Basic Mechanics notes

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Parallel tutorial session #1: Basic Mechanics

Welcome and introduction to GEM^4

- International, interdisciplinary, inter-institutional initiative started early 2006
- Focus: MIT, NSU, Harvard, Institut Pasteur
- Engineering, biology, medicine & public health intersected
- Paradigm for global cooperation through research, training & translation
- Networking opportunities
- Infrastructure capabilities

- Training program: Summer school (2007 in Singapore, focus on cancer)*
  Also offered by GEM^4: Distinguished lecture series
  Junior scientist program

*With the newly announced SMART: Singapore-MIT Alliance for Research and Technology Center in Singapore

GEM^4 co-sponsors the next worldwide meeting on biomechanics in 2010.

- Cell and molecular mechanics in biomedicine, with a focus on infectious diseases
  From a course developed at MIT by Prof. Patrick Doyle, Allan Grodzinsky & R. Kamm
  Lab info: http://www.openvnetware.org/wiki/GEM4 labs
  Breakdown of participants: 30% life scientists, 70% engineers
  Poster sessions to share research knowledge
  Research proposals to be developed during the summer school, presented in 3-4 pages

Direct questions to Maggie Sullivan or Roger Kamm: suhsmag @ mit.edu

Simple statistical mechanics for biological systems

- Questions: What is the goal?
  Starting with the central dogma in biology: DNA → RNA → proteins → organelles
  (Crick)
  (Ecosystem → organism → tissue → cells →)
  (and feedback), essentially increasing length scale

L. Meckelov

Simple statistical mechanics for biological systems
Hence, length and time scales and "out of equilibrium" principles matter.

**Length scales:**
- \( \Phi \) DNA size: \( 10^{-9} \) m
- Nucleus size: \( 10^{-1} \) m
- Cell (animal) size: \( 10^{-3} \) m
- Plant cell size: \( 10^{-3} \) m
- DNA length: \( 10^{-1} \) m
- Human size: \( 10^1 \) m
- Whale size: \( 10^3 \) m

Cells are the fundamental units of life: smallest to function independently, cell size a amount of DNA enclosed.

**Time scales:**
- Chemical reaction time: \( 10^{-6} \) s
- Action potential of E. Coli: \( 10^{-4} \) s
- Cell mobility: \( 10^{-2} \) s
- Life (Caenorhabditis): \( 10^2 \) s
- Life (human): \( 10^8 \) s

Out of equilibrium biology: soft, wet, dynamic, warm.

Information (encoded in DNA...), energy, matter.

We wish to couple energy and matter: biology is warm, hence in motion, hence energy (dynamic & directed).

**Energy scales:**
- Thermal energy used as a ruler.
- Energy / mole / K \( \sim \) \( \frac{RT}{k_B} \) (of ideal gas)
  \( R \) per degree of freedom
  \( (3 \text{ d.o.f.} \text{ for ideal gas}) \)
  \( \frac{8.3 \text{ J/mole} / \text{K}}{\text{for ideal gas}} \)
- Energy / molecule (and per degree of freedom)
  \( \sim \frac{RT}{k_B} \)
- Avogadro's number \( \Phi_A \) \( \sim 6 \times 10^{23} \) and Boltzmann's constant \( k_B \)
  \( \approx 1.38 \times 10^{-23} \text{ J/molecule/K} \)

\( U_{\text{molecule}} \approx 4 \times 10^{-24} \text{ J} \)

Hence force scale of pN and length scale of nm (pico Newtons, nanometers)

**Coupled interactions:**
- Chemical (physical)
- Electrical
- Mechanical

The grand goal is to understand how these interact (are organized) in space and time.
Energy scales:

- $10^1$: non-covalent bonds (in biology)
- $10^3$: photosynthesis (green light)
- $10^5$: glucose oxidation
- $10^7$: ATP hydrolysis
- $10^9$: C-C bond

Over the past decade, much progress has been made experimentally and technically. Down on small scales, biology is geometrically dominated by filaments and membranes which is connected with chemical mediatability which makes for physical complexity (nonlinearity).

Outline:
- random walks & diffusion
- drag, mobility, Boltzmann’s law, Stokes-Einstein
- biological forces & energies
- physics, mechanics and mechano-chemistry of polymers and membranes


A bacteria tumbles randomly in a homogeneous environment, then more directly in the presence of a chemotransmitter (response to a stimulus); when the chemotransmitter diffuses away, randomness reappears (adaptation).

Sensing and movement are coupled:

- in the absence of any active processes, what happens to a blob of chemotransmitter?
  - at random walks (in 1-D) and diffusion
  - microscopic and macroscopic

Maximize the disorder:

- statistical probability

$t = 0$ to $t \to \infty$
- from kinetic energy: \( \frac{1}{2} k_B T = \frac{1}{2} m \langle v^2 \rangle \)
\[ \langle v^2 \rangle = k_B T / m \]
mean squared velocity

for a lysozyme \( m \sim 14 \text{ kg / mole} \) and \( 6 \times 10^{23} \text{ molecules / mole} \)
\[ \sqrt{\langle v^2 \rangle} \sim 1 \text{ m / s} \]
very high!

but collisions and dissipation \( \Rightarrow \) no net motion of the lysozyme

velocity \( v \), step size \( \delta = \pm v c \) with \( c \): time between collisions.

\[-2\delta - \delta \quad 0 \quad +\delta \quad 2\delta\]

\begin{enumerate}
  \item probability of going in either direction \( p = 1/2 \)
  \item each step independent of others
\end{enumerate}

