

ETH

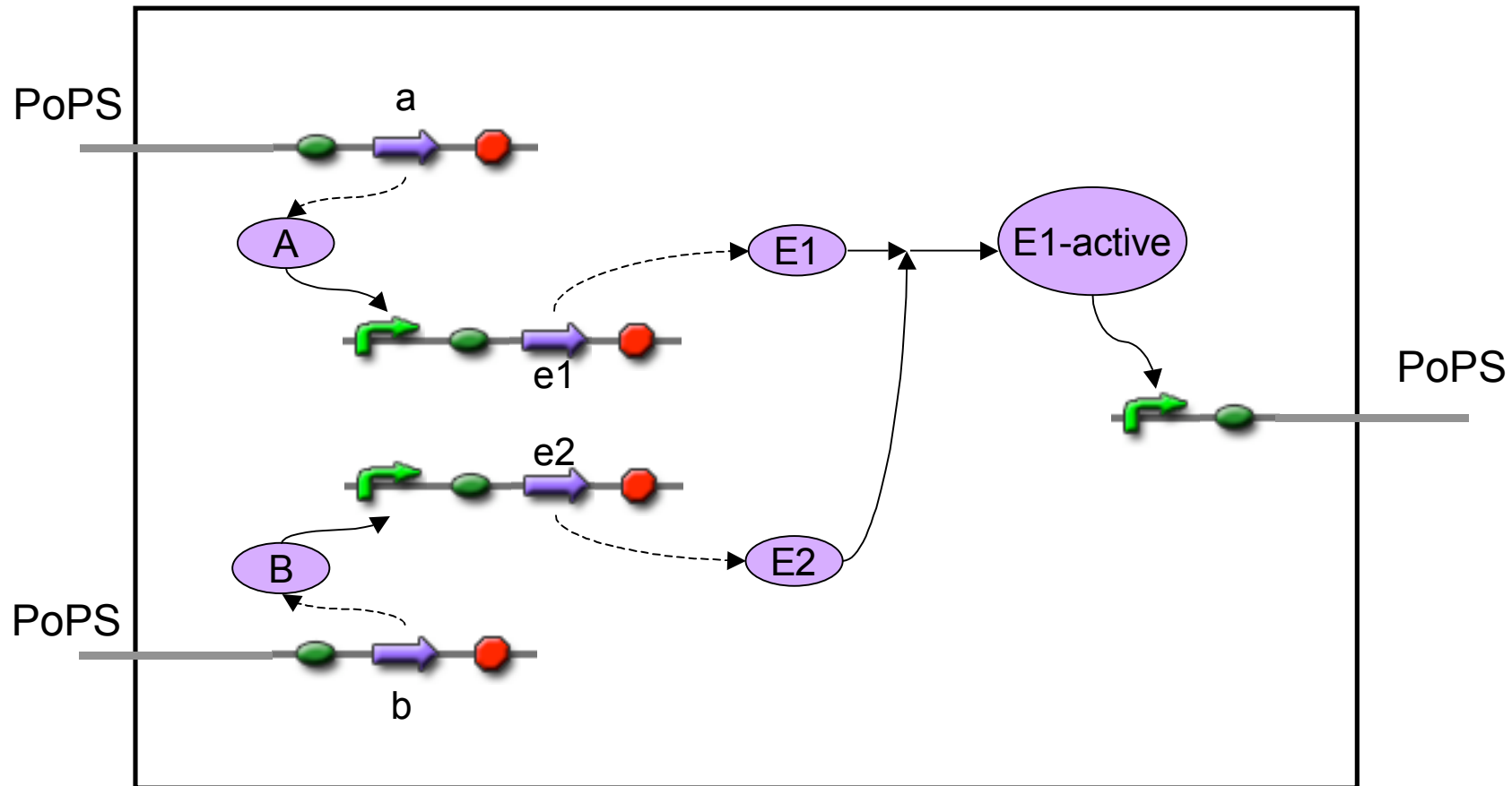
Eidgenössische Technische Hochschule Zürich
Swiss Federal Institute of Technology Zurich



