

Standardized description of simulation experiments: KiSAO, TEDDY, MIASE, SED-ML and NuML

An Introduction

15 AUG 2012 - COMBINE 2012

Dagmar Waltemath



**SYSTEMS BIOLOGY
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Traditio et Innovatio

BIOMD0000000127 - Izhikevich2003_SpikingNeuron

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Other formats (auto-generated)

Actions

Model

Overview

Math

Physical ex

Reference Publication

Publication ID: [18244602](#)

Izhikevich EM.
Simple model of spiking neurons.
IEEE Trans Neural Netw 2003;14(6):1569-72.
The Neurosciences Inst., San Diego, CA, USA

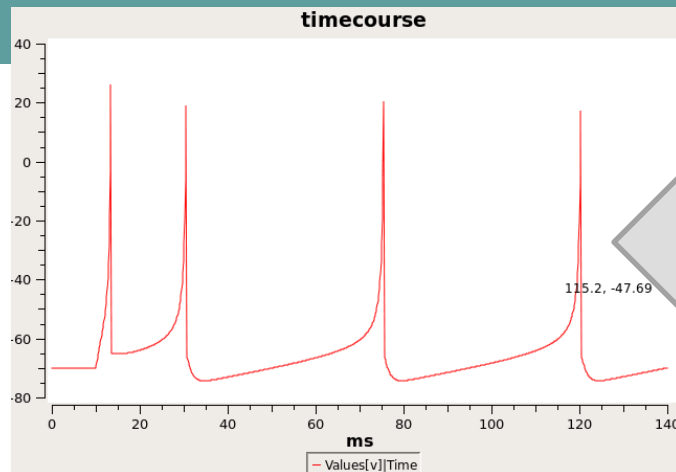


Fig.: Izhikevich (2003)

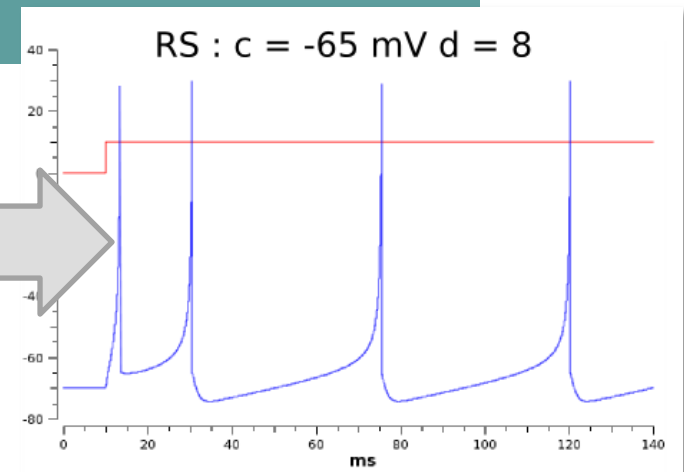


Fig.: COPASI simulation result

Use cases:

- Storing simulation experimental setups (“lab book”)
- Exchanging simulation experimental setups (collaborations)
- Using other people's simulation setups (published and standard models)
- Working with multiple simulation tools (import, export, re-import...)

Needs:

- Description of simulation setup
- Simulation algorithm
- Result data (?)
- Behavior of the model in a particular experiment

- Kinetic Simulation Algorithm Ontology (KiSAO)
- Terminology for the Description of Dynamics (TEDDY)
- Minimum Information About a Simulation Experiment (MIASE)
- Simulation Experiment Description Markup Language (SED-ML)
- Numerical Markup Language (NuML)

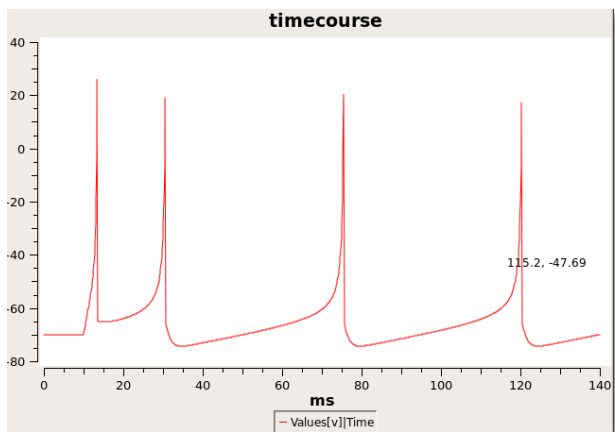


Fig.: Izhikevich (2003)

