HIERARCHICAL MODEL COMPOSITION

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CORE SBML MODELS

Biological Content:

Reactions

Species

Parameters

Compartments

Functions

Events

Math

Hierarchical Model Composition Models ('comp')

Biological Content:

Reactions

Species

Parameters

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Functions

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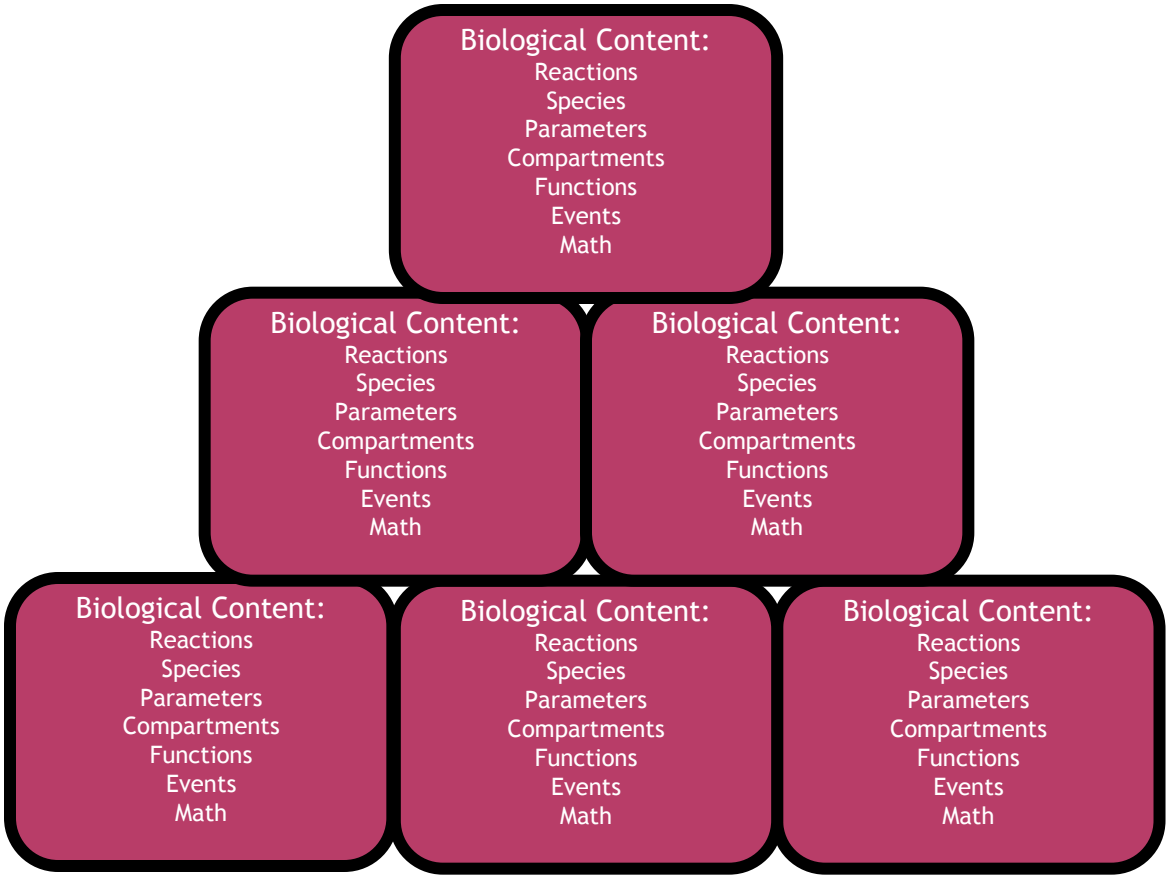
Math

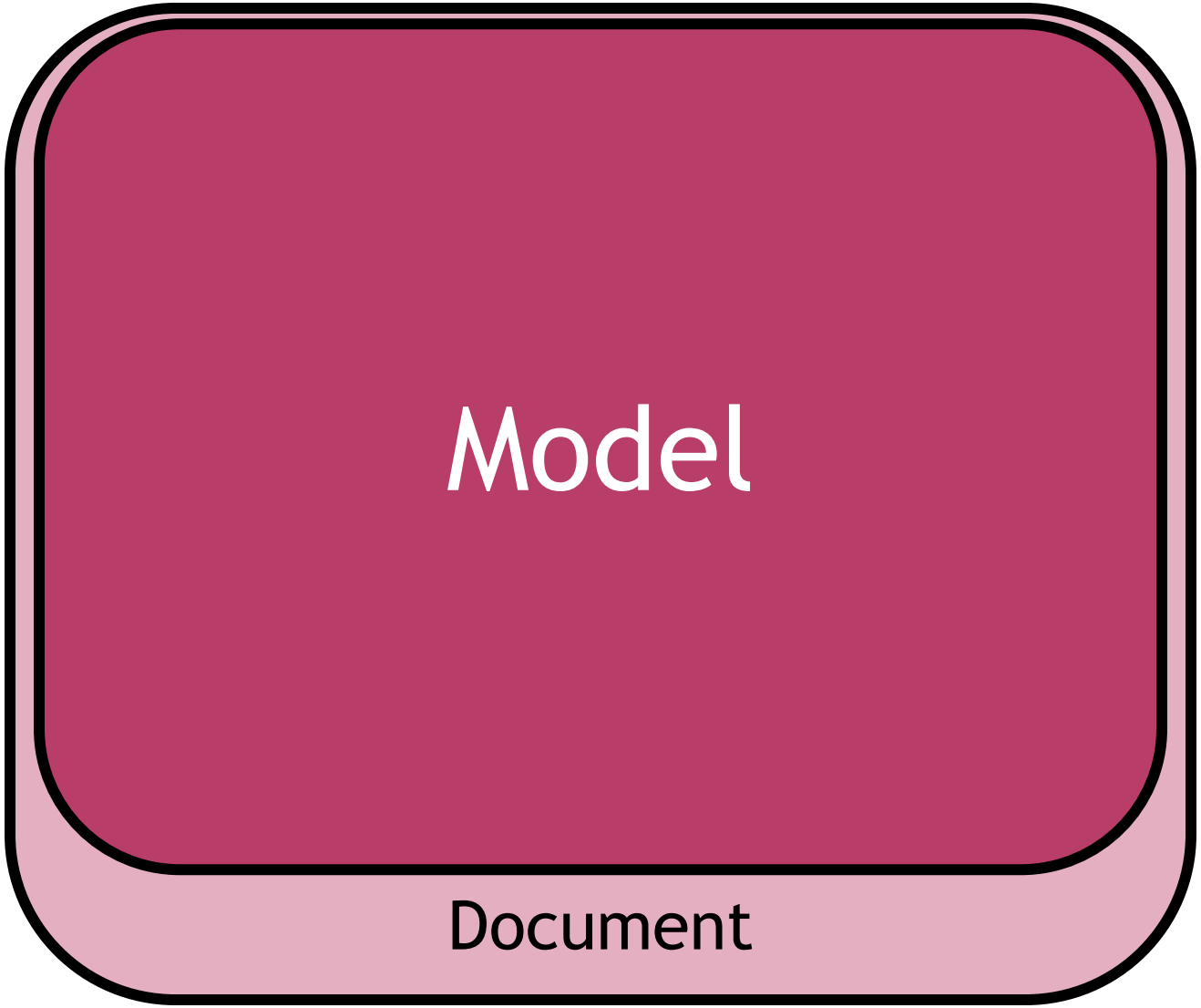
HIERARCHICAL MODEL COMPOSITION MODELS ('COMP')



Three basic tasks:

