DEB 2025

Synthesizing Units

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MARETEC
CENTRO DE CIÊNCIA E TECNOLOGIA DO AMBIENTE E DO MAR
TÉCNICO LISBOA

LARSyS
Laboratory of Robotics and Engineering Systems

School: 26 May - 3 Jun 2025

University of Crete, Heraklion, Greece

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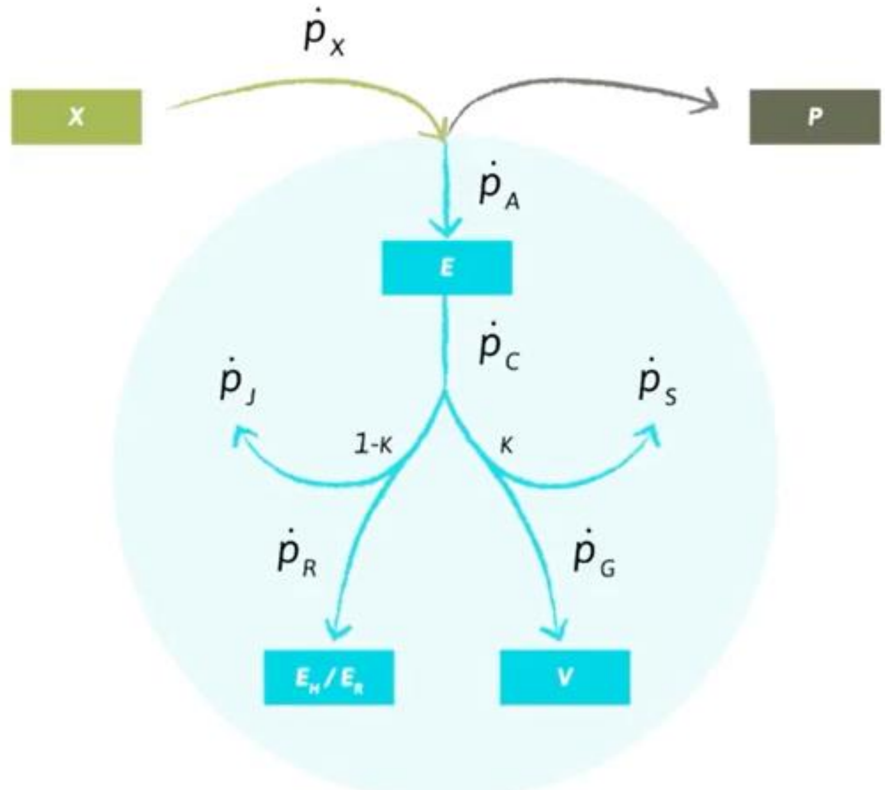
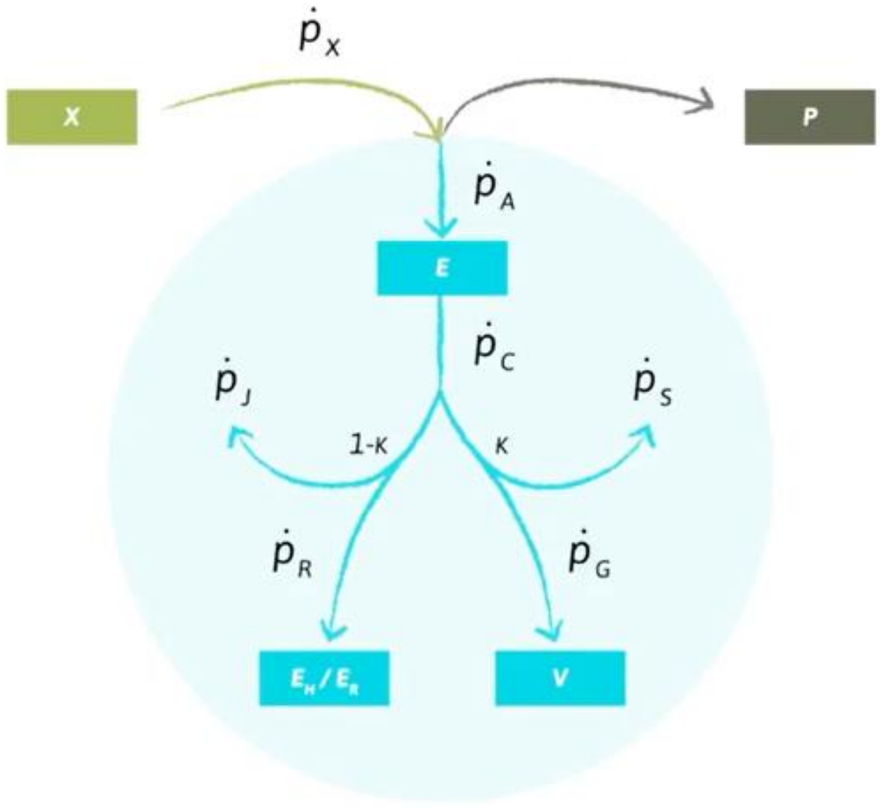
Conservation

