

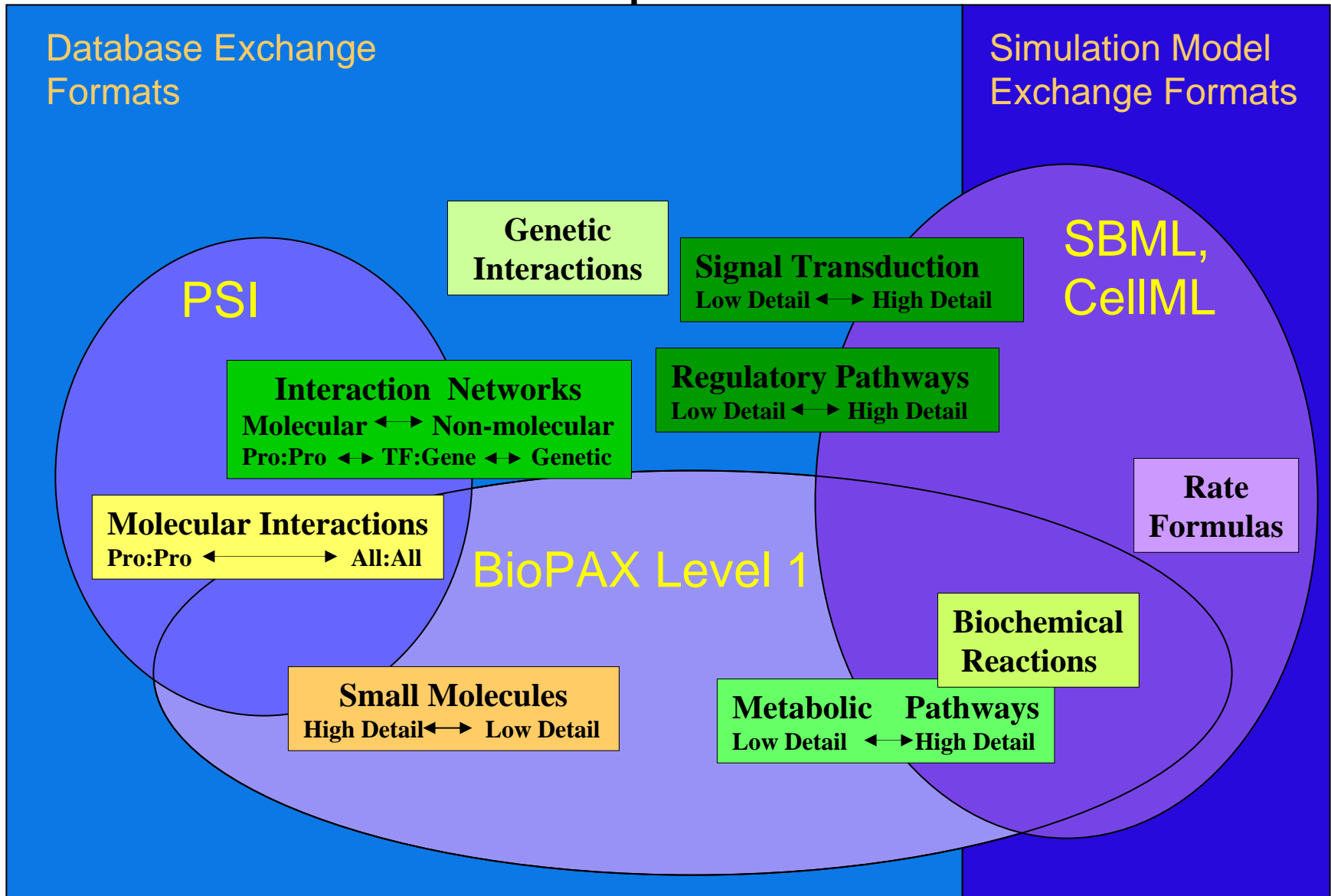
Model Integration in SBML Using the BioPAX Ontology

Jeremy Zucker and the rest of the
BioPAX Workgroup

BioPAX Goals

- BioPAX = Biological Pathway Exchange
- Ontology for representing pathway knowledge:
 - Metabolic pathways
 - Signaling pathways
 - Protein-protein interactions
 - Genetic regulatory pathways
- Abstract data model for integrating databases such as BioCyc, BIND, WIT, aMAZE, KEGG, etc. over 120 pathway databases
- Interoperate with existing standards (RDF/OWL, LSID, **SBML**, PSI, CellML Metadata Standard)

Scope of BioPAX Level 1 in the Pathway Data Space



How can BioPAX help SBML?

Addresses nasty data integration issues

- Different data types, same representation
- Same data, different representations
- External references...
- Synonyms...
- Provenance...