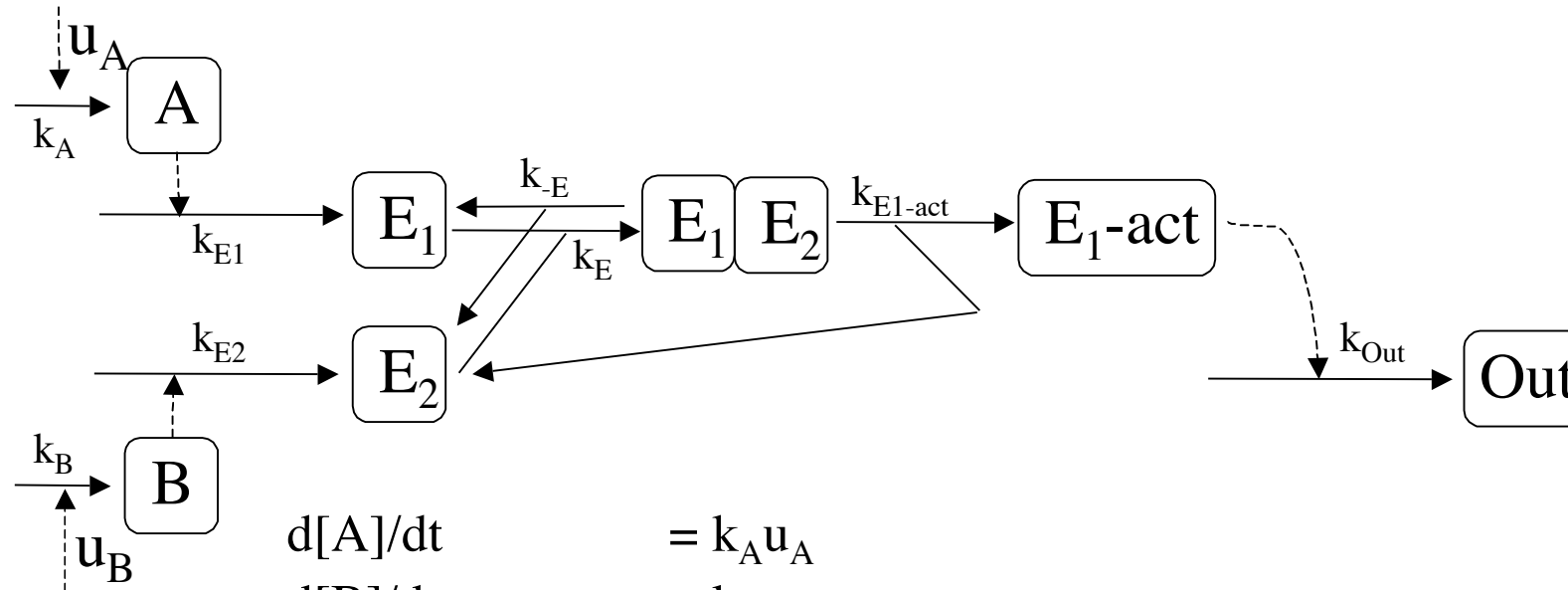
Half Adder - Modelling



AND – 1



AND – 1 (ODE's)



