

SBML Level 3 proposal for “Groups”

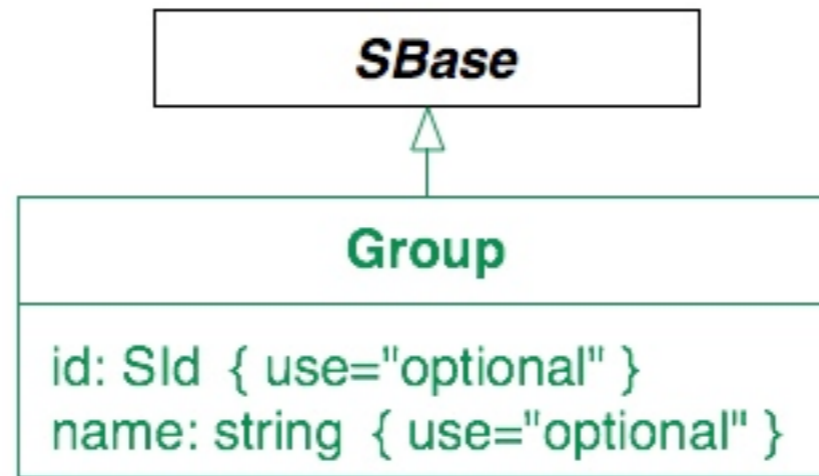
Mike Hucka

*California Institute of Technology
Pasadena, California, USA*

Goals of this proposal

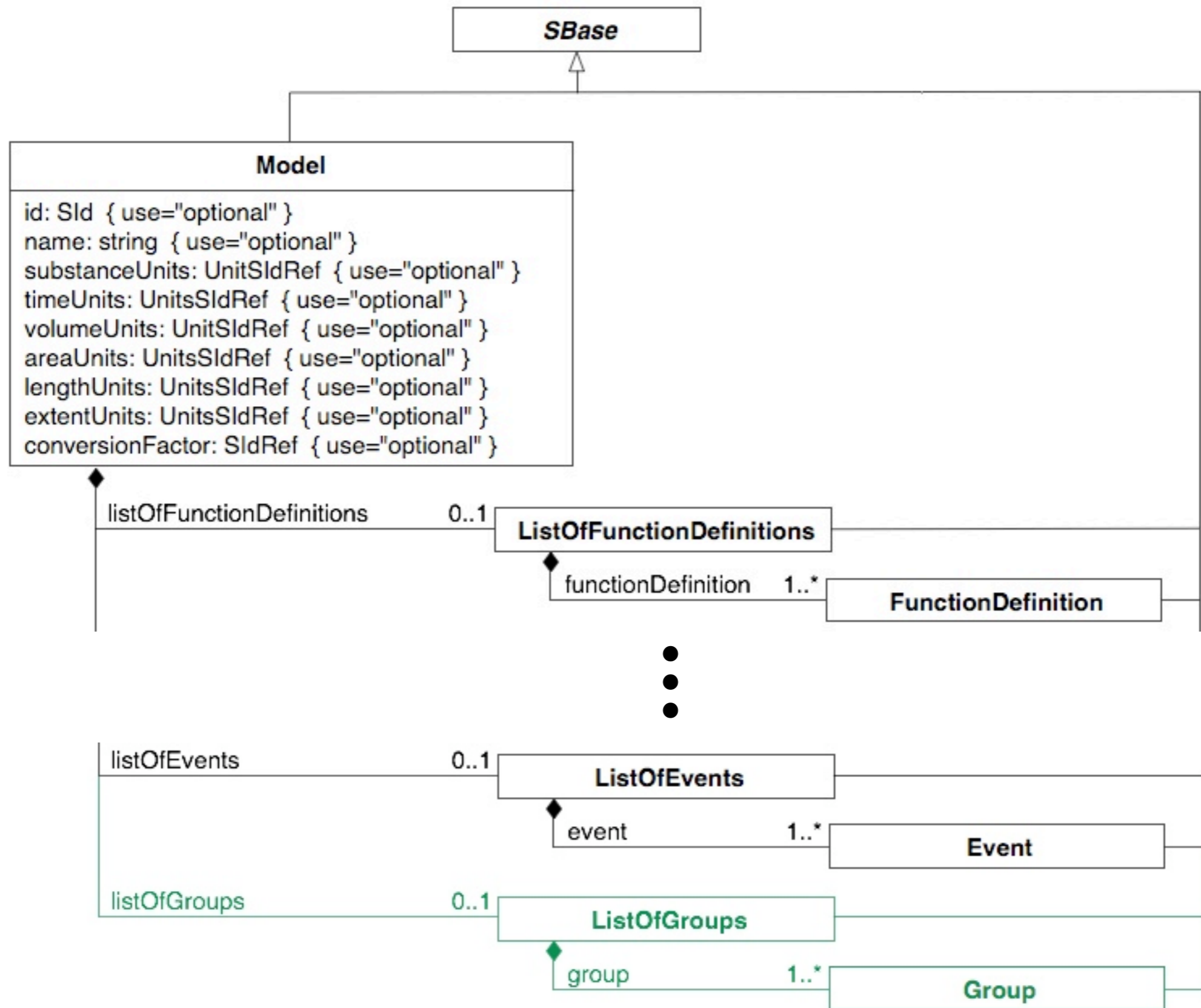
- ◎ Provide something akin to L2's *SpeciesType* and *CompartmentType*
 - But generalized to any entity: parameters, reactions, etc.
- ◎ Keep it simple
- ◎ Keep it flexible

