

Space in VCell ("Virtual Cell")

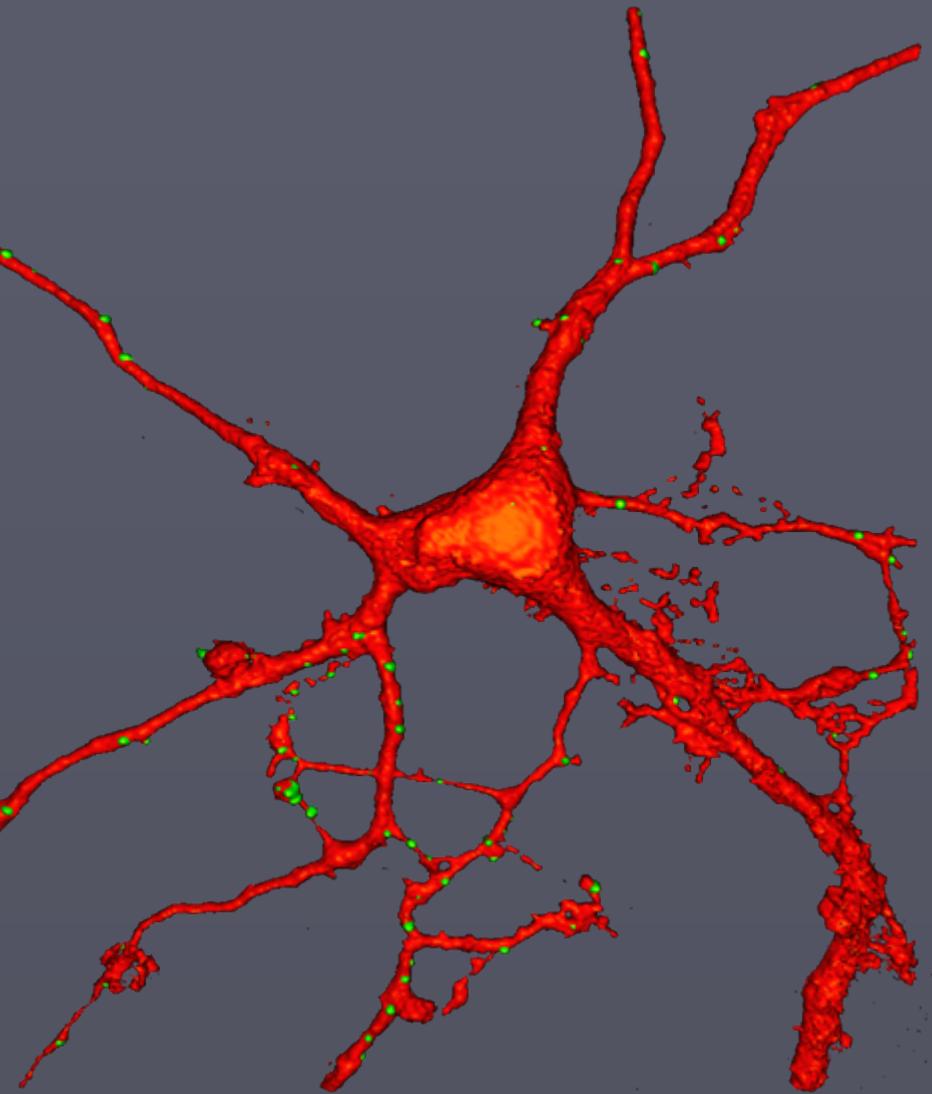
