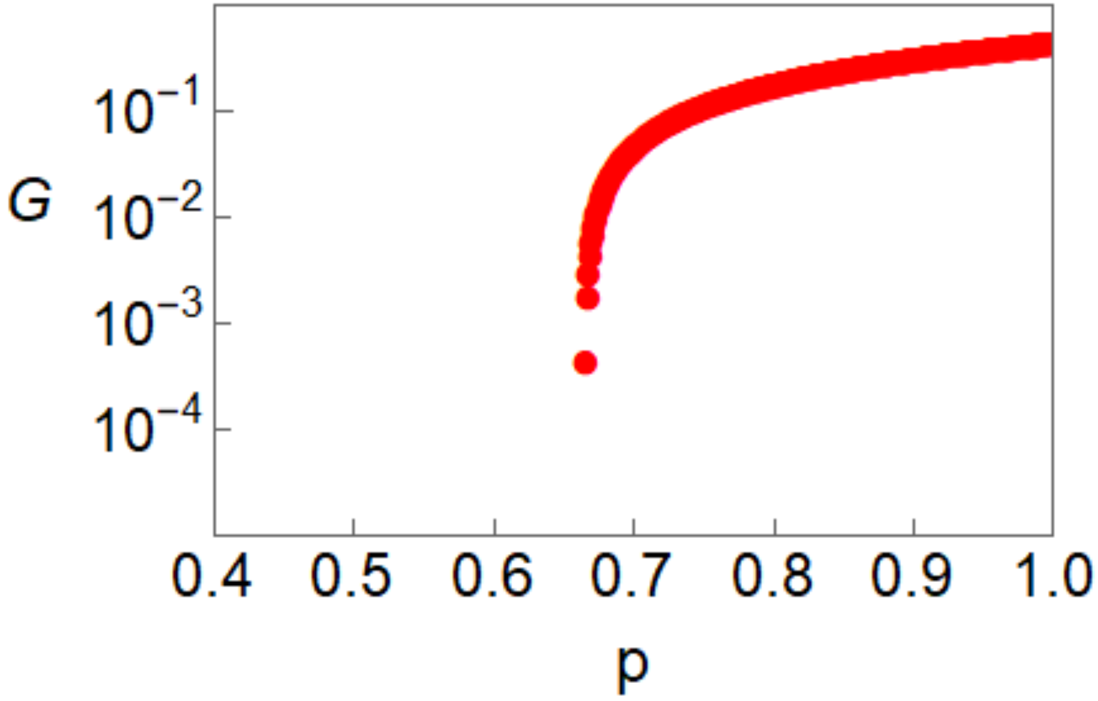
Also note: $a^* + b^* = \frac{2}{3}$

At the rigidity percolation threshold, p_c : $p_c + {p_c}^2 = \frac{2}{3}$. $\therefore\ p_c \approx 0.457$

MD, MacKintosh, Levine, PRL 2007, MD, D Quint, JM Schwarz, PloS One 2012, Broedersz et al Nature Ohys 0211

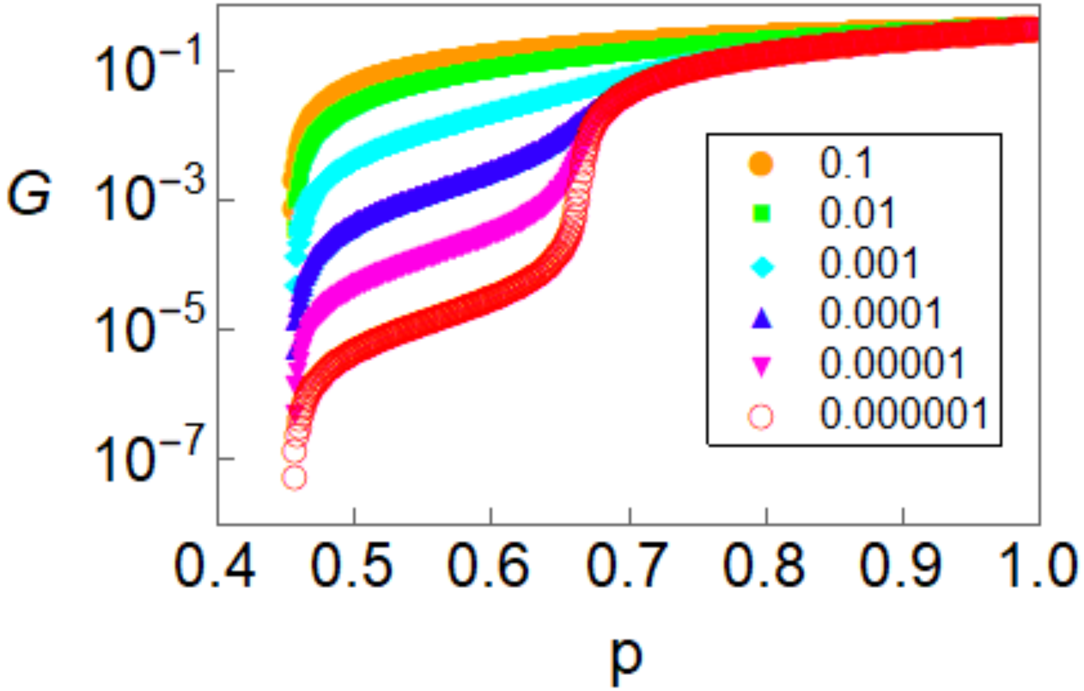
Rigidity Percolation in flexible and semiflexible networks on triangular lattice: EMT prediction of shear modulus G (G = $(\sqrt{3}/4)\ \alpha_m$)

