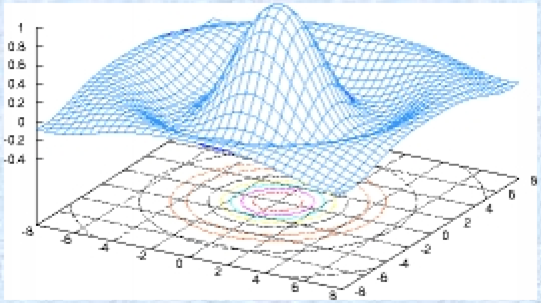
libSBML

Sarah Keating

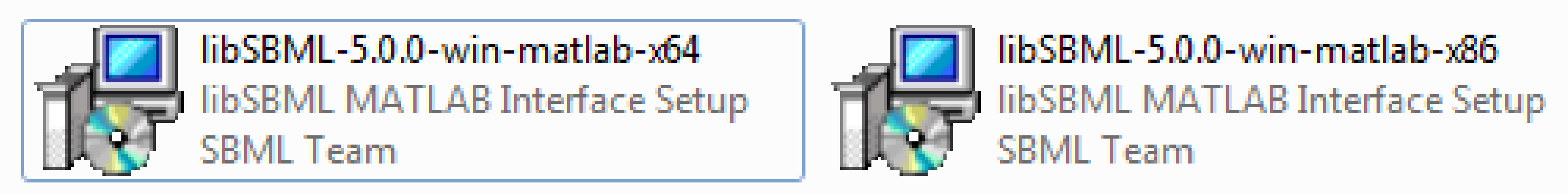
Using MATLAB/Octave ...



Installing libSBML MATLAB binding

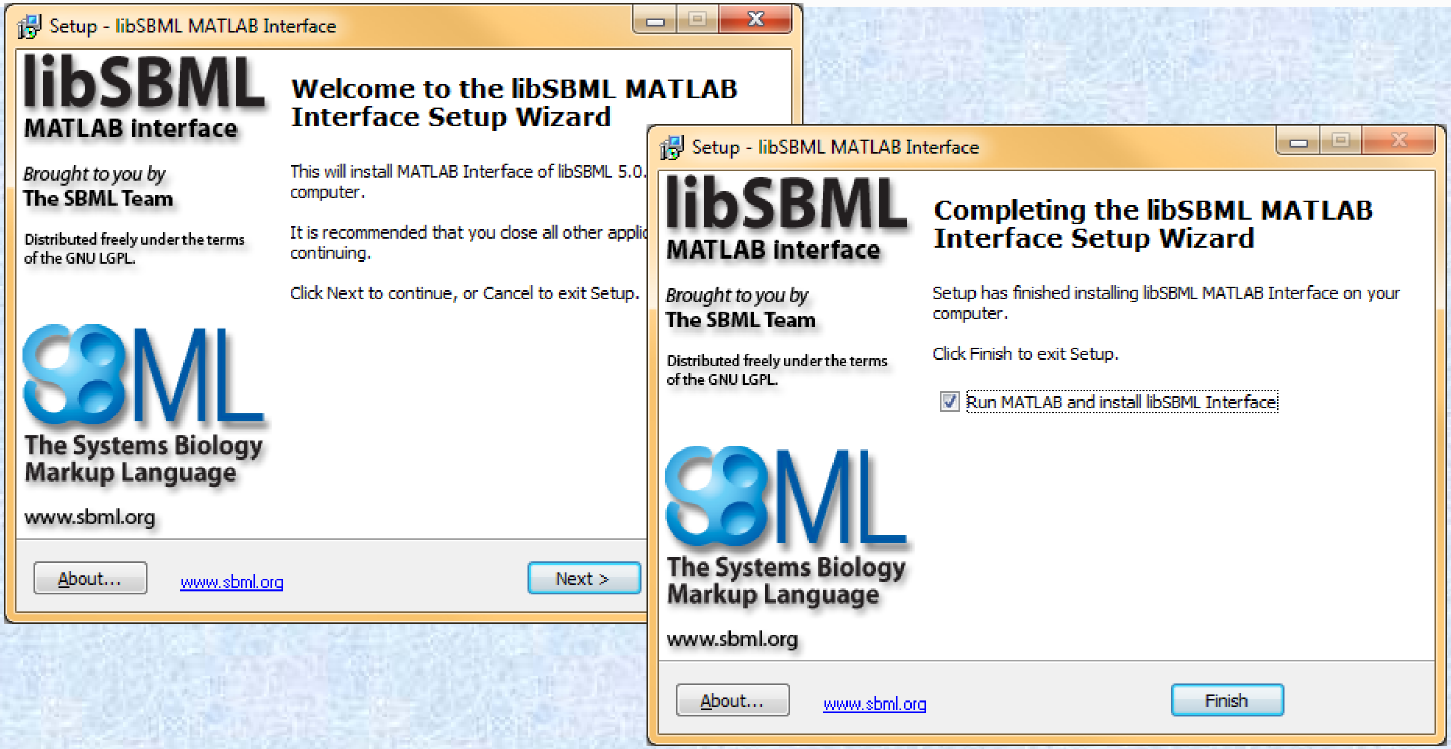
Installing libSBML MATLAB binding

on Windows



libSBML-5.0.0-win-matlab-x64
libSBML MATLAB Interface Setup
SBML Team

libSBML-5.0.0-win-matlab-x86
libSBML MATLAB Interface Setup
SBML Team



Setup - libSBML MATLAB Interface

libSBML
MATLAB interface

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The Systems Biology Markup Language

www.sbml.org

Welcome to the libSBML MATLAB Interface Setup Wizard

This will install MATLAB Interface of libSBML 5.0. computer.

It is recommended that you close all other applic continuing.

Click Next to continue, or Cancel to exit Setup.

Setup - libSBML MATLAB Interface

libSBML
MATLAB interface

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Completing the libSBML MATLAB Interface Setup Wizard

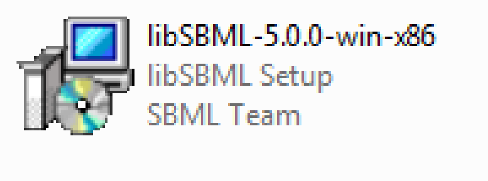
Setup has finished installing libSBML MATLAB Interface on your computer.

