BioPAX Overview - Harmony

Wednesday 20th April, 2011

Overview Sessions this morning

- Specification/Data
- Working Groups Overview - Work in Progress
- Software Tools
- Interoperability
- Controlled Vocabulary Requirements
- Additional Projects?

Specification/Data Introductory Session

- Data Normalization/Integration, Chairs: Emek and Arman
    - Goal: form groups of data providers to test data normalization and integration tools - ‘Can our data be integrated with their data?”
- Data Exchange - Level3, Chairs Peter and Gary
    - Goal: highlight known issues, collect additional issues from participants, organize people into workgroups to address those issues. Outcome: proposal for specification change or best practice to resolve issues. Prepare proposals to present to community and for subsequent discussion and decision by surveymonkey vote.
- Data Exchange Future Development, Chairs: Gary and Emek
    - Goal: try to get a complete list of requirements and issues, draft proposals to present to community. Target next combine for decision making and making things more concrete.

Harmony Data Integration Challenge, testing data exchange and integration in BioPAX Level 3

This session will provide an opportunity to test data exchange and integration of pathway data in BioPAX L3. If you have data in Level3 and you would like to spend some time testing exchange and integration of your data with other data providers please join us in this session. Topics of interest will include and not limited to:

- BioPAX Validation
- ID Normalisation
- Patch

Some background information on Paxtools and Patch can be found at http://bit.ly/paxtools_doc and at http://bit.ly/patch_overview

Data Exchange - Level3

- Inference rules, e.g., around dataSource (Provenance)
- pathwayOrder and particularly nextStep
- Multi-organism pathways
- Synchronize documentation between OWL file and other documentation
-

Data Exchange Future Development

- Level 4 Todo
    -

Working Groups Overview - Work in Progress

- Current Working Groups
    - Visualization and exchange Status: Started Point of Contact - Martijn Van Iersel
    - Semantics: Generics/polymers/logic/ Status: Initiated Point of Contact - Emek Demir
    - Semantic web/linking/CVs Status: Started - Point of Contact Andrea Splendiani
    - Validation and best practices Status: Initiated - Point of Contact Igor Rodchenkov
    - Quantitative modeling vs. static relationship /SBML/CellML/VirtualCell Status: Started - Point of Contact Oliver Ruebenacker

WIP - Visualization and exchange

- Martijn Proposal

WIP - Semantics: Generics/polymers/logic/

- Participants
  - Andrea Splendiani, Igor Rodchenkov, Nadia Anwar, Michel Dumontier, Camille Laibe, Nick Juty, Andrew Gibson, Alan Ruttenberg, Marco Antoniotti, Sujatha Mohan, Sorin Draghici, Michele Donato + others
- Conference Calls
- 3 Current proposals in progress
- Andrea slides

WIP - Semantic web/linking/CVs

- Andrea Slides

WIP - Validation and best practices

- rules and best practices overview
- writing rules, rule exchange: discuss other (than wiki or java) ways to define rules, e.g., regexp, SWRL, other rule languages
- equivalence: semantic equivalence vs. syntactic equivalence vs. java object equals vs. URI equals
- how to tell non-generic from generic (when neither element have unification xrefs, nor - any members; shall we have a new isGeneric property)
- whether to support "super rules" that look far beyond the BioPAX data in hands (for an external resource/warehouse); CV rules currently do.

WIP - Quantitative modeling vs. static relationship

1. Provide Tools to use pathway data to:
    - Create models
    - Annotate models
2. Provide tools to use model data to:
    - Extract pathways
    - Reference models and model elements
3. Extend BioPAX to support:
    - Concentrations and reaction rates
    - Rule-based pathways (like RB models)
    - Systems and views of systems

Coffee

Software Tools

- PaxTools - Emek
    - architecture
    - Goal:
- ChiBE - Ozgun
    - Goal: Reference BioPAX-SBGN PD implementation
- PathwayCommons - Ben
    - Goal: Pathway Commons website - transition to cpath2 web service

Software Tools - Paxtools

- Emek TODO

Software Tools - Chibe

- Ozgun TODO

Software Tools - PathwayCommons

- Ben TODO

Software Tools - Validator

- web and console application
- how to implement and test a rule (design, 'rule' beans and 'error' properties: code, category, behavior/level, messages)
- implement junit tests that also generate example BioPAX files for each rule
- how to integrate the validator into another project
- auto-fix and normalization (Normalizer)

WIP - Core Group

- Specification Modularization Proposal
    - introduce the idea of ontology modules within the BioPAX such as
    - x,y,z co-ordinates for visualization use cases,
    - high-level relations for semantic integration,
    - rules for validation,
    - initial conditions/parameters that can be used in modelling
- Community Organization - Proposal
    - BioPAX core group
    - Editorial Committee
    - Workgroups
    - Scientific Advisory Board

Interoperability

SBML/SBGN/BioPAX conversion
SBGN - BioPAX mapping

- Partial BioPAX to PD mapping
- Need to work on BioPAX to ER mapping

Goal: What topics to be discussed/ are people interested in?
What are the topics?

Controlled Vocabulary Requirements

Summary:

- Semantics of CV vs Xrefs in BioPAX (also, - can CV simply be a sub-class of RelationshipXref?)
- current CV recommendations/best practices
- overlap of CVs (different terms share synonyms (e.g., phosphorylation))
- use of CV's
- orphan CVs
- Controlled Vocabularies that are used by database groups and are not covered by BioPAX
- CV Integration Requirements
  - RelationshipTypeVocabulary
  - Small Molecule Vocabulary
- CV Integration Architecture options
  - MIREOT
  - CV Partitions/Fragments OntoPath

- **Goal: Create a CV working group**

Additional Projects?