

Spatial Extension for SBML Level 3

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Physiology

Compartment

CompartmentMapping

"local" reactions

diffusion

IC's

BC's

DomainType

cytosol

Domain

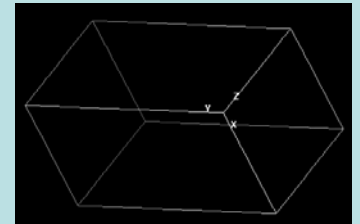
cytosol_1

Interior Points

Geometry

Coordinate System

bounding box
extent/origin

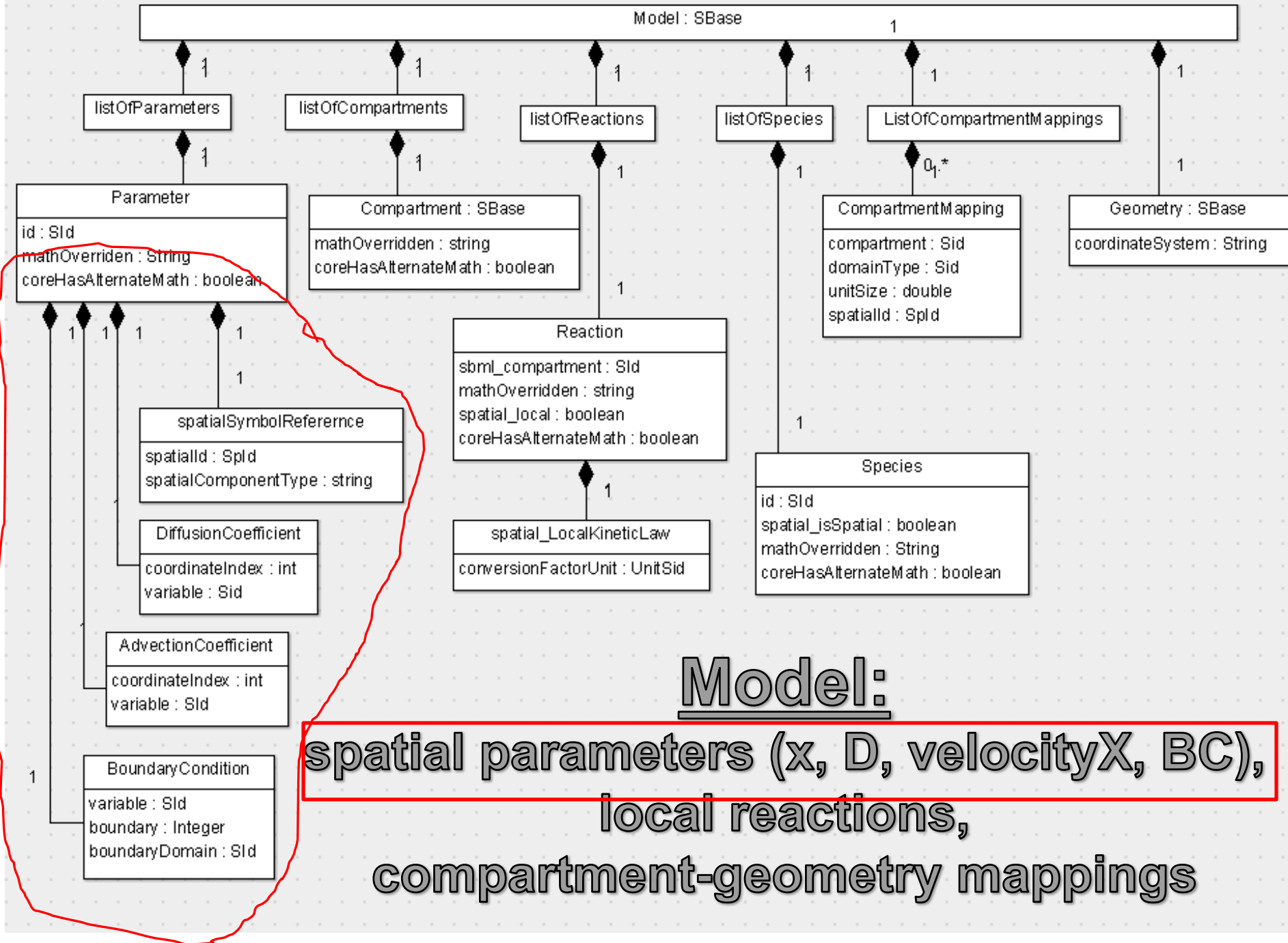


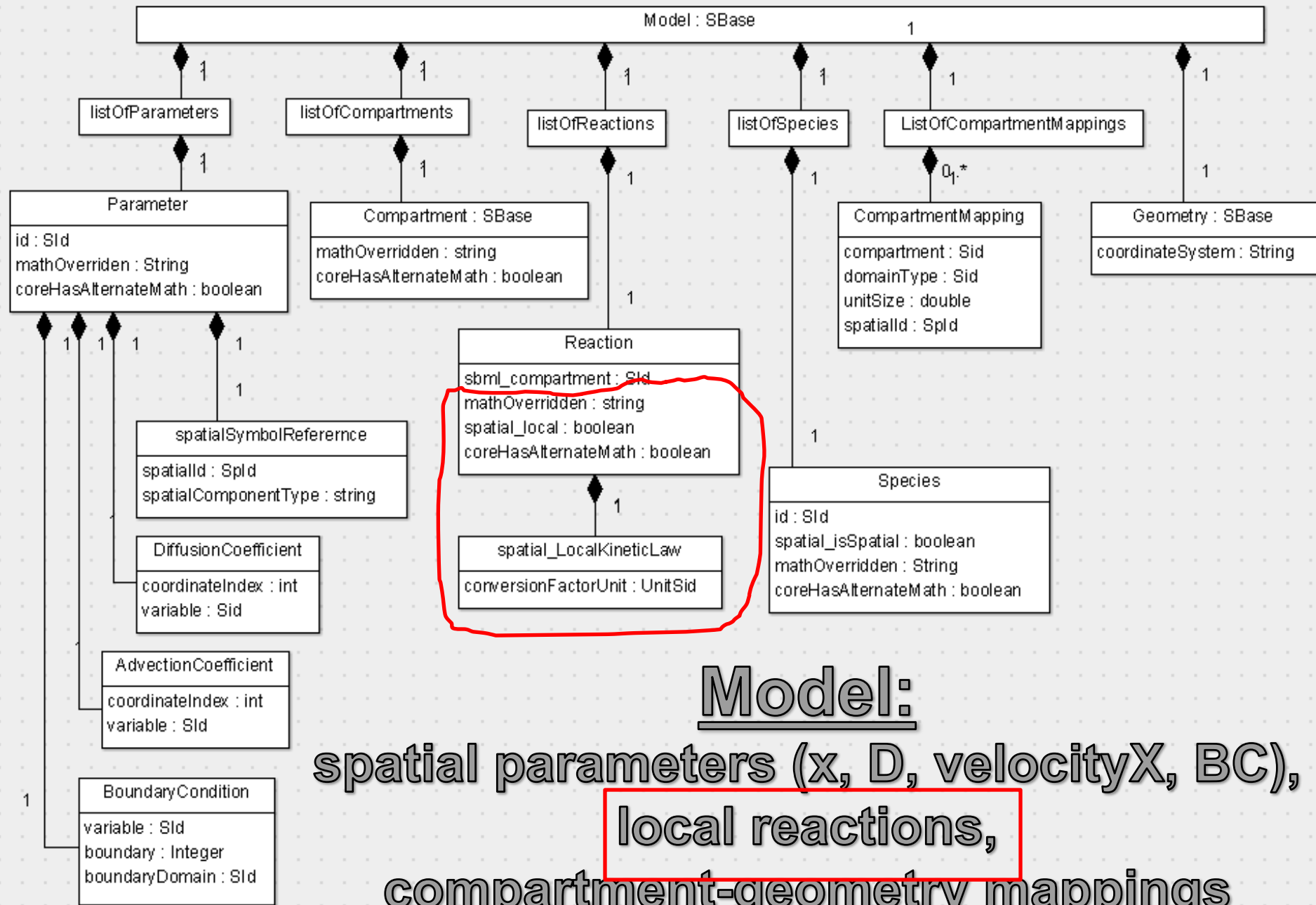
Analytic

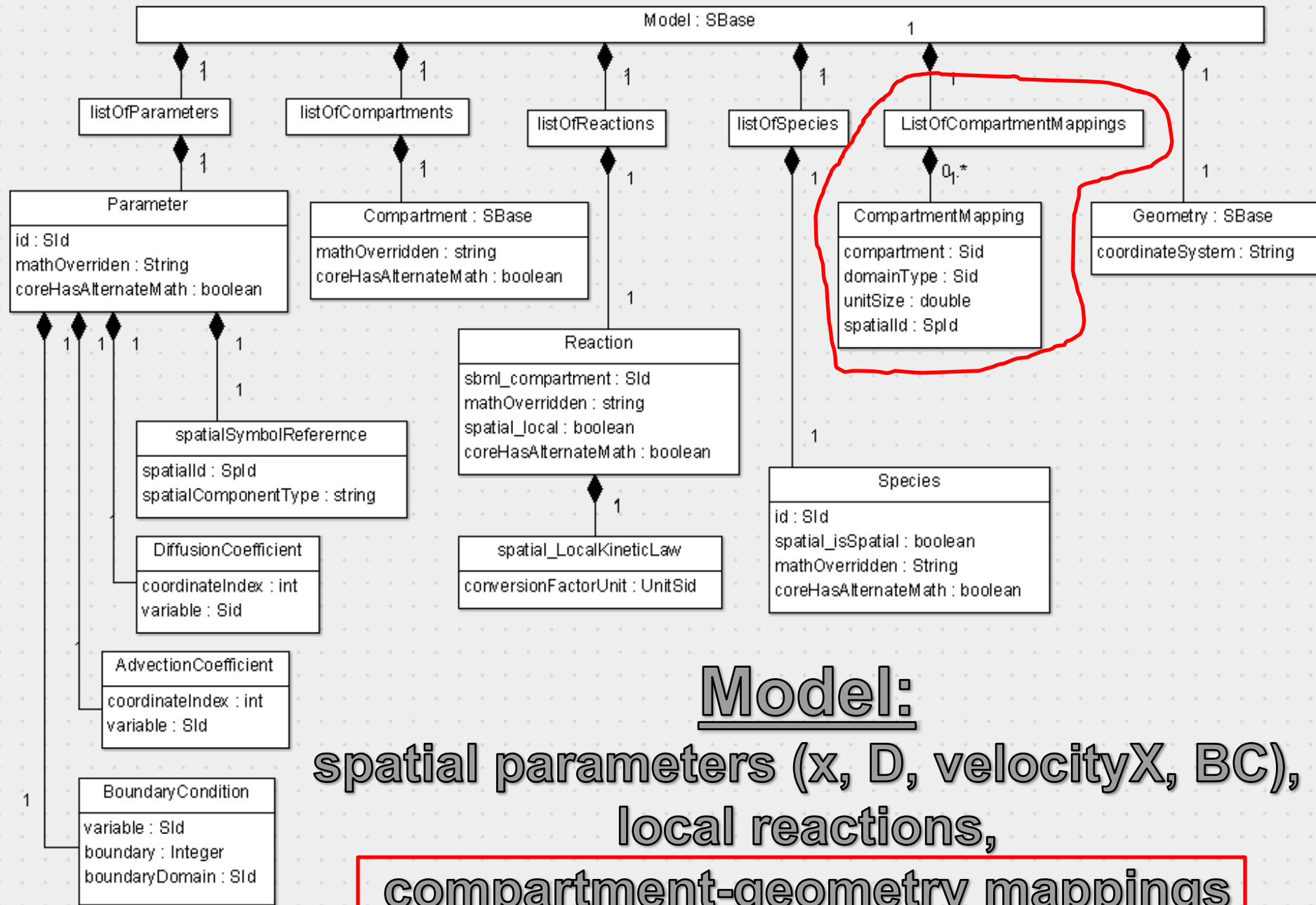
$$x^2 + y^2 + z^2 < R^2$$

Surface
