Slides, videos, links and more:
https://github.com/physicell-training/ws2021

Session 12: Intracellular Modeling

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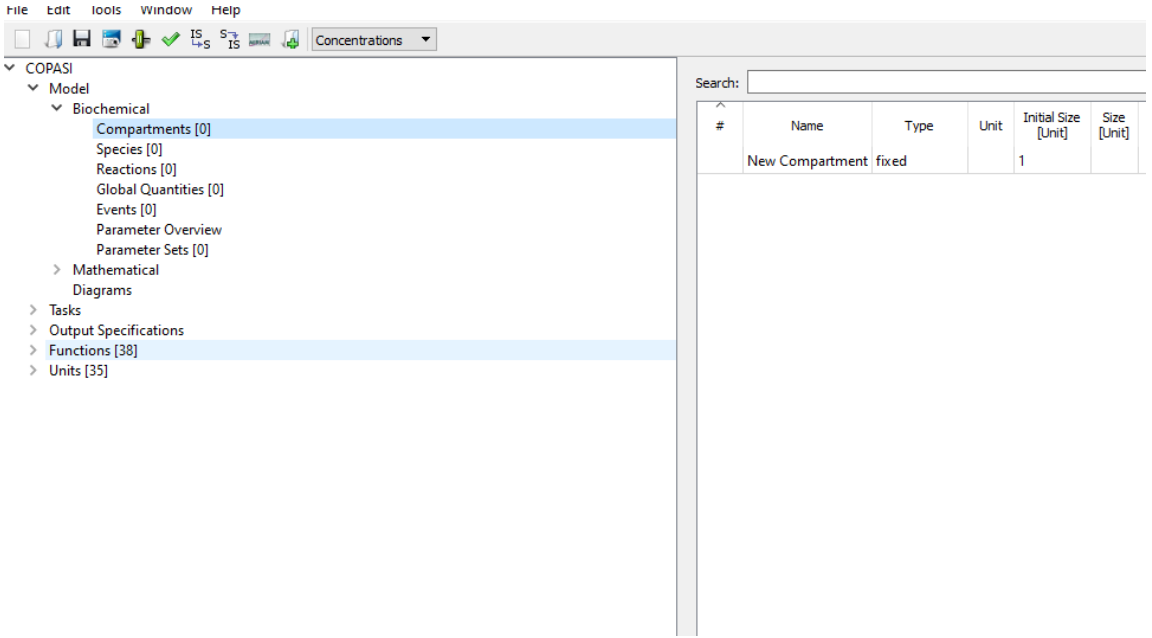
Agenda

- SBML Creation
- Populate ode-energy-sample
- Let’s remove some parts of the custom module.
- Let’s code together

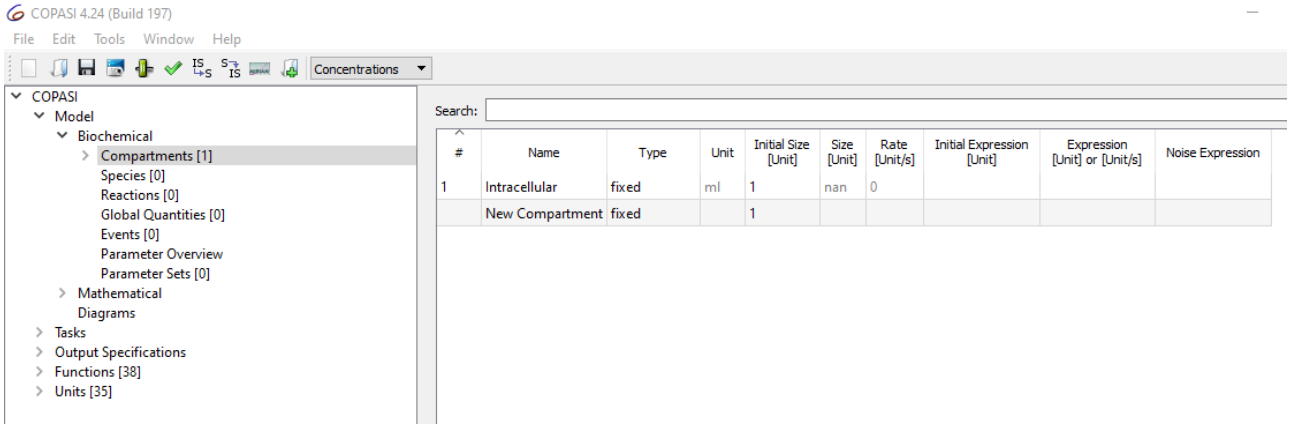
SBML Creation

- We need to create our SBML
- Let's start our Copasi



SBML Creation

- We will start with compartments
- Let's add "Intracellular" compartment
- Volume = 1.0



SBML Creation : Species

- There will be 8 Species

Search:

