

LECTURE 2: BIOCHEMICAL REACTION NETWORKS

Introduction to cellular system modelling
Daniel Georgiev

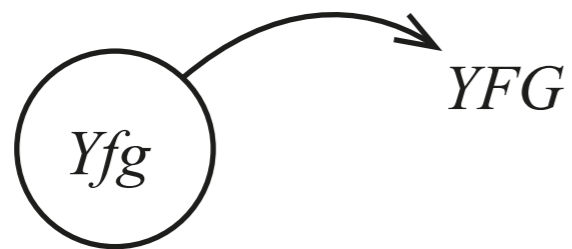
Summer 2015

OUTLINE

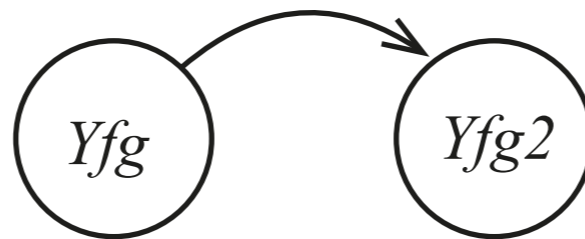
- Levels of abstraction in modelling
 - Reaction automata
 - Chemical reaction network
 - Mathematical models
- Levels of abstraction in design
 - Reaction automata
 - DNA schema
 - DNA sequences
- Chemical reaction network
 - Source
 - Inverter (single gene, double gene)
 - metabolism
 - signalling