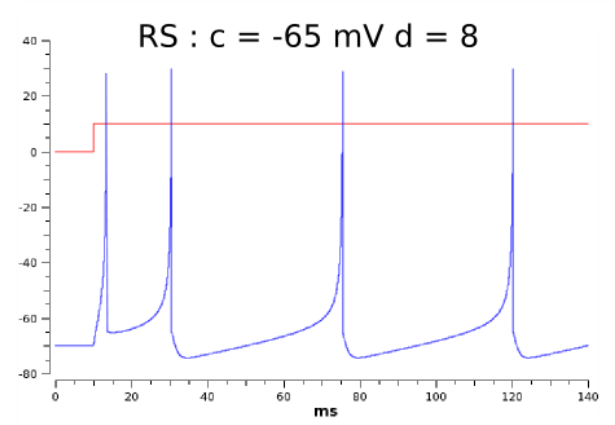


Fig.: COPASI simulation result

- Ontology for simulation algorithms used in computational biology
- OWL2 format
- <http://www.biomodels.net/kisao/>
- [biomodels-net-support @lists.sf.net](mailto:biomodels-net-support@lists.sf.net)
- *Courtot et al.*, Molecular Systems Biology (2011)



Browse KiSAO <http://bioportal.bioontology.org/ontologies/47524>

Kinetic Simulation Algorithm Ontology

Jump To:

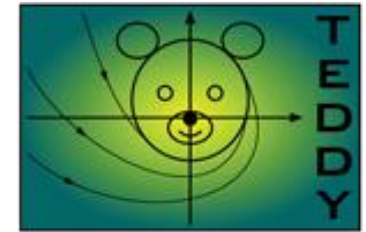
- modeling and simulation algorithm
 - modeling and simulation algorithm characteristic
 - hybridity
 - spatial description
 - symplecticness
 - type of domain geometry handling
 - type of method
 - type of problem
 - type of progression time step
 - type of solution
 - type of system behaviour
 - type of variable
 - modeling and simulation algorithm parameter
 - clusterization parameter
 - error control parameter
 - granularity control parameter
 - method switching control parameter
 - number of N-way partial least squares regression factors
 - number of partial least squares components
 - partitioning control parameter
 - type of validation
 - variables preprocessing parameter

Terms ▼

Details	Visualization	Notes (0)	Term Mappings (0)	Term Resources
Preferred Name	LSODA			
Synonyms (<i>skos:altLabel</i>)	Livermore solver for ordinary differential equations with automatic method switching			
Definitions (<i>skos:definition</i>)	LSODA solves systems $dy/dt = f$ with a dense or banded Jacobian when the problem is stiff, but it automatically selects between non-stiff (Adams [http://identifiers.org/biomodels.kisao/KISAO_0000289]) and stiff (BDF [http://identifiers.org/biomodels.kisao/KISAO_0000288]) methods. It uses the non-stiff method initially, and dynamically monitors data in order to decide which method to use.			
ID	kisao:KISAO_0000088			
Full Id	http://www.biomodels.net/kisao/KISAO#KISAO_0000088			
Creator	dk			
Label	LSODA			
See Also	http://identifiers.org/doi/10.1137/0904010 http://identifiers.org/isbn/978-0444866073 http://www.nea.fr/abs/html/uscd1227.html			
Alt Label	Livermore solver for ordinary differential equations with automatic method switching			
Definition	LSODA solves systems $dy/dt = f$ with a dense or banded Jacobian when the problem is stiff, but it automatically selects between non-stiff (Adams [http://identifiers.org/biomodels.kisao/KISAO_0000289]) and stiff (BDF [http://identifiers.org/biomodels.kisao/KISAO_0000288]) methods. It uses the non-stiff method initially, and dynamically monitors data in order to decide which method to use.			
Disjoint With	LSODPK LSOIBT LSODI LSODES			



- Ontology for dynamical behaviors, observable dynamical phenomena, and control elements in computational models
- OWL format



- <http://biomodels.net/teddy/>
- [biomodels-net-support @lists.sf.net](mailto:biomodels-net-support@lists.sf.net)
- *Courtot et al.*, Molecular Systems Biology (2011)

Explore TEDDY at <http://bioportal.bioontology.org/ontologies/46199>

Terminology for the Description of Dynamics

Jump To:

TEDDY entity

_obsolete

behaviour characteristic

behaviour diversification

functional motif

temporal behaviour

asymptotic behaviour

fixed point

limit behaviour

non-periodic orbit

periodic orbit

limit cycle

non-isolated cycle

Details

Visualization

Notes (0)

Term Mappings (0)

Term Resources

Preferred Name (*rdfs:label*)

limit cycle

Synonyms (*skos:altLabel*)

Grenzzyklus

isolated closed path

Definitions (*skos:definition*)

A closed orbit which is isolated, i.e. neighbouring orbits are not closed.

ID

TEDDY_0000051

Full Id

http://biomodels.net/teddy/TEDDY#TEDDY_0000051

Label

limit cycle

See Also

urn:miriam:isbn:0738204536

Alt Label

isolated closed path

Grenzzyklus

Definition

A closed orbit which is isolated, i.e. neighbouring orbits are not closed.

