Simulation Experiment Description Markup Language

Where we are and how we got there...

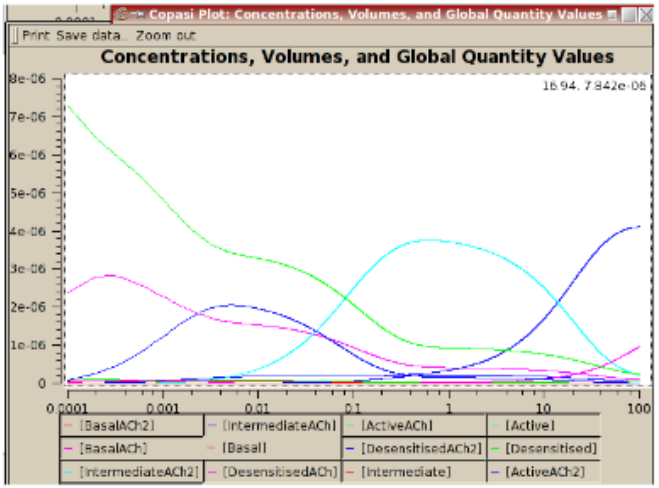
Dagmar Waltemath, COMBINE meeting, Heidelberg 2011

Motivation

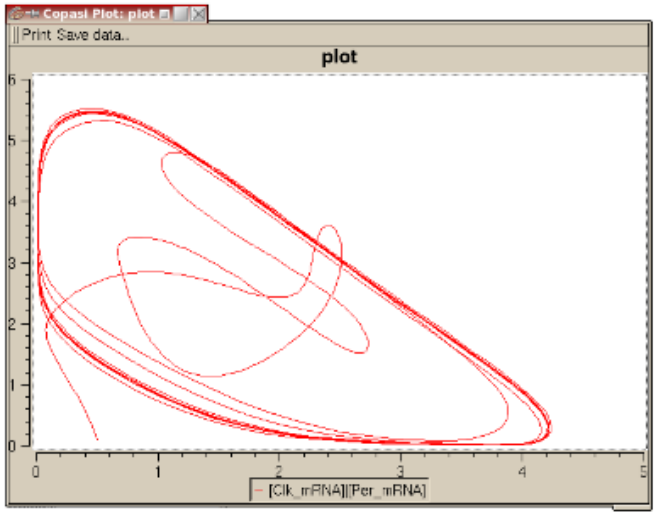
Figure: Nicolas Le Novère

Motivation

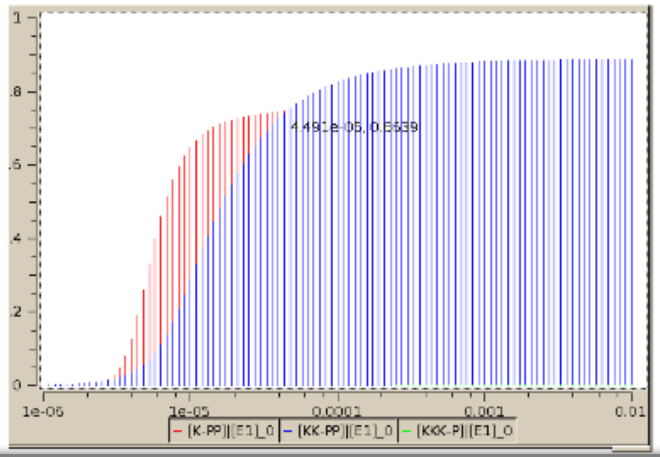
Edelstein et al 1996 (BIOMD0000000002)



Ueda, Hagiwara, Kitanol 2001 (BIOMD0000000022)



Huang & Ferrell (BIOMD0000000009)



Bornheimer et al 2004 (BIOMD0000000086)