Based

Geometric
Object
Definitions



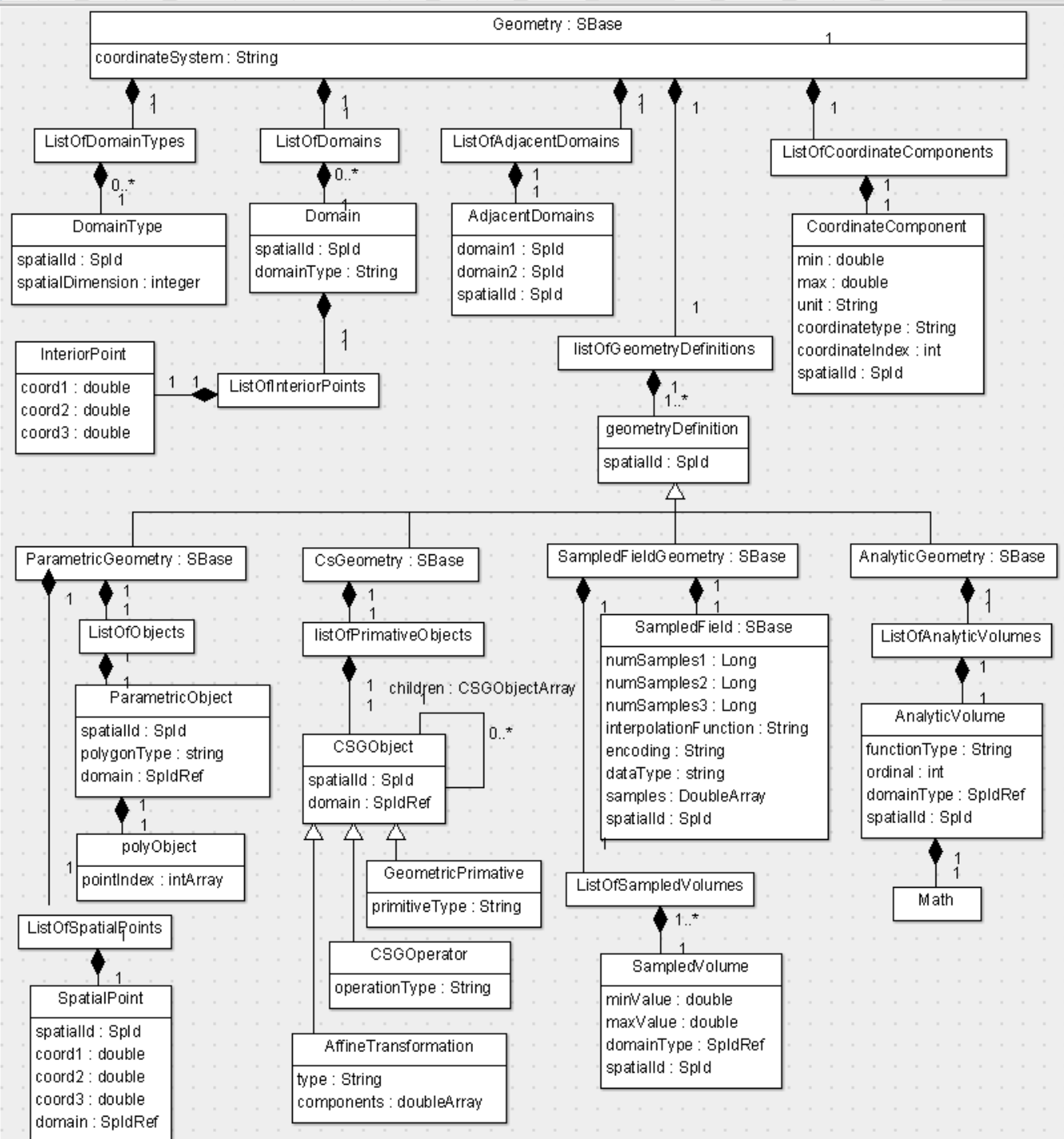




Geometry

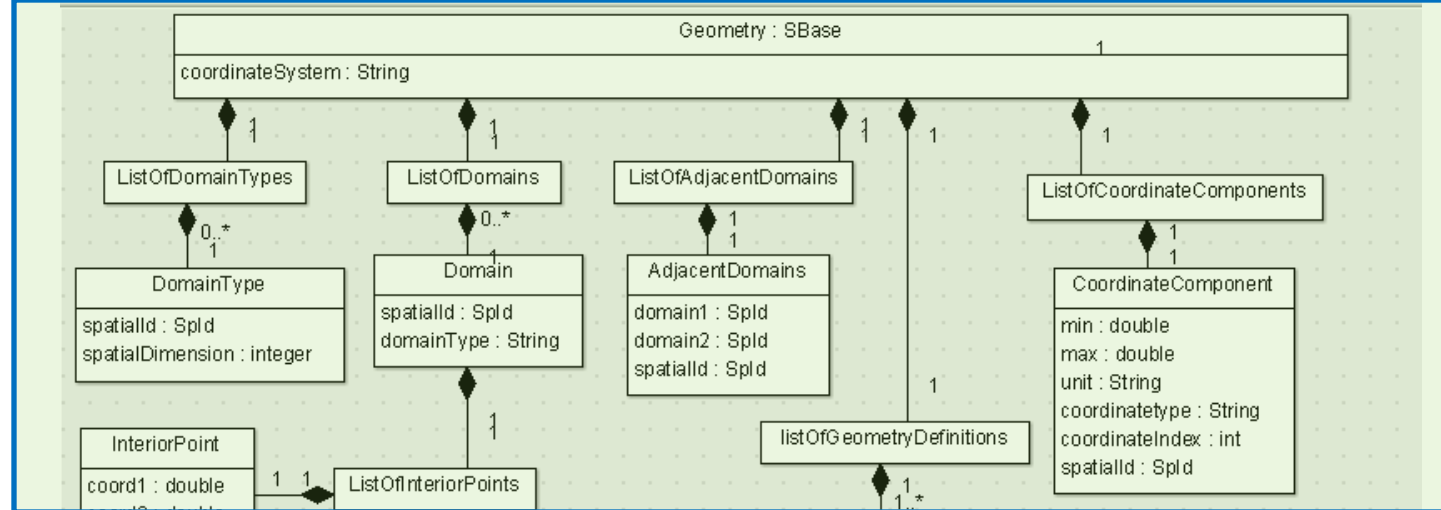
Geometry is reusable

