Interactions III : Vertex models

Note: I am skipping some other really nice models for tissues, including subcellular element models, cellular potts models, finite element models...

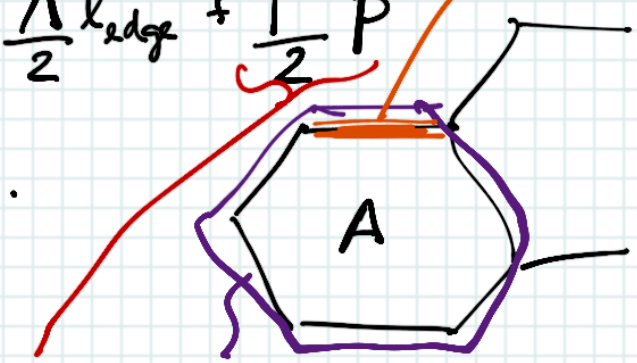
1. Zero-motility limit (no activity)

a. $E_{cell} = \frac{K_A}{2}(A - A_0)^2 + \sum_{edges} \frac{\Lambda}{2} l_{edge} + \frac{\Gamma}{2} P^2$

$P \equiv \sum_{edges} l_{edge}$.

interfacial tension

l_{edge}



3D incompressibility + height fluctuations

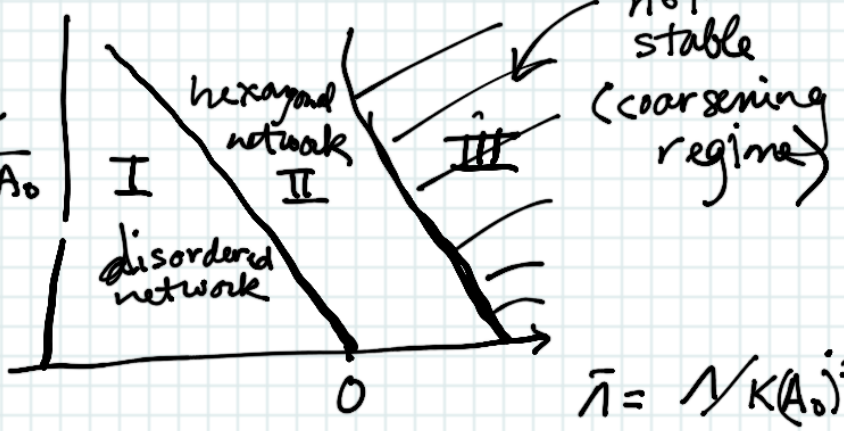
"contractility" P or "limited adhesion molecules"

Farhadifar et al Current Biology 17 2007

Note: lots of others before this. Honda, Hufnagel

b. Ground states:

$\bar{\Gamma} = \frac{\Gamma}{KA_0}$



c. For physicists, it is much easier in case where all Λ's are the same and so we can rewrite this as

$$E_{cell} = K_A (A - A_0)^2 + K_P (P - P_0)^2$$

where $P_0 = -\frac{\Lambda}{2\Gamma}$ and $K_A = \frac{K_A}{2}$

$$K_P = \frac{\Gamma}{2}$$

$$\mathcal{E}_{tot} = \frac{1}{K_A A_0^2} \sum_1^N E_i = \sum_1^N \left[(a_i - 1)^2 + \frac{1}{r} (p_i - p_0)^2 \right]$$

with $r = \frac{K_A A_0}{K_P}$ and $p_0 = \frac{P_0}{\sqrt{A_0}}$

r: stiffness ratio; p_0: shape index

Homework Exercise:

calculate the algebraic expressions for the lines shown in the phase diagram for the ground states.

Hint: In phase I $p_i = p_0$, $a_i = 1$ $\forall i$

In phase II p_i can be related to a_i $\forall i$

In phase III $p_i = 0$ $a_i = 0$

d. This is a good model for confluent tissues.

also really fun system for exploring disordered solidification in a system that is very different from spheres packings

e. Beyond ground states

→ biological tissues very rarely look ordered.