$\alpha = 1, \kappa = 0$



$p_c \approx 0.667$

$\alpha = 1, \kappa$ varied

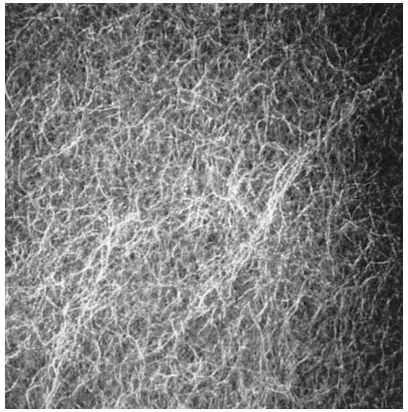


$p_c \approx 0.457$

MD, MacKintosh, Levine, PRL 2007, MD, D Quint, JM Schwarz, PloS One 2012, Broedersz et al Nature Ohys 0211

Rigidity Percolation in semiflexible networks: what happens when we have angle constraining crosslinks between crossing filaments?

F-actin/a-actinin network



Tseng, Wirtz 2001.

Filamin

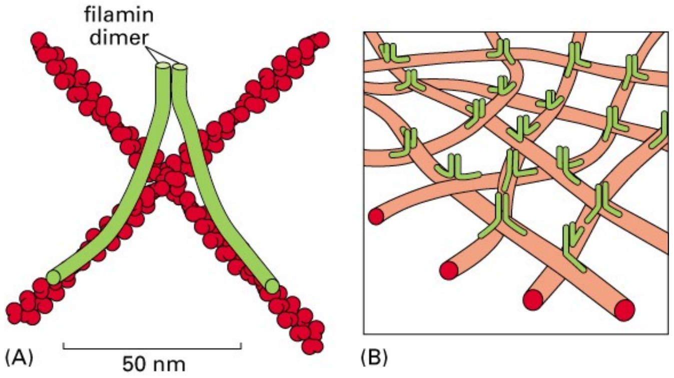
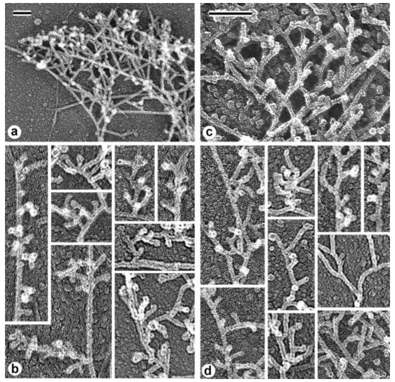


Figure 16–42. Molecular Biology of the Cell, 4th Edition.

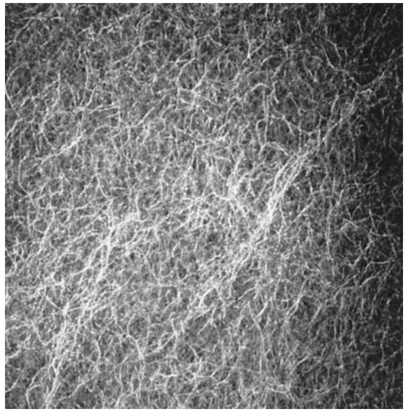
Arp 2/3



Svitkina and Borisy 1999.

Rigidity Percolation in semiflexible networks: what happens when we have angle constraining crosslinks between crossing filaments?

F-actin/a-actinin network



Tseng, Wirtz 2001.

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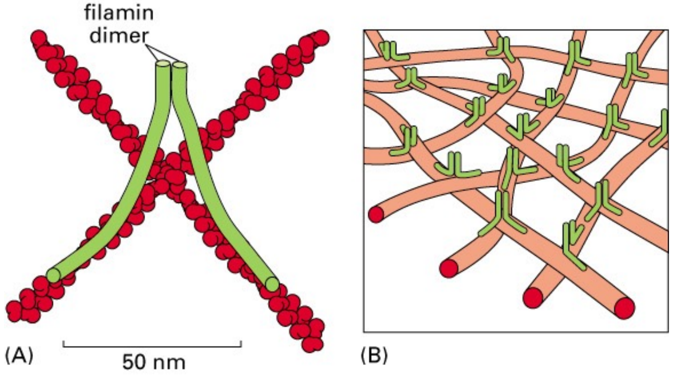
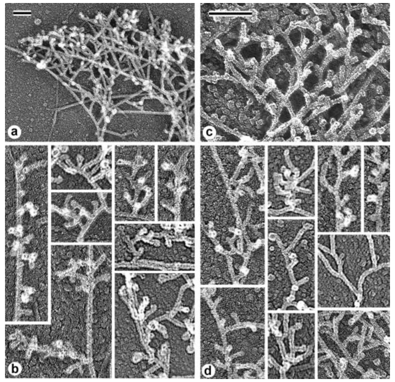


Figure 16–42. Molecular Biology of the Cell, 4th Edition.

