

# Spatial Extension for SBML Level 3

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# Physiology

Compartment

CompartmentMapping

"local" reactions

diffusion

IC's

BC's

DomainType

■ cytosol

Domain

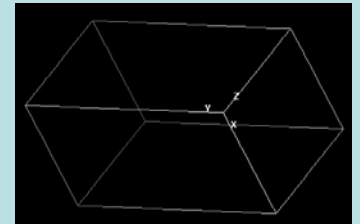
■ cytosol\_1

Interior Points

## Geometry

Coordinate System

bounding box  
extent/origin

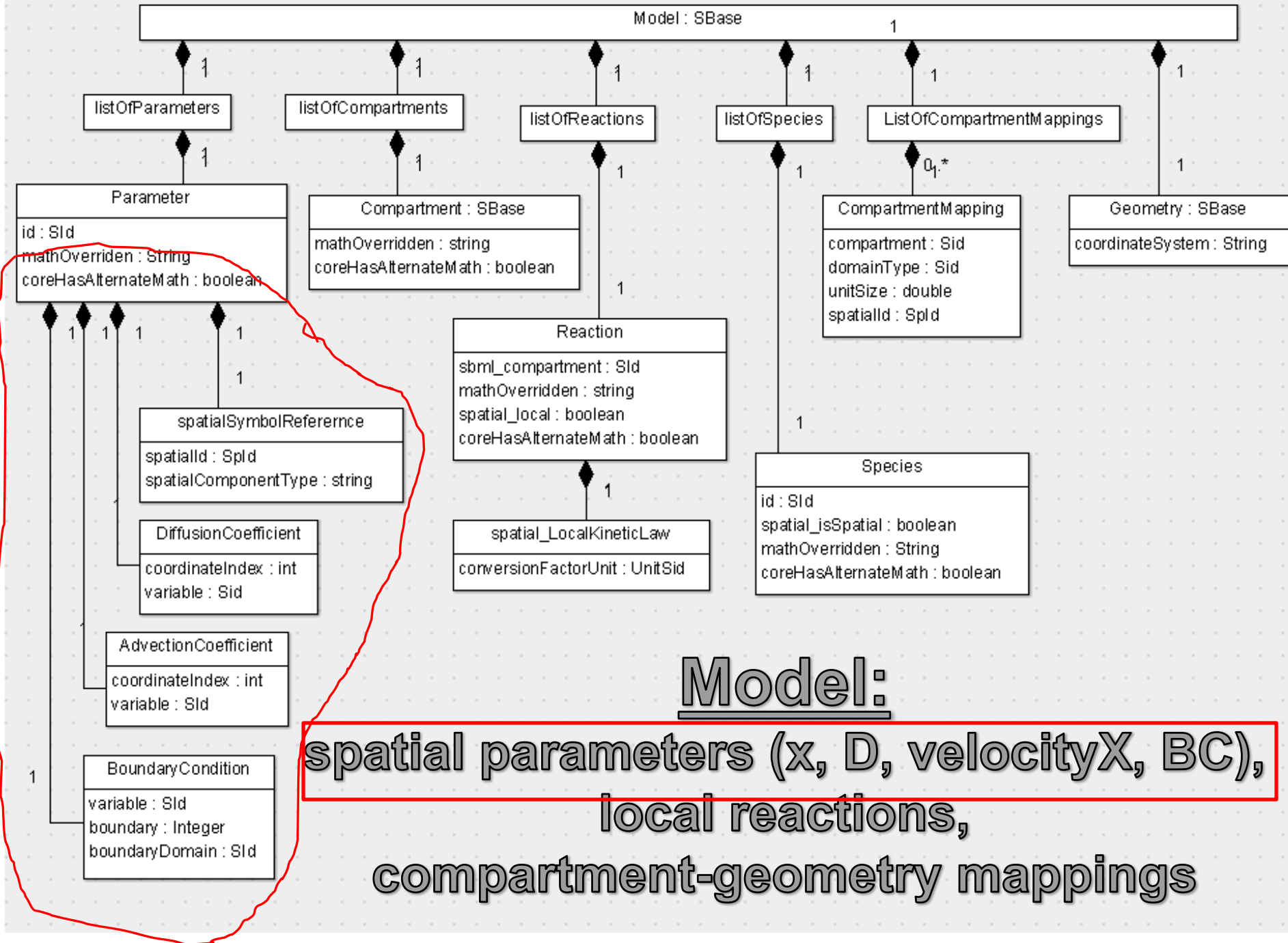


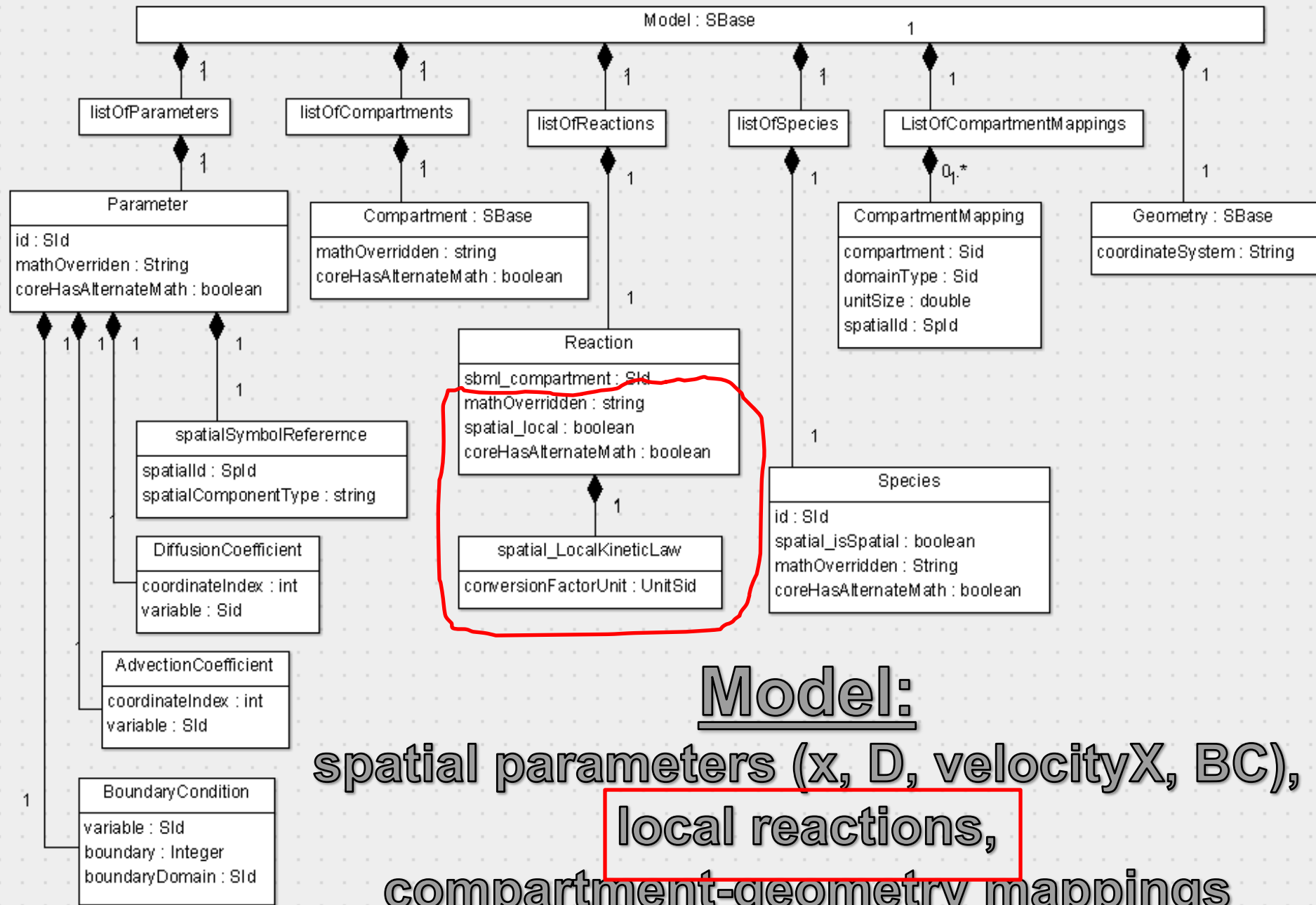
Analytic

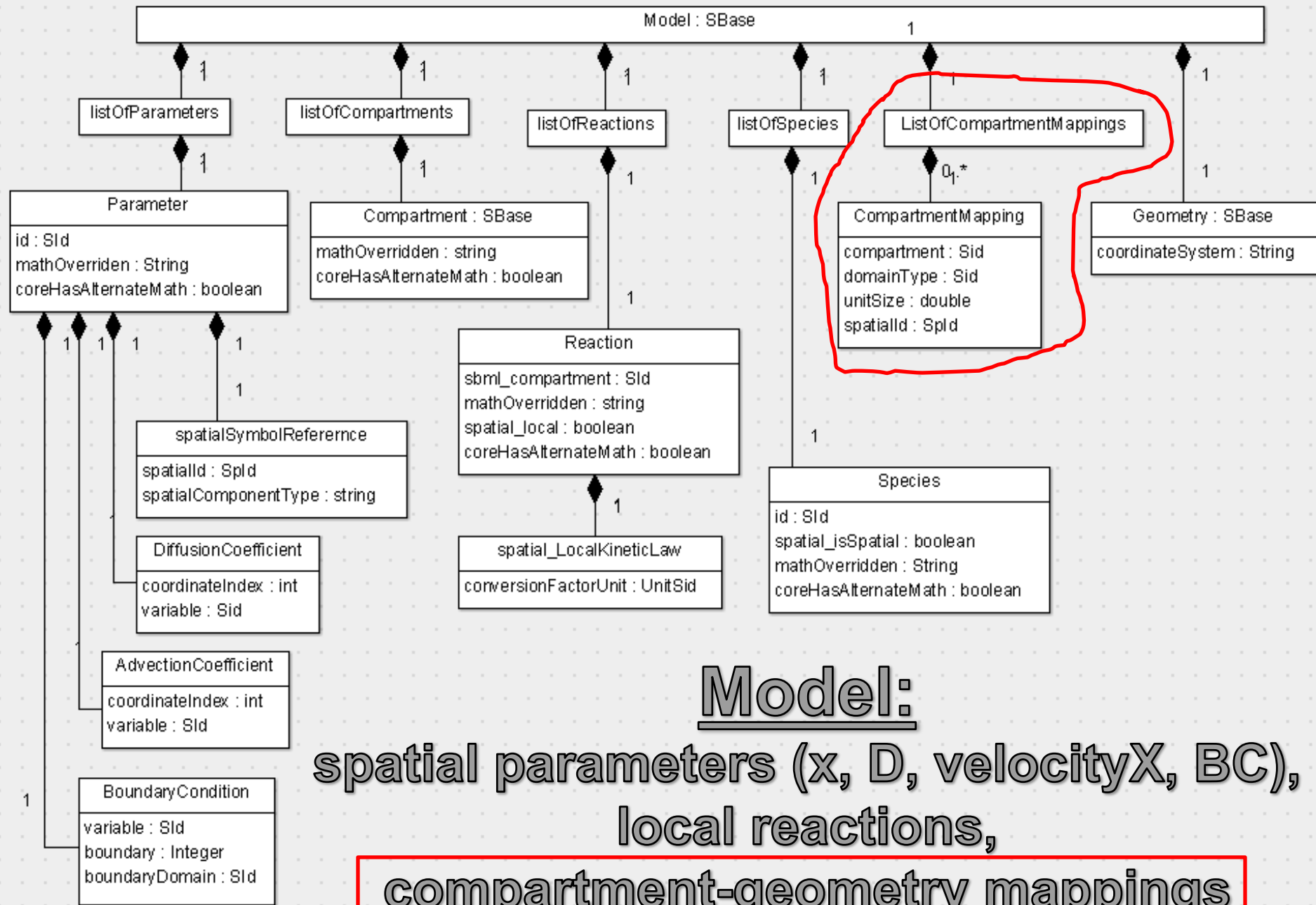
$$x^2 + y^2 + z^2 < R^2$$

Surface  
Based

Geometric  
