

Simulation Experiment Description Markup Language

Where we are and how we got there...



Dagmar Waltemath, COMBINE meeting, Heidelberg 2011

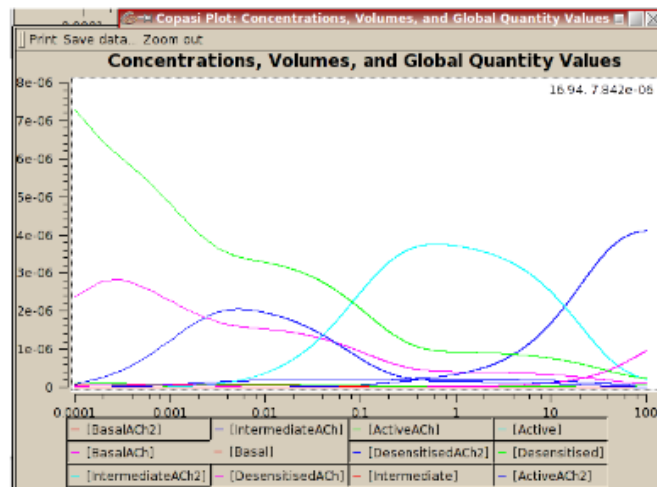
Motivation



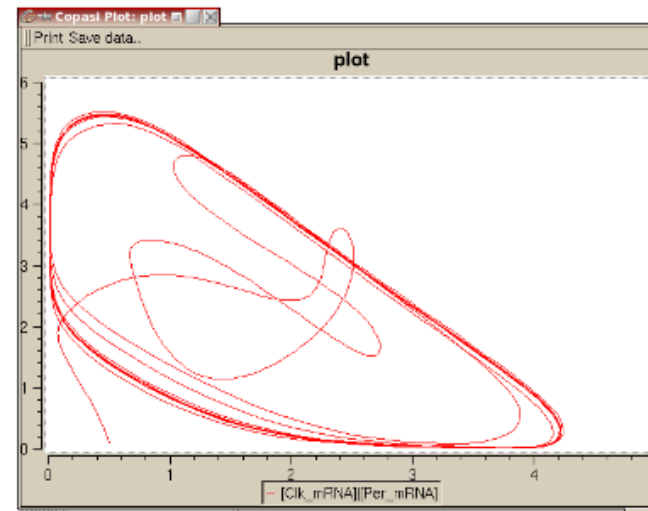
Figure: Nicolas Le Novère

Motivation

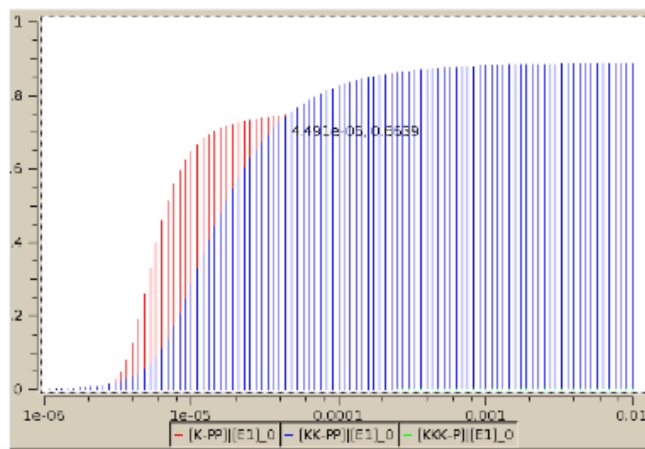
Edelstein et al 1996 (BIOMD0000000002)



Ueda, Hagiwara, Kitano 2001 (BIOMD0000000022)



Huang & Ferrell (BIOMD0000000009)



Bornheimer et al 2004 (BIOMD0000000086)

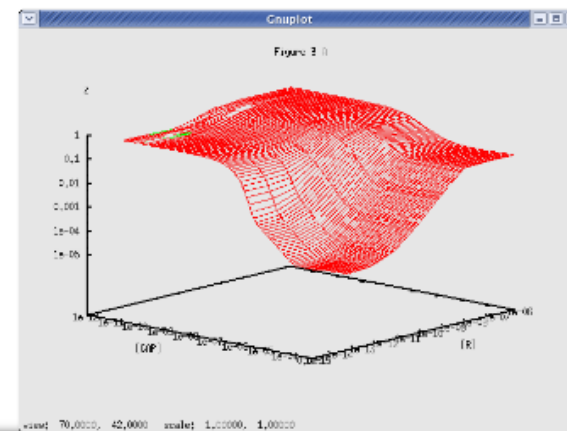


Figure: Nicolas Le Novère

Reproducible simulation setups

How it all began

Minimum Information About a Simulation Experiment (MIASE)

Toward the Repetition of Simulation Runs

Dagmar Koehn, Nicolas Le Novere



EBI is an Outstation of the European Molecular Biology Laboratory.

