Spatial Extension for SBML Level 3

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Geometric Object Definitions

Domain

DomainType
cytosol
cytosol_1

Coordinate System
bounding box
extent/origin

Geometry

Compartment Mapping

Compartment

Physiology

“local” reactions
diffusion
IC’s
BC’s

Interior Points

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

Surface Based

Geometric Object Definitions
Model: spatial parameters (x, D, velocityX, BC), local reactions, compartment-geometry mappings
Model:
spatial parameters \((x, D, \text{velocity}X, BC)\),
local reactions,
compartment-geometry mappings
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spatial parameters (x, D, velocityX, BC),
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Geometry

Geometry is reusable

Doesn’t refer to rest of model.
Abstract

Geometric Concepts
(domains/domainTypes)

Independent of particular geometric representation

Multiple Geometric Definitions in same model

Write as many as you can

Read the most convenient one.
Geometry (Abstraction)

domains, domainTypes, connectivity, coordinate system, geometry definition
required elements extension

- **Only SBML Core elements** (e.g. Parameters, Species, Compartments) *may define an identifier* for use within a MathML expression or as the target of a rule.

- But spatial models need to be able to define additional identifiers (x,y,z,domainSize,diffusionCoefficient) with semantics provided by the extension.

- Required Elements extension (Lucian Smith) allows other extensions to declare that they are changing the mathematical interpretation of an SBML Core element. So we can alter reactions to make them local and we can define new SBML Core parameters and but define them as attributes of the geometry.

```xml
<sbml xmlns="http://www.sbml.org/sbml/level3/version1/core" level="3" version="1"
    xmlns:req="http://www.sbml.org/sbml/level3/version1/requiredElements/version1"
    xmlns:spatial="http://www.sbml.org/sbml/level3/version1/spatial/version1"
    req:required="true" spatial:required="true">
    <sbml:parameter sbml:id="x" req:mathOverridden="spatial" req:coreHasAlternateMath="false">
        <spatial:spatialSymbolReference spatial:spatialReference="coord1"
            spatial:spatialType="coordinateComponent"/>
    </sbml:parameter>
</sbml>
```
Retooling VCell dogma

- Practical reconciliation of compartmental and spatial modeling
  - compartment topology only in geometry
  - Generalized spatial mapping (compartments/domains)
Richer prototype (VCell / Smoldyyn integration)

- **VCell**
  - explicit volumes (analytic or image-based)
  - implicit surfaces (compute approximate surfaces)
  - Deterministic modeling (pdes)
  - Concentration fields

- **Smoldyn**
  - Implicit volumes (with interior points)
  - explicit surfaces (polygonal)
  - Particle distributions (in progress).
libSBML 5.0 plugins

- **required elements (implemented)**
  - C++ and Swig Java binding

- **spatial extension (partial implementation)**
  - C++ and Swig Java binding
  - Partial model implementation
    - Compartment mappings
    - Other concepts via required elements package
  - Complete Abstract Geometry
  - Partial Concrete Geometry
    - Analytic only.
    - Images (sampledFields very soon).
Status

• **Documentation**
  – Draft proposal (12 pages and counting)
  – UML
  – XML Schema

• **Prototype implementation**
  – libSBML required elements extension (C++/Java)
  – libSBML spatial extension (C++/Java)
  – VCell Alpha / libSBML 5.0 / Smoldyn

• **Community**
  – Discussion (sbml-discuss → workshop)
  – Documentation (→ SBML wiki)
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