LAYERS OF ABSTRACTION - MODELLING

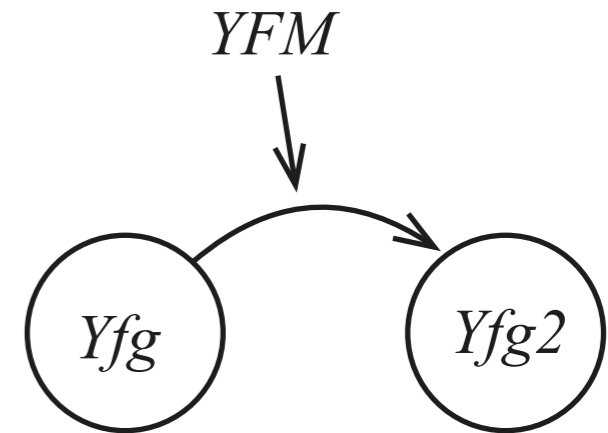
automata and chemical reaction networks



SOURCE



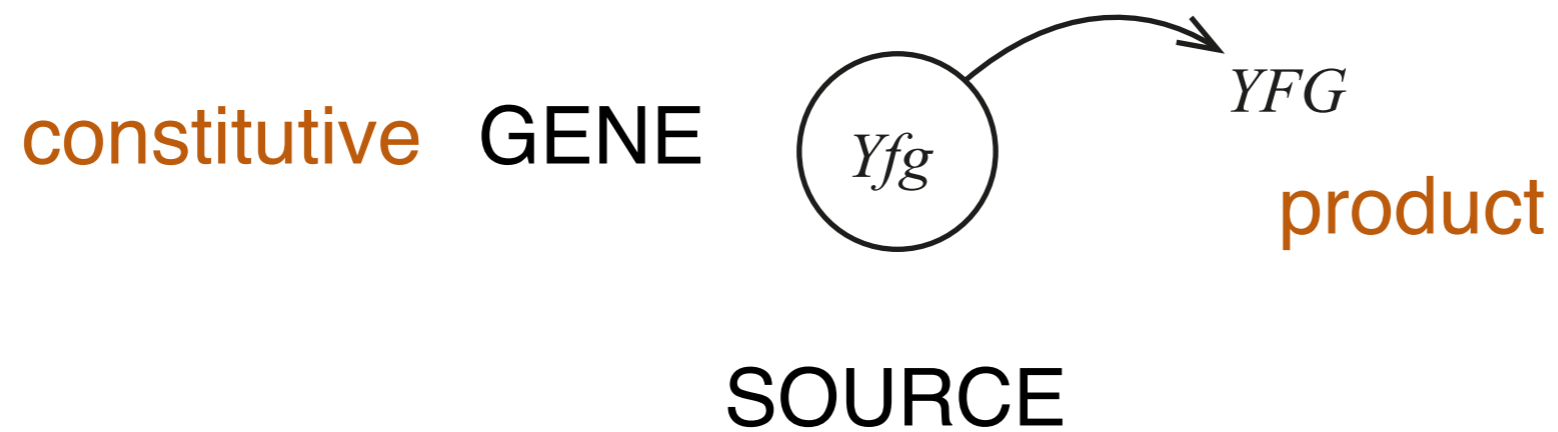
ACTIVATION



INDUCTION

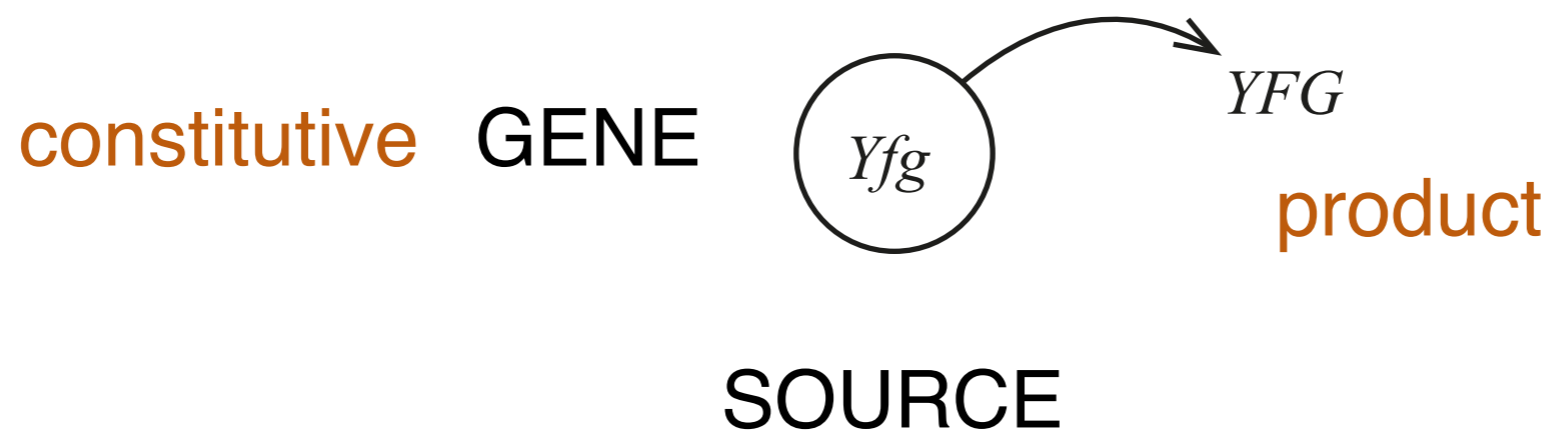
LAYERS OF ABSTRACTION - MODELLING

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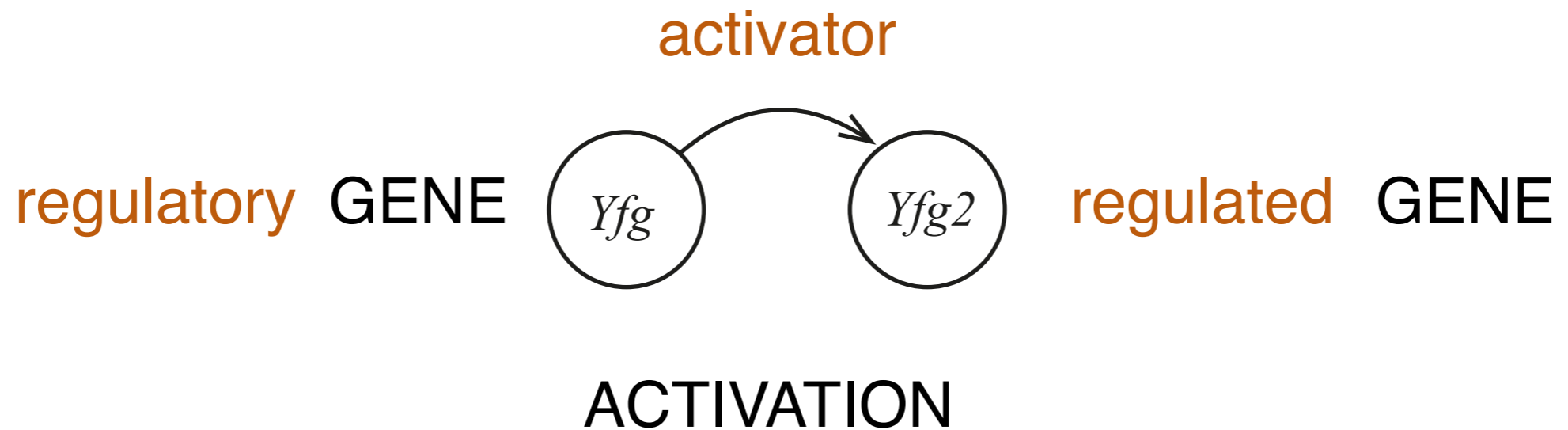
reaction rate



infinite source/sink molecular species

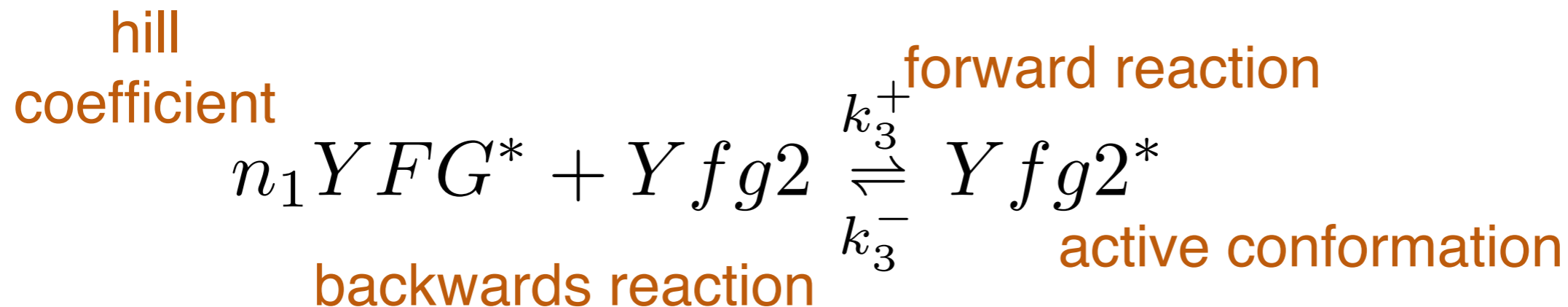
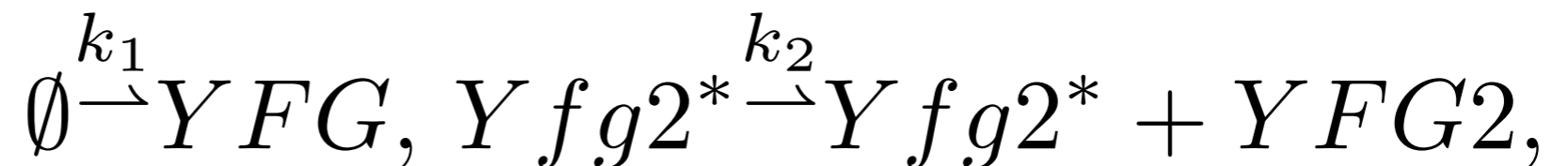
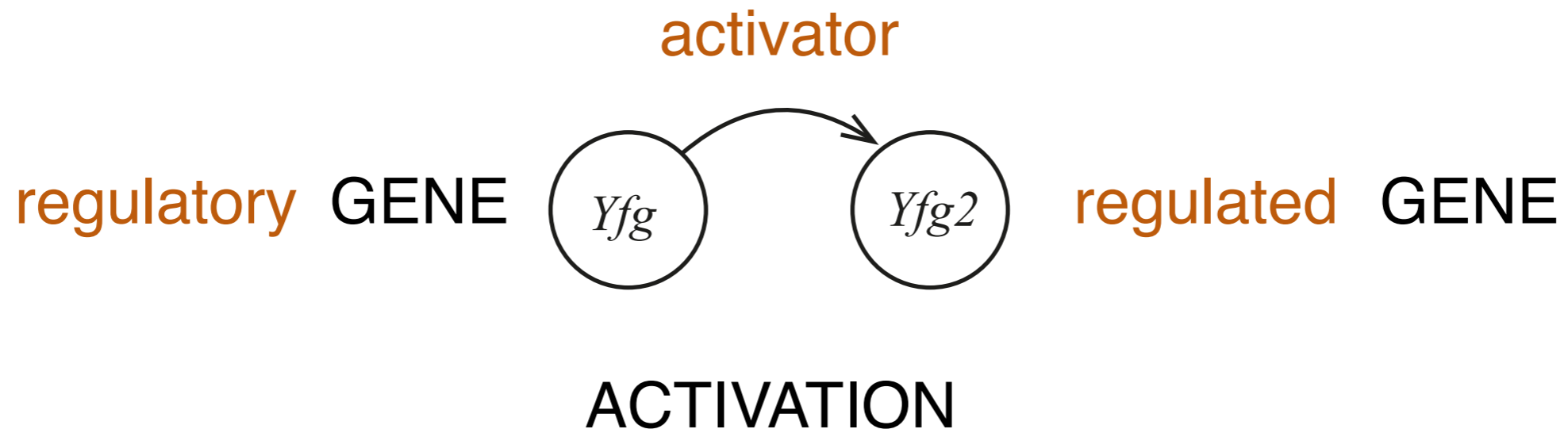
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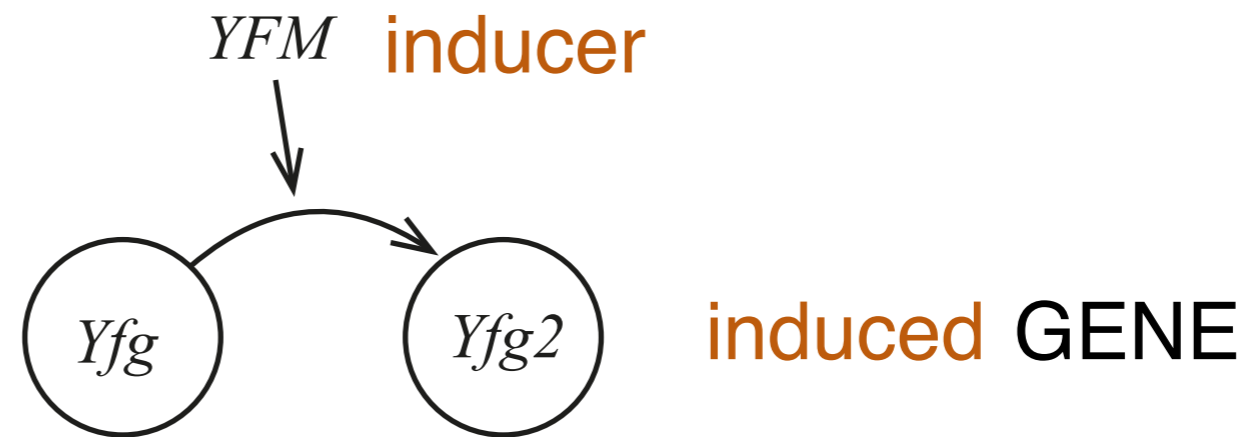
LAYERS OF ABSTRACTION - MODELLING

