

Tools for the Flux Balance Constraints Package

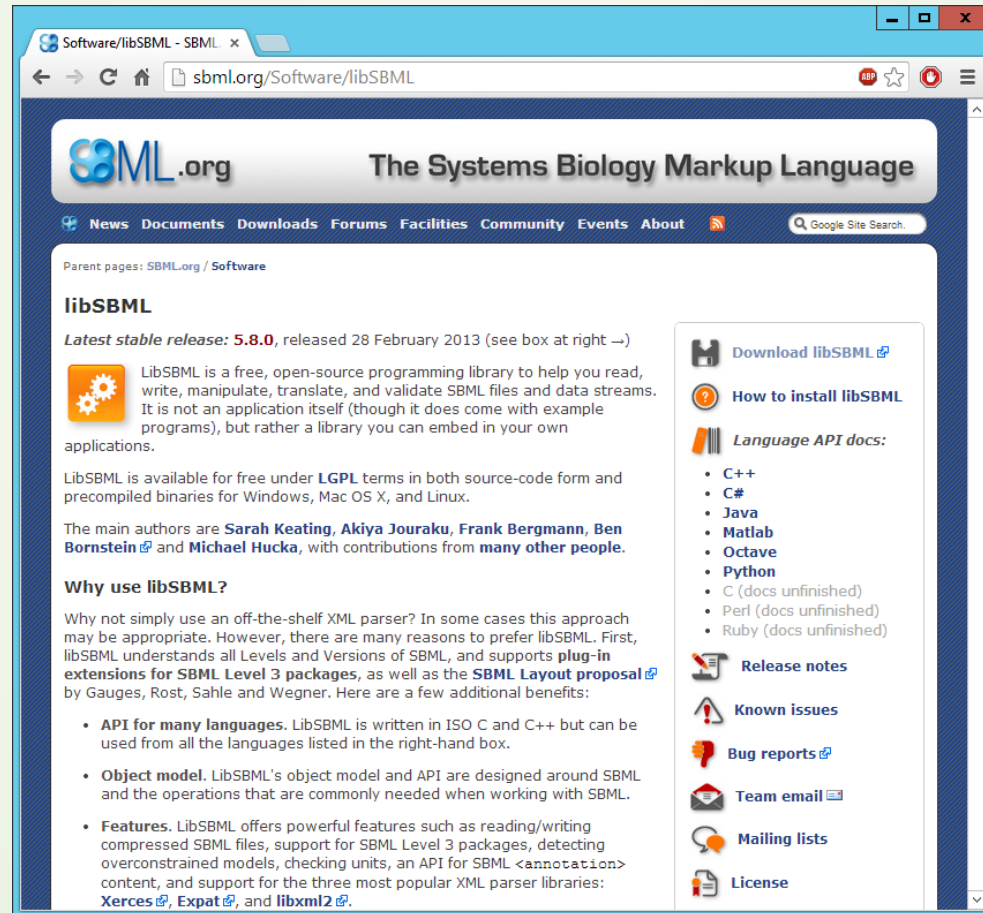


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libSBML

Overview



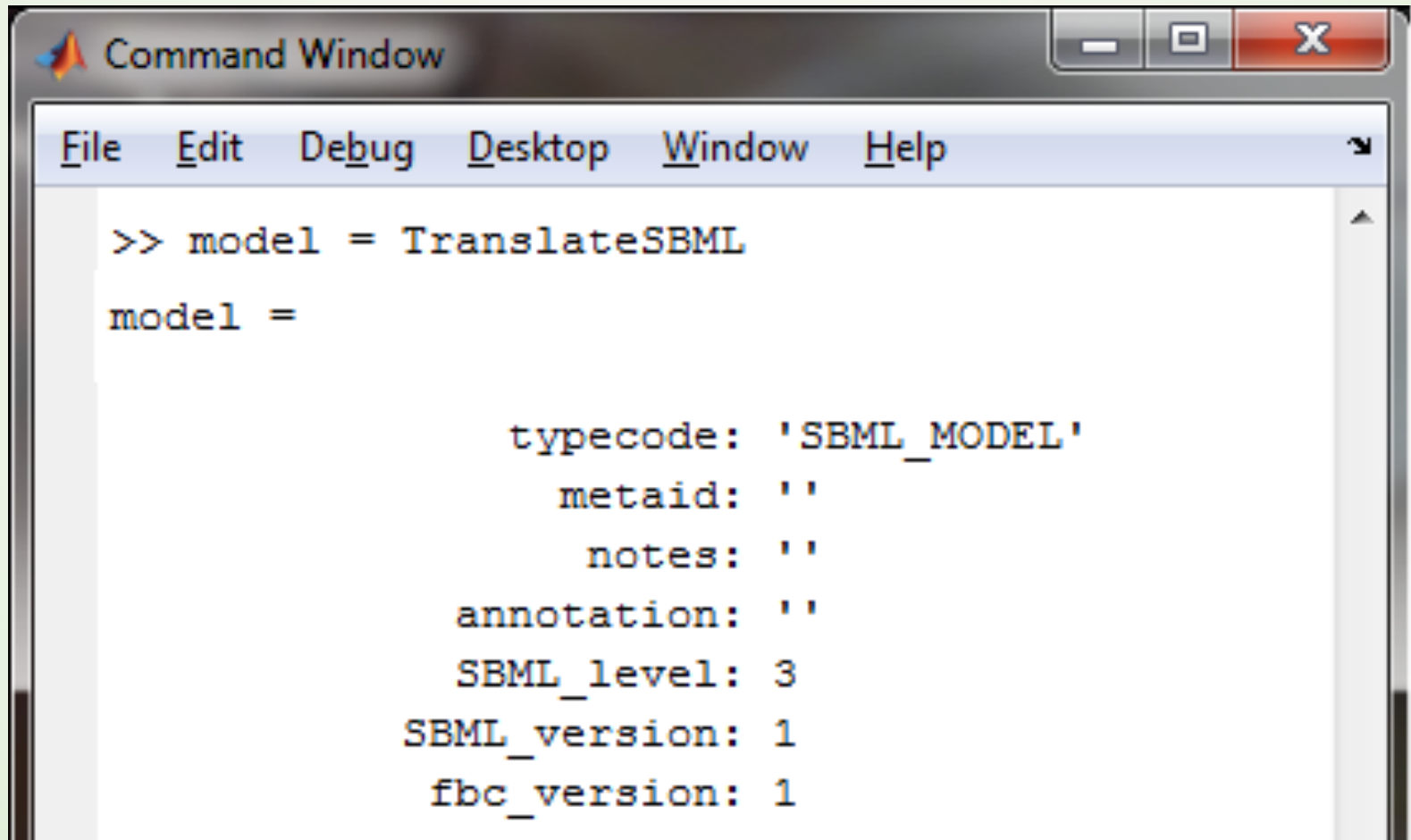
Converters

```
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

```
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
```

fx

>> |

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Matlab

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

fb =

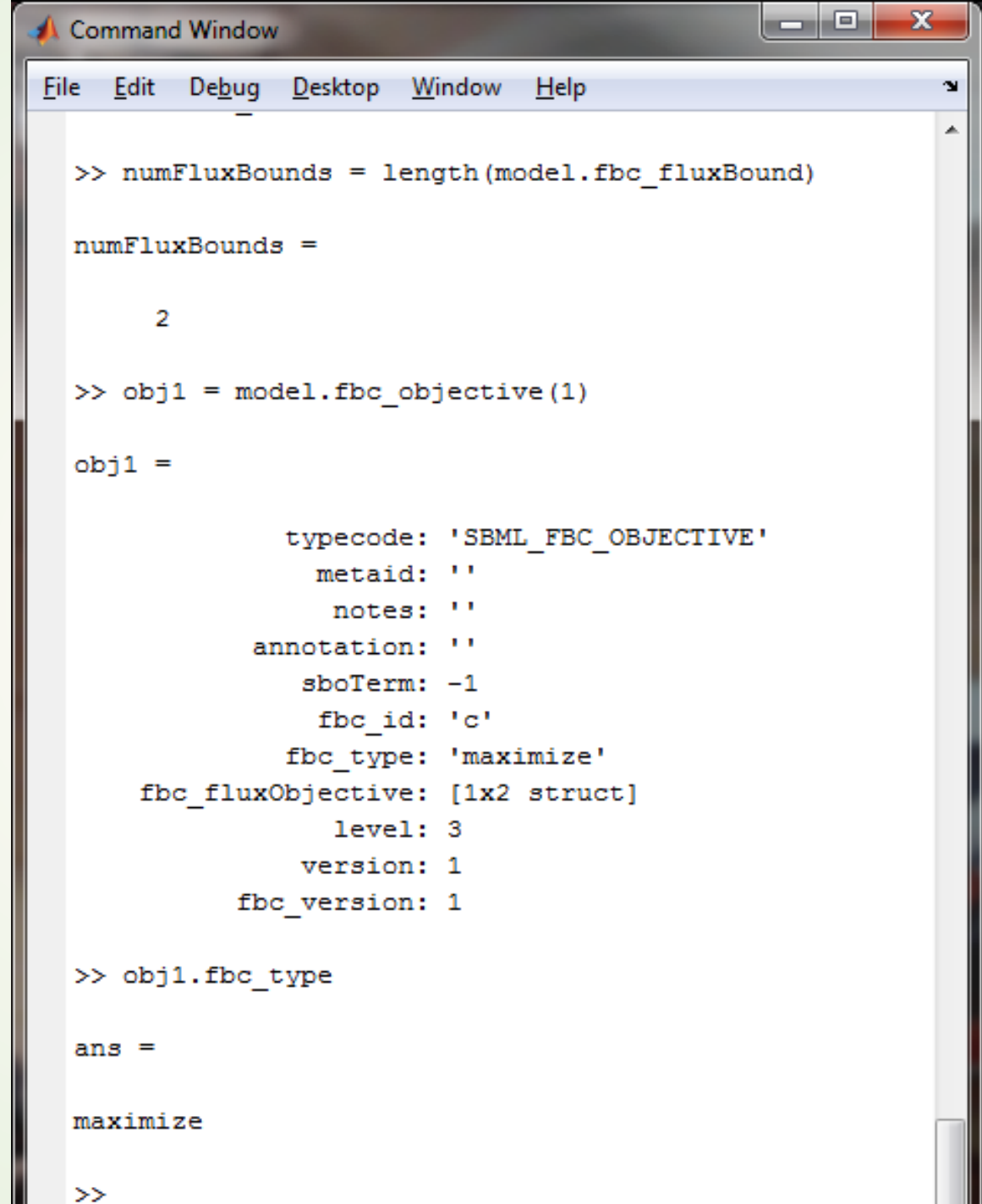
    typecode: 'SBML_FBC_FLUXBOUND'
    metaid: ''
    notes: ''
    annotation: ''
    sboTerm: -1
    fbc_id: ''
    fbc_reaction: ''
    fbc_operation: ''
    fbc_value: NaN
    isSetfbc_value: 0
    level: 3
    version: 1
    fbc_version: 1

>> 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