Different data types, same representation

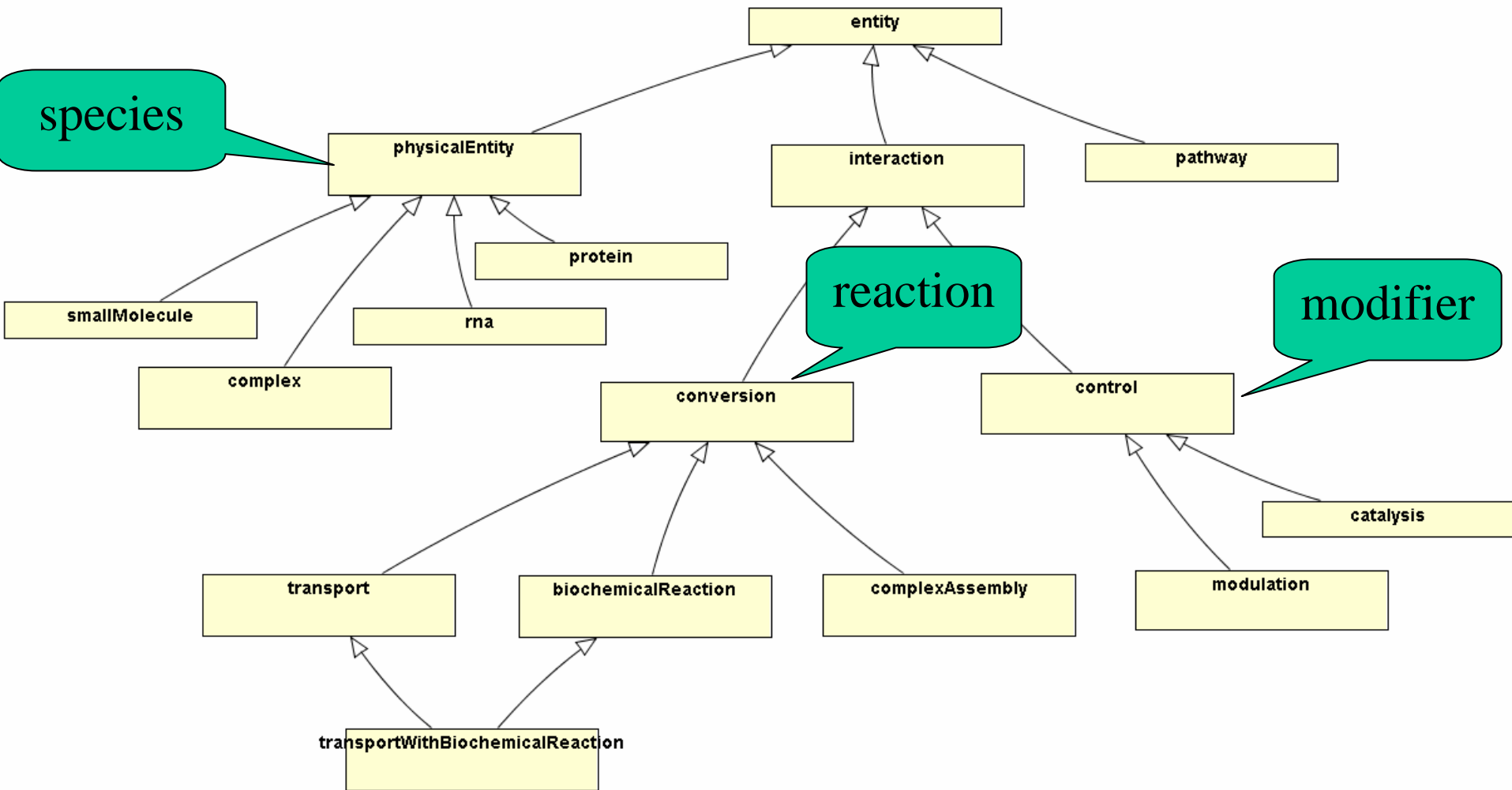
Protein-Protein Interaction

```
<reaction
  id="pyruvate_dehydrogenase_cplx
  "/>
<listOfReactants>
  <speciesRef species="PdhA" />
  <speciesRef species="PdhB" />
</listOfReactants>
<listOfProducts>
  <speciesRef
    species="Pyruvate_dehydrogenase
    _E1" />
</listOfProducts>
</reaction>
```

Biochemical Reaction

```
<reaction
  id="pyruvate_dehydrogenase_rxn" />
<listOfReactants>
  <speciesRef species="NADP+" />
  <speciesRef species="CoA" />
  <speciesRef species="pyruvate" />
</listOfReactants>
<listOfProducts>
  <speciesRef species="NADPH" />
  <speciesRef species="acetyl-CoA" />
  <speciesRef species="CO2" />
</listOfProducts>
<listOfModifiers>
  <modifierSpeciesRef
    species="pyruvate_dehydrogenase_E1"
  />
</listOfModifiers>
</reaction>
```