SBML Forum 2007 @ Long Beach

How it all began

Minimum Information About a
Simulation Experiment (MIASE)

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The MIASE-DM will provide a formal representation
of the minimum information description.

SBML Forum 2007 @ Long Beach

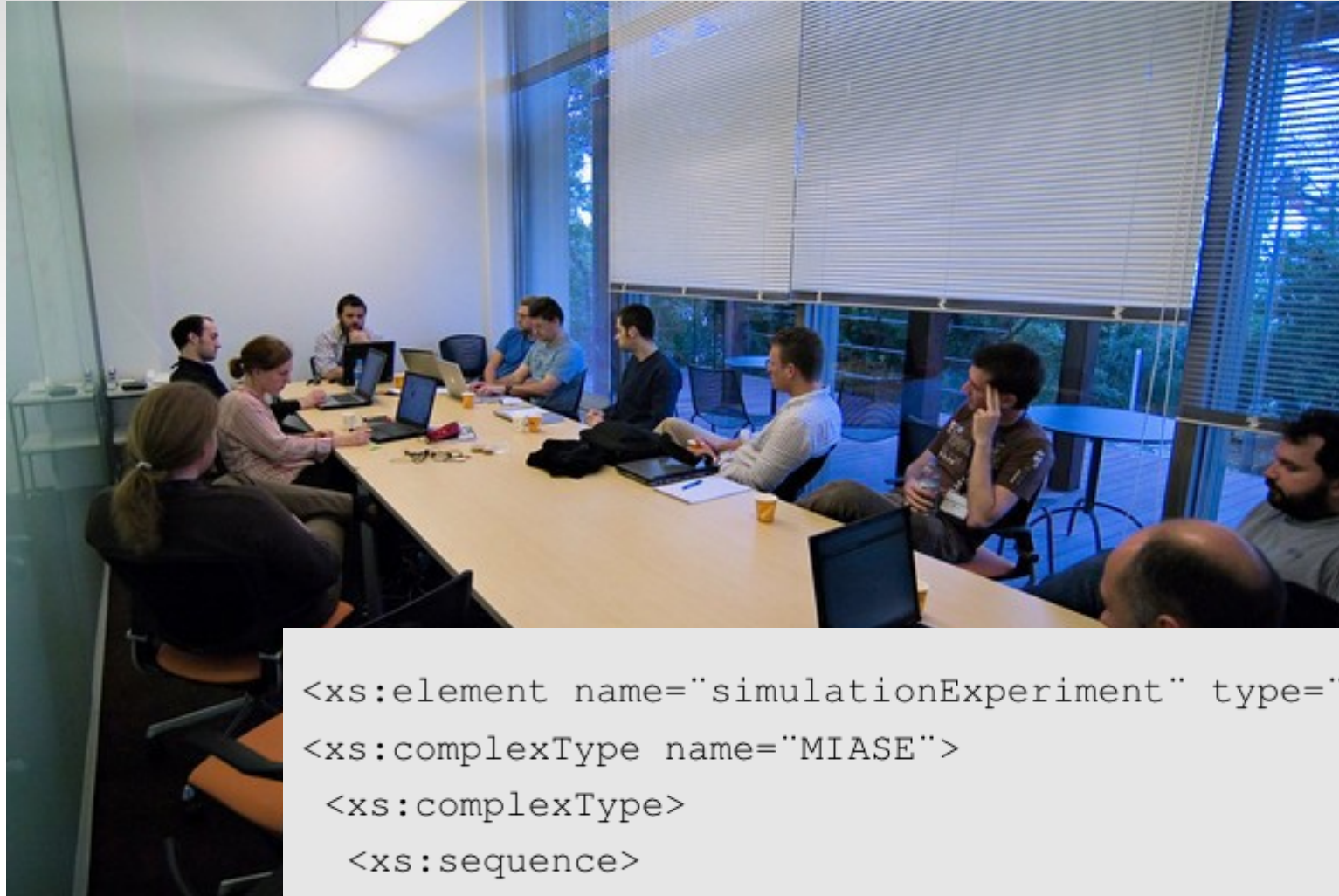