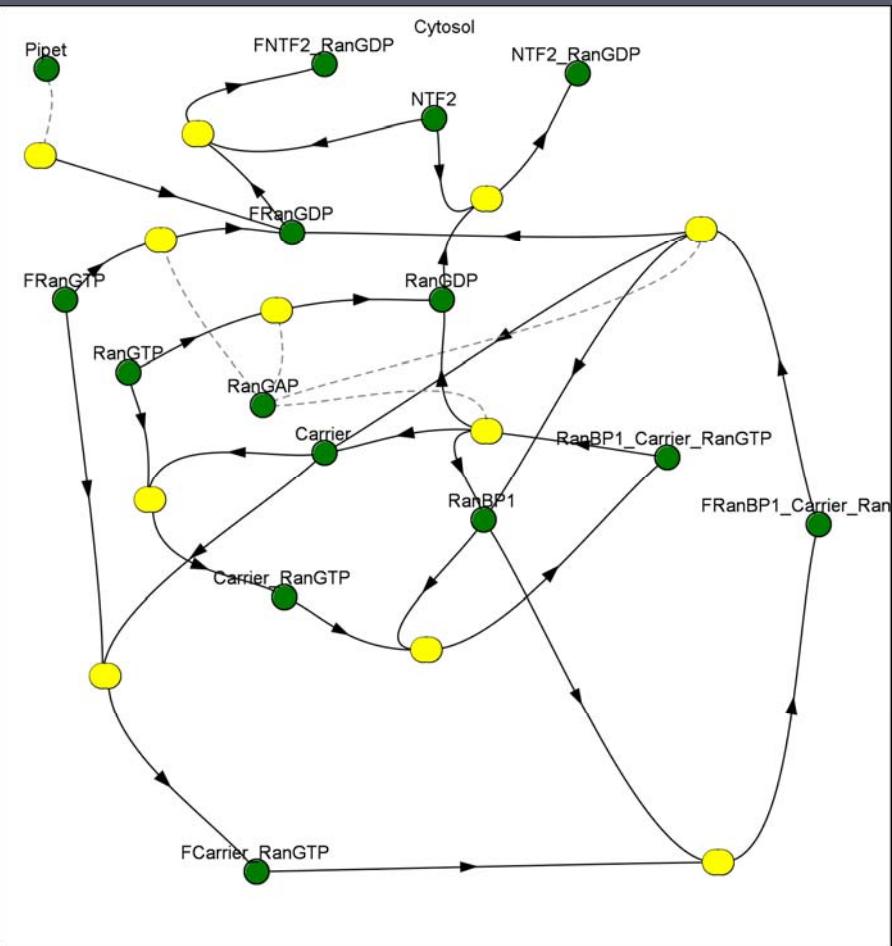
– Mapping Structures to Geometries –