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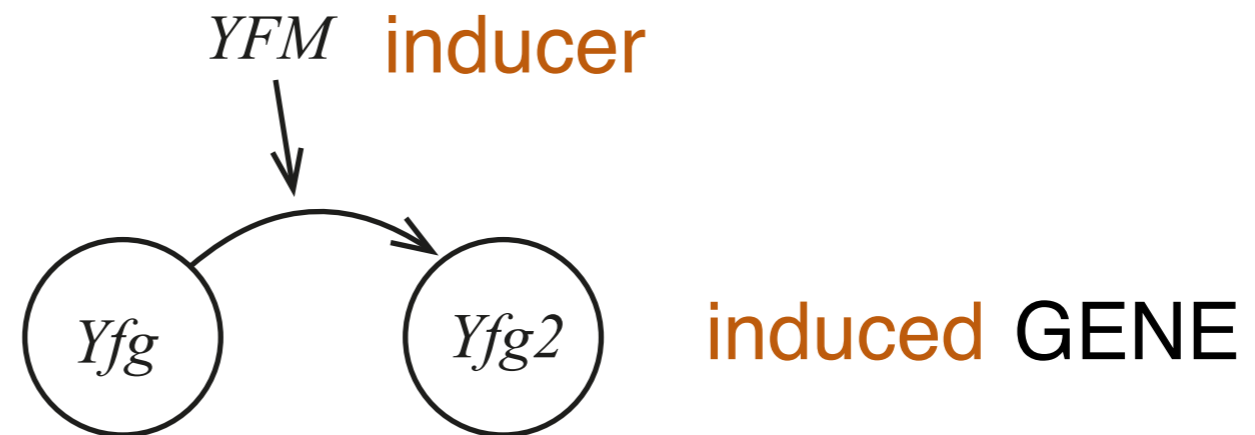
automata and chemical reaction networks



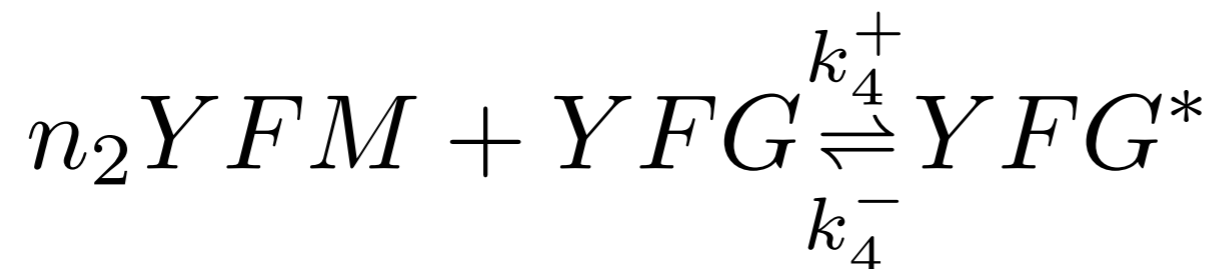
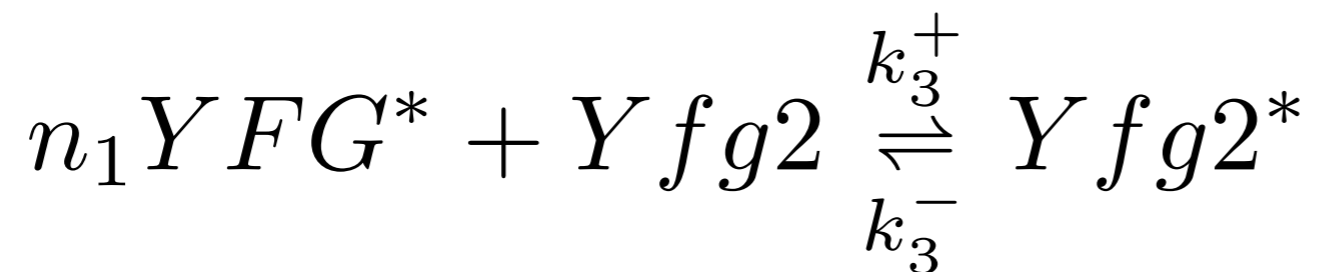
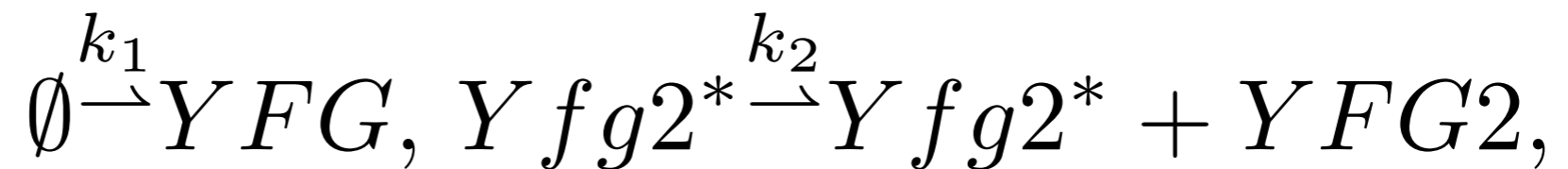
INDUCTION