How it all began



Picture: sbmlteam on smugmug

Superhackathon 2008 @ Okinawa

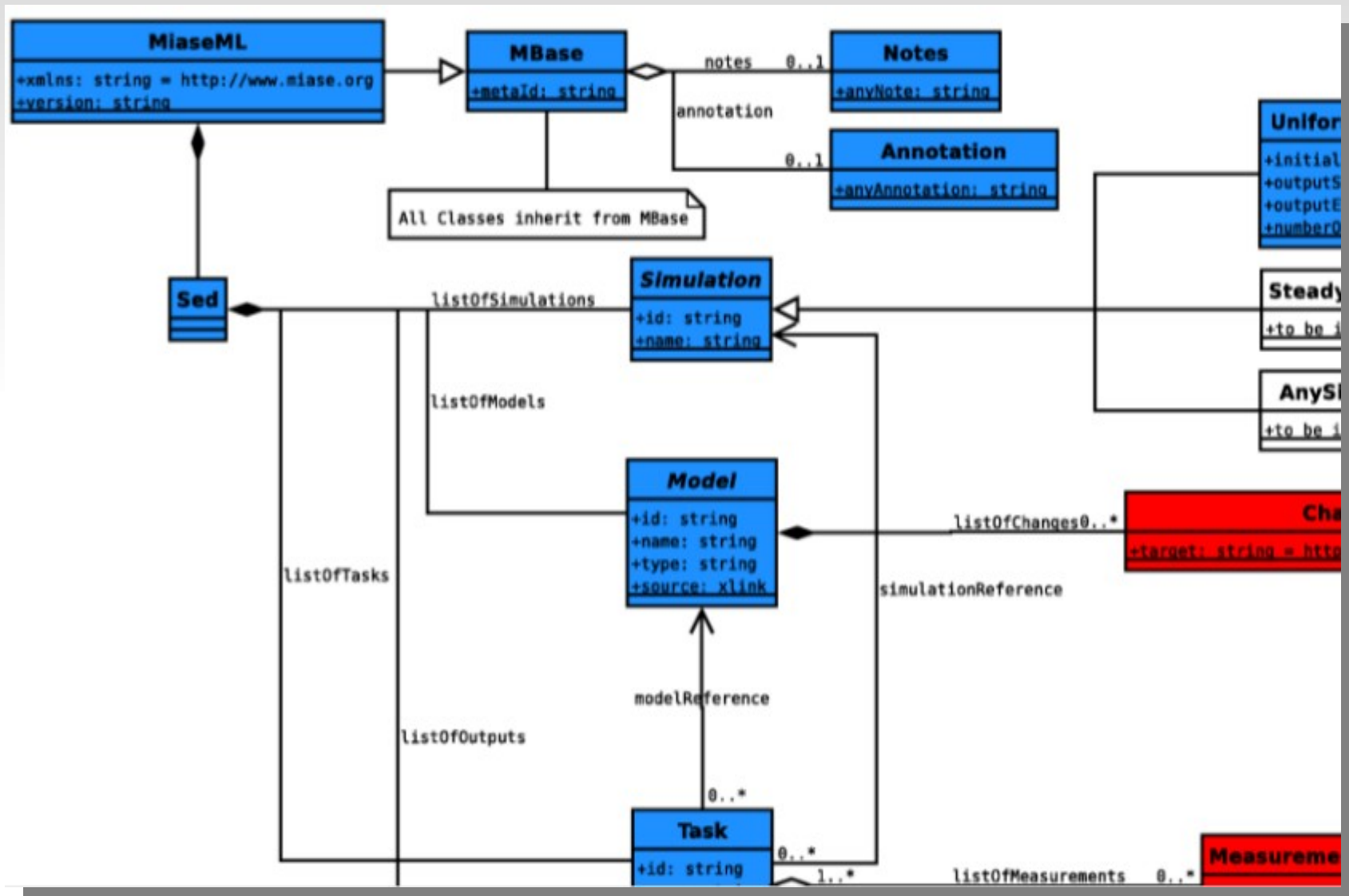
How it all began



```
<xs:element name="simulationExperiment" type="MIASE" />
<xs:complexType name="MIASE">
  <xs:complexType>
    <xs:sequence>
      <xs:element name="simulator" type="xs:string" />
```