- Define multiple models
- Import copies as submodels
- Connect their elements

1 DEFINE MULTIPLE MODELS



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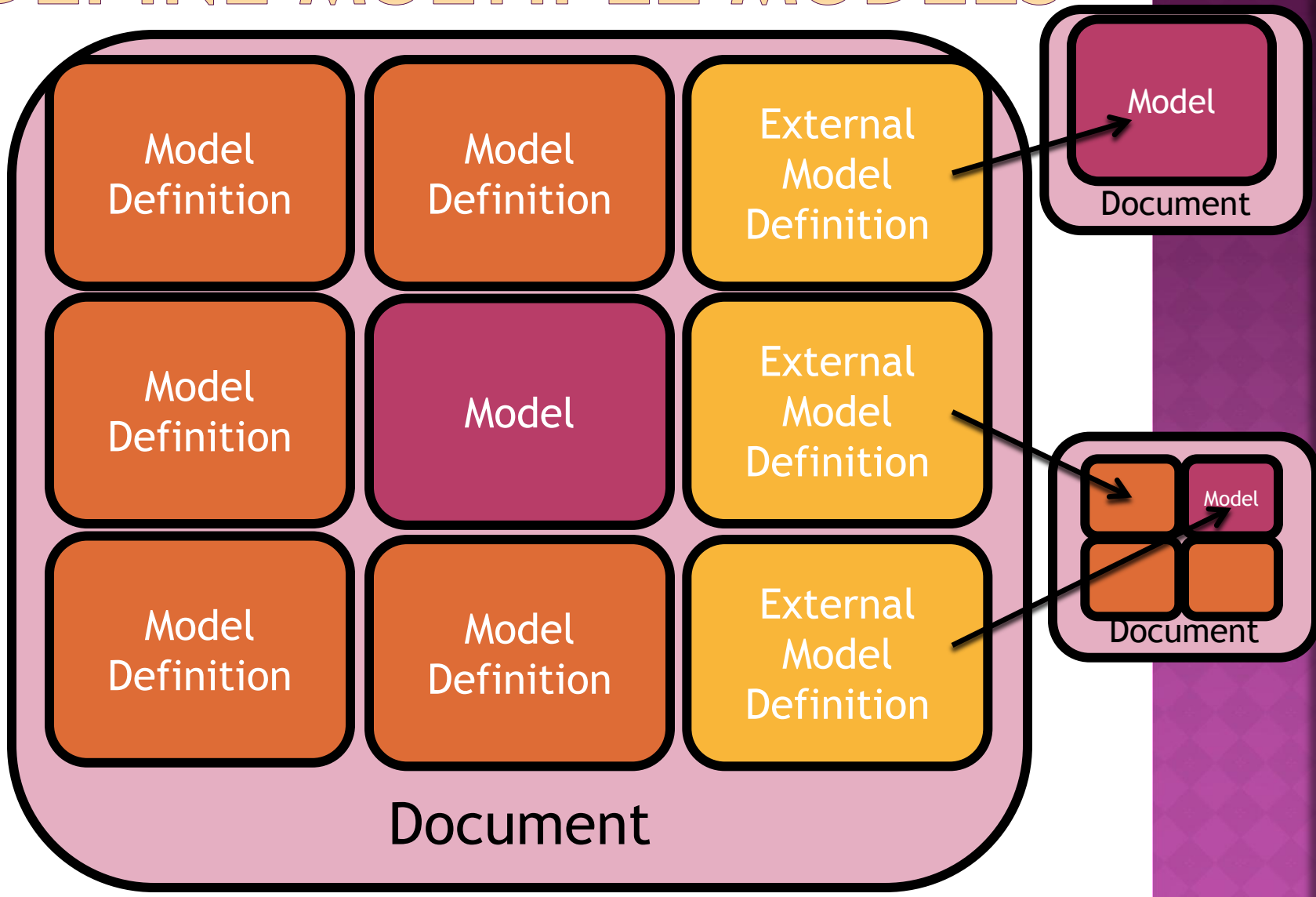
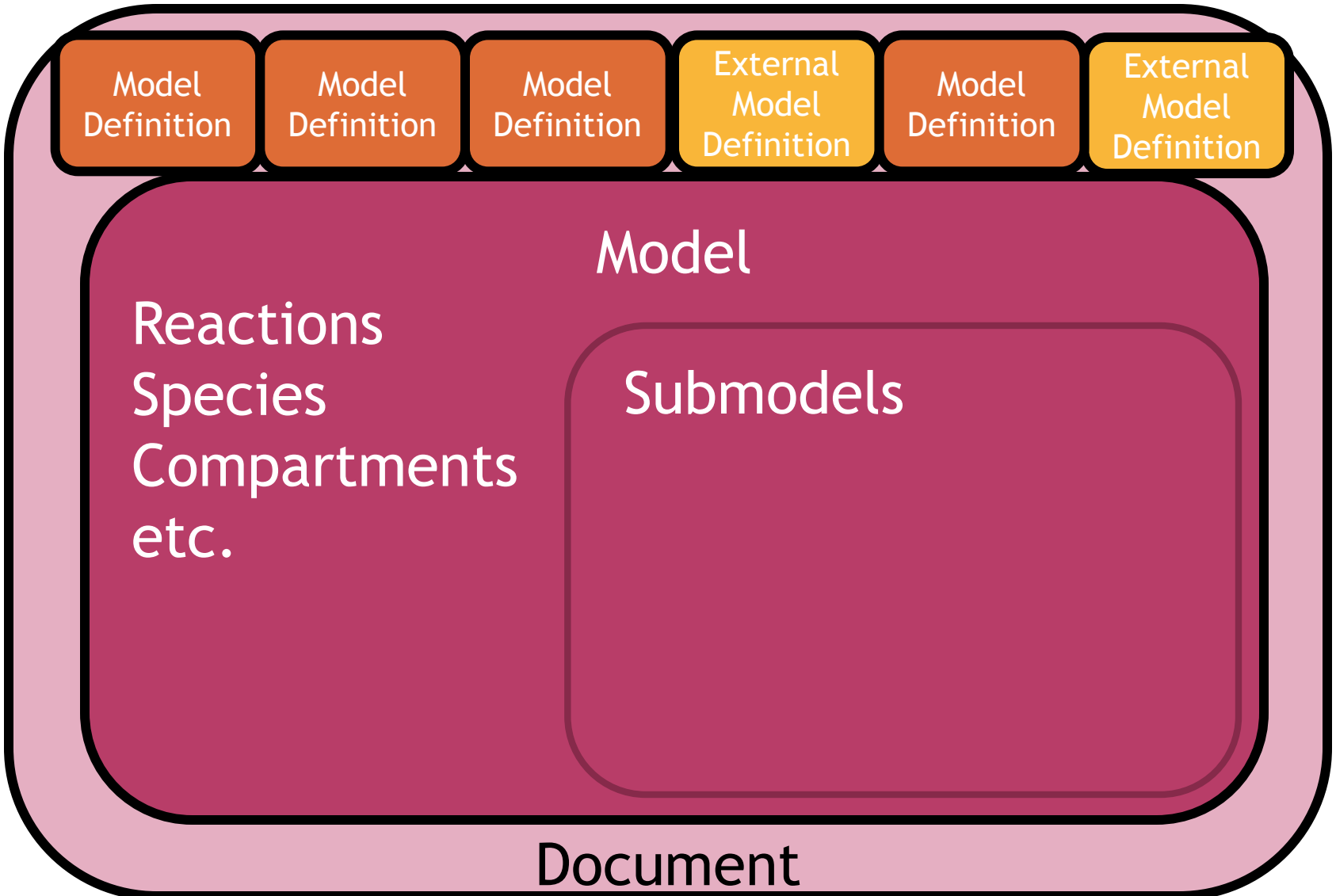


2 IMPORT COPIES AS SUBMODELS



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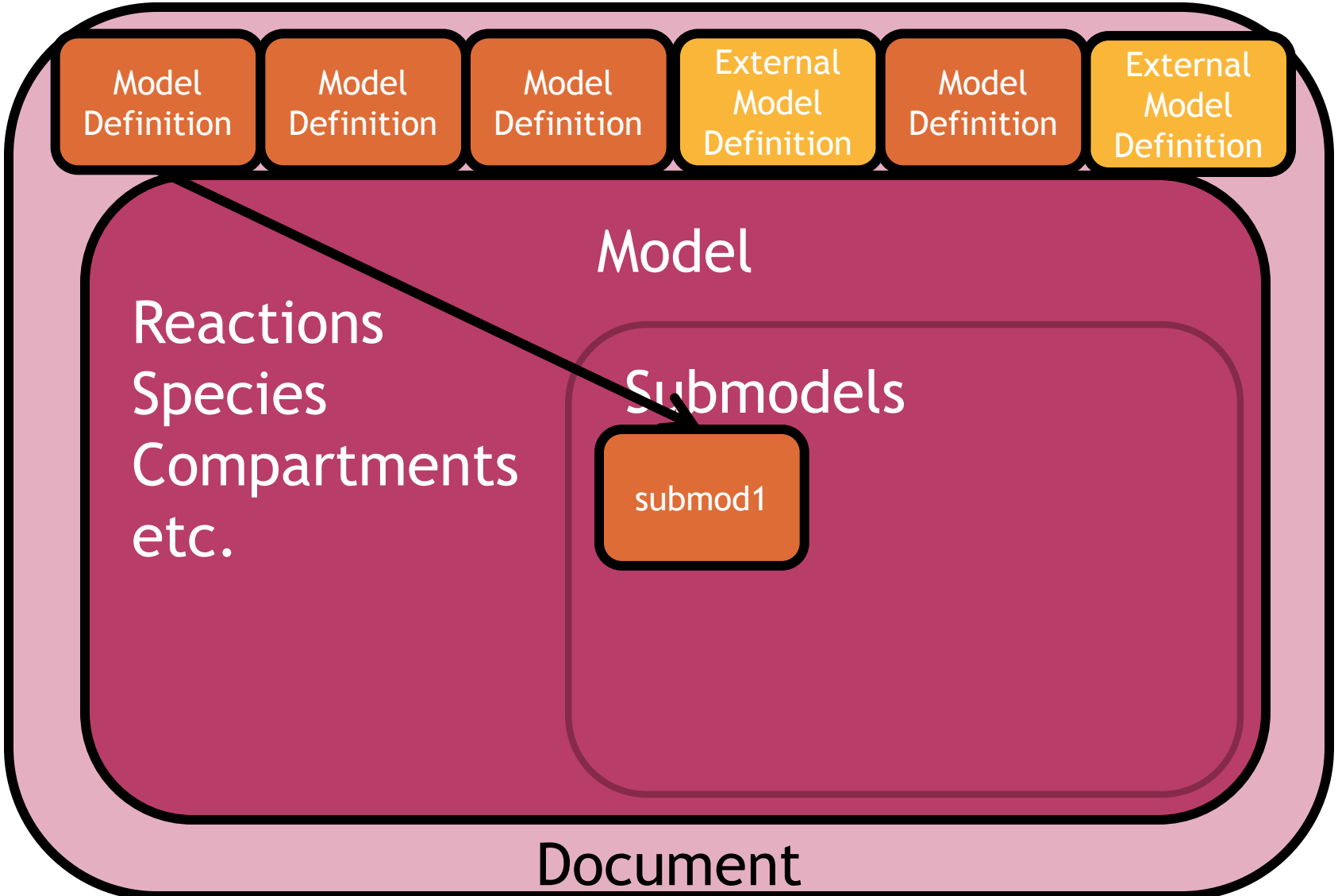

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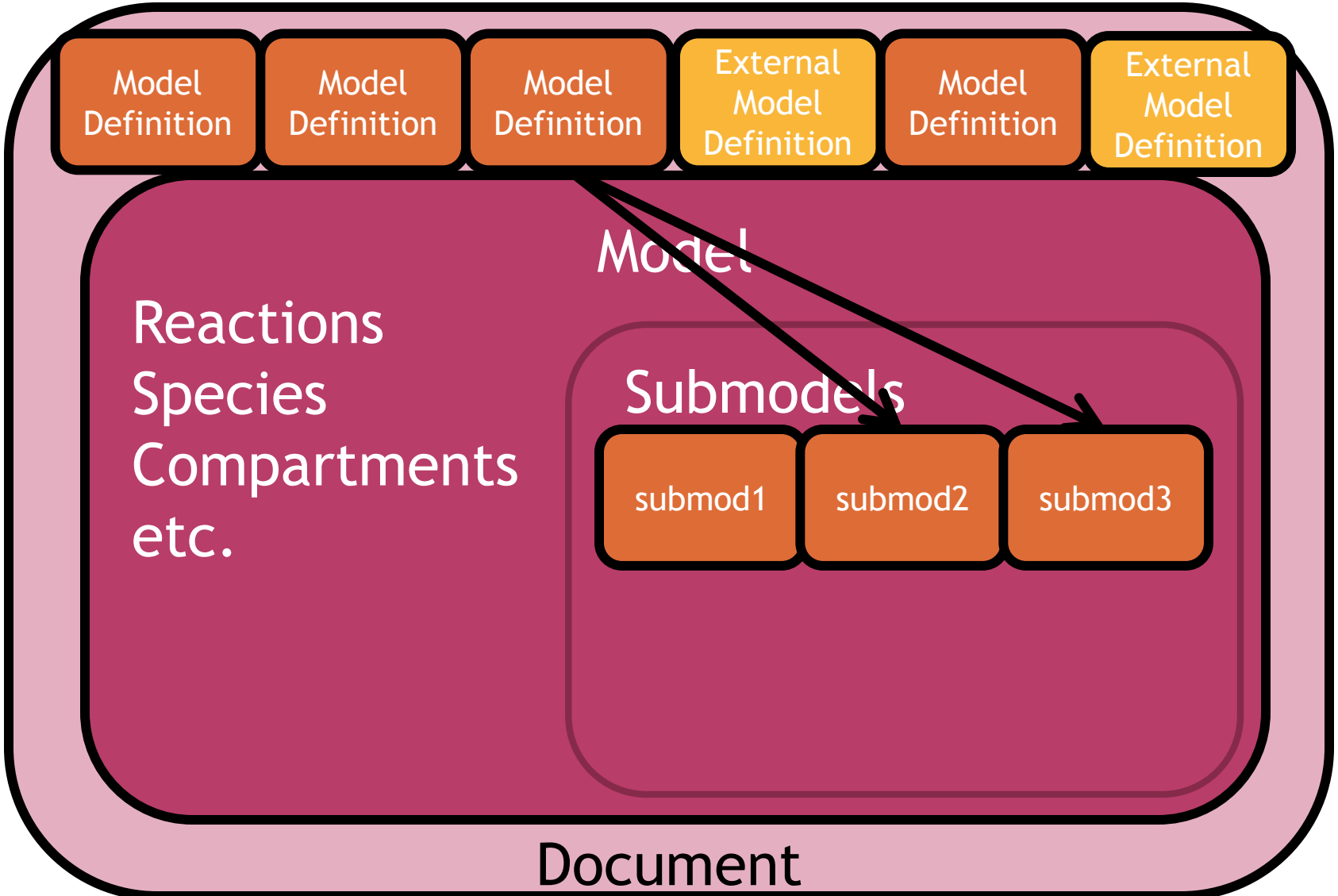

