Toymodel & Full FBA model

https://github.com/dagwa/wholecell-metabolism.git

Toymodel

https://github.com/dagwa/wholecell-metabolism/tree/master/mkoenig/python/metabolism/toymodel

toy_comp.xml

- toy_ode_model.xml
- toy_ode_update.xml
- toy_ode_bounds.xml

toy_fba.xml

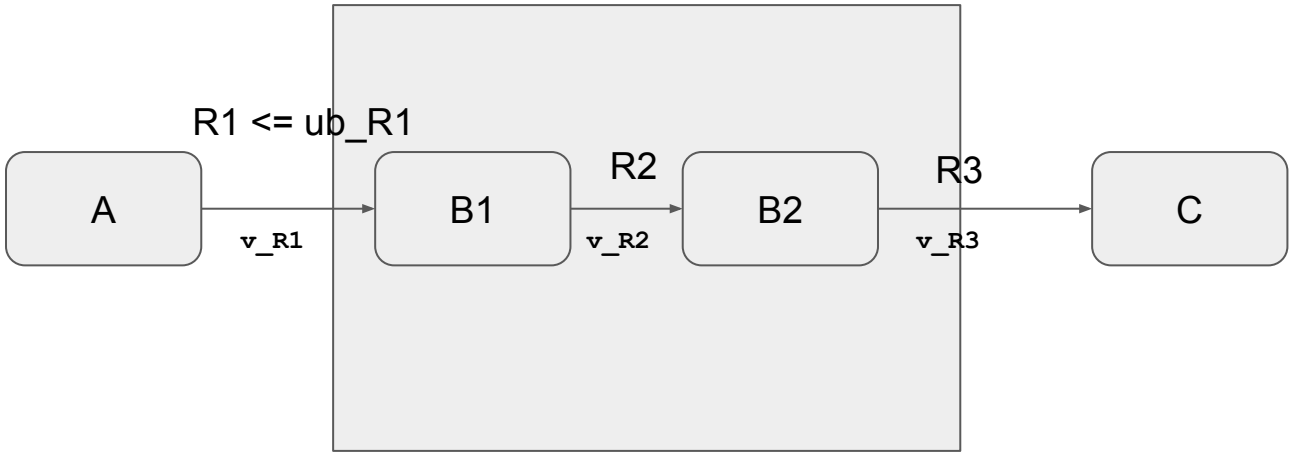
Full FBA model

https://github.com/dagwa/wholecell-metabolism/tree/master/mkoenig/results

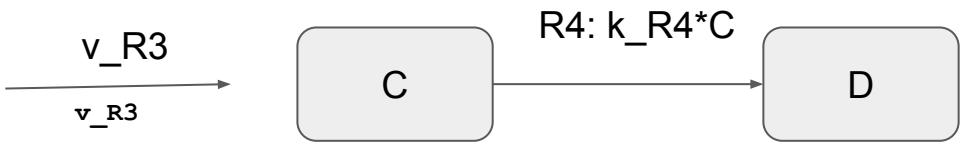
Metabolism_matrices_08_L3V1.xml

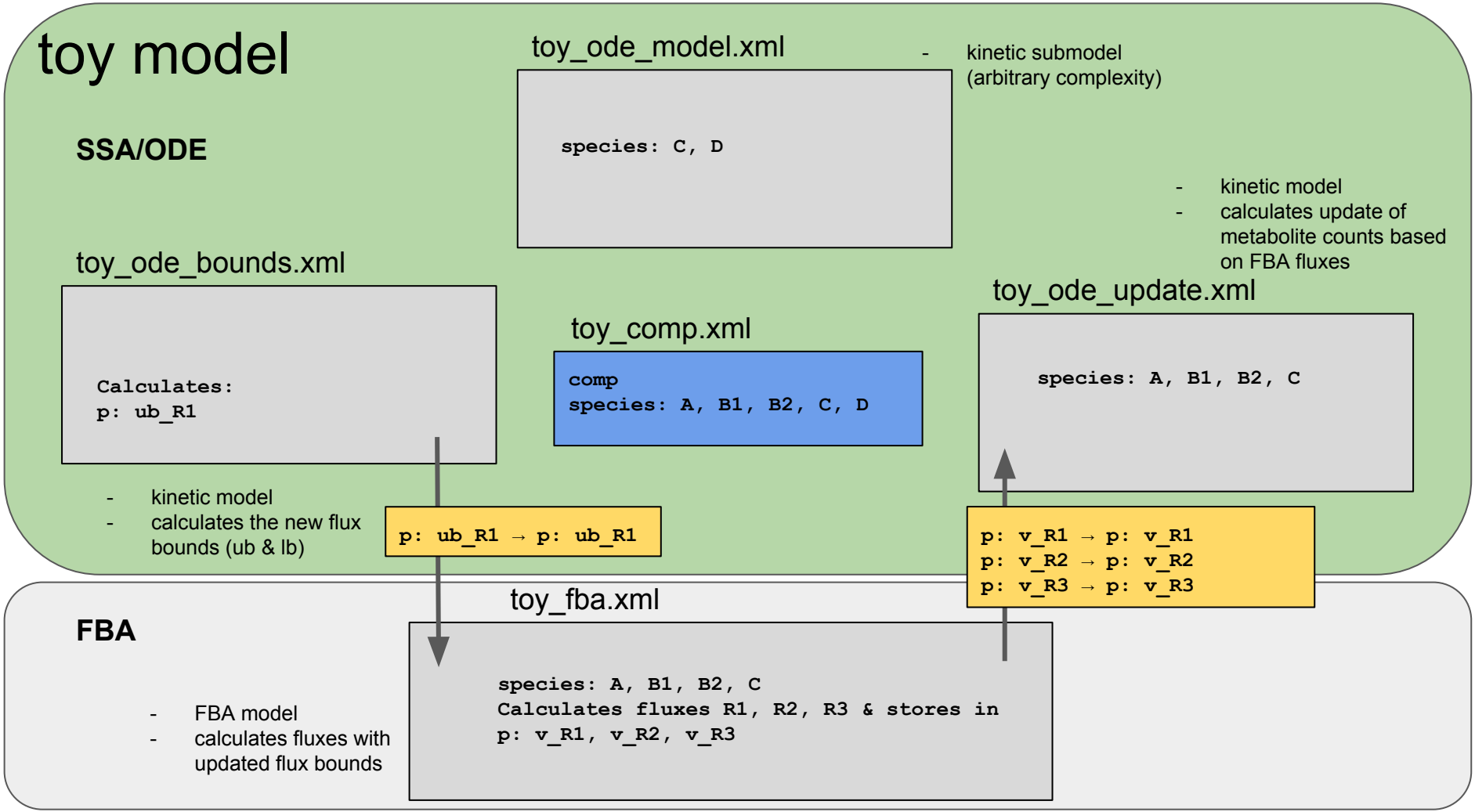
Metabolism_matrices_annotated_08_L3V1.xml

FBA Submodel

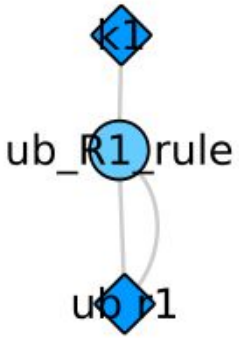


Kinetic Submodel