Superhackathon 2008 @ Okinawa

How it all began



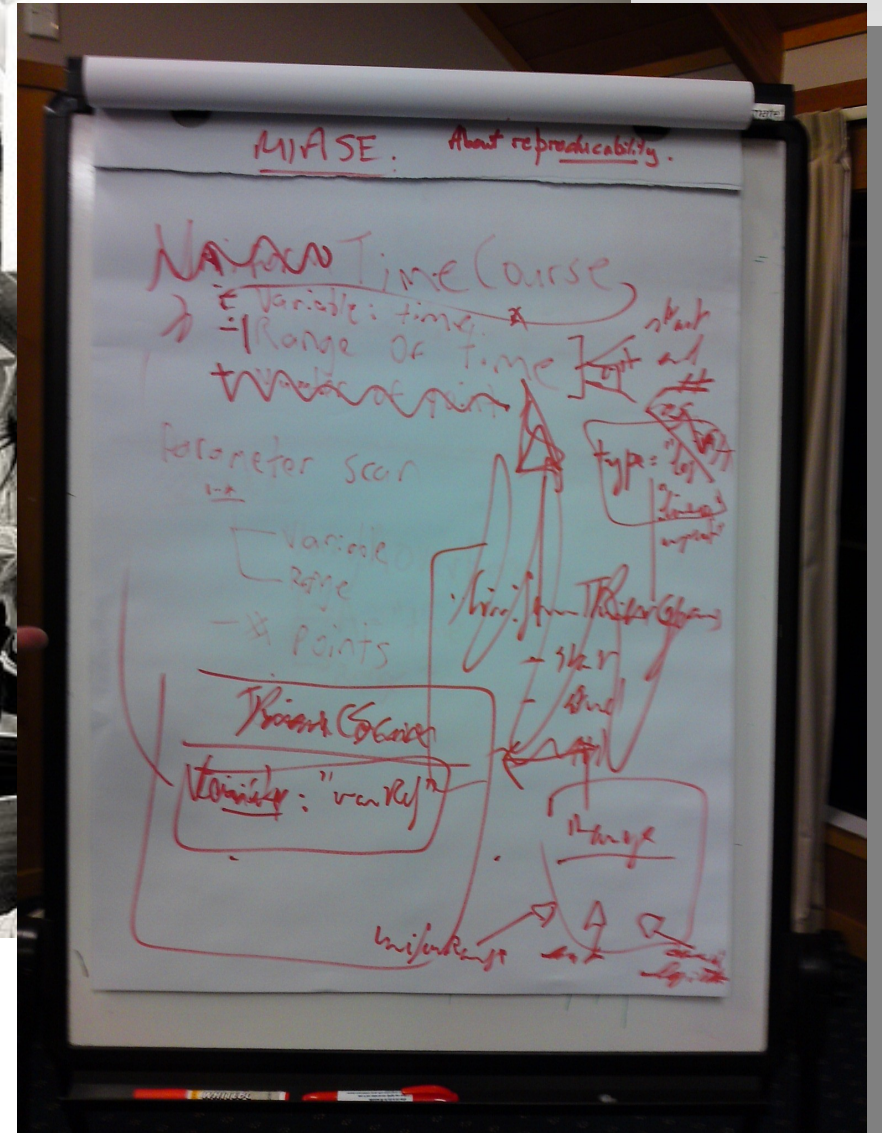
How it all began



Picture: francis_bacon on picasa

CellML workshop 2009 @ Waiheke

How it all began



CellML workshop 2009 @ Waiheke

How it all began



```
<model id="model1" name="Circadian Oscillations" type="SBML"
source="urn:miriam:biomodels.db:BIOMD0000000021" />
[...]  
<variable id="v1" taskReference="task1" target="/sbml/model/
listOfSpecies/species[@id='Mt']" />  
<plot2D> <listOfCurves>  
<curve xDataReference="time" yDataReference="tim1" />  
</listOfCurves> </plot2D>
```