Disjoint With

[double-positive feedback loop](#)

[two-node positive feedback loop](#)

[hyperbolicity](#)

[uniform stability](#)

[homoclinic orbit](#)


[heteroclinic orbit](#)

[stability characteristic](#)

[Poincaré stability](#)

[unstable degenerate node](#)

[non-periodic orbit](#)



Minimum Information About a Simulation Experiment (MIASE)

PERSPECTIVE



Minimum Information About a Simulation Experiment (MIASE)

Article

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Dagmar Waltemath¹, Richard Adams^{2,3}, Daniel A. Beard⁴, Frank T. Bergmann^{5,6}, Upinder S. Bhalla⁷, Randall Britten⁸, Vijayalakshmi Chelliah⁹, Michael T. Cooling⁸, Jonathan Cooper¹⁰, Edmund J. Crampin⁸, Alan Garny¹¹, Stefan Hoops¹², Michael Hucka¹³, Peter Hunter⁸, Edda Klipp¹⁴, Camille Laibe⁹, Andrew K. Miller⁸, Ion Moraru¹⁵, David Nickerson⁸, Poul Nielsen⁸, Macha Nikolski¹⁶, Sven Sahle¹⁷, Herbert M. Sauro⁵, Henning Schmidt^{18,19}, Jacky L. Snoep²⁰, Dominic Tolle⁹, Olaf Wolkenhauer¹⁸, Nicolas Le Novère^{9*}

1 Database and Information Systems, Graduate Research School dIEM
at SBIS, Bertoldi University, Bertoldi, Mecklenburg-Vorpommern, Germany, **2**

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Related Content

SED-ML L1 V1

Levels: major revisions containing substantial changes

Versions: minor revisions containing corrections and refinements

Editorial board: coordinates SED-ML development (elected by sed-ml-discuss members)

Scope:

- multiple models
- multiple simulation setups
- time course simulations

Simulation Experiment Description Markup Language (SED-ML) : Level 1 Version 1

March 25, 2011

Editors

Dagmar Waltemath	University of Rostock, Germany
Frank T. Bergmann	University of Washington, Seattle, USA
Richard Adams	University of Edinburgh, UK
Nicolas Le Novère	European Bioinformatics Institute, UK

The latest release of the Level 1 Version 1 specification is available at
<http://sed-ml.org/>

To discuss any aspect of the current SED-ML specification as well as language details, please send your messages to the mailing list
sed-ml-discuss@lists.sourceforge.net.

To get subscribed to the mailing list, please write to the same address
sed-ml-discuss@lists.sourceforge.net.

To contact the authors of the SED-ML specification, please write to
sed-ml-editors@lists.sourceforge.net



Simulation Experiment Description Markup Language (SED-ML)