<http://vcell.org>



Richard D. Berlin
Center for Cell Analysis and Modeling

What is a Model?

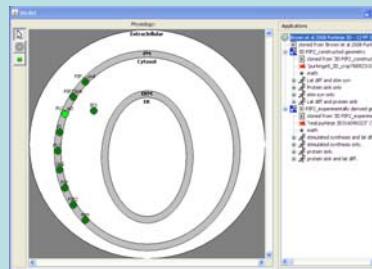


VCell Top-Level Documents

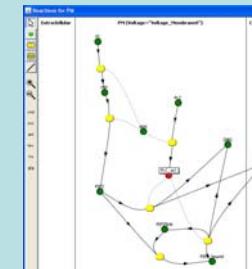
- Database object containers
 - BioModel
 - MathModel
 - Geometry
- Referential objects
 - ResultSet
 - FieldData

Physiology

Molecules
Structures
(topology)

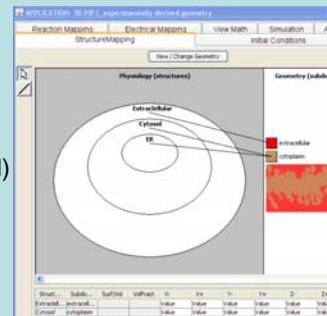


Reactions
Fluxes



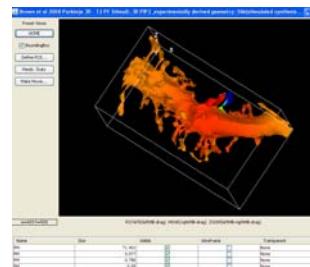
Applications

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



Species	Species Context	Structure	Clamped	Initial Conditions
IP3	IP3_Cyt	PM		0.16 (x < 4.32)
IP2	IP2_PM	PM		4000.0
IP1	IP1_PM	PM		2957.0
DAG	DAG_PM	PM		2000.0
PLC	PLC_PM	PM		100.0
