Spatial Modeling in SBML

Issues for Level 3

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VCell Project

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Perspective (space vs. time)

- Domain:
  - Time: t = 0 … Infinity; or (–Infinity … Infinity)
  - Space: defined by geometry (within bounding box?)

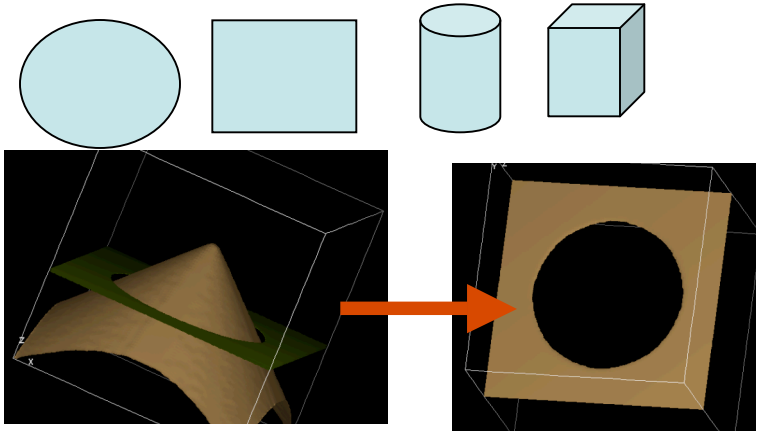
- Boundary Conditions:
  - Time: initial conditions, at t = 0, define value;
  - Space: at “edge” of geometry, define value, or flux, or periodic

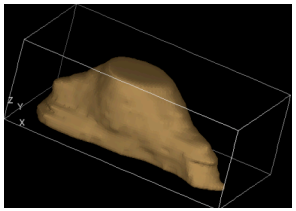
- Discontinuities
  - Time: events – discontinuous jumps across time
  - Space: (spatial discontinuities – e.g. membranes)

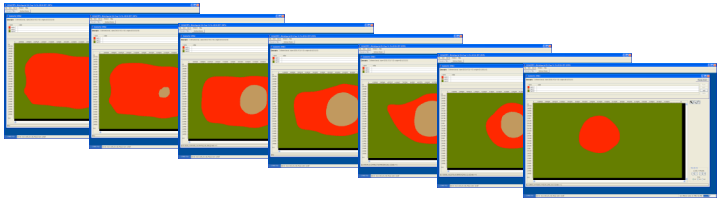
- Discretization
  - Time: outside SBML (**tool problem**: “integrator time step”)
  - Space: outside SBML (**tool problem**: “mesh”)

Geometric Description

- Geometric Primitives with
  - Sphere (center,radius)
- Implicit inside/outside functions
  - f(x,y,z) < 0
  - level-set image → [iso-surface, f()=0]
- Surface-based (polygonal)
- Segmented Images ?
  - Interpolate between slices
  - Need surface smoothing.
- Need common tools to convert between representations (libSPATIAL)
  - VCell ☺, ITK, VTK …







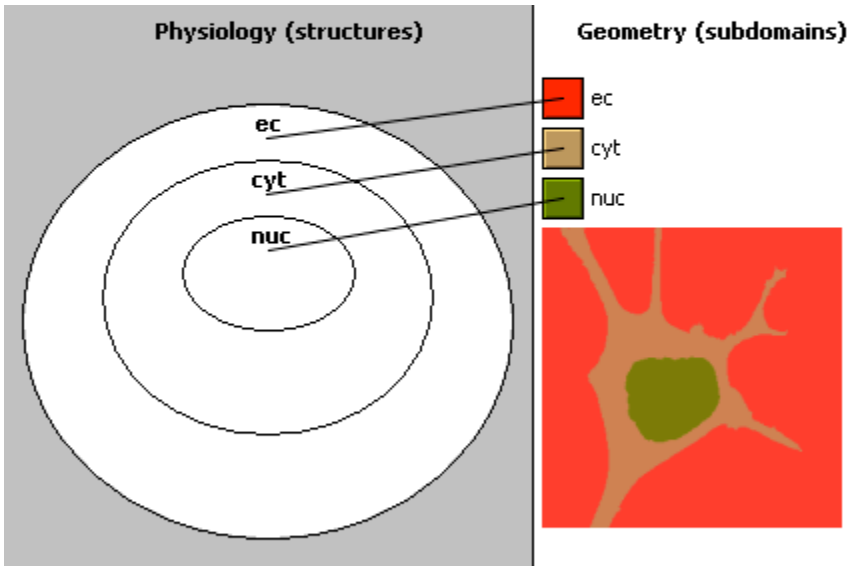
Spatial Domains (and types)

- Spatial domain types
  - 1D, 2D (water-tight membranes), 3D Geometric definitions (not meshes)
  - Set of domains with same biology (mapped from compartment)
  - Annotated for anatomical description.

