



Parallel session # 3 - CONTINUUM & STATISTICAL MECHANICS

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Simple statistical mechanics for biological systems (continued)

L. Mahadevan

* recommended reading: "Random walks in biology" by H. Berg

Random walks & diffusion: $\sqrt{\langle x^2(t) \rangle} = \sqrt{2Dt}$ with $D = v \delta \sim \frac{\delta^2}{\tau}$

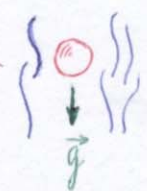
ballistic motion of constant velocity: $\sqrt{\langle x^2 \rangle} \sim vt$
 or if constant force $\sqrt{\langle x^2 \rangle} \sim at^2$

both fluctuation (associated with temperature) and dissipation (from movement in fluid) Einstein balances them: fluctuation \approx dissipation when the system is at equilibrium

- Fluid dynamics: "Archimedean" limit (very slow movement)

[F] ? dimension of a force with respect to basic dimensions: $\left. \begin{array}{l} L \text{ length, } T \text{ time, } M \text{ mass} \end{array} \right\} [F] = M \frac{L}{T^2}$

$F = C \mu a v$ and μ must have dimensions of $\left\{ \begin{array}{l} M / (LT) = [\mu] \\ \frac{MLT^{-2}}{L^2} \cdot T = [\mu] \\ \frac{\text{force}}{\text{area}} \cdot \text{time} = \text{Pa} \cdot \text{s} \end{array} \right.$
 μ is the viscosity of the fluid
 a and v characterize the sphere
 C is a constant dependent on shape ($C_{\text{sphere}} = 6\pi$)



here $F = 6\pi \mu a v = \Delta \rho g a^3 \frac{4\pi}{3}$
 μ is the only unknown and can be experimentally determined
 how much force should be exerted on the top plate to move it at constant velocity \vec{u} ?



$\sigma = F/A = \mu u/h$ (with \vec{u} shear velocity)

orders of magnitude: $\mu_{H_2O} \sim 10^{-3} \text{ Pa} \cdot \text{s}$
 $\mu_{\text{air}} \sim 10^{-5} \text{ Pa} \cdot \text{s}$

Reynold's number $Re = \frac{\rho_f U^2 L^2}{\mu UL} = \frac{\text{inertia}}{\text{viscosity}} = \frac{\rho_f UL}{\mu}$

Continuum and statistical mechanics - 2.

Reynold's number in biology

$$\left. \begin{aligned} L &\sim 10^{-6} \text{ m} = 1 \mu\text{m} \\ U &\sim 1 \mu\text{m/s} \\ \rho &\sim 10^3 \text{ kg/m}^3 \\ \mu &\sim 10^{-3} \text{ Pa}\cdot\text{s} \end{aligned} \right\} \text{Re} \sim 10^{-6} \ll 1$$

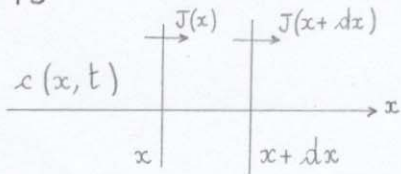
fluctuation \approx dissipation
Stokes - Einstein Smoluchowski

$$F \delta \sim k_B T$$

$$\mu a v \delta \sim k_B T \text{ or } v \delta \sim \mathcal{D} \sim \frac{k_B T}{\mu a} = \frac{k_B T}{\zeta}$$

ζ friction factor (drag)
 $1/\zeta$ mobility

- Macroscopically
in 1D



concentration $[c] = \# \text{ molecule / volume}$
flux $[J] = \# / \text{area} / \text{time}$

$$A dx \frac{\partial c}{\partial t} = (J|_x - J|_{x+dx}) dx A$$

$$\text{and } J|_{x+dx} \approx J|_x + \frac{\partial J}{\partial x} dx + \dots$$

one more equation needed:

$$J = - \mathcal{D} \frac{\partial c}{\partial x} \quad \text{dimensionally consistent: } [\mathcal{D}] = \frac{L^2}{T}$$

differential equation is the diffusion equation:

$$\frac{\partial c}{\partial t} = \mathcal{D} \frac{\partial^2 c}{\partial x^2}$$

