Tools for the Flux Balance Constraints Package

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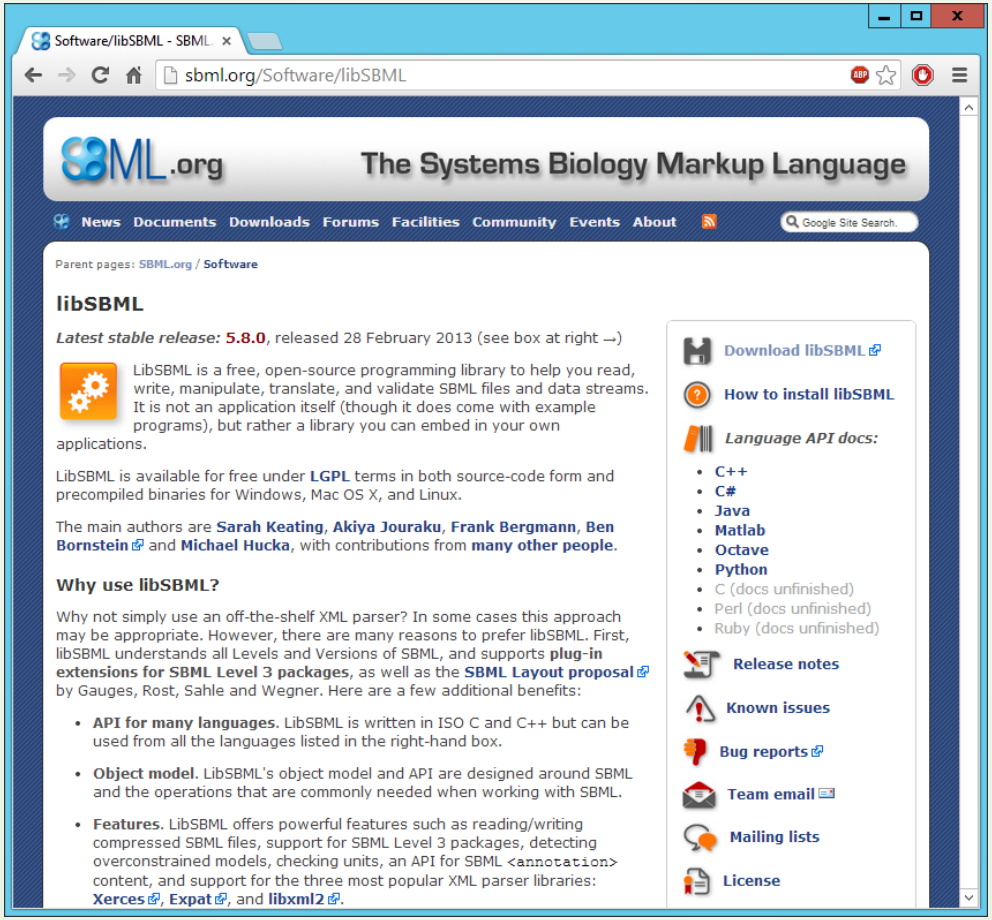
libSBML