BioPAX Ontology: Overview



Level 1 v1.0 (July 7th, 2004)

BioPAX solution: metadata

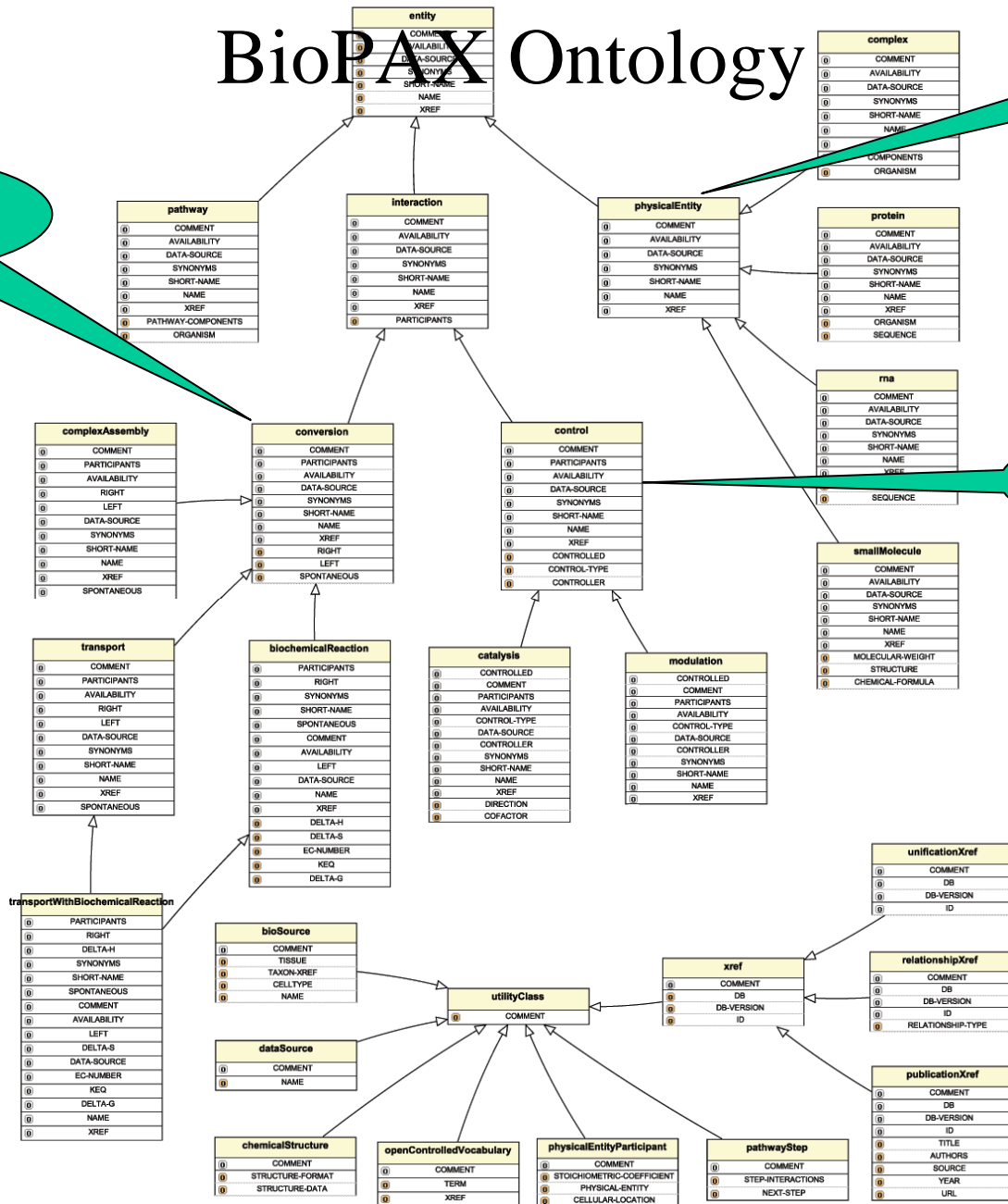
```
<sbml xmlns:bp="http://www.biopax.org/release1/biopax-release1.owl"
      xmlns:owl="http://www.w3.org/2002/07/owl#"
      xmlns:rdf="http://www.w3.org/1999/02/22-rdf-syntax-ns#">
<listOfSpecies>
  <species id="PdhA" metaid="PdhA">
    <annotation>
      <bp:protein rdf:ID="#PdhA"/>
    </annotation>
  </species>
  <species id="NADP+" metaid="NADP+">
    <annotation>
      <bp:smallMolecule rdf:ID="#NADP+"/>
    </annotation>
  </listOfSpecies>
<listOfReactions>
  <reaction id="pyruvate_dehydrogenase_cplx">
    <annotation>
      <bp:complexAssembly rdf:ID="#pyruvate_dehydrogenase_cplx"/>
    </annotation>
  </reaction>
  <reaction id="pyruvate_dehydrogenase_rxn" metaid="pyruvate_dehydrogenase_rxn">
    <annotation>
      <bp:biochemicalReaction rdf:ID="#pyruvate_dehydrogenase_rxn" />
    </annotation>
  </reaction>
</listOfReactions>
</sbml>
```