Doesn't refer to rest of model.



Abstract
Geometric
Concepts
(domains/
domainTypes

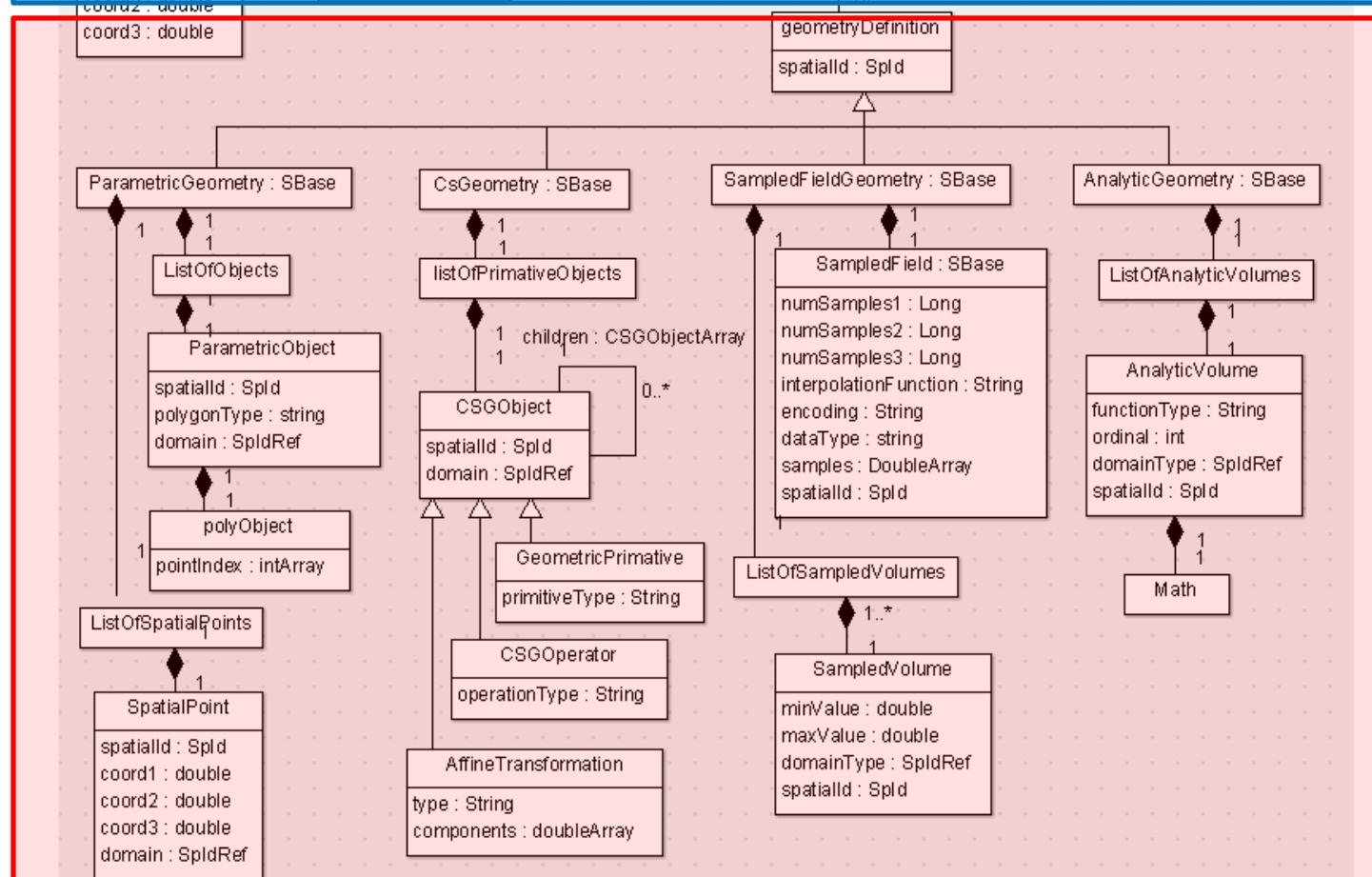
Independent of
particular
geometric
representation



