

# SBMLToolbox

## MATLAB\_SBML Structure

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This document describes the MATLAB\_SBML structure in detail. It lists the fields within each structure, the data types for each field and indicates the Levels and Versions of SBML for which each given field is appropriate.

For example:

### Component

| Fieldname                           | Type               |  |
|-------------------------------------|--------------------|--|
|                                     | C                  | MATLAB                                 |
| var                                 | int                | mxArray of int32                       |
| var2**                              | double             | mxArray of double                      |
| var3***                             | List Of structures | array of structures of type Component2 |
| ** L2V1 <div></div> *** L2V1 – L2V2 |                    |  |

Indicates that the Component has a field var which is of type int in C and an mxArray of type int32 in MATLAB. The field, which corresponds to an attribute on Component in SBML is present in all current levels and versions of SBML.

Component also has a field var2, of type double in C and an mxArray of type double in MATLAB. However, the attribute var2 is only present in SBML L2V1 and beyond.

The third field on Component, var3, represents a ListOf element from SBML. In this case var3 is a ListOf some other component Component2 which is a specialised ListOf structure in C and an array of structures in MATLAB. It should be noted that var3 only exists in L2V1 and L2V2 and has been removed from SBML in L2V3.

Details of each of the structures within the Model structure are given below.

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**Model**

| Fieldname                              | Type               |   |
|--|--------------------|---|
|  | C                  | MATLAB  |
| typecode                               | char *             | mxArray of char                                   |
| notes                                  | char *             | mxArray of char                                   |
| annotation                             | char *             | mxArray of char                                   |
| SBML_level                             | unsigned int       | mxArray of int32                                  |
| SBML_version                           | unsigned int       | mxArray of int32                                  |
| name                                   | char *             | mxArray of char                                   |
| id <sup>**</sup>                       | char *             | mxArray of char                                   |
| sboTerm <sup>***</sup>                 | unsigned int       | mxArray of int32                                  |
| functionDefinition <sup>**</sup>       | List of structures | array of structures of type<br>FunctionDefinition |
| unitDefinition                         | List of structures | array of structures of type<br>UnitDefinition     |
| compartmentType <sup>***</sup>         | List of structures | array of structures of type<br>CompartmentType    |
| speciesType <sup>***</sup>             | List of structures | array of structures of type<br>SpeciesType        |
| compartment                            | List of structures | array of structures of type<br>Compartment        |
| species                                | List of structures | array of structures of type<br>Species            |
| parameter                              | List of structures | array of structures of type<br>Parameter          |
| initialAssignment <sup>***</sup>       | List of structures | array of structures of type<br>InitialAssignment  |
| rule                                   | List of structures | array of structures of type<br>Rule               |
| constraint <sup>***</sup>              | List of structures | array of structures of type<br>Constraint         |
| reaction                               | List of structures | array of structures of type<br>Reaction           |
| event <sup>**</sup>                    | List of structures | array of structures of type<br>Event              |
| <sup>1</sup> time_symbol <sup>**</sup> | N/A                | mxArray of char                                   |
| namespaces                             | N/A                | array of structures with prefix & url             |
| <sup>**</sup> L2V1 <sup>***</sup> L2V2 |                    |   |

<sup>1</sup> if the MathML csymbol time has been used the symbol used is recorded in this field  
Multiple occurrences will be replaced with the symbol recorded here

## UnitDefinition

| Fieldname         | Type               |                                  |
|-------------------|--------------------|----------------------------------|
|                   | C                  | MATLAB                           |
| typecode          | char *             | mxArray of char                  |
| notes             | char *             | mxArray of char                  |
| annotation        | char *             | mxArray of char                  |
| sboTerm****       | unsigned int       | mxArray of int32                 |
| name              | char *             | mxArray of char                  |
| id**              | char *             | mxArray of char                  |
| unit              | List of structures | array of structures of type Unit |
| ** L2V1 **** L2V3 |                    |                                  |