→ need to generate an ensemble of higher energy states

skip

→ numerically, can do an "infinite temperature quench", take a Voronoi tessellation of uniformly distributed points, and find nearest minimum using gradient or conjugate gradient descent

$$\mu \dot{r}_i = -\nabla_i \mathcal{E}$$

μ: vertex position i

→ Program as "Surface Evolver" has built in functions to do this, or you can write your own

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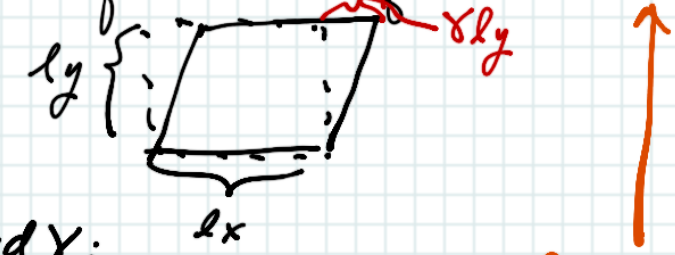
f. Linear Response: system becomes rigid when shear modulus $G > 0$

- Calculate the shear modulus around a minimum energy state
- For simple shear, describe deformation of the box γ



- $\mathcal{E} = \mathcal{E}(\{\vec{r}_i\}, \gamma)$

mechanically stable state at a fixed γ:

- $\mathcal{E}_{min}(\gamma) = \min_{\{r_i\}} \mathcal{E}(\{r_i\}, \gamma)$

extra degree of freedom: $(Nd + 1)$ DOF

Tutorial: Calculate shear modulus g

Merkel, Manning NJP 2018
Appendix A 7

$$g \equiv \frac{1}{V} \frac{d^2 \mathcal{E}_{min}(\gamma)}{d\gamma^2}$$

volume

$$g = \frac{1}{V}\left(\frac{\partial^2 \mathcal{E}}{\partial \gamma^2} + \sum_{k,\beta}' \frac{\partial^2 \mathcal{E}}{\partial r_k^\beta \partial \gamma} \dot{r}_k^{min,\beta} \right) \quad (\star)$$

$\dot{r}_k^{min,\beta} = \frac{dr_k^{min,\beta}}{d\gamma}$

vertex index $(1 \ldots N)$

dimension index (x, y)

→ Want to re-write this in terms of the dynamical matrix

$$D_{j\alpha,k\beta} \equiv \frac{\partial^2 \mathcal{E}}{\partial r_j^\alpha \partial r_k^\beta}$$

labels dimensions

labels vertices

eigenvalues ≥ 0

$$= \sum_m' \omega_m^2 \, \mathcal{U}_{j\alpha}^m \mathcal{U}_{k\beta}^m$$

eigenvectors

$m = (1 \ldots Nd)$

but force balance means

$$0 = \frac{\partial \mathcal{E}\left(r^{min}(\gamma), \gamma\right)}{\partial r_j^\alpha}$$

taking total derivative of this equation with respect to γ:

$$0 = \sum_{k,\beta}' D_{j\alpha,k\beta} \dot{r}_k^{min,\beta} + \frac{\partial^2 \mathcal{E}}{\partial r_j^\alpha \partial \gamma} \quad (\star\star)$$

Let $\bar{D}_{pq} = \dfrac{\partial^2 \mathcal{L}}{\partial z_p \partial z_q}$ where $z_p = (\vec{r}_1 \cdots \vec{r}_N, \gamma)$

$3N+1$ – dimensional

$$\bar{D}_{pq} = \sum_m \bar{\omega}_m^2 \, \bar{u}_p^m \, \bar{u}_q^m$$

and $\dot{z}^{min} \equiv (\dot{r}_1^{min} \cdots \dot{r}_{Nd}^{min}, 1)$.

Note that using (★★), we can re-write (★) as:

$$V_g \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ \vdots \\ 1 \end{bmatrix} = \begin{bmatrix} & & & \frac{\partial^2 \mathcal{L}}{\partial \gamma \partial r_1} \\ & D_{jd,k\beta} & & \vdots \\ & & & \\ \frac{\partial^2 \mathcal{L}}{\partial r_1 \partial \gamma} & \cdots & \cdots & \frac{\partial^2 \mathcal{L}}{\partial \gamma^2} \end{bmatrix} \begin{bmatrix} \dot{r}_1^{min} \\ \vdots \\ \dot{r}_{Nd}^{min} \\ 1 \end{bmatrix}$$

OR

$$V_g \, \delta_{\gamma p} = \bar{D}_{pq} \, \dot{z}_q^{min}$$

Take scalar product with $\bar{u}_p^m$:

$$V_g \, \bar{u}_\gamma^m = \bar{\omega}_m^2 \sum_q u_q^m \, \dot{z}_q^{min} \qquad \forall m \qquad (\star\star\star)$$

γ^{th} entry in the eigenmode $\tilde{m}$

Comment 1: if $\exists$ a zero mode $\tilde{m}$ with $u_\gamma^{\tilde{m}} \neq 0$ (e.g. non-zero overlap with shear DOF)

then $g = 0$.