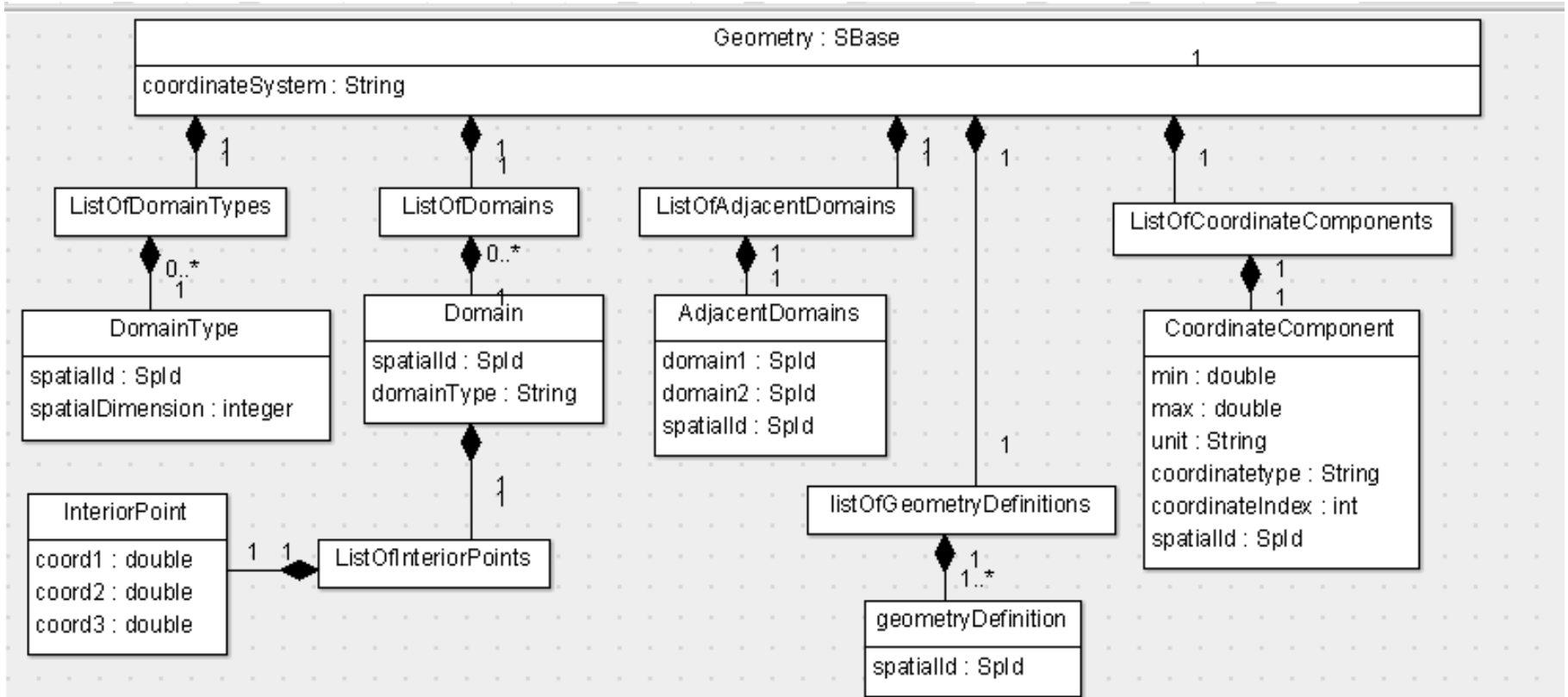
Multiple
Geometric
Definitions in
same model

Write as many as
you can

Read the most
convenient one.

