University of Connecticut Health Center

Space in VCell ("Virtual Cell")

– Mapping Structures to Geometries –

http://vcell.org

National Institute of General Medical Sciences

NIH Roadmap

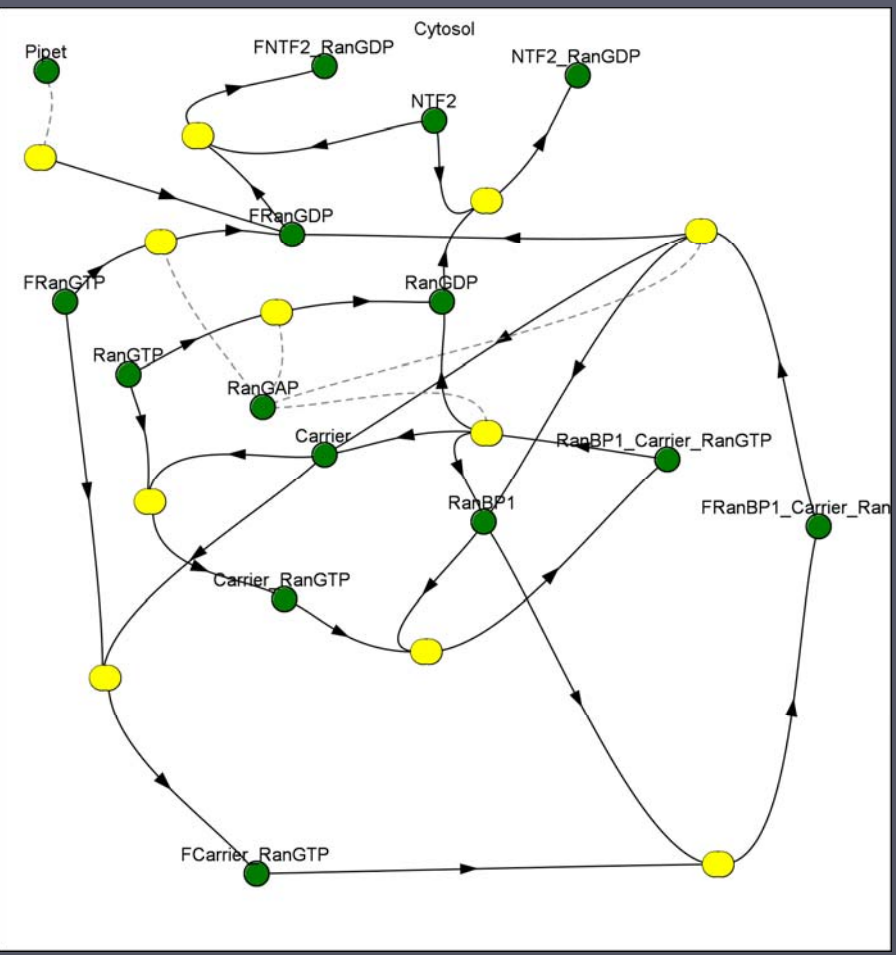
National Center for Research Resources

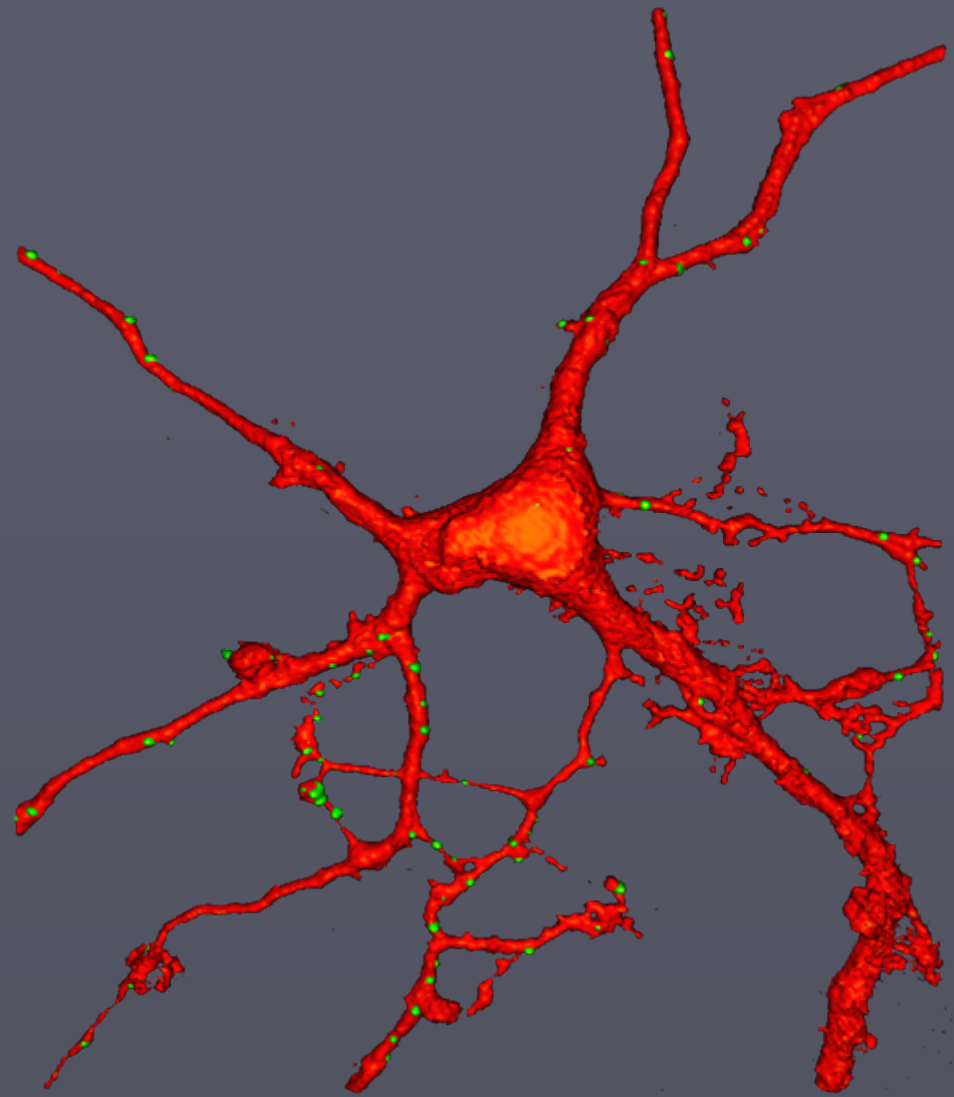
Richard D. Berlin

Center for Cell Analysis and Modeling

National Technology Center for Networks and Pathways

What is a Model?



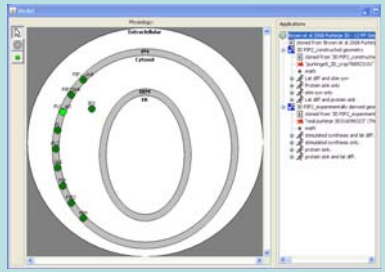


VCell Top-Level Documents

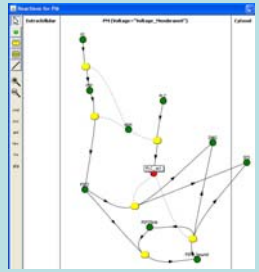
- Database object containers
  - BioModel
  - MathModel
  - Geometry
- Referential objects
  - ResultSet
  - FieldData

Physiology

Molecules
Structures
(topology)

