

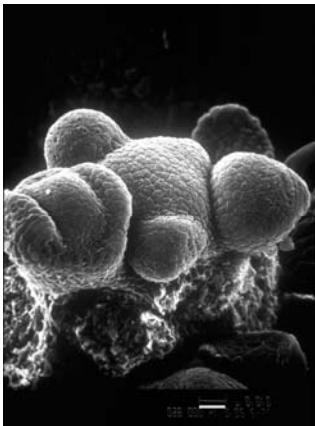
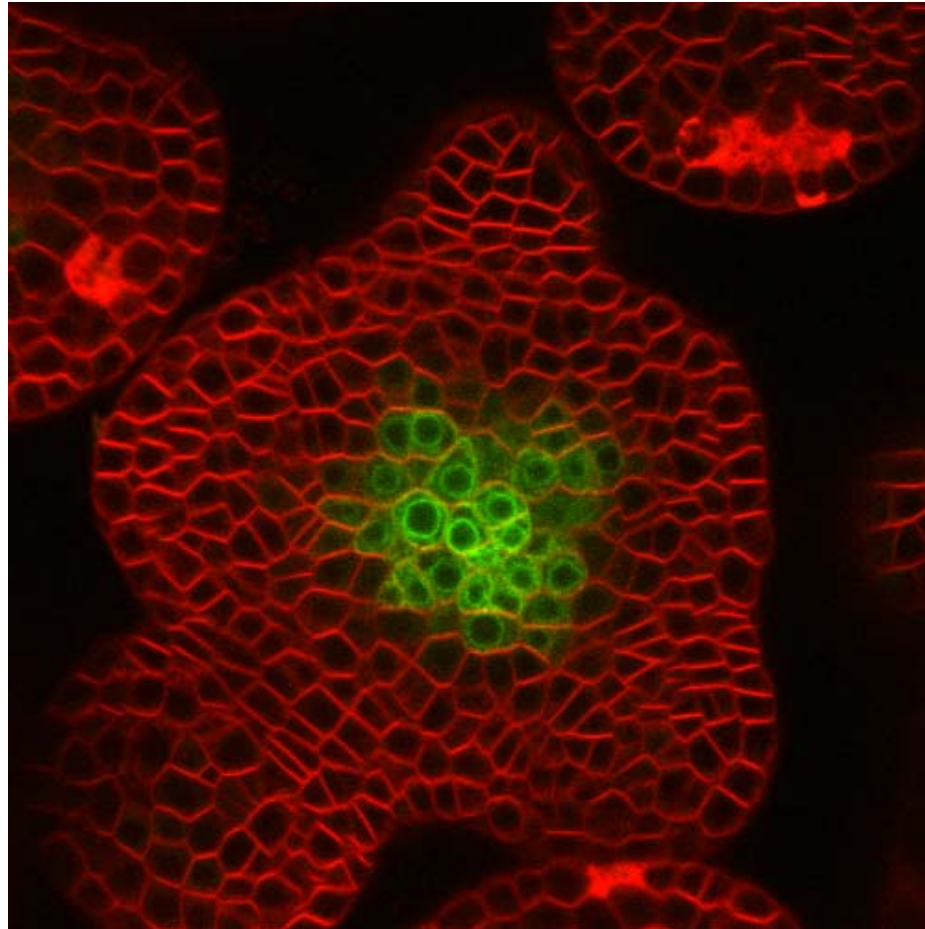
# Array Implementations in MathSBML and The Computable Plant

Bruce E Shapiro

bshapiro@caltech.edu

# Arrays: Level 3 Proposal

- <http://www.sbml.org/wiki/arrays>
  - Proposal 1 May 2003 by Andrew Finney *et al*
  - (One) Goal: Support developmental models of multicellular systems including dynamic arrays of compartments and other objects
- MathSBML: <http://sbml.org/software/mathsbml/>
  - *Mathematica* package for SBML model manipulation & simulation
  - Includes partial implementation of *Array Proposal*
- Computable Plant Project: [www.computableplant.org](http://www.computableplant.org)
  - Observe and model plant meristems
  - *Cellerator (Mathematica)* models
  - MathSBML for SBML