The screenshot shows a web browser window titled "Online SBML Validator" with the URL "sbml.org/Facilities/Validator/". The page features the SBML.org logo and the text "The Systems Biology Markup Language". A navigation bar includes links for News, Documents, Downloads, Forums, Facilities, Community, Events, and About, along with a Google Site Search bar. The main content area explains the validator's purpose: testing syntax and internal consistency of SBML files. It provides a "Sign in or Register" link and a section for retrieving results from a previously scheduled validation using a key. Below this, there are three tabs: "Upload File", "Submit URL", and "Paste SBML". The "Upload File" tab is active, showing a "Browse" button to select a file from the computer. A "Clear Queue" button is also present. To the right, there are "Validate now" and "Schedule for Validation" buttons. A "Validation options" section lists several checkboxes, most of which are checked, including checks for measurement units, identifiers, MathML expressions, SBO identifiers, static analysis, modeling practices, and general consistency checks. The page also includes a "Limitations" section and a "Please refer to the privacy notice" link. At the bottom, there is a small text block crediting the developers: Frank T. Bergmann, Michael Hucka, Benjamin J. Bornstein, and Akiya Jouraku.

Online SBML Validator

sbml.org/Facilities/Validator/

SBML.org The Systems Biology Markup Language

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Parent pages: SBML.org / Facilities / Online SBML Validator

This system can test the syntax and internal consistency of an SBML file. Passing this validator doesn't *guarantee* a file is 100% correct SBML, but it's the best automated assessment available.