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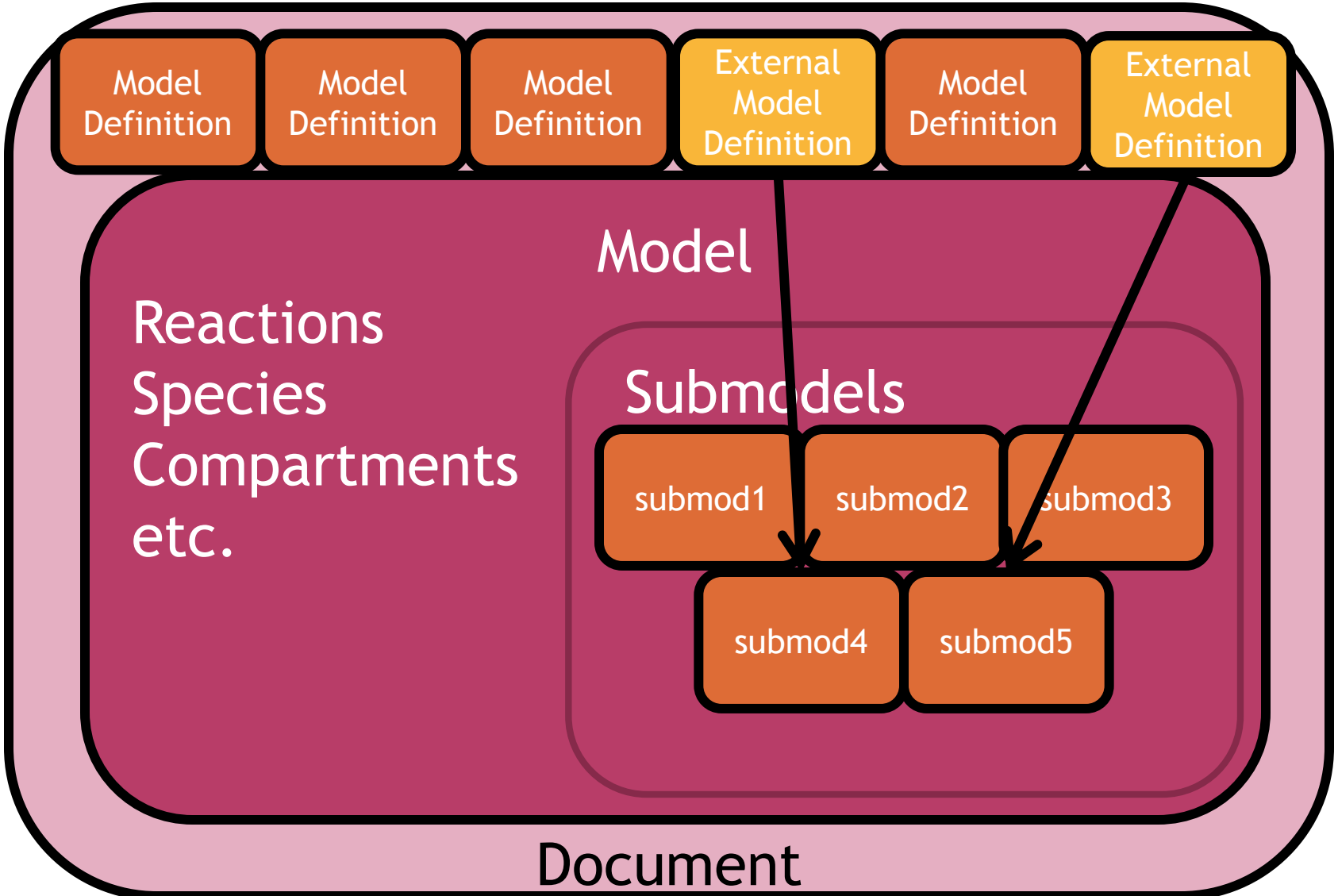

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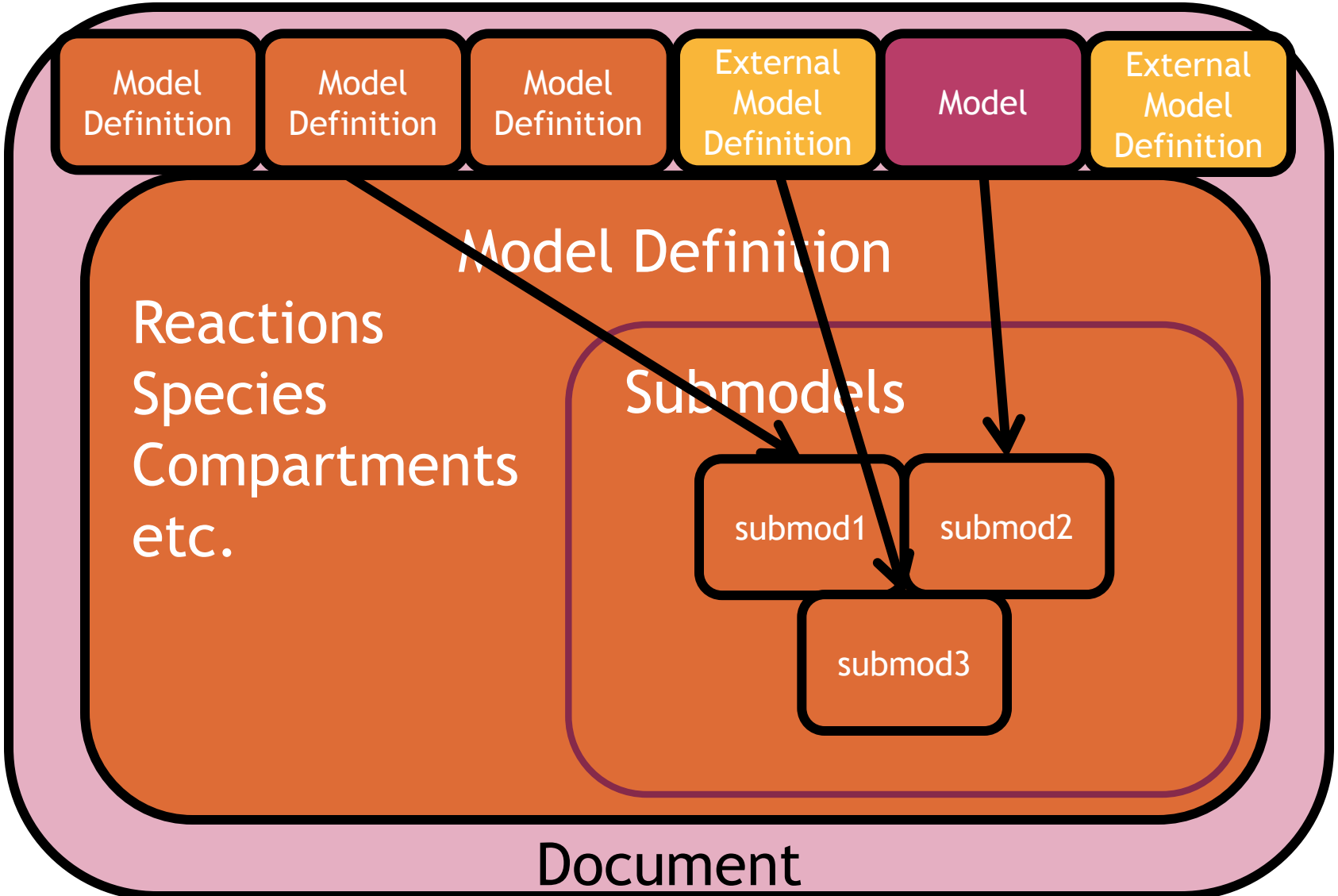