Overview



http://sbml.org/Software/libSBML

Converters

Cobra -> FBC

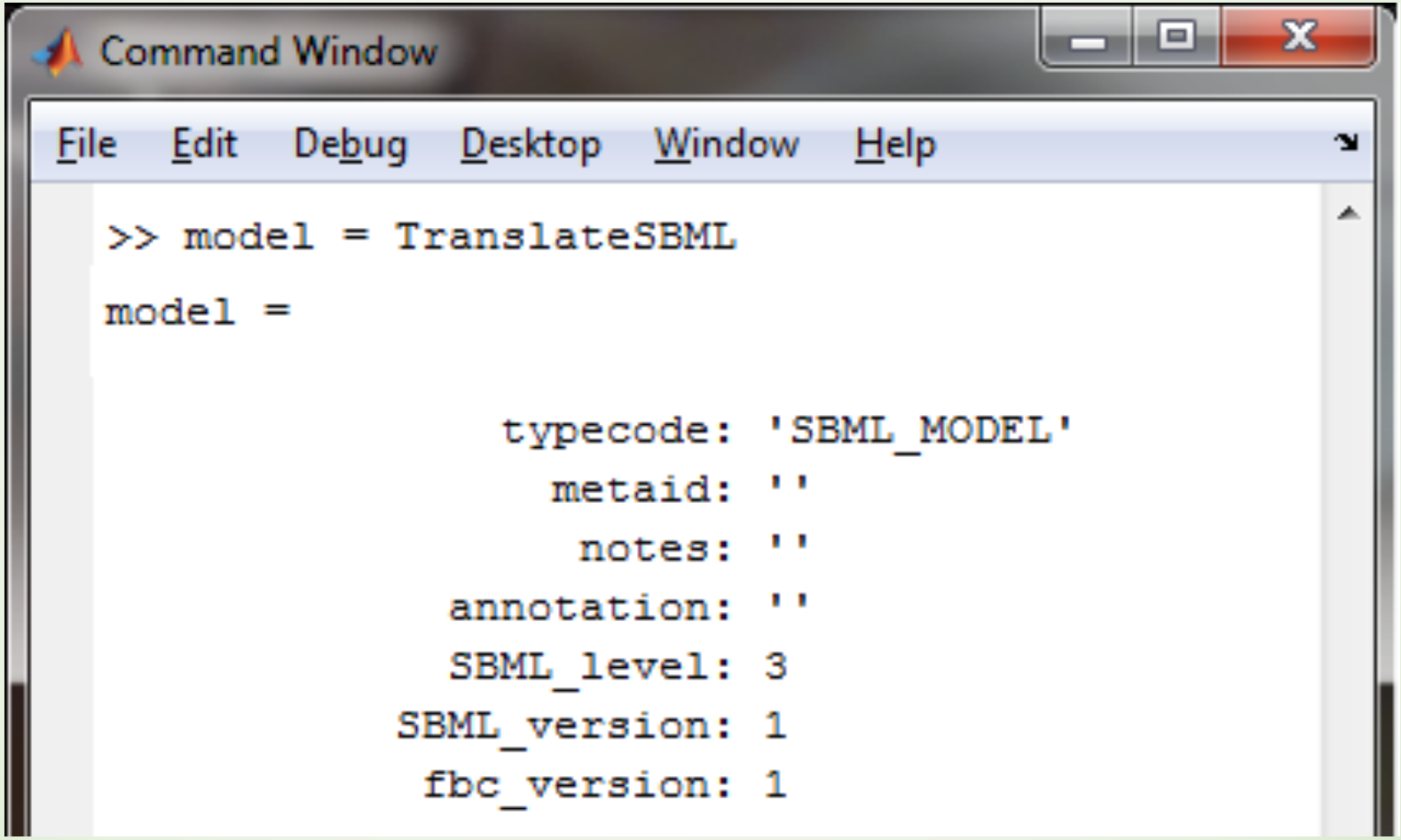
```
sbmldoc = libsbml.readSBML (filename)
props = libsbml.ConversionProperties()
props.addOption("convert cobra", True,
                "Convert Cobra model")
result = sbmldoc.convert(props)
if (result != libsbml.LIBSBML_OPERATION_SUCCESS):
  print("[Error] Conversion failed... ")
  sys.exit(1)
```

Converters

FBC -> Cobra

```
sbmldoc = libsbml.readSBML (filename)
props = libsbml.ConversionProperties()
props.addOption("convert fbc to cobra", True,
            "Convert FBC model to Cobra model”)
result = sbmldoc.convert(props)
if (result != libsbml.LIBSBML_OPERATION_SUCCESS):
  print("[Error] Conversion failed... ")
  sys.exit(1)
```