- with \( N \) particles at origin \( x = 0 \)
  \[ x_i(n) = x_i(n-1) \pm \delta \]
  \( i \): particle label
  \( n \): number of steps \( = t / \tau \)

\[ \langle x(n) \rangle = \frac{1}{N} \sum_{i=1}^{N} x_i(n) = \langle x_i(n-1) \rangle = \ldots = \langle x_i(0) \rangle = 0 \]

\[ \langle x(n) \rangle = 0 \]
mean location of particles

- spread of distribution: variance
  \[ x_i^2(n) = x_i^2(n-1) + \delta^2 + 2\delta x_i(n-1) \]

\[ \langle x_i^2(n) \rangle = \langle x_i^2(n-1) \rangle + \delta^2 = n\delta^2 \]

\[ \langle x^2(t / \tau) \rangle = \frac{1}{2} \cdot 2\delta^2 / \tau \cdot t = 2D \cdot t \]
mean squared proportional to time

\[ \sqrt{\langle x^2(t / \tau) \rangle} \sim t^{1/2} \quad \text{slow (diffusion)} \]

\[ D \sim \sqrt{\langle v^2 \rangle} \delta \sim 10^{-3} \text{ m / s} \quad 10^{-9} \text{ m}^2 / \text{s} \text{ or } 10^{-5} \text{ cm}^2 / \text{s} \]

\[ \tau \sim 10^{-4} \text{ s} \sim 1 \text{ um} \sim 10^{-8} \text{ m} / (10^{-9} \text{ m}^2 / \text{s}) \sim 10^{-3} \text{ s} \quad \text{quick on small scale} \]

\[ \tau \sim 1 \text{ um} \sim 10^{4} \text{ s} \text{ or } 10 \text{ hours} \quad \text{slow on large scale} \]
Newton's law \( \mathbf{F} = m \frac{d\mathbf{v}}{dt} \) was noted to be the most important human discovery. It is at the core of biology (force & velocity related).

A major part of mechanics today is to understand and measure forces.

**Forces**

What should the mass \( m \) be in biology? Neighboring cells influence one cell.

Newton's law is not as useful in this discrete form as in engineering.

Interaction between discrete identifiable objects.

But another definition of force / interaction is needed in biology.

**Stress**

\[
\frac{dS}{n} = \text{surface area}
\]

\[
\frac{\mathbf{v}}{\mathbf{n}} = \text{outer normal}
\]

\[
\lim_{\Delta S \to 0} \frac{\Delta T}{\Delta S} = \frac{\mathbf{v}}{\mathbf{n}}
\]

and with \( \mathbf{v} \parallel x_1 \) axis:

\[
\mathbf{v} \parallel x_2 \text{ axis } : \quad \mathbf{v} \parallel x_3 \text{ axis }
\]

\[
\mathbf{T} = \begin{pmatrix} 
\tau_{11} & \tau_{12} & \tau_{13} \\
\tau_{21} & \tau_{22} & \tau_{23} \\
\tau_{31} & \tau_{32} & \tau_{33}
\end{pmatrix}
\]

**Stress tensor**

- Normal stress:
  - \( \tau_{11} \), \( \tau_{22} \), \( \tau_{33} \)
  - \( \tau_{12} \), \( \tau_{13} \), \( \tau_{23} \)

- Shear stress:
  - \( \tau_{ij} \), \( i \neq j \)

**Pressure**

\[
\text{Pressure} = -\frac{1}{3} \left( \tau_{11} + \tau_{22} + \tau_{33} \right)
\]

**Principal Stress**

Starting with an analogy with vectors.

Coordinates depend on set of axes.

In principal coordinates system (one and only one exists):

\[
\begin{pmatrix}
\tau_{11} & 0 & 0 \\
0 & \tau_{22} & 0 \\
0 & 0 & \tau_{33}
\end{pmatrix}
\]

**Stress Deviators**

The solutions to certain problems are independent of normal stresses.

\[
\begin{cases}
\bar{\tau}_{ij} = \tau_{ij} - \frac{1}{3} \left( \tau_{11} + \tau_{22} + \tau_{33} \right) \\
\delta_{ij} = \tau_{ij} + P \delta_{ij}
\end{cases}
\]

**Mean Normal Stress**
Residual stress

Deformation strain strain rate

The unloaded state is not necessarily stress-free without residual stress.

Displacement $u_i = x_i - a_i$

Final - initial

Includes deformation and translation.

Hooke: change in length measures deformation alone.

Change of length $s^2 - s_0^2 = \text{strain} \times 2 \times \text{initial distance}$

Deformation gradients $\frac{\partial x_k}{\partial a_j}$

\[
E_{ij} = \frac{1}{2} \left( \frac{\partial x_k}{\partial x_j} \cdot \frac{\partial x_k}{\partial x_i} - \delta_{ij} \right)
\]

Deformation strain $E_{ij} = \frac{1}{2} \left( \frac{ds^2}{ds_0^2} - 1 \right)$

Sketch ratio $\lambda = \frac{ds}{ds_0}$

$E_{12} \approx \tan \alpha$

Reference states in biology are debatable, difficult to define (because deformable materials).

In a fluid, what quantity is proportional to the applied stress? Strain rate.

$F \sim \mu \frac{\partial v_i}{\partial x_j}$

Velocity gradient or strain rate

Spatial velocity gradients $\frac{\partial v_i}{\partial x_j}, \frac{\partial v_i}{\partial x_2}, \frac{\partial v_i}{\partial x_3}$