PL	PL_Cyt	PM		142857.0
PLC_act	PLC_act_PM	PM		0.0
PLC_2act	PLC_2act_PM	PM		2947.0
PL2_bound	PL2_bound_PM	PM		36003.0

Results



Simulations

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

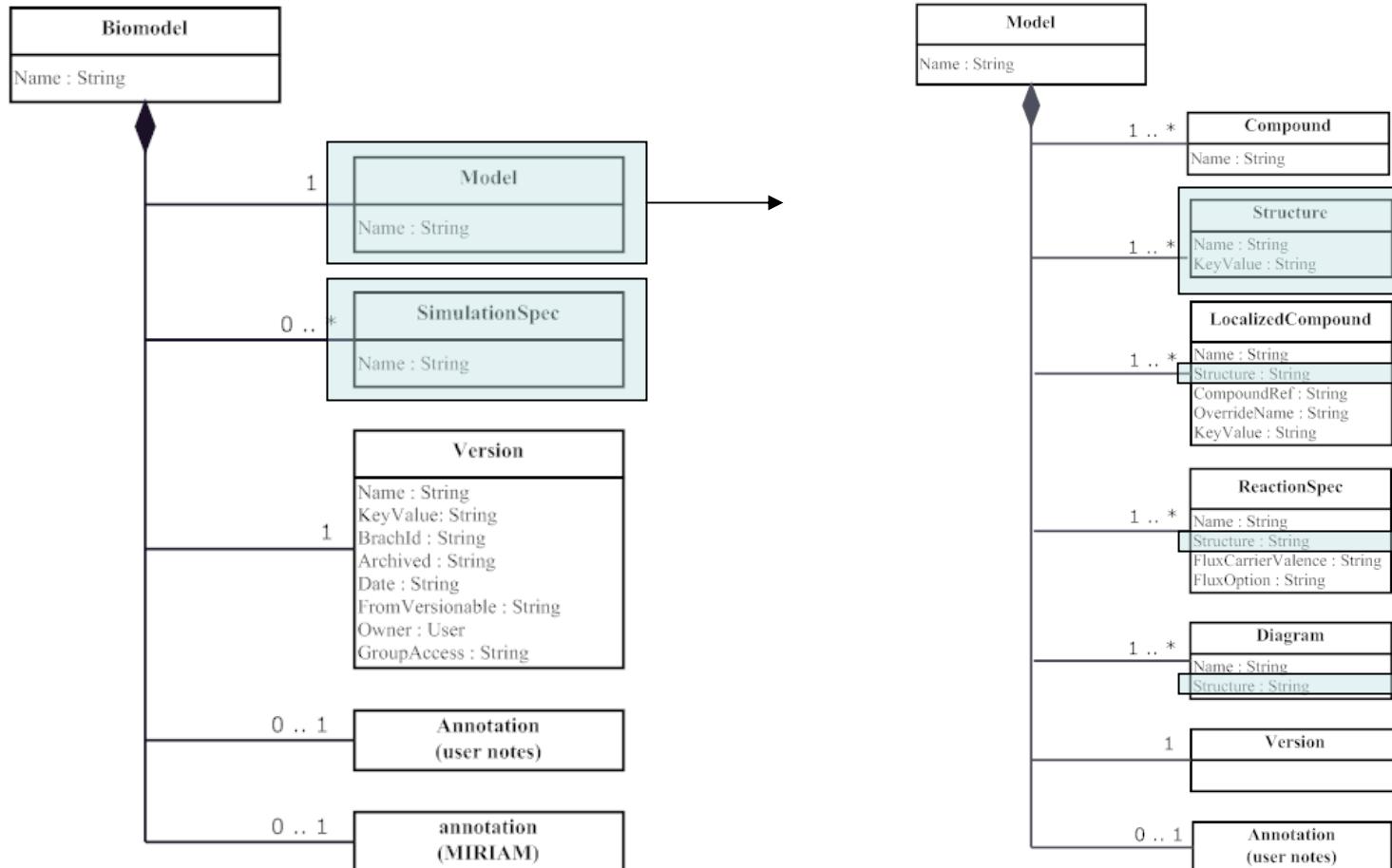
Specify non-default parameter values or scan over a range of values:			
Parameter Name	Default Value	Change Value	Scan
Sal_P0_cyt	2000.0		
IP3_cyt	0.16		
IP2_cyt	4000.0		
IP1_cyt	2957.0		
DAG_cyt	2000.0		
PLC_cyt	100.0		
PL_cyt	142857.0		
PLC_act_cyt	0.0		
PLC_2act_cyt	2947.0		
PL2_bound_cyt	36003.0		
IP3_cyt	0.16	0.05	
IP2_cyt	4000.0	0.0	
IP1_cyt	2957.0	0.0	
DAG_cyt	2000.0	0.0	
PLC_cyt	100.0	0.0	
PL_cyt	142857.0	0.0	
PLC_act_cyt	0.0	0.0	
PLC_2act_cyt	2947.0	0.0	
PL2_bound_cyt	36003.0	0.0	