Click Finish to exit Setup.

☑ Run MATLAB and install libSBML Interface

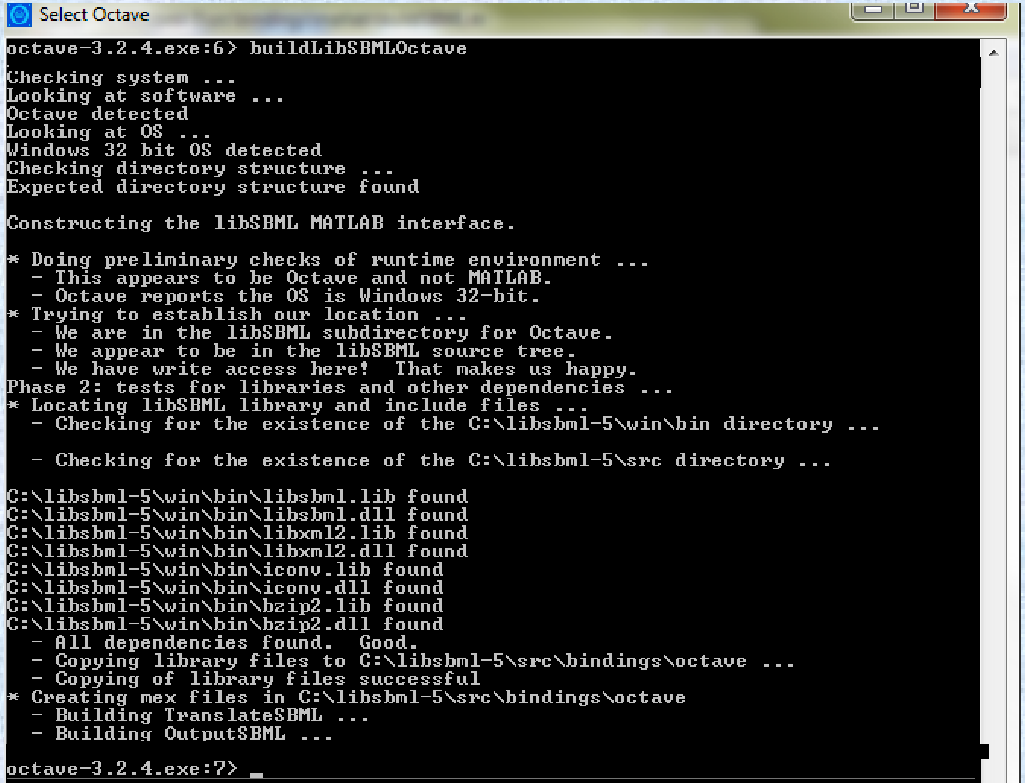
Installing libSBML Octave binding

on Windows



libSBML-5.0.0-win-x86
libSBML Setup
SBML Team

- Install libSBML using the windows installer.
- Open Octave and navigate to the binding/octave directory
- Run buildLibSBMLOctave



```
octave-3.2.4.exe:6> buildLibSBMLOctave

Checking system ...
Looking at software ...
Octave detected
Looking at OS ...
Windows 32 bit OS detected
Checking directory structure ...
Expected directory structure found

Constructing the libSBML MATLAB interface.

* Doing preliminary checks of runtime environment ...
  - This appears to be Octave and not MATLAB.
  - Octave reports the OS is Windows 32-bit.
* Trying to establish our location ...
  - We are in the libSBML subdirectory for Octave.
  - We appear to be in the libSBML source tree.
  - We have write access here!  That makes us happy.
Phase 2: tests for libraries and other dependencies ...
* Locating libSBML library and include files ...
  - Checking for the existence of the C:\libsbml-5\win\bin directory ...

  - Checking for the existence of the C:\libsbml-5\src directory ...

C:\libsbml-5\win\bin\libsbml.lib found
C:\libsbml-5\win\bin\libsbml.dll found
C:\libsbml-5\win\bin\libxml2.lib found
C:\libsbml-5\win\bin\libxml2.dll found
C:\libsbml-5\win\bin\iconv.lib found
C:\libsbml-5\win\bin\iconv.dll found
C:\libsbml-5\win\bin\bzip2.lib found
C:\libsbml-5\win\bin\bzip2.dll found
  - All dependencies found.  Good.
  - Copying library files to C:\libsbml-5\src\bindings\octave ...
  - Copying of library files successful
* Creating mex files in C:\libsbml-5\src\bindings\octave
  - Building TranslateSBML ...
  - Building OutputSBML ...

octave-3.2.4.exe:7> _
```

Installing libSBML MATLAB binding

on Linux/Mac

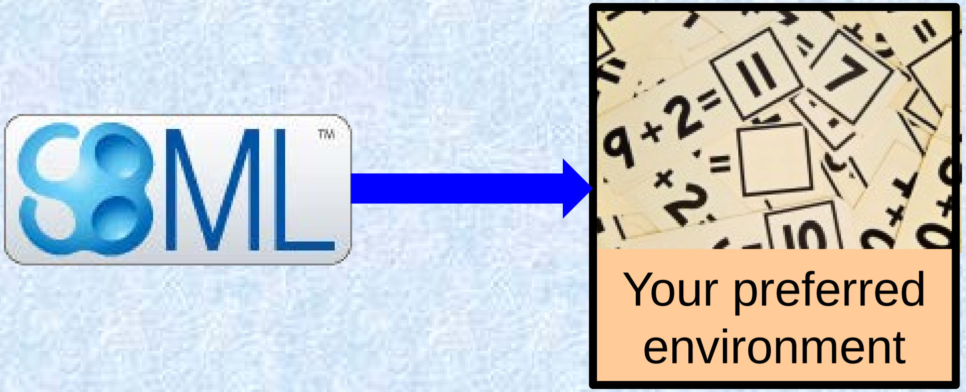
```
./configure –-with-matlab
make
sudo make install
```