$$d[A]/dt = k_A u_A$$

$$d[B]/dt = k_B u_B$$

$$d[E_1]/dt = k_{E1}[A] - k_E[E_1][E_2] + k_{-E}[E_1E_2]$$

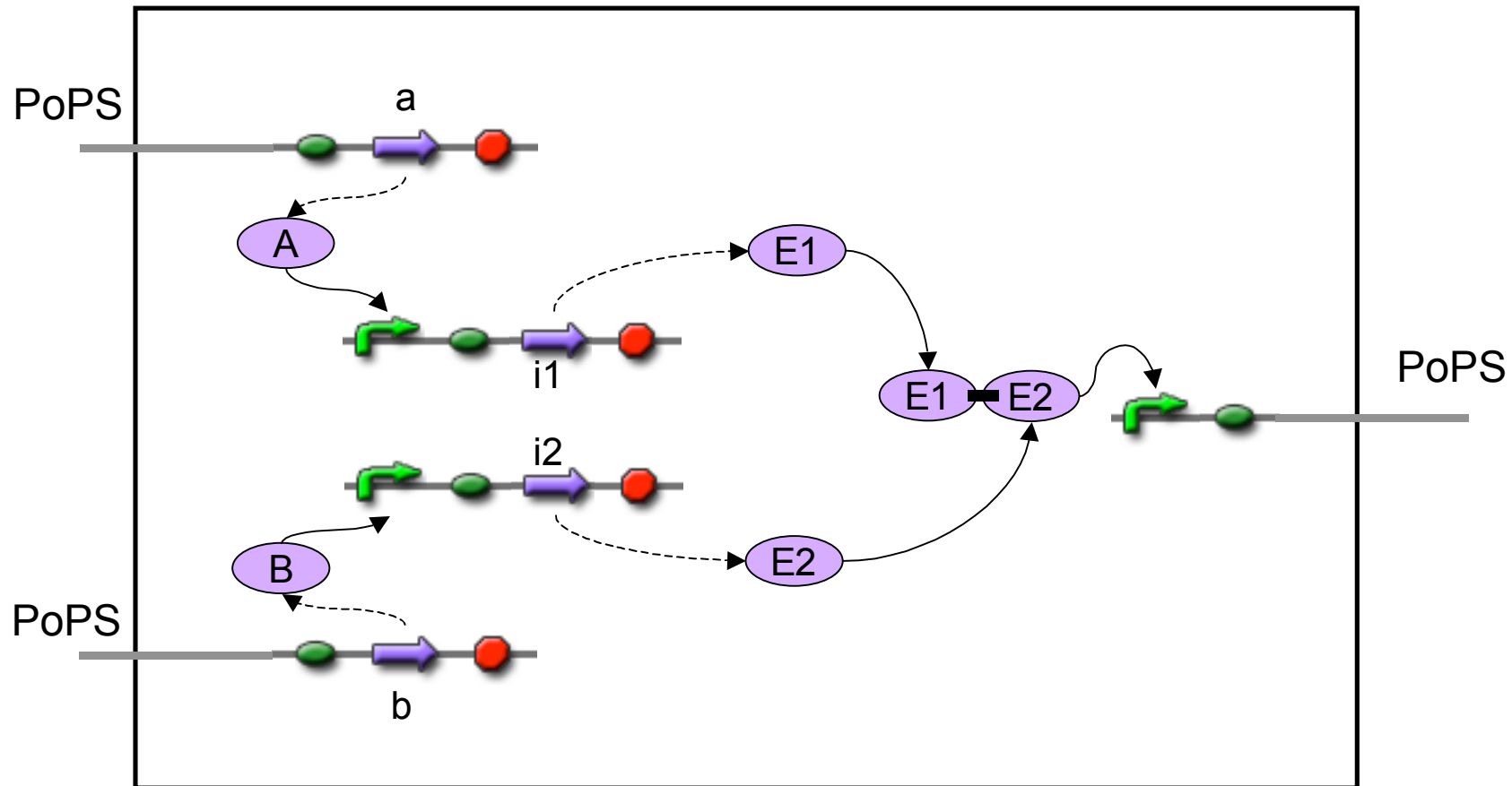
$$d[E_2]/dt = k_{E2}[B] - k_E[E_1][E_2] + k_{-E}[E_1E_2] + k_{E1-act}[E_1E_2]$$