Mathematical Description
(view-only, automatically generated)

```
# This file contains the mathematical description of the model, generated automatically by the software. It includes the system of differential equations and boundary conditions.
```

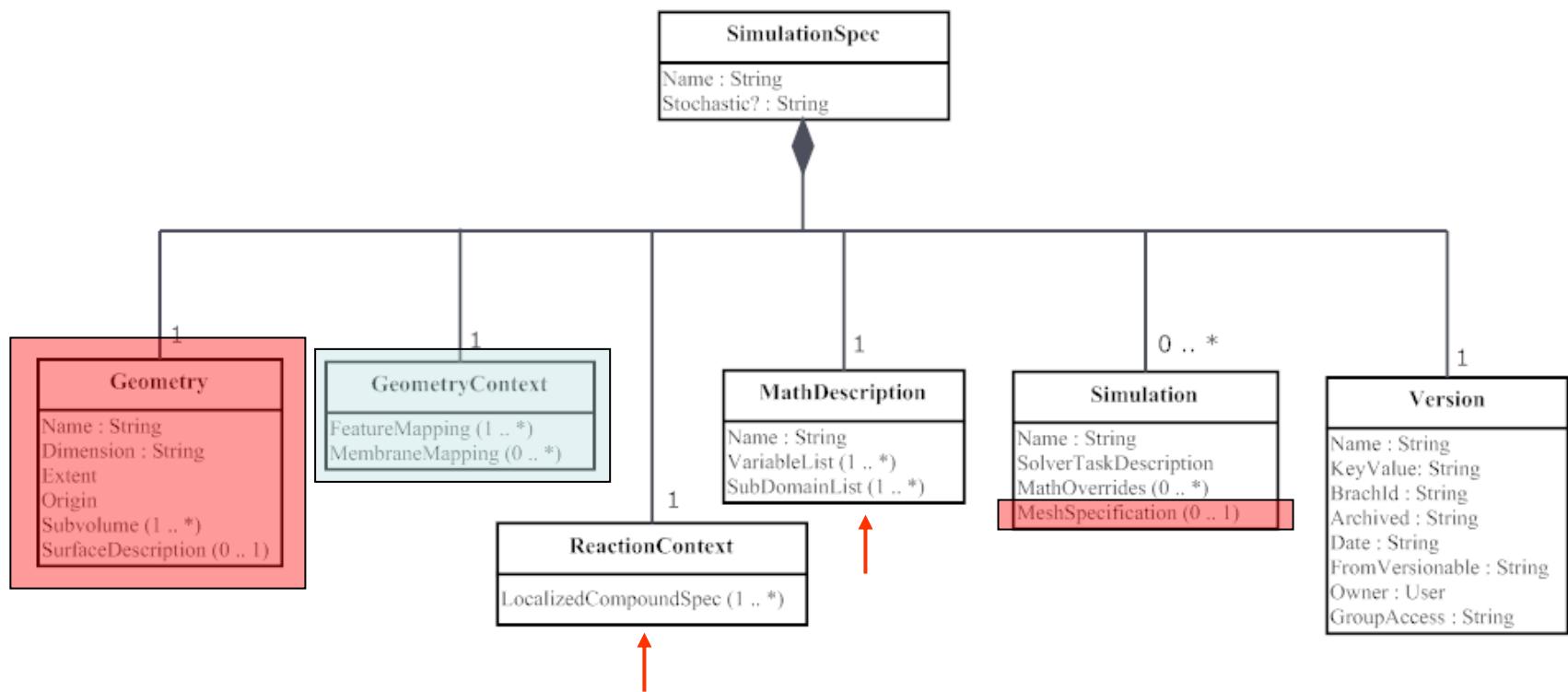
$$\frac{\partial}{\partial t} [IP3]_P = -k_{IP3_act} [IP3]_P + k_{IP3_2act} [IP2]_P^2 - k_{IP3_bind} [IP3]_P [PLC]_P + k_{IP3_diss} [IP3]_P$$
$$\frac{\partial}{\partial t} [IP2]_P = k_{IP3_act} [IP3]_P - 2k_{IP2_act} [IP2]_P^2 + k_{IP2_bind} [IP2]_P [PLC]_P - k_{IP2_diss} [IP2]_P$$
$$\frac{\partial}{\partial t} [IP1]_P = k_{IP2_act} [IP2]_P^2 - k_{IP1_act} [IP1]_P + k_{IP1_bind} [IP1]_P [PLC]_P - k_{IP1_diss} [IP1]_P$$
$$\frac{\partial}{\partial t} [DAG]_P = k_{IP1_act} [IP1]_P - k_{DAG_act} [DAG]_P + k_{DAG_bind} [DAG]_P [PLC]_P - k_{DAG_diss} [DAG]_P$$
$$\frac{\partial}{\partial t} [PLC]_P = k_{IP1_bind} [IP1]_P [PLC]_P - k_{PLC_act} [PLC]_P + k_{PLC_2act} [PLC]_2 [PLC]_P - k_{PLC_diss} [PLC]_P$$
$$\frac{\partial}{\partial t} [PL]_P = k_{PLC_act} [PLC]_P - k_{PL_diss} [PL]_P$$
$$\frac{\partial}{\partial t} [PLC_act]_P = k_{PLC_act} [PLC]_P - k_{PLC_2act} [PLC]_2 [PLC]_P$$
$$\frac{\partial}{\partial t} [PLC_2act]_P = k_{PLC_2act} [PLC]_2 [PLC]_P - k_{PLC_act} [PLC]_P$$
$$\frac{\partial}{\partial t} [PL2_bound]_P = k_{PL2_bind} [PL2]_P [PL]_P - k_{PL2_diss} [PL2_bound]_P$$

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

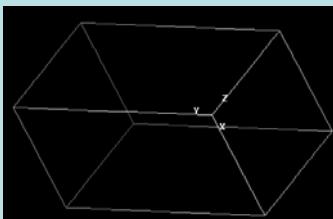
(graph of all volume/surface instances
with adjacency and size metrics)