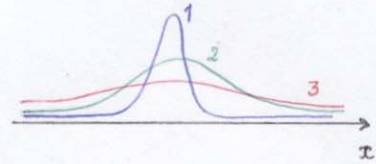
macroscopic diffusion \equiv microscopic random walk

$$\frac{c}{T} \sim \mathcal{D} \frac{c}{x^2} \text{ or } x^2 \sim \mathcal{D} t$$

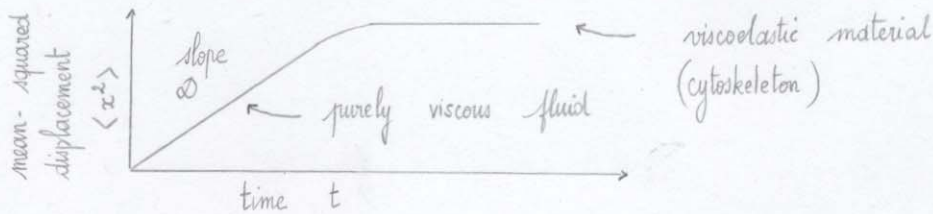
- what if a flux due to fluid velocity was added to the flux due to concentration

$$J = - \frac{\partial c}{\partial x} \mathcal{D} + v c \quad \text{and Stokes - Einstein would be recovered [differences?]$$

as a function of time, diffusion equation solution:



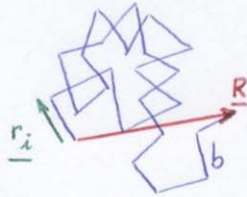
- the viscosity of a fluid can be determined experimentally:



- Boltzmann's statistics : random walk as a model for a polymer (DNA e.g.)



modeled
as



all "steps" of length "b" (N links)
all independent, equally likely
polymer \equiv random walk in space

no energy associated with bending or twisting or crowding (enthalpy)
but entropic energy : how many different ways can I arrange this molecule?
free energy

$$G = H - TS$$

enthalpy - temperature * entropy (or disorder)

to define disorder :

$P(\text{wavy}) < P(\text{coiled})$ calculate these probabilities

Boltzmann

$$S = k_B \ln P$$

extensive quantity

entropy adds up, but # of states gets multiplied \Rightarrow ln needed

random walk has mean of 0
variance of Nb

$$P = \exp\left(\frac{-|R|^2}{3Nb^2 \times 2}\right)$$

$$G = -TS = \frac{Tk_B |R|^2}{3Nb^2}$$

$$G = \frac{1}{2} \cdot \frac{k_B T}{3Nb^2} \cdot |R|^2$$

$$U = \frac{1}{2} k (l - l_0)^2$$

polymer = spring of reference length zero
of constant directly dependent on temperature
that gets more sloppy as $N \uparrow$

polymer \equiv entropic spring

Foundations of continuum mechanics : elastic & viscoelastic response

- stress : τ_{ij} force per unit area
- strain : E_{ij} change of length between 2 neighboring points
 $E_{ii} = \frac{1}{2} (\lambda_{ii}^2 - 1)$ normal component, E_{12} shear component
 λ_{ii} is the stretch ratio = final length \div initial length
- strain rate : $\frac{\partial v_i}{\partial x_j}$ velocity gradient, directly proportional to $\frac{\partial E_{ij}}{\partial t}$

* recommended reading : Y. C. Fung : A first course in continuum mechanics

- solid material $\tau_{ij} \propto E_{ij}$ stress proportional to strain
- fluid material $\tau_{ij} \propto \dot{E}_{ij} = \frac{\partial v_i}{\partial x_j}$ " " strain rate
- viscoelastic material $\tau_{ij} \propto E_{ij}$ and \dot{E}_{ij}

- Solids : τ_{ij} linearly proportional to E_{ij} : Hookean materials

$$\tau_{ij} = \underbrace{C_{ijkl}}_{31 \text{ coefficients}} E_{kl} \rightarrow \text{repetition of indices} = \text{summation convention}$$