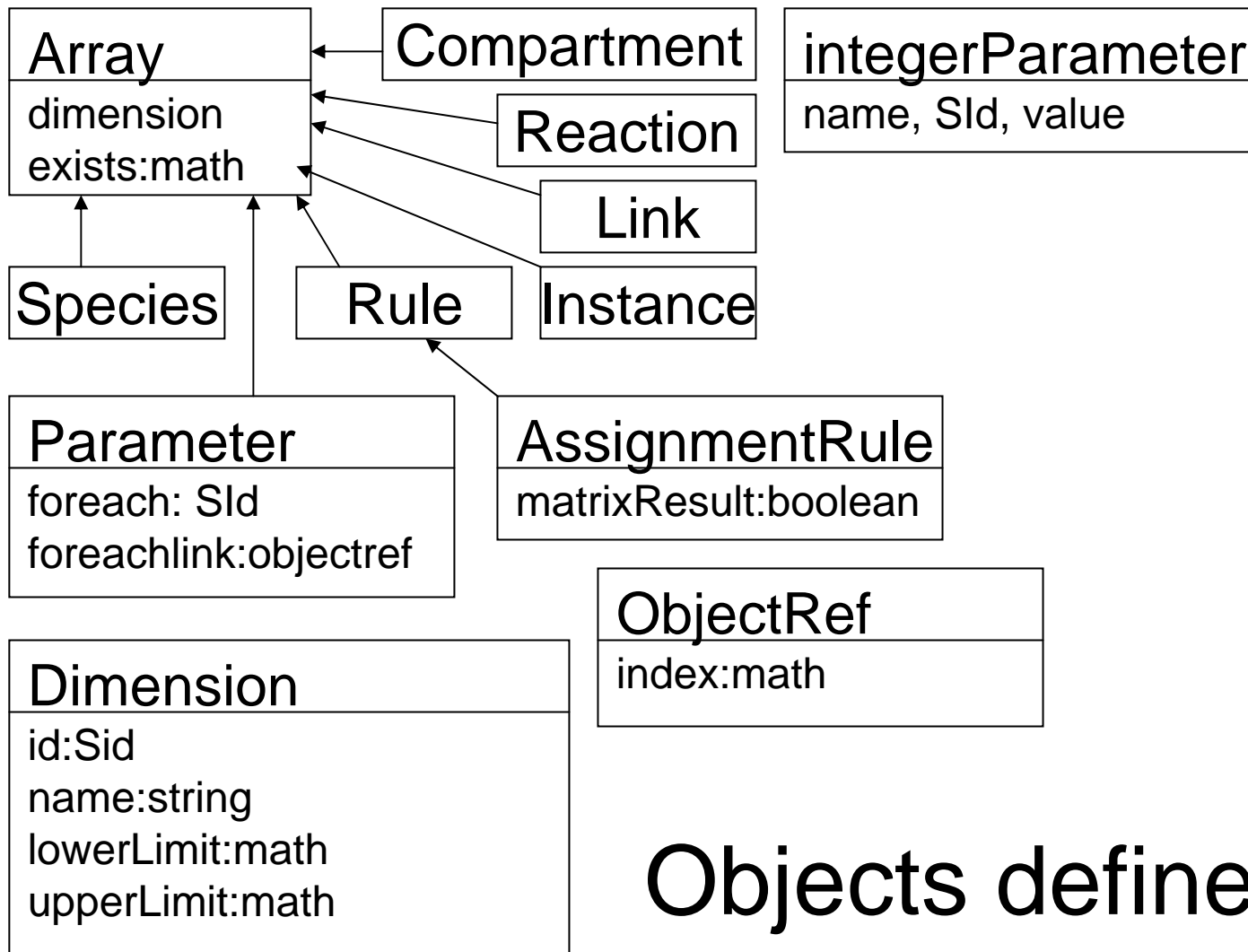


## A multicellular model of a feedback network regulating spatial gene expression domains in the shoot apical meristem

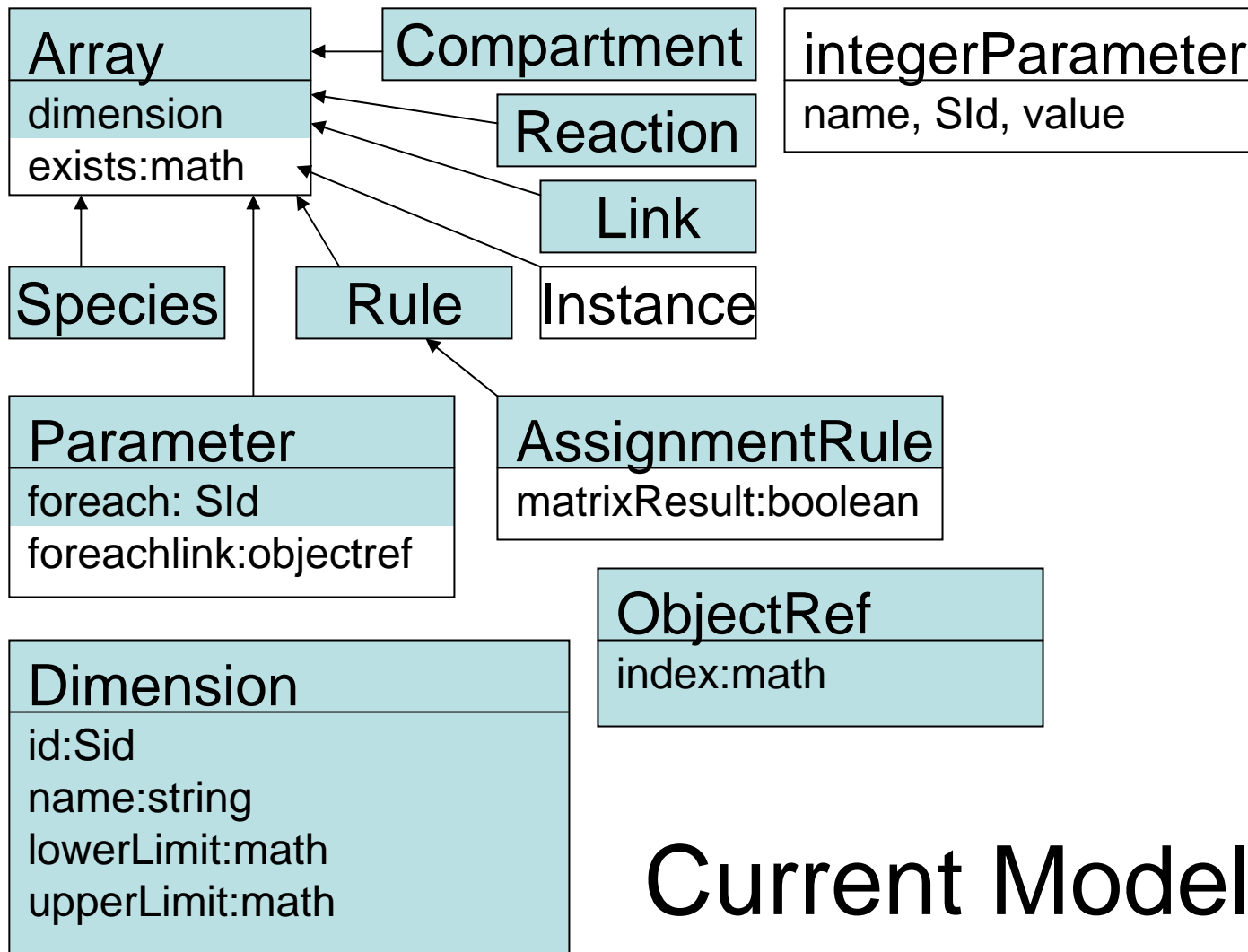
Henrik Jönsson<sup>1</sup>, Bruce E. Shapiro<sup>2</sup>, Victoria Gor<sup>2</sup>, G. Venugopala Reddy<sup>3</sup>, Marcus Heisler<sup>3</sup>,  
Elliot M. Meyerowitz<sup>3</sup> and Eric Mjolsness<sup>4</sup>