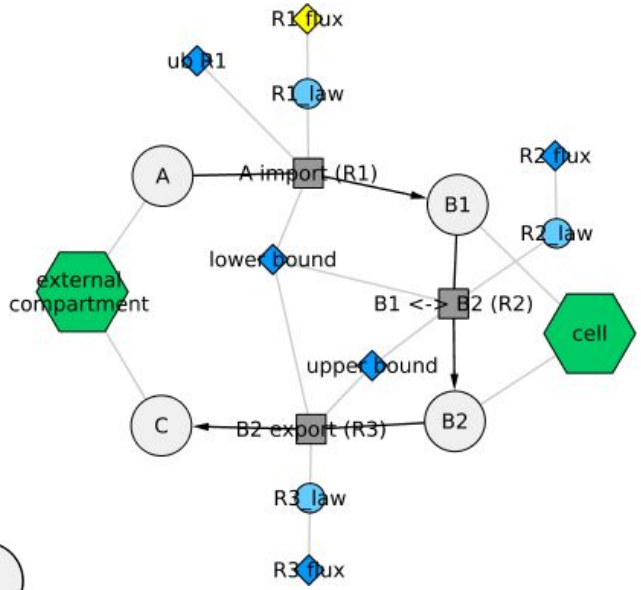



toy model
SSA/ODE
toy_ode_model.xml
species: C, D
- kinetic submodel (arbitrary complexity)
- kinetic model
- calculates update of metabolite counts based on FBA fluxes
toy_ode_update.xml
species: A, B1, B2, C
toy_ode_bounds.xml
Calculates:
p: ub_R1
toy_comp.xml
comp
species: A, B1, B2, C, D
- kinetic model
- calculates the new flux bounds (ub & lb)
p: ub_R1 → p: ub_R1
p: v_R1 → p: v_R1
p: v_R2 → p: v_R2
p: v_R3 → p: v_R3
FBA
toy_fba.xml
species: A, B1, B2, C
Calculates fluxes R1, R2, R3 & stores in
p: v_R1, v_R2, v_R3
- FBA model
- calculates fluxes with updated flux bounds