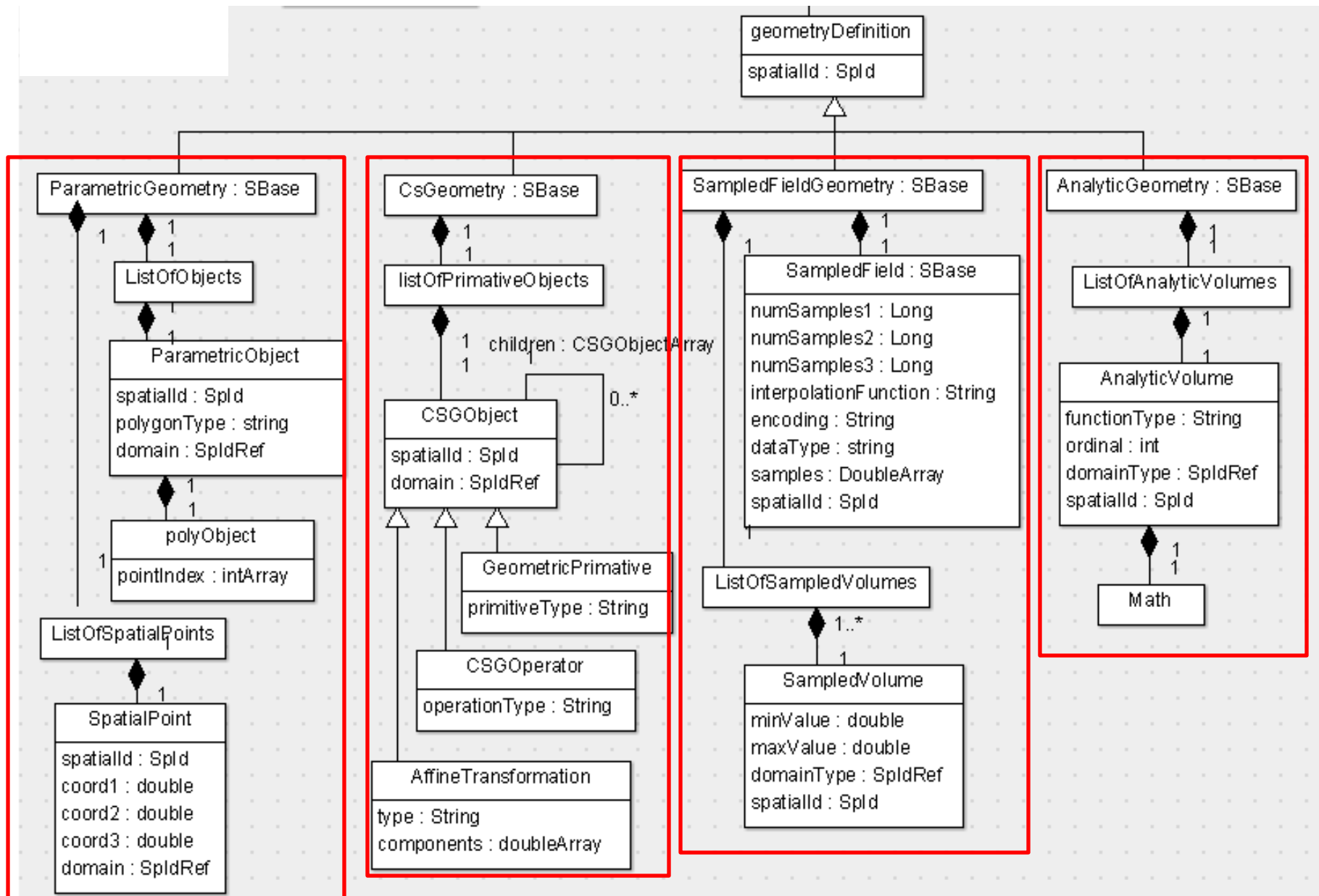


Geometry (Abstraction)



