

BioPAX Work Group
March 31, 2004 Conference Call Minutes

Participants: Gary Bader, Michael Cary, Peter Karp, Terri Klein, Joanne Luciano, Natalia Maltsev, Suzanne Paley, Imran Shah, Jeremy Zucker

Overview:

1. Grants
 - a. Draft text sent to list
 - b. Draft budget coming soon
2. Roadmap
 - a. EcoCyc → BioPAX (in GKB) converter done
 - b. GKB → OWL still needs work
 - c. Other converters not started yet
3. Recent issues
 - a. Location – add location slot to (and rename) stoichiometry class
 - b. Transport – Suzanne will draft proposal
 - c. Coefficients – in stoichiometry class
 - d. Reversibility – removed from reaction
4. Next meeting
 - a. Tentative: June 3,4 at U. Chicago
5. External meetings
 - a. ISMB poster (deadline = 4/19/04)

Summary:

Grants

Gary and Mike revised Joanne's original version of the grant and sent it out to the pax list. Imran plans to read it and will send comments back to Gary and Mike. After Chris reviews the budget, Gary and Mike will send it out. Joanne commented that some of the funding in the DOE grant was to be used to support BPC activities.

Roadmap

The first draft of the EcoCyc → BioPAX converter is finished. The GKB → OWL converter is still in progress; Peter estimated that it would require another week at least. Jeremy offered to help but Peter felt that it wouldn't be worthwhile to bring in an external programmer at this stage.

Suzanne outlined her approach for the EcoCyc→BioPAX converter: she first created a BioPAX KB, then translated data from EcoCyc into this BioPAX KB. The last step will be to use the GKB→OWL converter (unfinished) to translate the BioPAX KB into OWL.

Natalia asked for assistance in mapping BioPAX to WIT; she agreed to send an XML version of the WIT format to the group for us to review. She also suggested that we look at the issue (mapping of BioPAX→ WIT) during the next face-to-face meeting.

Teri's group is still getting up to speed on BioPAX and will likely ask Peter for help when they need it (Note: Mark Woon will be doing most of work on the BioPAX → PharmGKB converter).

Recent Issues

Location: Gary made a few changes to the ontology based on recent discussions. The only change he made to location (currently a slot on physical entity) was to constrain the cardinality to one. This was due to discussion about general vs. specific location. General location refers to all of the possible locations that a physical entity is known to occur, while specific location refers to the single location of a particular instance. The location slot was meant to capture specific location, so its cardinality should be limited to one. We will not represent general location in Level 1.

Peter said that he still felt that we were jumping the gun by putting specific location in physical entity, and that the best solution for now was to modify the stoichiometry class to capture both coefficients and location in level 1. Gary asked if there were other slots that Peter thought should also use this new utility class. Peter said that it looked like it would make sense to use it for a few other slots (e.g. CONTROLLER in enzyme catalysis) as well.

Mike pointed out that complexes can currently take instances of the stoichiometry class as components, if we add a location slot to stoichiometry then complexes could contain location information. This would break the principle that location not be stored in physical entities.

Imran asked how our target databases for Level 1 encode specific location. EcoCyc stores location information as an annotation (similar to a utility class) on the participants of the reaction; WIT also stores location in reactions. Imran asked if storing location in reactions in Level 1 would preclude us from storing it in physical entities in later levels.

Gary said that if we added location to physical entity later, then it would be in two places (it would be necessary to preserve it in the conversion class in order to maintain backward compatibility). This will result in two ways of encoding the same data.

For this reason, Peter disfavors putting location in two places in later levels, he would rather us move the slot (if we deemed that necessary). But he pointed out that we were working on Level 1, not Level 2, and that we could not definitively say what we will want to do in Level 2 at present.

Imran suggested we go with the modified stoichiometry class solution for now, and make a comment that there were valid alternatives that were considered and could perhaps be adopted in later levels. Gary said he felt strongly (as did Mike) that location would need to be attached to physical entities (perhaps via states) in future levels in order to represent signal transduction pathways. He also said that we should avoid changing things in future levels because it leads to compatibility issues (he cited the SBML "specie" → "species" example).

Gary asked if there were any specific advantage for putting location in the conversion class rather than in physical entities. Suzanne said that one major reason was that if you created separate copies of an instance for each location then you had no way of knowing when two different physical entities were actually the same one. This point appeared to shift the balance in favor of storing location in the modified stoichiometry utility class.

Conclusion: We will move the LOCATION slot to the stoichiometry subclass, which will be renamed to reflect its expanded role (providing information about a physical entity that is specific for its participation in some interaction).

Transport: Jeremy asked how we were going to handle transports that modified the physical entities. Suzanne questioned the need for the transport class, given the modified stoichiometry class. Mike pointed out that some of the biochemical reaction slots would not make sense for transports that did not involve chemical changes. Imran said that it would not make any sense to have a transport class that would preclude us from capturing a significant number of transport reactions.

Gary suggested we come up with a proposal for how to handle transport (given the modified stoichiometry subclass) – do we need a separate transport and reaction class? Suzanne volunteered to draft this proposal and send it to the pax list for comment.

Coefficients: The solution Jeremy proposed (the stoichiometry utility class) has been implemented. It will be expanded and renamed to include location (see above).

Reversibility: We removed the reversibility slot from conversion because it was superfluous. This issue was discussed by Mike and Suzanne on the pax list.

Next Meeting

There was preference for holding the meeting on May 20 & 21, but the first week of June (3rd & 4th) seemed to have broader appeal. We will decide the exact date via the pax list; the location has been chosen: University of Chicago.

External Meetings

The ISMB-04 poster deadline is April 19th; we plan to present a poster during the main session. Joanne will get back to the list with details on the BPC SIG meeting.