Object  
Definitions



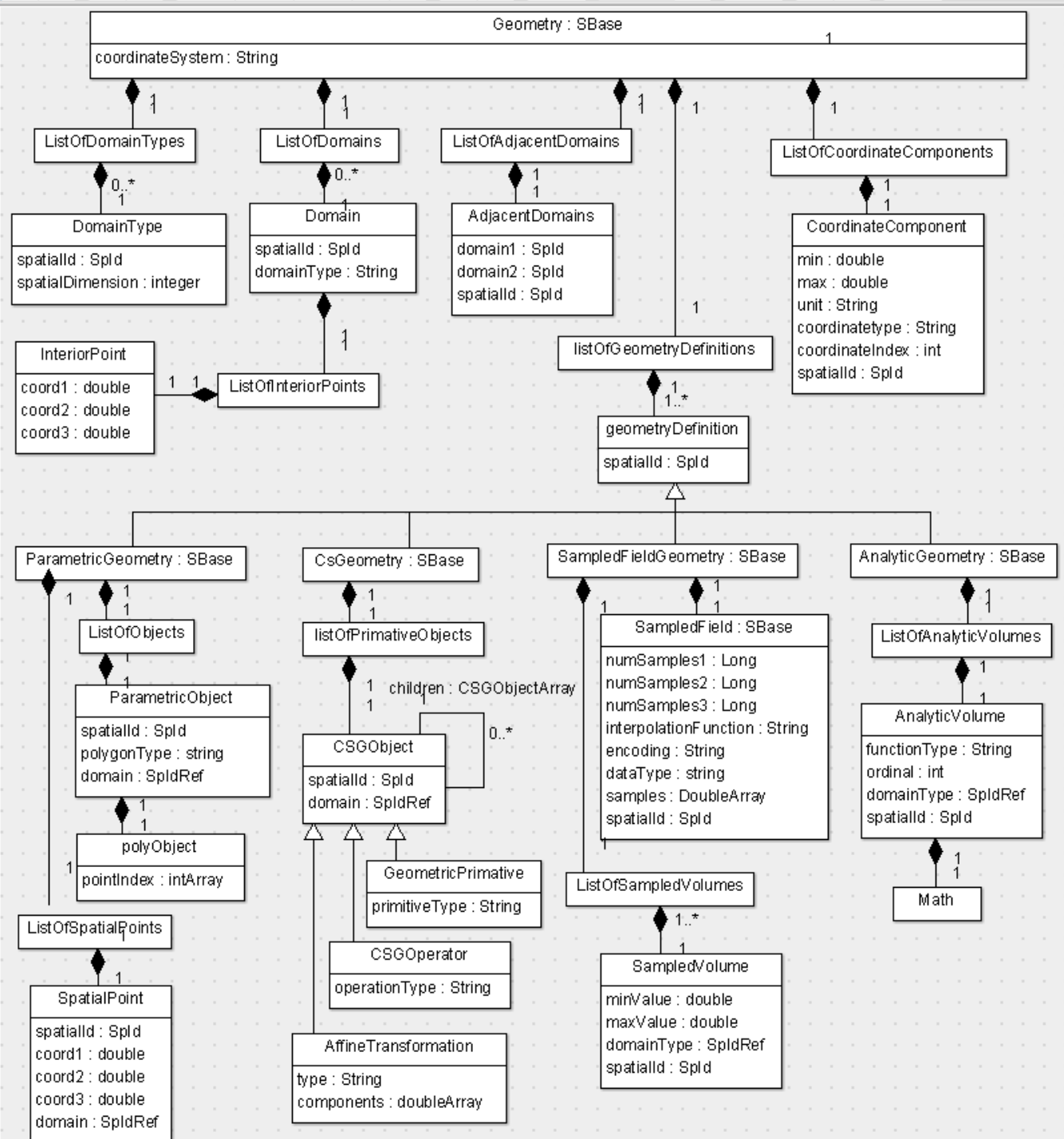




# Geometry

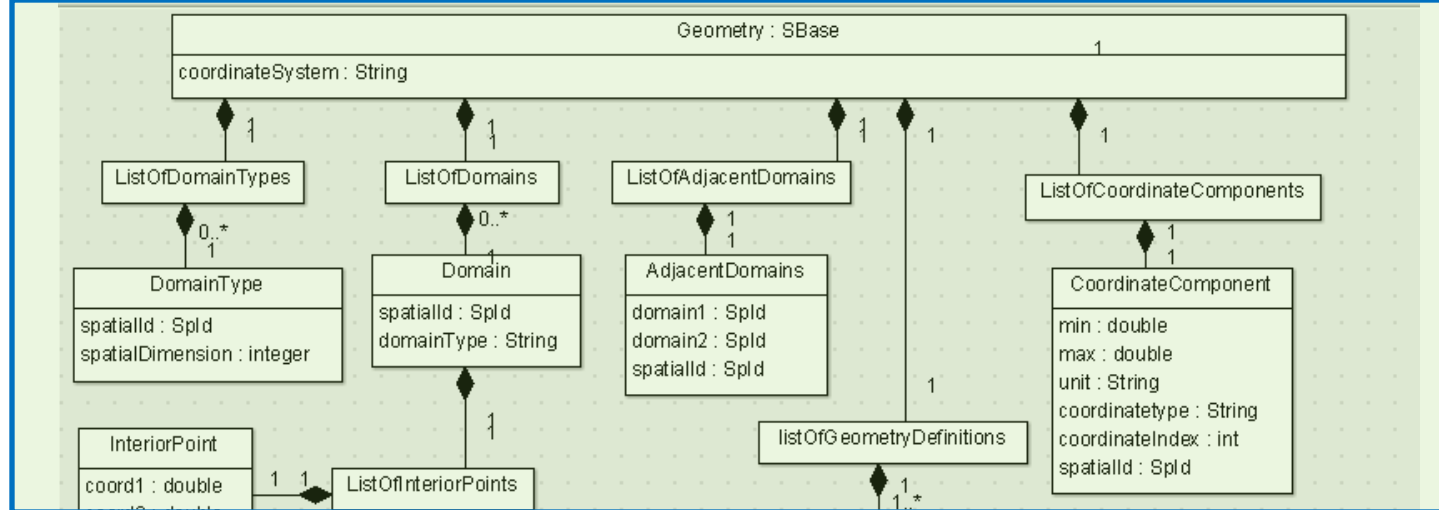
Geometry is reusable

Doesn't refer to rest of model.