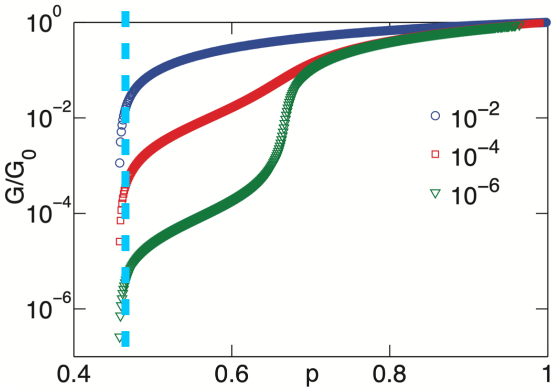
Arp 2/3



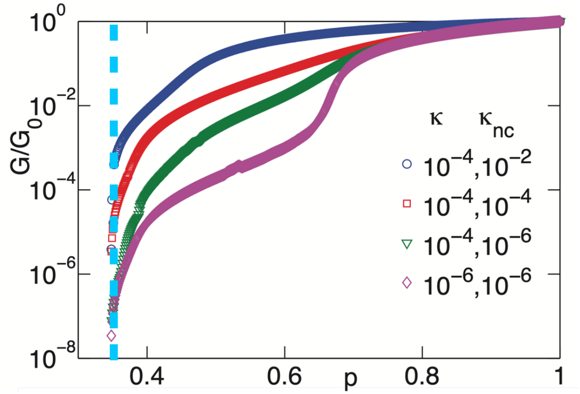
Svitkina and Borisy 1999.