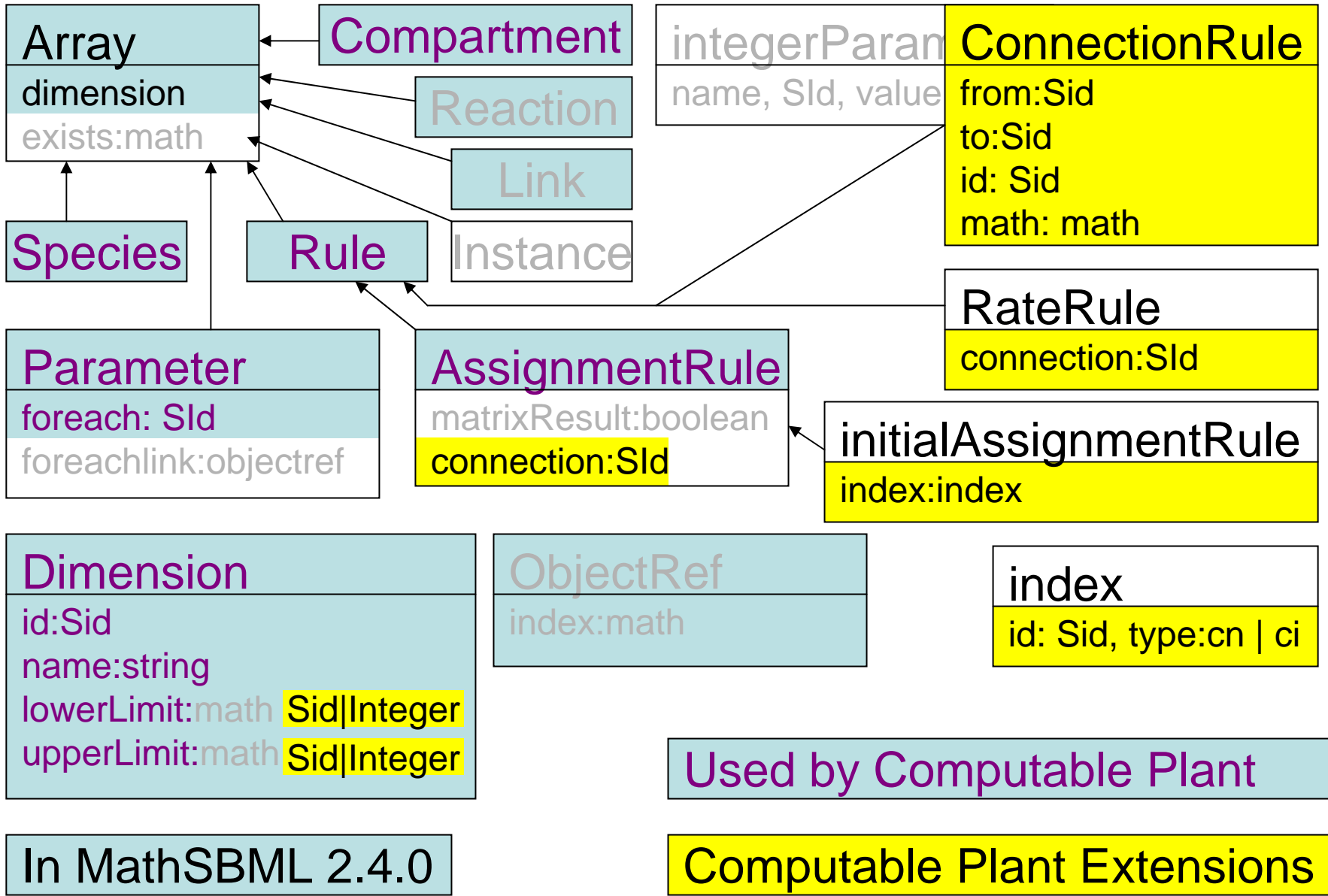


# Objects defined in the Array Proposal



# Current Model Builder Implementation

In MathSBML 2.4.0



# Array features in MathSBML

- Options for `newModel`  
`Arrays->False,`  
`ArraysAreAnnotations->True`
- Options for `addx` or `xToSBML`  
`ArrayDimensions->`  
`{i->{imin,imax}, j->{jmin,jmax},`  
`k->{kmin,kmax},...}`

where `x=compartment,species,parameter,rule,`  
(`reaction` under development)

# New lower level features

`dimensionToSBML` `dimensionToSBML`

generates `<dimension ... >`, `<listOfDimensions...>`

`indexToSBML`, `indicesToSBML`

generates `<index...>`, `<listOfIndices ...>`

`vectorToSBML`, `matrixToSBML`

generates vector or Matrix MathML

`dimensionToSymbolicSBML`, `indexToSymbolicSBML`

generates `XMLElement ["dimension", {...}, {...}]`,  
`XMLElement ["index", {...}, {...}]`

# array of species $x_5, \dots, x_{10}$

```
Input: setAnnotationPackage ["arrays"];
       setAnnotationURL ["http://www.foo.com"];
       speciesToSBML[x, compartment -> C,
                    ArrayDimensions -> {foo -> {5,10}}]
```

Output:

```
<species id="x" name="x" compartment="C"
  boundaryCondition="false" constant="false"
  substanceUnits="substance" hasOnlySubstanceUnits="false">
  <annotation xmlns:foo="http://www.myfoo.com">
    <listOfDimensions>
      <dimension id="foo" lowerLimit="5" upperLimit="10"/>
    </listOfDimensions>
  </annotation>
</species>
```

MathSBML allows  
arrays to be  
annotations if desired

# parameter $x_{ijk}, i=0..4, j=0..5, k=0..9$

**Input:** parameterToSBML[x,  
    ArrayDimensions -> {foo -> {0, 4},  
                          moo -> {0, 5},  
                          goo -> {0, 9}}]

## Output:

```
<parameter id="x" name="x">  
  <listOfDimensions>  
    <dimension id="foo" lowerLimit="0" upperLimit="4"/>  
    <dimension id="moo" lowerLimit="0" upperLimit="5"/>  
    <dimension id="goo" lowerLimit="0" upperLimit="9"/>  
  </listOfDimensions>  
</parameter>
```