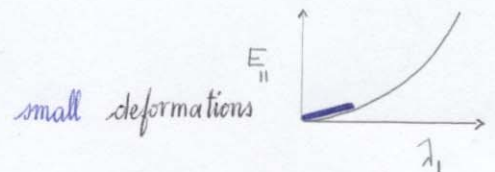
$$a_i b_i = \sum_{i=1}^3 a_i b_i = a_1 b_1 + a_2 b_2 + a_3 b_3$$

isotropic materials

$$\tau_{ij} = \lambda \epsilon_{kk} \delta_{ij} + 2\mu E_{ij}$$

$$E_{ij} \propto \epsilon_{ij} \text{ such that } E_{ii} = \frac{1}{2} (\lambda_i^2 - 1) = \lambda_i - 1 = \epsilon_{ii}$$

inverse ①
$$\epsilon_{ii} = \frac{1}{E} (\tau_{ii} - \nu (\tau_{22} + \tau_{33}))$$



writing it out :
$$\tau_{ii} = \lambda \epsilon_{kk} + 2\mu \epsilon_{ii}$$

$$\tau_{12} = 2\mu \epsilon_{12} \text{ because } \delta_{12} = 0$$

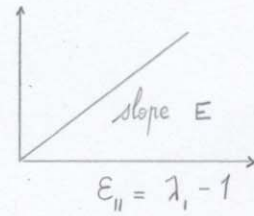
since $\epsilon_{kk} = \epsilon_{11} + \epsilon_{22} + \epsilon_{33} \propto \Delta V / V_0$ change of volume

if $\epsilon_{kk} = 0$ incompressible material and only shear effects

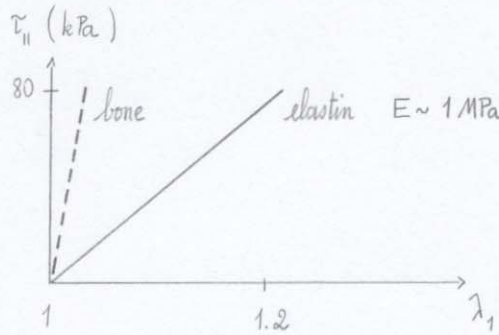
2 material coefficients for linear viscoelastic materials : λ and μ , or E and ν
 μ : shear modulus (sometimes G)

inverse ②
$$\epsilon_{12} = \frac{1+\nu}{E} \tau_{12} = \frac{1}{2G} \tau_{12}$$

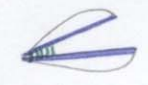
ν : Poisson's ratio (compressibility) τ_{11}
 E : Young's modulus



examples:

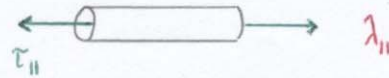
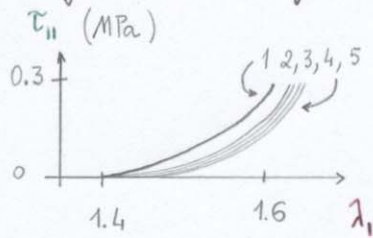


$E_{\text{collagen}} \sim 10^3 \text{ MPa}$
 $E_{\text{bone}} \sim 10^4 \text{ MPa}$
 $E_{\text{rubber}} \sim 1.4 \text{ MPa}$


 in muscles
 adductin \approx elastin

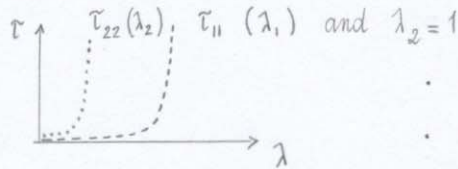
$0 \ll \nu \ll 0.5$ compressibility (incompressible materials have $\nu = \frac{1}{2}$)

dog carotid artery:



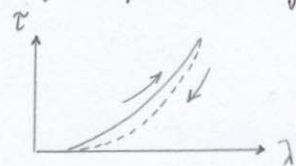
- preconditioning necessary for stress-strain curves to become reproducible.
- what plot is more relevant? 1 or 2,3,4,5?