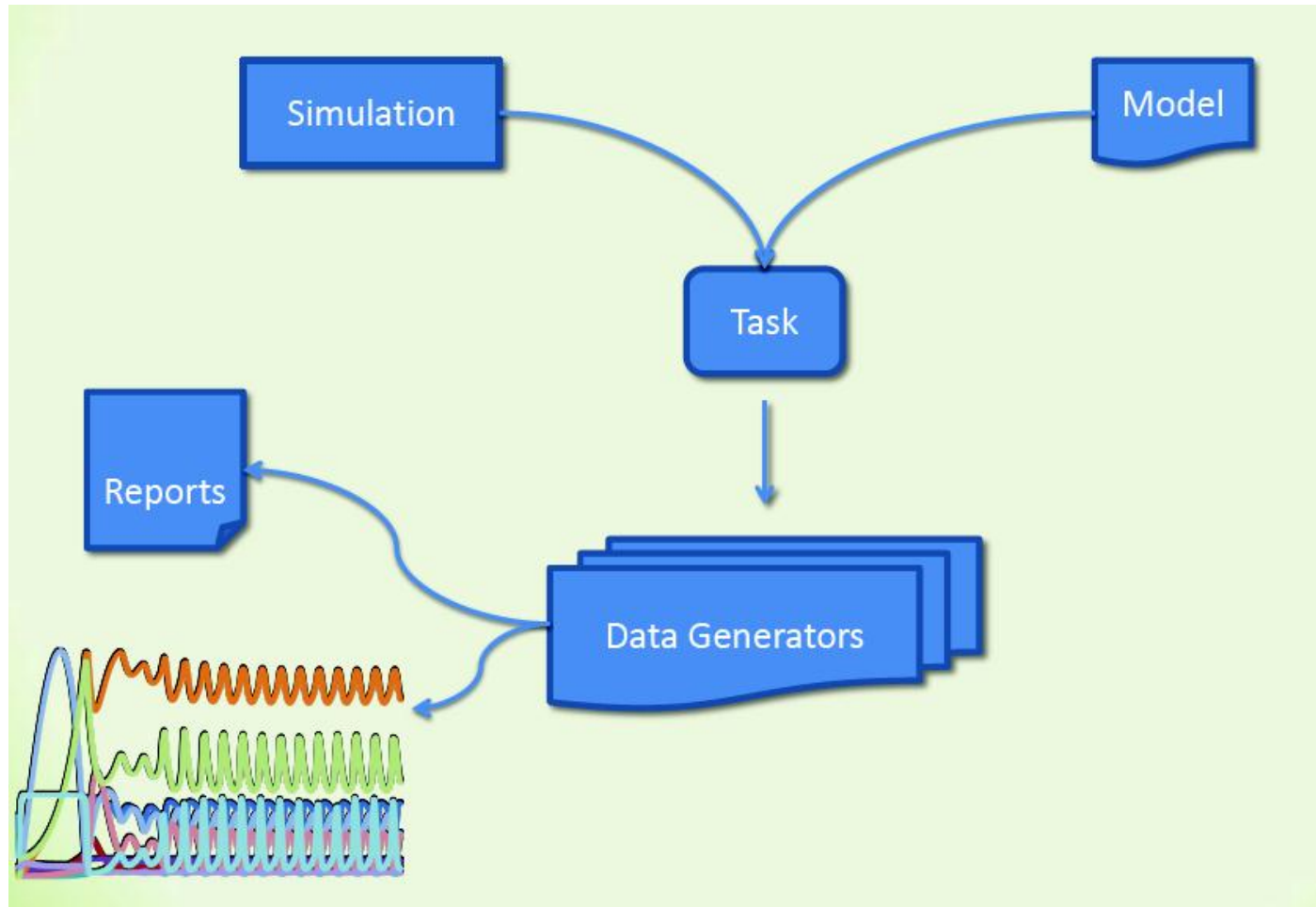


Fig.: SED-ML structure *Waltemath et al., BMC SysBiol (2011)*

Model class

- unambiguous link to a model in an open repository
- model preprocessing, e.g. updated or additional model parameter, substituted mathematical function

```
<model id="model1" name="spiking neuron"
  language="urn:sedml:language:sbml.level-2.version-3"
  source="urn:miriam:biomodels.db:BIOMD0000000127">
  <listOfChanges>
    <changeAttribute
      target="/sbml/model/listOfParameters/parameter
        [@name='c']/@value" newValue="-55">
    </changeAttribute>
  </listOfChanges>
</model>
```

Model class

- unambiguous link to a model in an open repository
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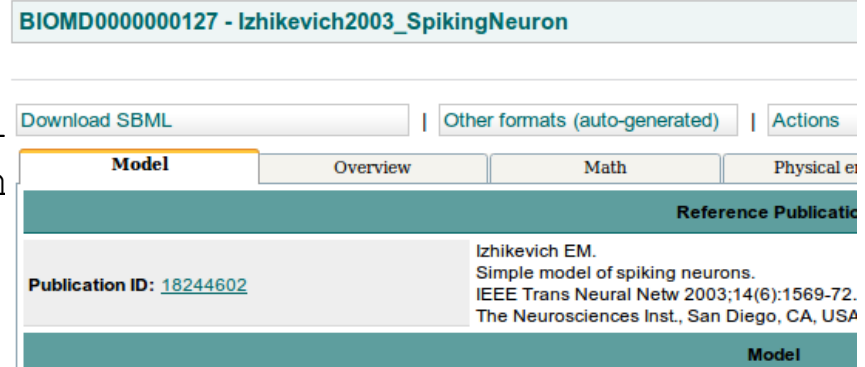
```
<model id="model1" name="spiking neuron"
  language="urn:sedml:language:sbml.level-2.version-3"
  source="urn:miriam:biomodels.db:BIOMD0000000127":
    <listOfChanges>
      <changeAttribute
        target="/sbml/model/listOfParameters/parameter
          [@name='c']/@value" newValue="-55">
      </changeAttribute>
    </listOfChanges>
  </model>
```



Model class

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<model id="model1" name="spiking neuron"
  language="urn:sedml:language:sbml.level-2.version-3"
  source="urn:miriam:biomodels.db:BIOMD0000000127">
  <listOfChanges>
    <changeAttribute
      target="/sbml/model/1
      [@name='c']/@value" n
    </changeAttribute>
  </listOfChanges>
</model>
```



BIOMD0000000127 - Izhikevich2003_SpikingNeuron

Download SBML | Other formats (auto-generated) | Actions

Model Overview Math Physical e

Reference Publication

Publication ID: [18244602](#)

Izhikevich EM.
Simple model of spiking neurons.
IEEE Trans Neural Netw 2003;14(6):1569-72.
The Neurosciences Inst., San Diego, CA, USA

Model

Model class

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        [@name='c']/@value" newValue="-55">
    </changeAttribute>
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```

Simulation class

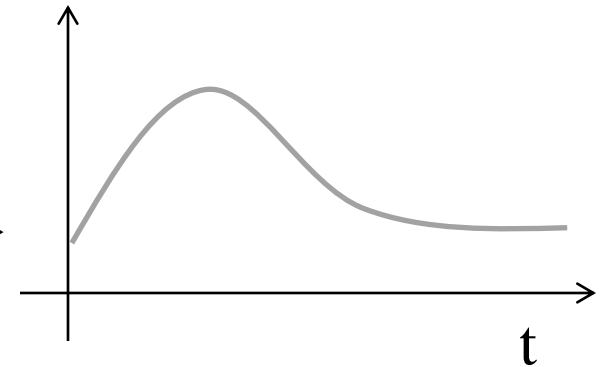
- type of simulation
- simulation algorithm to apply and its settings

