Spatial processes and geometry

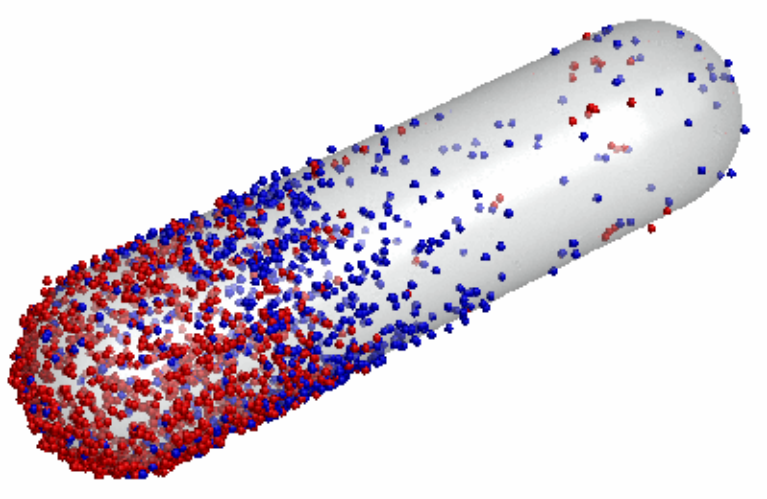
What?

Why?

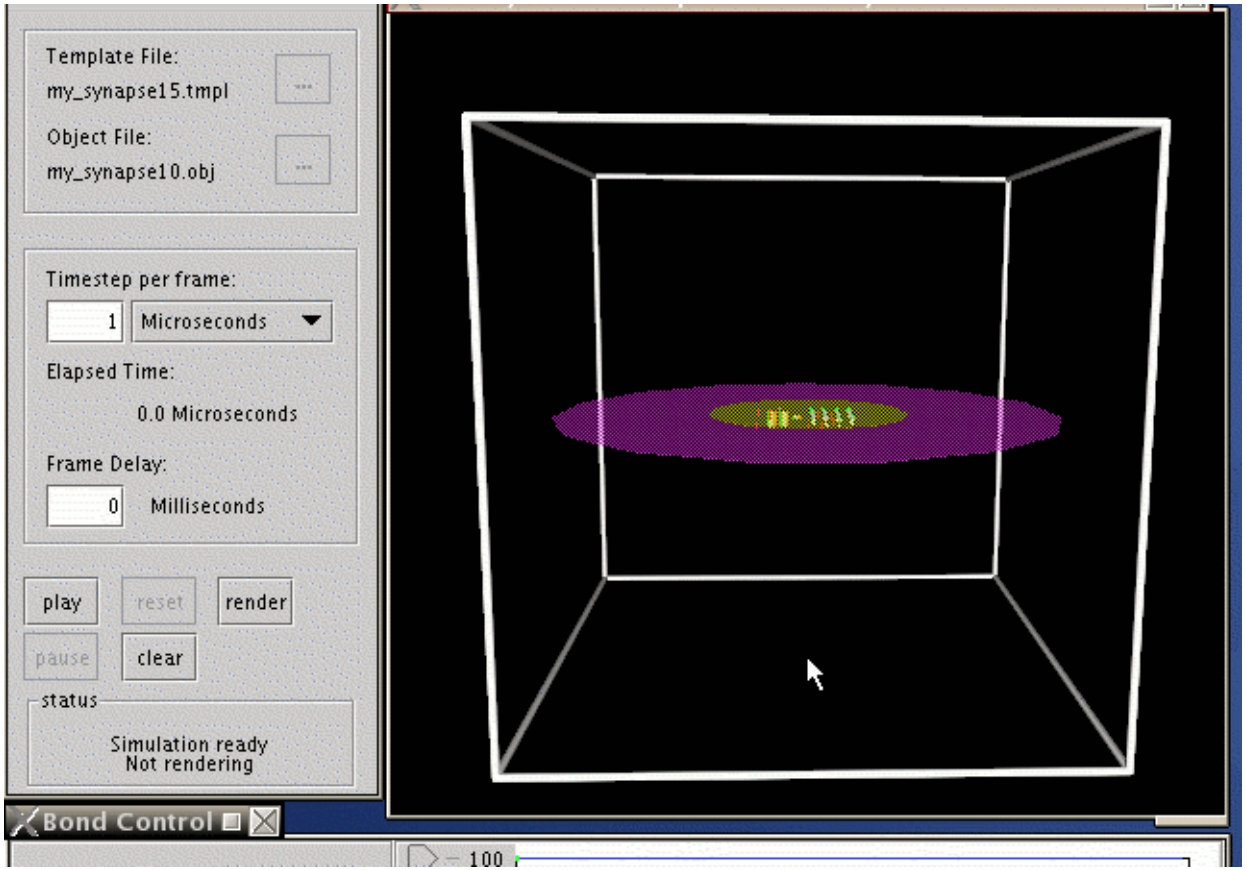
How?