- Energy



Conservation

- Energy
- Mass



Conservation

- Energy
- Mass
- Time

What is an SU?

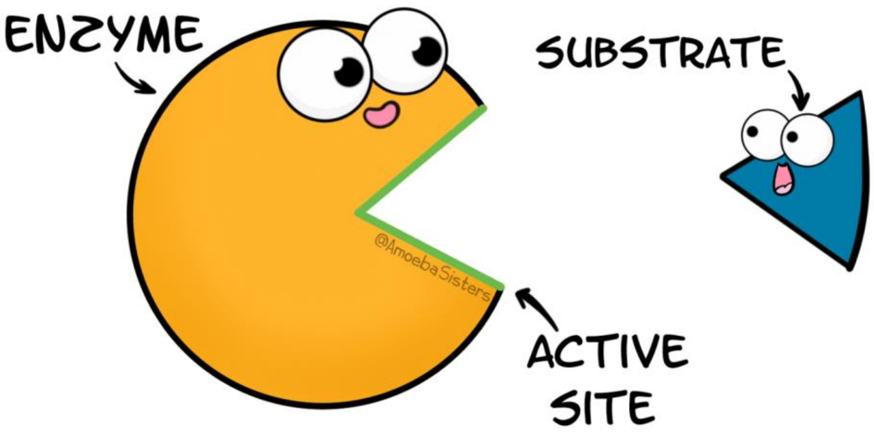
An entity that gets substrate(s)
and processes them into product(s)

- Enzyme
- Organism
- Factory

What is an SU?

An entity that **gets** substrate(s)
and processes them into product(s)

Passive



What is an SU?

An entity that **gets** substrate(s)
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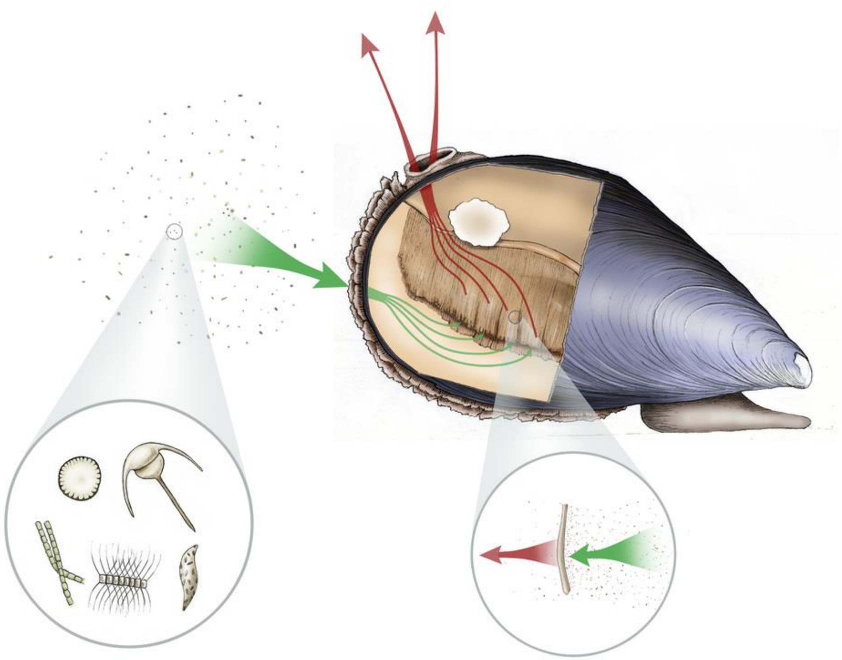