$$d[E_1E_2]/dt = k_E[E_1][E_2] - k_{-E}[E_1E_2] - k_{E1-act}[E_1E_2]$$

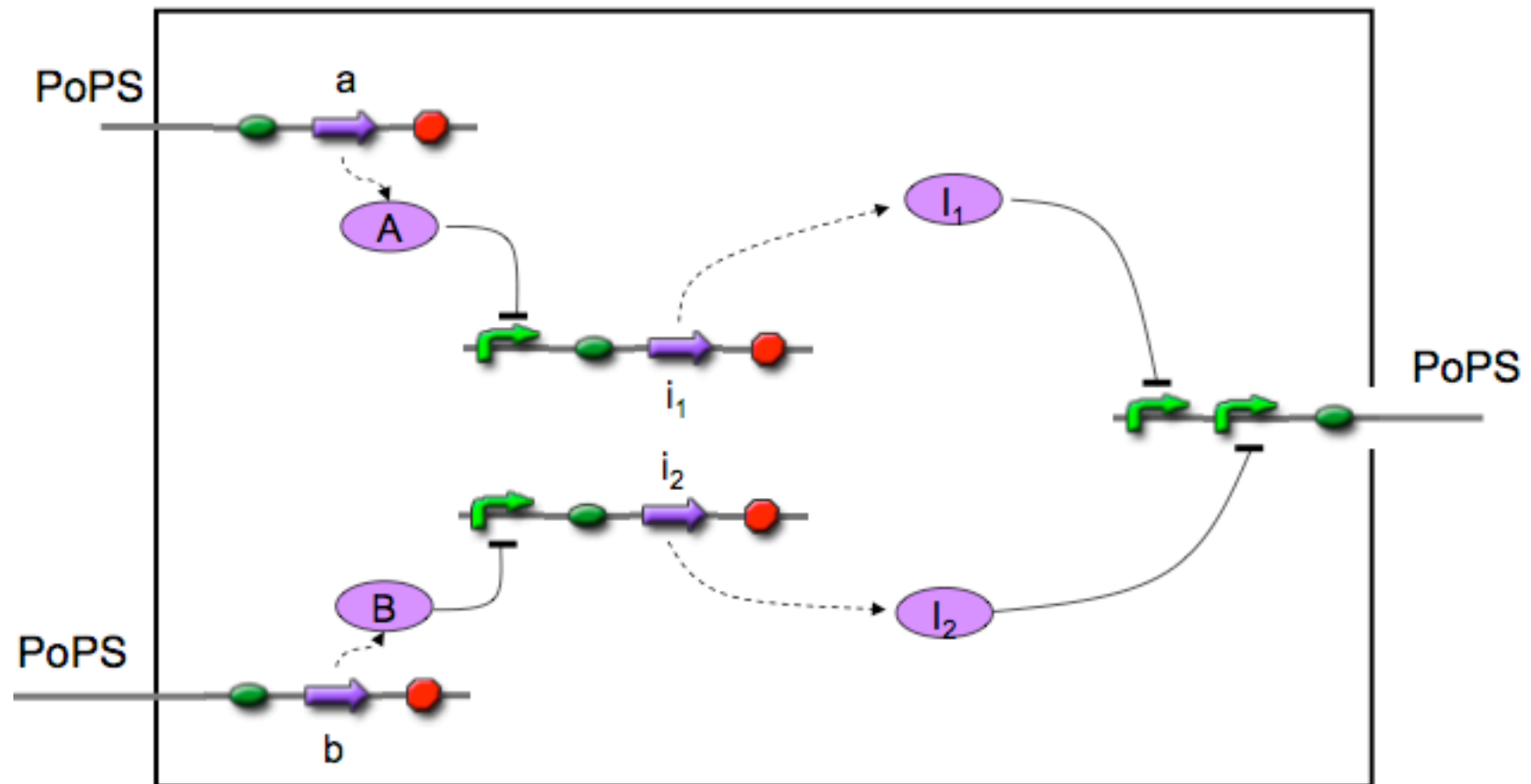
$$d[E_1-act]/dt = k_{E1-act}[E_1E_2]$$