```
<uniformTimeCourse id="simulation1"  
  initialTime="0"  
  outputStartTime="0"  
  outputEndTime="1000"  
  numberOfPoints="1000">  
  <algorithm kisaoID="KISAO:0000088" />  
</uniformTimeCourse>
```


Simulation class

- type of simulation
- simulation algorithm to apply and its settings

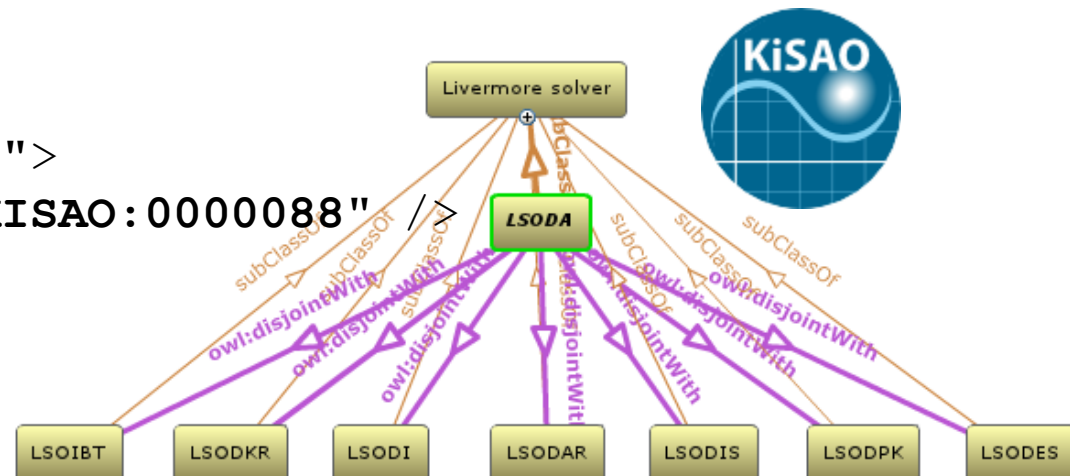
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<uniformTimeCourse id="simulation1"  
  initialTime="0"  
  outputStartTime="0"  
  outputEndTime="1000"  
  numberOfPoints="1000">  
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</uniformTimeCourse>
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Simulation class

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```
<uniformTimeCourse id="simulation1"  
  initialTime="0"  
  outputStartTime="0"  
  outputEndTime="1000"  
  numberOfPoints="1000">  
  <algorithm kisaoID="KISAO:0000088" />  
</uniformTimeCourse>
```



Task class

- groups 1 simulation and 1 model at a time

```
<listOfTasks>  
  <task id="task1" name="spiking with initial  
    parameters" modelReference="model1"  
    simulationReference="simulation1" />  
  
  <task id="task2" name="spiking with updated  
    parameters" modelReference="model2"  
    simulationReference="simulation1" />  
</listOfTasks>
```

DataGenerator class

- entities needed for output
- post-processing of result data after simulation
- use: explicitly defined model entities and predefined variables, e.g., sed-ml:time

```
<dataGenerator id="v" name="voltage">
  <listOfVariables>
    <variable id="v1" taskReference="task1" target="/sbml/
      model/listOfParameters/parameter[@id='v']"/>
  </listOfVariables>
  <math:math>
    <math:ci>v1</math:ci>
  </math:math>
</dataGenerator>
```

DataGenerator class

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  </listOfVariables>  
  <math:math>  
    <math:ci>v1</math:ci>  
  </math:math>  
</dataGenerator>
```

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  </listOfVariables>
  <math:math>
    <math:ci>v1</math:ci>
  </math:math>
</dataGenerator>
```