Abstract  
Geometric  
Concepts  
(domains/  
domainTypes

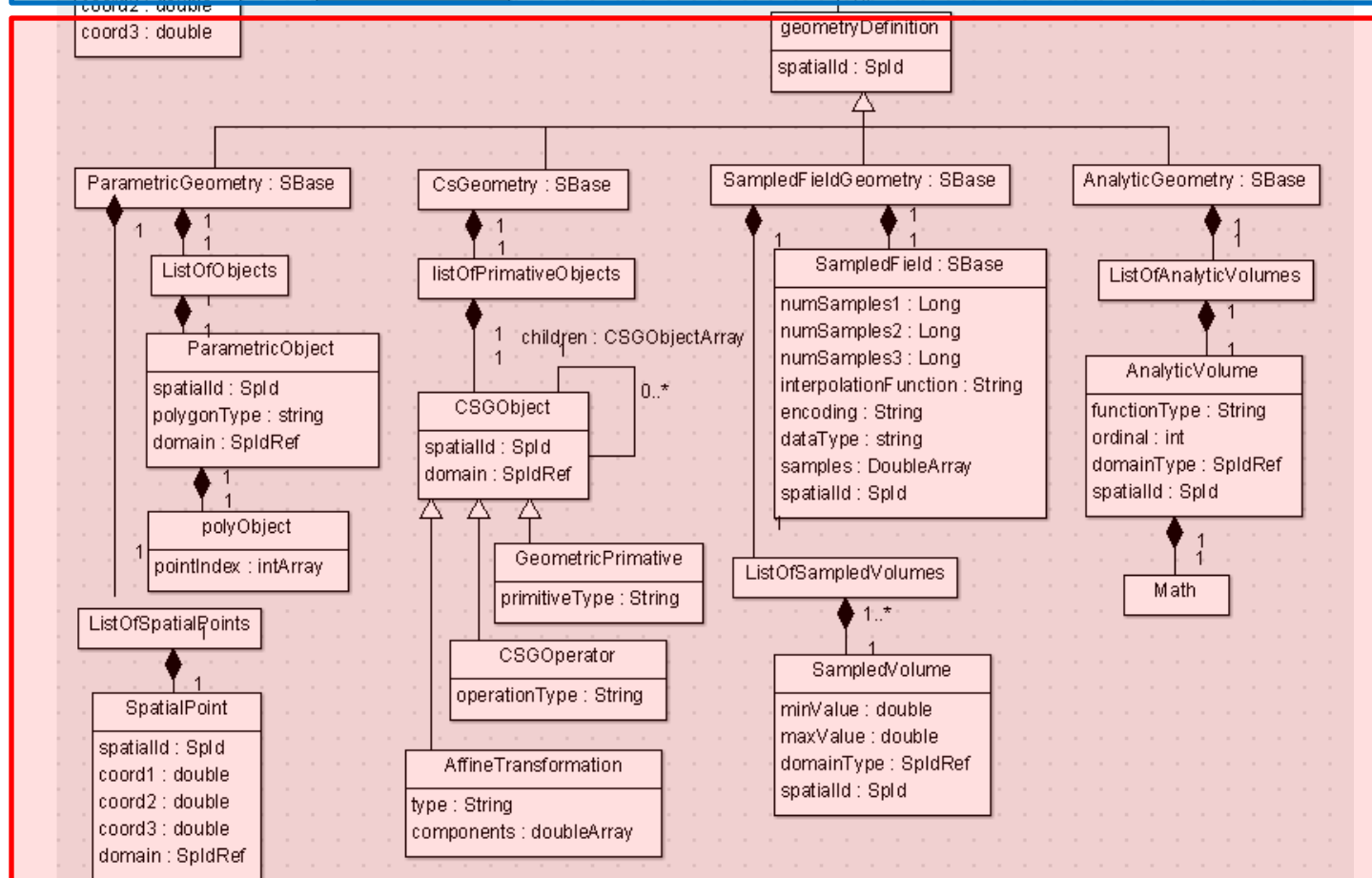
Independent of  
particular  