skipped in lecture

Comment 2: otherwise, all zero modes have vanishing overlap with the shear degree of freedom so the shear must be the sum over remaining e-vectors:

$$\delta_{\gamma q} = \sum_{\substack{m \text{ with} \\ \text{nonzero } \omega_m}} \bar{u}_\gamma^m \bar{u}_q^m \quad \Rightarrow \quad 1 = \sum_{m,q}^{m \text{ non-zero}} \bar{u}_\gamma^m \bar{u}_q^m \dot{z}_q^{min}$$

(because $\dot{z}_\gamma^{min} = 1$)

Define $\{\tilde{m}\}$ as m s.t. $\omega_m \neq 0$.

Inserting eq ~~AAAA~~ we find

$$1 = \sum_{\tilde{m}} \bar{u}_\gamma^m \underbrace{\sum_q u_q^m \dot{z}_q^{min}}_{\frac{V_q u_\gamma^m}{\bar{\omega}_m^2}} \Rightarrow \quad 1 = V_q \sum_{\tilde{m}} \frac{\bar{u}_\gamma^m}{\bar{\omega}_m^2}$$

$$\Rightarrow \boxed{g = \frac{1}{V}\left[\sum_{\tilde{m}} \frac{(\bar{u}_\gamma^m)^2}{\bar{\omega}_m^2}\right]^{-1}}$$

if no non-trivial zero modes.

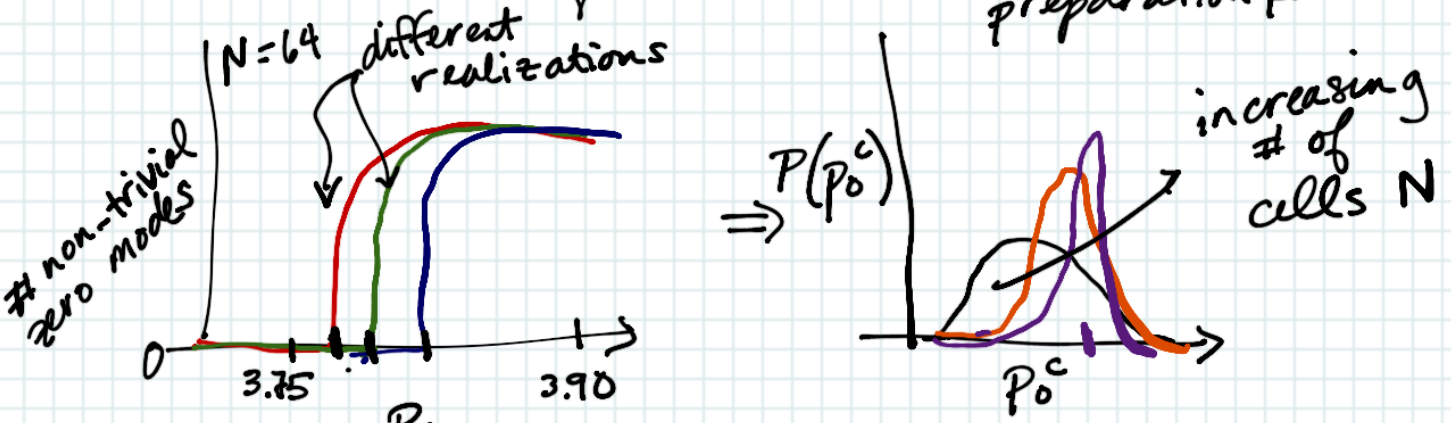
Result

$$g = \begin{cases} 0 \text{ if } \exists \text{ a nontrivial zero mode} \\ \text{otherwise, its a weighted sum of overlaps of eigenvectors with shear D.O.F} \end{cases}$$

Easiest to quantify the number of non-trivial zero modes:

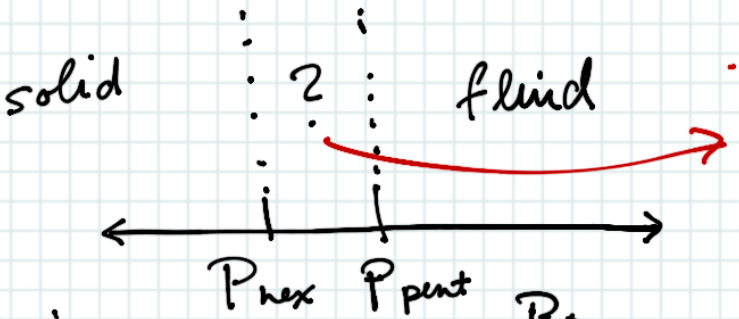
for ordered ground states, Staple et al EPJE 2010 demonstate that the system is linearly stable below $P_0 = P_{hex} \cong 3.72$

