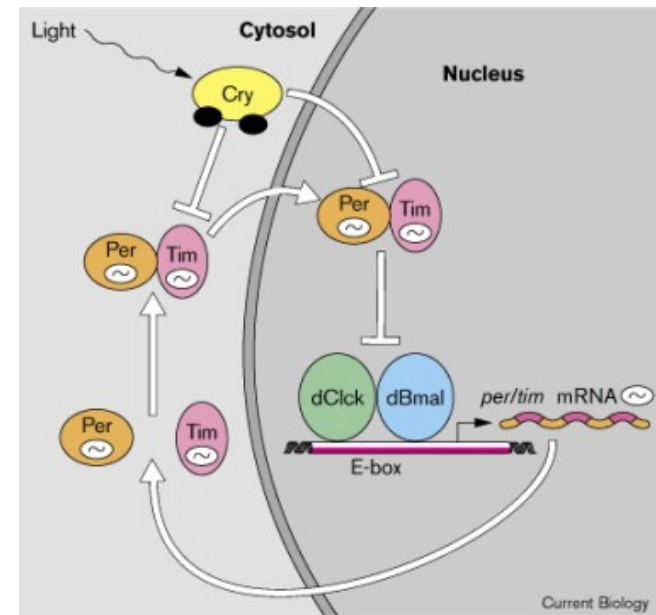


CS341: Lecture 3 Slides

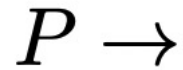
Equations Capturing Chemical Kinetics

- Goal 1: simulate mathematical model of biological system based on understanding of molecular mechanisms.
- Goal 2: develop an intuition for how the rate of a reaction relates to the dynamics over time of the molecules (e.g. proteins)
- We use the language of chemistry to to this.
- Chemical kinetics: the study of rates of chemical processes
- Law of mass action: the rate of a reaction is proportional to the product of the concentrations of the reactants
- Degradation: the process by which a molecule “dies”
- Dimerize: to form a dimer (complex) of two molecules, such as two proteins. Also say they “bind” to each other.

Dimerization in the Fruit Fly Circadian Clock



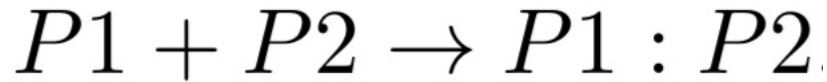
(Lucas & Foster, Curr Biol, 1999)



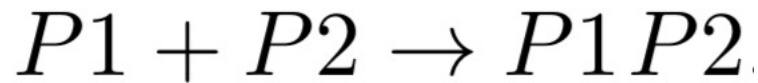
P is degraded, so the product of this process is nothing. We start with P and end with nothing

Under the assumptions that the reactions are occurring continuously and that the system is well-stirred (i.e. that the molecules are arranged uniformly in the space), we write this as a continuous reaction rate equation. The rate at which the concentration of P (denoted $[P]$) decreases with respect to time is the product of a rate constant k and $[P]$, i.e.

$$\frac{d[P]}{dt} = -k[P]$$



2 notations for the
same chemical
reaction



P1 and P2 form a
dimer P1P2 (or P1:P2)

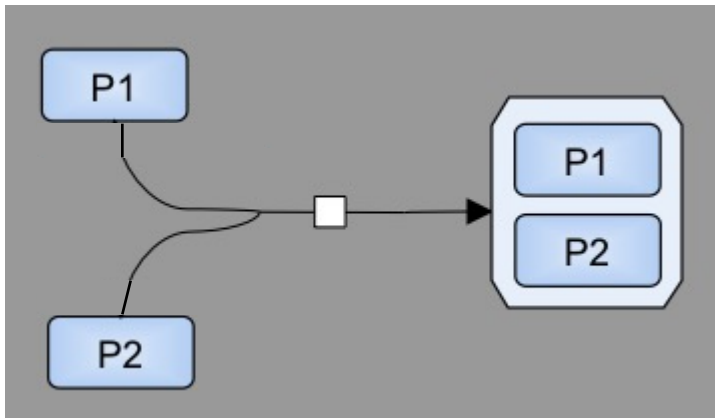
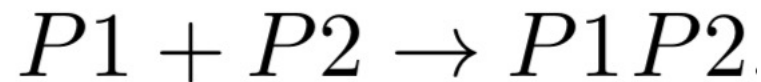
Under the assumptions that the reactions are occurring continuously and that the system is well-stirred (i.e. that the molecules are arranged uniformly in the space), we write this as a continuous reaction rate equation. The rate at which the concentration of P1P2 (denoted [P1P2]) increases with respect to time is the product of a rate constant k , [P1], and [P2], i.e.

$$\frac{d[P1P2]}{dt} = k[P1][P2]$$

Need to model all 3 proteins

In general, for every thing (e.g. protein or mRNA) we are modeling, we define a differential equation

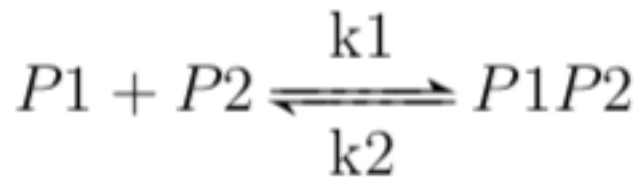
$$\frac{dP}{dt} = \text{rate_of_production} - \text{rate_of_consumption}$$