Shear modulus

freely rotating x-links



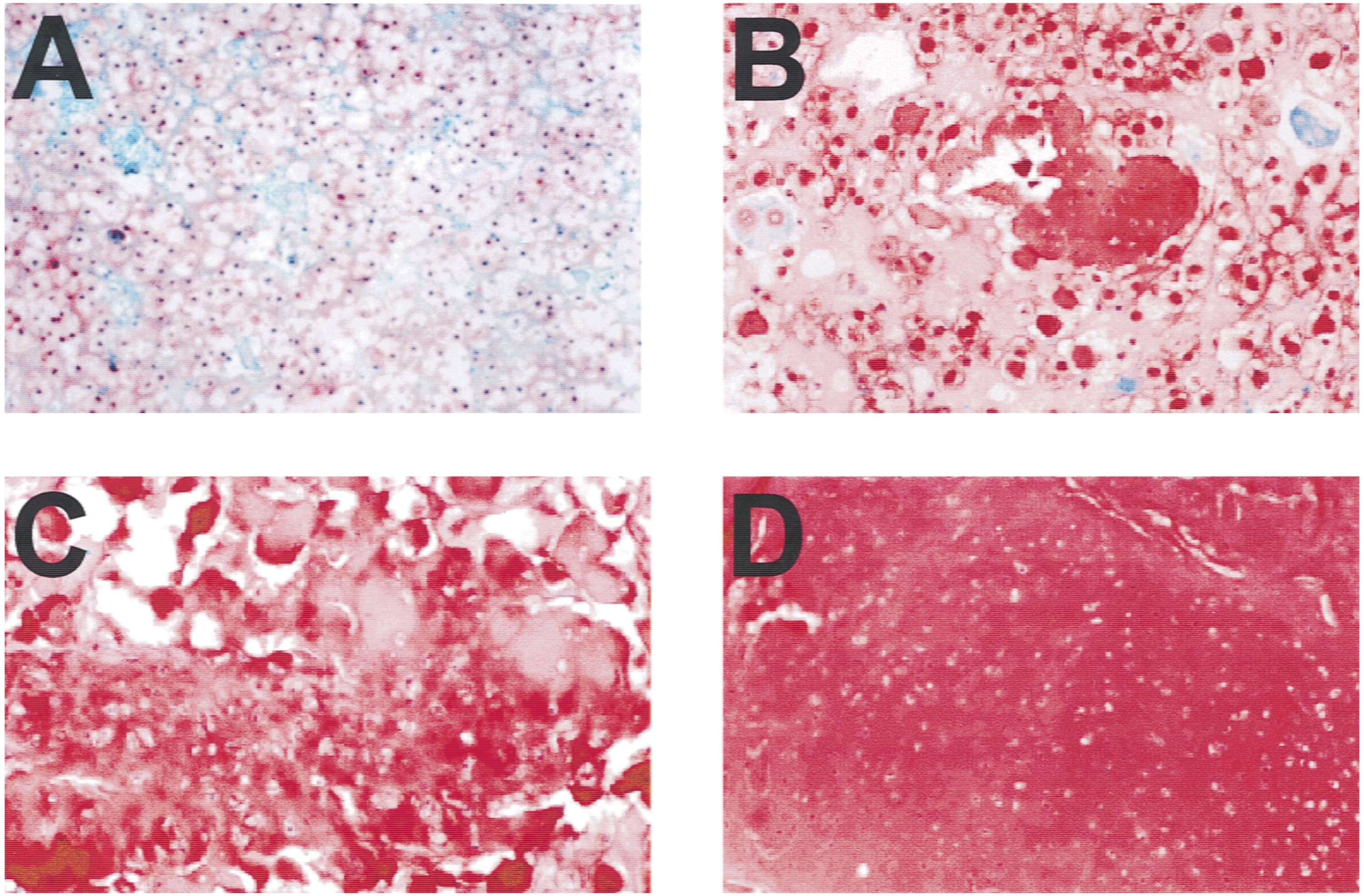
angle constraining xlinks



Bond occupation probability

MD, Quint, and, Schwarz, PLOS One 2012

Rigidity Percolation in semiflexible networks: what happens when the network has spatial inhomogeneity?



