

# The Virtual Cell and XML

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Pasadena, May 31.





# Our Goals:

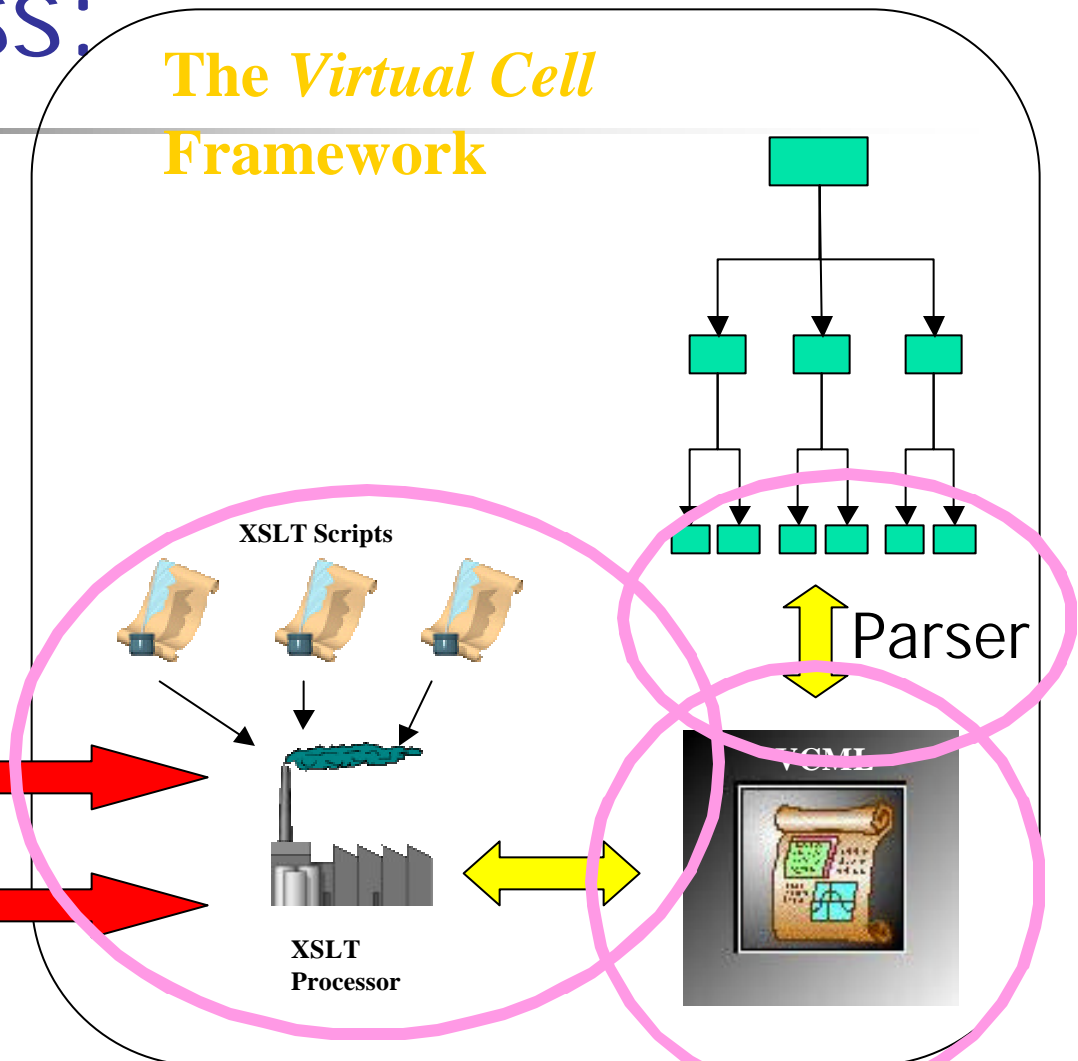
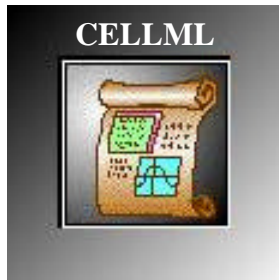
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The project of applying XML to the Virtual Cell is mainly composed by the following parts:

- ✍ Participate in the specification of the SBML.
- ✍ Implement a XML Java parser for the virtual Cell.