$$d[Out]/dt = k_{out}[E_1-act]$$

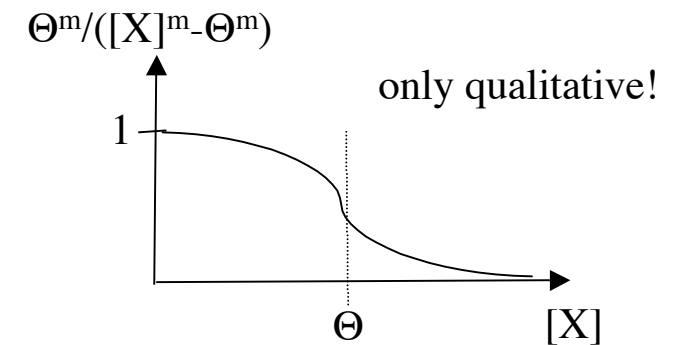
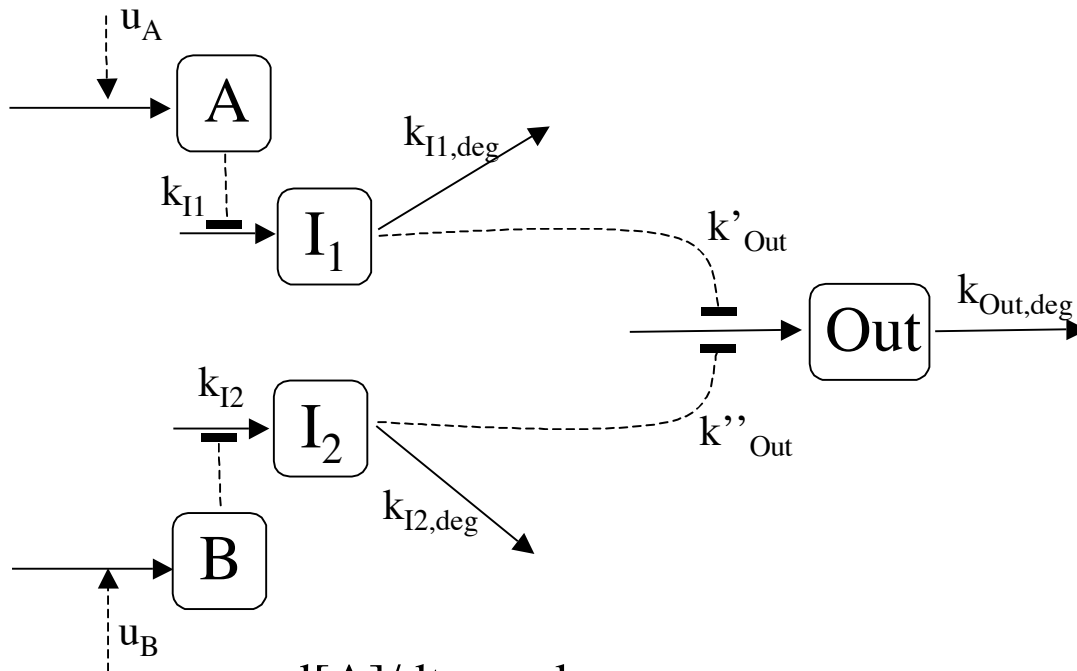
AND – 2



AND – 3



AND – 3 (ODE's)