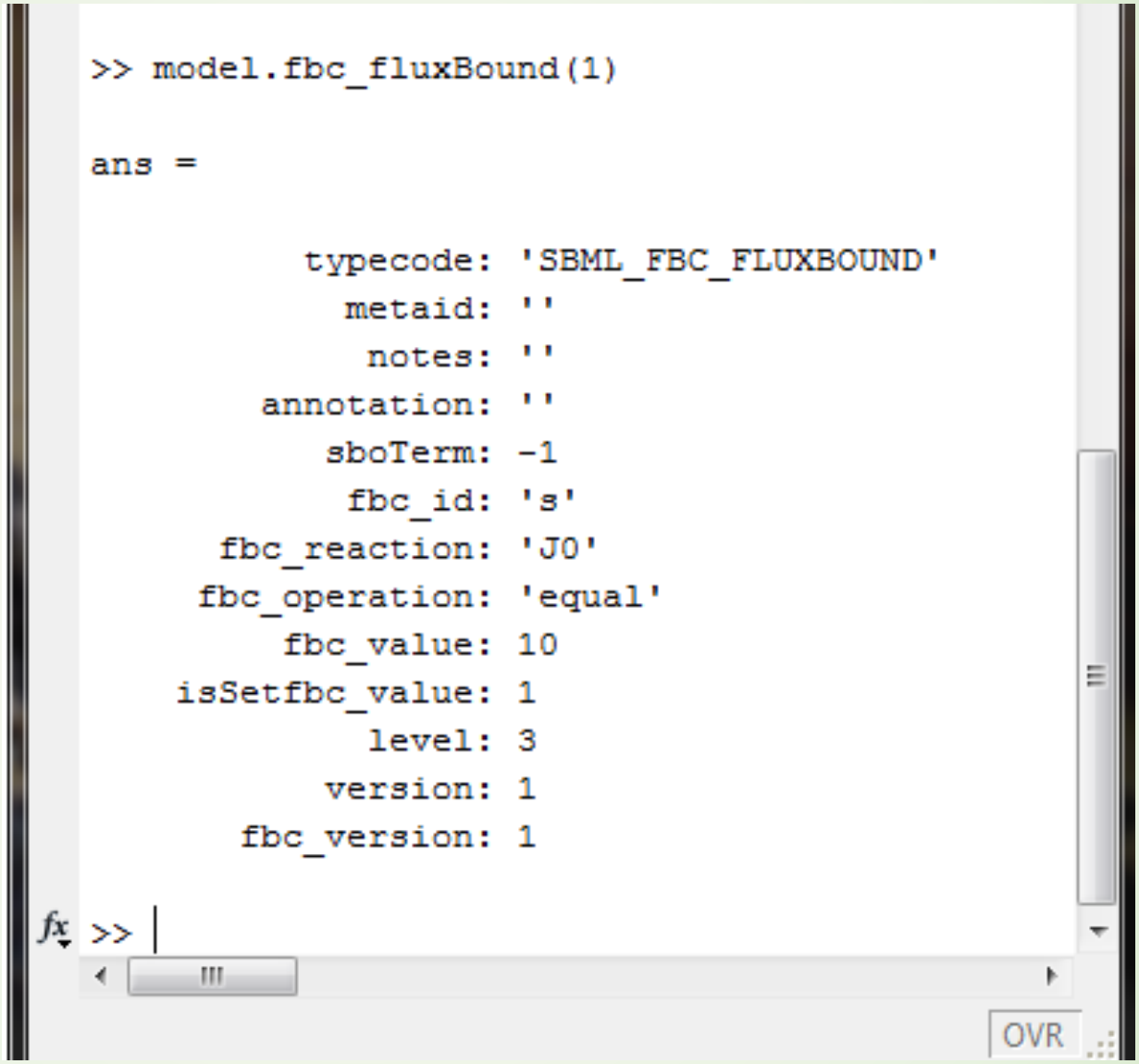
Matlab


Command Window
File Edit Debug Desktop Window Help
>> model = TranslateSBML
model =
typecode: 'SBML_MODEL'
metaid: ''
notes: ''
annotation: ''
SBML_level: 3
SBML_version: 1
fbc_version: 1

Matlab

```
        functionDefinition: [1x0 struct]
            unitDefinition: [1x1 struct]
               compartment: [1x1 struct]
                   species: [1x5 struct]
                 parameter: [1x0 struct]
          initialAssignment: [1x0 struct]
                      rule: [1x0 struct]
                constraint: [1x0 struct]
                  reaction: [1x2 struct]
                     event: [1x0 struct]
           fbc_fluxBound: [1x2 struct]
           fbc_objective: [1x1 struct]
      fbc activeObjective: 'obj1'
```

Matlab


>> model.fbc_fluxBound(1)
ans =
typecode: 'SBML_FBC_FLUXBOUND'
metaid: ''
notes: ''
annotation: ''
sboTerm: -1
fbc_id: 's'
fbc_reaction: 'J0'
fbc_operation: 'equal'
fbc_value: 10
isSetfbc_value: 1
level: 3
version: 1
fbc_version: 1
>>
OVR

Matlab

```
>> fb = FluxBound_create(3,1,1)

fb =

          typecode: 'SBML_FBC_FLUXBOUND'
            metaid: ''
             notes: ''
        annotation: ''
           sboTerm: -1
            fbc_id: ''
      fbc_reaction: ''
     fbc_operation: ''
         fbc_value: NaN
    isSetfbc_value: 0
             level: 3
           version: 1
       fbc_version: 1

>> fb = FluxBound_setId(fb, 'fb1')

fb =

          typecode: 'SBML_FBC_FLUXBOUND'
            metaid: ''
             notes: ''
        annotation: ''
           sboTerm: -1
            fbc_id: 'fb1'
      fbc_reaction: ''
     fbc_operation: ''
         fbc_value: NaN
    isSetfbc_value: 0
             level: 3
           version: 1
       fbc_version: 1
```