Installing libSBML Octave binding

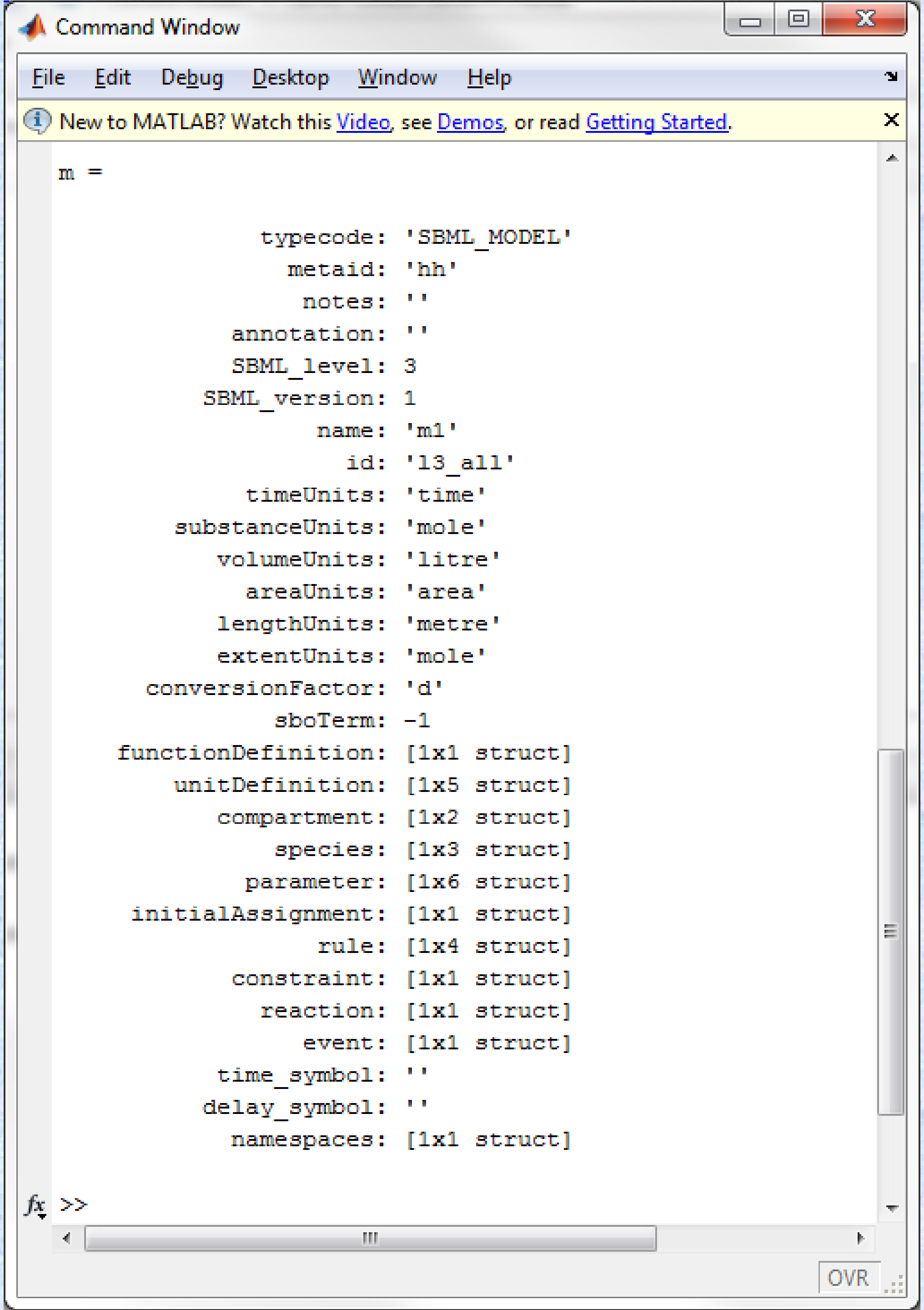
on Linux/Mac

```
./configure –with-octave
make
sudo make install
```

Import SBML



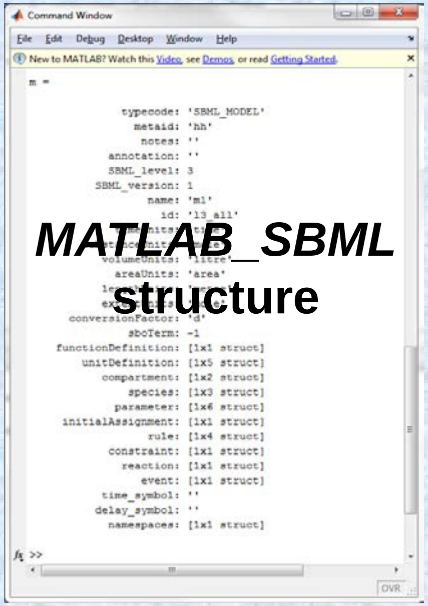
Your preferred environment


Command Window
File Edit Debug Desktop Window Help
New to MATLAB? Watch this Video, see Demos, or read Getting Started.
OVR

```
m = 

              typecode: 'SBML_MODEL'
                metaid: 'hh'
                 notes: ''
            annotation: ''
            SBML_level: 3
          SBML_version: 1
                  name: 'm1'
                    id: 'l3_all'
             timeUnits: 'time'
        substanceUnits: 'mole'
           volumeUnits: 'litre'
             areaUnits: 'area'
           lengthUnits: 'metre'
           extentUnits: 'mole'
      conversionFactor: 'd'
               sboTerm: -1
    functionDefinition: [1x1 struct]
        unitDefinition: [1x5 struct]
           compartment: [1x2 struct]
               species: [1x3 struct]
             parameter: [1x6 struct]
     initialAssignment: [1x1 struct]
                  rule: [1x4 struct]
            constraint: [1x1 struct]
              reaction: [1x1 struct]
                 event: [1x1 struct]
           time_symbol: ''
          delay_symbol: ''
            namespaces: [1x1 struct]

>> 
```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```
m =