$$d[A]/dt = k_A u_A$$

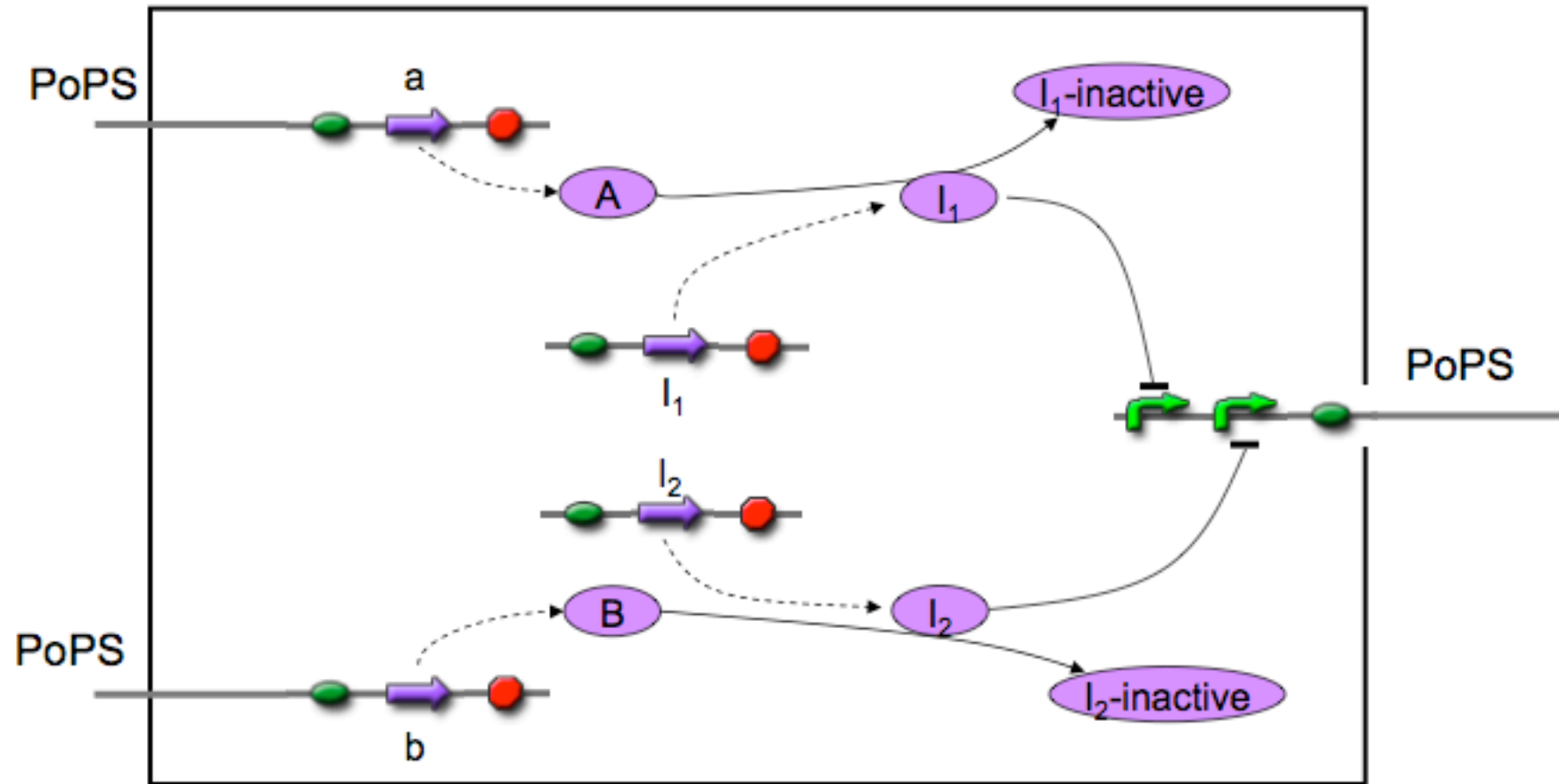
$$d[B]/dt = k_B u_B$$

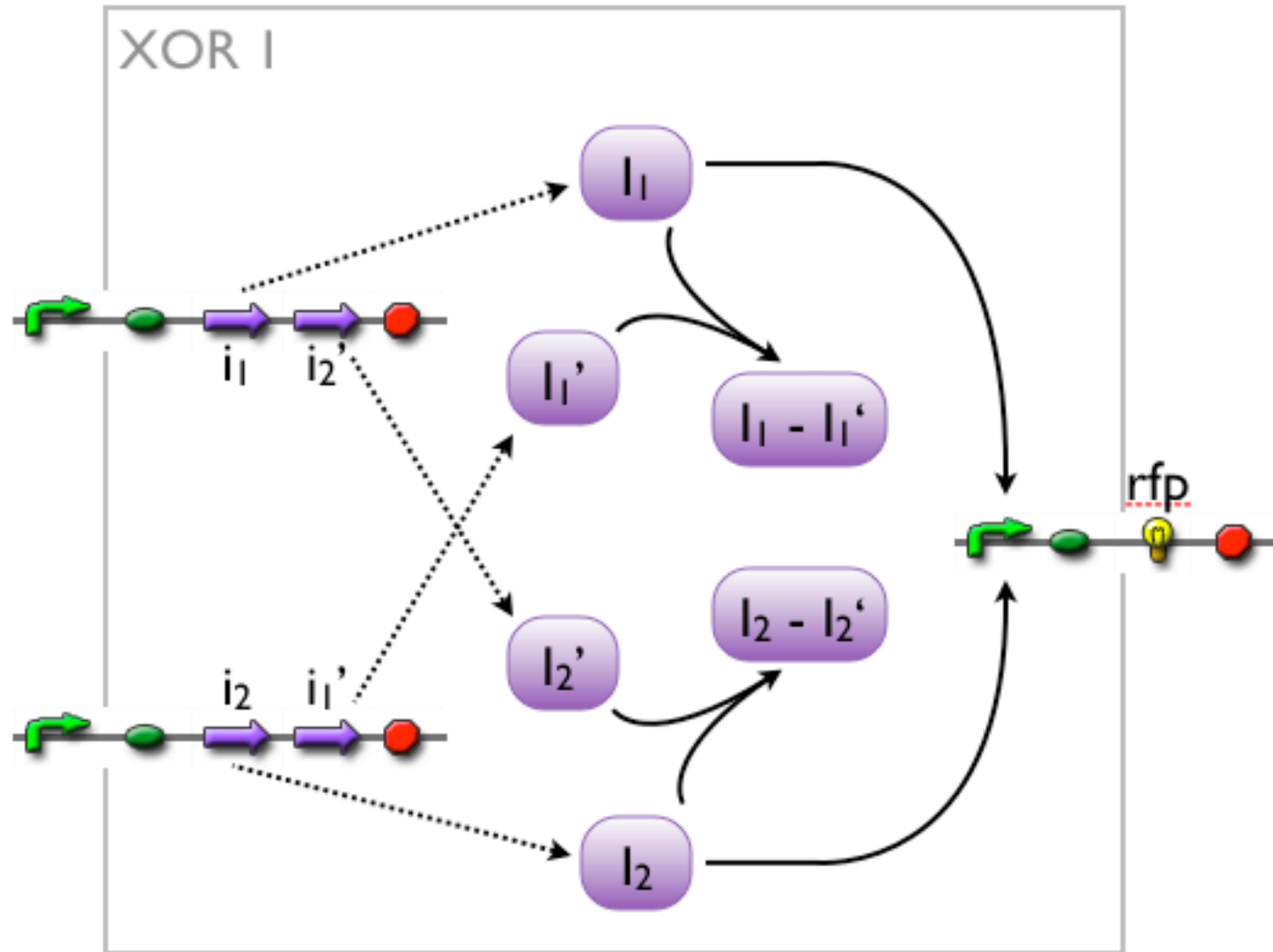
$$d[I_1]/dt = k_{I1} \frac{\Theta^{m1}}{[A]^{m1} - \Theta^{m1}} - k_{I1,deg} [I_1]$$

$$d[I_2]/dt = k_{I2} \frac{\Theta^{m1}}{[B]^{m1} - \Theta^{m1}} - k_{I2,deg} [I_2]$$

