Continuum and Statistical Mechanics notes

Parallel session # 3 - CONTINUUM & STATISTICAL MECHANICS

08/08/2006

Simple statistical mechanics for biological systems (continued)

L. Mahadevan

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

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

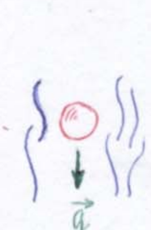
ballistic motion of constant velocity : $\sqrt{\langle x^2 \rangle} \sim v\,t$
or if constant force $\sqrt{\langle x^2 \rangle} \sim a\,t^2$

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

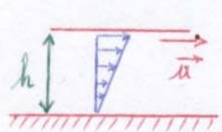
- Fluid dynamics : " Archimedean " limit (very slow movement)
  [F] ? dimension of a force with respect to basic dimensions : L length , T time , M mass $\Big\}$ $[F] = M \frac{L}{T^2}$

$F = C\,\mu\,a\,v$ and μ must have dimensions of
μ is the viscosity of the fluid
a and v characterize the sphere
C is a constant dependent on shape ($C_{sphere} = 6\pi$)

$$\left\{\begin{array}{l} M/(LT) = [\mu] \\ \frac{M L T^{-2}}{L^2}\cdot T = [\mu] \\ \frac{\text{force}}{\text{area}}\cdot \text{time} \equiv \text{Pa.s} \end{array}\right.$$



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 : $\mu_{H_2O} \sim 10^{-3}$ Pa.s
$\mu_{air} \sim 10^{-5}$ Pa.s

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

Continuum and statistical mechanics _ 2.

Reynold's number in biology

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

inertia negligible

fluctuation $\approx$ dissipation

Stokes - Einstein Smoluchowski

$F\,\delta \sim k_B T$

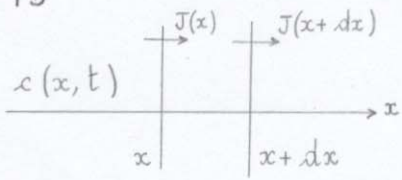
$\mu\, a\, v\, \delta \sim k_B T$ or $v\delta \sim \boxed{\mathcal{D} \sim \dfrac{k_B T}{\mu a} = \dfrac{k_B T}{\zeta}}$

ζ friction factor (drag)

$1/\zeta$ mobility

_ Macroscopically

in 1D



concentration $[c]$ = # molecule / volume

flux $[J]$ = # / area / time

$$\left.\begin{array}{l} A\, dx\, \dfrac{\partial c}{\partial t} = \left(J|_x - J|_{x+dx} \right) dx\, A \\ \text{and} \quad J|_{x+dx} \approx J|_x + \dfrac{\partial J}{\partial x}\, dx + \ldots \end{array}\right\} \quad \frac{\partial c}{\partial t} = - \frac{\partial J}{\partial x}$$

one more equation needed :

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

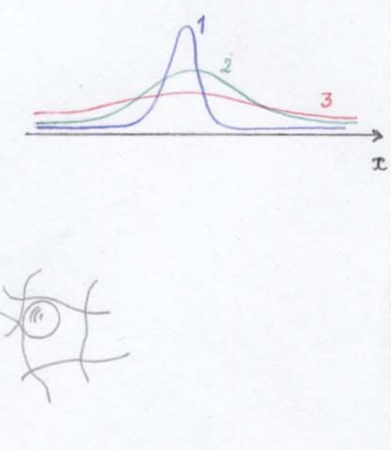
differential equation is the diffusion equation : $\dfrac{\partial c}{\partial t} = \mathcal{D}\, \dfrac{\partial^2 c}{\partial x^2}$

macroscopic diffusion $\equiv$ microscopic random walk $\dfrac{c}{T} \sim \mathcal{D}\, \dfrac{c}{x^2}$ or $x^2 \sim \mathcal{D} t$

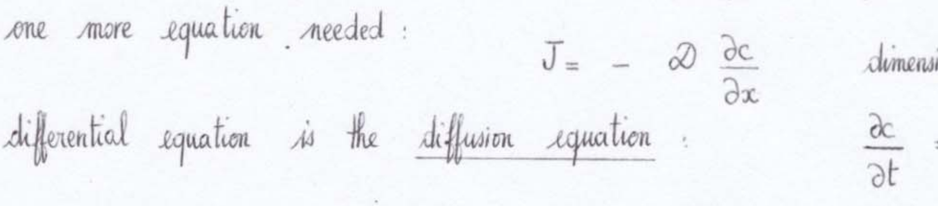
- what if a flux due to fluid velocity was added to the flux due to concentration

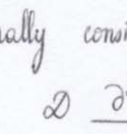
$J = - \dfrac{\partial c}{\partial x}\, \mathcal{D} + v\, c$ and Stokes - Einstein would be recovered [differences ?

as a function of time , diffusion equation solution :

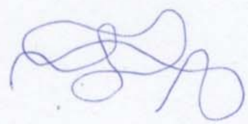


- the viscosity of a fluid can be determined experimentally :

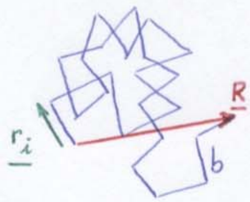




- <u>Boltzmann's statistics</u> : random walk as a model for a polymer (DNA e.g.)