           typecode: 'SBML_MODEL'
             metaid: 'hh'
              notes: ''
         annotation: ''
         SBML_level: 3
       SBML_version: 1
               name: 'm1'
                 id: '13_all'
          timeUnits: 'time'
     substanceUnits: 'mole'
        volumeUnits: 'litre'
          areaUnits: 'area'
        lengthUnits: 'metre'
        extentUnits: 'mole'
   conversionFactor: 'd'
            sboTerm: -1
 functionDefinition: [1x1 struct]
     unitDefinition: [1x5 struct]
        compartment: [1x2 struct]
            species: [1x3 struct]
          parameter: [1x6 struct]
  initialAssignment: [1x1 struct]
               rule: [1x4 struct]
         constraint: [1x1 struct]
           reaction: [1x1 struct]
              event: [1x1 struct]
        time_symbol: ''
       delay_symbol: ''
         namespaces: [1x1 struct]

fx >>
```

***MATLAB_SBML* structure**

User conversion

The COBRA Toolbox

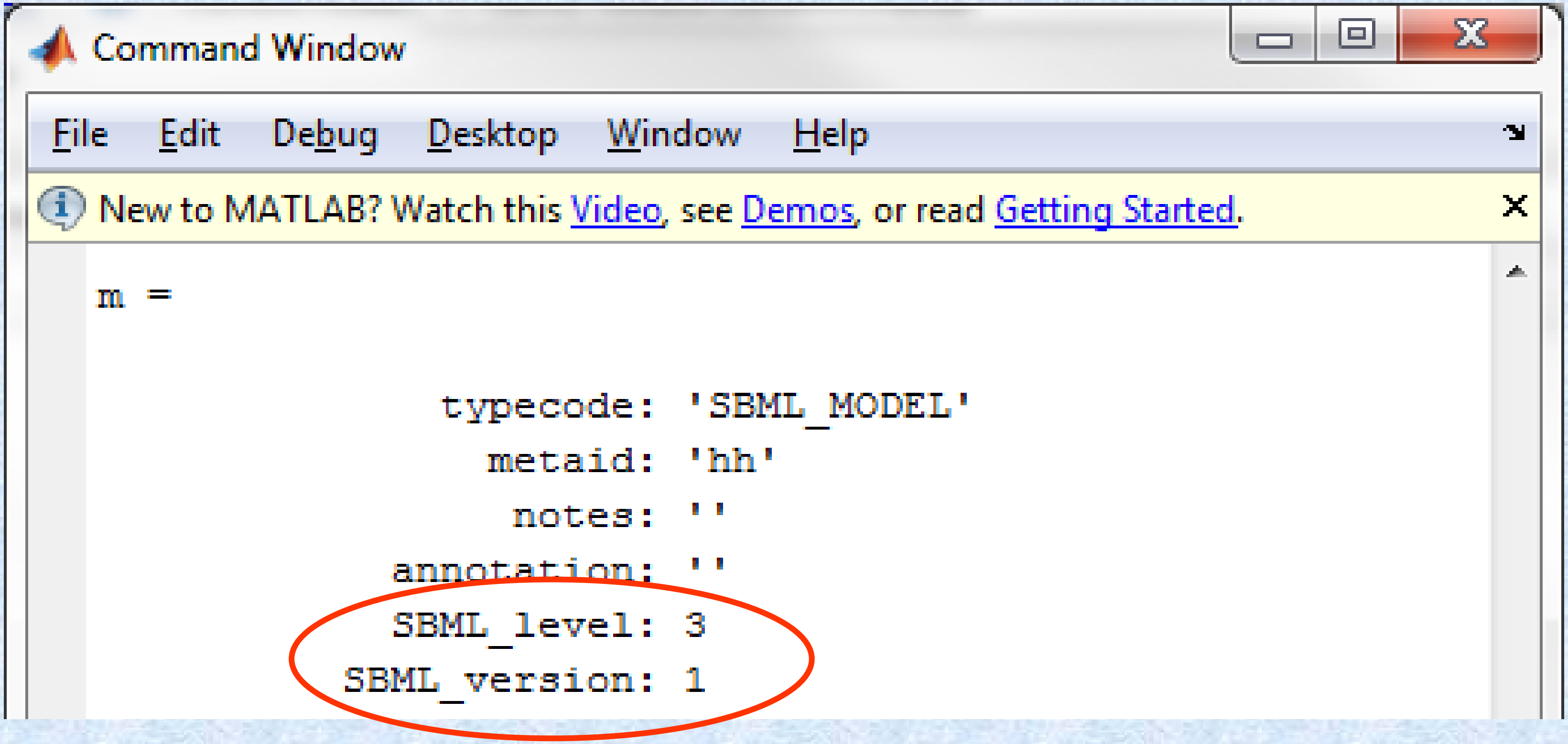
POTTERSWHEEL
Mathematical Modeling

sbtoolbox2

SBMLToolbox

…

MATLAB_SBML structure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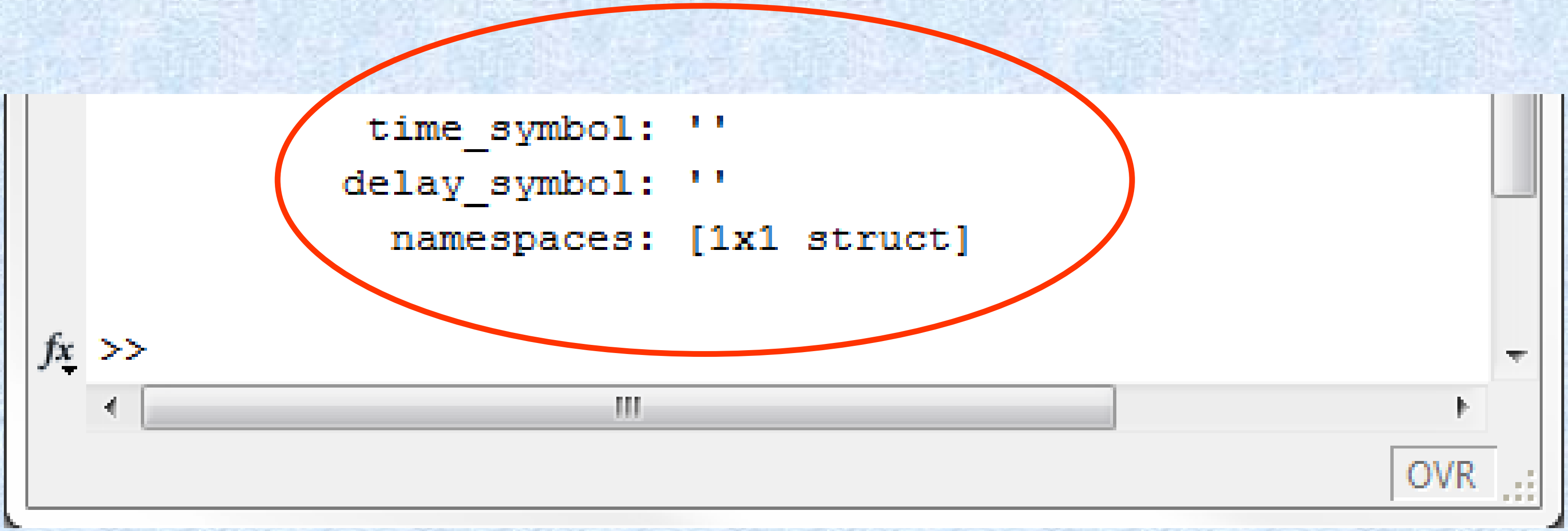
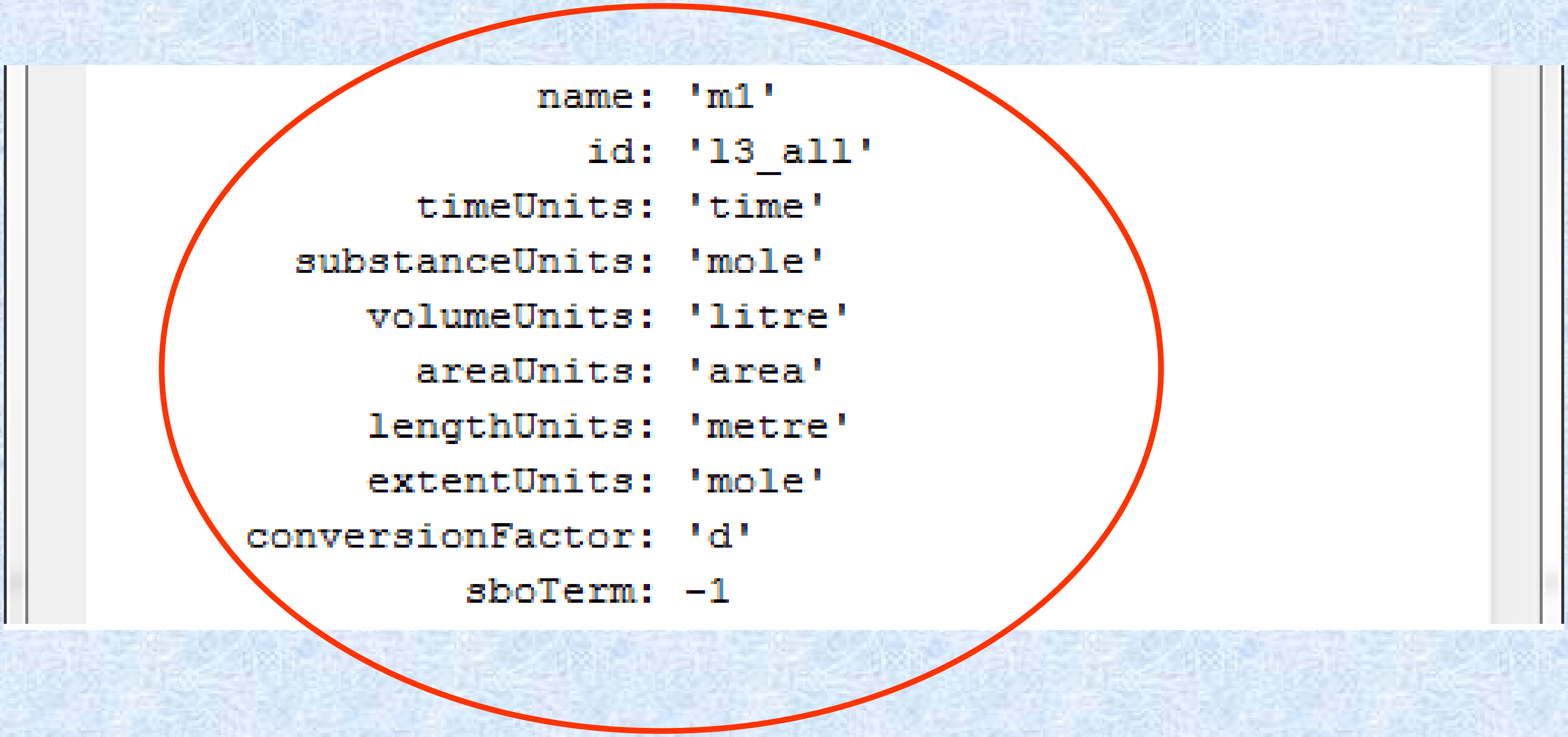
```
m =