- ✍ Develop a XML Schema for internal usage, compliant with the BioModel and MathModel objects (VCML).
- ✍ Implement a XML Document comparison tool.
- ✍ Begin the specification of XSLT scripts for transforming reading and writing

# The Process:

## The *Virtual Cell* Framework



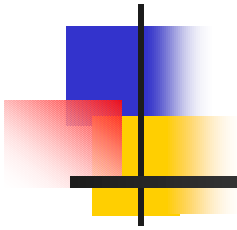


# XSLT Script(VCML->SBML):

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```
<?xml version="1.0" ?>
<!--Generated by XSLWiz, the XSLT generator from EBProvider Inc.-->
  <xsl:stylesheet xmlns:xsl="http://www.w3.org/1999/XSL/Transform"
version = "1.0">
  <xsl:template match = "/">
    <xsl:variable name = "name_9_var1" select = "/BioModel/@Name"/>
    <xsl:variable name = "name_9_position_var1" select = "position()"/>
    <xsl:element name = "sbml">
      <xsl:attribute name = "level">
        <xsl:value-of select = "'1'"/>
      </xsl:attribute>
      <xsl:attribute name = "version">
        <xsl:value-of select = "'1'"/>
      </xsl:attribute>
      <xsl:element name = "model">
        <xsl:if test = "not(normalize-space($name_9_var1)='')">
          <xsl:attribute name = "name">
            .
          </xsl:attribute>
        </xsl:if>
      </xsl:element>
    </xsl:element>
  </xsl:template>
</xsl:stylesheet>
```

# Geometry Proposal



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Pasadena, May 31, 2001.





# Overview:

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- ✍ Fundamental concepts
- ✍ Volume-based Geometries
- ✍ Surface-Based Geometries
- ✍ Vcell Geometry
- ✍ Proposed SBML Geometry



# Fundamental Concepts

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- ✍ Parametric units (of  $u, v, w$ ) (? m, radians, degrees)
- ✍ Coordinates systems
  - ✍ Cartesian, Polar, Spherical, Cylindrical
- ✍ Dimension of space (1D, 2D, 3D)
- ✍ Metrics about the geometry (Areas, Volumes, lengths) ... store these?



# Fundamental Concepts

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- ✍ Set operations (Constructive solid geometry)
  - ✍ union, intersection, difference
- ✍ Coordinate “Affine” Transformations
  - ✍ rotation/translations...?



# Fundamental Concepts

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- ✍ Identification of “Contiguous Regions” (volume/surface)
  - ✍ Topological relationships (check validity with respect to geometry? or just annotation)
  - ✍ Connected graph representation of topological relationships?
  - ✍ Identity (e.g. anatomical)
  - ✍ Properties (e.g. geometric measurements)



# Volume-based Geometry

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- ✍ Implicit representation of surfaces.
- ✍ Volume samples
  - ✍ 2,3-dimensional experimental images (z-series)
  - ✍ Segmentated images throw away information
    - ✍ Ambiguous surfaces, convex-hulls provide staircase, need better.
- ✍ Volume Analytic
  - ✍ Inequalities  $f(u,v,w) < 0$  (e.g.  $x^2 + y^2 + z^2 < R^2$ )
  - ✍ Geometric primitives (spheres, cones...)
  - ✍ Constructive solid geometry?