-Surface sampling – visualization params

Provides
Volume
Sampling
Function

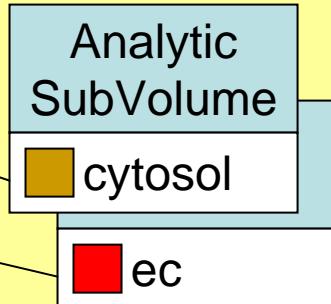
OR

bounding box
extent/origin



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

1.0



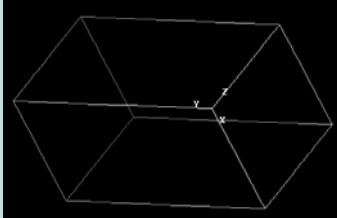
x, y, z



SubVolume

Geometry Specification

bounding box
extent/origin



VCell
Image

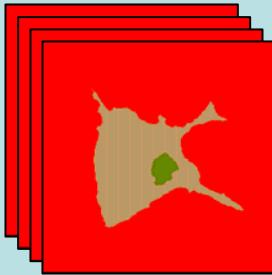


Image
SubVolume

nucleus

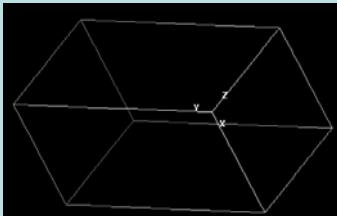
cytosol

ec

Provides
Volume
Sampling
Function

OR

bounding box
extent/origin



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

1.0

Analytic
SubVolume

cytosol

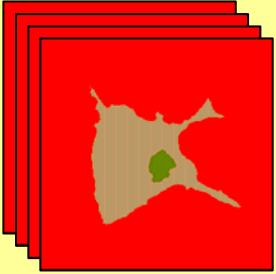
ec



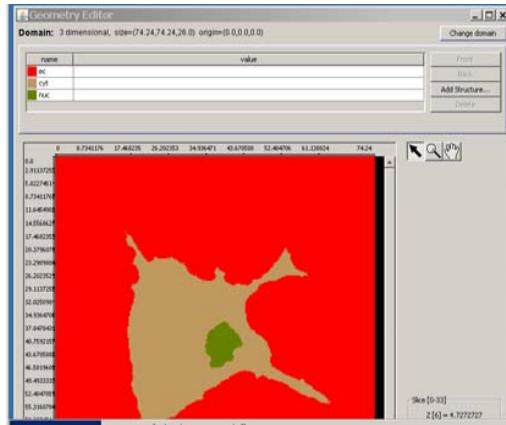
SubVolume

Geometry Visualization

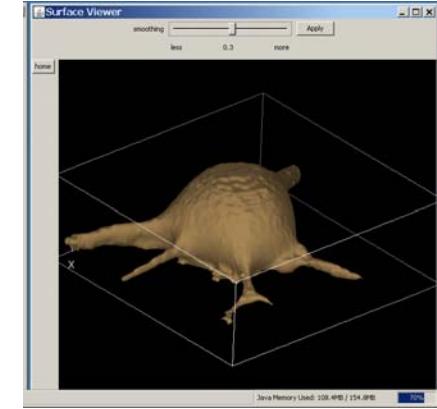
Image-based Geometry



Sampled at
original image
resolution



Sampled
Volume

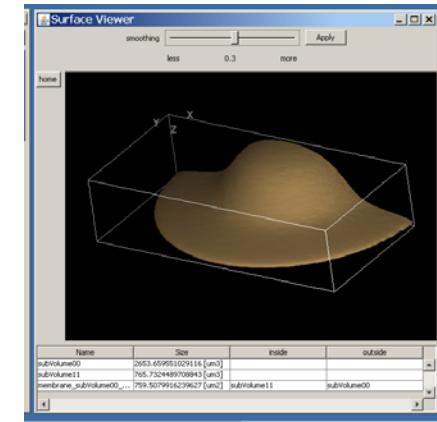
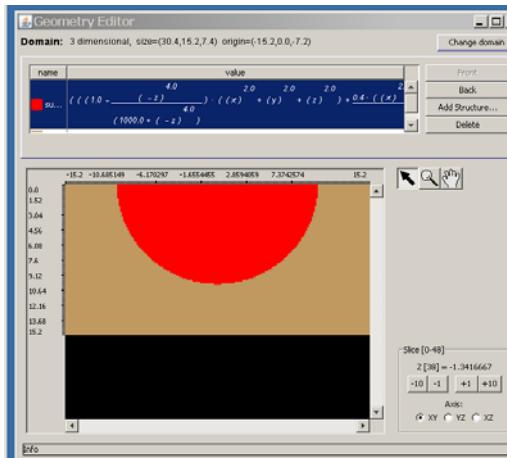