         typecode: 'SBML_MODEL'
           metaid: 'hh'
            notes: ''
       annotation: ''
       SBML_level: 3
     SBML_version: 1
```

MATLAB_SBML structure



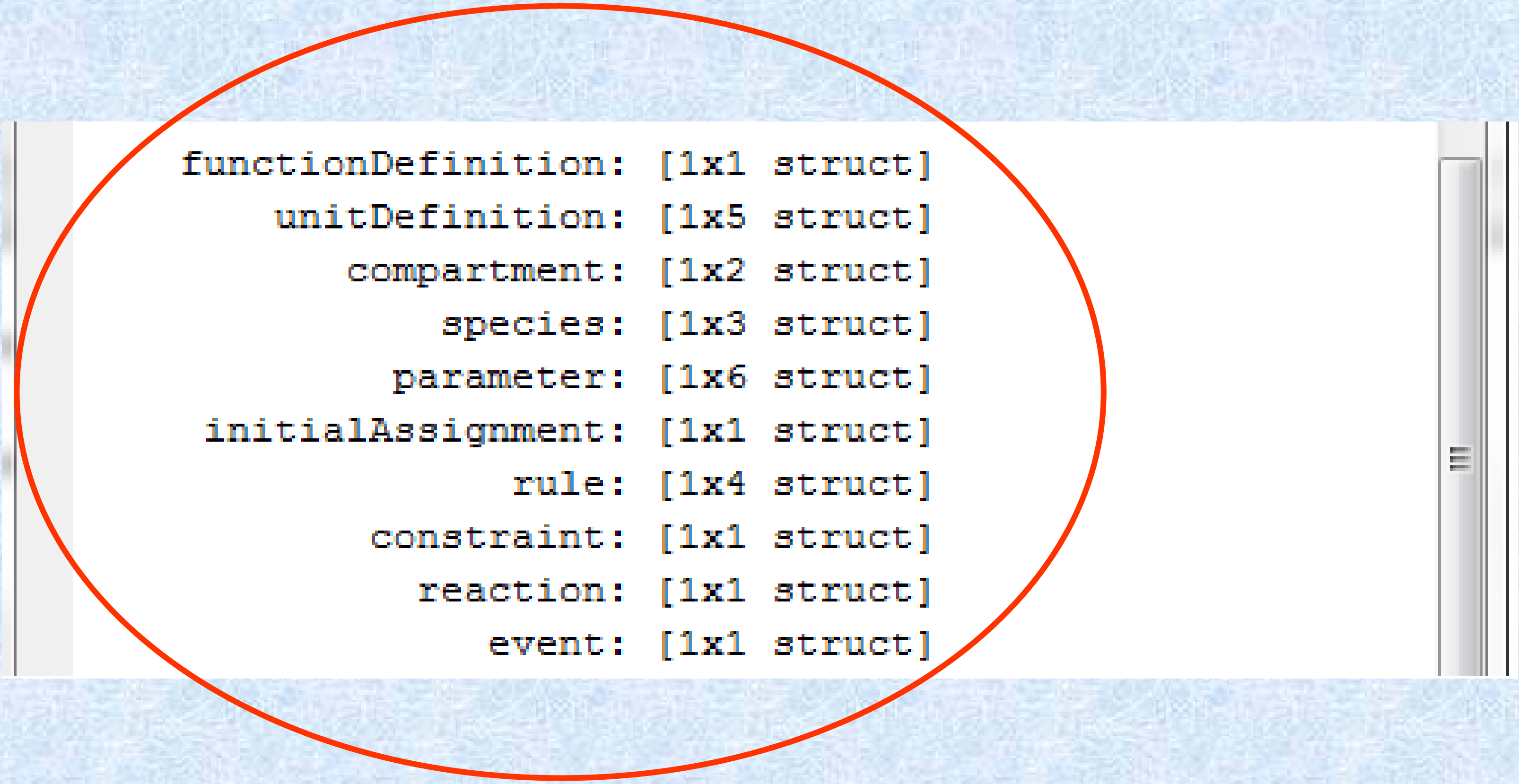
```
  time_symbol: ''
 delay_symbol: ''
   namespaces: [1x1 struct]

