Space in VCell ("Virtual Cell")

- Mapping Structures to Geometries -

http://vcell.org
What is a Model?
VCell Top-Level Documents

• Database object containers
  – BioModel
  – MathModel
  – Geometry

• Referential objects
  – ResultSet
  – FieldData
SimulationSpec Element

– a.k.a. “Application” wizard, a.k.a. SimulationContext object –
Spatially Resolved Species

• Initial Concentrations:
  – PDE:
    • Concentration FIELD
  – Stochastic:
    • Spatial distribution function FIELD

• Boundary Conditions:
  – PDE:
    • specified concentration FIELD (Dirichlet)
    • specified concentration FIELD (Neumann)
    • Periodic
  – Stochastic:
    • specified flux density probability FIELD
    • Periodic

• Diffusion Coefficient:
  – PDE & Stochastic:
    • (An)isotropic (optionally) spatially varying FIELD
VCell Geometry

GeometrySpec
(image-based or analytic)
Provides volume sampling
(surfaces are implicit)

GeometrySurfaceDesc
- Region Image
  (discriminates disjoint regions of same type)
- Volume/Membrane Regions
  (graph of all volume/surface instances with adjacency and size metrics)
- Surface sampling – visualization params

OR

bounding box extent/origin

\[ x^2 + y^2 + z^2 < R^2 \]

Analytic SubVolume
- cytosal
- ec

Provides Volume Sampling Function

x, y, z

SubVolume
Geometry Specification

Provides Volume Sampling Function

OR

bounding box extent/origin

VCell Image

Image SubVolume
- nucleus
- cytosol
- ec

Analytic SubVolume
- cytosol
- ec

\[ x^2 + y^2 + z^2 < R^2 \]

x, y, z

SubVolume
Geometry Visualization

Image-based Geometry

Sampled at original image resolution

Analytic Geometry

Sampled at “arbitrary” resolution

Sampled Volume

Generated Surfaces (smoothed staircase “quads”)
Summary – 2 separate domains
...spatial model elements… (~“L3 spatial”)
...geometry descriptions… (~“L3 geom”)

```xml
<vcspatial:listOfSpatials
  xmlns:vcspatial="http://spatial.vcell.org/sbml/level3">
  <vcspatial:spatial>
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  </vcspatial:spatial>
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