

Spatial Extension Progress

- Language support
 - libSBML 3.1 C++ extensions (**abandoned**)
 - Java Abstraction Layer (libSBML/VCell) (**abandoned**)
 - Java libSBML (4.0 API) with Spatial prototype
- Comparison of geometric representations of many spatial modeling packages
 - see Wiki <http://ntcnp.org/twiki/bin/view/VCell/SpatialSBML>
- VCell branch as reference implementation for SBML Spatial
 - generalized topology (e.g. “outside”)
 - generalized component-domain mappings (SizePerUnitSize)
 - Mixing lumped/distributed reactions, species

model

listOfCompartmentMappings

CompartmentMapping

compartment
domainType

geometry

listOfCoordinateComponents

CoordinateComponent

Id (symbol e.g. x,y,z)
Unit (e.g. um, radians)
Min (min bounds)
Max (max bounds)
Type (polygonal_tessellation, csg, level_set)

listOfDomainTypes

DomainType

Id (e.g. "cytosol")
Dimension (0,1,2,3)

listOfDomains

Domain

Id (e.g. "cyt1")
domainType

InsideOutsideMath

CSG (via objects)

listOfObjects

Compartment Mapping

```
<spatial:listOfCompartmentMappings>  
  <spatial:compartmentMapping  
    Id:    (unitSize)  
    spatial:compartment="ec"  
    spatial:domainType="subVolume1"  
    spatial:unitSize="1.0" />  
</spatial:listOfCompartmentMappings>
```

Geometry Elements

```
<spatial:geometry id="3D uniform"  
  spatial:coordinateSystem="cartesian"  
  spatial:geometryType="analytic">  
  <spatial:listOfCoordinateComponents>  
    <spatial:coordinateComponent  
      id="x" spatial:type="X"  
      spatial:min="0.0" spatial:max="10.0"  
      spatial:unit="um" />  
    <spatial:coordinateComponent id="y" .../>  
    <spatial:coordinateComponent id="z" .../>  
  </spatial:listOfCoordinateComponents>  
  <spatial:listOfDomainTypes>  
    <spatial:domainType id="cytosol" spatial:dim="3" />  
  </spatial:listOfDomainTypes>  
  <spatial:listOfDomains>  
    <spatial:domain id="cytosol1" spatial:type="cytosol"/>  
  </spatial:listOfDomains>  
  .....  
</spatial:geometry>
```

Reactions need location if “spatial”

Reaction extent needs to be concentration/time
... look into ReactionDensity??

Species can be “pools” or “distributed”

Diffusion rate

Advection velocities

Boundary conditions

Internal

External

Coordinate bounds (surfaces defined by $x=\min$, ...)