>>
```

MATLAB_SBML structure



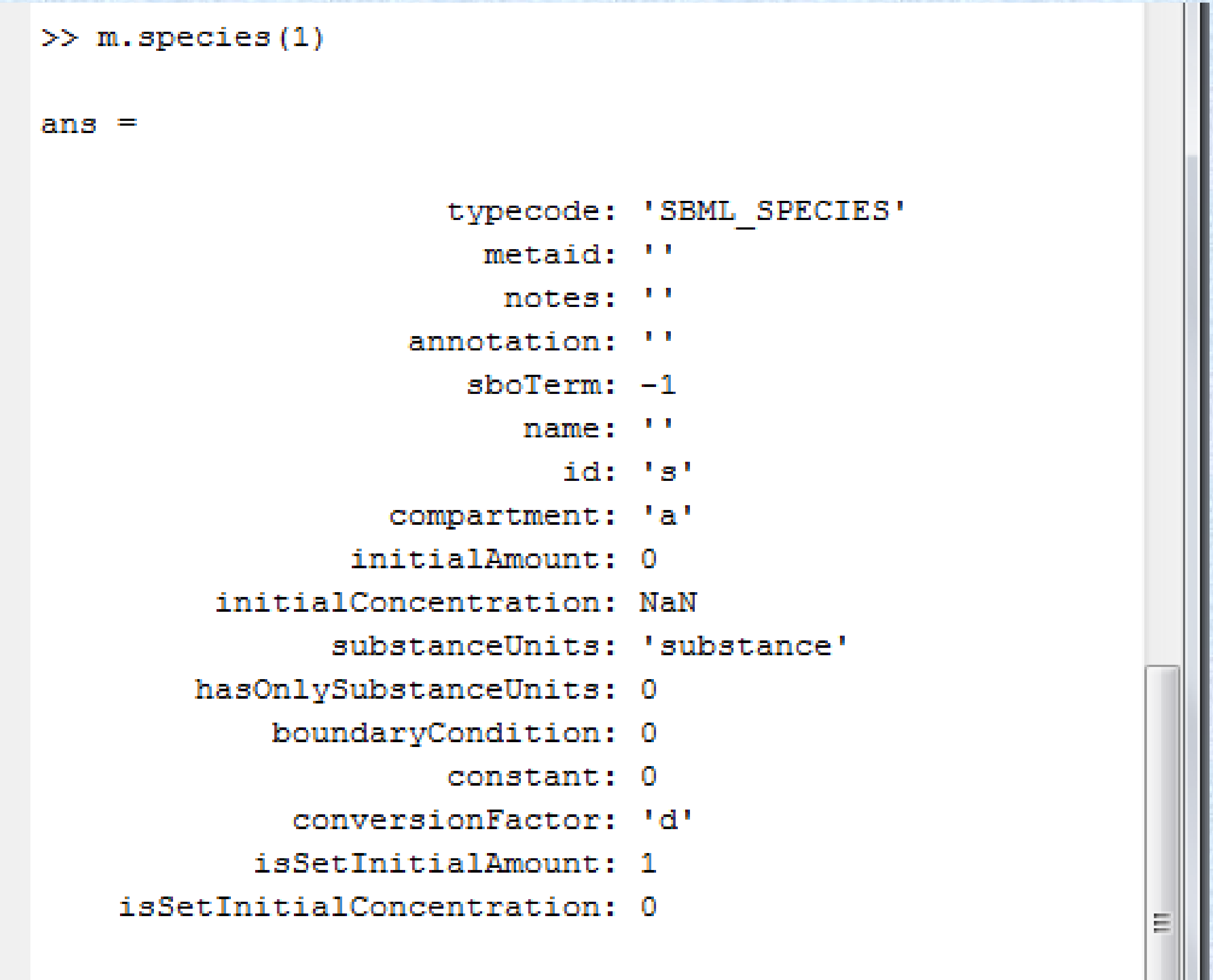
```
             name: 'm1'
               id: 'l3_all'
        timeUnits: 'time'
   substanceUnits: 'mole'
      volumeUnits: 'litre'
        areaUnits: 'area'
      lengthUnits: 'metre'
      extentUnits: 'mole'
 conversionFactor: 'd'
          sboTerm: -1
```

MATLAB_SBML structure



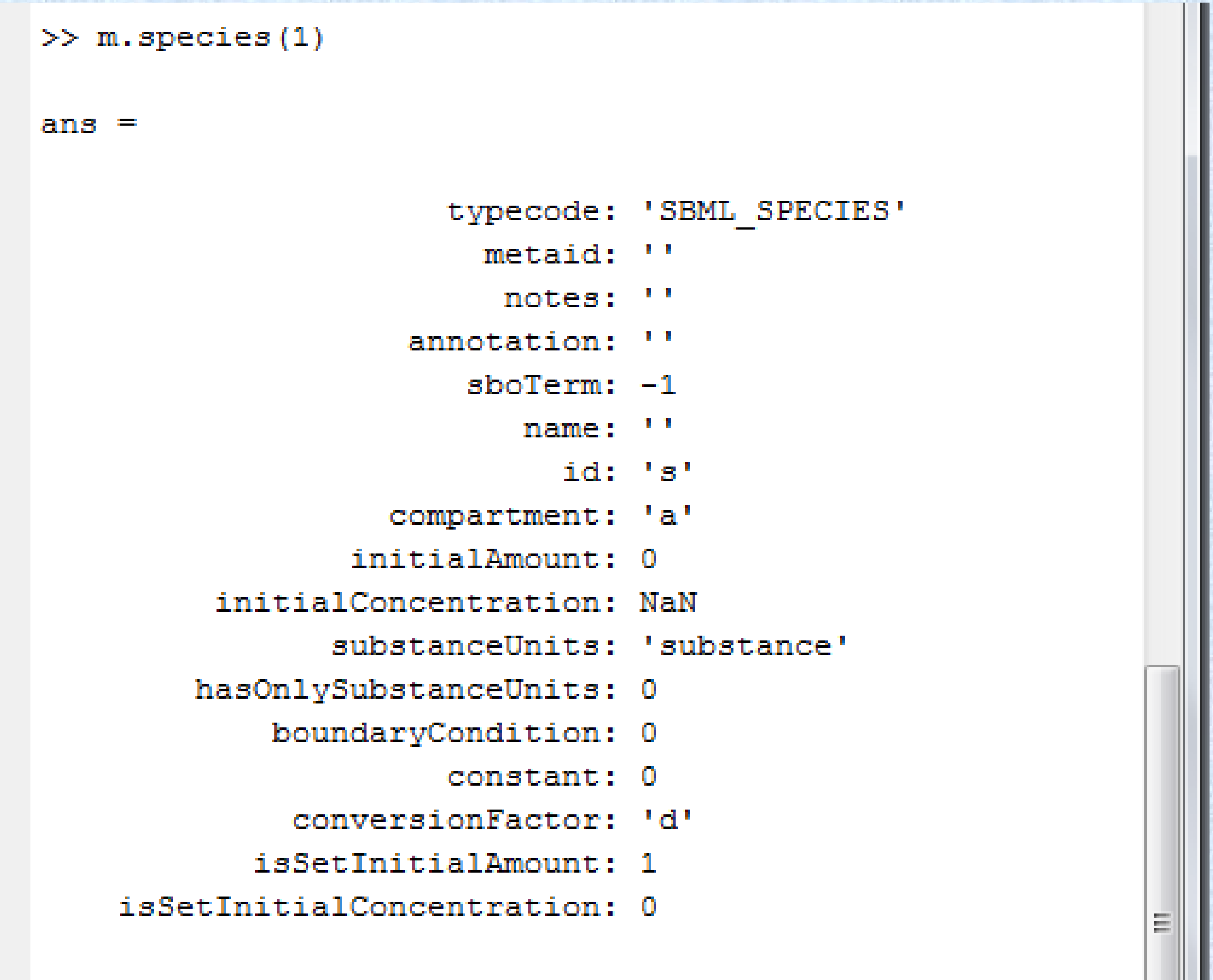