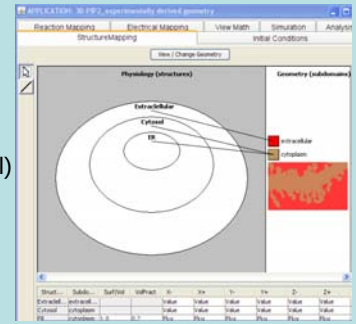


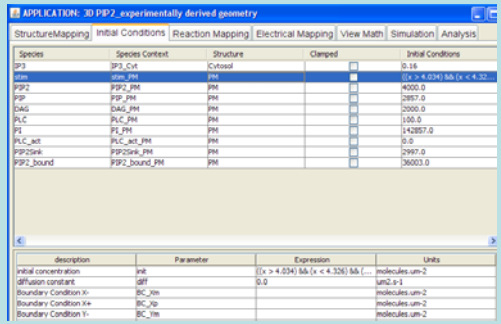
Reactions
Fluxes



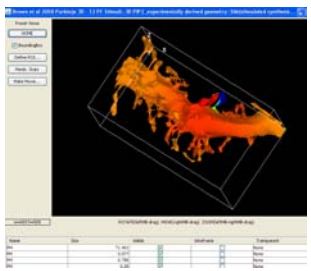
Applications

Structure mapping
(topology to geometry)
Initial Conditions
Boundary conditions
Diffusion constants (if spatial)
Electrophysiology protocols
Enable/disable reactions
Fast reactions
Model analysis
Stochastic rate conversion





Results

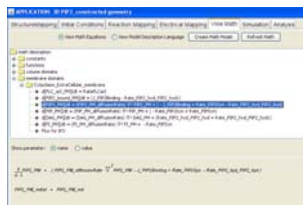


Simulations

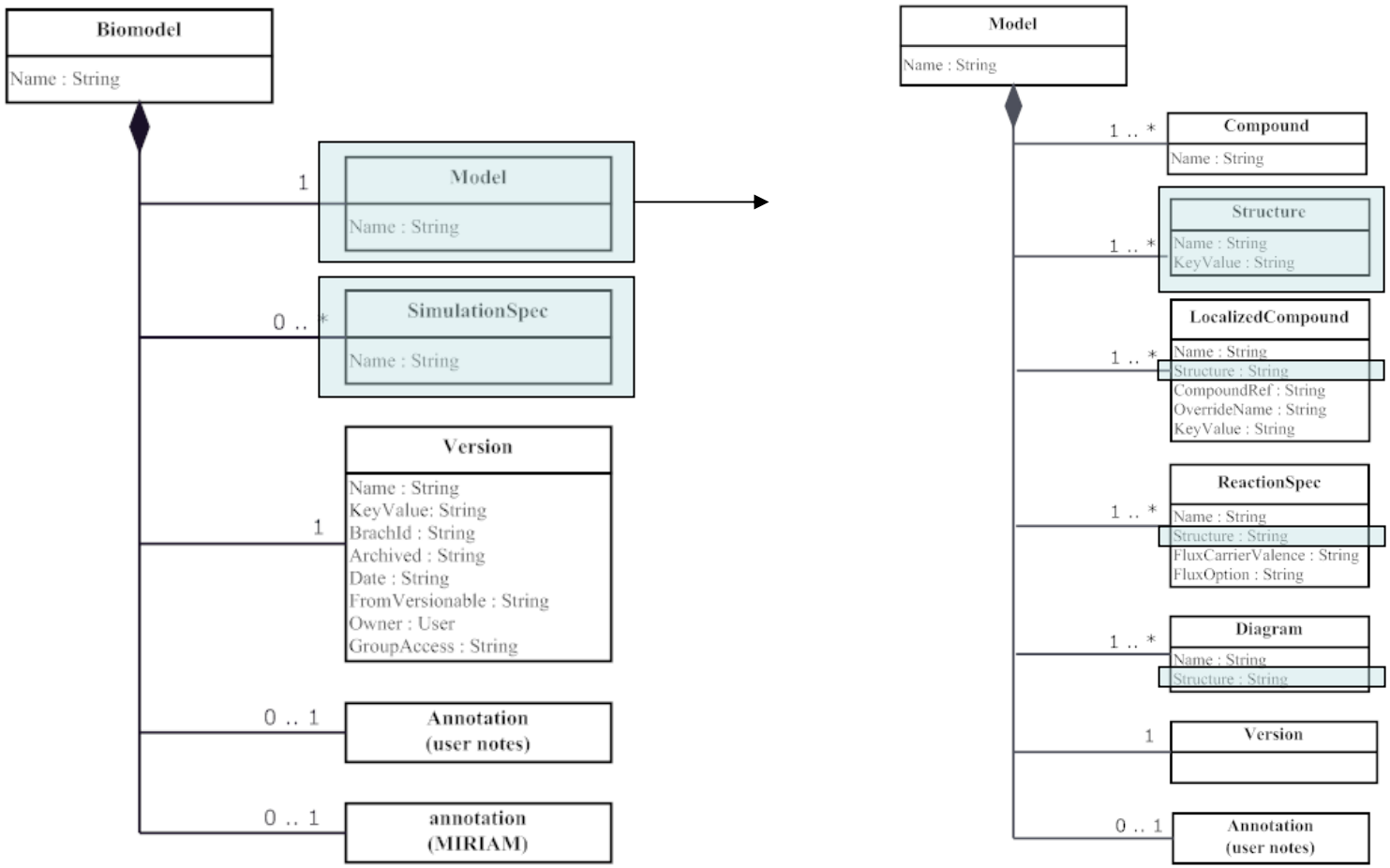
Timecourse
Timestep
Mesh size
Solver type
Solver settings
Parameter changes
Parameter scans
Parameter sensitivity