# Explicit Membrane Determination

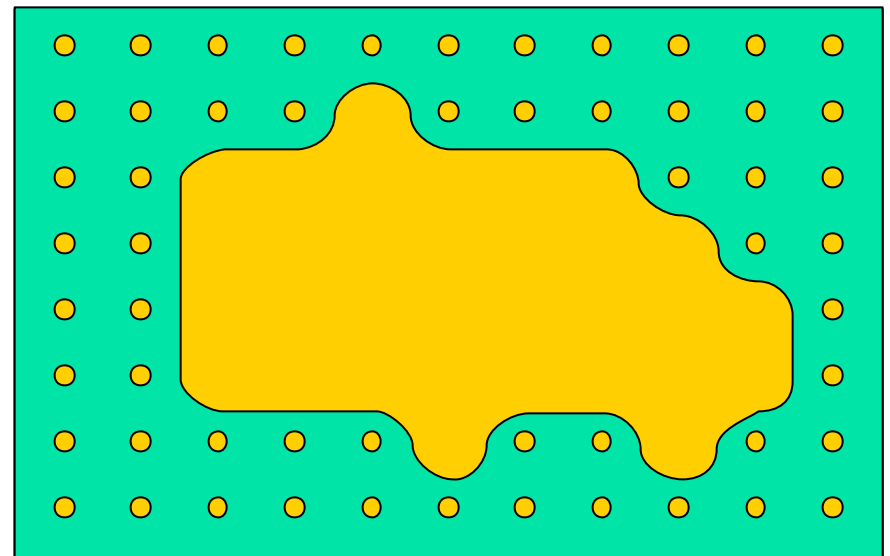
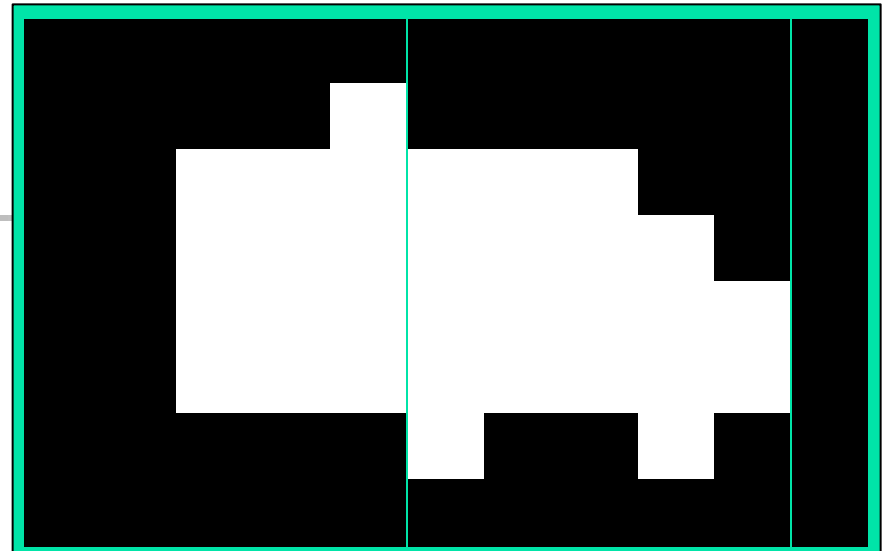
Membranes are currently defined implicitly as border between dissimilar pixels.

Consider image as point samples instead of pixels

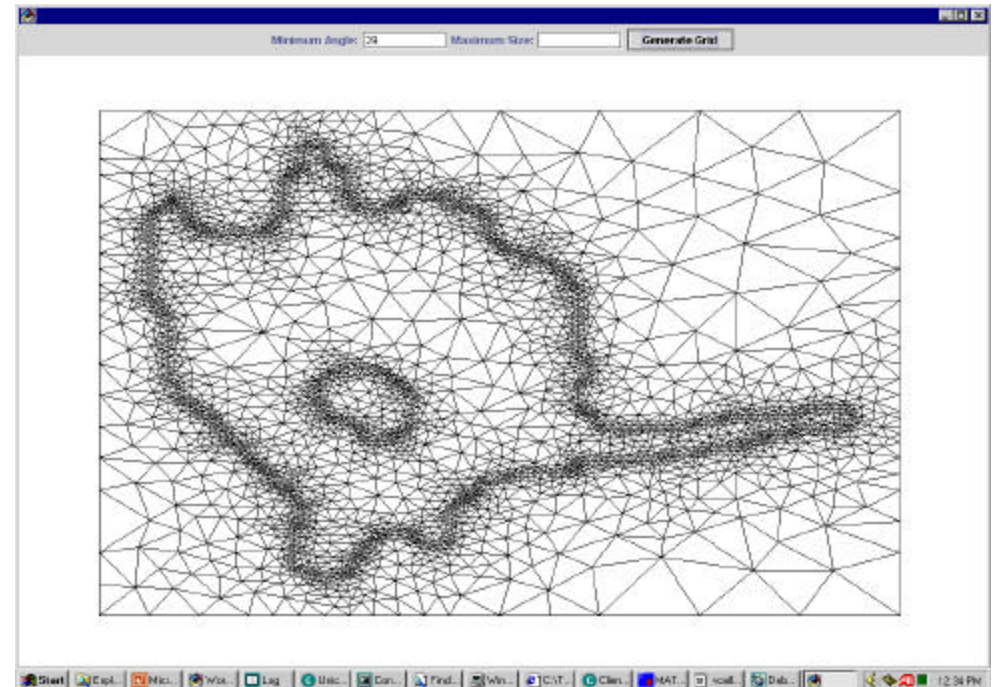
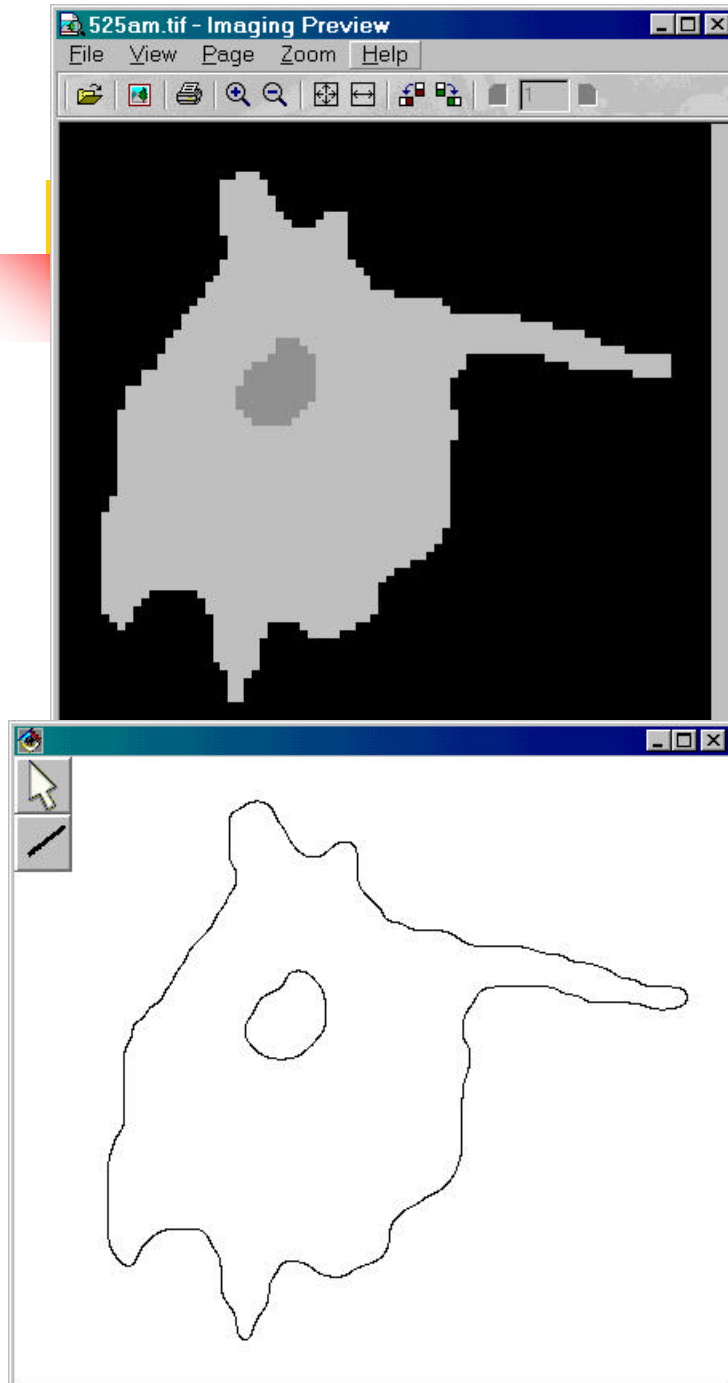
Choose more optimal boundary based on curvature, feature size