Passive

Active

What is an SU?

An entity that **gets** substrate(s)
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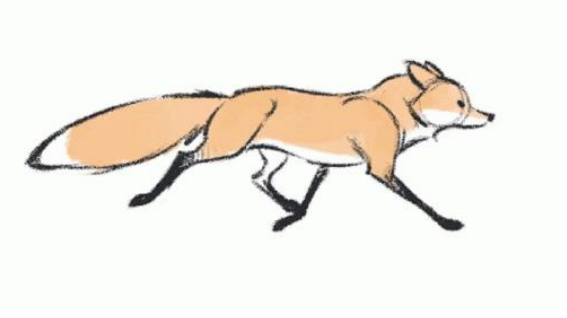
Passive

Active



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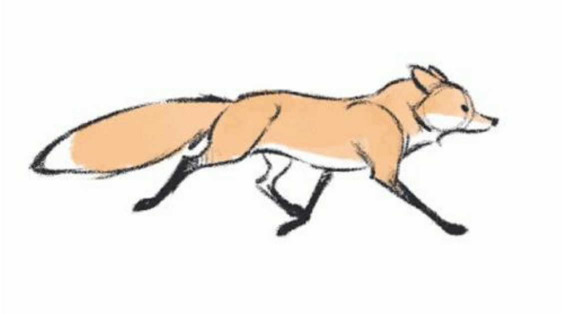
Passive

Active



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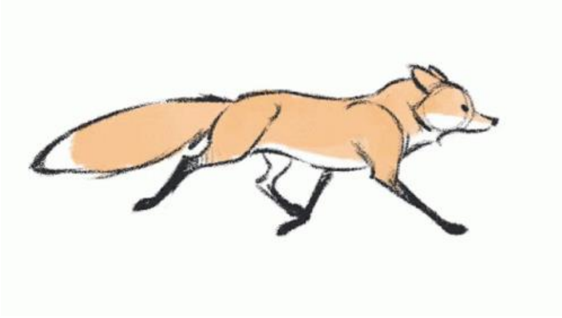
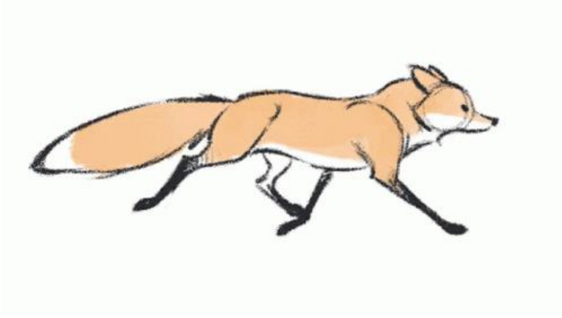


What is an SU?

An entity that **gets** substrate(s)
and processes them into product(s)