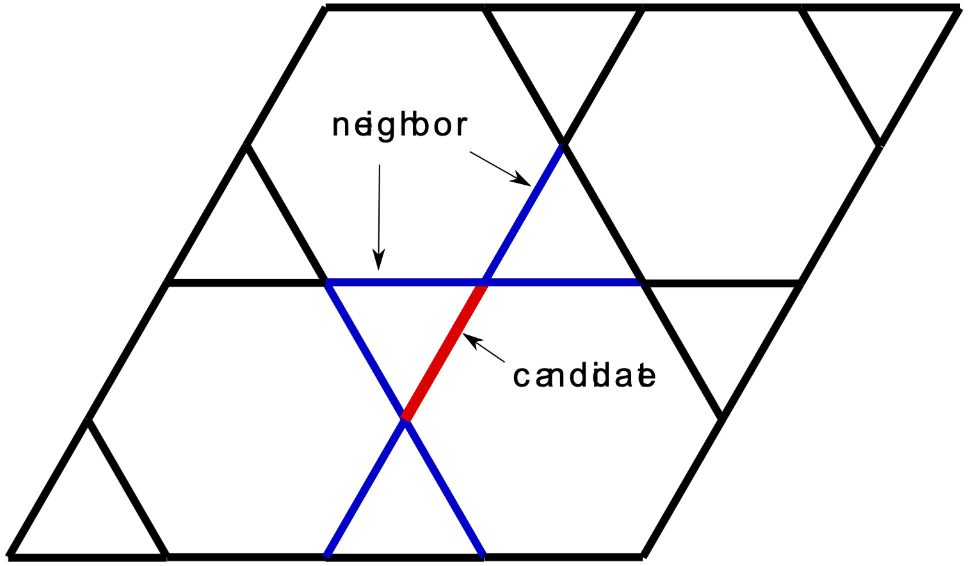
Chang, et al., J. Biomed. Res., 2001

Model: Kagome-lattice based network with structural correlation

- Include randomly chosen bond with acceptance probability $P = (1 - c)^{6-nn}$

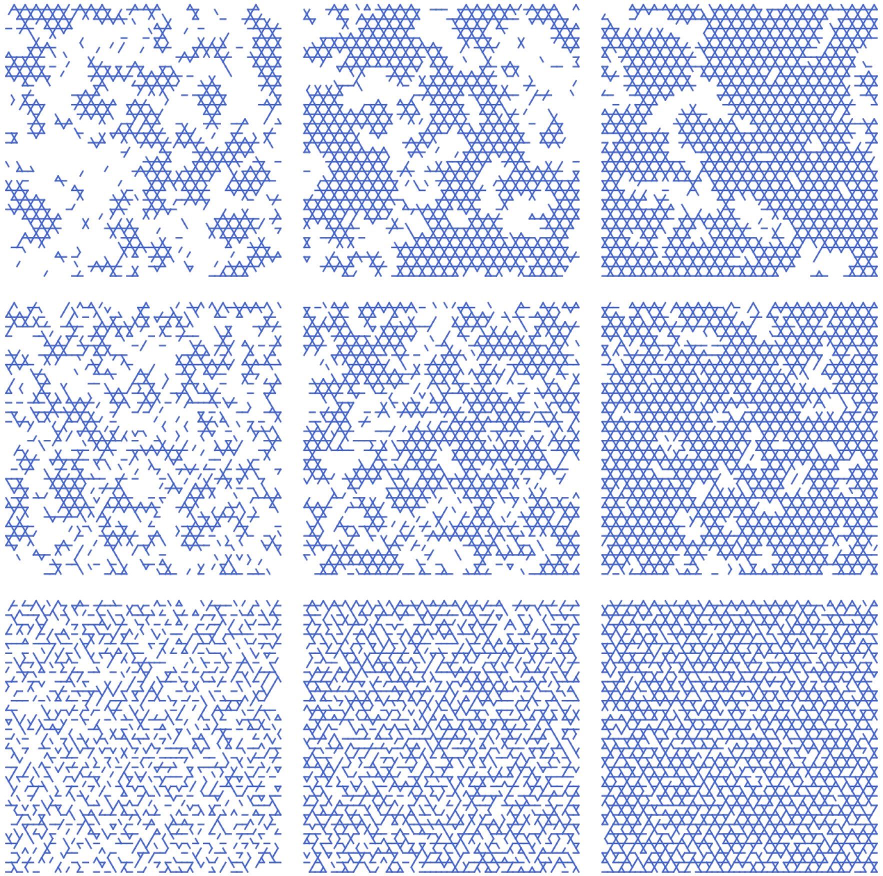
- c sets the strength of correlation

- Larger values of correlation strength yield patchier structures



J Michel, ++, MD, Phys Rev R, 2022