CellML workshop 2009 @ Waiheke

How it all began

SED-ML L1 V1

- SED-ML Spec is on the way
- preliminary version available from Sourceforge
- Feel free to read, bug report and start implementing :-)

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

April 27, 2010

Editors

Dagmar Waltemath
Nicolas Le Novère
Frank T. Bergmann

*Rostock University, Germany
European Bioinformatics Institute, UK
University of Washington, Seattle, USA*

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 dagmar.waltemath@uni-rostock.de

SBML-biomodels.net Hackathon 2010 @ Seattle

The logo question



Questioning the name

- SED-ML
- MIASE-ML
- SEDML
- SedML
- sedML
- sedml

SED-ML L1 V1

- Publication of specification

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

March 25, 2011

Editors

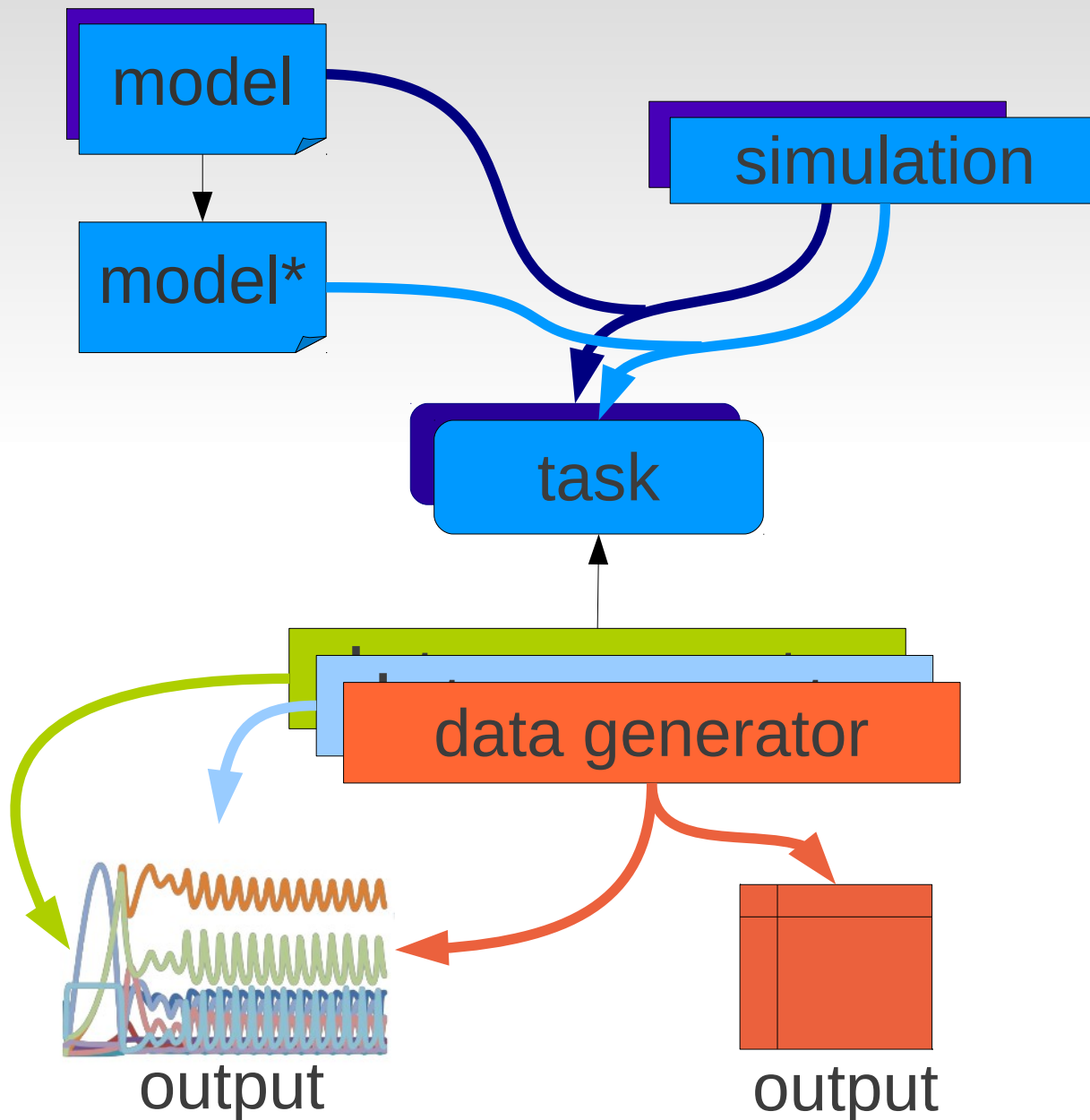
Dagmar Waltemath
Frank T. Bergmann
Richard Adams
Nicolas Le Novère