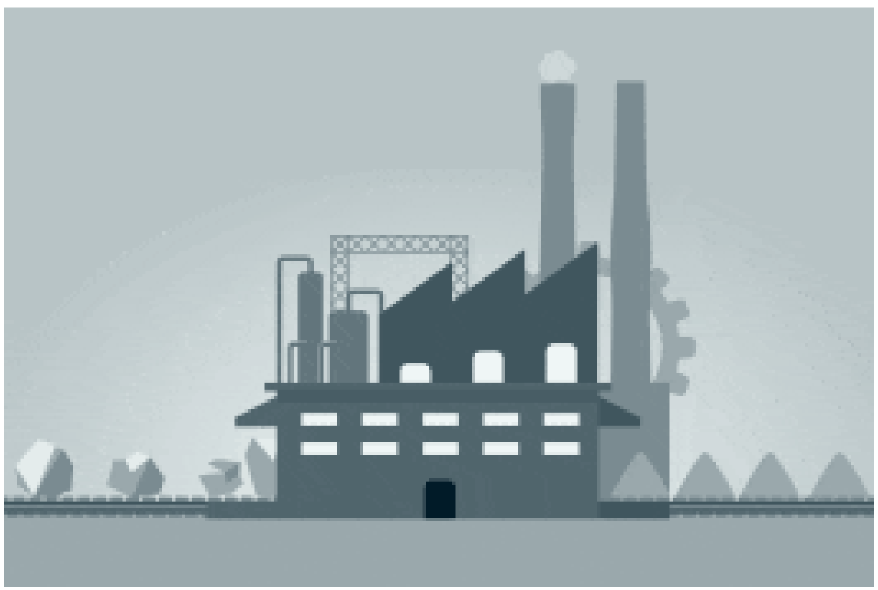
~~Passive~~

~~Active~~



What is an SU?

An entity that **gets** substrate(s)
and processes them into product(s)



~~Passive~~

~~Active~~

Unconstrained

What is an SU?

An entity that **gets** substrate(s)
and processes them into product(s)

Handshake protocols
- Open
- Closed

See section 7.1

~~Passive~~

~~Active~~

Unconstrained

What is an SU?

An entity that **gets** substrate(s)
and **processes** them into product(s)

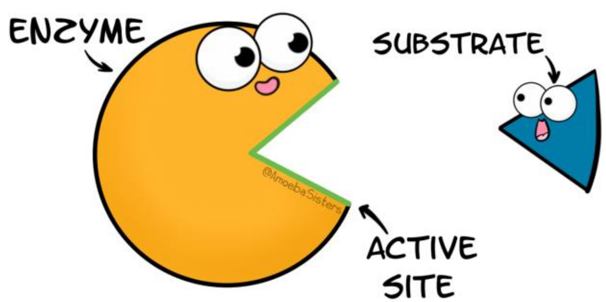
Handshake protocols for carriers

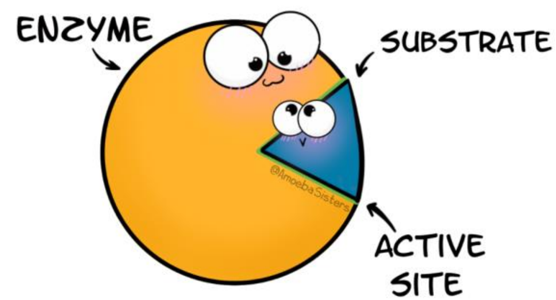
- Open
- Closed

See section 7.1

What is an SU?

An entity that **gets** substrate(s)
and **processes** them into product(s)





