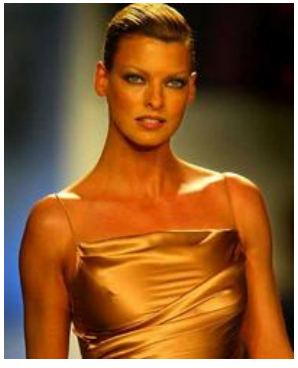
Outline

- Modeling intro
- First order chemical kinetics.
- Second order chemical kinetics.

Modeling

- A model is an abstract representation of an object, system, or process, usually idealizing some features and neglecting others.

For a population with heritable variation in some characteristic that influences an individual's capacity to reproduce or success in reproduction, the frequency of those phenoptypes that reproduce most successfully will increase.



$$\frac{\partial u}{\partial t} = D\nabla^2 u$$

Modeling and theories

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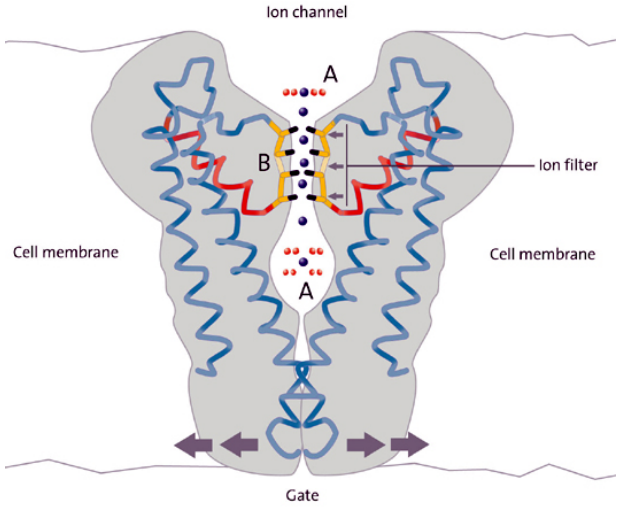
- Example: Assume that the size of a population of bacteria grows at a rate proportional to its current size (our assumption). Translating into an equation, we get $dp/dt = rp$ (the assumption restated in our mathematical language). Solving this equation (an acceptable means of drawing conclusions), we find that the population grows exponentially. To determine if we've got a good theory, we must look at data.

Chemical kinetics

First order kinetics

- A reaction whose rate depends on the concentration of only one reactant.
- Example: an ion channel undergoing a conformation change (closed to open).

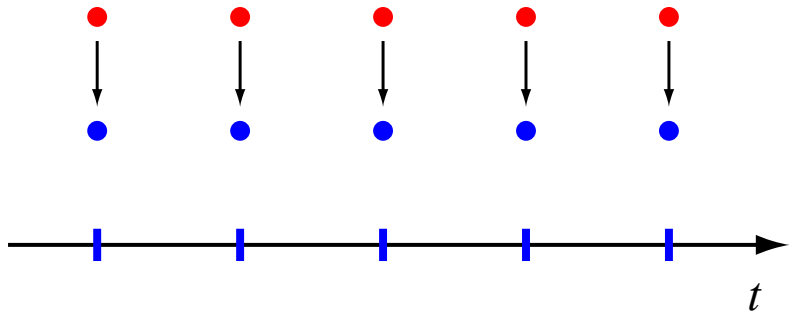


(From `http://www.bio.miami.edu/~cmallery/150/memb/ion_channels.htm`)

Chemical kinetics

First order kinetics

- When is it reasonable to claim that for a collection of 100 molecules, we can determine the average rate of the reaction?



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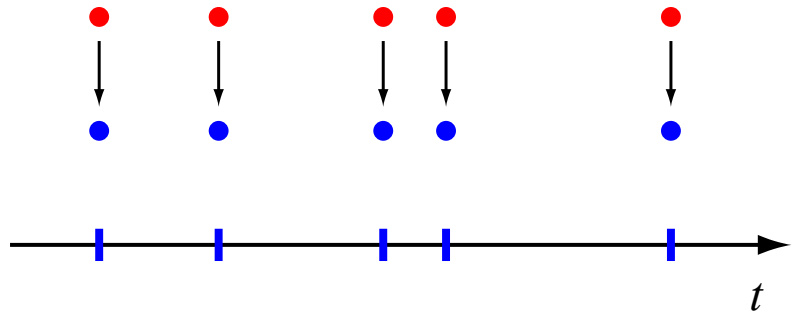