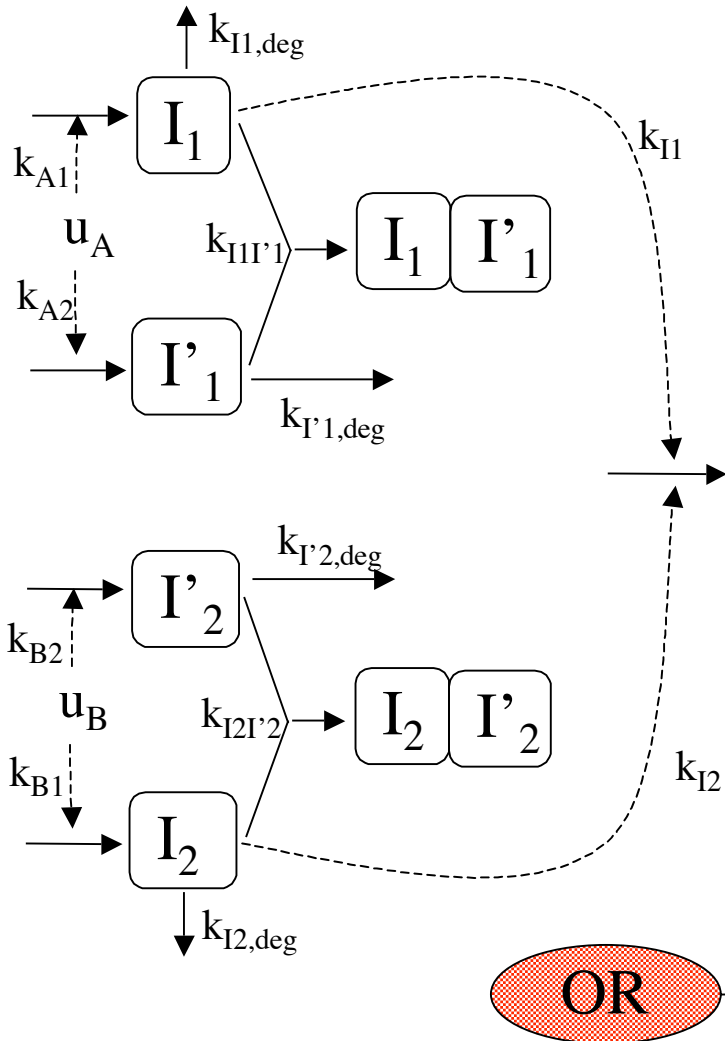
$$d[Out]/dt = k'_{Out} \frac{\Theta^{m3}}{[I_1]^{m3} - \Theta^{m3}} - k''_{Out} \frac{\Theta^{m4}}{[I_2]^{m4} - \Theta^{m4}} - k_{Out,deg} [Out]$$

AND – 4





XOR – 1 (ODE's)



Question: Should $k_{I1I'1}$ and $k_{I2I'2}$ be modelled as reversible reactions?

$$\begin{aligned}
 \frac{d[I_1]}{dt} &= k_{A1}u_A - k_{I1I'1}[I_1][I'_1] - k_{I1,deg}[I_1] \\
 \frac{d[I'_1]}{dt} &= k_{A2}u_A - k_{I1I'1}[I_1][I'_1] - k_{I'1,deg}[I'_1] \\
 \frac{d[I_2]}{dt} &= k_{B1}u_B - k_{I2I'2}[I_2][I'_2] - k_{I2,deg}[I_2] \\
 \frac{d[I'_2]}{dt} &= k_{B2}u_B - k_{I2I'2}[I_2][I'_2] - k_{I'2,deg}[I'_2] \\
 \frac{d[I_1I'_1]}{dt} &= k_{I1I'1}[I_1][I'_1] \\
 \frac{d[I_2I'_2]}{dt} &= k_{I2I'2}[I_2][I'_2] \\
 \frac{d[Out]}{dt} &= k_{I1}(1 - \Theta^{m1}/([I_1]^{m1} - \Theta^{m1})) \\
 &\quad + k_{I2}(1 - \Theta^{m2}/([I_2]^{m2} - \Theta^{m2})) - k_{Out,deg}[Out]
 \end{aligned}$$

OR