binding phase prossessing phase

One substrate

$\theta_{\cdot}$

$\theta_{\cdot}$ proportion in binding

θ_S

θ_S proportion in processing

One substrate

$\theta_{.}$

$\theta_{.}$ proportion in binding

θ_S

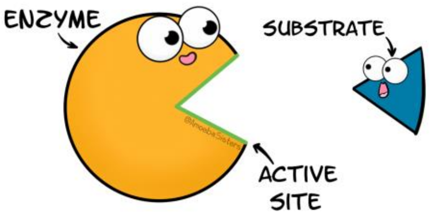
θ_S proportion in processing

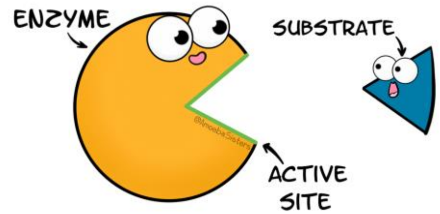
proportion

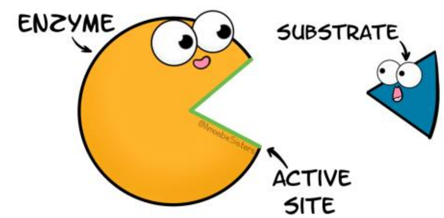
of time of one SU in state

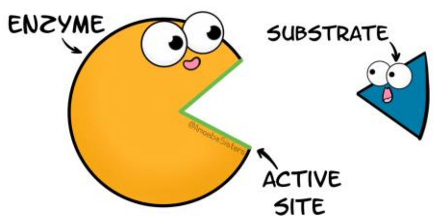
of number of SUs in state

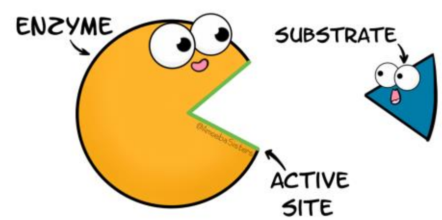
Examples of SUs



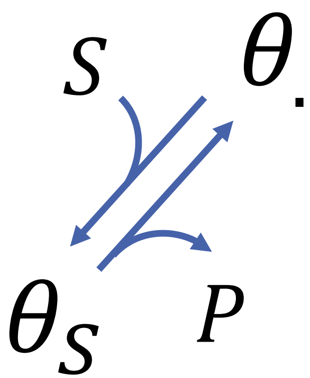








One substrate



$\theta_{.}$ proportion in binding

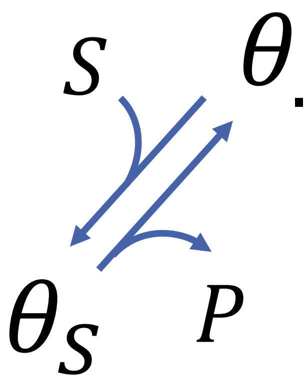
θ_S proportion in processing

of time of one SU in state

proportion

of number of SUs in state