Matlab

Command Window

File Edit Debug Desktop Window Help

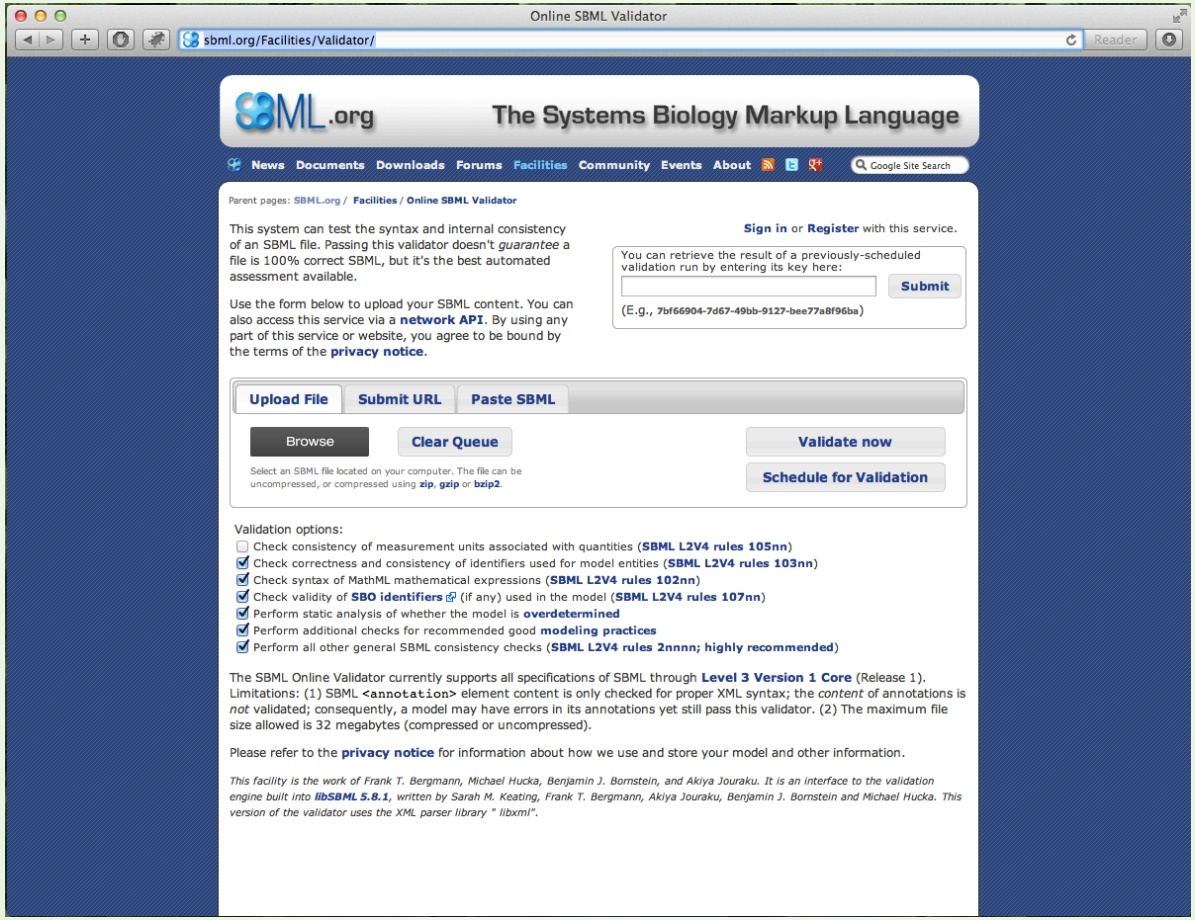
```
>> numFluxBounds = length(model.fbc_fluxBound)

numFluxBounds =

     2

>> obj1 = model.fbc_objective(1)

obj1 =

             typecode: 'SBML_FBC_OBJECTIVE'
               metaid: ''
                notes: ''
           annotation: ''
              sboTerm: -1
               fbc_id: 'c'
             fbc_type: 'maximize'
    fbc_fluxObjective: [1x2 struct]
                level: 3
              version: 1
          fbc_version: 1

>> obj1.fbc_type

ans =

maximize

>>
```

Matlab

```
>> id = Objective_getId(obj1)

id =

c

>> rn = FluxBound_getReaction(fb)

rn =

J0

>> op = FluxBound_getOperation(fb)

op =

lessEqual
```