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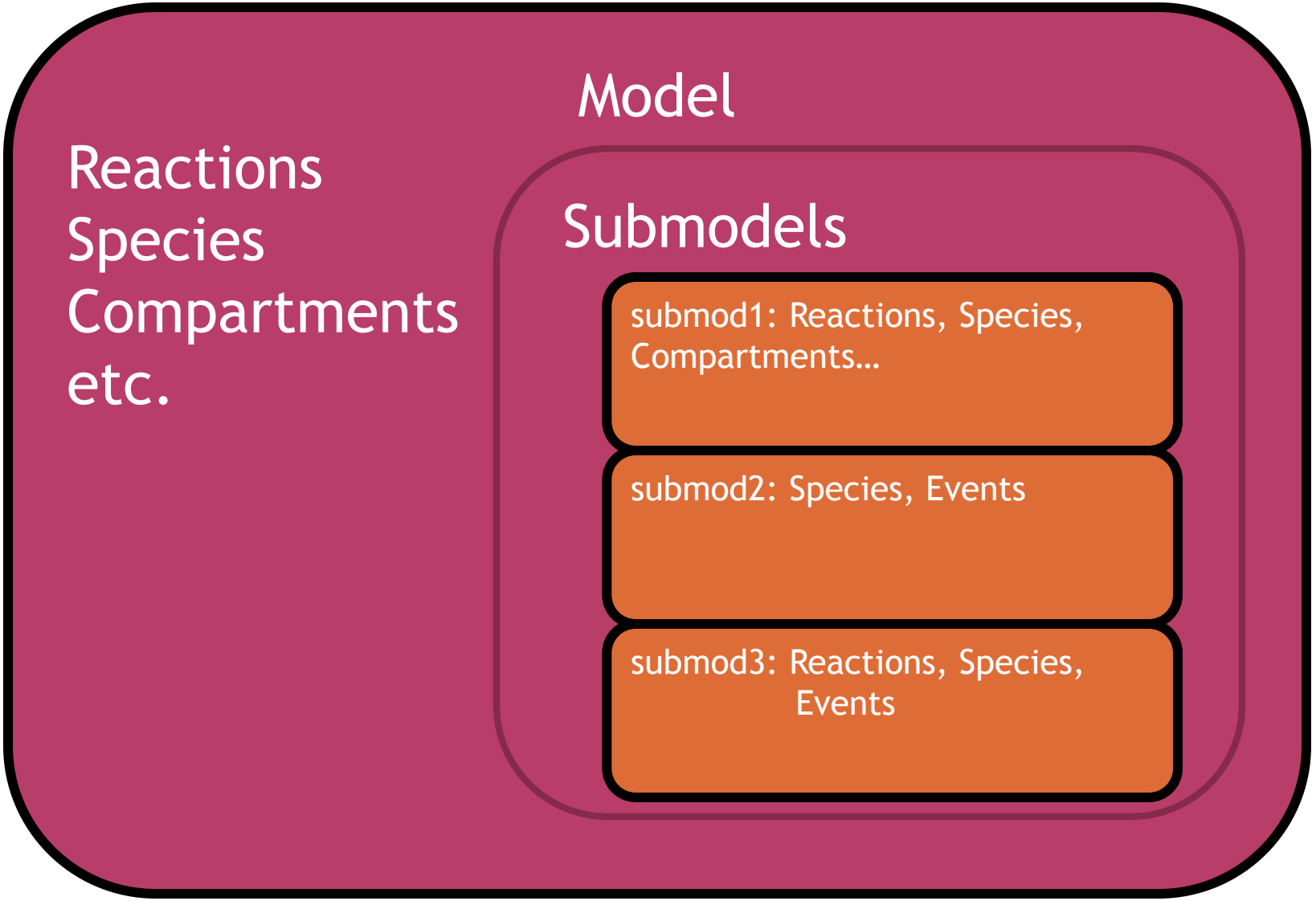
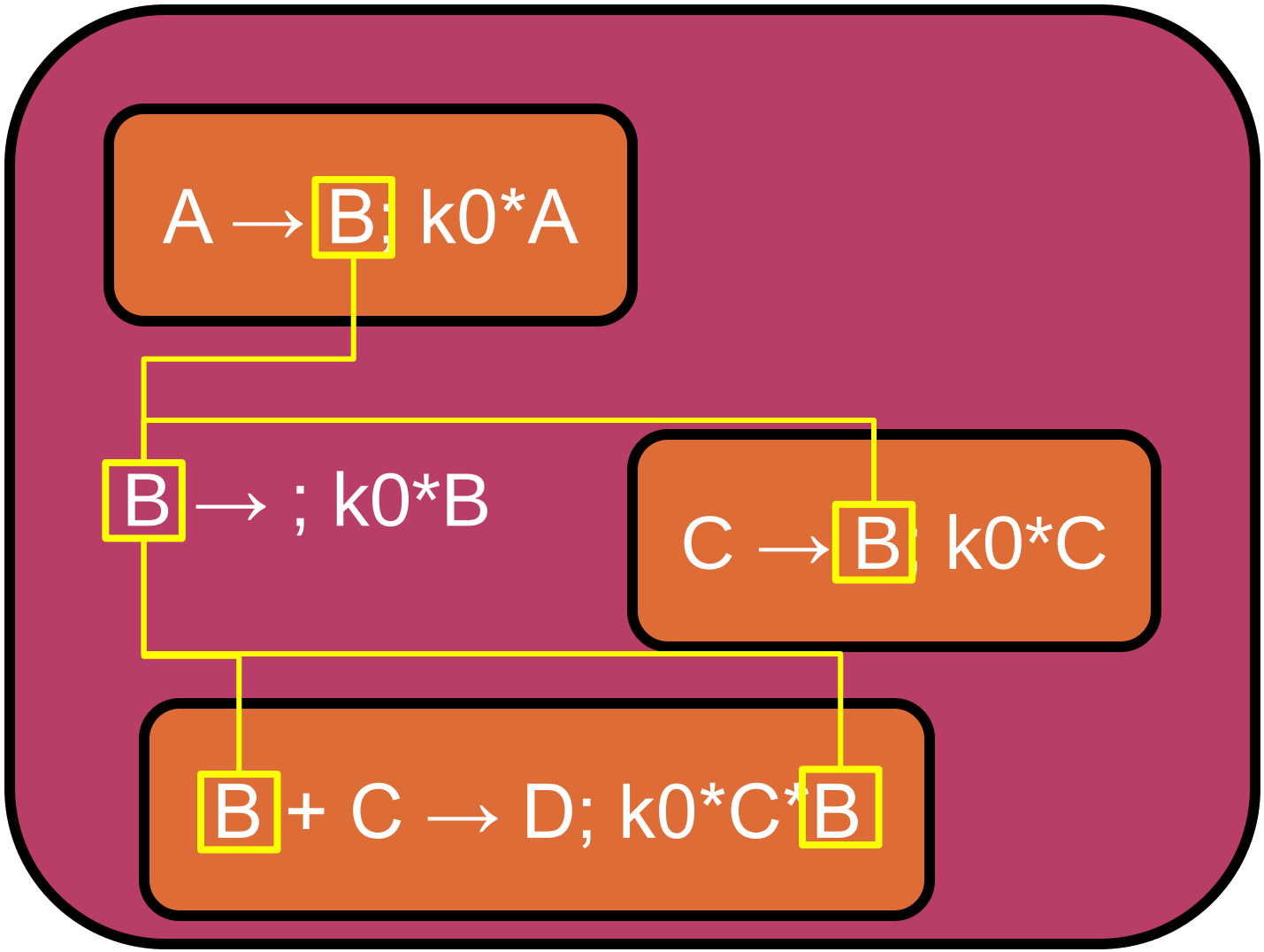


3 CONNECT THEIR ELEMENTS



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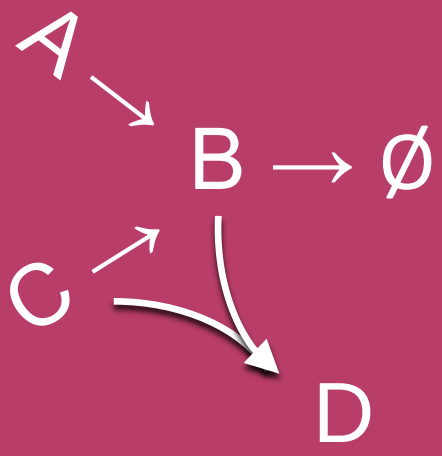
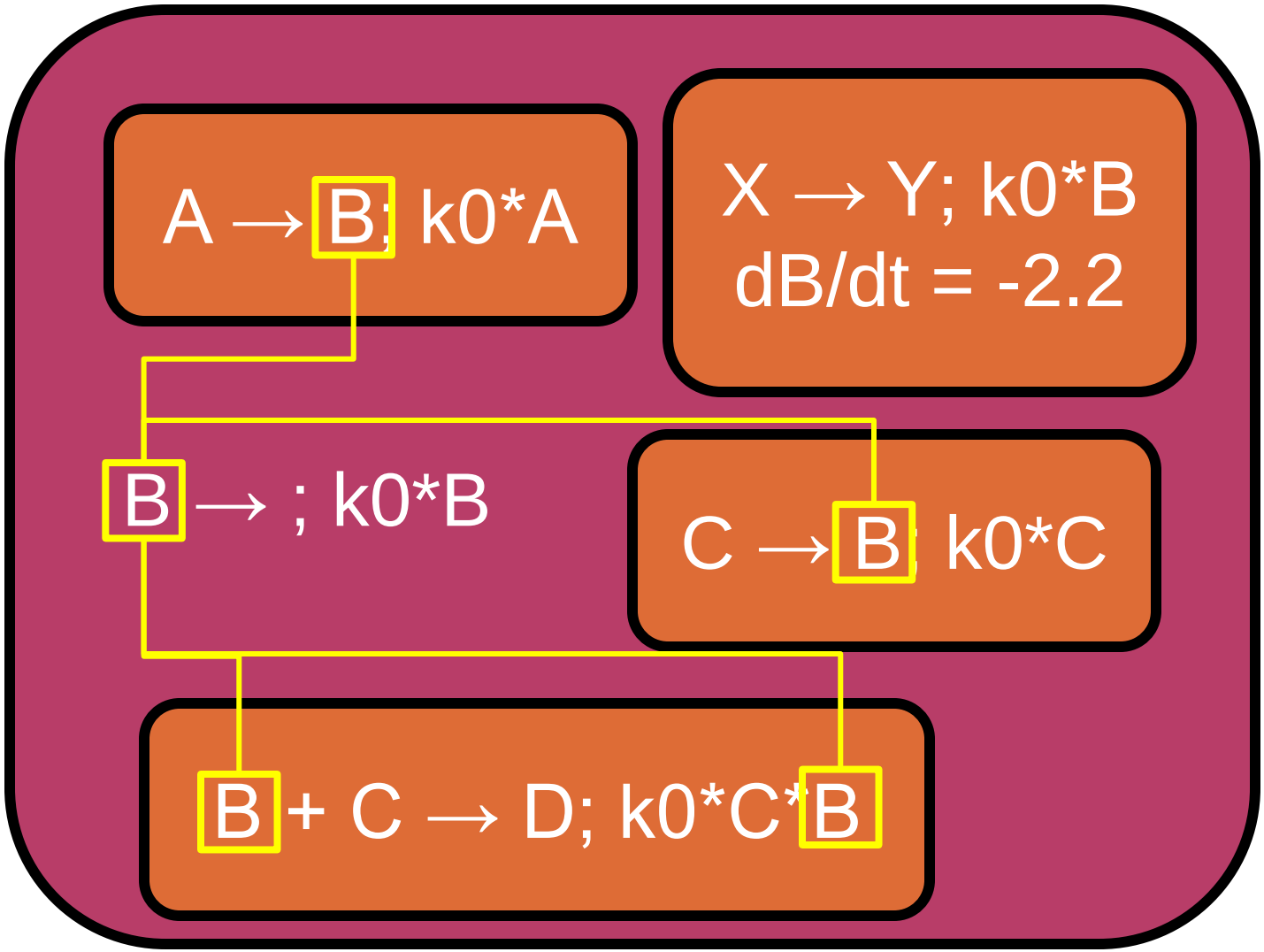