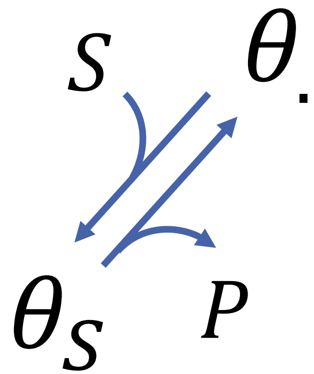
One substrate



Conservation

$$\theta_{\cdot} + \theta_S = 1$$

One substrate

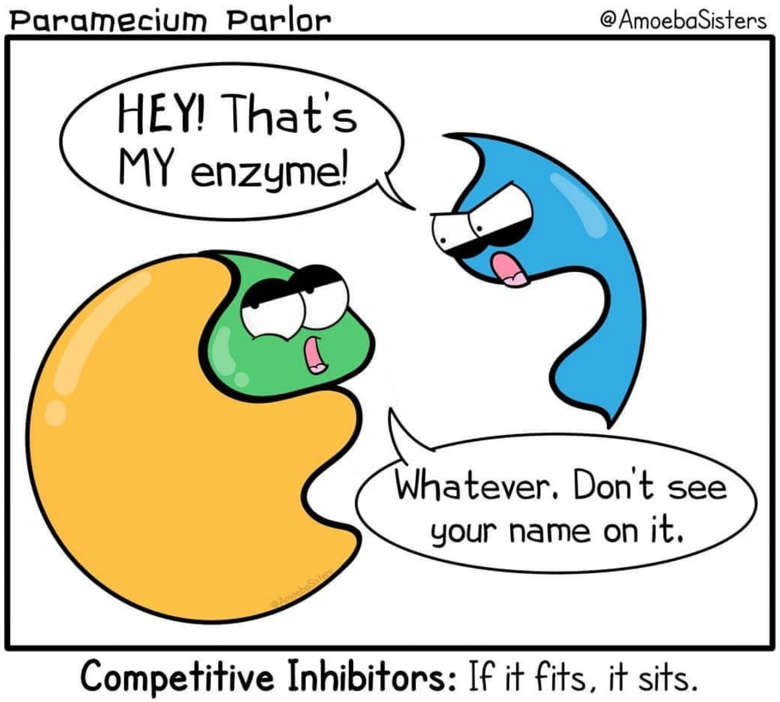


Conservation

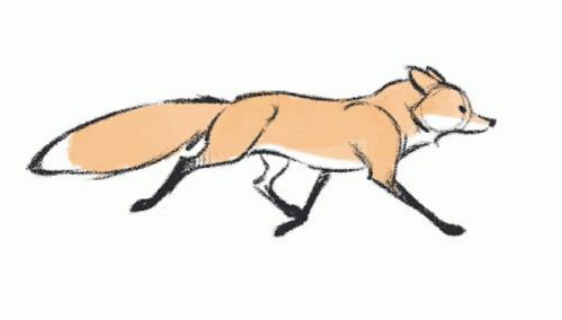
$$\theta_{.} + \theta_S = 1$$

$$j_P = \left(\frac{1}{\dot{k}} + \frac{1}{\dot{b} S} \right)^{-1}$$

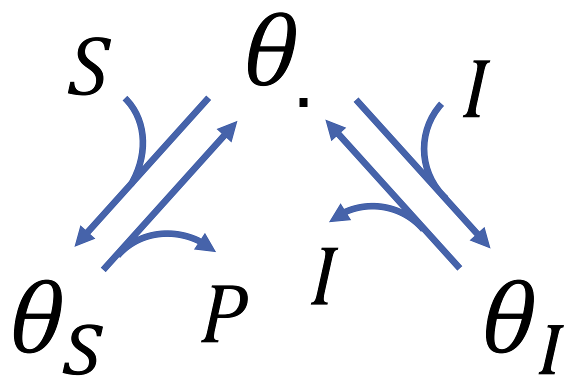
Inhibition example



Inhibition example

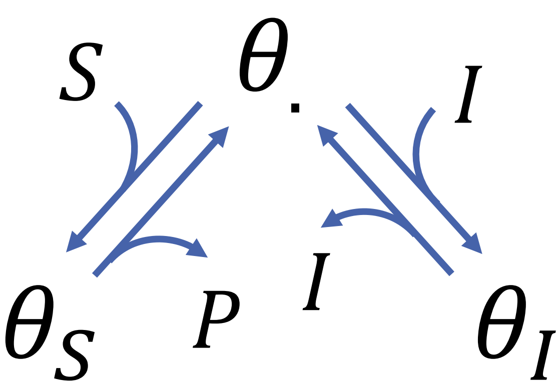


Inhibition example



Inhibition example

$$\frac{d\theta_{\cdot}}{dt} =$$

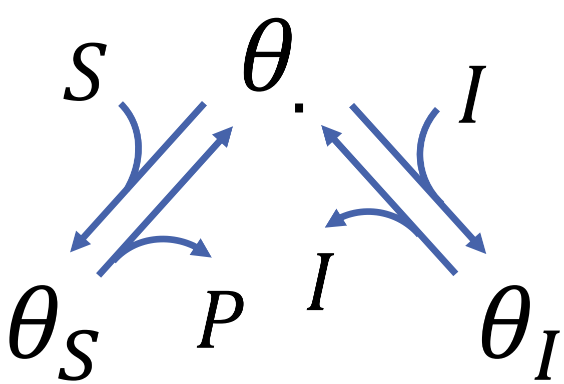


$$\frac{d\theta_S}{dt} =$$

$$\frac{d\theta_I}{dt} =$$

Inhibition example

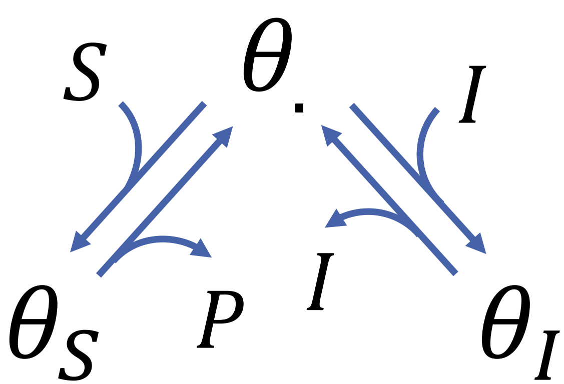
$$\frac{d\theta_{\cdot}}{dt} = -\dot{b}_S S \theta_{\cdot}$$