geometric  
representation



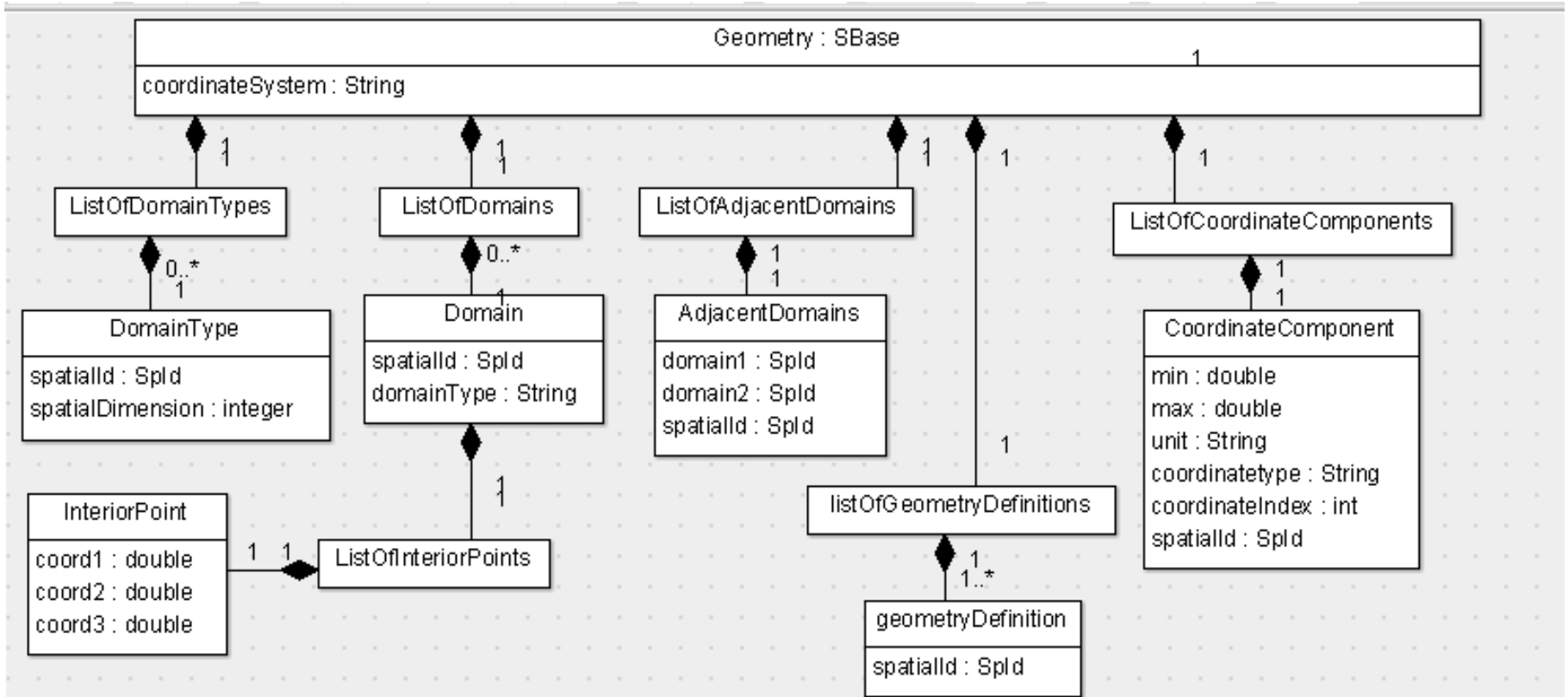
Multiple  
Geometric  
Definitions in  
same model