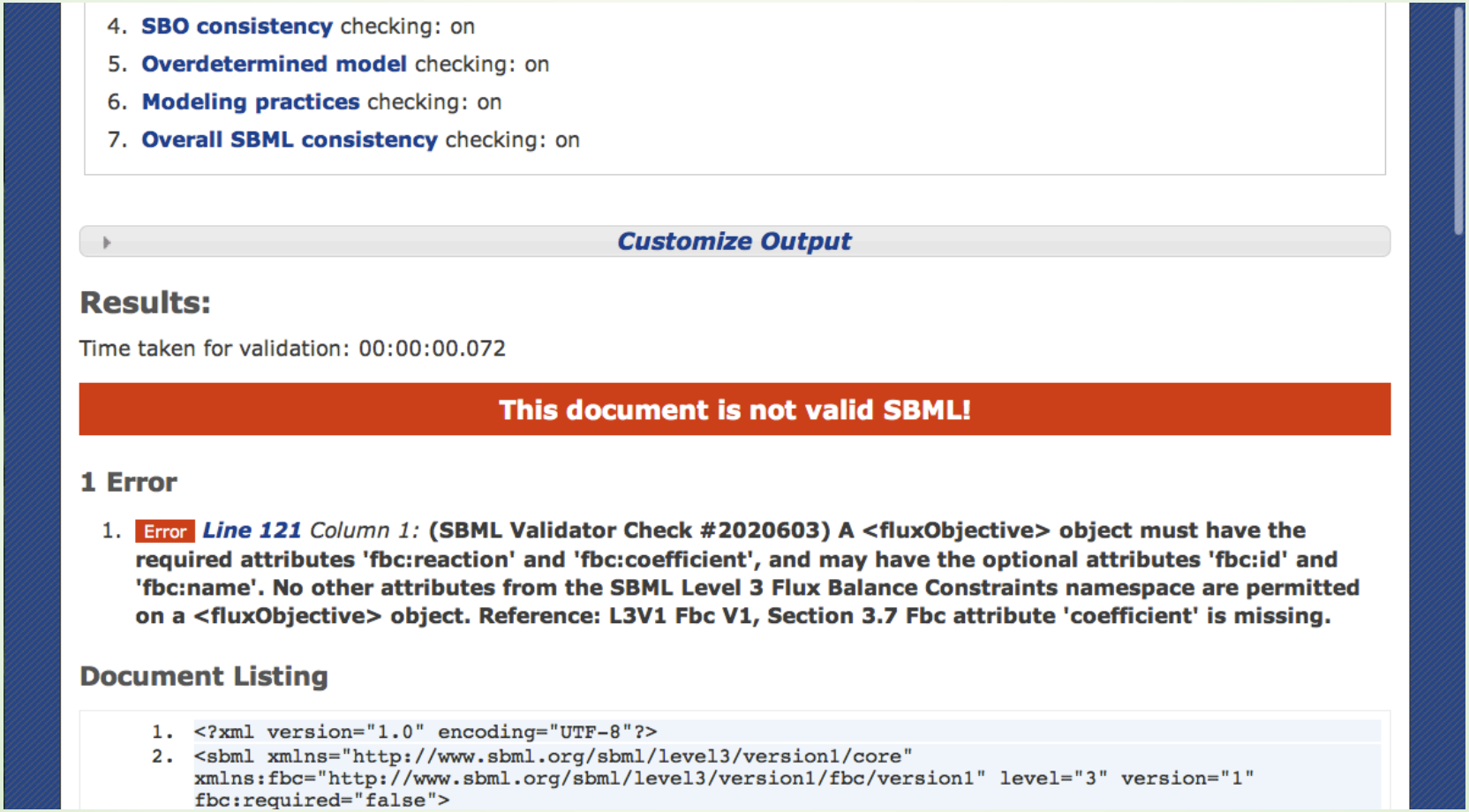
Online Validator

Online Validator



http://sbml.org/Facilities/Validator/

Online Validator



4. **SBO consistency** checking: on
5. **Overdetermined model** checking: on
6. **Modeling practices** checking: on
7. **Overall SBML consistency** checking: on

Customize Output

Results:

Time taken for validation: 00:00:00.072

This document is not valid SBML!