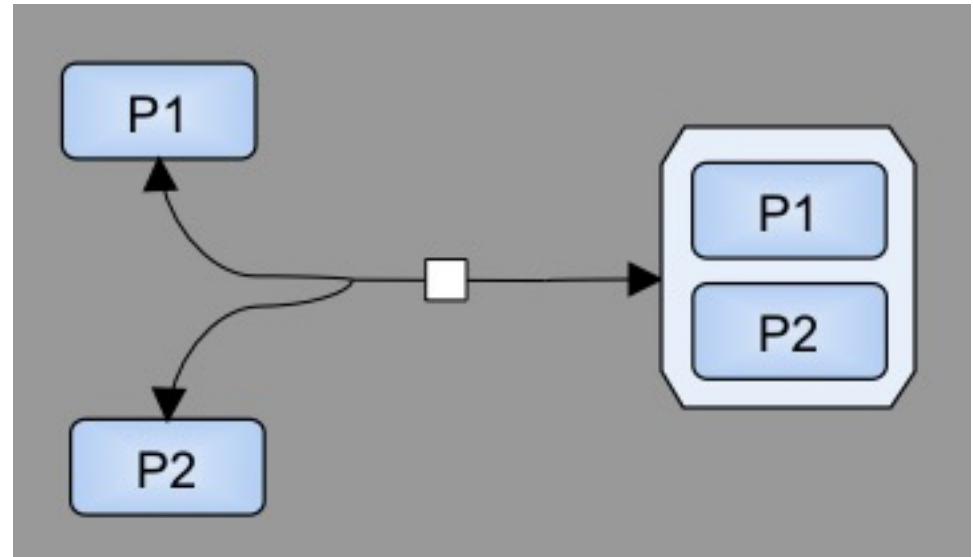
$$\begin{aligned}\frac{d[P1]}{dt} &= -k[P1][P2] \\ \frac{d[P2]}{dt} &= -k[P1][P2] \\ \frac{d[P1P2]}{dt} &= k[P1][P2]\end{aligned}$$

Reversible Dimerization
Represented
3 Ways

Chemical Reactions



Network Diagram



Ordinary Differential Equations (ODEs)

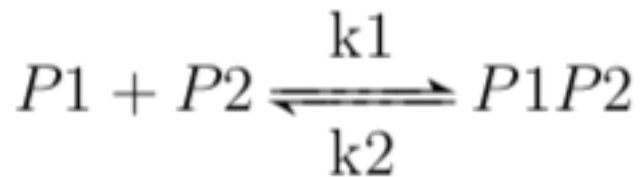
$$\frac{dP1}{dt} = .$$

$$\frac{dP2}{dt} = .$$

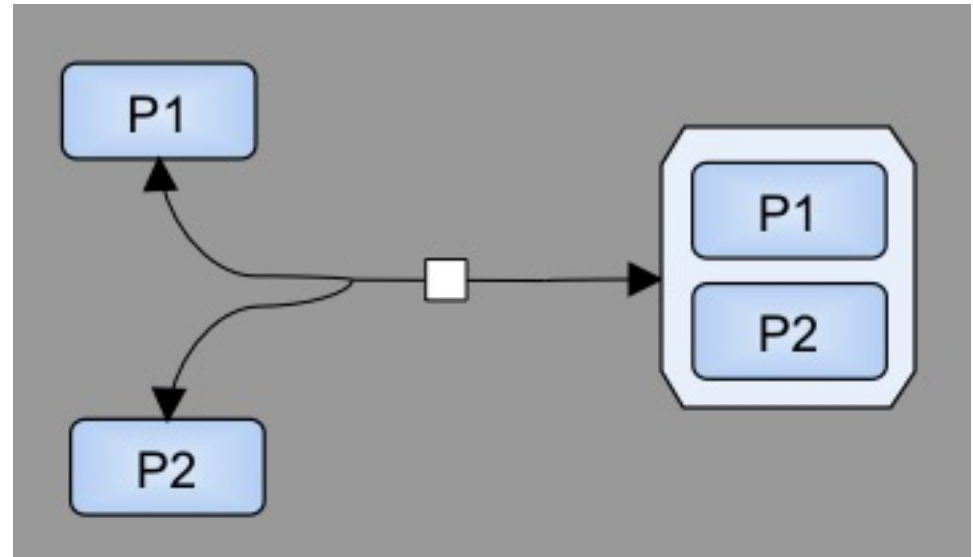
$$\frac{dP1P2}{dt} =$$

Reversible Dimerization
Represented
3 Ways

Chemical Reactions



Network Diagram



Ordinary Differential Equations (ODEs)

$$\frac{dP1}{dt} = -k1 \cdot P1 \cdot P2 + k2 \cdot P1P2$$

$$\frac{dP2}{dt} = -k1 \cdot P1 \cdot P2 + k2 \cdot P1P2$$

$$\frac{dP1P2}{dt} = -k2 \cdot P1P2 + k1 \cdot P1 \cdot P2$$