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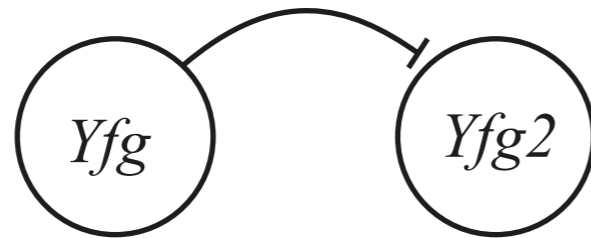


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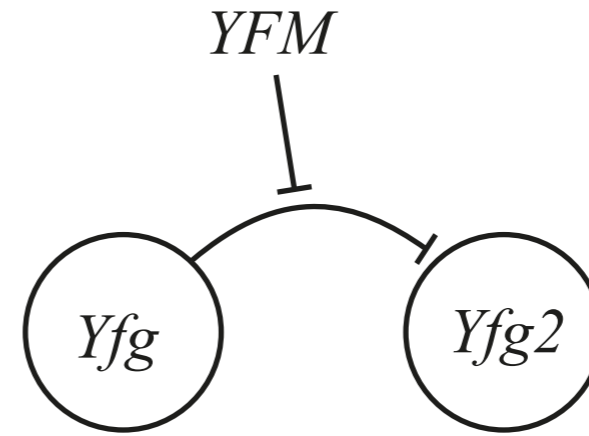


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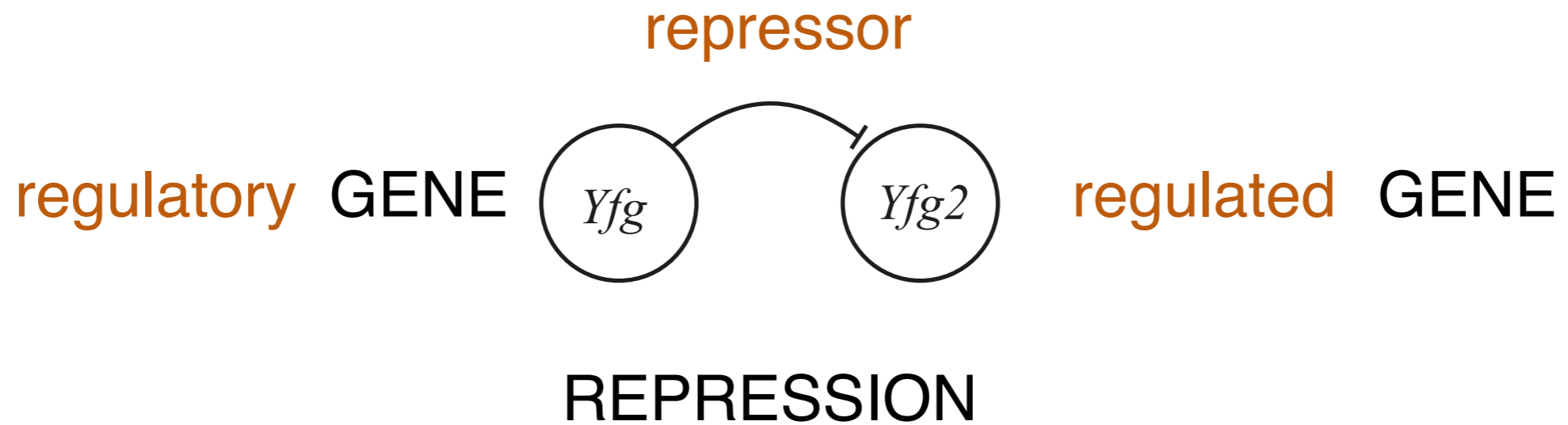
REPRESSION