Increasing correlation yields dense clusters

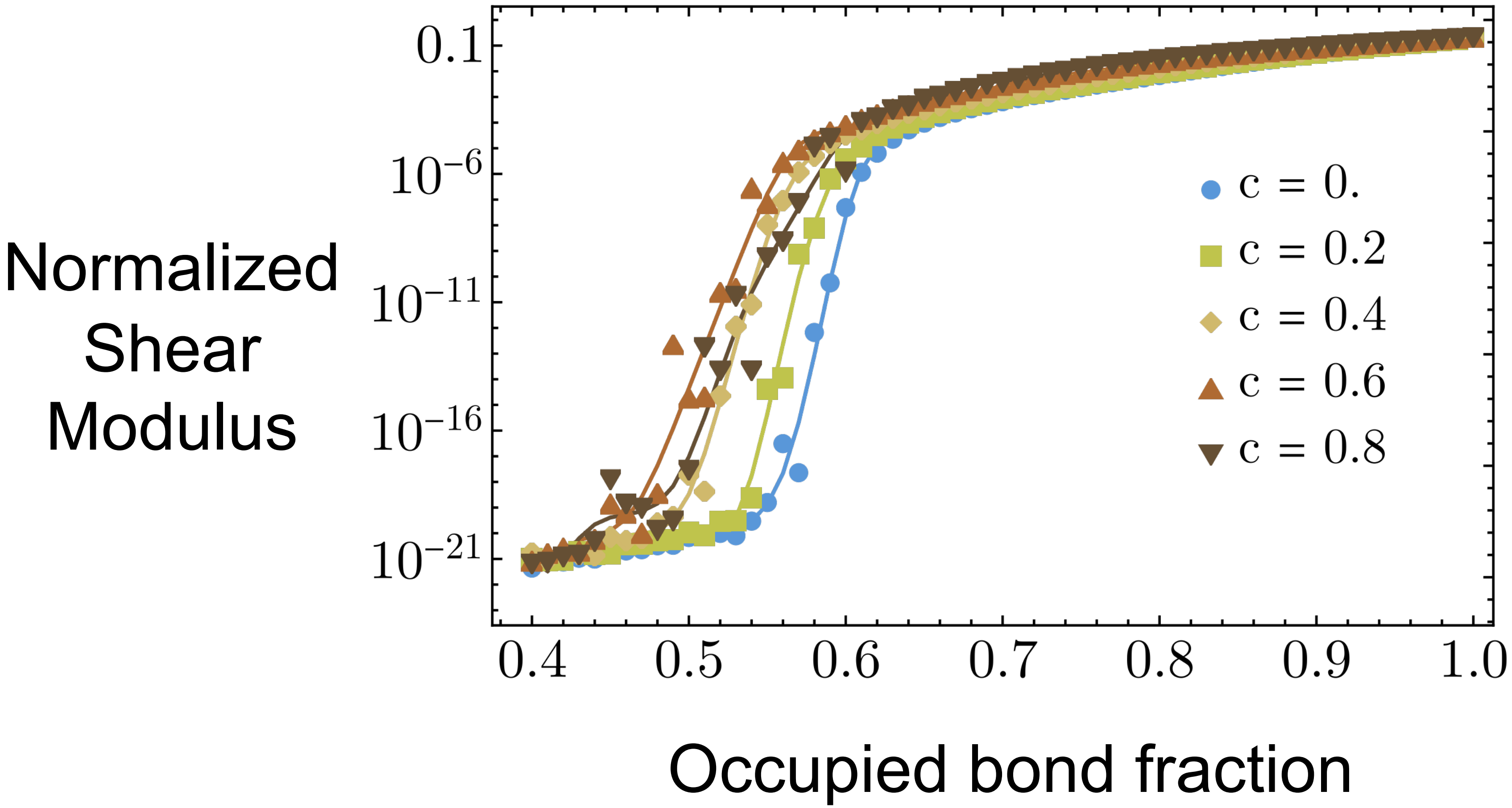


Increasing correlation

Increasing fraction of occupied bonds

J Michel, ++, MD, Phys Rev R, 2022

Threshold for Rigidity Depends varies Non-monotonically with Correlation



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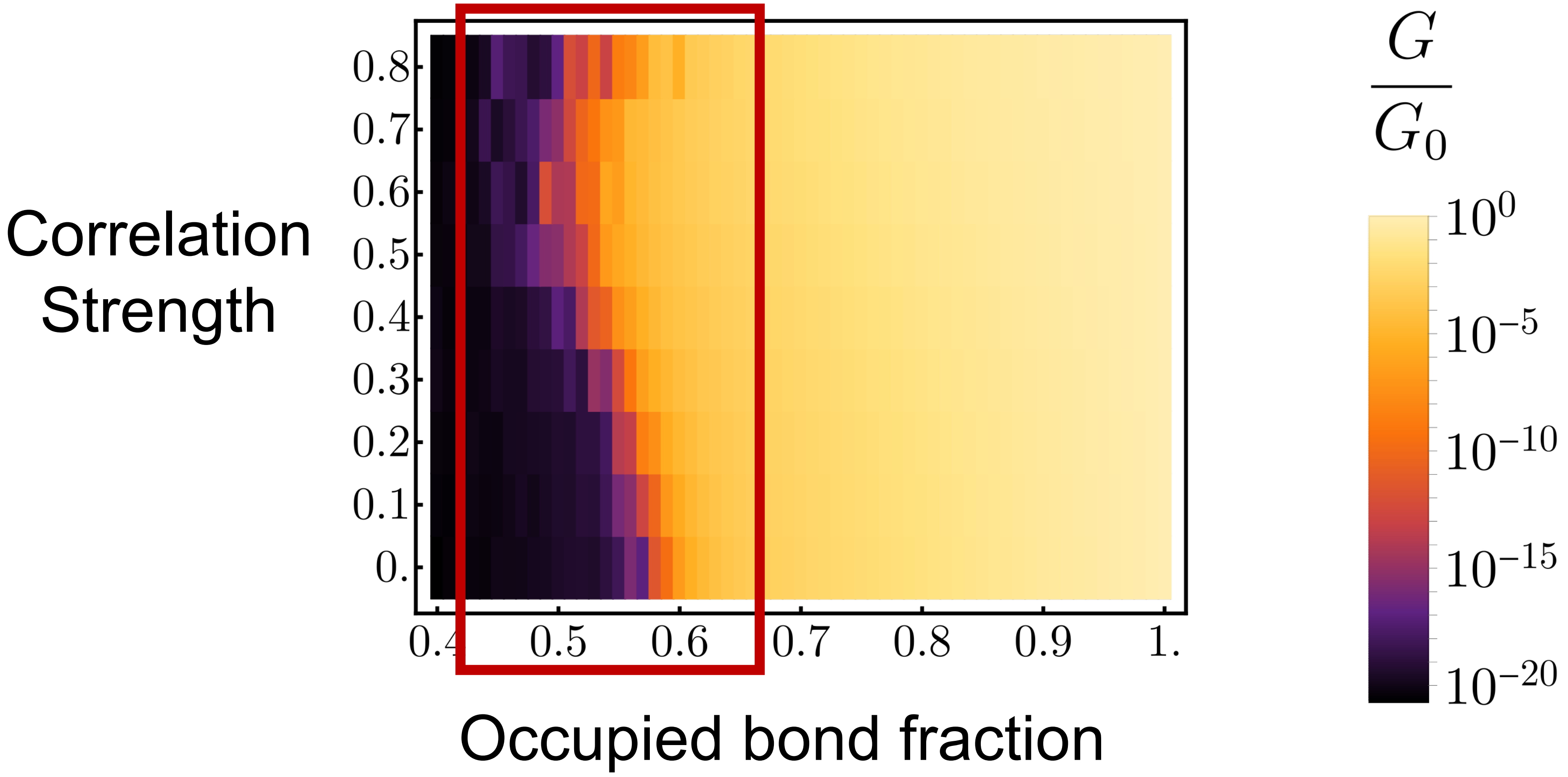
Threshold for Rigidity Depends varies Non-monotonically with Correlation