DataGenerator class

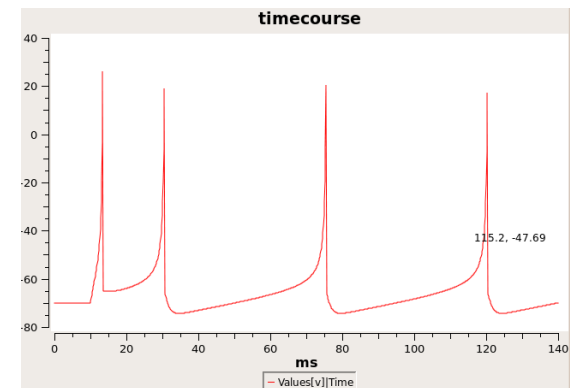
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  </listOfVariables>
  <math:math>
    <math:ci>v1</math:ci>
  </math:math>
</dataGenerator>
```

Output class

- output type
- plot definition

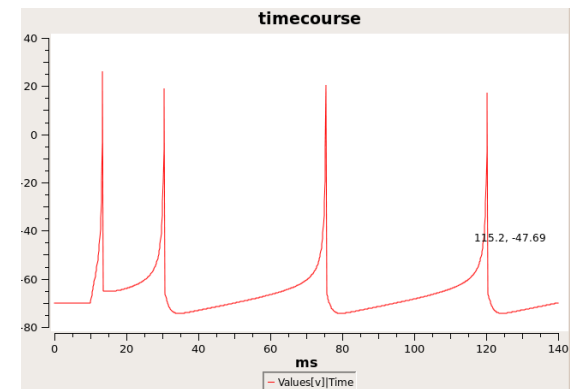
```
<plot2D id="plot1_Basic" name="voltage change over time">  
  <listOfCurves>  
    <curve id="c1" logX="false" logY="false"  
      xDataReference="timeDG" yDataReference="v" />  
  </listOfCurves>  
</plot2D>
```



Output class

- output type
- plot definition

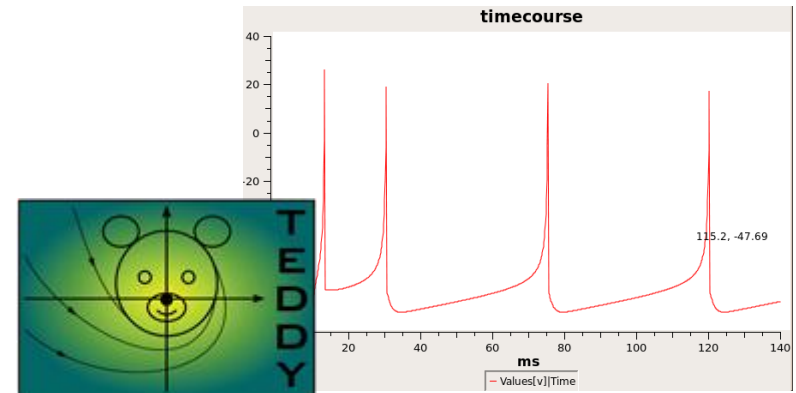
```
<plot2D id="plot1_Basic" name="voltage change over time">  
  <listOfCurves>  
    <curve id="c1" logX="false" logY="false"  
      xDataReference="timeDG" yDataReference="v" />  
  </listOfCurves>  
</plot2D>
```



Output class

- output type
- plot definition

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<plot2D id="plot1_Basic" name="voltage change over time">  
  <listOfCurves>  
    <curve id="c1" logX="false" logY="false"  
      xDataReference="timeDG" yDataReference="v" />  
  </listOfCurves>  
</plot2D>
```



SED-ML in model repositories.

An OpenCell 0.8 session file is available. [SED-ML](#) can also be used to simulate this model, the simulation description is in [Lorenz_1963_sedml.xml](#), and the simulation experiment can be run using the [SED-ML Web Tools](#). The figures below show the results from OpenCell and from using [SED-ML](#).

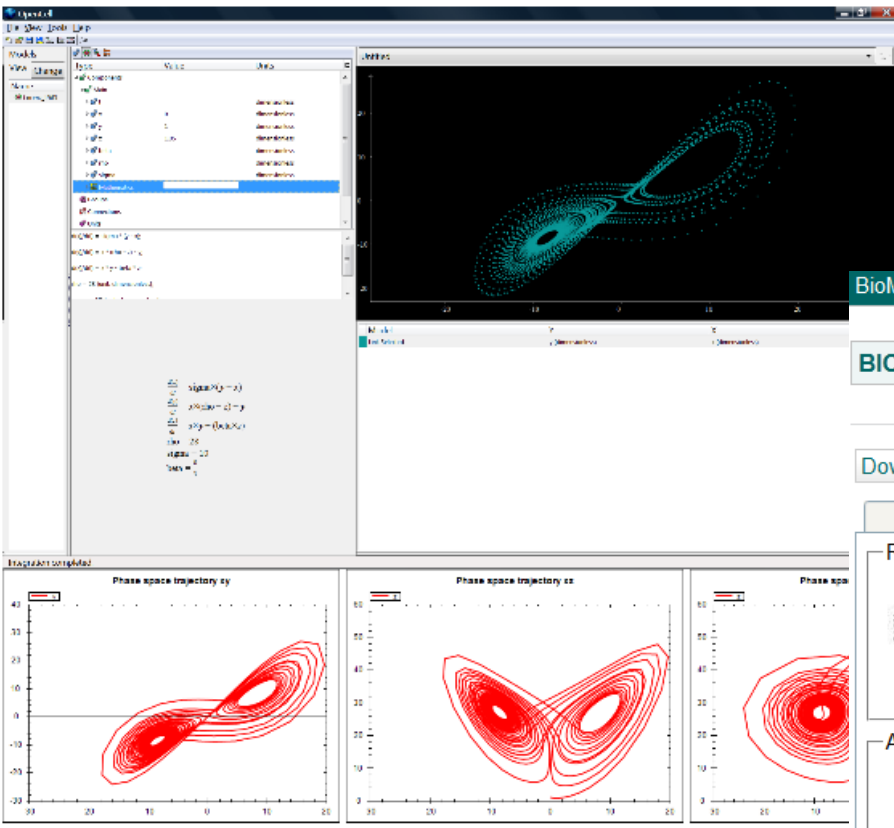


Fig.: CellML models in PMR2 with supplementary SED-ML files.

