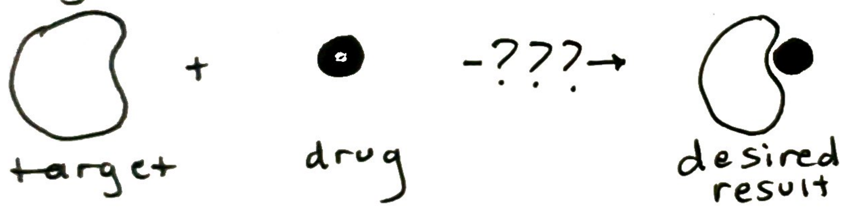
Intro to Biological Thermodynamics
Summer HSSP 2020
Notes - 7/11/2020

What is thermodynamics?

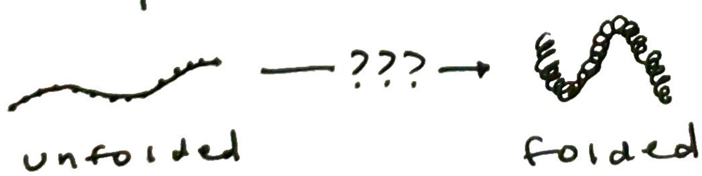
Studies how energy interacts/transfers between molecules or collections of molecules, especially how they contribute to larger processes

Why should you care?

- pharmaceuticals: determines if candidate drug binds to its target



- protein folding: used to characterize and compare proteins' structures, including predicting folding temperature and final protein form



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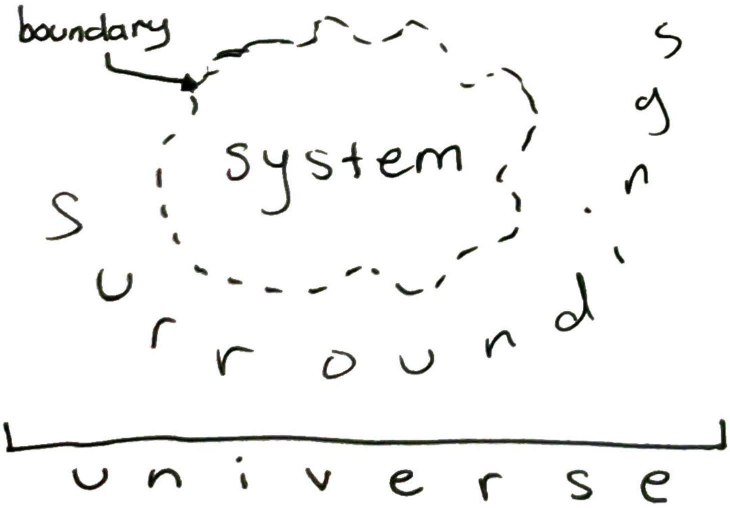
Energy

Internal energy = all ways energy can be stored
↳ noted as "U"

$$U_{total} = U_{KE} + U_{PE} + U_{vibration} + U_{\text{[redacted]} CE} + \ldots$$

Energy units: 1 Joule (J) = $1 \frac{kg \cdot m^2}{s^2}$

Systems and Surroundings



types of systems:
- isolated = no energy exchange, no mass exchange
- closed = energy exchange, no mass [redacted] exchange
- open: energy exchange, mass exchange

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1st Law of Thermodynamics

$$\Delta U_{universe} = \Delta U_{system\ (sys)} + \Delta U_{surroundings\ (surr)} = 0$$

means that energy cannot be created or destroyed! only transferred

Work and heat

- heat [redacted] = random particle motion
  ↳ noted as "q"
- work = non-random (e.g. directional) particle motion
  ↳ noted as "w"

$$\underbrace{\Delta U}_{stored} = \underbrace{q + w}_{transferred}$$

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Variables and equations

- 2 types of variables:
  - state variables (path - [redacted] independent) = do not depend on the history of the system, only dependent on the current state of the system
    - examples: T (temperature)
      P (pressure)
      U (internal energy)
      H (enthalpy)
      S (entropy)
      ... and more!
  - path-dependent = depend and change based on the changes made to the system
    - examples: u (heat)
      w (work)

- use variables to form equations of state:

generic:

$V = f(n, P, T)$

$P = f(n, V, T)$

→ specific:

$PV = nRT$

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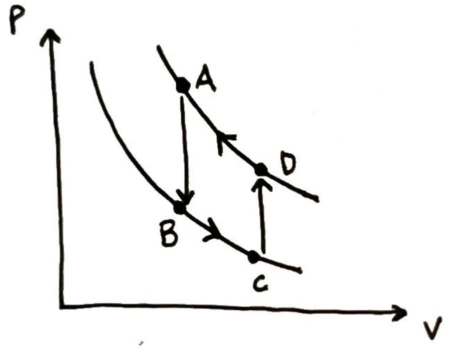
Processes

- involves a change in the state functions defining a system
- describes <u>how</u> a transition occurs
- example:



☆ fact: each line on a PV diagram represents a process at equilibrium: the variables remain [redacted] uniform throughout the system

Reversible vs. Irreversible Transitions

Reversible	Irreversible
- process can be "reversed" through infitessimal changes to system	- process that is fully "non-reversible"
- no loss or dissipation of energy	- can never reach the original state from its final state
- does not exist in the real world, only theore[redacted]tical	- system passes through a series of non-equilibrium states
	- all real-world processes

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Kinetic Theory of Gases

- translational kinetic energy = energy due to motion from one location to another
- formula: $E = \frac{3}{2} k_B T$

  T = temperature
  k_B = Boltzmann's constant
  $= 1.38 \times 10^{-23}$ $m^2 kg s^{-2} K^{-1}$

Ideal Gas Law

- formula: $PV = nRT$
- [redacted] to be an ideal gas...
  1) gas molecules do not attract or repel each other
  2) gas molecules do not take up volume
  3) volume of the individual gas particles is negligible compared to the volume of the gas as a whole
  4) collisions between gas particles and container walls are elastic, meaning the total kinetic energy remains the same.