Explicit piece-wise analytic functions define “REAL” geometry

Meshing algorithms / User feedback



# 2D Unstructured Mesh Development



Geometry Service (Forms Bezier curves)

Meshing Service (uses “Triangle”)



# Surface-based Geometry

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- ✎ Analytic (implicit representation)
  - ✎ Equations  $f(u,v,w)=0$  (e.g.  $x^2+y^2+z^2=R^2$ )
  - ✎ difficult to sample directly into membranes
- ✎ Piecewise analytic (explicit representation)
  - ✎ (e.g. polygons, bicubic patches)
  - ✎ Easy to sample into membranes

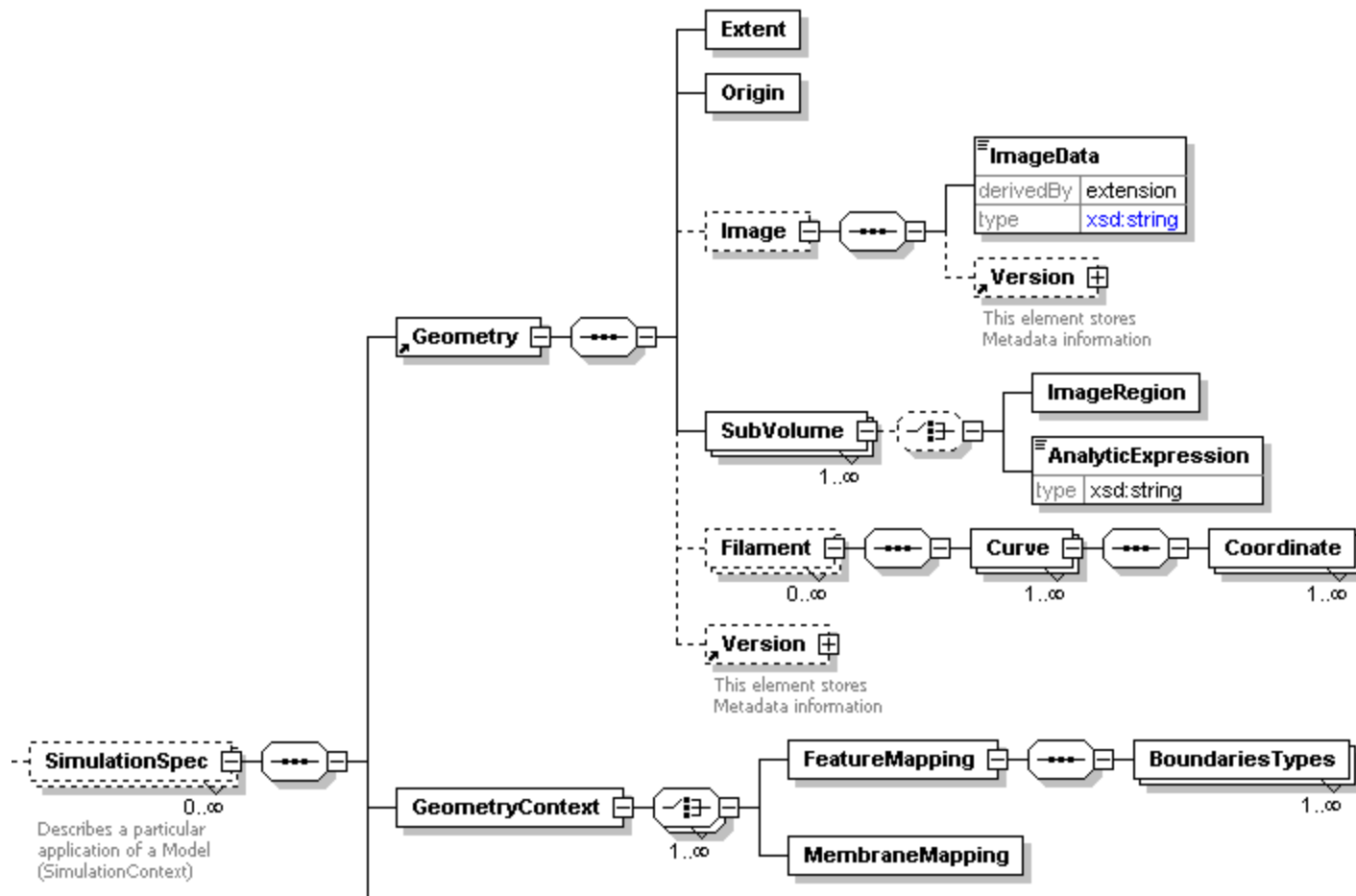


# Current Vcell Geometry

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- ✍ Image-based volume sampled
- ✍ Analytic volume
- ✍ Implicit boundaries (volumes form basis)