1 Error

1. Error ***Line 121*** *Column 1:* **(SBML Validator Check #2020603) A <fluxObjective> object must have the required attributes 'fbc:reaction' and 'fbc:coefficient', and may have the optional attributes 'fbc:id' and 'fbc:name'. No other attributes from the SBML Level 3 Flux Balance Constraints namespace are permitted on a <fluxObjective> object. Reference: L3V1 Fbc V1, Section 3.7 Fbc attribute 'coefficient' is missing.**

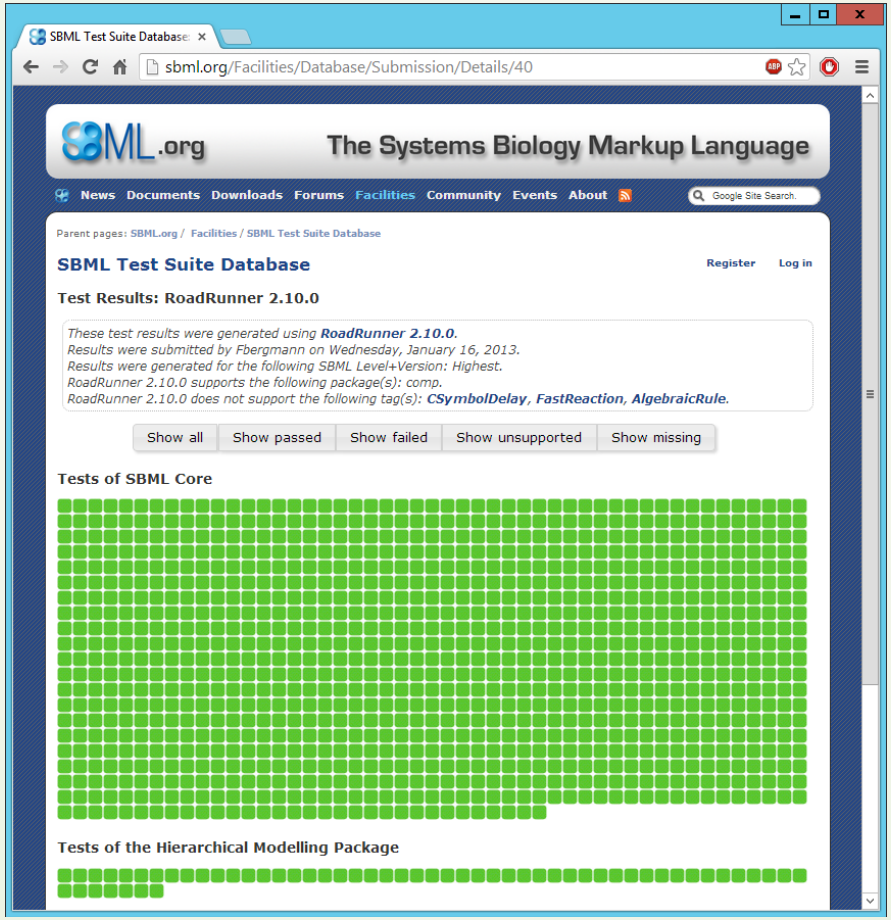
Document Listing

```
1. <?xml version="1.0" encoding="UTF-8"?>
2. <sbml xmlns="http://www.sbml.org/sbml/level3/version1/core"
   xmlns:fbc="http://www.sbml.org/sbml/level3/version1/fbc/version1" level="3" version="1"
   fbc:required="false">
```