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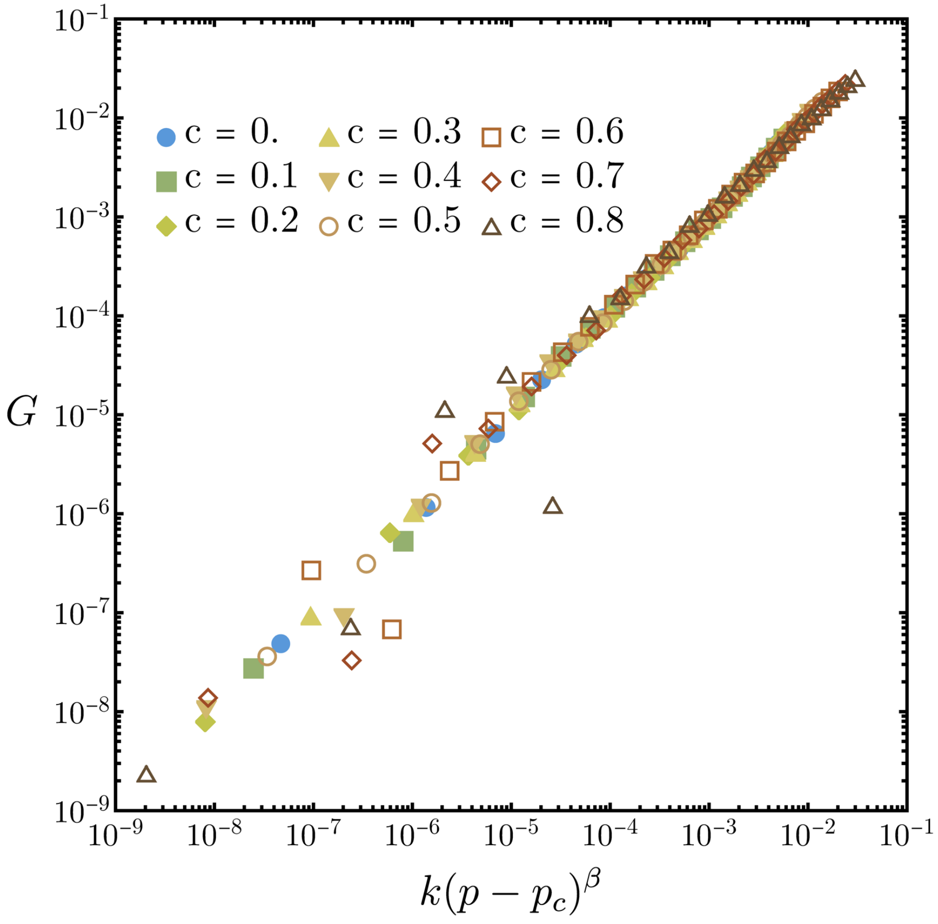
Computing percolation thresholds

- Fit shear modulus around percolation threshold to power law
- $G = k(p - p_c)^{\beta}$
  - p_c denotes the percolation thresholds (depends on c)
  - β is a critical exponent found by fitting



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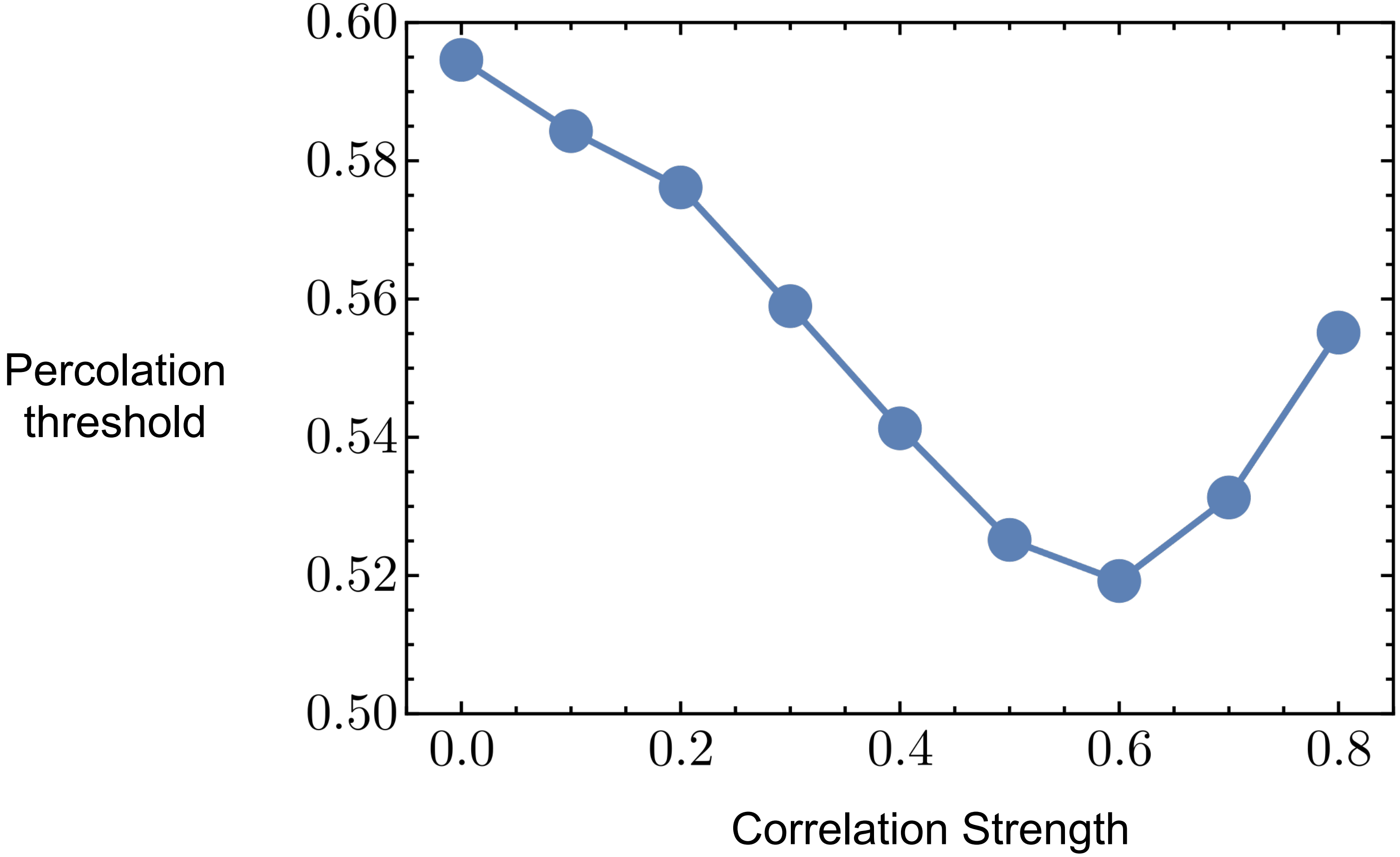
p_c exhibits reentrance