For disordered states, we can numerically calculate the number of zero modes as a function of p_0 for different realizations of the disorder with a given preparation protocol



extrapolate and find $\lim_{N\to\infty} \overline{p_0^c} = p_0^* \cong 3.81 \cong p_0^{pent}$

But, preparation protocol matters!
↳ see slide

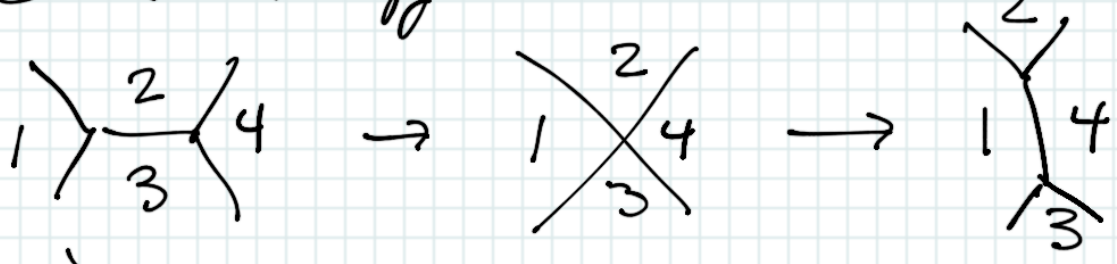


. hexagons linearly unstable
but disordered states linearly stable

Preeti Sahu Kang
arXiv 1905.12714

g. Nonlinear response:

Calculate energy barriers for localized rearrangements

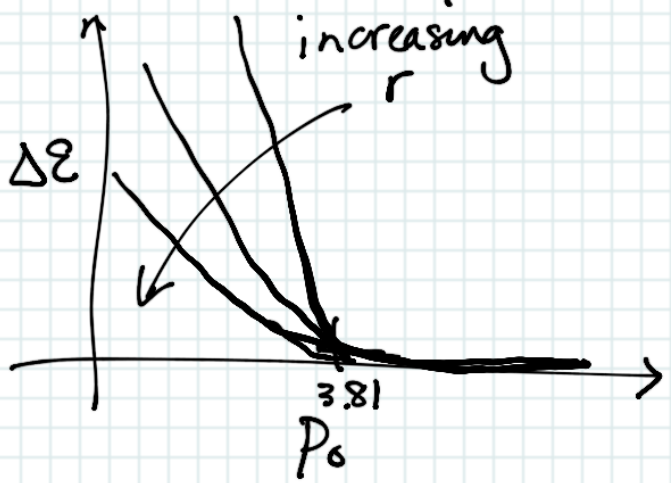


T_1 transition

→ execute T_1 transition by shortening 1 edge + extending in other direction (other transition paths possible)

