Exercises for BSS 2024 – Lisa Manning

I. CONCRETE PROBLEMS:

Emergent mechanical properties of the vertex model for confluent biological tissues

1. The goal of this problem is to write an expression for a macroscopic mechanical response (in this case the shear modulus G of a network of vertices) as an expansion in terms of normal modes of the dynamical matrix (discussed earlier by Prof. Das in her Lecture 2 and also by Lisa in her Lecture 1)

   (a) The formal definition of the shear modulus is:

$$G = \frac{1}{V}\frac{d^2U(\mathbf{r_i})}{d\gamma^2}, \tag{1}$$

   where U is the potential energy, $\mathbf{r_i}$ is the vector location of the i^{th} vertex (N vertices total in d dimensions), and we parameterize the change of shape of the "box" or the "boundaries" by the shear strain γ. Write an expression for G in terms of partial derivatives with respect to γ instead of the full derivative.

   (b) Note that force balance requires

$$0 = \frac{\partial U}{\partial r_{i\alpha}}, \tag{2}$$

   where α indexes the dimension, e.g. x, y. Write an expression for the total derivative of this equation with respect to γ.

   (c) Let's view the shape of the box, parameterized by the shear strain γ, as an extra degree of freedom. Then let z be a column vector of all the $dN + 1$ degrees of freedom, e.g. all of the $r_{i\alpha}$'s, and then the last entry is γ. Then define an extended dynamical matrix $\bar{D}_{qp}$, which is the second derivatives of the energy U with respect to z_p and z_q. Using your result from part (b), demonstrate that you can re-write (a) as $VG\delta_{\gamma p} = \bar{D}_{qp}\left(\partial z_q/\partial\gamma\right)$.

   (d) Assume that all normal modes of the dynamical matrix with zero frequency have vanishing overlap with the shear degree of freedom. Then use your result from (c) to demonstrate that $G = \frac{1}{V}\left[\sum_m u_{\gamma,m}^2/\omega_m^2\right]^{-1}$, where m is an index over eigenvectors of the dynamical matrix. Hints: take the scalar product with an entry of the normal mode, $u_{p,m}$, and write an expression for $\delta_{\gamma p}$ in terms of the normal modes.

   (e) What happens if there is a normal mode of zero frequency that does have a non-zero overlap with the shear degree of freedom?

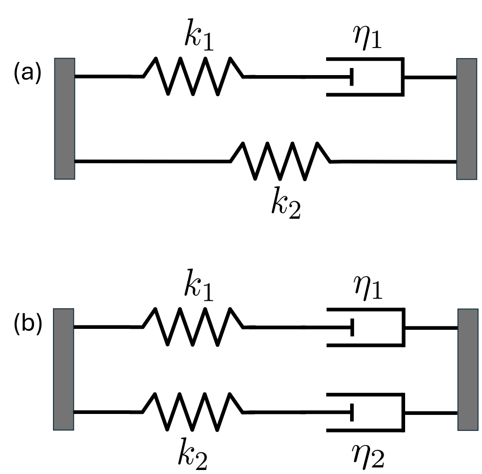

Figure 1. (a) Standard linear solid or Zener model. (b) Standard linear liquid or Burgers model

2. It has been shown [Sijie Tong, Navreeta K Singh, Rastko Sknepnek, Andrej Kosmrlj, PLOS Comp Bio 2022] that the finite-frequency linear response of the vertex model is like Burgers model in the regime where the zero-frequency network response is floppy, and like the Zener model when the network is rigid. Schematics for the two different models are shown in the figure.
   (a) Derive the complex modulus G^*, as well as the storage G' and loss G'' moduli for the Zener model, and discuss the scaling behavior in the low-frequency limit. Does it make sense?
   (b) Derive the complex modulus G^*, as well as the storage G' and loss G'' moduli for Burgers model, and discuss the scaling behavior in the low-frequency limit. Does it make sense?

II. OPEN-ENDED PROBLEM:

In the lectures, we focused almost exclusively on mechanical response of biological tissues in the athermal limit (temperature or active fluctuations going to zero) An interesting set of open problems are thinking about the finite-temperature or finite-fluctuation response of mechanical networks, especially when those fluctuations are not simply thermal, but have a memory kernel or persistence.

In second-order rigid spring networks, fluctuations can open up interesting critical phases, c.f.

- M. Dennison, M. Sheinman, C. Storm, and F. C. MacKintosh, Phys. Rev. Lett. 111, 095503 (2013).
- L. Zhang and X. Mao, Phys. Rev. E 93, 022110 (2016).
- Arzash, S., Gannavarapu, A., and MacKintosh, F. C. Physical Review E, 108(5)(2023).

In vertex models and particle-based models for dense groups of cells, active forcing with a memory kernel robustly gives rise to velocity-velocity correlations that overlap the low-frequency normal modes of the material, c.f.

- Henkes, S., Kostanjevec, K., Collinson, J. M., Sknepnek, R., and Bertin, E. (2020). Dense active matter model of motion patterns in confluent cell monolayers. Nature communications, 11(1), 1405.

One interesting open question is how fluctuations with memory kernels might alter the behavior of these critical phases that emerge in second order rigid systems at finite temperature. A pretty challenging problem is to attempt to derive for yourself Equation 6 from Henkes et al:

$$\left\langle |\mathbf{v}(\mathbf{q})|^2 \right\rangle = \sum_m \frac{v_0^2}{2(1+\omega_m^2 \tau/\xi)} |\mathbf{u_m}(\mathbf{q})|^2, \tag{3}$$

where we've used the same notation as above for normal modes $\mathbf{u_m}$ of the dynamical matrix with frequency ω_m, and τ is the persistence time of an active self-propulsion of magnitude v_0 with damping ξ.

A longer term project would be to understand how these correlations, which are absent in systems where $\tau \to 0$, impact the mechanical behavior right at the critical strain? One could use published software for vertex models

- Barton, Daniel L., et al. "Active vertex model for cell-resolution description of epithelial tissue mechanics." PLoS computational biology 13.6 (2017): e1005569.
- Sussman, Daniel M. "cellGPU: Massively parallel simulations of dynamic vertex models." Computer Physics Communications 219 (2017): 400-406.

to analyze the behavior of the finite difference shear modulus with τ and v_0.