Use the form below to upload your SBML content. You can also access this service via a **network API**. By using any part of this service or website, you agree to be bound by the terms of the **privacy notice**.

Sign in or Register with this service.

You can retrieve the result of a previously-scheduled validation run by entering its key here:

Submit

(E.g., 7bf66904-7d67-49bb-9127-bee77a8f96ba)

Upload File **Submit URL** **Paste SBML**

Browse **Clear Queue** **Validate now** **Schedule for Validation**

Select an SBML file located on your computer. The file can be uncompressed, or compressed using **zip**, **gzip** or **bzip2**.

Validation options:

- ☐ Check consistency of measurement units associated with quantities (**SBML L2V4 rules 105nn**)
- ☒ Check correctness and consistency of identifiers used for model entities (**SBML L2V4 rules 103nn**)
- ☒ Check syntax of MathML mathematical expressions (**SBML L2V4 rules 102nn**)
- ☒ Check validity of **SBO identifiers** (if any) used in the model (**SBML L2V4 rules 107nn**)
- ☒ Perform static analysis of whether the model is **overdetermined**
- ☒ Perform additional checks for recommended good **modeling practices**
- ☒ Perform all other general SBML consistency checks (**SBML L2V4 rules 2nnnn**; **highly recommended**)

The SBML Online Validator currently supports all specifications of SBML through **Level 3 Version 1 Core** (Release 1).

Limitations: (1) SBML **<annotation>** element content is only checked for proper XML syntax; the *content* of annotations is *not* validated; consequently, a model may have errors in its annotations yet still pass this validator. (2) The maximum file size allowed is 32 megabytes (compressed or uncompressed).

Please refer to the **privacy notice** for information about how we use and store your model and other information.

This facility is the work of Frank T. Bergmann, Michael Hucka, Benjamin J. Bornstein, and Akiya Jouraku. It is an interface to the validation engine built into **libSBML 5.8.1**, written by Sarah M. Keating, Frank T. Bergmann, Akiya Jouraku, Benjamin J. Bornstein and Michael Hucka. This version of the validator uses the XML parser library "libxslt".

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">`

SBML Test Suite

SBML Test Suite Database

The screenshot displays the SBML Test Suite Database website. The browser's address bar shows the URL sbml.org/Facilities/Database/Submission/Details/40. The website header includes the SBML.org logo and the text "The Systems Biology Markup Language". A navigation menu contains links for News, Documents, Downloads, Forums, Facilities, Community, Events, and About. A search bar labeled "Google Site Search" is also present. Below the header, the page title is "SBML Test Suite Database" with links for "Register" and "Log in". The main content area is titled "Test Results: RoadRunner 2.10.0". It contains a text box with the following information: "These test results were generated using RoadRunner 2.10.0. Results were submitted by Fbergmann on Wednesday, January 16, 2013. Results were generated for the following SBML Level+Version: Highest. RoadRunner 2.10.0 supports the following package(s): comp. RoadRunner 2.10.0 does not support the following tag(s): CSymbolDelay, FastReaction, AlgebraicRule." Below this text box are five buttons: "Show all", "Show passed", "Show failed", "Show unsupported", and "Show missing". The page then shows two sections of test results: "Tests of SBML Core" and "Tests of the Hierarchical Modelling Package". Each section is represented by a grid of green squares, indicating successful test results. The "Tests of SBML Core" section shows a large grid of approximately 1000 green squares, while the "Tests of the Hierarchical Modelling Package" section shows a smaller grid of approximately 100 green squares.

SBML.org The Systems Biology Markup Language

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Parent pages: SBML.org / Facilities / SBML Test Suite Database

SBML Test Suite Database Register Log in

Test Results: RoadRunner 2.10.0

These test results were generated using RoadRunner 2.10.0.
Results were submitted by Fbergmann on Wednesday, January 16, 2013.
Results were generated for the following SBML Level+Version: Highest.
RoadRunner 2.10.0 supports the following package(s): comp.
RoadRunner 2.10.0 does not support the following tag(s): CSymbolDelay, FastReaction, AlgebraicRule.