Mathematical Description

(view-only, automatically generated)

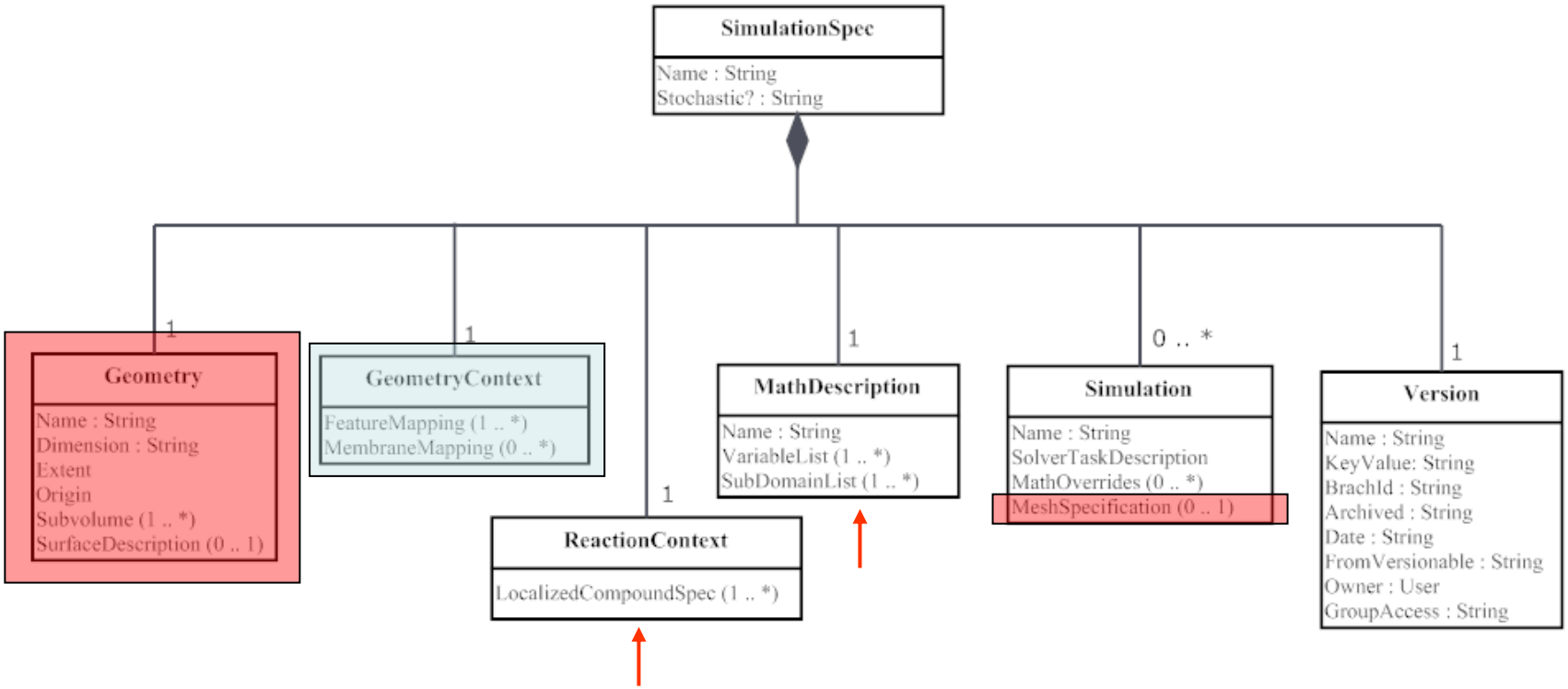


BioModel Object Hierarchy



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

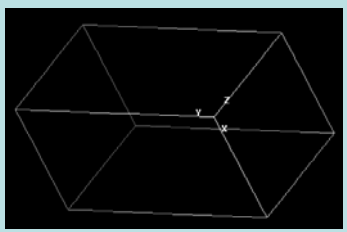
(graph of all volume/surface instances with adjacency and size metrics)