INDUCTION

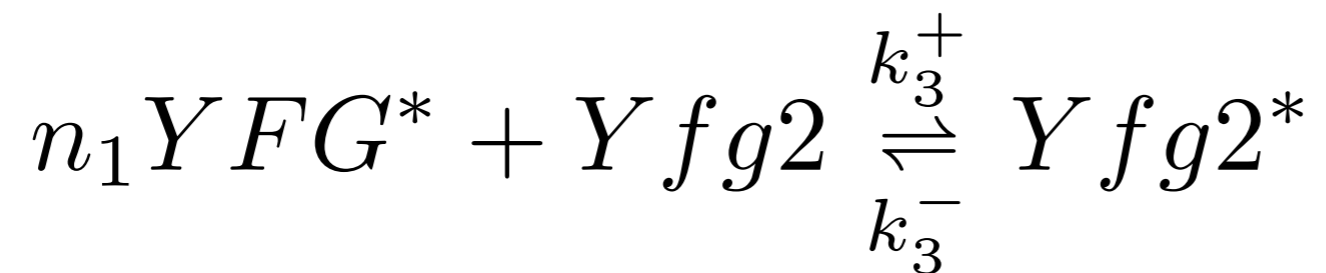
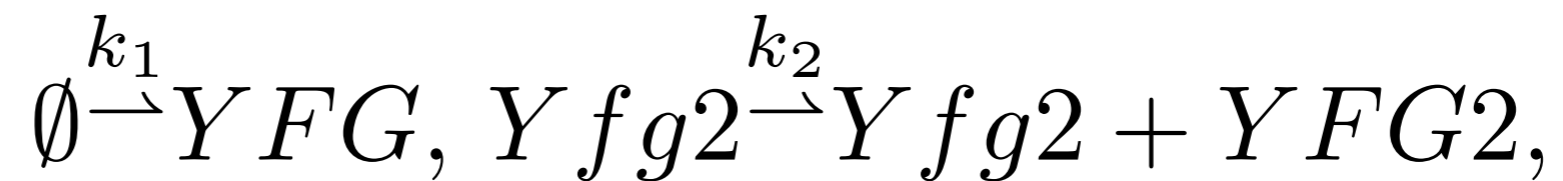
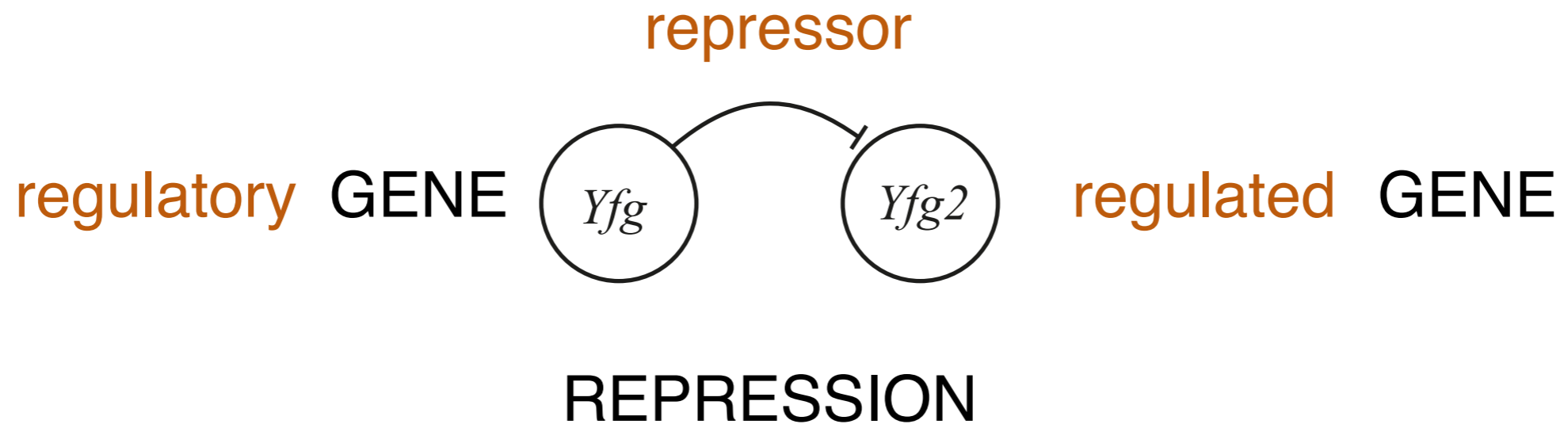
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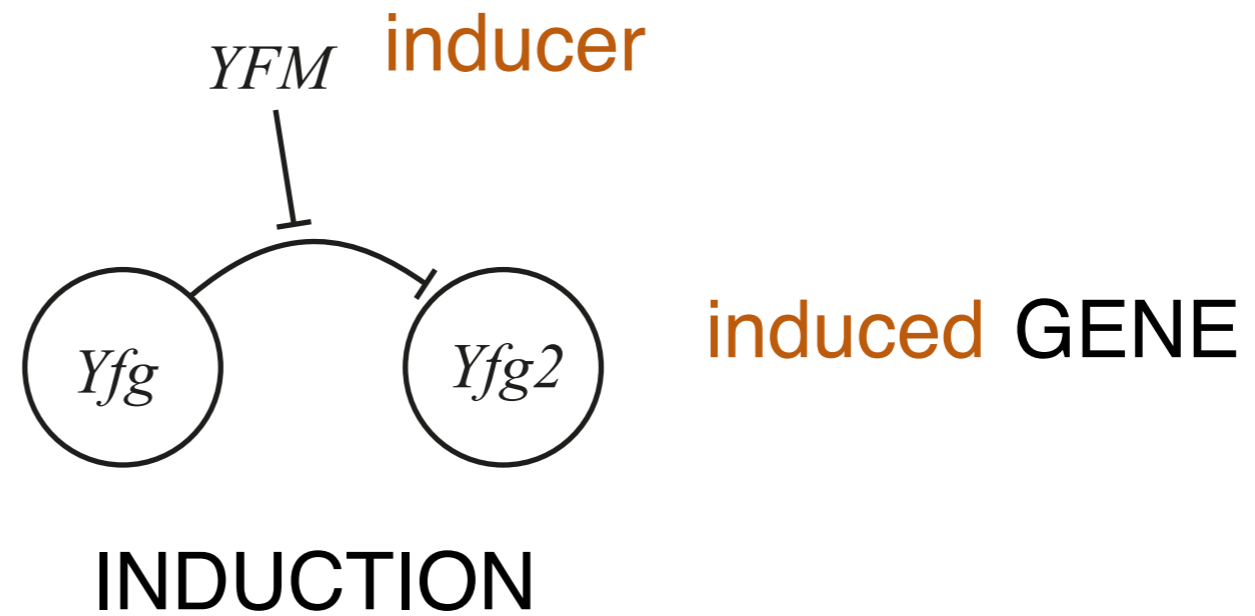
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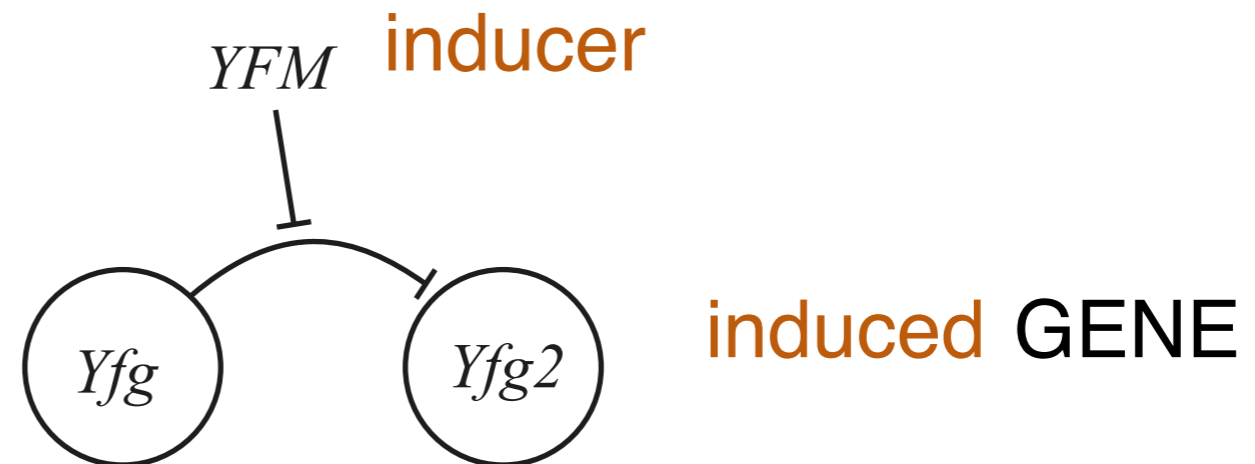
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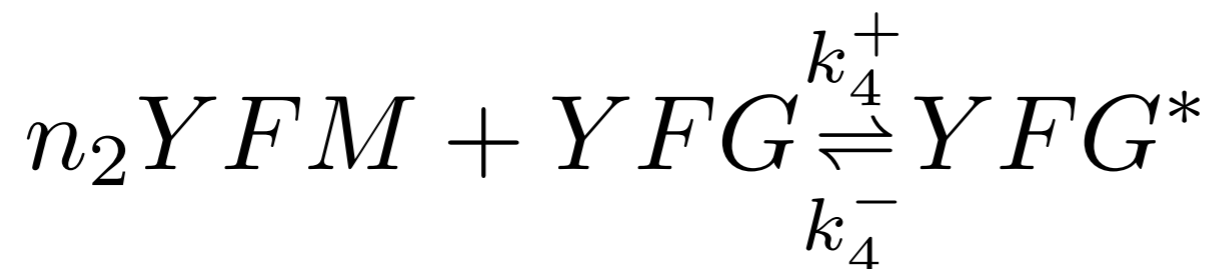
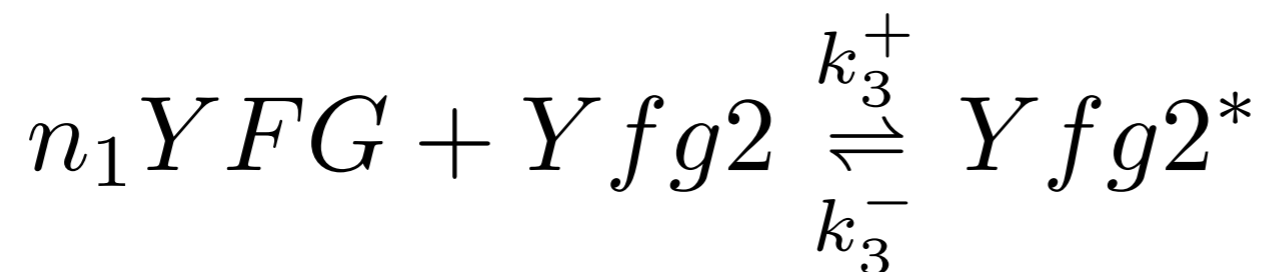
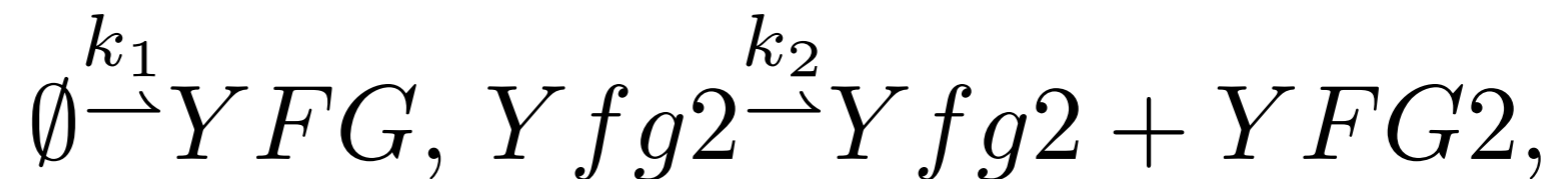