```
functionDefinition: [1x1 struct]
    unitDefinition: [1x5 struct]
       compartment: [1x2 struct]
           species: [1x3 struct]
         parameter: [1x6 struct]
 initialAssignment: [1x1 struct]
              rule: [1x4 struct]
        constraint: [1x1 struct]
          reaction: [1x1 struct]
             event: [1x1 struct]
```

MATLAB_SBML structure

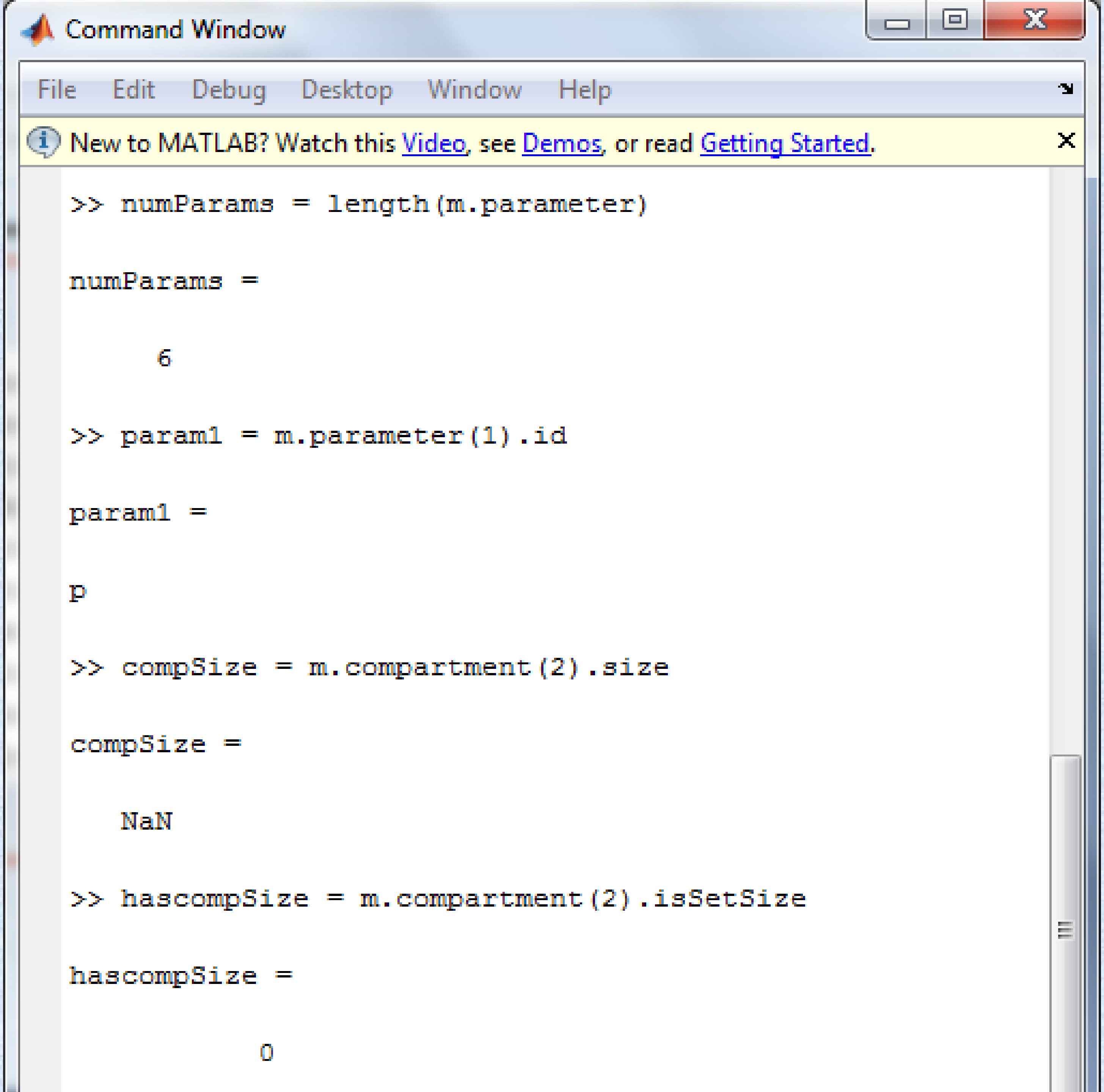