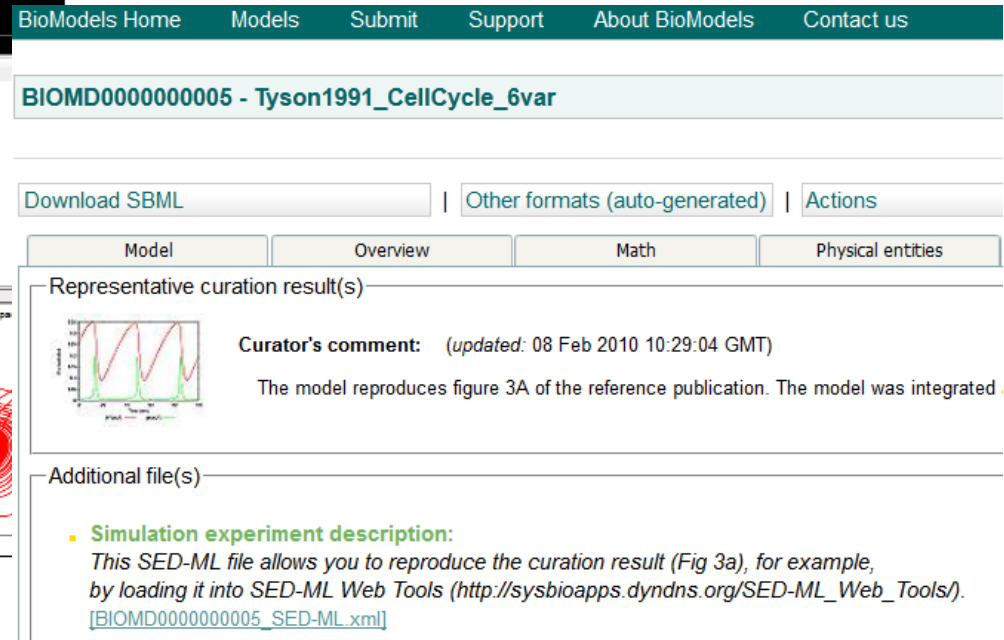


Fig.: SBML models in BioModels Database with supplementary SED-ML files.

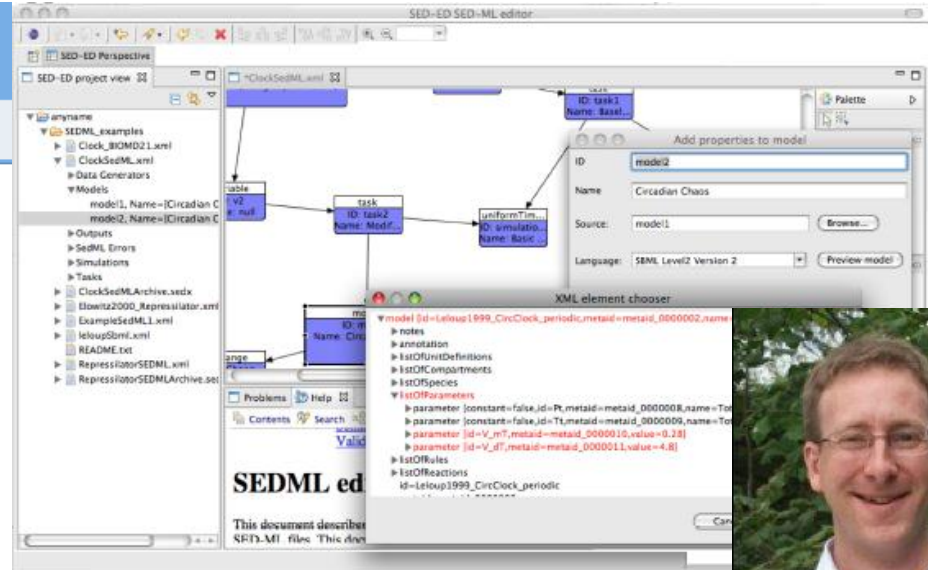
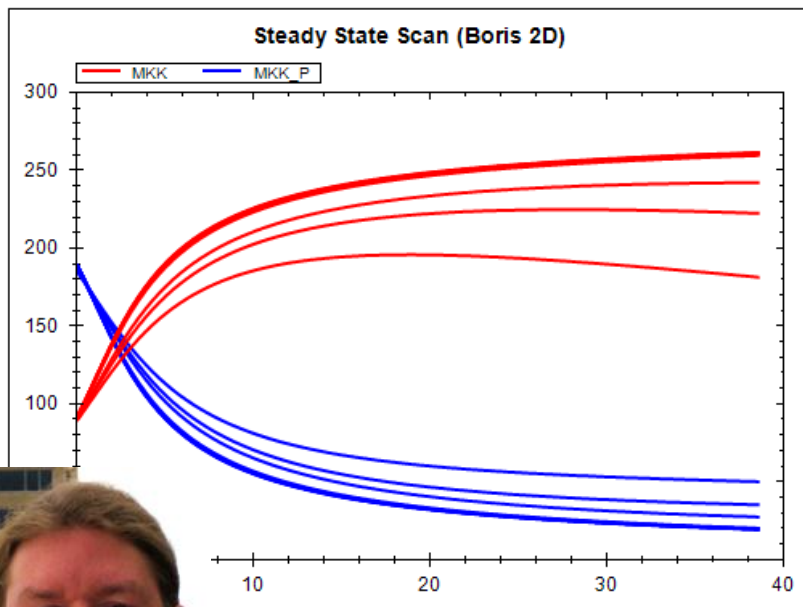
SED ML Web Tools