- Mapping of compartments to spatial domain types
  - Dimensions of geometry may be < 3D.
    - compartment "cytosol" mapped to spatial domain type 2D
    - IMPORTANT ASSUMPTIONS of missing 3rd dimension … make explicit?

- Multiple instances spatial domains of spatial domain types.
  - e.g. multiple cells.
  - Bounding box?

- Topology of spatial domains
  - spatial⇔nonspatial



Definition: Field

- Scalar valued function of position defined over a domain
  - Coordinate system (e.g. Cartesian, cylindrical, spherical)
  - F(**x**,t,**p**,**u**) where
    - **x** is a position (x,y,z) or (r,theta),
    - **p** are parameters,
    - **u** are variables,
    - t is time
  - image/lookup table (with basis function for interpolation)
- Examples:

– Example 1:	sin(x)*cos(y)	**explicit function of space**
– Example 2:	sin(x)*cos(y)*t	**explicit function of space and time**
– Example 3:	(x<3)?(5):(0)	**discontinuous function of space**
– Example 4:	4*calcium	**if "calcium" is a field**
– Example 5:	<image ref>, scale, offset, size, bilinear interpolation	**image**

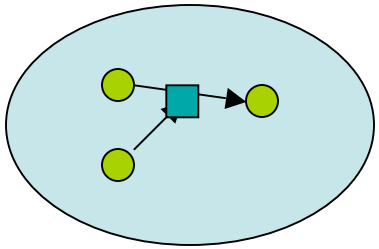
Spatially Resolved Species

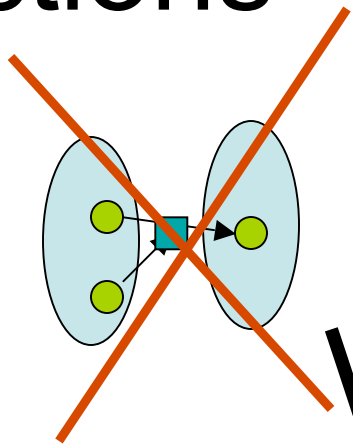
- Initial Conditions:
  - PDE:
    - Concentration **FIELD**
  - Stochastic:
    - "Spatial Distribution Function" **FIELD**
    - List of initial positions (orientation?) for each individual
- Boundary Conditions:
  - PDE:
    - specify concentration **FIELD** (Dirichlet)
    - specify flux **FIELD** (Neumann)
    - periodic
  - Stochastic:
    - specify flux density probability **FIELD**
    - periodic

Spatially Resolved Species (continued)

- Diffusion Coefficient:
  - PDE:
    - **FIELD - defined everywhere, could spatially vary. (Could also be a function of local environment)**
  - Stochastic:
    - **FIELD – defined everywhere, could spatially vary.**

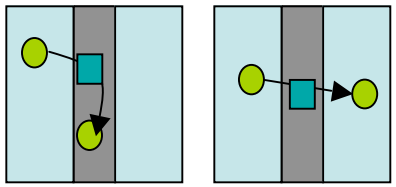
Spatially Resolved Reactions

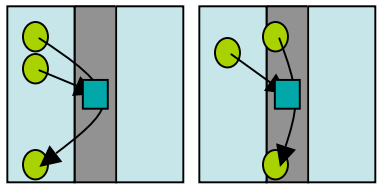


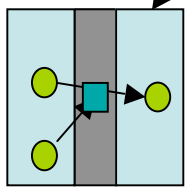


- Reaction locations needed
- Volume Reactions:
  - Reaction Rate:
    - Deterministic: concentration per time
    - Stochastic: function of true radii and “reactivity”???
  - Reactants/Products/Modifiers in same volume

- Membrane Reactions:
  - Reaction Rate:
    - Deterministic: surface density per time (or flux density)
    - Stochastic: function of true radii and “reactivity”???
  - Reactants/Products/Modifiers in same “membrane” or adjacent volumes.







Related efforts

- Geometry Specifications:
  - CAD formats (e.g. IGES)
  - AVS/UCD, STL, VTK, ITK
- Spatial Modeling Languages
  - CellML/FieldML
  - VCML, … other spatial simulation descriptions.
- Other Spatial Modeling Frameworks
  - lattice models
  - tissue/morphogenesis modeling
  - Agent-based populations of cells

Summary

- Geometry definition - not meshes
- Spatial distributions - functions or lookup tables
- All Reactions localized.
- Reactions rate in density/time for continuous
- Map compartments to SpatialDomainType
- Need shared geometry processing libraries (libSPATIAL)

- Spatial Proposal from community input.
- Start wiki at http://ntcnp.org/ … move to http://sbml.org