#	Name	Compartment	Type	Unit	Initial Concentration [Unit]	Concentration [Unit]	Rate [Unit/min]	Initial Expression [Unit]	Expression [Unit] or [Unit/min]	Noise Expression
1	Glucose	Intracellular	reactions	mmol/ml	100	nan	nan			
2	Oxygen	Intracellular	reactions	mmol/ml	100	nan	nan			
3	Energy	Intracellular	reactions	mmol/ml	450	nan	nan			
4	Lactate	Intracellular	reactions	mmol/ml	0	nan	nan			
5	apoptosis_rate	Intracellular	reactions	mmol/ml	0	nan	nan			
6	migration_speed	Intracellular	reactions	mmol/ml	0	nan	nan			
7	Lac_Secretion_Rate	Intracellular	reactions	mmol/ml	0	nan	nan			
8	Transition_Rate	Intracellular	reactions	mmol/ml	0	nan	nan			
	New Species	Intracellular	reactions	mmol/ml	1					

SBML Creation : Reactions

- There will be three Reactions

Search:

#	Name	Reaction	Rate Law	Flux [mmol/min]	Noise Expression
1	Aerobic	Glucose + 6 * Oxygen -> 38 * Energy	Mass action (irreversible)	nan	
2	Anaerobic	Glucose -> 2 * Energy + Lactate	Mass action (irreversible)	nan	
3	Energy_Usage	Energy ->	Mass action (irreversible)	nan	
	New Reaction				

SBML Creation : Global Quantities

- There will be 6 Global Quantities

Search:

#	Name	Type	Unit	Initial Value [Unit]	Transient Value [Unit]	Rate [Unit/min]	Initial Expression [Unit]	Expression [Unit] or [Unit/min]	Noise Expression
1	k_aer	fixed	?	0.01	nan	0			
2	k_ane	fixed	?	0.00018	nan	0			
3	k_usage	fixed	?	0.0023	nan	0			
4	energy_move_thresh	fixed	?	440	nan	0			
5	energy_death_thresh	fixed	?	430	nan	0			
6	energy_prolif_thresh	fixed	?	445	nan	0			
	New Quantity	fixed		0					

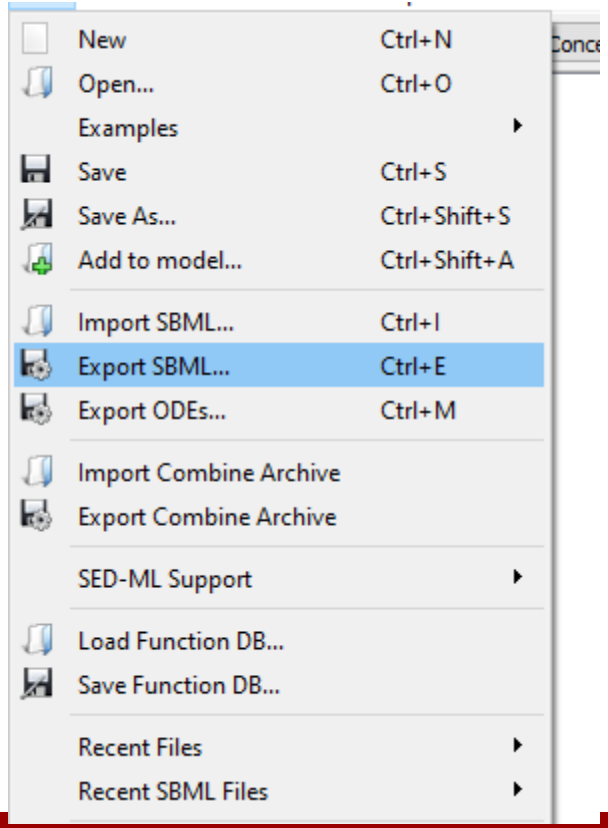
SBML Creation: Events

- 6 Events to create

Search:

#	Name	Trigger Expression	Delayed	Delay Expression	Assignment Target	Assignment Expression
1	die	[Energy] lt Values[energy_death_thresh]	Assignment	0	apoptosis_rate	8.9999999999999999e+99
2	do_not_move	[Energy] gt Values[energy_move_thresh]	Assignment	0	migration_speed	0
3	move	[Energy] lt Values[energy_move_thresh]	Assignment	0	migration_speed	10
4	Lac_Sec	[Lactate] gt 0.01	Assignment	0	Lac_Secretion_Rate	0.0001
5	divide	[Energy] gt Values[energy_prolif_thresh]	Assignment	0	Transition_Rate	0.00016666660000000001
6	do_not_divide	[Energy] lt Values[energy_prolif_thresh]	Assignment	0	Transition_Rate	0
	New Event					

SBML Creation : Save



Populate

- make clean
- make data-cleanup
- make reset
- make list-projects
- make ode-sample-project
- make

Let’s remove important part

- In the custom module
- Browse through the setup tissue() function
- Remove the inner code of the for loop
  - Starting with Line #166 to #183
- Remove the inner part of update_intracellular() function
  - Starting with Line #192 to #263
- That’s all

Coding together

- Let’s code together…

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