-Surface sampling – visualization params

Provides Volume Sampling Function

OR

bounding box extent/origin



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

1.0

Analytic SubVolume

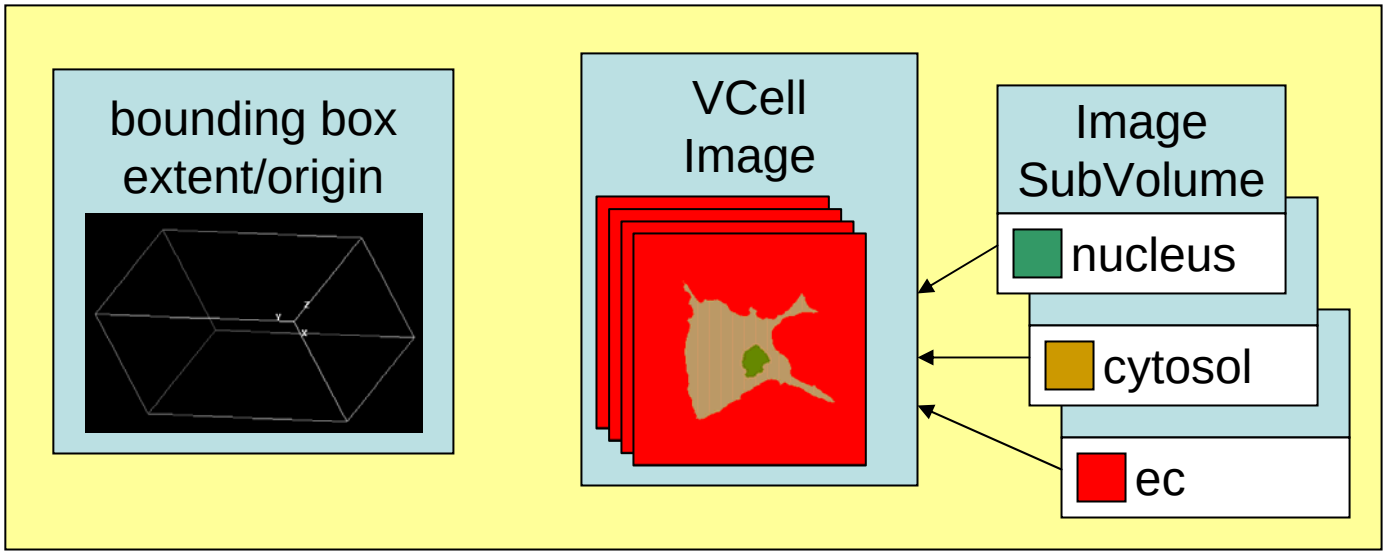
cytosol

ec

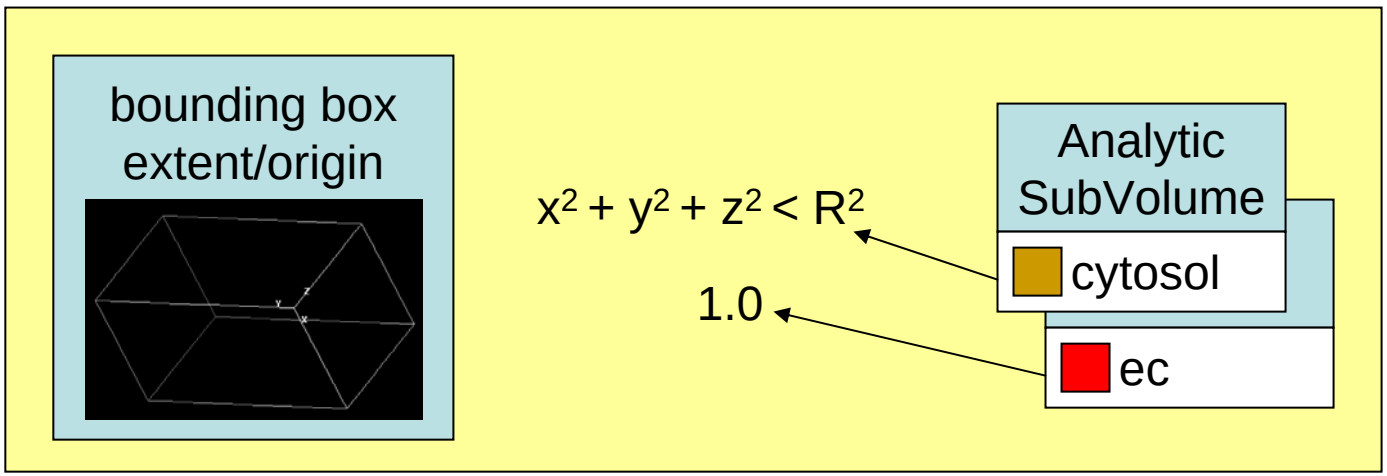
x, y, z

SubVolume

Geometry Specification



OR



Provides Volume Sampling Function