BioPAX Ontology

reaction








species

Modifier



BioPAX Ontology: Root

- Root class: Entity
 - Any concept referred to as a discrete biological unit when describing pathways. This is the root class for all biological concepts in the ontology, which include pathways, interactions and physical entities

entity	
	SYNONYMS
	COMMENT
	DATA-SOURCE
	SHORT-NAME
	AVAILABILITY
	NAME
	XREF

BioPAX: External References

```
<species id="pyruvate" metaid="pyruvate">
<annotation
  xmlns:bp="http://biopax.org/release1/biopax-release1.owl">
  <bp:smallMolecule rdf:ID="#pyruvate">
    <bp:Xref>
      <bp:unificationXref rdf:ID="#unificationXref119">
        <bp:DB>LIGAND</bp:DB>
        <bp:ID>c00022</bp:ID>
      </bp:unificationXref>
    </bp:Xref>
  </bp:smallMolecule>
</annotation>
</species>
```

BioPAX: Synonyms

```
<species id="pyruvate" metaid="pyruvate">
<annotation
  xmlns:bp="http://biopax.org/release1/biopax_release1.owl"/>
<bp:smallMolecule rdf:ID="#pyruvate" >
  <bp:SYNONYMS>pyroracemic acid</bp:SYNONYMS>
  <bp:SYNONYMS>2-oxo-propionic acid</bp:SYNONYMS>
  <bp:SYNONYMS>alpha-ketopropionic acid</bp:SYNONYMS>
  <bp:SYNONYMS>2-oxopropanoate</bp:SYNONYMS>
  <bp:SYNONYMS>2-oxopropanoic acid</bp:SYNONYMS>
  <bp:SYNONYMS>BTS</bp:SYNONYMS>
  <bp:SYNONYMS>pyruvic acid</bp:SYNONYMS>
</bp:smallMolecule>
</annotation>
</species>
```

Complementary approaches

- Semantic validation
- Semantic consistency checks
- Modularization of SBML
- Level 3 features
- Controlled vocabularies
- Other ontologies

Coming soon...

- Biocyc, KEGG, WIT, aMAZE => BioPAX
- libBioPAX (apologies to Ben)
- BioPAX 2 SBML
- BioPAX 2 BioWarehouse
- BioPAX hackathons, Forums, conference calls

To join: biopax-discuss@biopax.org

BioPAX Ontology

conversion	
0	COMMENT
0	PARTICIPANTS
0	AVAILABILITY
0	DATA-SOURCE
0	SYNONYMS
0	SHORT-NAME
0	NAME
0	XREF
0	RIGHT
0	LEFT
0	SPONTANEOUS

control	
0	COMMENT
0	PARTICIPANTS
0	AVAILABILITY
0	DATA-SOURCE
0	SYNONYMS
0	SHORT-NAME
0	NAME
0	XREF
0	CONTROLLED
0	CONTROL-TYPE
0	CONTROLLER

biochemicalReaction	
0	PARTICIPANTS
0	RIGHT
0	SYNONYMS
0	SHORT-NAME
0	SPONTANEOUS
0	COMMENT
0	AVAILABILITY
0	LEFT
0	DATA-SOURCE
0	NAME
0	XREF
0	DELTA-H
0	DELTA-S
0	EC-NUMBER
0	KEQ
0	DELTA-G

catalysis	
0	CONTROLLED
0	COMMENT
0	PARTICIPANTS
0	AVAILABILITY
0	CONTROL-TYPE
0	DATA-SOURCE
0	CONTROLLER
0	SYNONYMS
0	SHORT-NAME
0	NAME
0	XREF
0	DIRECTION
0	COFACTOR

modulation	
0	CONTROLLED
0	COMMENT
0	PARTICIPANTS
0	AVAILABILITY
0	CONTROL-TYPE
0	DATA-SOURCE
0	CONTROLLER
0	SYNONYMS
0	SHORT-NAME
0	NAME
0	XREF



Same data, Same model

- Different SBML representation
- Modules UML-based

Same model, different data

Same data, different model

- BioPAX solution:
- `<reaction id=“`

Different data, different model

- BioPAX solution