Definitions

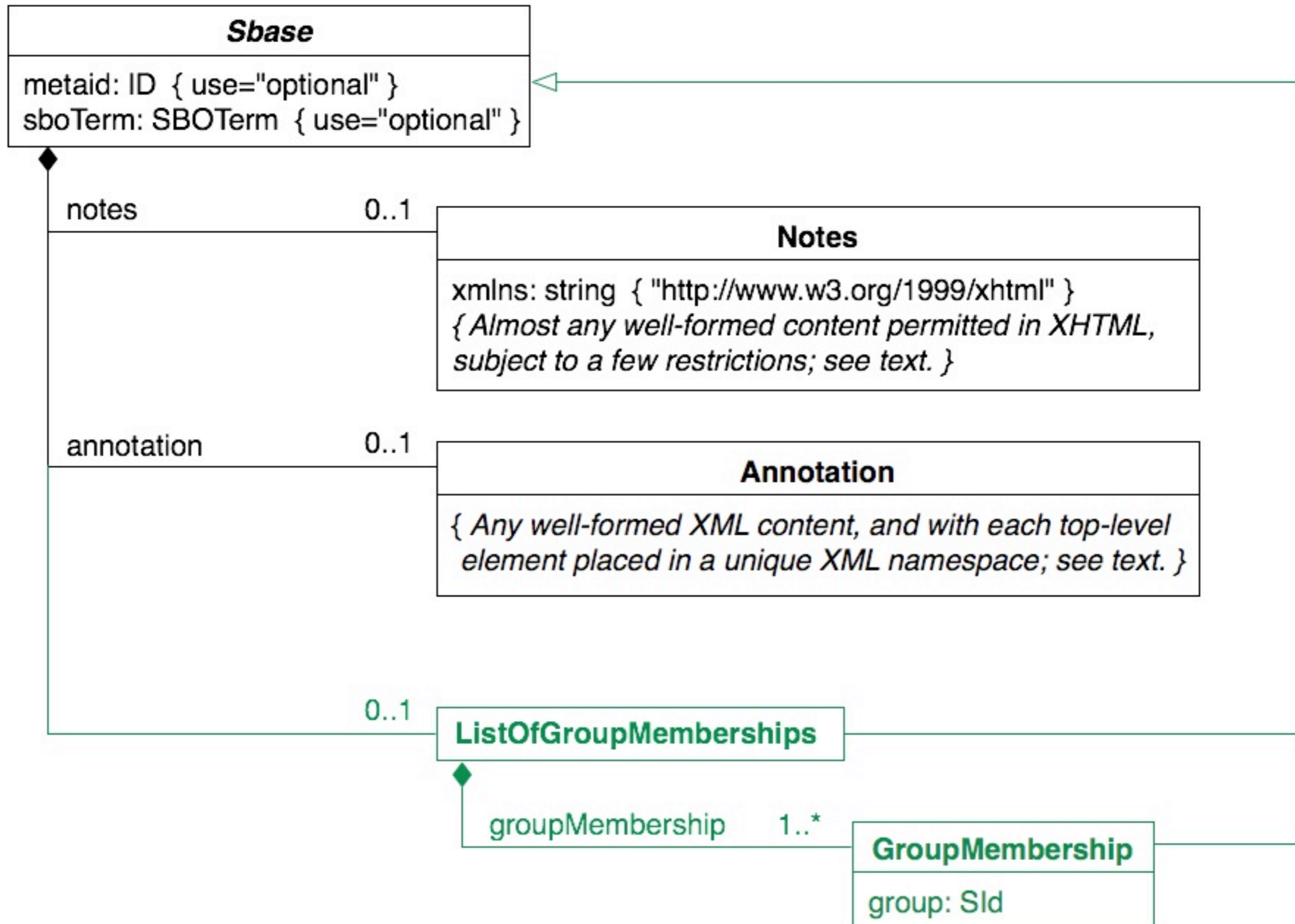


- A group is just a label—an identifier
 - But may have SBO term & MIRIAM annotations attached
 - This can provide machine-readable semantics

More definitions



Yet more definitions



Interpretation

- An entity (species, compartment, etc.) indicates it is a member of one or more groups by listing them

```
<listOfGroups>
  <group id="intermediates">
  <group id="cytoplasmic">
  ...
</listOfGroups>
...
<species id="S1" ...>
  <listOfGroupMemberships>
    <groupMembership group="intermediates">
    <groupMembership group="cytoplasmic">
  </listOfGroupMemberships>
</species>
```

- Meaning of group membership:

- For entity X and group G :

“Entity X is conceptually related to other members of group G ”

- Nature of relationship is not prescribed

- Members can be anything, including diff. elements (species, compart.)

Implications

- ◎ “Groups” are more like tags or labels than types
 - No mathematical implications
 - Presumably a model reader can safely ignore them
- ◎ Entities can be part of multiple groups
 - But this not really multiple inheritance
 - No behaviors are associated with groups

Unresolved issues

- ◎ Should this cover behavior of L2's SpeciesTypes?
 - Have rules about {species, species type} combos in compartments?
- ◎ How should this interact with L3 multi* ?
- ◎ What are implications of annotating group definitions?
 - E.g., if group "A" has "isa" relationship to something, and group "B" is part of group "A", what does it mean?