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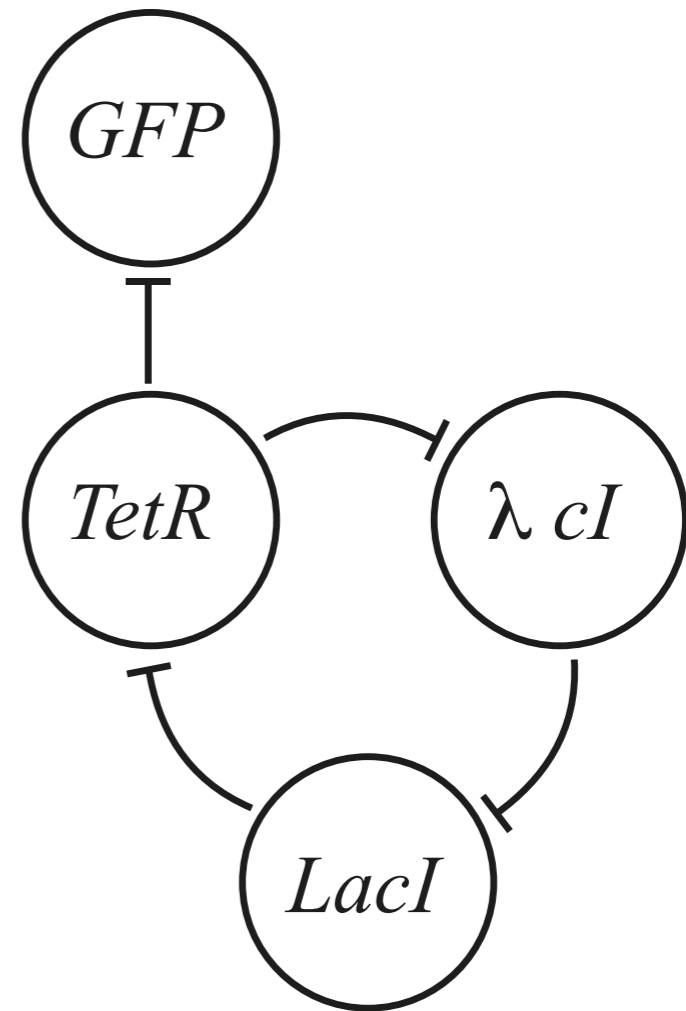
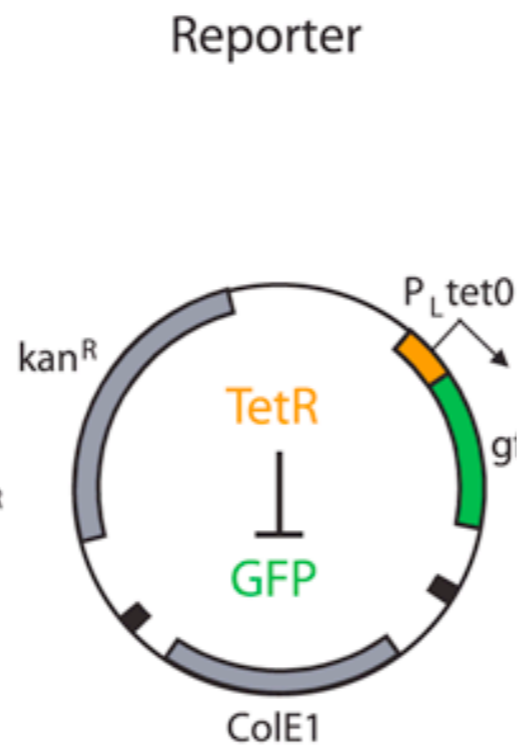
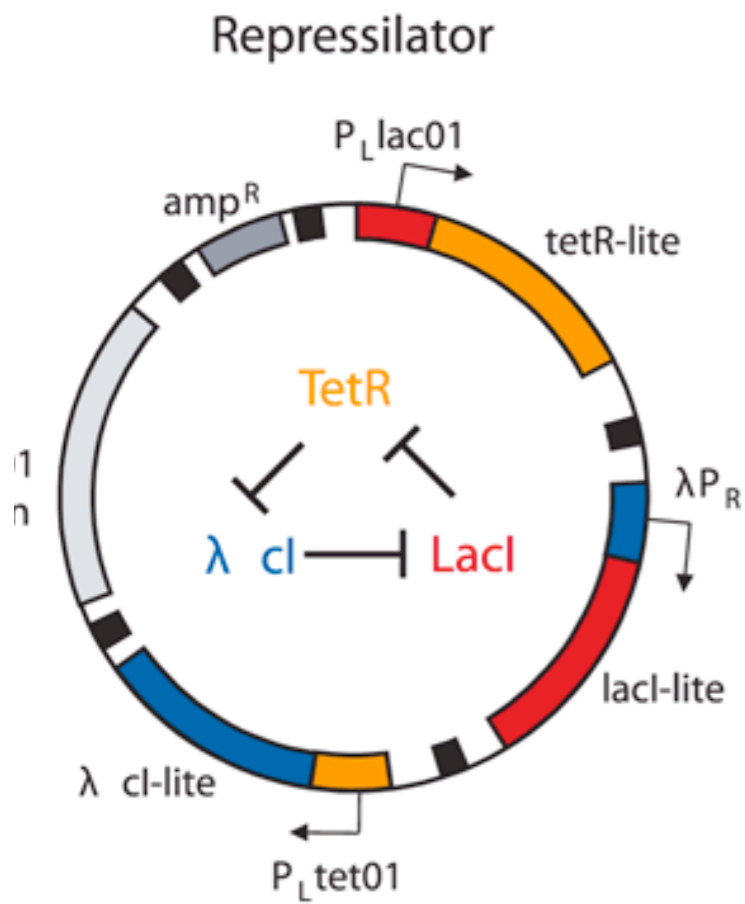