$$\frac{d\theta_S}{dt} = \dot{b}_S S \theta_{\cdot}$$

$$\frac{d\theta_I}{dt} =$$

Inhibition example



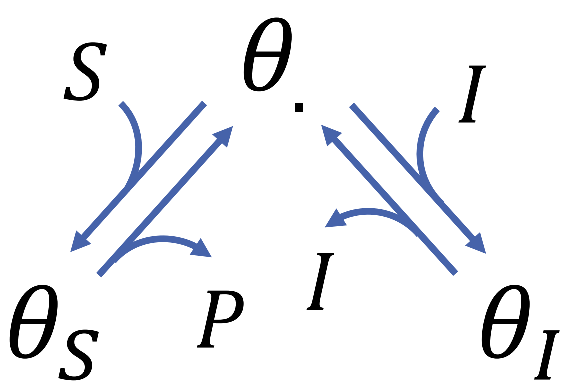
$$\frac{d\theta_{\cdot}}{dt} = -\dot{b}_S S\theta_{\cdot} + \dot{k}_s\theta_S$$

$$\frac{d\theta_S}{dt} = \dot{b}_S S\theta_{\cdot} - \dot{k}_s\theta_S$$

$$\frac{d\theta_I}{dt} =$$

Inhibition example

$$\frac{d\theta_{\cdot}}{dt} = -\dot{b}_S S\theta_{\cdot} + \dot{k}_s\theta_S - \dot{b}_I I\theta_{\cdot}$$

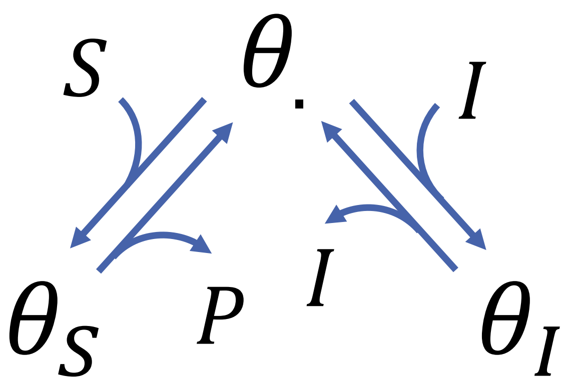


$$\frac{d\theta_S}{dt} = \dot{b}_S S\theta_{\cdot} - \dot{k}_s\theta_S$$

$$\frac{d\theta_I}{dt} = \dot{b}_I I\theta_{\cdot}$$

Inhibition example

$$\frac{d\theta_{\cdot}}{dt} = -\dot{b}_S S \theta_{\cdot} + \dot{k}_s \theta_S - \dot{b}_I I \theta_{\cdot} + \dot{k}_I \theta_I$$



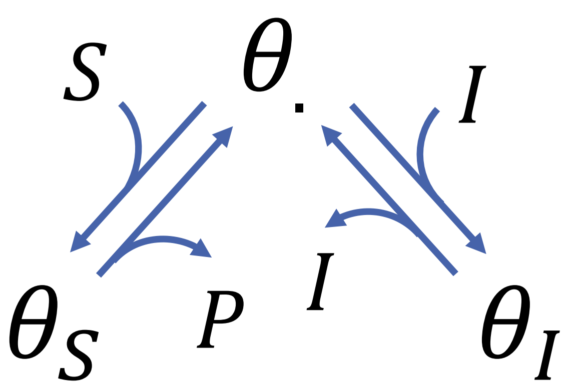
$$\frac{d\theta_S}{dt} = \dot{b}_S S \theta_{\cdot} - \dot{k}_s \theta_S$$

$$\frac{d\theta_I}{dt} = \dot{b}_I I \theta_{\cdot} - \dot{k}_I \theta_I$$

Inhibition example

Fast dynamics assumption

$$0 = -\dot{b}_S S\theta_. + \dot{k}_s\theta_S - \dot{b}_I I\theta_. + \dot{k}_I\theta_I$$