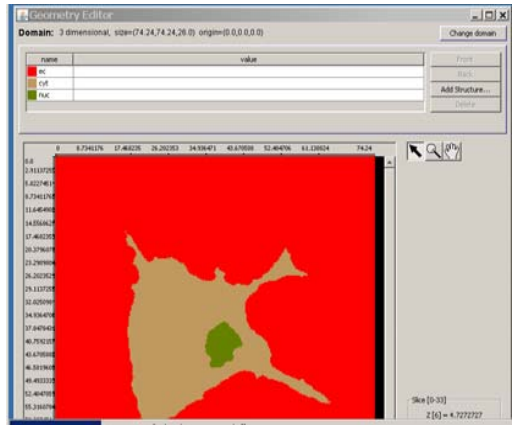
x, y, z

SubVolume

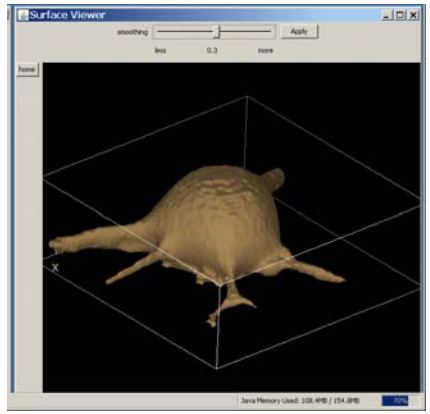
Geometry Visualization

Image-based Geometry

Sampled at original image resolution



Sampled Volume

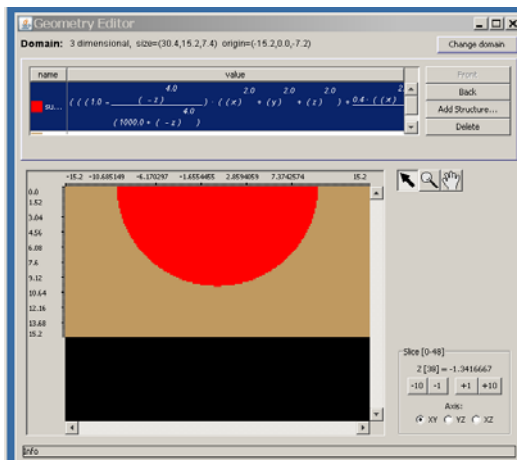


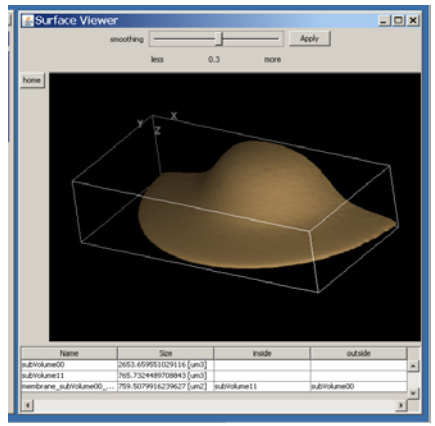
Generated Surfaces (smoothed staircase "quads")