## Compartment

| Fieldname                              | Type         |                   |
|--|--------------|-------------------|
|  | C            | MATLAB            |
| typecode                               | char *       | mxArray of char   |
| notes                                  | char *       | mxArray of char   |
| annotation                             | char *       | mxArray of char   |
| sboTerm****                            | unsigned int | mxArray of int32  |
| name                                   | char *       | mxArray of char   |
| id**                                   | char *       | mxArray of char   |
| compartmentType***                     | char *       | mxArray of char   |
| spatialDimensions**                    | unsigned int | mxArray of int32  |
| size**                                 | double       | mxArray of double |
| volume*                                | double       | mxArray of double |
| units                                  | char *       | mxArray of char   |
| outside                                | char *       | mxArray of char   |
| constant**                             | int          | mxArray of int32  |
| isSetSize**                            | unsigned int | mxArray of int32  |
| isSetVolume                            | unsigned int | mxArray of int32  |
| * L1V1–L1V2 ** L2V1 *** L2V2 **** L2V3 |              |                   |

## Species

| Fieldname   | Type         |                   |
|---|--------------|-------------------|
|   | C            | MATLAB            |
| typecode  | char *       | mxArray of char   |
| notes   | char *       | mxArray of char   |
| annotation  | char *       | mxArray of char   |
| sboTerm****   | unsigned int | mxArray of int32  |
| name  | char *       | mxArray of char   |
| id**  | char *       | mxArray of char   |
| speciesType***  | char *       | mxArray of char   |
| compartment   | char *       | mxArray of char   |
| initialAmount   | double       | mxArray of double |
| initialConcentration**  | double       | mxArray of double |
| substanceUnits**  | char *       | mxArray of char   |
| spatialSizeUnits <sup>1*</sup>  | char *       | mxArray of char   |
| hasOnlySubstanceUnits**   | int          | mxArray of int32  |
| units*  | char *       | mxArray of char   |
| boundaryCondition   | int          | mxArray of int32  |
| charge  | int          | mxArray of int32  |
| constant**  | int          | mxArray of int32  |
| isSetInitialAmount  | unsigned int | mxArray of int32  |
| isSetConcentration**  | unsigned int | mxArray of int32  |
| isSetCharge   | unsigned int | mxArray of int32  |
| *L1V1–L1V2      **L2V1      ***L2V2 <sup>1*</sup> L2V1–L2V2      ****L2V3 |              |                   |

## Parameter

| Fieldname        | Type         |                   |
|------------------|--------------|-------------------|
|                  | C            | MATLAB            |
| typecode         | char *       | mxArray of char   |
| notes            | char *       | mxArray of char   |
| annotation       | char *       | mxArray of char   |
| sboTerm***       | unsigned int | mxArray of int32  |
| name             | char *       | mxArray of char   |
| id**             | char *       | mxArray of char   |
| value            | double       | mxArray of double |
| units            | char *       | mxArray of char   |
| constant**       | int          | mxArray of int32  |
| isSetValue       | unsigned int | mxArray of int32  |
| ** L2V1 *** L2V2 |              |                   |

## Rule

| Fieldname              | Type         |                  |
|------------------------|--------------|------------------|
|                        | C            | MATLAB           |
| typecode               | char *       | mxArray of char  |
| notes                  | char *       | mxArray of char  |
| annotation             | char *       | mxArray of char  |
| sboTerm***             | unsigned int | mxArray of int32 |
| type***                | char *       | mxArray of char  |
| formula                | char *       | mxArray of char  |
| variable               | char *       | mxArray of char  |
| species                | char *       | mxArray of char  |
| compartment            | char *       | mxArray of char  |
| name                   | char *       | mxArray of char  |
| units                  | char *       | mxArray of char  |
| * L1V1 – L1V2 *** L2V2 |              |                  |

