Simulation / Graph metadata in OpenCell

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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?

- 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 \(<\text{known1}> = <\text{unknown}> * <\text{known2}>\) which tells us the units on \(<\text{unknown}>\) are \(<\text{known1}>/ <\text{known2}>\). This gives us the units on \((3 + 5)\)
- Then we have a pattern for \(<\text{known}> = <\text{unknown1}> + <\text{unknown2}>\), i.e. \(<\text{unknown1}>\) and \(<\text{unknown2}>\) have the same units as \(<\text{known}>\).
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.