

# Simulation / Graph metadata in OpenCell

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# Principles

- OpenCell is closely tied to the format of the data it edits – everything that can be changed in OpenCell is represented in either CellML or metadata (including non-standard OpenCell specific metadata).
- The simulation settings UI in OpenCell therefore acts as a simulation metadata editor.
- The graph control in OpenCell acts as a graph metadata editor.



# Questions & Discussion

Questions and discussion about OpenCell's support for metadata?

# Converting from SBML to CellML

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# Why?

- SBML describes models of biochemical reaction networks.  
CellML describes mathematical models.
- CellML is more general.
- It is useful to go from the more specific format to the more general format so systems biology models can be integrated with other models.

# Complexities of translation

- Different level of abstraction – SBML primarily describes reactions, while CellML describes the system in terms of ODEs.
- Functions – SBML supports these, but CellML doesn't (yet).
- Types – CellML requires types everywhere. SBML doesn't.

# SBML2CellML Approach

- Convert all SBML rules and reactions into equations in CellML.
- Functions are expanded inline in the CellML output.
- Time is added into the model.
- Missing units are automatically inferred when possible.



# Units inference

- Say we have  $x \text{ [mol/L]} = (3 + 5) * y \text{ [mol/L/s]}$
- CellML needs to know the units on the constants 3 and 5.
- We can infer this by using a pattern like  $\langle \text{known1} \rangle = \langle \text{unknown} \rangle * \langle \text{known2} \rangle$  which tells us the units on  $\langle \text{unknown} \rangle$  are  $\langle \text{known1} \rangle / \langle \text{known2} \rangle$ . This gives us the units on  $(3 + 5)$
- Then we have a pattern for  $\langle \text{known} \rangle = \langle \text{unknown1} \rangle + \langle \text{unknown2} \rangle$ , i.e.  $\langle \text{unknown1} \rangle$  and  $\langle \text{unknown2} \rangle$  have the same units as  $\langle \text{known} \rangle$ .

# Units inference

- SBML2CellML has inference rules for the entire CellML subset of MathML.
- In many, but not all cases, SBML2CellML will automatically infer the unit.
- SBML models often miss out constants of factor 1 which serve no purpose other than to convert units, which units inference won't insert.
- Automatically 'fixing' units does create a risk that we mask units problems by fudging the units to make them fit.

# Next steps

- SBML2CellML is only a prototype and is very slow.
- We need to handle metadata so models can be converted to SBML to CellML and back without losing anything.
- SBML reactions will become CellML equations + CellML metadata describing the reaction.

# Questions / Discussion

- Questions / comments / discussion on SBML2CellML...
- Discussion about the problem of converting between model representation and metadata formats generally.