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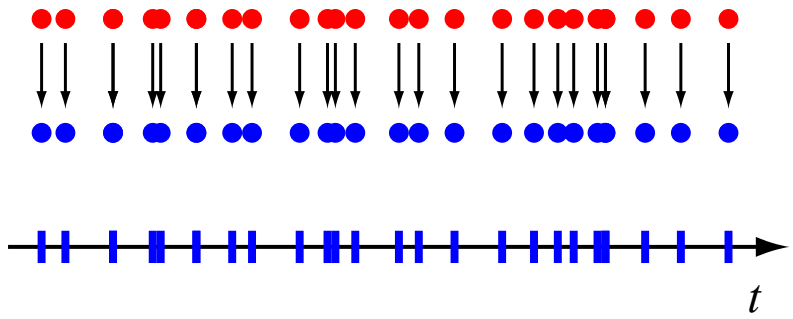

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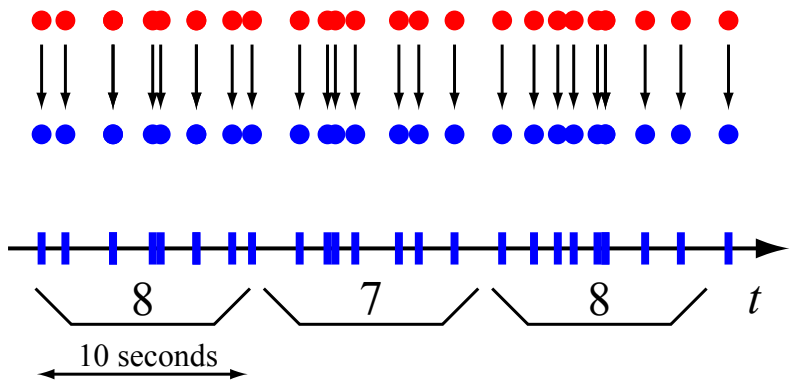

Estimate of reaction rate: $\lambda = 7.7$ reactions per 10 seconds per 100 molecules $= 0.077$ s^{-1} molecule^{-1}

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- In the limit $\Delta t \longrightarrow 0$,

$$\frac{dN}{dt} = -\lambda N.$$

  Valid only for periods of time long enough for the average rate to give a good approximation of the number of reactions. More molecules $\Rightarrow$ short time intervals are ok.

- What determines λ, the average rate?

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First order kinetics

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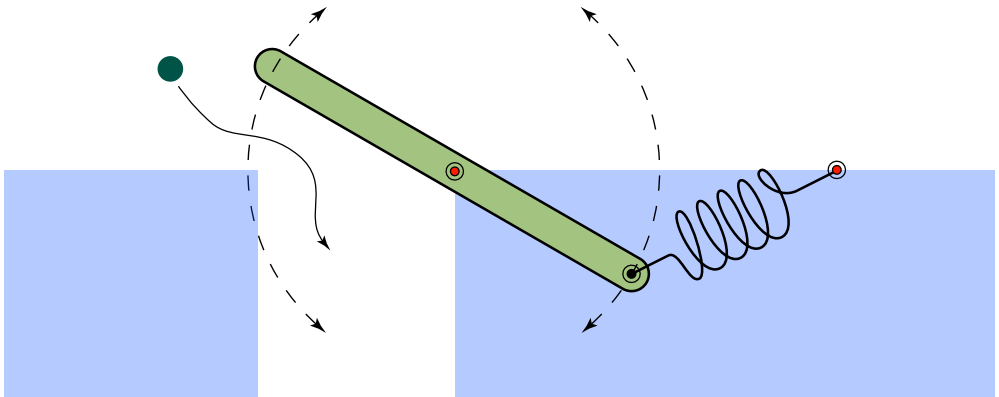