## Reaction

| Fieldname                             | Type               |  |
|---------------------------------------|--------------------|--|
|                                       | C                  | MATLAB   |
| typecode                              | char *             | mxArray of char                                      |
| notes                                 | char *             | mxArray of char                                      |
| annotation                            | char *             | mxArray of char                                      |
| sboTerm***                            | unsigned int       | mxArray of int32                                     |
| name                                  | char *             | mxArray of char                                      |
| id**                                  | char *             | mxArray of char                                      |
| reactant                              | List of structures | array of structures of type SpeciesReference         |
| product                               | List of structures | array of structures of type SpeciesReference         |
| modifier**                            | List of structures | array of structures of type ModifierSpeciesReference |
| kineticLaw                            | structure          | structure of type KineticLaw                         |
| reversible                            | int                | mxArray of int32                                     |
| fast                                  | int                | mxArray of int32                                     |
| isSetFast**                           | unsigned int       | mxArray of int32                                     |
| ** L2V1                      *** L2V2 |                    |  |

## KineticLaw

| Fieldname   | Type               |                                       |
|---|--------------------|---------------------------------------|
|   | C                  | MATLAB                                |
| typecode  | char *             | mxArray of char                       |
| notes   | char *             | mxArray of char                       |
| annotation  | char *             | mxArray of char                       |
| sboTerm***  | unsigned int       | mxArray of int32                      |
| name  | char *             | mxArray of char                       |
| formula   | char *             | mxArray of char                       |
| math**  | char *             | mxArray of char                       |
| parameter   | List of structures | array of structures of type Parameter |
| timeUnits <sup>2*</sup>   | char *             | mxArray of char                       |
| substanceUnits <sup>2*</sup>                                    | char *             | mxArray of char                       |
| ** L2V1 <sup>2*</sup> L2V1 – L2V1                      *** L2V2 |                    |                                       |



## SpeciesReference

| Fieldname   | Type                                     |                                       |
|---|--|---------------------------------------|
|   | C  | MATLAB                                |
| typecode  | char *                                   | mxArray of char                       |
| notes   | char *                                   | mxArray of char                       |
| annotation  | char *                                   | mxArray of char                       |
| sboTerm <sup>***</sup>  | unsigned int                             | mxArray of int32                      |
| species   | char *                                   | mxArray of char                       |
| id <sup>***</sup>   | char *                                   | mxArray of char                       |
| name <sup>***</sup>   | char *                                   | mxArray of char                       |
| stoichiometry   | int <sup>*</sup><br>double <sup>**</sup> | mxArray of int32<br>mxArray of double |
| demoninator <sup>2*</sup>   | int                                      | mxArray of int32                      |
| stoichiometryMath <sup>**</sup>   | char *                                   | mxArray of char                       |
| <sup>*</sup> L1V1–L1V2 <sup>**</sup> L2V1 <sup>***</sup> L2V2 <sup>2*</sup> L2V1–L2V1 |  |                                       |

## Unit

| Fieldname   | Type         |                   |
|---|--------------|-------------------|
|   | C            | MATLAB            |
| typecode  | char *       | mxArray of char   |
| notes   | char *       | mxArray of char   |
| annotation  | char *       | mxArray of char   |
| sboTerm <sup>****</sup>   | unsigned int | mxArray of int32  |
| kind  | char *       | mxArray of char   |
| exponent  | int          | mxArray of int32  |
| scale   | int          | mxArray of int32  |
| multiplier <sup>**</sup>  | double       | mxArray of double |
| offset <sup>2*</sup>  | double       | mxArray of double |
| <sup>**</sup> L2V1 <sup>****</sup> L2V3 <sup>2*</sup> L2V1 – L2V1 |              |                   |

**FunctionDefinition (Level 2 ONLY)**

| Fieldname              | Type         |                  |
|------------------------|--------------|------------------|
|                        | C            | MATLAB           |
| typecode               | char *       | mxArray of char  |
| notes                  | char *       | mxArray of char  |
| annotation             | char *       | mxArray of char  |
| sboTerm <sup>***</sup> | unsigned int | mxArray of int32 |
| name                   | char *       | mxArray of char  |
| id                     | char *       | mxArray of char  |
| math                   | char *       | mxArray of char  |
| *** L2V2               |              |                  |