Show all Show passed Show failed Show unsupported Show missing

Tests of SBML Core

Tests of the Hierarchical Modelling Package

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

SBML Test Suite Database

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Select additional tests related to SBML 3 packages:

- ☐ Include Tests For L3 Core
- ☐ Include Tests For Comp
- ☒ Include Tests For FBC

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Choose other miscellaneous options:

- ☐ Exclude Results from Archive
- ☐ Exclude SED-ML Descriptions from Archive

Download

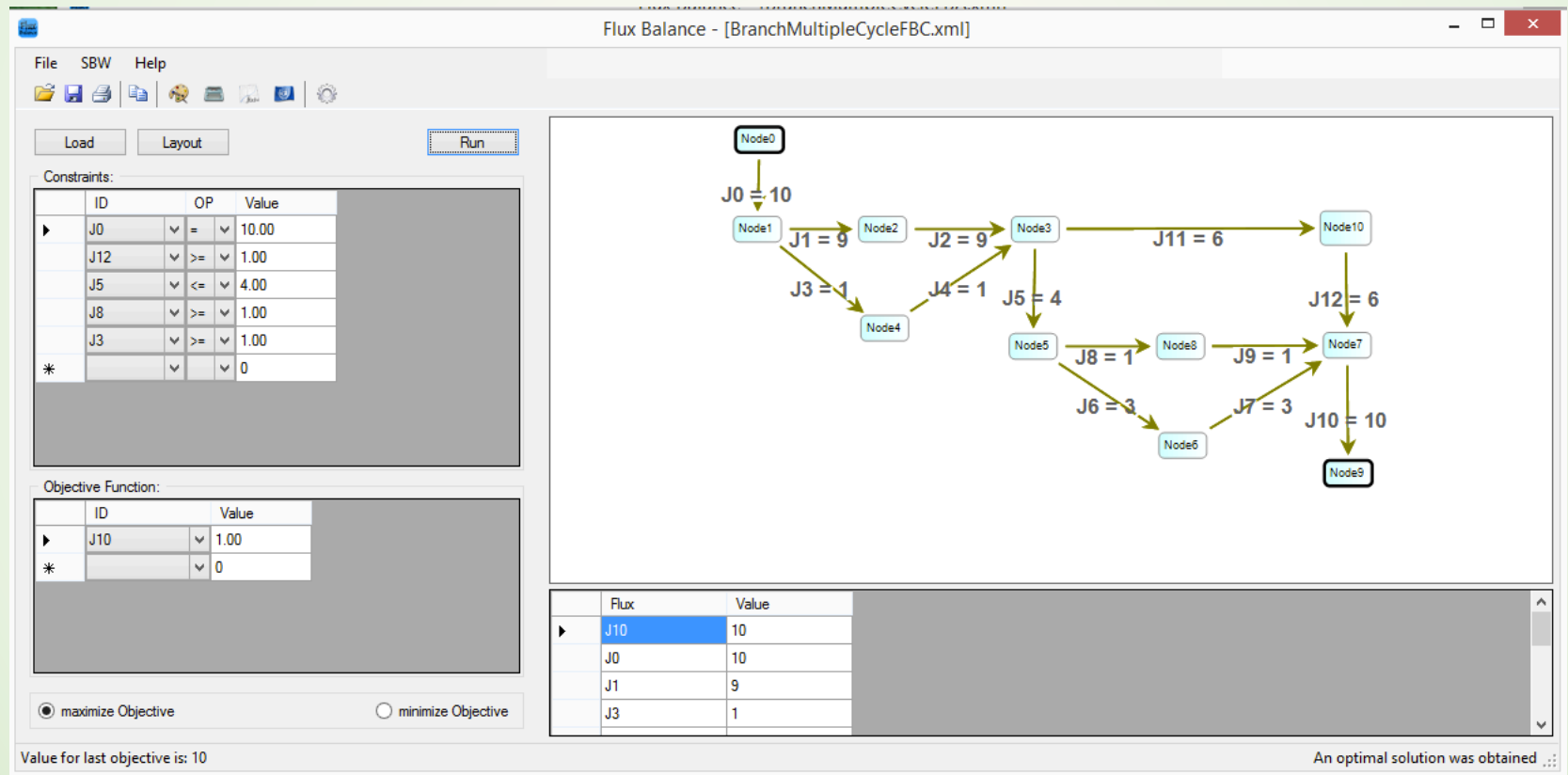
Reset

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

Flux Balance Tool

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



Acknowledgements

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