*University of Rostock, Germany
University of Washington, Seattle, USA
University of Edinburgh, UK
European Bioinformatics Institute, UK*

- Election of editorial board

sed-ml-editors@lists.sourceforge.net

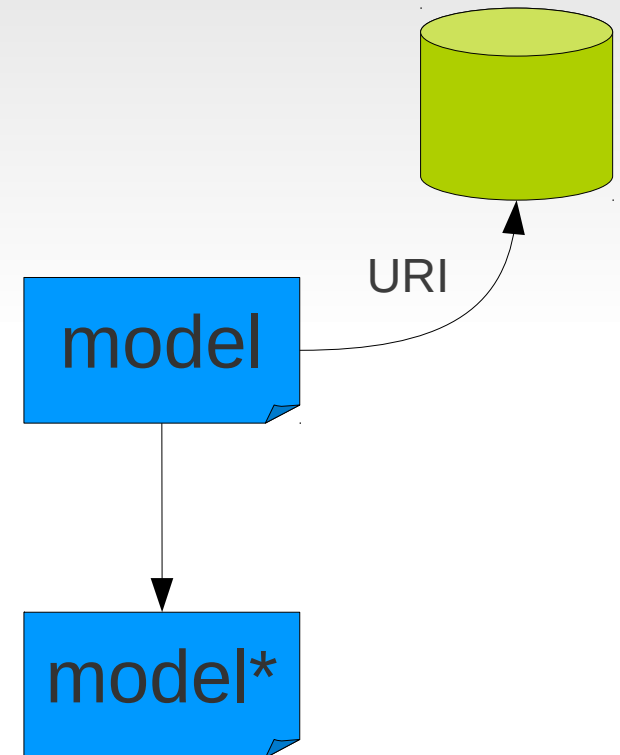
Language overview



- **Model Class**
References models used during the experiment
- **Simulation Class**
Defines simulation settings and steps
- **Output Class**
Specifies the result output

Model definition

- Link to model code
 - in standard format
 - using unambiguous reference (e.g. MIRIAM identifiers)
- Encoding language
 - using SED-ML language URNs
- Model pre-processing (e.g. update in model parametrisation or structure)



Simulation definition

- Simulation setup
- Experiment type
 - Currently: time course simulations
- Algorithm
 - KiSAO