Analytic Geometry

$$\left(\left(1.0 - \frac{4.0}{(1000.0 + (-z))}\right) \cdot (x)^{2.0} + (y)^{2.0} + (z)^{2.0}\right)$$

Sampled at "arbitrary" resolution

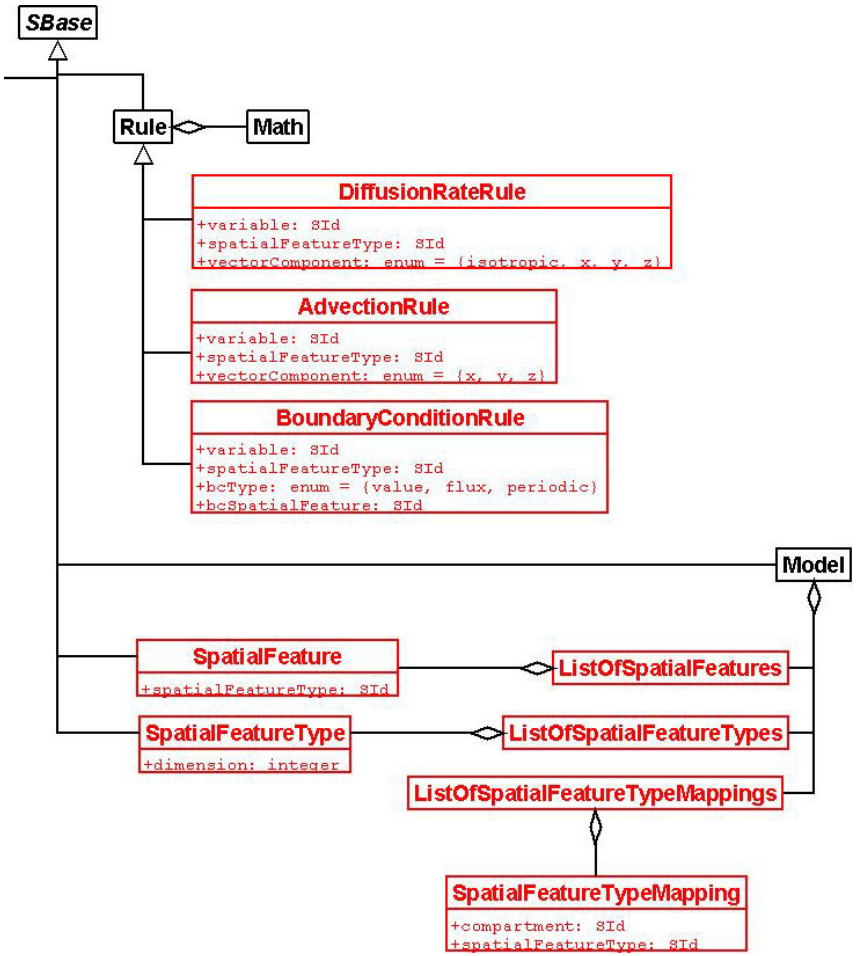




Summary – 2 separate domains

…spatial model elements… (~“L3 spatial”)

…geometry descriptions… (~“L3 geom”)

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