COMPLICATION 1: DELETIONS



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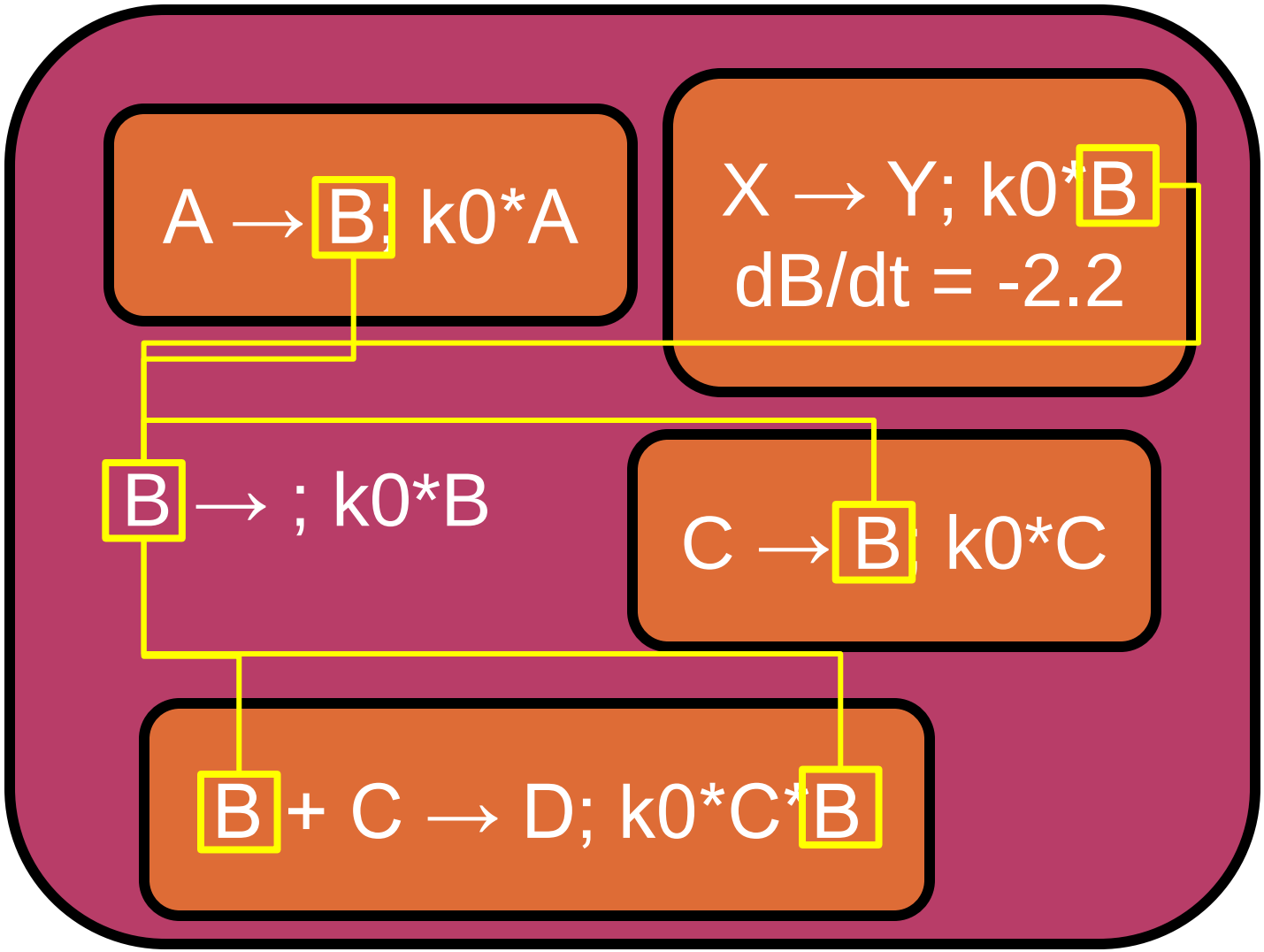

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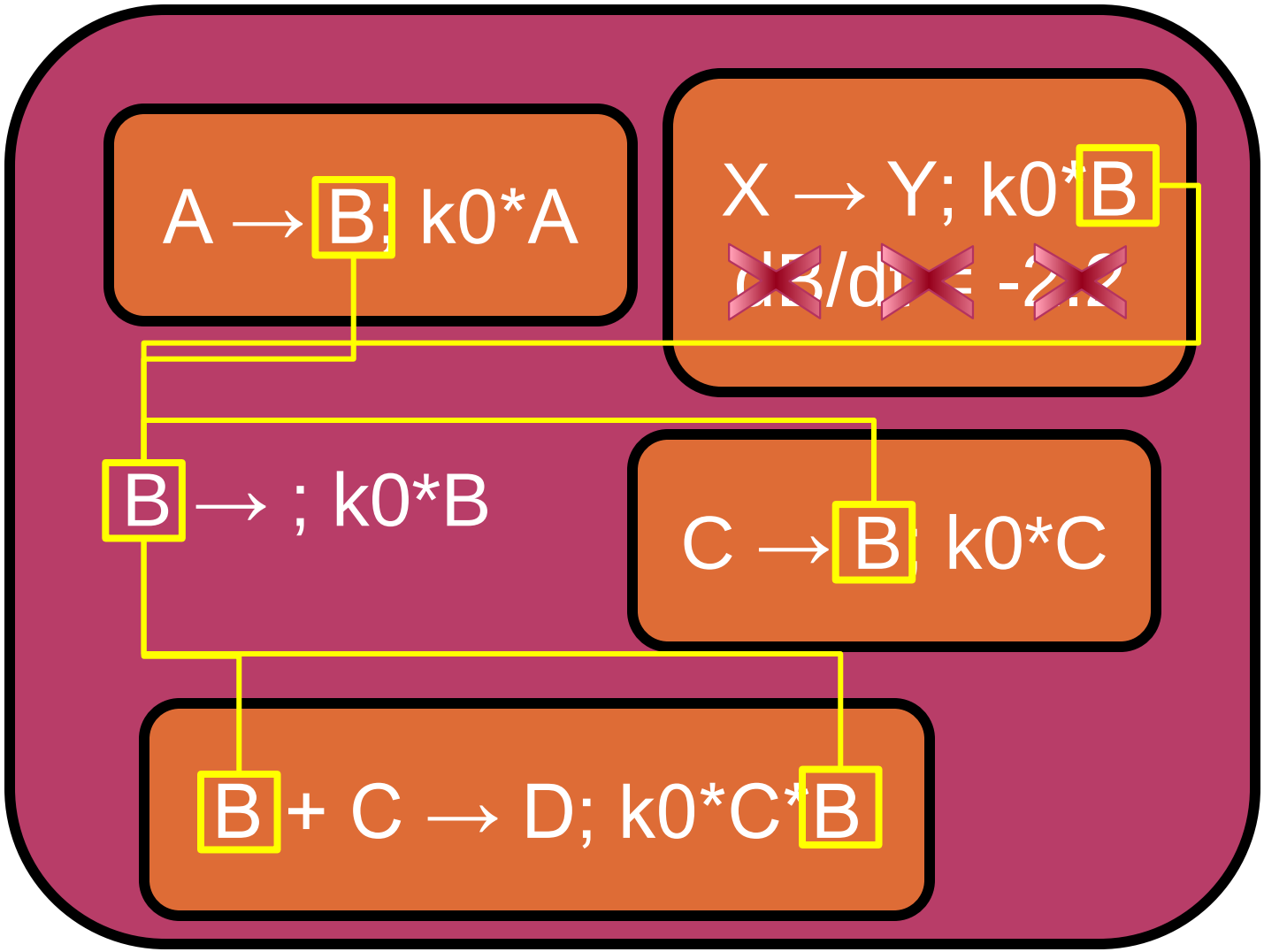
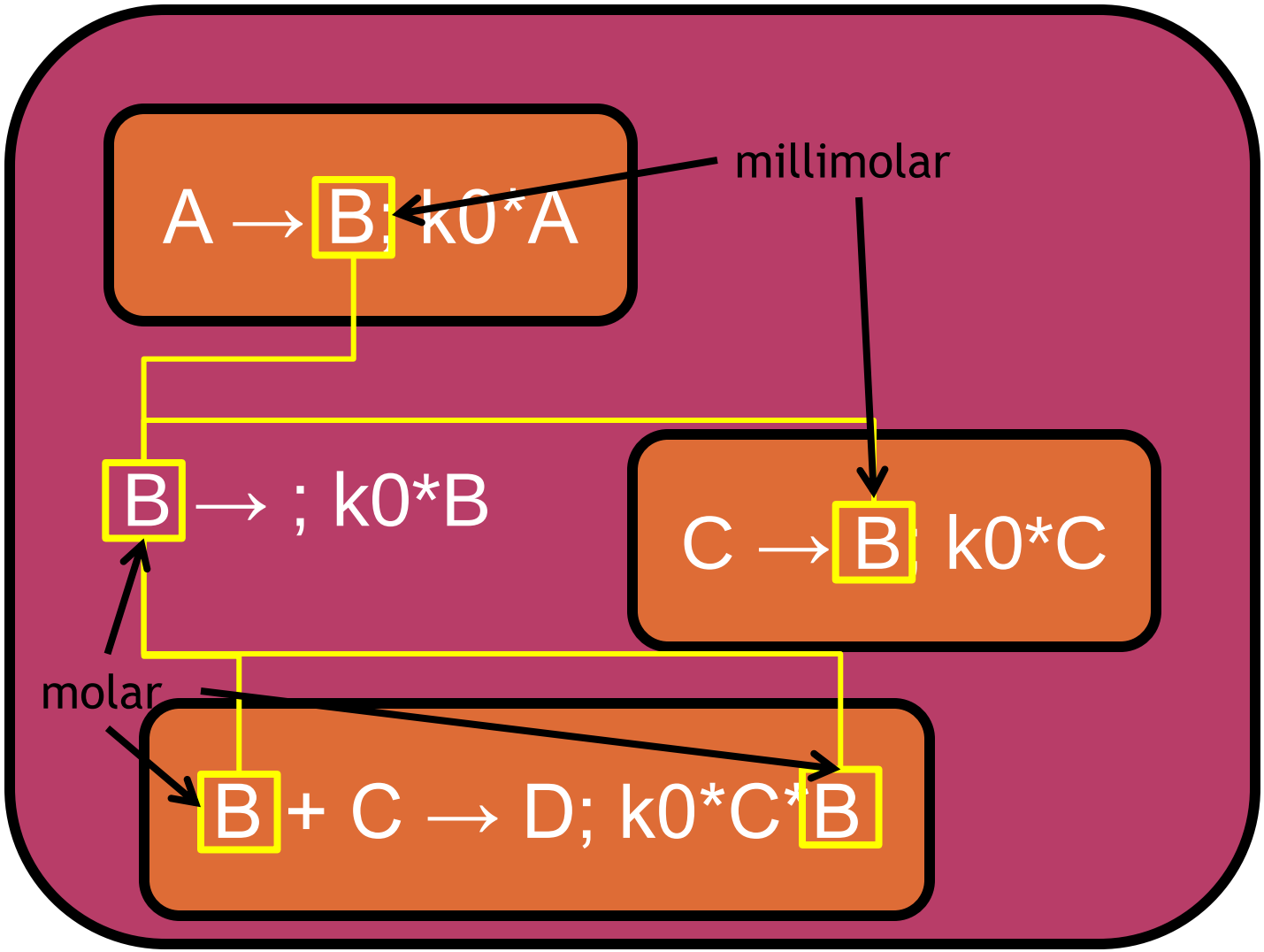