http://sbml.org/Facilities/Validator/

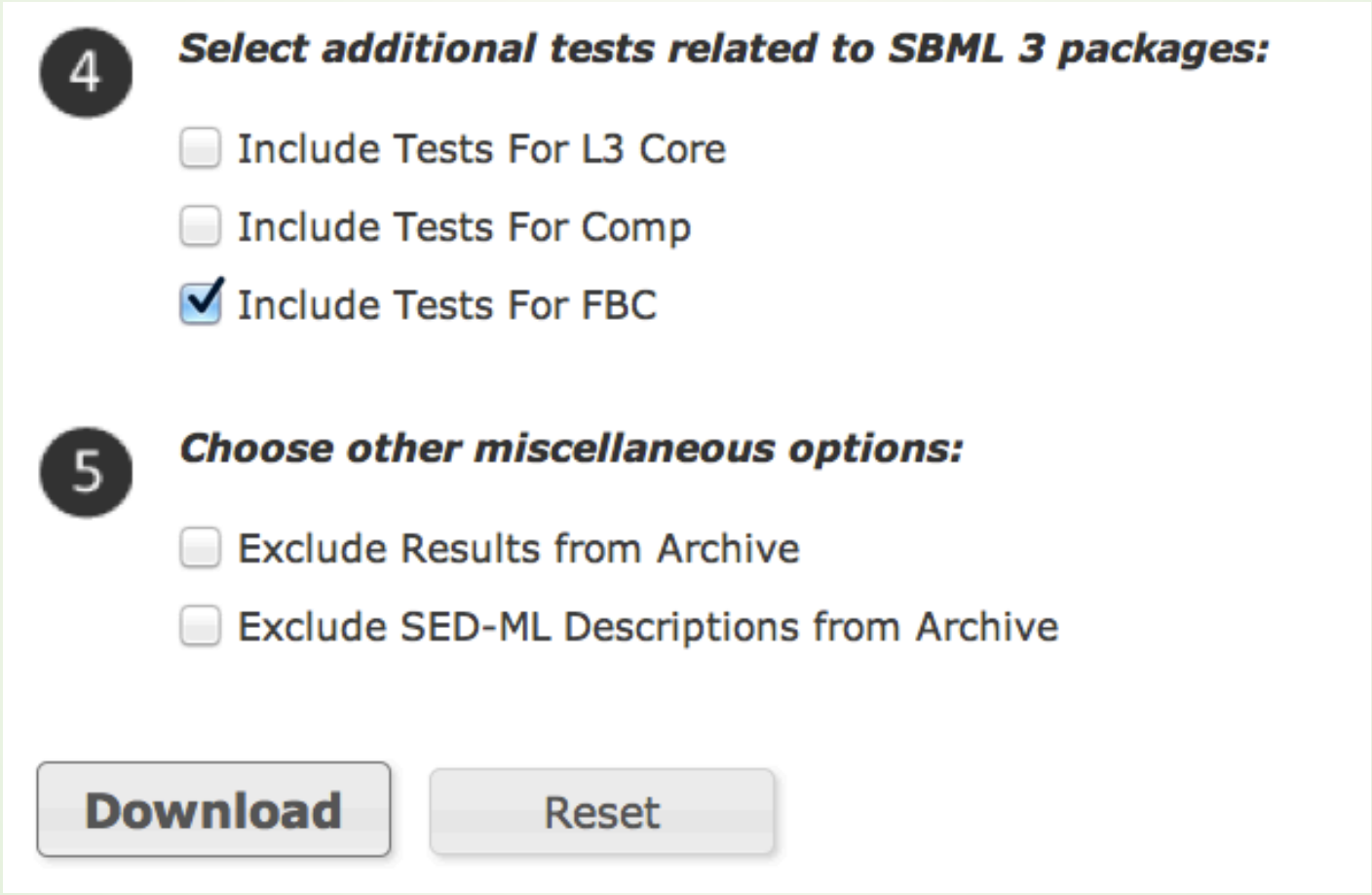
SBML Test Suite

SBML Test Suite Database



http://sbml.org/Facilities/Database/

SBML Test Suite Database



http://sbml.org/Facilities/Database/

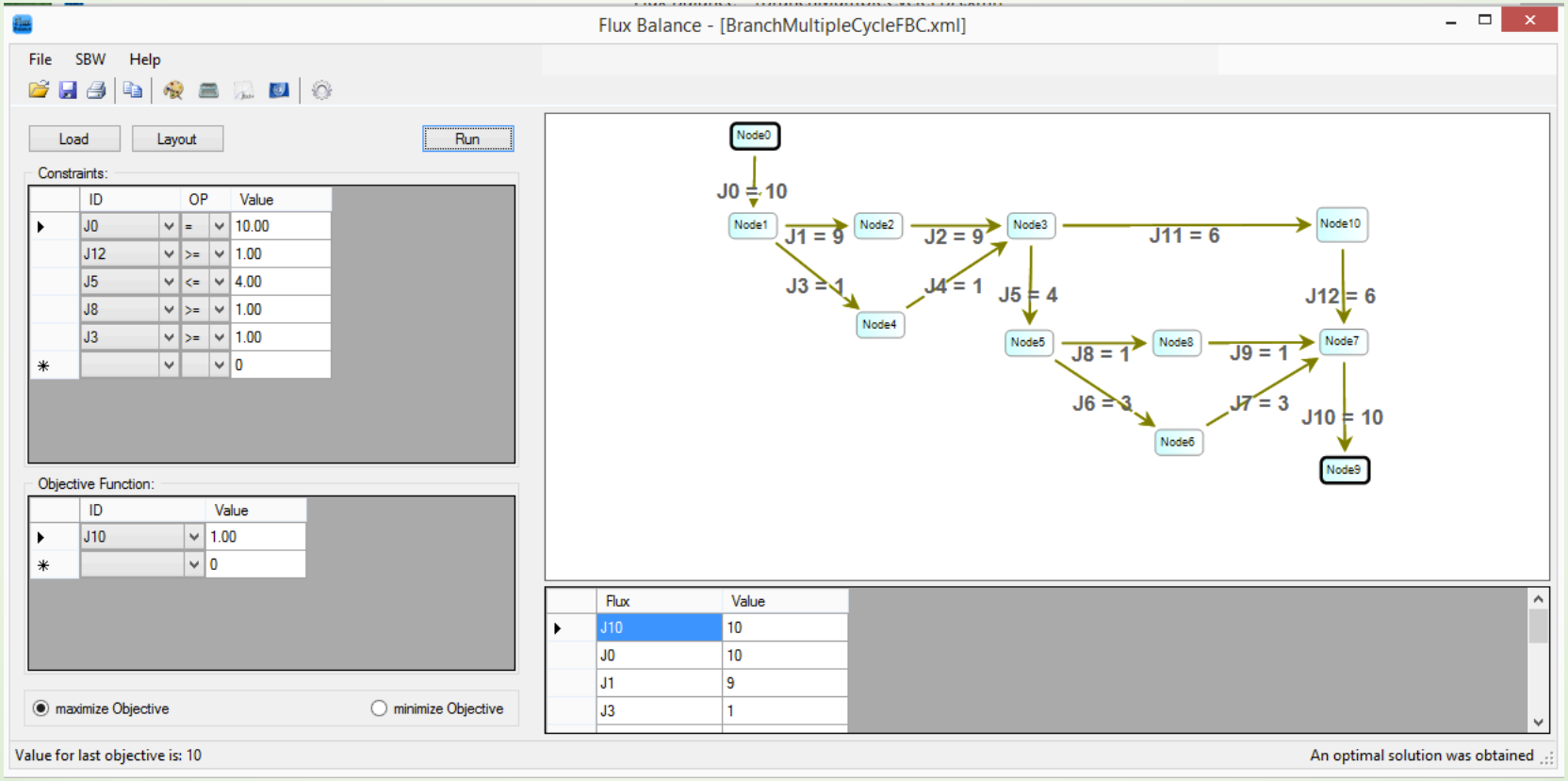
SBML Test Suite Database

Name	Component tags	Test tags	Brief summary of model
01186	Compartment, Reaction, Species, fbc:FluxBound, fbc:Objective, fbc:FluxObjective,	fbc:MaximizeObjective,	Maximize single objective function, hard bounds.
01187	Compartment, Reaction, Species, fbc:FluxBound, fbc:Objective, fbc:FluxObjective,	fbc:MinimizeObjective,	Minimize single objective function, hard bounds.
01188	Compartment, Reaction, Species, fbc:FluxBound, fbc:Objective, fbc:FluxObjective,	fbc:MaximizeObjective,	Maximize single objective function, infinite bounds.
01189	Compartment, Reaction, Species, fbc:FluxBound, fbc:Objective, fbc:FluxObjective,	fbc:MinimizeObjective,	Minimize single objective function, infinite bounds.
01190	Compartment, Reaction, Species, fbc:FluxBound, fbc:Objective, fbc:FluxObjective,	fbc:MaximizeObjective,	Maximize single objective function, non-unitary objective flux coefficient