INDUCTION



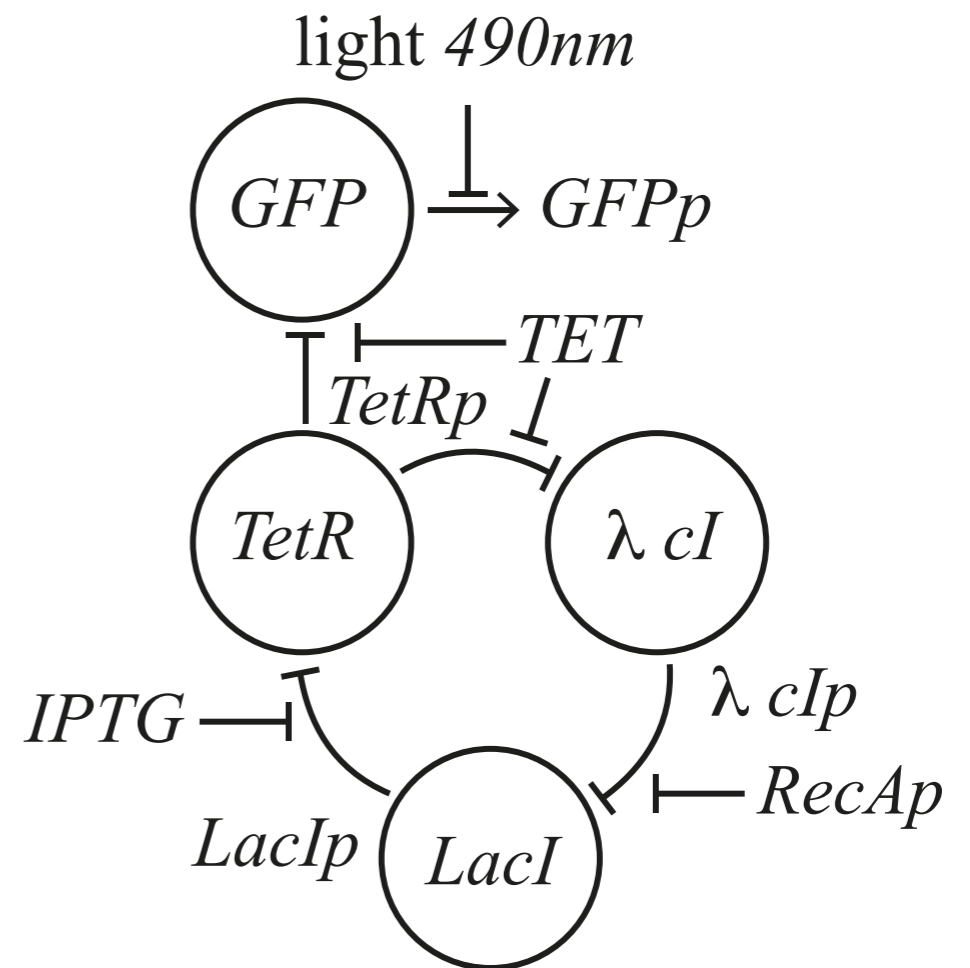
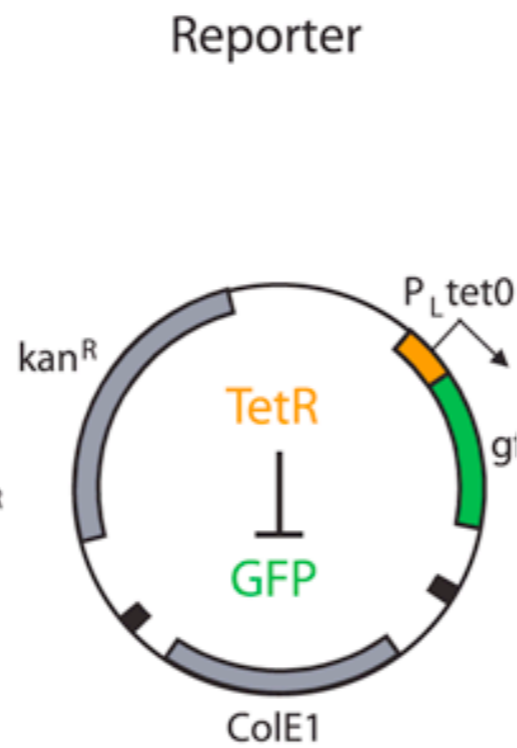
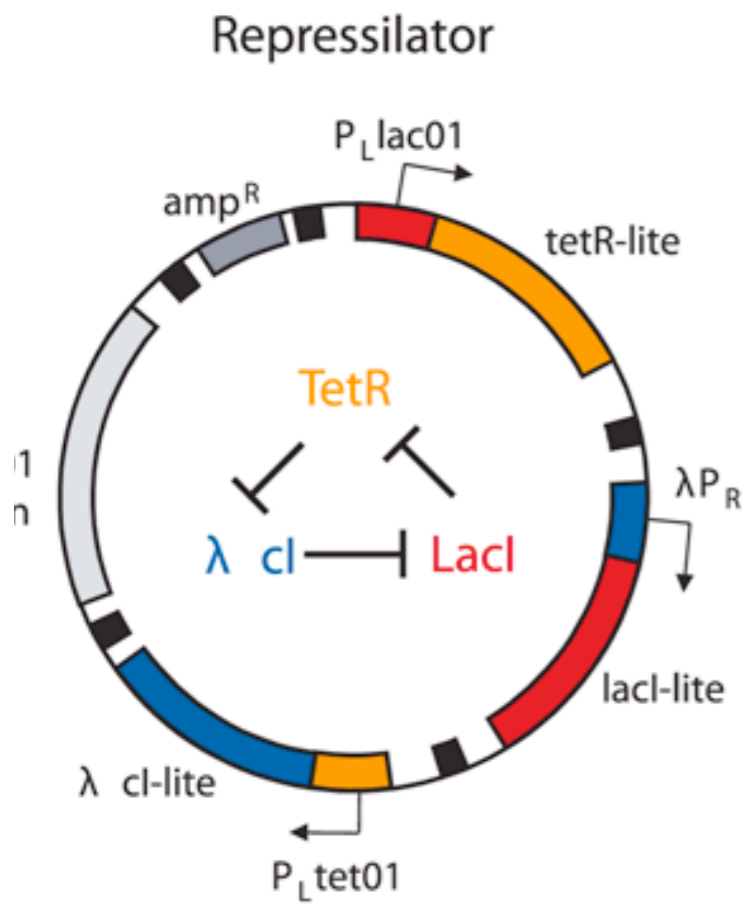
EXAMPLE