COMPLICATION 2: CONVERSION FACTORS



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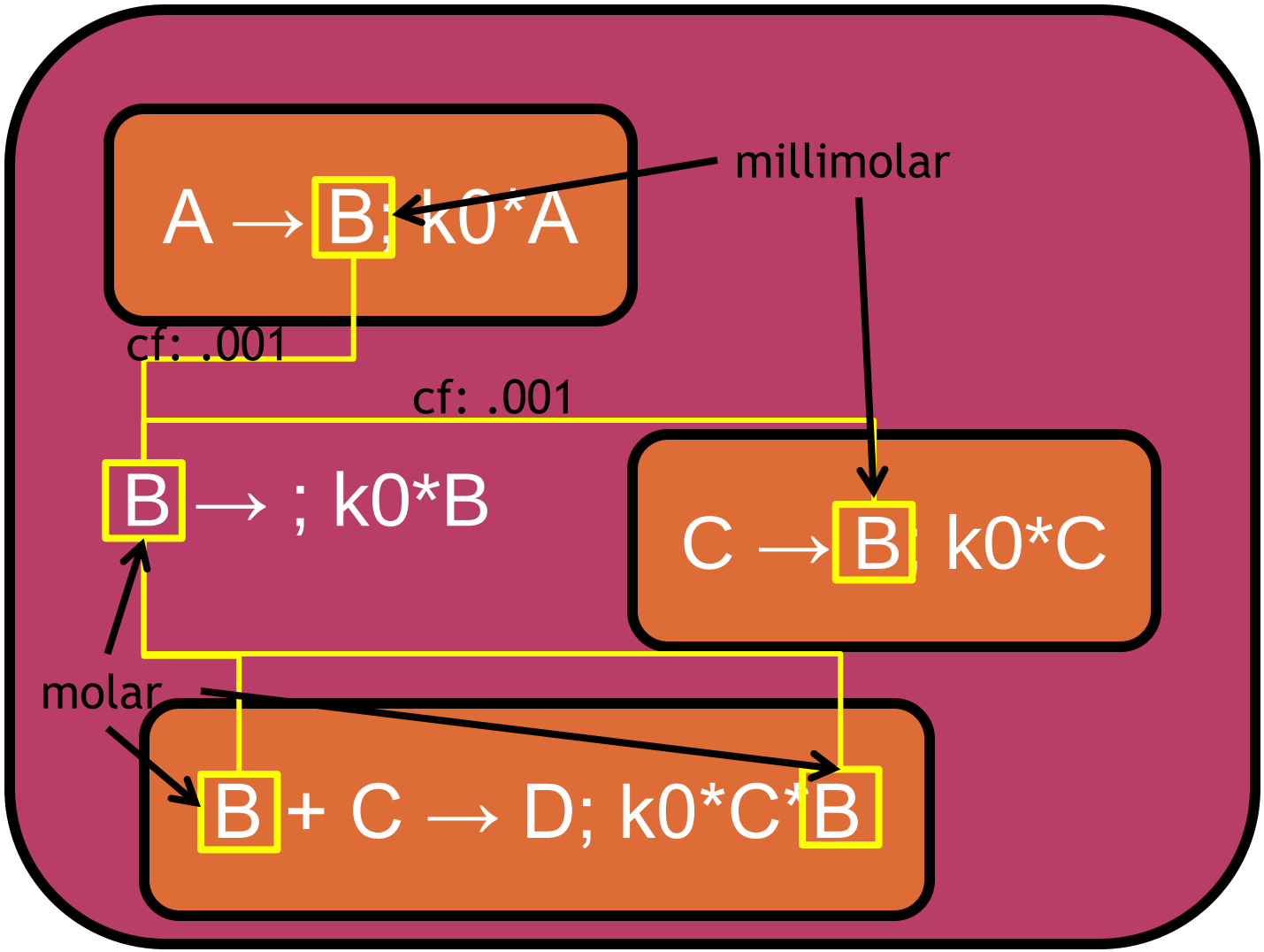
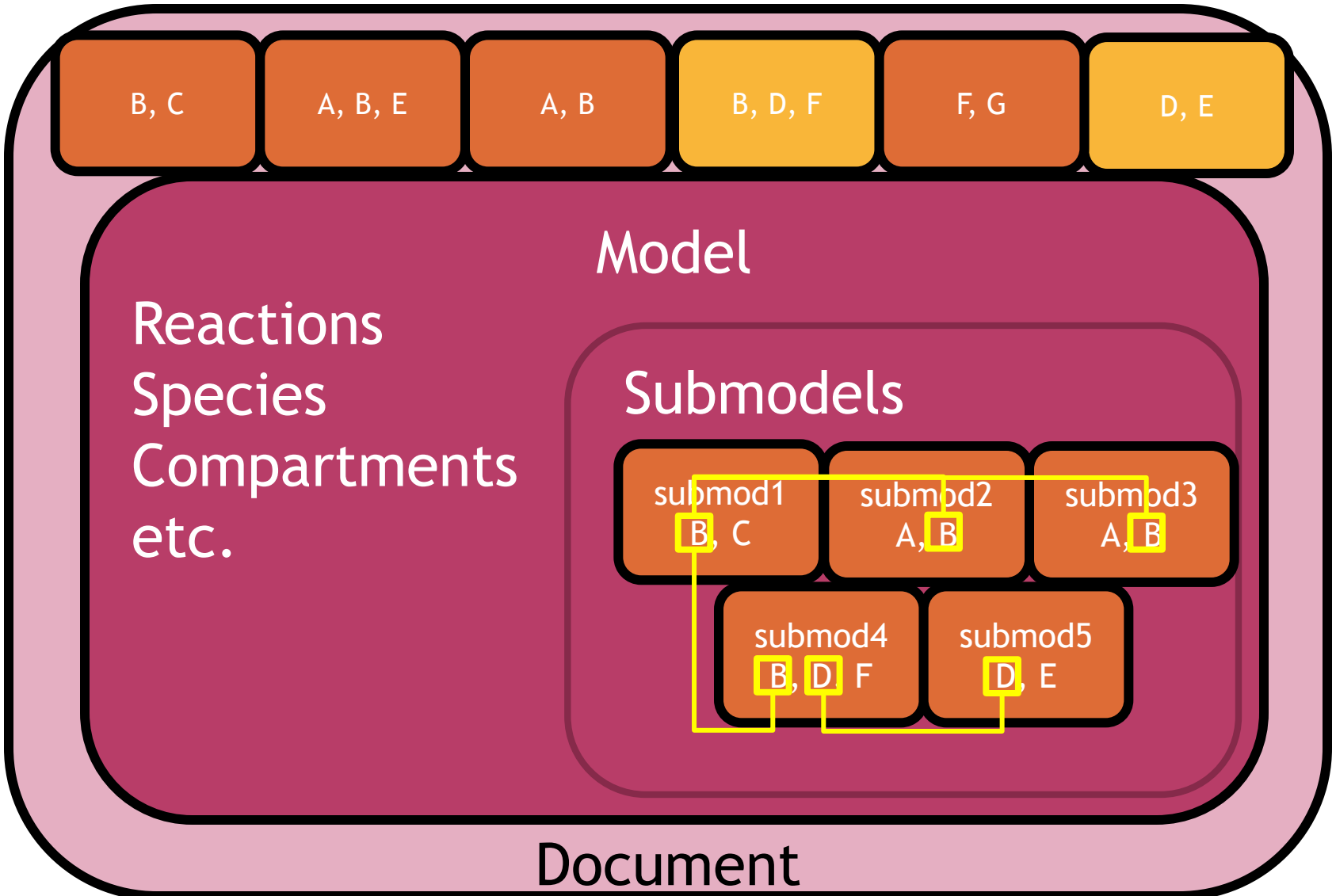
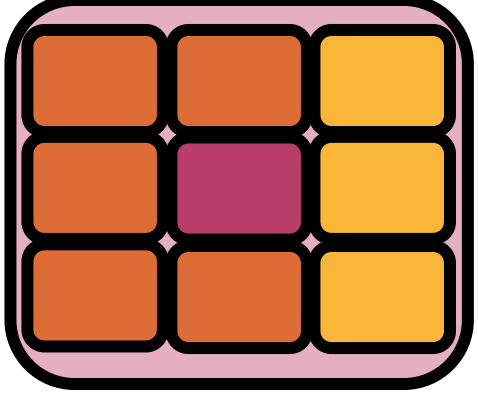
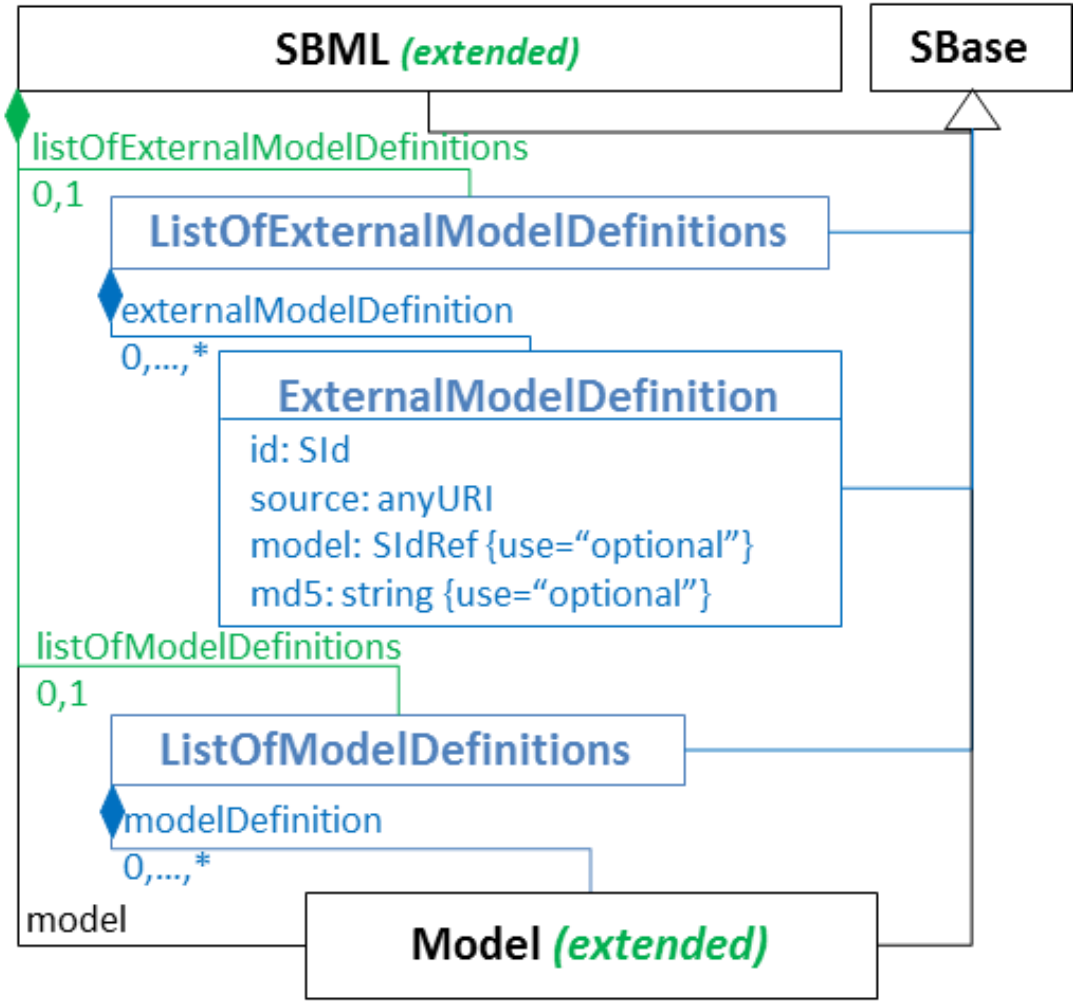


