

Cell Models

Definition

- We already have GO terms and PEP.location attribute for specifying compartments in BioPAX.
- It would be nice if we could also define containment and neighborhood relations between compartments.

Uses

- **Extra validation at model level:**
 - All members of a non-transport conversion must be in a single compartment or a single compartment and its neighbors.
 - Transport conversions must be between adjacent compartments.
 - Complexes can only span adjacent compartments.
- **Visualization and Layout**
 - Allows visualizing compartments and transportation events
 - Greatly improves automated layout
 - Helps preserving mental maps even with modified / re-layed out graphs
- **Complexity Management**
 - You can fold/hide compartments for managing complexity

Requirements

- An optional external resource
- Handle different cell types. e.g. bacteria, lymphocytes, neurons.
- Map sub trees of the GO
- Represent topology and neighborhood relations.

Implementation proposal

- In BioPAX file something like
 - `<uses org.reactome.defaultCellModel/>` OR
 - `<uses org.ecocyc.EColiModel/>`

! What is the best way to this in owl/rdf?
- CellModel file would be another owl file specifying relations
- Only a single optional line in BioPAX file, entity entries are untouched.

Implementation Cntd.

- Compartment definition:
 - GOTerm
 - Name
 - Type (Membrane, Space, Wall, Subregion)
- Relations between compartments:
 - *Membrane k* surrounds *Space y*
 - *Space y* contains *Membrane l* and *m*
 - *Subregion a* is a part of *Space y*
 - *Membrane l* is neighbor of *Membrane m*

Example