**Event (Level 2 ONLY)**

| Fieldname                                    | Type               |  |
|--|--------------------|--|
|  | C                  | MATLAB   |
| typecode                                     | char *             | mxArray of char                                |
| notes  | char *             | mxArray of char                                |
| annotation                                   | char *             | mxArray of char                                |
| sboTerm <sup>***</sup>                       | unsigned int       | mxArray of int32                               |
| name   | char *             | mxArray of char                                |
| id   | char *             | mxArray of char                                |
| trigger                                      | char *             | mxArray of char                                |
| delay  | char *             | mxArray of char                                |
| timeUnits <sup>1*</sup>                      | char *             | mxArray of char                                |
| eventAssignment                              | List of structures | array of structures of type<br>EventAssignment |
| *** L2V2                      1* L2V1 – L2V2 |                    |  |

**ModifierSpeciesReference (Level 2 ONLY)**

| Fieldname  | Type         |                  |
|------------|--------------|------------------|
|            | C            | MATLAB           |
| typecode   | char *       | mxArray of char  |
| notes      | char *       | mxArray of char  |
| annotation | char *       | mxArray of char  |
| sboTerm*** | unsigned int | mxArray of int32 |
| species    | char *       | mxArray of char  |
| id***      | char *       | mxArray of char  |
| name***    | char *       | mxArray of char  |
| *** L2V2   |              |                  |

**EventAssignment (Level 2 ONLY)**

| Fieldname  | Type         |                  |
|------------|--------------|------------------|
|            | C            | MATLAB           |
| typecode   | char *       | mxArray of char  |
| notes      | char *       | mxArray of char  |
| annotation | char *       | mxArray of char  |
| sboTerm*** | unsigned int | mxArray of int32 |
| variable   | char *       | mxArray of char  |
| math       | char *       | mxArray of char  |
| *** L2V2   |              |                  |

**CompartmentType (L2V2 onwards)**

| Fieldname   | Type         |                  |
|-------------|--------------|------------------|
|             | C            | MATLAB           |
| typecode    | char *       | mxArray of char  |
| notes       | char *       | mxArray of char  |
| annotation  | char *       | mxArray of char  |
| sboTerm**** | unsigned int | mxArray of int32 |
| name        | char *       | mxArray of char  |
| id          | char *       | mxArray of char  |
| **** L2V3   |              |                  |

**SpeciesType (L2V2 onwards)**

| Fieldname   | Type         |                  |
|-------------|--------------|------------------|
|             | C            | MATLAB           |
| typecode    | char *       | mxArray of char  |
| notes       | char *       | mxArray of char  |
| annotation  | char *       | mxArray of char  |
| sboTerm**** | unsigned int | mxArray of int32 |
| name        | char *       | mxArray of char  |
| id          | char *       | mxArray of char  |
| **** L2V3   |              |                  |

**InitialAssignment (L2V2 onwards)**

| Fieldname  | Type         |                  |
|------------|--------------|------------------|
|            | C            | MATLAB           |
| typecode   | char *       | mxArray of char  |
| notes      | char *       | mxArray of char  |
| annotation | char *       | mxArray of char  |
| sboTerm    | unsigned int | mxArray of int32 |
| symbol     | char *       | mxArray of char  |
| math       | char *       | mxArray of char  |

**Constraint (L2V2 onwards)**

| Fieldname  | Type         |                  |
|------------|--------------|------------------|
|            | C            | MATLAB           |
| typecode   | char *       | mxArray of char  |
| notes      | char *       | mxArray of char  |
| annotation | char *       | mxArray of char  |
| sboTerm    | unsigned int | mxArray of int32 |
| math       | char *       | mxArray of char  |
| message    | char *       | mxArray of char  |