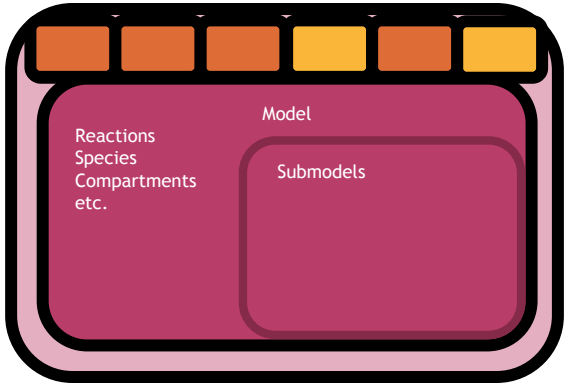
COMPLICATION 3: PORTS

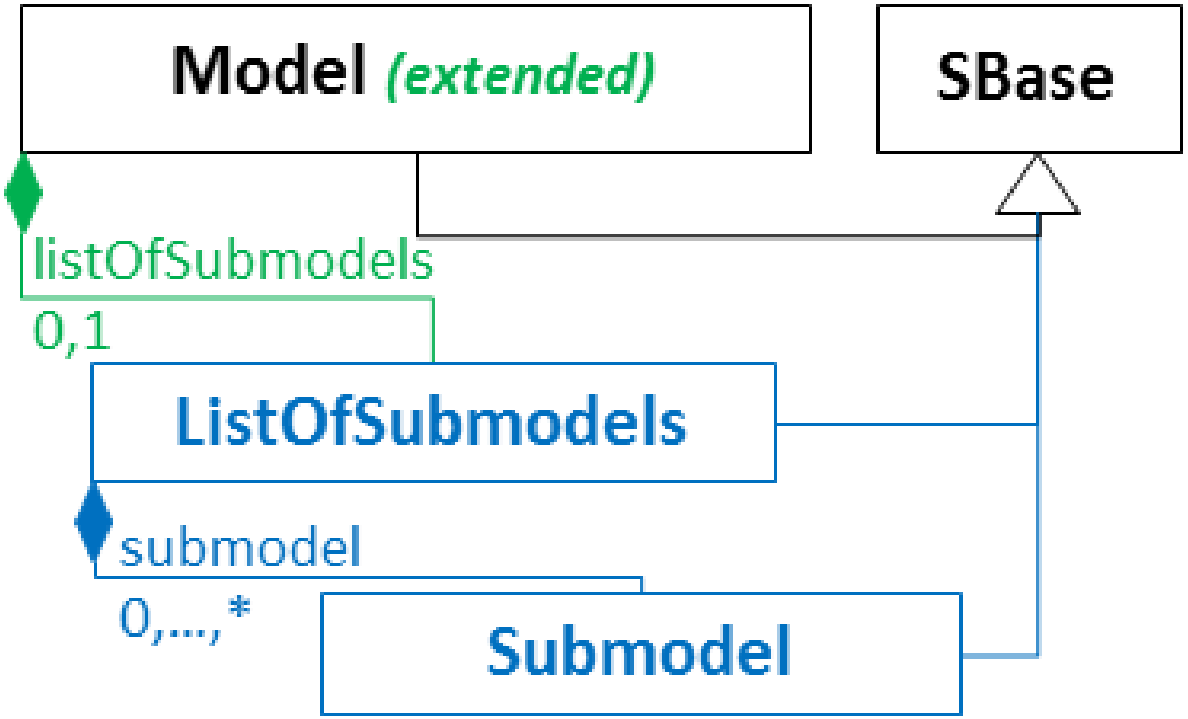


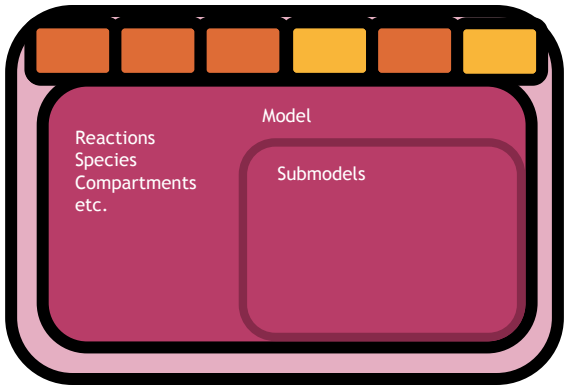
PART II: XML STRUCTURES




SBML (extended)
SBase
listOfExternalModelDefinitions
0,1
ListOfExternalModelDefinitions
externalModelDefinition
0,…,*
ExternalModelDefinition
id: SId
source: anyURI
model: SIdRef {use="optional"}
md5: string {use="optional"}
listOfModelDefinitions
0,1
ListOfModelDefinitions
modelDefinition
0,…,*
model
Model (extended)


Model
Reactions
Species
Compartments
etc.
Submodels


Model (extended)
SBase
listOfSubmodels
0,1
ListOfSubmodels
submodel
0,…,*
Submodel



Submodel

id: SId
modelRef: SIdRef
lengthConversionFactor: SIdRef {use="optional"}
areaConversionFactor: SIdRef {use="optional"}
volumeConversionFactor: SIdRef {use="optional"}
substanceConversionFactor: SIdRef {use="optional"}
timeConversionFactor: SIdRef {use="optional"}
extentConversionFactor: SIdRef {use="optional"}