01191	Compartment, Reaction, Species, fbc:FluxBound, fbc:Objective, fbc:FluxObjective,	fbc:MaximizeObjective,	Multiple objectives defined, optimize active one (maximize)
01192	Compartment, Reaction, Species, fbc:FluxBound, fbc:Objective, fbc:FluxObjective,	fbc:MaximizeObjective,	Single objective, multiple flux objectives
01193	Compartment, Reaction, Species, fbc:FluxBound, fbc:Objective, fbc:FluxObjective,	fbc:MaximizeObjective, fbc:BoundGreaterEqual,	Single objective, test R07 GE 0.5, R10 GE 0.5
01194	Compartment, Reaction, Species, fbc:FluxBound, fbc:Objective, fbc:FluxObjective,	fbc:MaximizeObjective, fbc:BoundLessEqual,	Single objective, test R07 LE 0.2, R10 LE 0.3
01195	Compartment, Reaction, Species, fbc:FluxBound, fbc:Objective, fbc:FluxObjective,	fbc:MaximizeObjective, fbc:BoundEqual,	Single objective, test: R07 EQ 0.2, R10 EQ 0.2, R25 EQ 0.6
01196	Compartment, Reaction, Species, fbc:FluxBound, fbc:Objective, fbc:FluxObjective,	fbc:MaximizeObjective,	Infeasible solution, should return a nan

http://sbml.org/Facilities/Database/

Flux Balance Tool

Teaching Tool: explore fluxes along a network, define flux bounds, run fba.



http://fbergmann.github.io/FluxBalance/

Acknowledgements

- Sarah Keating, Mike Hucka, Ursula Kummer, Herbert Sauro