```
>> m.species(1)

ans = 

                     typecode: 'SBML_SPECIES'
                       metaid: ''
                        notes: ''
                   annotation: ''
                      sboTerm: -1
                         name: ''
                           id: 's'
                  compartment: 'a'
                initialAmount: 0
         initialConcentration: NaN
               substanceUnits: 'substance'
        hasOnlySubstanceUnits: 0
            boundaryCondition: 0
                     constant: 0
             conversionFactor: 'd'
          isSetInitialAmount: 1
   isSetInitialConcentration: 0
```

MATLAB_SBML structure



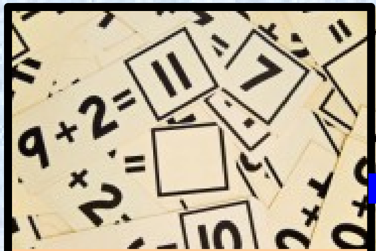
```
>> m.species(1)

ans =

                     typecode: 'SBML_SPECIES'
                       metaid: ''
                        notes: ''
                   annotation: ''
                      sboTerm: -1
                         name: ''
                           id: 's'
                  compartment: 'a'
                initialAmount: 0
         initialConcentration: NaN
               substanceUnits: 'substance'
        hasOnlySubstanceUnits: 0
            boundaryCondition: 0
                     constant: 0
             conversionFactor: 'd'
           isSetInitialAmount: 1
    isSetInitialConcentration: 0
```



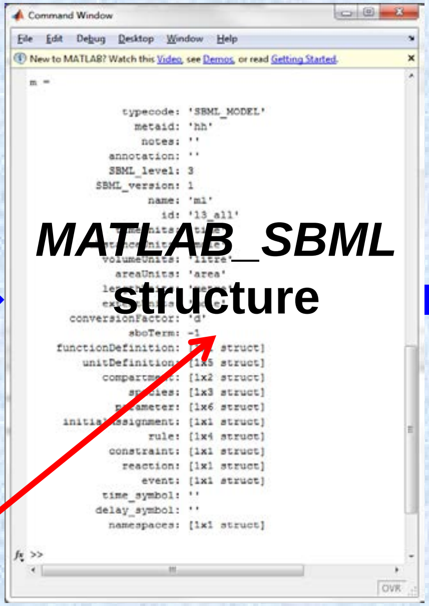
New to MATLAB? Watch this Video, see Demos, or read Getting Started.

```
>> numParams = length(m.parameter)

numParams =

     6

>> param1 = m.parameter(1).id

param1 =

p

>> compSize = m.compartment(2).size

compSize =

   NaN

>> hascompSize = m.compartment(2).isSetSize

hascompSize =

           0
```

Export SBML



Your preferred environment



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```
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            extentUnits: 'mole'
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         unitDefinition: [1x5 struct]
            compartment: [1x2 struct]
                species: [1x3 struct]
              parameter: [1x6 struct]
      initialAssignment: [1x1 struct]
                   rule: [1x4 struct]
             constraint: [1x1 struct]
               reaction: [1x1 struct]
                  event: [1x1 struct]
            time_symbol: ''
           delay_symbol: ''
             namespaces: [1x1 struct]

fx >>
```

MATLAB_SBML **structure**

Must be a structure of the required format

Use the ‘isSBML_Model’ script to determine whether the structure is as expected.

Export SBML

Checking the structure

isSBML_Model

✓checks typecode

✓all required fields present

✓have appropriate types of data

Acknowledgements

Akiya Jouraku

Keio, Japan

Frank Bergmann

Caltech, USA

Mike Hucka

Caltech, USA

National Institute of General Medical Sciences