$$G = k(p - p_c)^{\beta}$$



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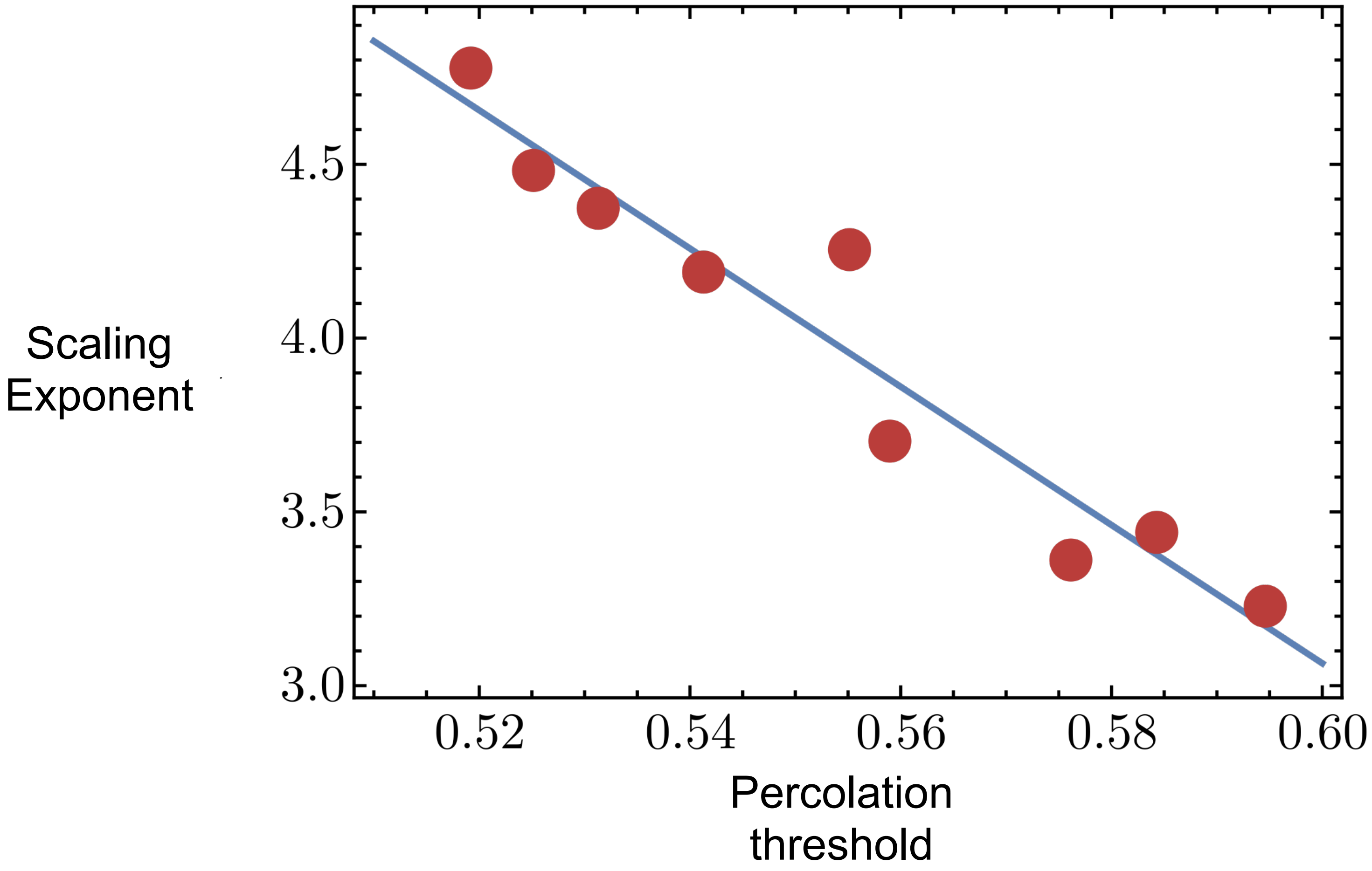
Scaling Exponents Decreases Linearly with Rigidity Threshold



J Michel, ++, MD, Phys Rev R, 2022