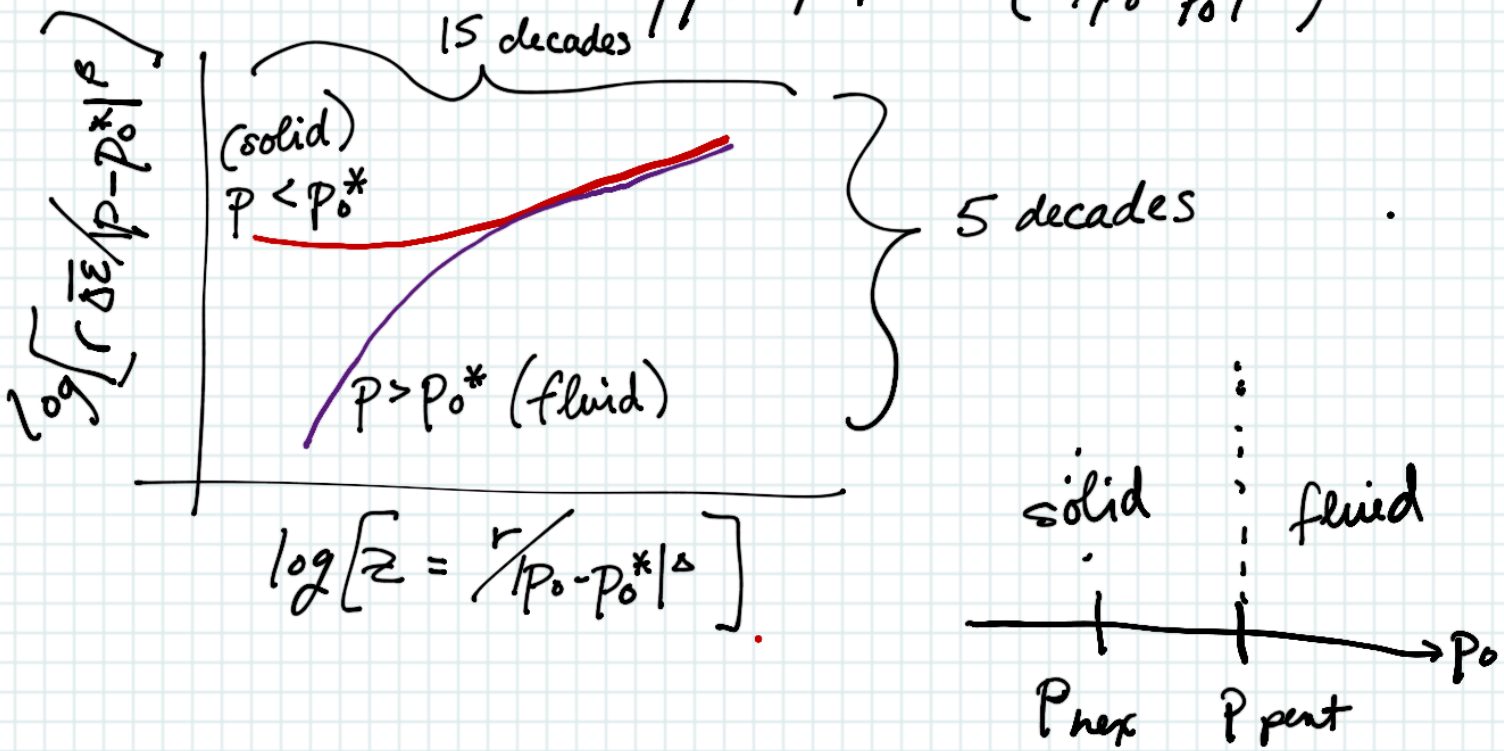
→ minimize global energy (allowing passive T_1 transitions elsewhere)

Result



Scaling ansatz: just like $(m, h, T - T_c)$ in Ising model $(r\Delta\bar{\mathcal{E}}, r, P_0 - P_0^*)$ here ⇒

$$r\,\Delta\bar{\mathcal{E}} = |P_0 - P_0^*|^{\beta} f_{\pm}\left(\frac{r}{|P_0 - P_0^*|^{\Delta}}\right)$$