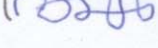
modeled as



all "steps" of length "b" (N links)
all independent, equally likely
<u>polymer ≡ random walk in space</u>

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() < P () calculate these propabilities

Boltzmann $S = k_B \ln P$
extensive quantity
entropy adds up , but # of states gets multiplied => ln needed

random walk has mean of 0, variance of N b $\Big\}$ $P = \exp\left(\dfrac{-|\underline{R}|^2}{3Nb^2 \times 2}\right)$

$$G = -TS = \frac{T k_B |\underline{R}|^2}{3Nb^2}$$

$$\left.\begin{array}{l} G = \dfrac{1}{2} \cdot \dfrac{k_B T}{3Nb^2} \cdot |\underline{R}|^2 \\[2ex] U = \dfrac{1}{2}\, k\, (l - l_0)^2 \end{array}\right\}$$

polymer ≡ spring of reference length zero
of constant directly dependent on temperature
that gets more sloppy as N ↗

<u>polymer ≡ entropic spring</u>

Geert Schmid-Schönbein

Foundations of continuum mechanics : elastic & viscoelastic response

- stress : τ_{ij} force per unit area
- strain : E_{ij} change of length between 2 neighboring points
  $E_{11} = \frac{1}{2}\left(\lambda_{11}^2 - 1\right)$ normal component , E_{12} shear component
  λ_{11} is the stretch ratio = final length ÷ 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 mechanic

- 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

$$\tau_{ij} = \underbrace{C_{ijkl}}_{81 \text{ coefficients}} E_{kl}$$

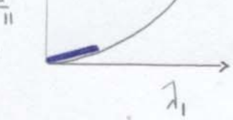
→ repetition of indices = summation convention $\qquad a_i b_i = \sum_{i=1}^{3} a_i b_i = a_1 b_1 + a_2 b_2 + a_3 b_3$

isotropic materials $\tau_{ij} = \lambda\, \varepsilon_{kk}\, \delta_{ij} + 2\mu\, \varepsilon_{ij}$

$E_{ij} \propto \varepsilon_{ij}$ such that $E_{11} = \frac{1}{2}\left(\lambda_1^2 - 1\right) = \lambda_1 - 1 = \varepsilon_{11}$

inverse ① $\varepsilon_{11} = \frac{1}{E}\left(\tau_{11} - \nu\left(\tau_{22} + \tau_{33}\right)\right)$

small deformations



writing it out : $\tau_{11} = \lambda\, \varepsilon_{kk} + 2\mu\, \varepsilon_{11}$

$\tau_{12} = 2\mu\, \varepsilon_{12}$ because $\delta_{12} = 0$

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

if $\varepsilon_{kk} = 0$ 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 $\varepsilon_{12} = \frac{1+\nu}{E}\,\tau_{12} = \frac{1}{2G}\,\tau_{12}$

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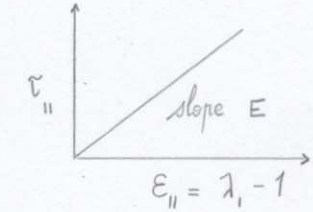
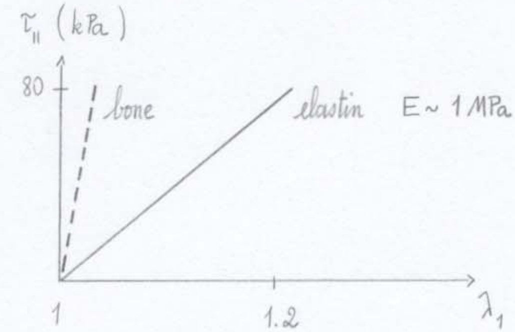
ν : Poisson's ratio (compressibility)

E : Young's modulus



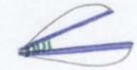
examples :

- 

  $E_{collagen} \sim 10^3$ MPa

  $E_{bone} \sim 10^4$ MPa

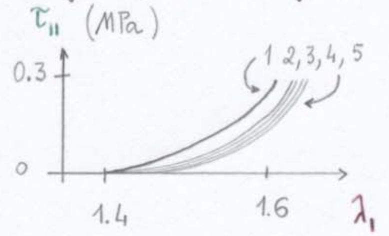
  $E_{rubber} \sim 1.4$ MPa

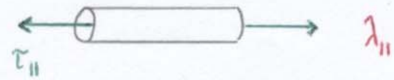
  

  [in mussels adductin $\approx$ elastin

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

- dog carotid artery :

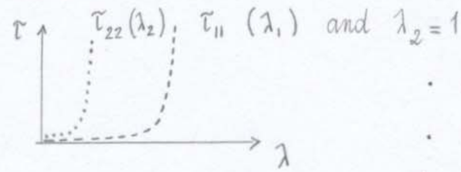
  

  . preconditioning necessary for stress - strain curves to become reproducible.