Generated Surfaces
(smoothed staircase
“quads”)

Analytic Geometry

$$\left(\left(1.0 - \frac{4.0}{(-z)} \right) \cdot \left((x)^2 + (y)^2 + (z)^2 \right) \right)$$

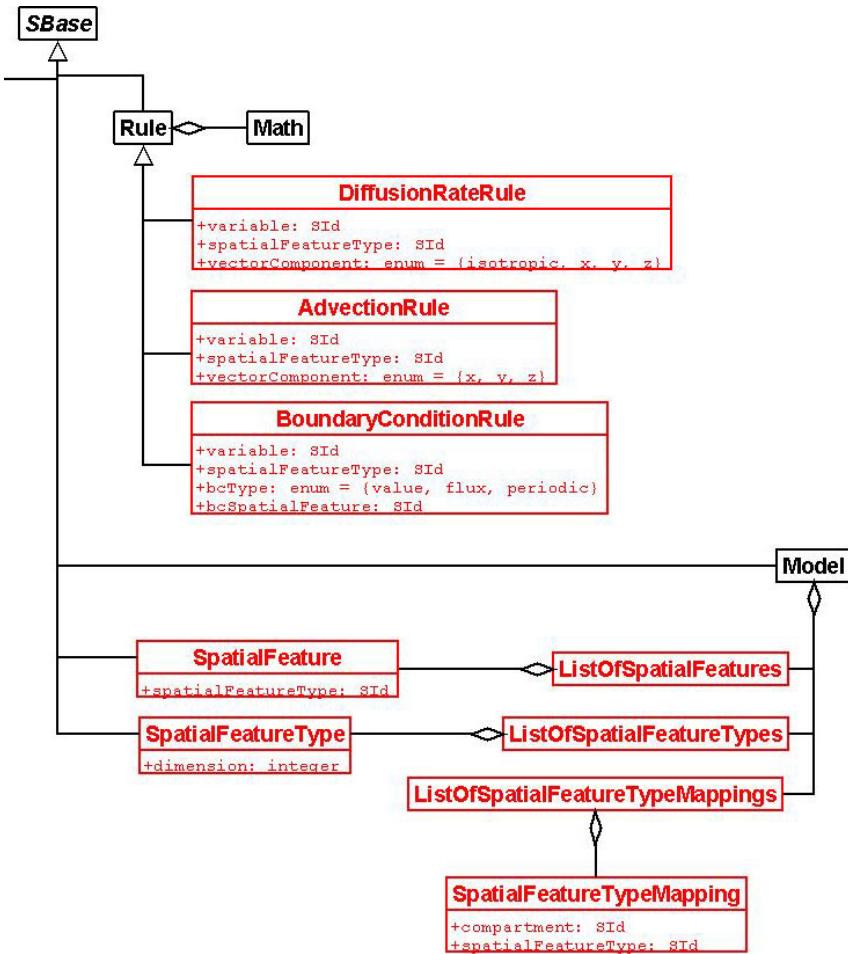
Sampled at
“arbitrary”
resolution



Generated Surfaces
(smoothed staircase
“quads”)

Summary – 2 separate domains

- ... spatial model elements... (~“L3 spatial”)
- ... geometry descriptions... (~“L3 geom”)



```

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      <vcspatial:domain name="ec1" id="ec1" domainType="extracellular"/>
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