- ✍ Regions are still implicit and are identified in mesh generation (numerics)
- ✍ Topology is identified in mesh generation (numerics)

# Current Vcell Geometry





# Properties not supported

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- ✍ Rendering info (material properties)
- ✍ Explicit anatomical taxonomy



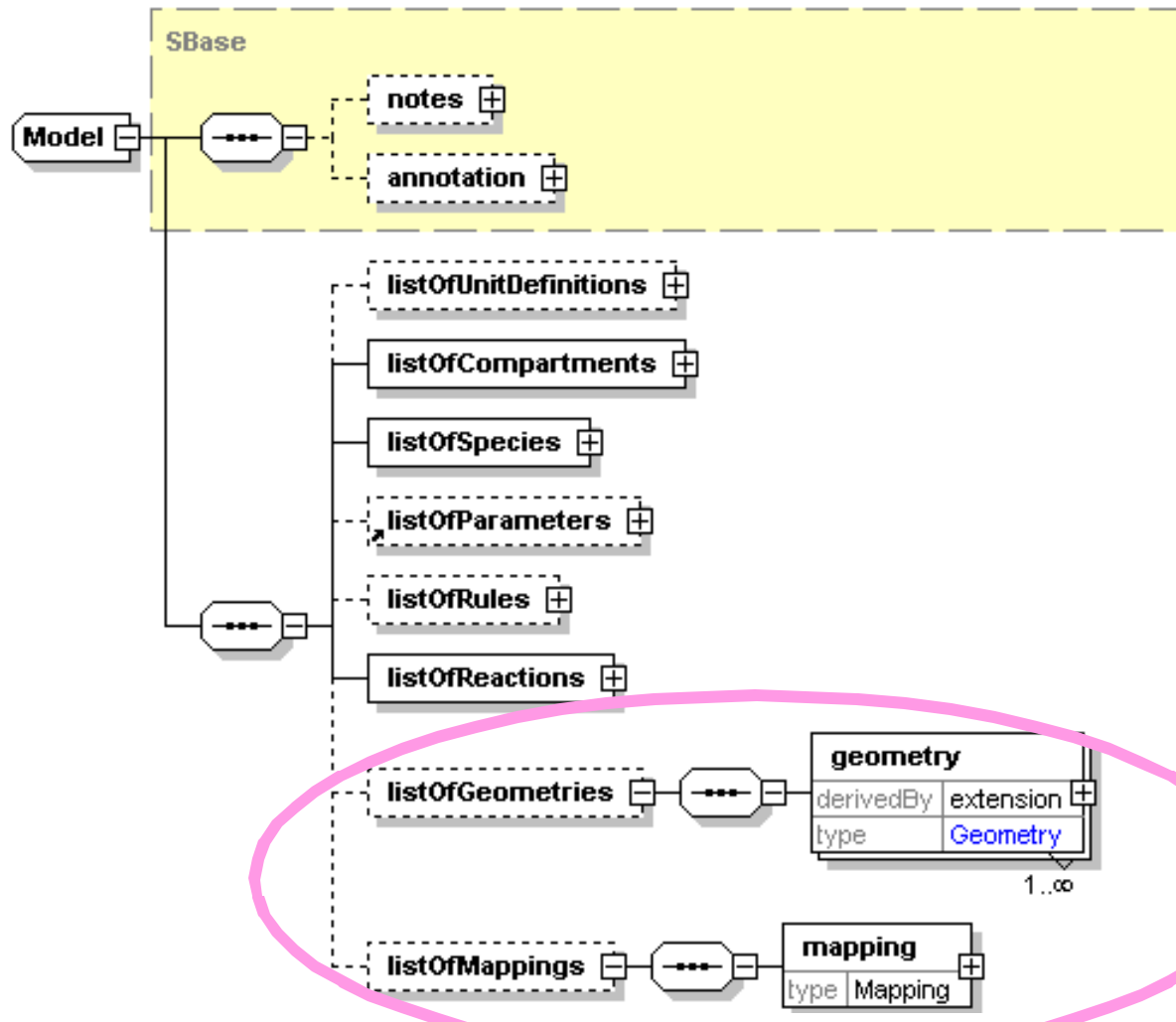
# Proposed SBML Geometry

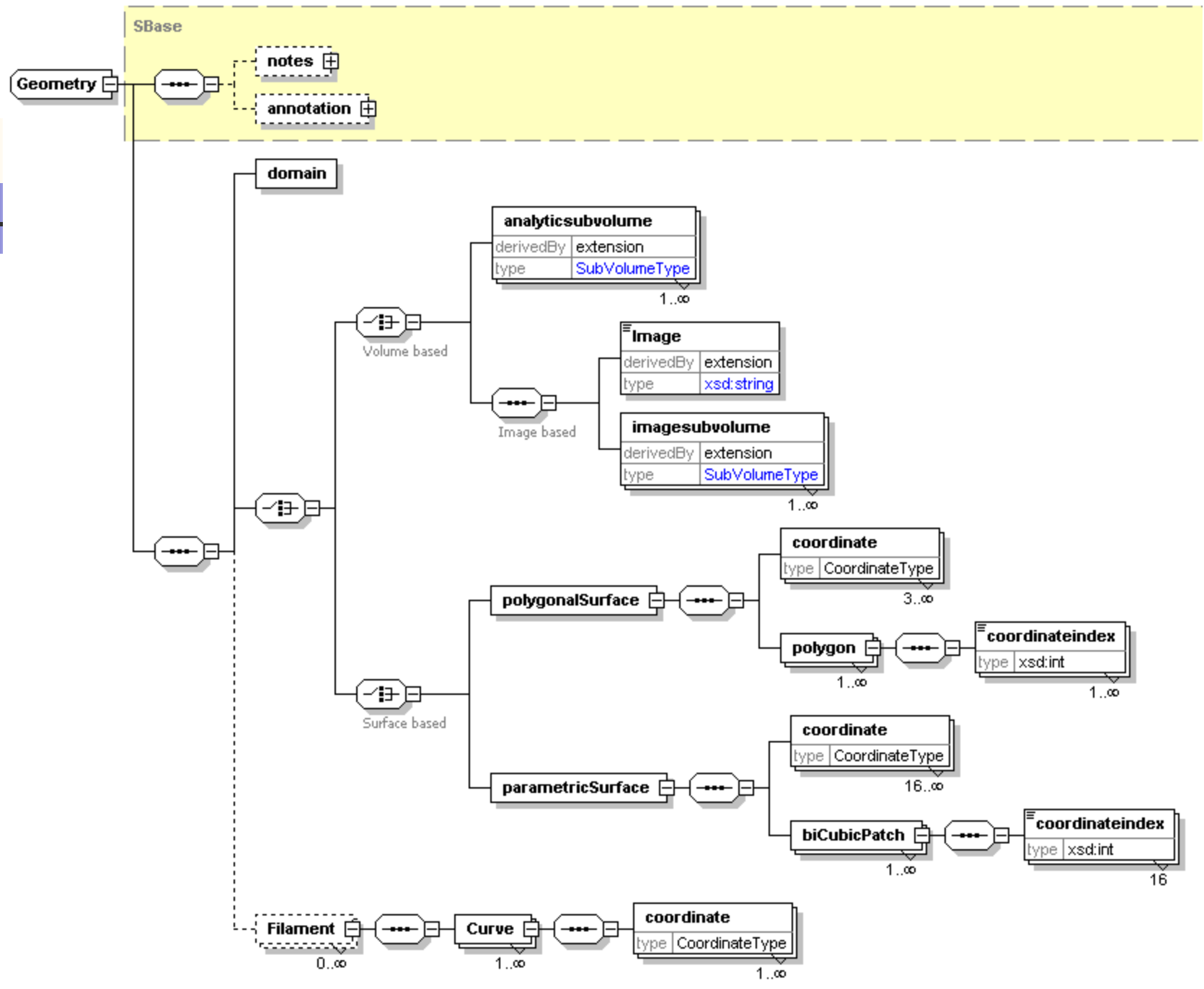
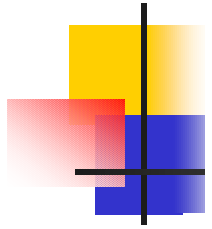
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This proposal includes the following concepts:

- Surface-based geometries
- Volume-based geometries
- Filaments
- Mappings

# Proposed SBML Geometry







Our web site:

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[www.nrcam.uchc.edu](http://www.nrcam.uchc.edu)