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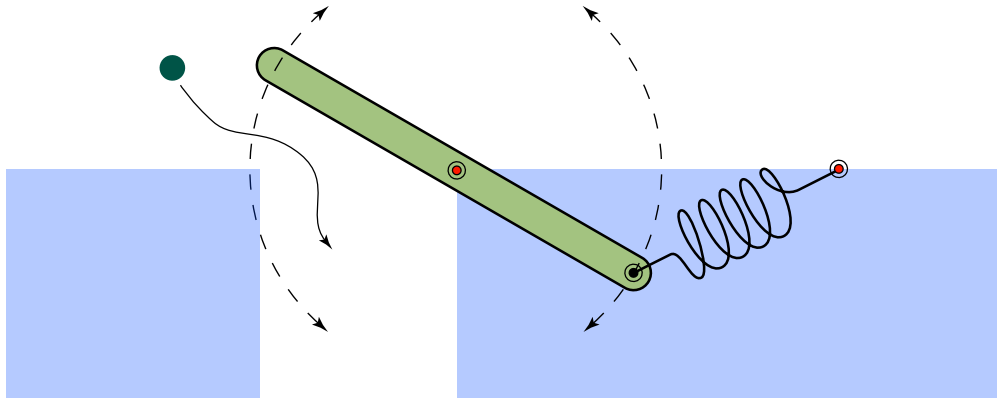
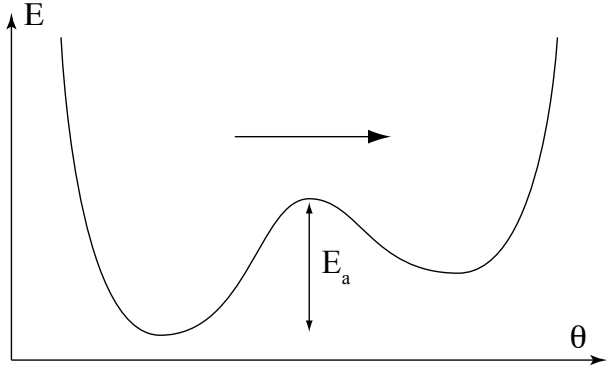


- Energy as a function of gate angle:



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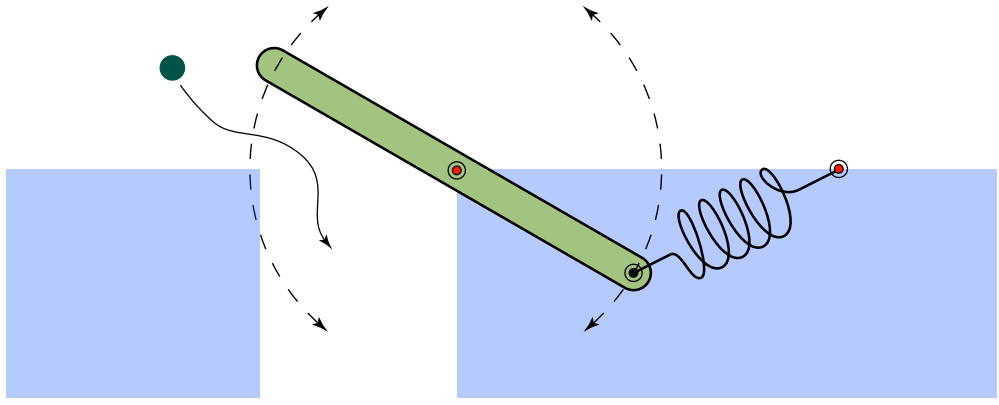

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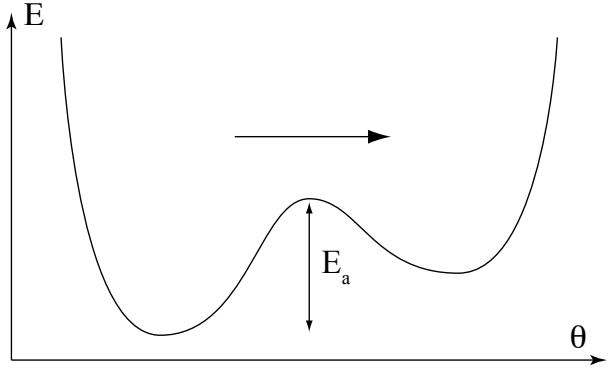

- Average rate $\propto e^{-E_a/kT}$. Matlab movies...

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- The reaction rate equation:

$$\frac{dN}{dt} = -kN^2.$$