

BioPAX Work Group
April 21, 2004 Conference Call Minutes

Participants: Gary Bader, Michael Cary, Peter Karp, Terri Klein, Joanne Luciano, Elizabeth Marland, Suzanne Paley, Jeremy Zucker

Overview:

1. Roadmap
 - a. GKB → OWL converter: works, but installer still has bugs
 - b. EcoCyc → BioPAX conversion: waiting for final version of ontology
2. Recent ontology updates
 - a. Control subclasses changed to: modulation, catalysis
 - b. Implemented transport proposal #4 (created dual subclass of transpt and rxn)
 - i. This class will cover transports with ANY covalent change (even just ATP→ADP)
3. Remaining Level 1 issues
 - a. Restrict CONTROLLED slot in modulation to catalyses? Yes
 - b. Set value of CONTROL-TYPE slot in catalysis to “activation”? Yes
 - c. Require use of physicalEntityParticipant class? Yes
 - d. Split stoichiometry to separate class? No
4. Release to-do items
 - a. Pre-release (v0.99) for community comment? No
 - b. Updating comments, will then add to spec. doc.
 - c. BioCyc→BioPAX conversion should be done in time
 - i. EcoCyc will be open access!
5. External Meetings
 - a. Various conversations with: Bernard Moret, Aneil Mallavarapu, Susie Stephens, Minoru Kanehisa
 - b. Gary attended PSI meeting
 - i. They are expanding to interactions with other molecule types, should be compatible with BioPAX level 2.
6. Grants
 - a. DOE – waiting for budget review by Chris
 - b. NSF – Sylvia Spengler expressed interest in BioPAX
7. Paper – wait for more database buy-in
8. Next meeting: June 3-4, U. Chicago

Summary:

Roadmap

The GKB→OWL converter is working, but the installer isn't (it would be too complicated to create it as a patch to version 8 of the pathway tools). John sent out the latest OWL version of the ontology during the call. Suzanne is holding off on finishing the BioCYC→BioPAX conversion until the ontology is final.

Ontology updates

Mike briefly went over the changes to the ontology that have been implemented since the last conference call: 1) Control subclasses changed to modulation and catalysis; 2) Implemented Suzanne's fourth transport proposal (created a subclass of both transport and biochemical reaction).

We discussed how we should classify various types of transports and decided that all transports that involve any covalent changes (including just the hydrolysis of ATP) should be instances of the new transportWithBiochemicalReaction class.

Jeremy asked if we planned to implement generic chemical structures (e.g. "an alcohol") in BioPAX. This subject has come up in the past but we have not done much work in this area as of yet, so generic structures will not likely be part of BioPAX in the near future (unless there is a mechanism in SMILES or CML to create generic structures). Suzanne said that there are a lot of pathways in EcoCyc that involve generic small molecules, but they do not capture structural information for these.

Jeremy also asked about the possibility of creating classes of compounds and then creating instances of those classes. Gary said that this could be handled via equivalence classes (similar to what PATIKA does), but we agreed this should be put off until a later level.

Remaining Level 1 Issues

We agreed to restrict the CONTROLLED slot in the modulation class to instances of the catalysis class. We also agreed to set the value of the CONTROL-TYPE slot in catalysis to "activation".

In the latest version, we limited the LEFT and RIGHT slots in conversions to the physicalEntityParticipant class (rather than also allowing straight physicalEntities). Allowing physicalEntities directly would create ambiguity with interaction locations (e.g. if a user did not use the participant class, does that mean they meant for the location to be the cytoplasm or does it mean they didn't know the location? Or did they mean to create a generic interaction that can occur anywhere?). Since there are GO terms for e.g. "unspecified" and "cell", we decided that it would be OK to require location (i.e. use of the physicalEntityParticipant). We will explain how to represent various ambiguous locations (e.g. somewhere in the cell, or totally unknown) in the documentation.

Jeremy mentioned splitting STOICHIOMETRY from the participant class in an email. This could have a number of advantages, including a) fewer instances of the participants class would be required, and b) it would be more compatible with SBML. We decided to keep the participants class as-is for Level 1.

Jeremy asked how stoichiometry would be represented for polymerization reactions. Suzanne said this was more of a physical entities question (e.g. glycogen + UDP-glucose → glycogen + UDP), i.e. the process would be represented by an unbalanced reaction. Gary said this should be added to the documentation.

Release to-do items

We decided to not release a 0.99 version. Mike has been updating all of the comments in the ontology; these will be sent to the pax list for review in the near future, then added to the specification document.

Suzanne said she should be able to have the BioCyc→BioPAX conversion done in time for the release. Peter announced that EcoCyc is now an open database, and that the BioPAX version of EcoCyc would be freely available. This should be part of our Level 1 release announcement.

External Meetings

Liz attended the RECOMB conference and talked to people who might be interested in BioPAX. She spoke with Bernard Moret, from the CIPRes project (<http://www.phylo.org/>), and pointed him toward our website. She plans to contact him to follow up.

Jeremy spoke with Aneil Mallavarapu at Harvard. He is working on a biomodeling language called B. Jeremy showed him the GKB version of BioPAX and it looks like it would be straightforward to import BioPAX instances into B (where they would be classes). Jeremy said Aneil might use BioPAX in the future.

Joanne met with Susie Stephens of Oracle's Life Science department. They have a contingent in Japan that works with KEGG; Joanne said there may be a connection there where we can get KEGG more involved in BioPAX.

Peter spoke with Minoru Kanehisa recently; he disavowed any knowledge of a project called BioPACS. BioPACS is a conversion utility that converts pathways in KEGG and BioCyc into a format readable by Genomic Object Net (GON), "a software tool for representing and simulating interactions and processes in biopathways." The project appears to be inactive.

Gary attended the PSI meeting in Nice, France. The PSI-MI format was expanded to Level 2 during the meeting. Level 2 expands the format to include molecular interactions involving small molecules, DNA, and RNA. Their interaction ontology looks like it will be easily compatible with BioPAX.

The ISMB poster abstracts have been submitted.

Grants

The remaining to-do item for the DOE grant is review of the budget by Chris, then sending it out for review by the core group. Chris has been out-of-office for the past two weeks but Mike and Gary will try to get him to do this in the near future. The text of the grant is complete; comments from Peter and Imran have been incorporated. The target date set by Chris and Joanne for submitting the DOE grant was April 19th.

Joanne mentioned that Sylvia Spengler expressed interest in providing us with some funding. She will coordinate with Chris to contact Sylvia and find out more about this.

Paper

Gary mentioned that the PSI group will begin working on a paper soon and we briefly discussed submitting a paper on Level 1; we agreed that it would be preferable to have two or three databases support BioPAX before submitting a paper.

June Meeting

We agreed to conduct the next meeting on June 3-4 in Chicago.