Home

Create

Simulate

Steady State Scan (Boris 2D)



SED-ED (Bioinformatics. 2012 Feb 25)

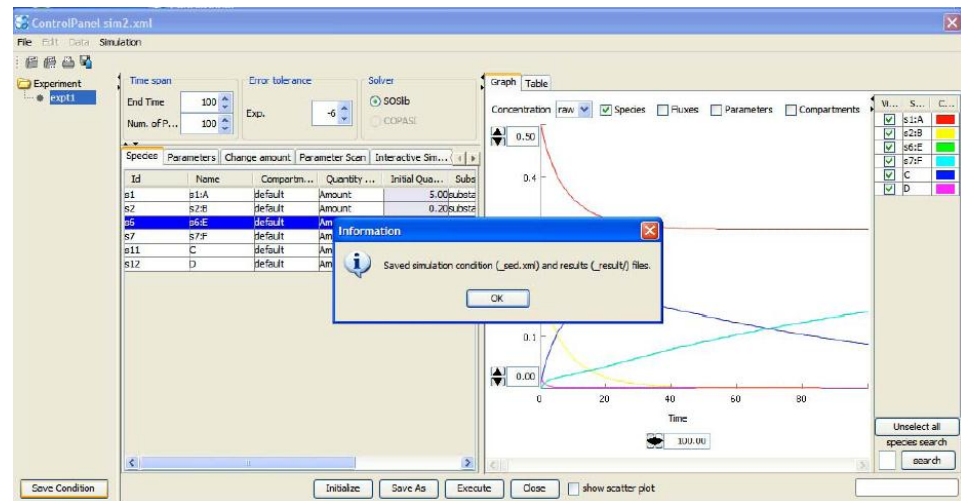


Fig.:SED-ML import/export in CellDesigner.

- Changes at runtime
- Linking to experimental/simulation data - NuML
 - XML format
 - Standardized exchange of numerical results
 - <http://code.google.com/p/numl/>
 - <http://groups.google.com/group/numl-discuss/>
- Improved post-processing / working with > 1 models
- Nested simulations
- What else?

1. Have a look at the current SED-ML L1 V1.
Specification document on <http://sed-ml.org>
2. Try out some examples.
<http://sed-ml.org>, <http://sourceforge.net/projects/libsedml>
3. Identify what is missing for you to encode your simulation experimental setups.
What can you *not* express?
4. Submit a feature request & post it on the list.
feature request tracker: <http://sourceforge.net/projects/sed-ml>
mailing list: sed-ml-discuss@lists.sourceforge.net
5. ... submit a proposal with example files and prototype.
proposal tracker: <http://sourceforge.net/projects/sed-ml>

Needs:

- Description of simulation setup
- Simulation algorithm
- Result data
- Behavior of the model in a particular experiment



NuML



SED-ML editors

Frank Bergmann
Jonathan Cooper
David Nickerson
Nicolas Le Novère
Dagmar Waltemath
Richard Adams
Andrew Miller

NuML developers

Joseph Dada,
Frank Bergmann,
Nicolas Le Novère

TEDDY developers

Christian Knüpfer
Anna Zhukova
Nicolas Le Novère

KiSAO developers

Anna Zhukova
Nicolas Le Novère
Dagmar Waltemath

MIASE co-authors

Dagmar Waltemath, Richard Adams,
Daniel A Beard, Frank Bergmann,
Upi Bhalla, Randall Britten,
Vishi Chelliah, Mike Cooling,
Jonathan Cooper, Edward Crampin,
Alan Garny, Stefan Hoops,
Mike Hucka, Peter Hunter,
Edda Klipp, Camille Laibe,
Andrew Miller, Ion Moraru , David
Nickerson, Poul Nielsen, Masha
Nikolski, Sven Sahle, Herbert Sauro,
Henning Schmidt, Jacky Snoep,
Dominic Tolle, Olaf Wolkenhauer,
Nicolas Le Novère

<http://biomodels.net>