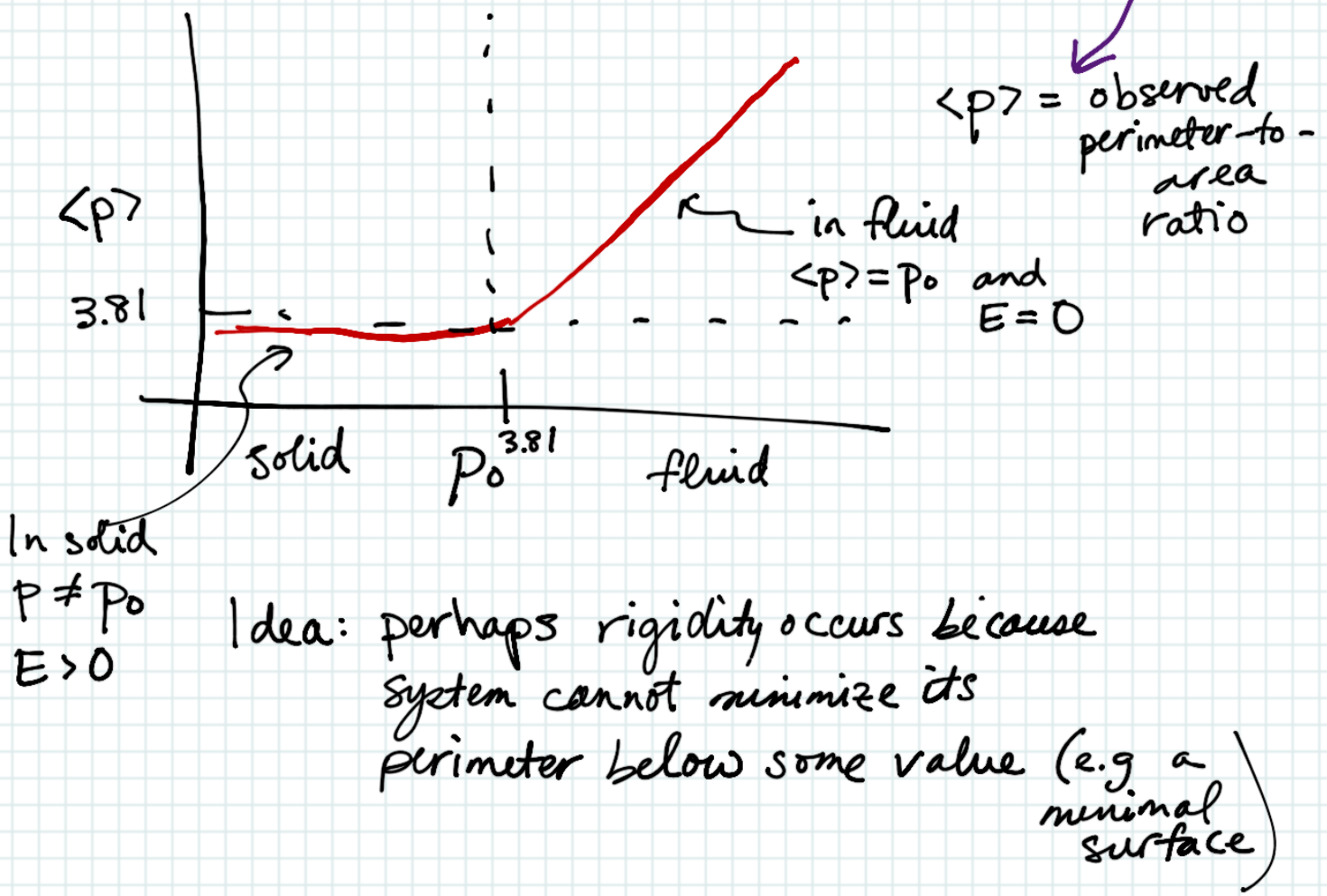


Interesting: energy barriers seem to go to zero at same location as shear modulus goes to zero.

Sahu et al: New result (energy barriers → 0 at ~3.81 for ordered solids)

h. Structural Order parameter:

Unlike particulate matter, vertex models have a structural order parameter for the transition:



Idea: perhaps rigidity occurs because system cannot minimize its perimeter below some value (e.g. a minimal surface)

2. Adding activity — Czajkowski arXiv 1905.01603

→ Self-propelled Vertex:

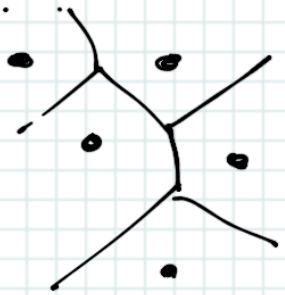
→ developed voronoi models to simplify activity

E. Voronoi models:

1. Model description.

DOF are cell centers: $\vec{r}_i$

cell shapers are given by a voronoi tessellation (Wigner-Seitz cell)



- interactions are driven by cell shapes according to usual energy functional:

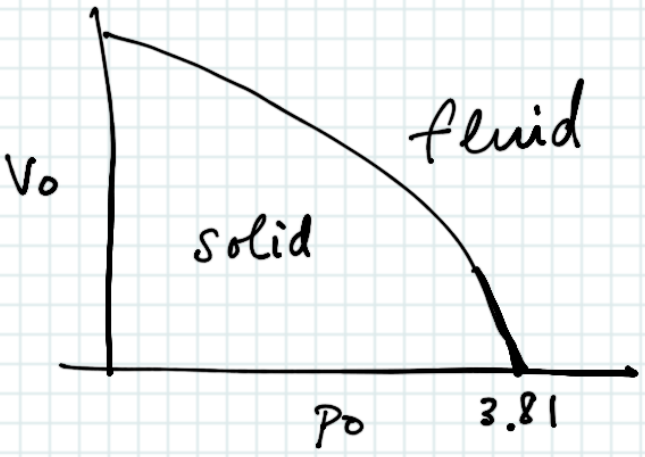
$$E = \sum_i^N \left[K_A (A - A_0)^2 + K_P (P - P_0)^2 \right]$$