Write as many as  
you can

Read the most  
convenient one.

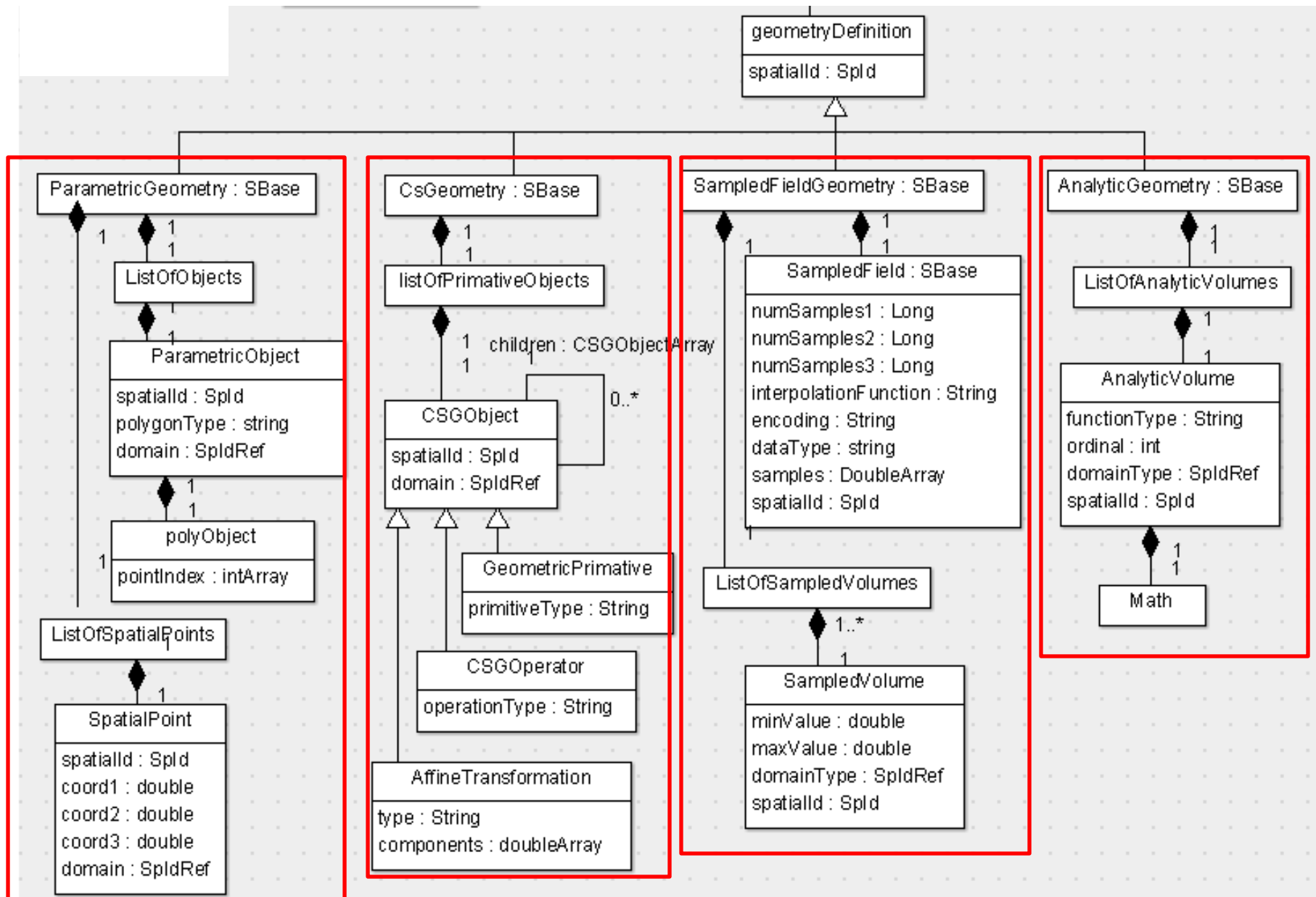


# Geometry (Abstraction)



domains, domainTypes, connectivity,  
coordinate system, geometry definition

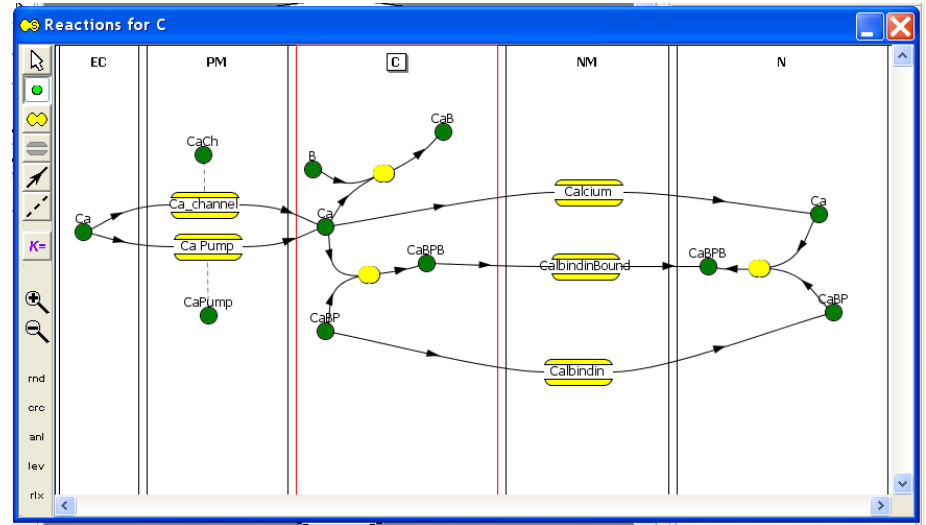
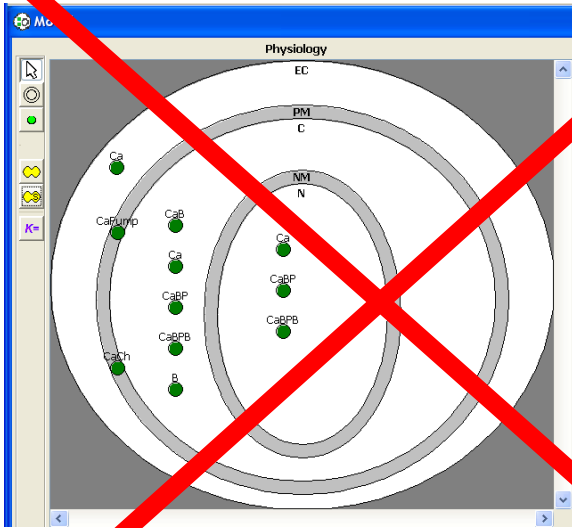
# Geometry (Description)



# 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)

# Acknowledgements

- Fei Gao (VCell software developer)
- Sarah Keating (libSBML 5.0 plugin arch.)
- Steve Andrews (Smoldyn)
  
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- NIH/NCRR VCell funding