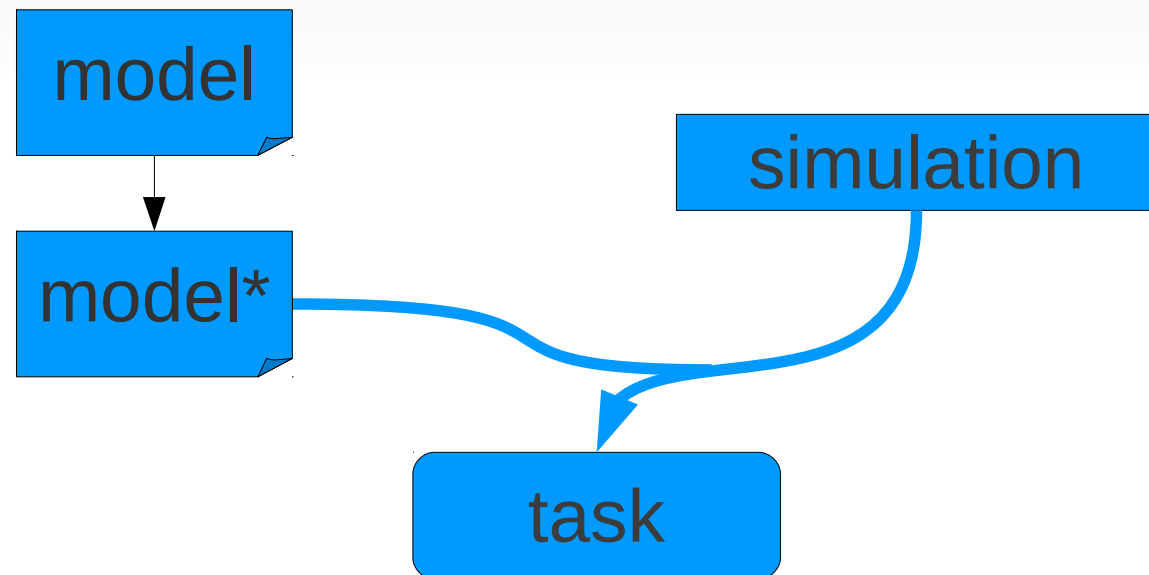
<http://www.biomodels.net/kisao/>

simulation



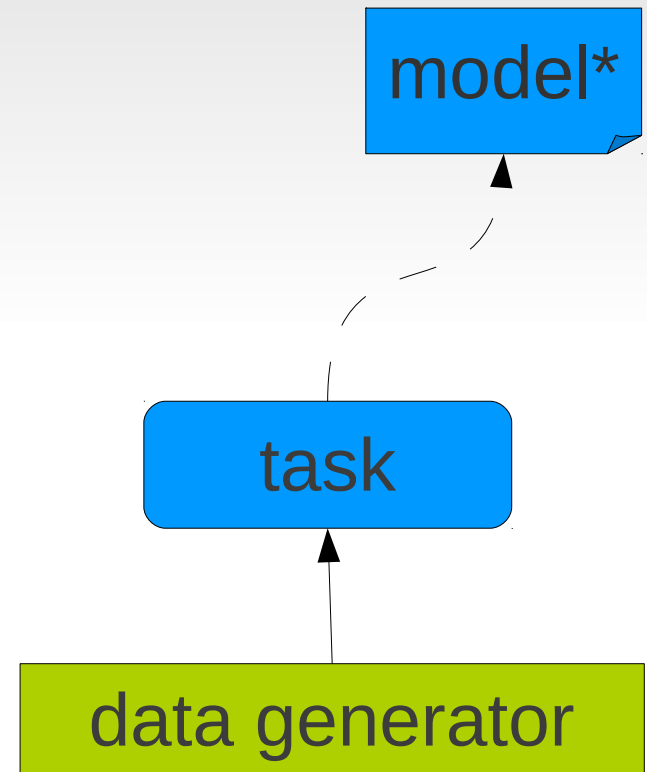
Task definition

- Link model and simulation



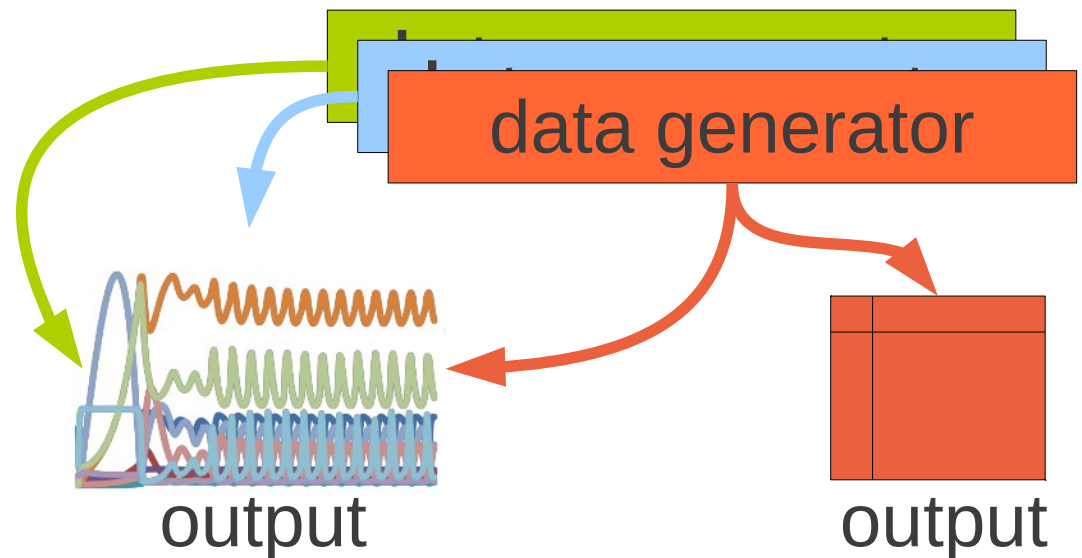
Data generator definition

- Post-processing of simulation output
- Parameter definition
- Variable references (task)
 - XPath
- Implicit variables
 - SED-ML symbols
 - URNs