http://sbml.org/wiki/Spatial_Features

Finite elements



Individual particles



Geometry extension

- Aim: Describe the topology and the deformation of SBML physical entities: compartments and species
- Use examples:
  - The morphology of neuronal compartments is central to the treatment of signals, whether electrical or calcium diffusion.
  - The topology of supra-macromolecular structures in the post-synaptic junction affects the signal transduction.
- What it codes:
  - space associated with the model
  - Initial geometry of objects
  - Deformation laws
  - Rules

Geometry extension

- What it does not code:
  - MesoRD: We think it is a good idea to describe geometry independent of the particular algorithm that will be used to analyze the SBML model.
- constraints
  - JS: rather than use "outside compartment", we need adjacency lists. This enables us to encode non-tree (cyclic) topologies and those that have no parent/child relationships.
  - JS: we need a relative spatial domain (xmin,ymin,zmin,xmax,ymax,zmax) and associated coordinate system (with reserved symbols for spatial coordinates) or some other notion to size/origin of world. polar and cartesian.

Thoughts on possible Geometric representations

by James Schaff

1) geometric primatives with constructive solid geometry (union/intersection/difference of spheres, cones, planes, ...

2) implicit surfaces/volumes using inequalities in x,y,z

3) implicit surfaces/volumes using level sets

4) a set of piecewise analytic functions (e.g. polygonal surfaces ... WHICH IS TREATED AS A GEOMETRIC DEFINITION AND NOT A MESH) might provide an alternative mechanism for interchange that is easy to understand and unambiguous.

5) images are not geometries (without further interpretation). Under some circumstances, the uncertainty of surface location from images may be tolerable ... but rarely

6) One could provide services to generate (4) from (1)(2)(3)(5).

Link to other proposals

- Core arrays: if every Sid in SBML can represent an array in addition to a scalar, things become MUCH simpler
- Sets and bunches
- Parameter sets and distributions

Spatial processes

- Aim: support mathematical description using spatial concepts: PDE, but also finite elements, single-particle models etc.
- Use examples:
  - Differential location of a given species in subcellular compartments affects its function, e.g. the CaMKII differential phosphorylation in post-synaptic density and in cytosol
  - Hysteresis generated by the differential location of kinases and phosphatases.
  - MAPK cascade from the membrane to the nucleus.
- What it codes:
  - initial positions
  - movement laws
  - deformation laws
  - spatially variable parameters
  - boundary conditions

Spatial features

- What it does not code:
  - JS: meshes are not part of the model, rather part of the solution. However a separate mechanism for mesh interchange would be very useful.
  - MesoRD: We would not like if a specific spatial discretization is given in the SBML model.
- Constraints
  - Spatial operators (if we are going to allow "rate rules" for spatial models) du/dt = div(D*grad(u)).
  - We should be able to run the model without space representation and get something.

Dependencies on other packages

- Arrays and/or sets
- multi-component species
- parameter distributions
  - initial positions: uniform, gaussian, gradient distrib etc.
  - problem: arbitrary distributions, including originating from images or other complex (and huge) datasets.
  - See FieldML, morohML for info.
  - Do-we include all the info or do-we externalise some.
  - Interoperability?