skin



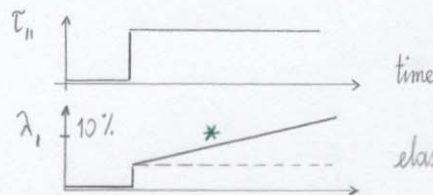
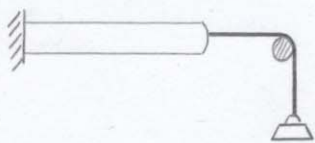
- skin is anisotropic
- skin is extremely nonlinear: from soft to stiff

after preconditioning:



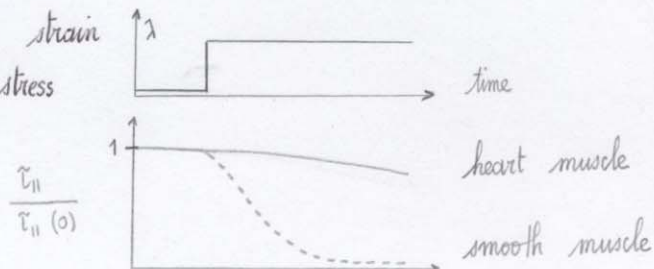
- loading curve vs. "stress decreased" = unloading curve
- hysteresis
- loop changes with frequency of loading?

- creep test: apply τ_{11} , observe λ_1



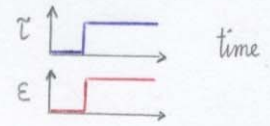
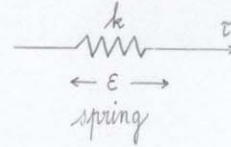
* heart muscle, arteries, ...

relaxation experiment: constant strain observe stress

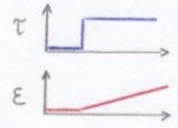
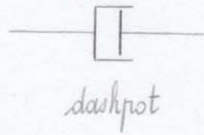


Viscoelasticity : stress τ as a function of strain ϵ and strain rate $\dot{\epsilon}$ in a linear viscoelastic material

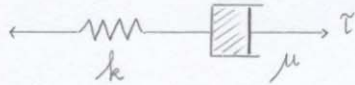
$\tau = k \epsilon$
elastic solid



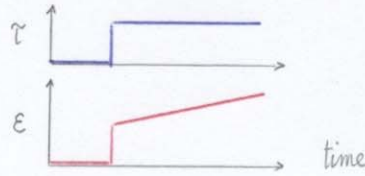
$\tau = \mu \dot{\epsilon}$
viscous fluid



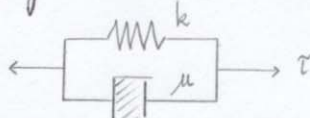
Maxwell fluid



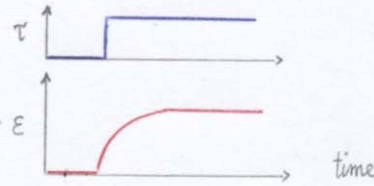
$$\frac{\tau}{\mu} + \frac{1}{k} \frac{d\tau}{dt} = \frac{d\epsilon}{dt}$$



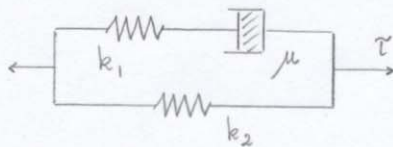
Voigt body



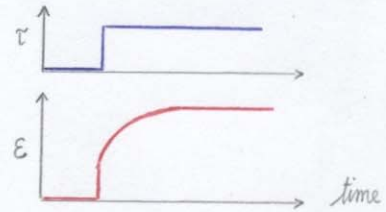
$$\tau = k \epsilon + \mu \dot{\epsilon}$$



Standard solid



$$\tau + \frac{\mu}{k_1} \dot{\tau} = k_2 \epsilon + \mu \left(1 + \frac{k_2}{k_1}\right) \dot{\epsilon}$$



goes back to its original state
good model for cells if small deform.

in fact cells continue to creep, they don't reach a steady state like standard solids. biological materials have "a spectrum of coefficients (k, μ) ".