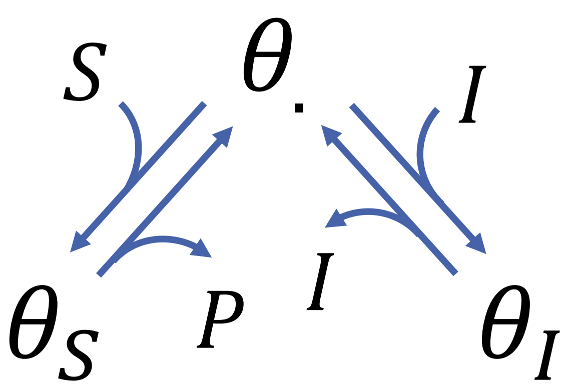


$$0 = \dot{b}_S S\theta_. - \dot{k}_s\theta_S$$

$$0 = \dot{b}_I I\theta_. - \dot{k}_I\theta_I$$

Inhibition example

$$\theta_{\cdot} + \theta_S + \theta_I = 1$$

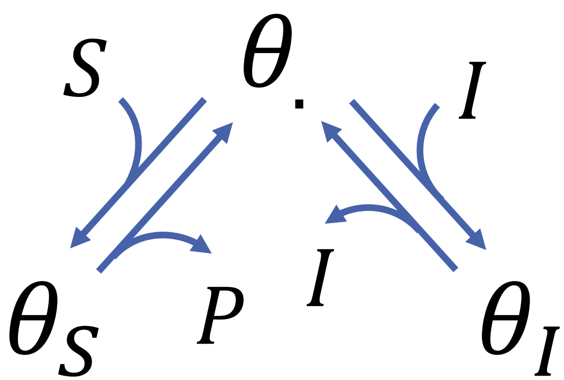


$$0 = \dot{b}_S S \theta_{\cdot} - \dot{k}_s \theta_S$$

$$0 = \dot{b}_I I \theta_{\cdot} - \dot{k}_I \theta_I$$

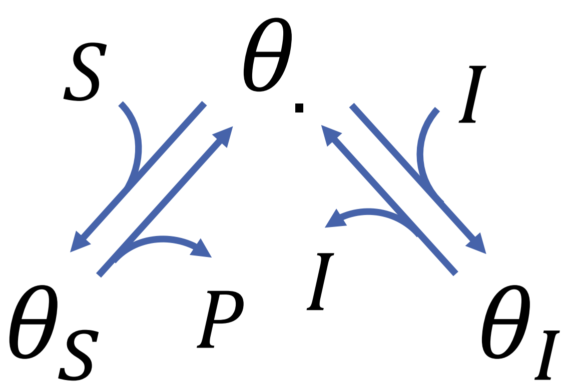
Inhibition example

$$j_P = \dot{k}_s \theta_S$$



Inhibition example

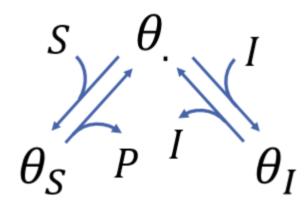
$$j_P = \dot{k}_s \theta_S = \left(\frac{1}{\dot{k}_s} + \frac{1}{\dot{b} S} \left(1 + \frac{\dot{b}_I}{\dot{k}_I} I \right) \right)^{-1}$$



$I = 0$

$$j_P = \left(\frac{1}{\dot{k}} + \frac{1}{\dot{b} S} \right)^{-1}$$

Step-by-step summary



1. Draw the scheme
2. Write the equations
3. Use the fast dynamics assumption
4. Add the conservation constraint
5. Compute the flux
6. Check consistency of the solution