repressilator



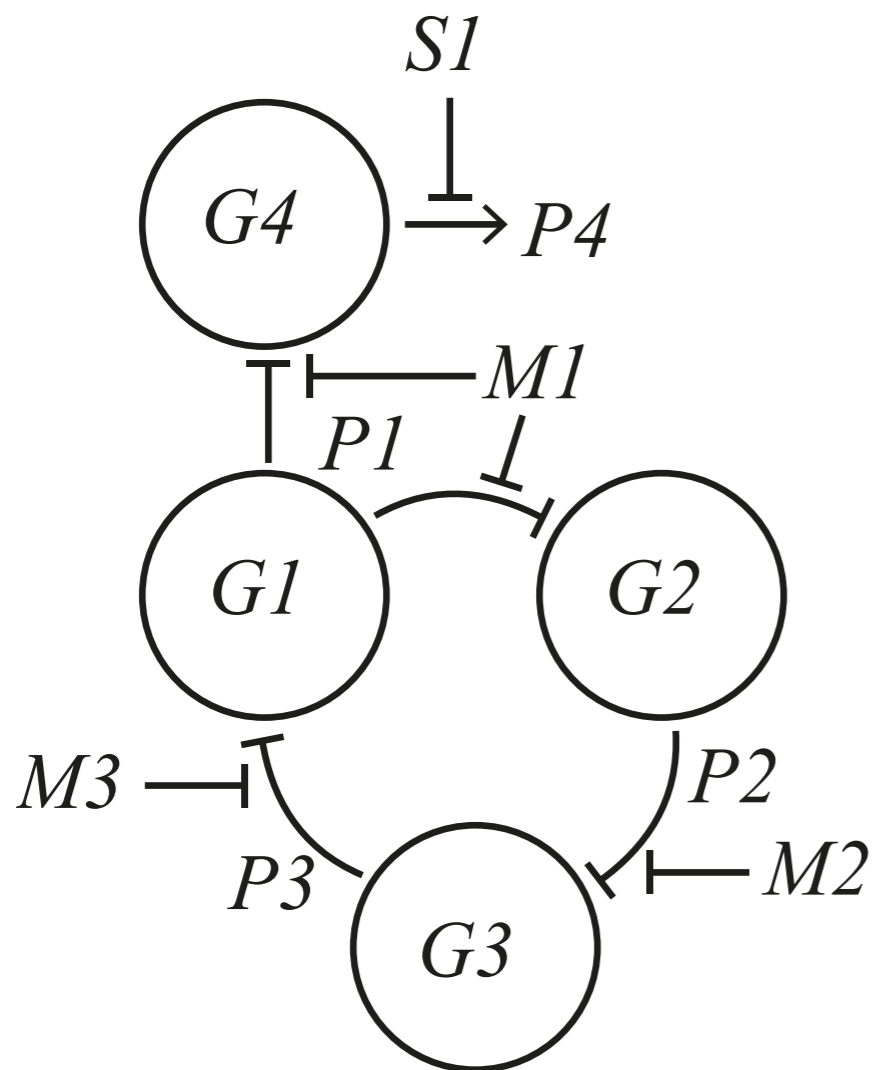
EXAMPLE

repressilator



EXAMPLE

repressilator



WRITE DOWN THE CORRESPONDING CRN

HOW MANY REACTIONS?

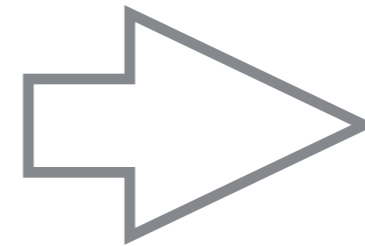
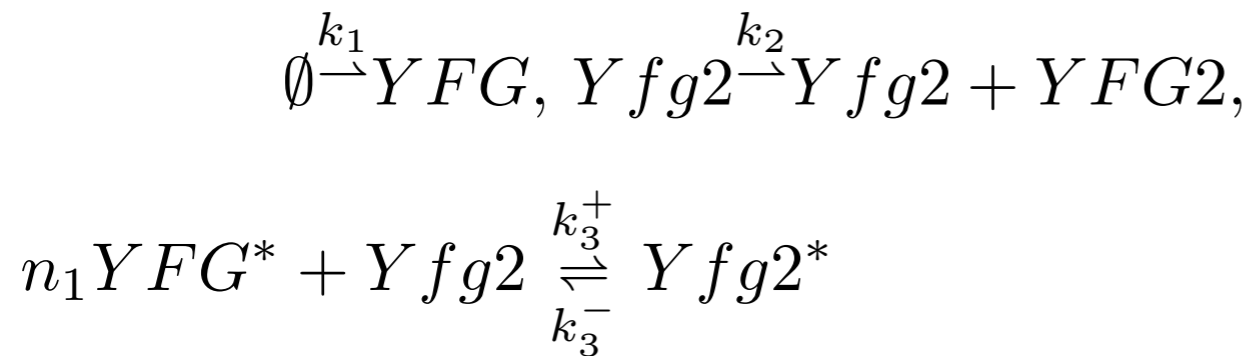
HOW MANY SPECIES?

WHAT HILL COEFFICIENTS DID YOU USE?

WHAT MAJOR SIMPLIFICATIONS
WERE MADE?

NEXT TIME

mathematical modelling and simulation



$$\frac{dx}{dt} = f(x, k)$$



RuleBender is a powerful simulation tool we'll be using throughout the course.

DOWNLOAD AND INSTALL BEFORE NEXT LECTURE!!!

RuleBender

```
--
56 begin reaction rules
57
58 G(b~0) -> G(b~0) + R() kpR
59 G(b~1) -> G(b~1) + R() kpR
60 R() -> Null() kdR
61 R() -> R() + P() kpP
62 P() -> Null() kdP
63 P() + G(b~0) -> G(b~1) kfow
64 G(b~1) -> P() + G(b~0) kbac*10
65 P() + G(b~1) -> G(b~2) kfow
66 G(b~2) -> P() + G(b~1) kbac
67
68 end reaction rules
69 end model
--
```