SBase

listOfDeletions
0,1

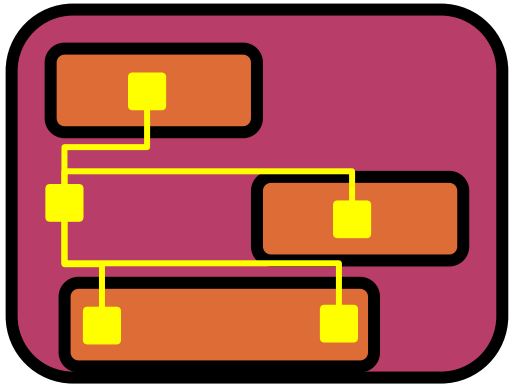
ListOfDeletions

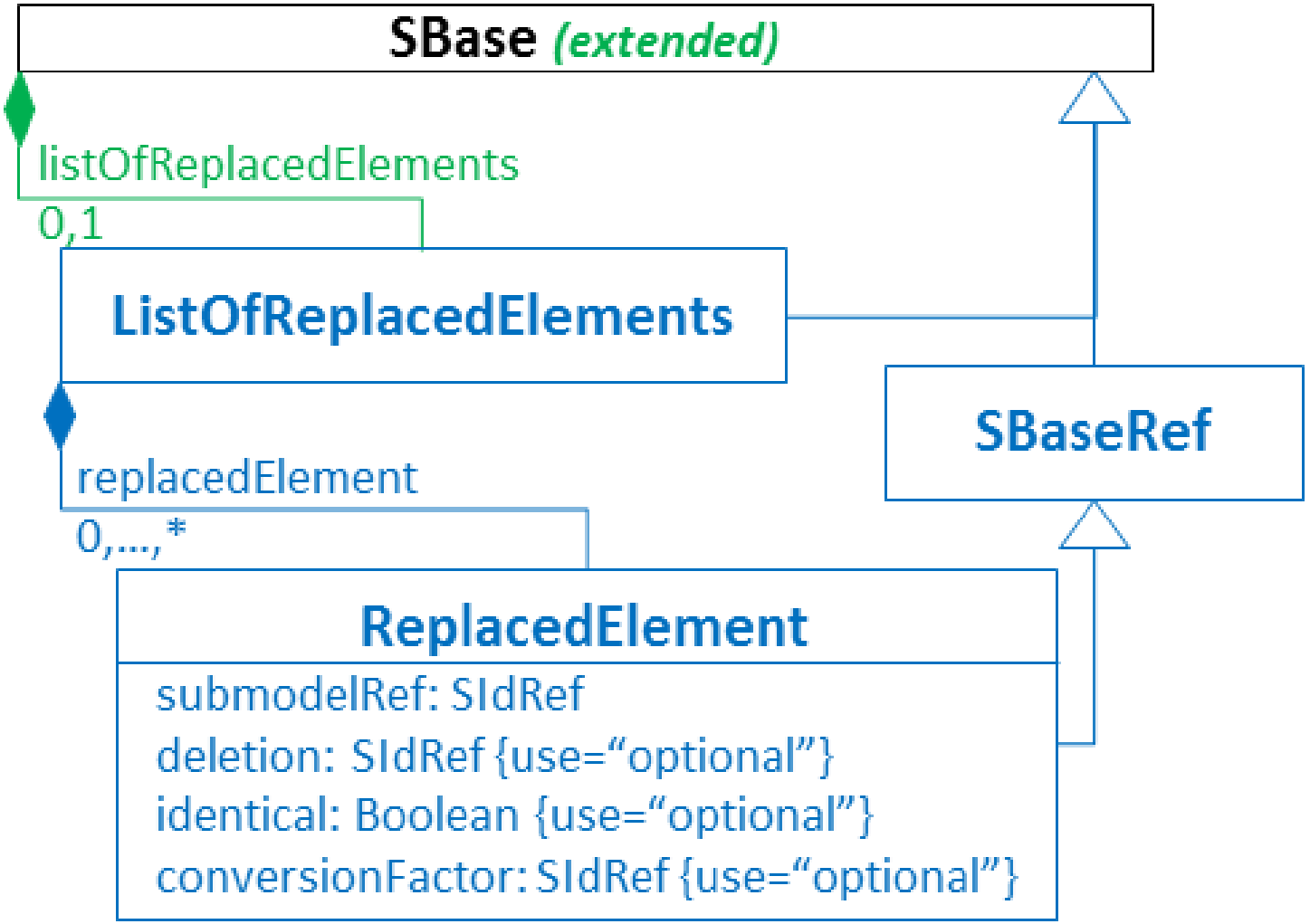
deletion
0,...,*

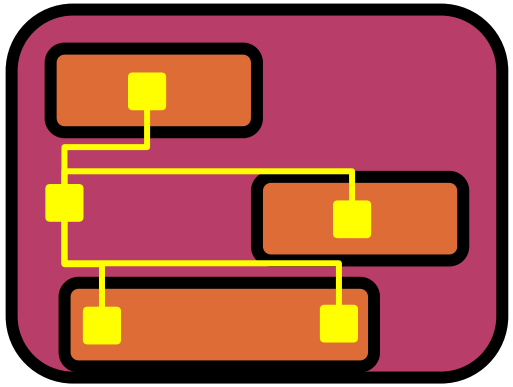
SBaseRef

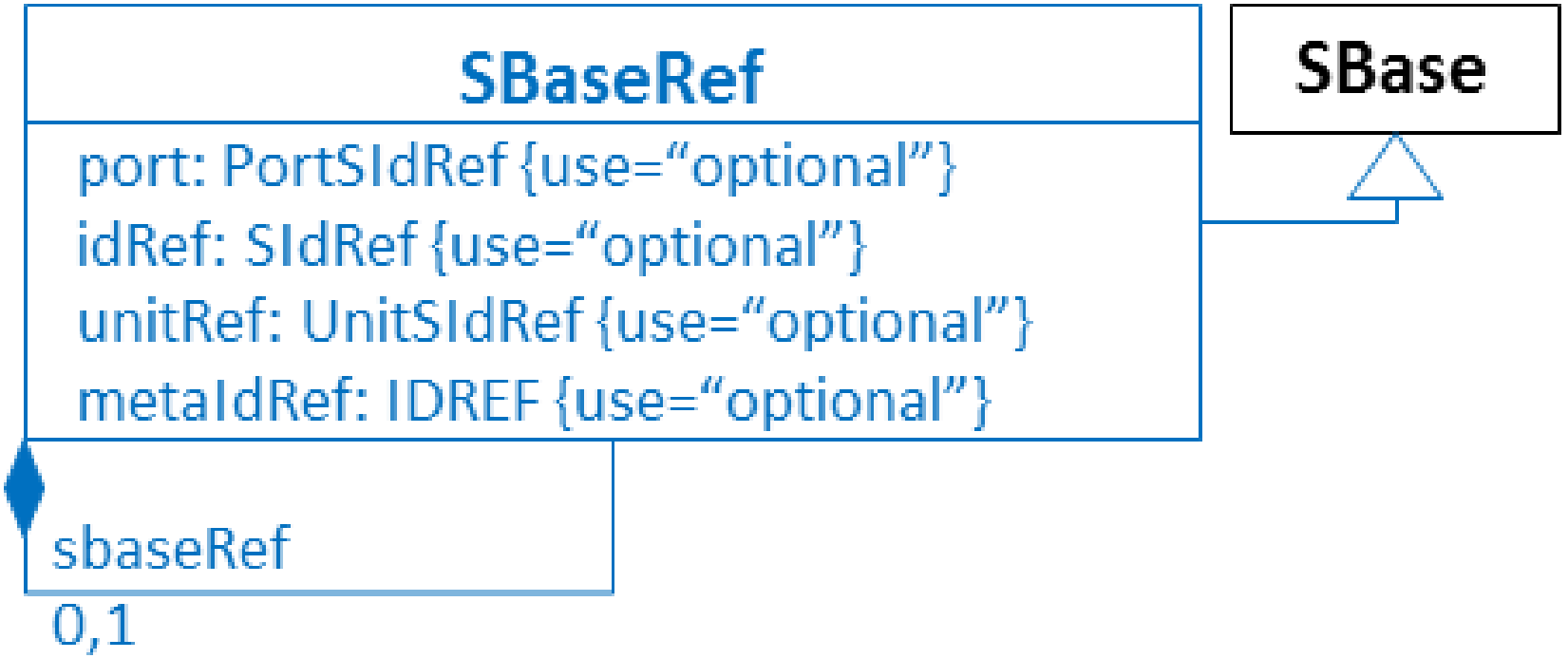
Deletion

id: SId {use="optional"}




SBase (extended)
listOfReplacedElements
0,1
ListOfReplacedElements
SBaseRef
replacedElement
0,…,*
ReplacedElement
submodelRef: SIdRef
deletion: SIdRef {use="optional"}
identical: Boolean {use="optional"}
conversionFactor: SIdRef {use="optional"}




SBaseRef
port: PortSIdRef {use="optional"}
idRef: SIdRef {use="optional"}
unitRef: UnitSIdRef {use="optional"}
metaIdRef: IDREF {use="optional"}
SBase
sbaseRef
0,1

Potential Issue: Conversion Factors

Component	Attribute value	Automatic conversion factor
AlgebraicRule	*(All)*	1
AssignmentRule	*(All)*	*Conversion factor for referenced object*
Compartment	`spatialDimensions="1"`	`lengthConversionFactor`
Compartment	`spatialDimensions="2"`	`areaConversionFactor`
Compartment	`spatialDimensions="3"`	`volumeConversionFactor`
Compartment	`spatialDimensions` not equal to "1", "2", or "3"	1
Constraint	*(All)*	*(None needed)*
Delay	*(All)*	`timeConversionFactor`
EventAssignment	*(All)*	*Conversion factor for referenced object*
FunctionDefinition	*(All)*	1
InitialAssignment	*(All)*	*Conversion factor for referenced object*
KineticLaw	*(All)*	$\frac{\texttt{extentConversionFactor}}{\texttt{timeConversionFactor}}$
Implied rate of change of a species	*(All)*	$\frac{\texttt{substanceConversionFactor}}{\texttt{timeConversionFactor}}$
Parameter	*(All)*	1
Priority	*(All)*	1
RateRule	*(All)*	$\frac{\textit{Conversion factor for referenced object}}{\texttt{timeConversionFactor}}$
Species	`hasOnlySubstanceUnits="true"`	`substanceConversionFactor`
Species	`hasOnlySubstanceUnits="false"`	$\frac{\texttt{substanceConversionFactor}}{\textit{Conversion factor for referenced object}}$
Species	`hasOnlySubstanceUnits="true"` replaced by a **Species** having `hasOnlySubstanceUnits="false"`	$\frac{\texttt{substanceConversionFactor}}{\textit{Compartment size}}$
Species	`hasOnlySubstanceUnits="false"` replaced by a **Species** having `hasOnlySubstanceUnits="true"`	$\frac{\texttt{substanceConversionFactor}\cdot\textit{(Compart. size)}}{\textit{Conversion factor for compartment}}$
SpeciesReference	*(All)*	1
Trigger	*(All)*	*(None needed)*
(Unknown)	*(All)*	1

Table 3: *Conversion factors used for the different components defined by SBML Level 3 Core.*

Potential Issue: Conversion Factors

- Perhaps remove conversion factors for submodels?
- Retain conversion factors for replacements
- Parameters unconverted anyway…

PART III: EXISTING IMPLEMENTATIONS

LIBSBML-COMP

- All classes implemented
- Get/set all attributes
- Add/remove all children
- Requires libSBML 5.1.0
- libsbml/5.1-packages-beta/comp-5.1.0-beta-1.zip

- In-progress: convenience functions
  - Flattening
  - Submodel instantiation

ANTIMONY

- Read/write hierarchical models!

- In-progress:
  - Replace rules more robustly
  - Introduce deletions
- Can only ‘replace’ elements with ids.

ACKNOWLEDGEMENTS

Contributor	Affiliation	City and Country
Stefan Hoops	Virginia Bioinformatics Institute	Blacksburg, Virginia, US
Nicolas Le Novère	EMBL-European Bioinformatics Institute	Hinxton, Cambridge, UK
Andrew Finney	(Independent)	Oxford, UK
Martin Ginkel	Max Planck Institute for Dynamics of Complex Technical Systems	Magdeburg, DE
Wolfram Leibermeister	Max Planck Institute for Molecular Genetics	Berlin, DE
Ranjit Randhawa	Dept. of Computer Science, Virginia Tech.	Blacksburg, VA, US
Jonathan Webb	BBN Technologies	Cambridge, MA, US

Table 1: *List of individuals who made significant contributions to the development of prior SBML proposals that influenced the present version of hierarchical model composition.*

- …and members of sbml-discuss and sbml-comp