Or

Require explicit geometric objects

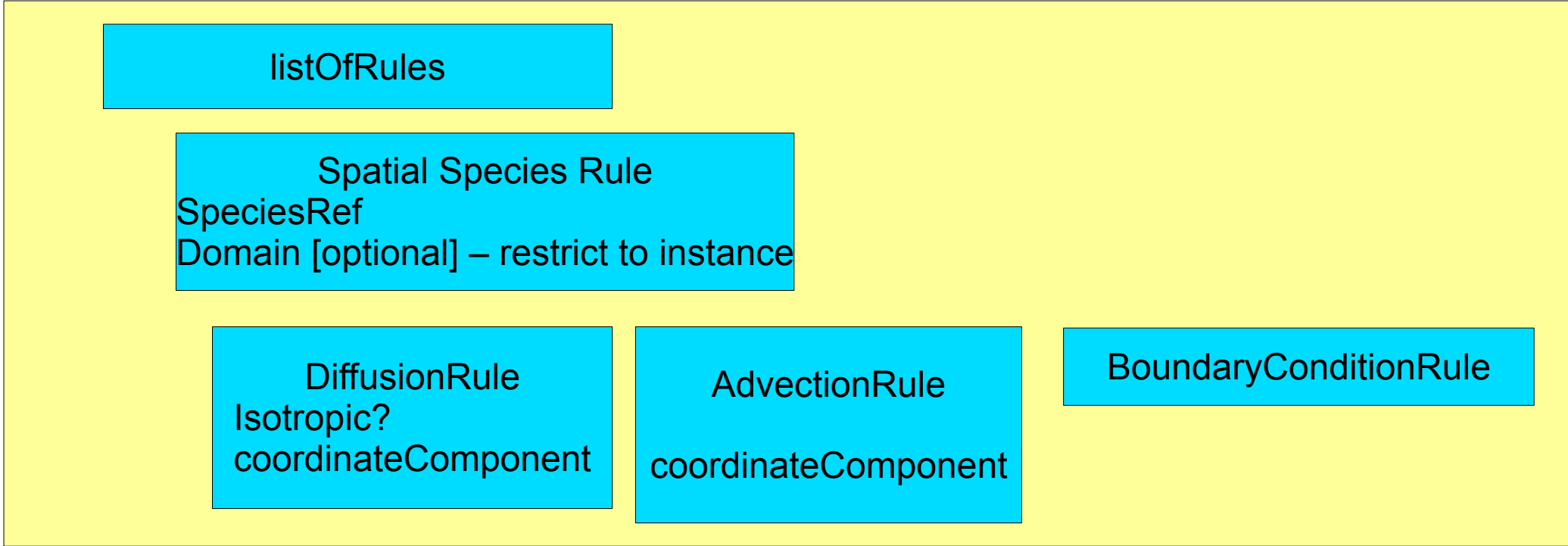
Reaction

“Spatial” flag
Reaction density???

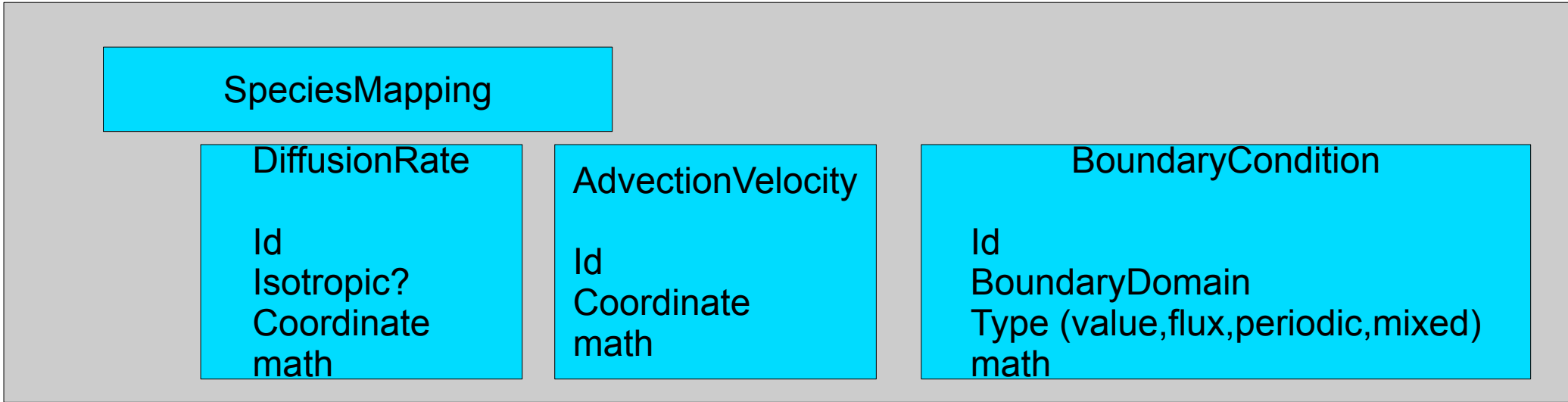
Species

spatialFlag

Where to put spatial operators and boundary conditions?



OR



Plan

Complete working prototype (Sept 2009) of
“java libSBML spatial” and Vcell
(test against 1000's of existing spatial models).

Distribute initial L3 proposal (Nov 2009)

Update Wiki with latest ideas and solicit contributions from
community (Sept 2009)

Video/Tele Workshops for Spatial Modeling
(1st quarter 2010)

Distribute draft Level 3 Proposal (summer 2010)

Develop libSBML 5.0 C++ implementation (summer 2010)