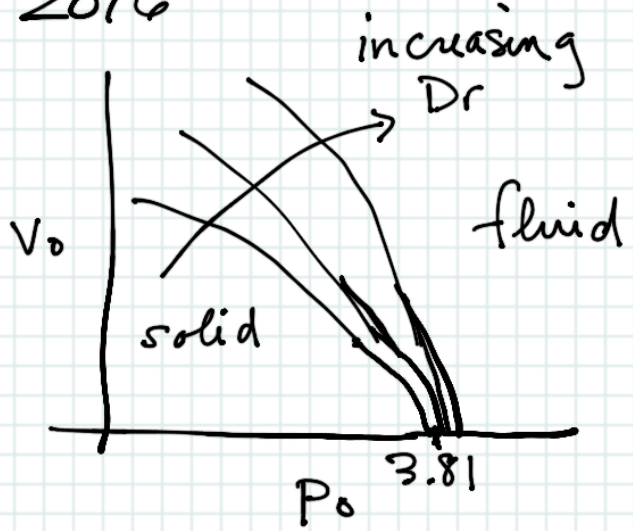
- cells move according to overdamped dynamics + self-propelled part:

$$\frac{d\vec{r}_i}{dt} = \mu \vec{F}_i + v_0 \hat{n}_i$$

$$\vec{F}_i = -\vec{\nabla}_i E \qquad \partial_t \theta_i = \text{white noise with strength } D_r.$$

2. 2D Results: Bi et al PRX 2016





Comment 1: similar to SPP models

→ increasing Dr enhances fluidization

→ can apply same argument as in Lecture 3 to show displacements are highly weighted by low frequency normal modes.

Comment 2: Structural order parameter still works.

MSD (dynamical data)
matches
shape index <p7

Slide: phase diagram

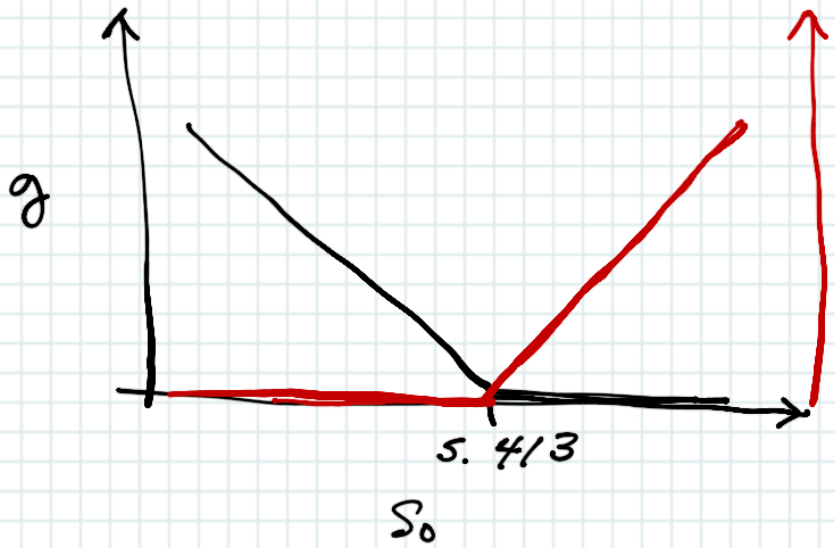
3. 3D Results : Merkel & Manning, ArXiv 2017

"zero temperature" → $v_0 = 0$

$$E = \sum_i \left[K_v (v_i - v_0)^2 + K_s (s_i - s_0)^2 \right]$$

$$s_0 = \frac{S_0}{\langle V \rangle^{2/3}} = \text{3D shape index} \qquad \langle s \rangle = \frac{\langle s_i \rangle}{\langle v \rangle^{2/3}}$$

Same as in 2D ⇒



$\langle s \rangle$ structural order parameter.

= average observed shape index

4. Rigidity in these systems different from jamming.

When do the number of constraints = number DOF?

$$2N \left(\begin{matrix} 1 \text{ volume constraint} \\ 1 \text{ surface constraint} \end{matrix} \text{ per cell} \right) = \underbrace{3N}_{\text{SPV in 3D}}$$

underconstrained?

Better:

$$\bar{D}_{pq} = 2 \sum_i \Bigg[\underbrace{\frac{\partial s_i}{\partial z_p} \frac{\partial s_i}{\partial z_q} + K_v \frac{\partial v_i}{\partial z_p} \frac{\partial v_i}{\partial z_q}}_{\text{spring terms}} + \underbrace{(s_i - s_0) \frac{\partial^2 s_i}{\partial z_p \partial z_q} + K_v (v_i - 1) \frac{\partial^2 v_i}{\partial z_p \partial z_q}}_{\text{residual stresses}} \Bigg]$$

surface tension

pressure

Merkel et al PNAS 2019

Large class of models are all very similar:

→ vertex, voronoi models for cells in 2D*, 3D

→ spring + fiber network models

Observation

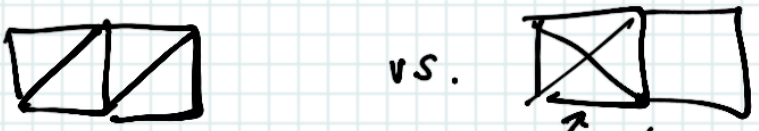
SPV in 3D : 3N DOF

vertex model in 2D: 4N DOF (for 3-fold coord network)

cellular potts models: arbitrary DOF

all seem to exhibit <u>same</u> rigidity transition

Another important contribution to rigidity: states of self stress



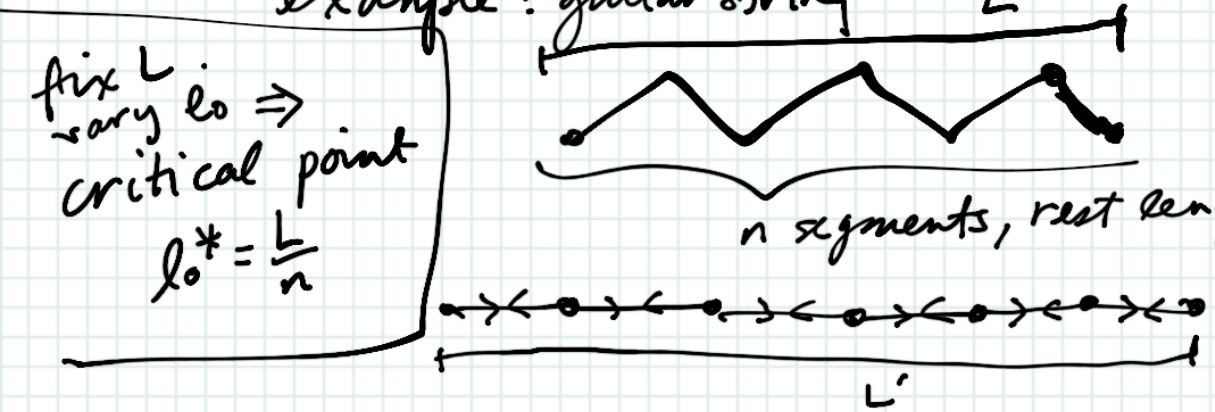
vs.

↑ state of self stress

(stresses that do not result in node displacement)

A self-stress can be created by **geometric incompatibility**.

example: guitar string



For spring networks (and vertex models)

energy $E = N\left((\bar{\ell} - \ell_0)^2 + \sigma_e^2\right)$

system needs to compromise b/w minimizing $|\bar{\ell} - \ell|$ and σ_e. How?

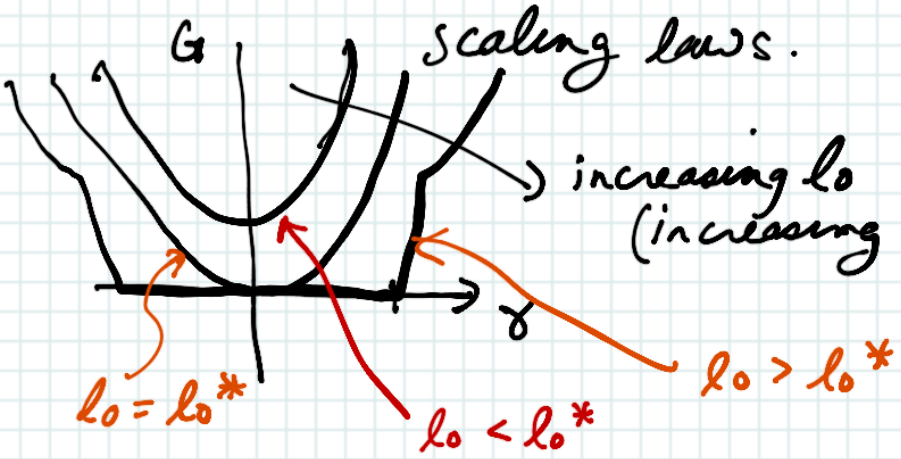
One can show analytically that the geometrically induced self-stress gives

$\bar{\ell}_{min}(\sigma_e) = \ell_0^* - a_e \sigma_e + b_e \gamma^2$

(a_e: constants; γ: strain)

then E can be written as a function of ℓ_0^*, ℓ_0, γ only!

and we can take derivatives and compute scaling laws.



Different path to rigidity than jamming

(where #DOF = #constraints at rigidity)