# initialAssignmentRule

**input:** ruleToSBML[type -> "initialAssignmentRule",  
variable->u, data->{{2,4,6}, {3,6,9}}]

**output:**

```
<initialAssignmentRule variable="u">  
<math xmlns="http://www.w3.org/1998/Math/MathML">  
<matrix>  
<matrixrow>  
<cn>2</cn>  
<cn>4</cn>  
<cn>6</cn>  
</matrixrow>  
<matrixrow>  
<cn>3</cn>  
<cn>6</cn>  
<cn>9</cn>  
</matrixrow>  
</matrix>  
</math>  
</initialAssignmentRule>
```

$$u = \begin{pmatrix} 2 & 4 & 6 \\ 3 & 6 & 9 \end{pmatrix}$$

# Matrix initialAssignmentRule

## The Computable Plant

```
<initialAssignmentRule variable="u" >
  <math xmlns="http://www.w3.org/1998/Math/MathML">
    <cn type="integer">2</cn>
  </math>
  <listOfIndices>
    <index id="0" type="cn"/>
    <index id="0" type="cn"/>
  </listOfIndices>
</initialAssignmentRule>
<initialAssignmentRule variable="u" metaid="rule2">
  <math xmlns="http://www.w3.org/1998/Math/MathML">
    <cn type="integer">4</cn>
  </math>
  <listOfIndices>
    <index id="0" type="cn"/>
    <index id="1" type="cn"/>
  </listOfIndices>
</initialAssignmentRule> ...
```

$$u_{0,0} = 2$$

$$u_{0,1} = 4$$

# connectionRule

In the Computable Plant

- expresses a connection between compartments

```
<connectionRule from="cell" to="cell" metaid="embnbrfar">
  <math xmlns="http://www.w3.org/1998/Math/MathML">
    ...
    _____
    (from < to)  $\wedge$   $\left( \sqrt{(x_{from} - x_{to})^2 + (y_{from} - y_{to})^2} < k_1(r_{from} + r_{to}) \right)$ 
  </math>
  </connectionRule>
  _____
   $\wedge$   $\left( k_2(r_{from} + r_{to}) < \sqrt{(x_{from} - x_{to})^2 + (y_{from} - y_{to})^2} \right)$ 
  ...
  <rateRule variable="x" metaid="x_from_far" connection="embnbrfar">
    <listOfIndices>
      <index id="i" type="ci"/>
    </listOfIndices>
    <math xmlns="http://www.w3.org/1998/Math/MathML">
      ...
      _____
      </math>
      _____
       $\frac{dr_i}{dt} = k_3(x_i - x_j) \frac{1 - k_4(r_i + r_j)}{\sqrt{(x_i - x_j)^2 + (y_i - y_j)^2}}$ 
    </rateRule>
```

# Array Implementation Summary

	Proposal	MathSBML Model Builder	Computable Plant
compartment arrays	✓	✓	✓
species arrays	✓	✓	✓
parameter arrays	✓	✓	✓
Implied via foreach	✓	✓	✓
rule arrays			
rateRule	✓	✓	✓
assignmentRule	✓	✓	✓
algebraicRule	✓	✓	
initialAssignmentRule	✓	✓	▼ [a]
connectionRule		✓	▼ [d]
Birth/death rule			●
matrixResult	✓	●	
reaction arrays	✓	◆	●
MathML matrix/vector	✓	✓	
Objects as annotations	Level 3	✓◆ (optional)	
<index>	MathML	MathML,C	▼[b,e]; C (●MathML)
<dimension> limits	MathML	MathML,C	▼[b,e] C (●MathML)
objectLinks	✓	✓	▼ [c]
<exists>	✓	●	
integerParameter object	✓	●	▼ [e]

✓ Implemented; ◆ Under Development; ● Planned

▼ Implementation deviates from array proposal. (a) no matrix/vector support; some syntactic differences (b) \*<index> replaces <dimensions> in rules; (c) implied arrays without object links (looks for specific index references) (d) uses reserved fields "from" and "to" as implied indices; (e) Allows any parameter for integer parameter

# Discussion





**<!-- Systems Biology Markup Language -->**



```
<sbml xmlns="http://sbml.org/"
  <model id="SBMLWorkshop9"
    name="Heidelberg, Germany, 2004">
  ...
</model>
</sbml>
```

[http://www.zazzle.com/contributors/products/gallery/browse\\_results.asp?cid=238769197763420286](http://www.zazzle.com/contributors/products/gallery/browse_results.asp?cid=238769197763420286)