  . what plot is more relevant ? 1 or 2,3,4,5 ?

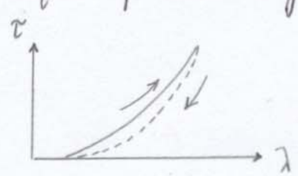
- skin

  . skin is anisotropic

  . skin is extremely nonlinear : from soft to stiff

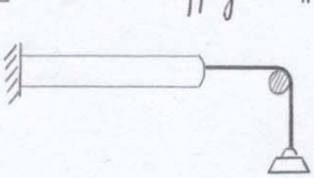
- after preconditioning : loading curve vs. "stress decreased" = unloading curve

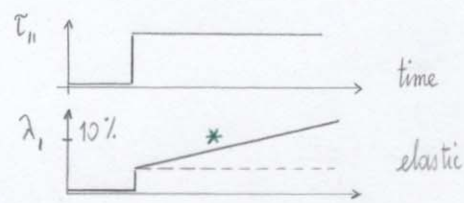
  

  . hysteresis

  . loop changes with frequency of loading ?

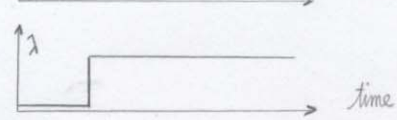
_ creep test : apply τ_{11} , observe λ_1

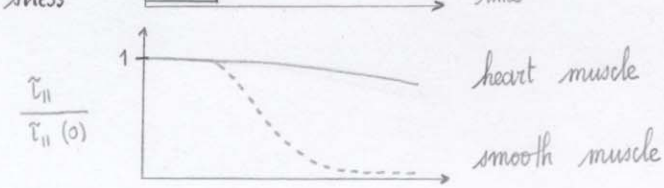




* heart muscle, arteries , ...

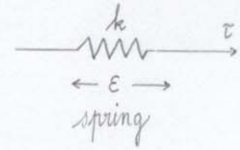
relaxation experiment : constant strain observe stress

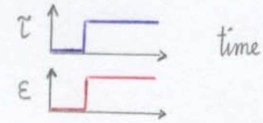




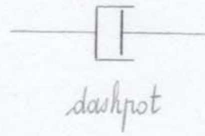
<u>Viscoelasticity</u> : stress τ as a function of strain ε and strain rate $\dot{\varepsilon}$ in a linear viscoelastic material

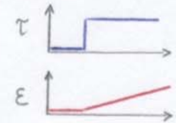
$\tau = k\,\varepsilon$
elastic solid



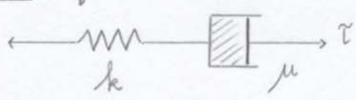


$\tau = \mu\,\dot{\varepsilon}$
viscous fluid

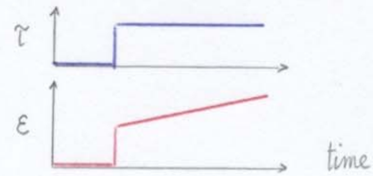




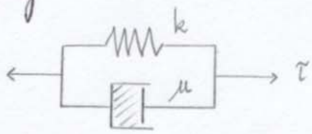
<u>Maxwell fluid</u>



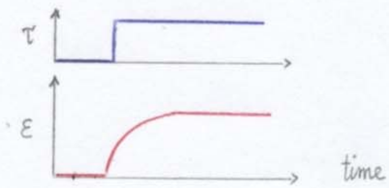
$$\frac{\tau}{\mu} + \frac{1}{k}\,\frac{d\tau}{dt} = \frac{d\varepsilon}{dt}$$



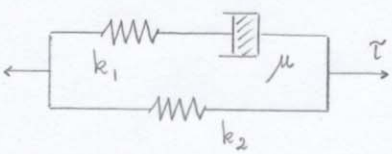
<u>Voigt body</u>



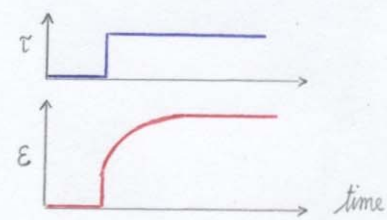
$$\tau = k\,\varepsilon + \mu\,\dot{\varepsilon}$$



<u>Standard solid</u>



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



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)".