domains, domainTypes, connectivity,
coordinate system, geometry definition

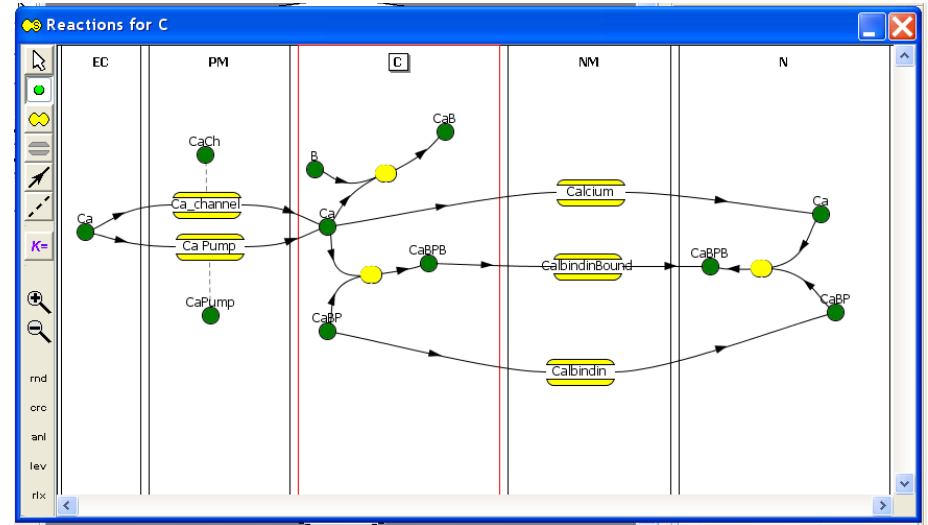
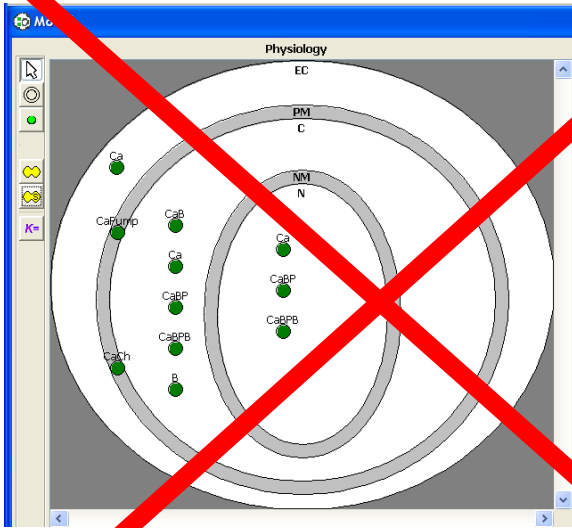
Geometry (Description)



required elements extension

- **Only SBML Core elements** (e.g. Parameters, Species, Compartments) **may define an identifier** for use within a MathML expression or as the target of a rule.
- But spatial models need to be able to define additional identifiers (x,y,z,domainSize,diffusionCoefficient) with semantics provided by the extension.
- Required Elements extension (Lucian Smith) allows other extensions to declare that they are changing the mathematical interpretation of an SBML Core element. So we can alter reactions to make them local and we can define new SBML Core parameters and but define them as attributes of the geometry.
- ```
<sbml xmlns="http://www.sbml.org/sbml/level3/version1/core" level="3" version="1"
 xmlns:req="http://www.sbml.org/sbml/level3/version1/requiredElements/version1"
 xmlns:spatial="http://www.sbml.org/sbml/level3/version1/spatial/version1"
 req:required="true" spatial:required="true">
```
- ```
<sbml:parameter sbml:id="x" req:mathOverridden="spatial" req:coreHasAlternateMath="false">
  <spatial:spatialSymbolReference spatial:spatialReference="coord1"
  spatial:spatialType="coordinateComponent"/>
</parameter>
```

Retooling VCell dogma



- Practical reconciliation of compartmental and spatial modeling
 - compartment topology only in geometry
 - Generalized spatial mapping (compartments/domains)

Richer prototype (VCell / Smoldyn integration)

- VCell
 - explicit volumes (analytic or image-based)
 - implicit surfaces (compute approximate surfaces)
 - Deterministic modeling (pdes)
 - Concentration fields
- Smoldyn
 - Implicit volumes (with interior points)
 - explicit surfaces (polygonal)
 - Particle distributions (in progress).

libSBML 5.0 plugins

- **required elements (implemented)**
 - C++ and Swig Java binding
- **spatial extension (partial implementation)**
 - C++ and Swig Java binding
 - Partial model implementation
 - Compartment mappings
 - Other concepts via required elements package
 - Complete Abstract Geometry
 - Partial Concrete Geometry
 - Analytic only.
 - Images (sampledFields very soon).

Status

- Documentation
 - Draft proposal (12 pages and counting)
 - UML
 - XML Schema
- Prototype implementation
 - libSBML required elements extension (C++/Java)
 - libSBML spatial extension (C++/Java)
 - VCell Alpha / libSBML 5.0 / Smoldyn
- Community
 - Discussion (sbml-discuss → workshop)
 - Documentation (→ SBML wiki)

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- Steve Andrews (Smoldyn)

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