

BIOPAX Work Group
6/18/03 Conference Call Minutes

Participants: Gary Bader, Michael Cary, Joanne Luciano, Suzanne Paley.

Purpose of call: Review ontology work, discuss preparation for ISMB.

Overview:

1. Ontology work
 - a. GKB questions
 - b. Next steps for ontology development
 - i. Documentation
 - ii. Inclusion of states
 - iii. Adding slots to all relevant classes
 - iv. Problem: Pathways as interactions?
2. ISMB preparation
 - a. Presentation module repository on PM site
3. Genome Technology article – no formal reply needed
4. PSI Paper – submitted for publication
5. Next conference call date: 1st or 2nd week of July

Summary:

The call began with Gary asking Suzanne a few technical questions about using GKB. She agreed to email him instructions on how to create “OR” and “ONE OF” constructs in slot definitions.

Gary mentioned that he planned to put up a CVS server, in order to make collaborating on the ontology development easier.

We waited a bit longer than usual for participants, but the only Gary, Joanne, Mike, and Suzanne called in. Since these four were also at the May 23 meeting, we decided to skip the first part of the agenda, in which we planned to review the progress we made with the ontology at that meeting.

Instead, we discussed what the next steps should be in the ontology development process. The day before the call, Gary had sent out some documentation on the class structure that was agreed upon at the May 23. He said that we next needed to incorporate states into the ontology. The solution to the states problem that the states subgroup came up with was to create a separate class (i.e. not in the sub-tree of *Entity*), called *State*, which contained a reference to an *Entity* and some additional descriptive information. Interactions would then be allowed to occur between both *States* and *Entities*. Combinations of multiple *States* (e.g. “phosphorylated on ser-15” AND “phosphorylated on thr-35”) could be created using the *Equivalence Class*. Gary and Mike will work together to document these ideas and add them to the ontology.

We next discussed the problem that Suzanne brought up at the end of the May 23 meeting regarding the distinction between interactions and pathways. Briefly, the problem is that many pathways are in a sense themselves interactions (as we have defined them). For example, one type of interaction we have is a *Conversion* (e.g., a biochemical reaction), in which some entity A is physically converted to come other entity B. Most metabolic pathways, however, are also conversions (e.g. glycolysis converts glucose to pyruvate), albeit multi-step conversions. The same holds true for other types of pathways – they can be thought of abstractly as simple interactions between the starting molecule(s) and the ending molecule(s). The problem is given even more weight when one considers the fact that many interactions in existing databases may have intermediates that are yet to be discovered. What do we do when new intermediates are found - “promote” the old interactions to pathways?

Suzanne suggested we could move the *Pathway* class under *Interactions*. While this would allow pathways to be interactions, the interaction subtypes would not propagate to the *Pathway* class, so we could only have generic “inputs” and “outputs” slots on pathways. Also, we could create these slots on *Pathway* without making it a subclass of *Interactions*.

Mike offered that we could eliminate the *Pathway* class, and just allow all *Interactions* to have “intermediates” (which would be a slot containing other interactions). When a new intermediate interaction was discovered, it could be added to this slot. Gary felt it would be dangerous to allow an *Interaction* to represent both a single interaction and a set of interactions.

Mike then asked Suzanne if, in a formal ontology, an instance could be an instance of multiple classes (just as a class can be a sub-class of multiple parent classes). For example, could an instance called “glycolysis” be of type *Interaction* AND of type *Pathway*, inheriting the slots of both classes? Suzanne said that this could be done in GKB, but wasn’t sure about OWL and ontologies in general. We agreed that this problem would need further consideration and moved on to the next issue.

Mike then mentioned a number of items that still needed to be dealt with in the ontology: in addition to finalizing the *State* recommendation, he said we need to figure out how to handle provenance, evidence, and timing. Gary said that most of that had been dealt with, conceptually at least, in our earlier documents. The problem at hand is merely translating what we decided into the ontology.

We then talked about the steps we were taking to prepare for ISMB. Mike, Gary, and Joanne had broken the presentation materials into 12 separate topic-specific modules (e.g. Introduction, Use Cases, Related Efforts, etc.), of 1-10 slides each. They were depositing these on the project management site and planned to assemble them into the two presentations and two posters when they were done.

They had shown one module, a brief ontology tutorial, to Peter for him to review; he said

he approved of it. At the time of the call, about half of the modules were complete. They planned to finish the remaining ones in the next day or so.

There was no news about Subgroups, except that Joanne said she was in the processing of gathering several use cases for the Examples subgroup. Mike said he didn't have a clear understanding of the difference between a "use case" and an "example". Joanne and Gary agreed that a use case was more general, and described some scenario where a software product (in this case, the BioPAX exchange format) would be of practical value to a user. Examples, on the other hand, are more specific and would typically involve actual data. It occurred to Mike that one might think of use cases as classes, while examples could be considered instances of those classes – but he didn't voice this thought because he thought it might confuse the issue.

Gary reviewed what had been discussed on the pax list about Nat's Genome Technology article. In that discussion, we said we agreed with the points Nat made – which is one of the reasons why we're building BioPAX in the first place (to give order to the pathways database space). We said our best response to Nat's slightly negative comments would be to make BioPAX available as soon as possible.

Gary said that PSI had submitted their paper for publication, and he offered to send copies of it to anyone who'd be interested in reading it (as long as they promised not to disseminate it further).

We agreed to hold our next call in July after ISMB. The subject of the call will likely be by Joanne's travels from now till then. We did not set a firm date, as Joanne's schedule was still unknown.

Action Items:

Suzanne – email Gary instructions on how to do "OR" and "ONE OF" constructs in GKB.

Gary and Mike – add *States* to ontology, along with documentation.

Gary, Mike, and Joanne – prepare presentation materials (2 talks, 2 posters) for ISMB.

Gary – send PSI paper to Mike, Suzanne, and Joanne (or to pax list).