Output definition

- Relevant data to be represented in the output
- 2D-plot, 3D-plot, data tables
- No result data encoding → SBRML
- No layout description

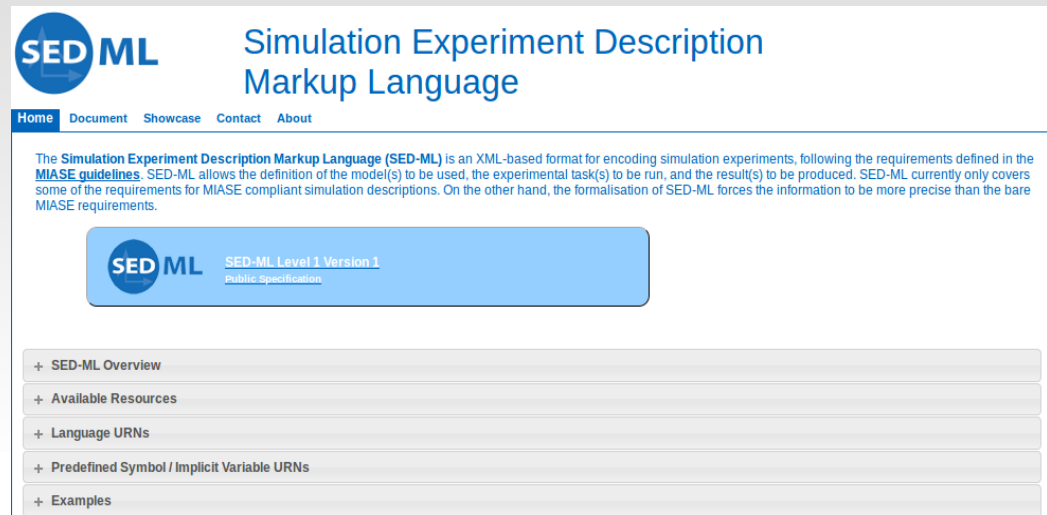


Resources

- SED-ML homepage

<http://sed-ml.org>

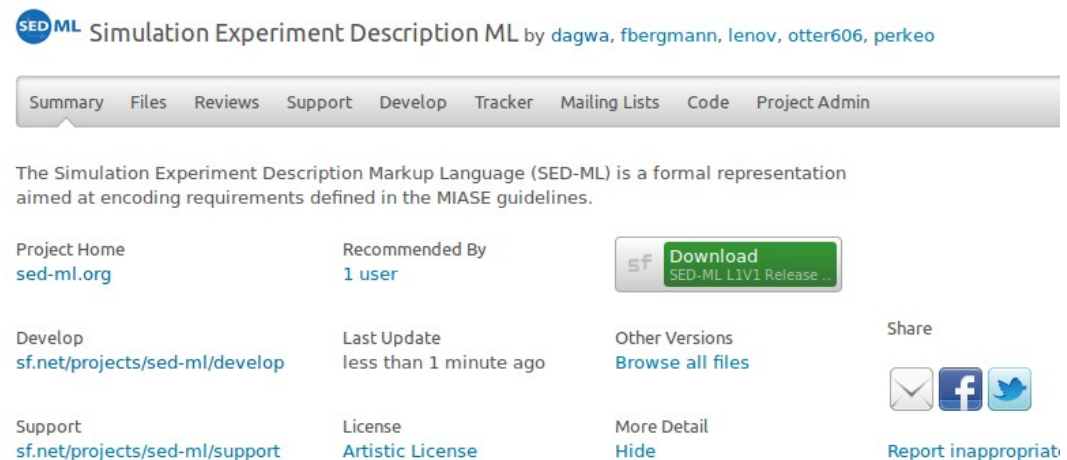
- Specification



- SED-ML development

<https://sourceforge.net/projects/sed-ml/>

- bug tracker
- mailing list



Thank you!

- Fellow SED-ML editors
 - Richard Adams
 - Frank Bergmann
 - David Nickerson
 - Andrew Miller
 - Nicolas Le Novère
- sed-ml-discuss members