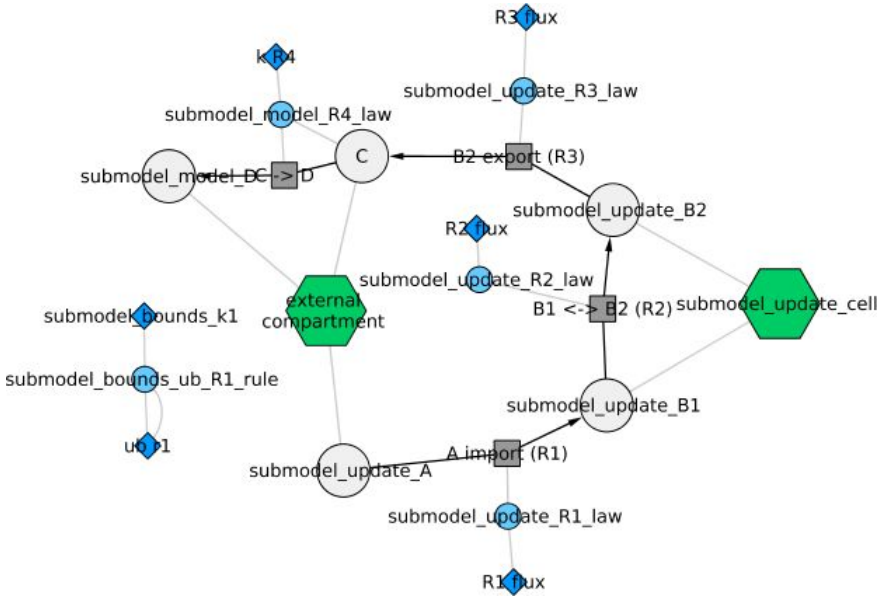
toy_bounds.xml



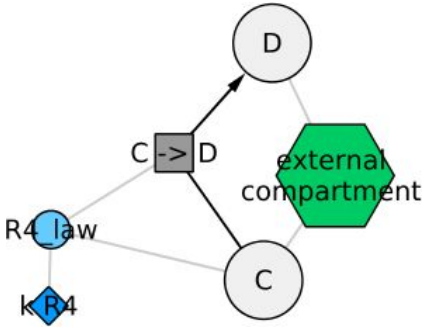
toy_fba.xml & toy_ode_update.xml

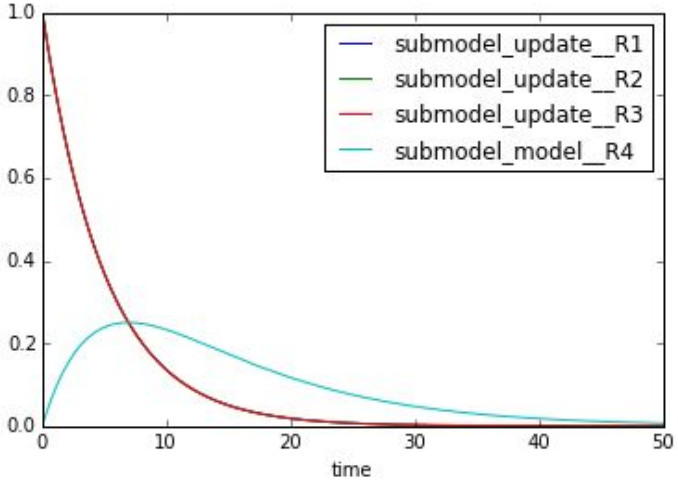


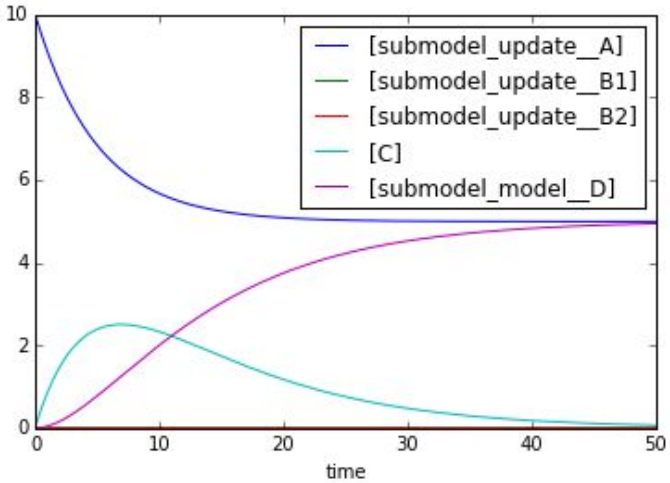
toy_comp.xml (flattened)



toy_model.xml







Version: 61004733ca7

Solution for
simulate(tend=50.0, step_size=0.01)

Initial Values

Parameters

ub_R1 = 1.0
ub = 1000
lb = 0

Species

A = 10.0
B1 = 0.0
B2 = 0.0
C = 0.0
D = 0.0

Compartments

ext = 1.0
cell = 1.0

FluxBounds

lb <= R1 <= r1
lb <= R2 <= ub
lb <= R3 <= ub

Objective

maximize : 1.0*R3