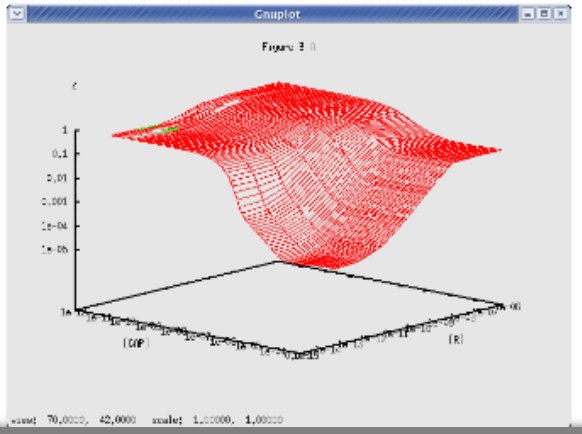
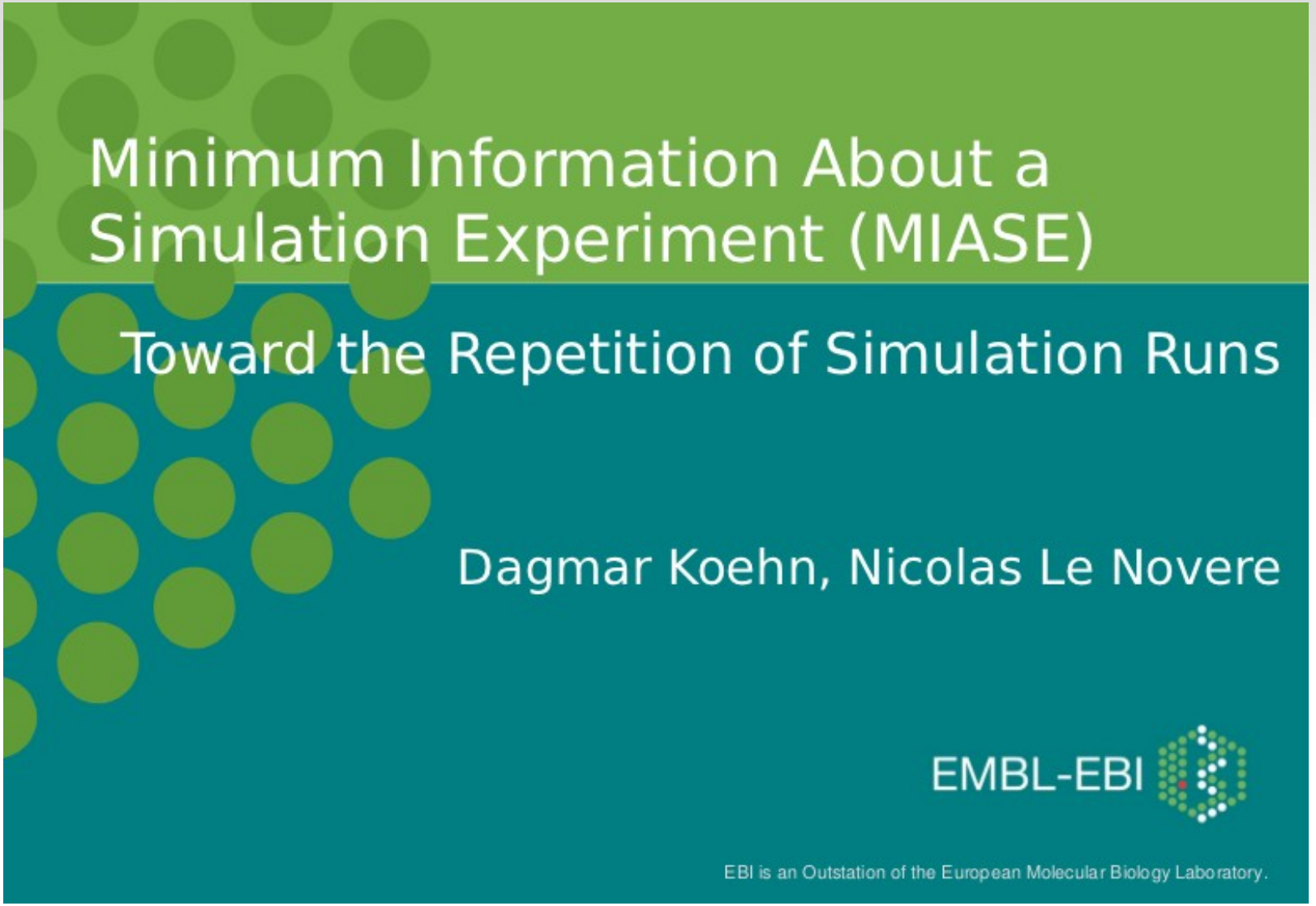


Figure: Nicolas Le Novère

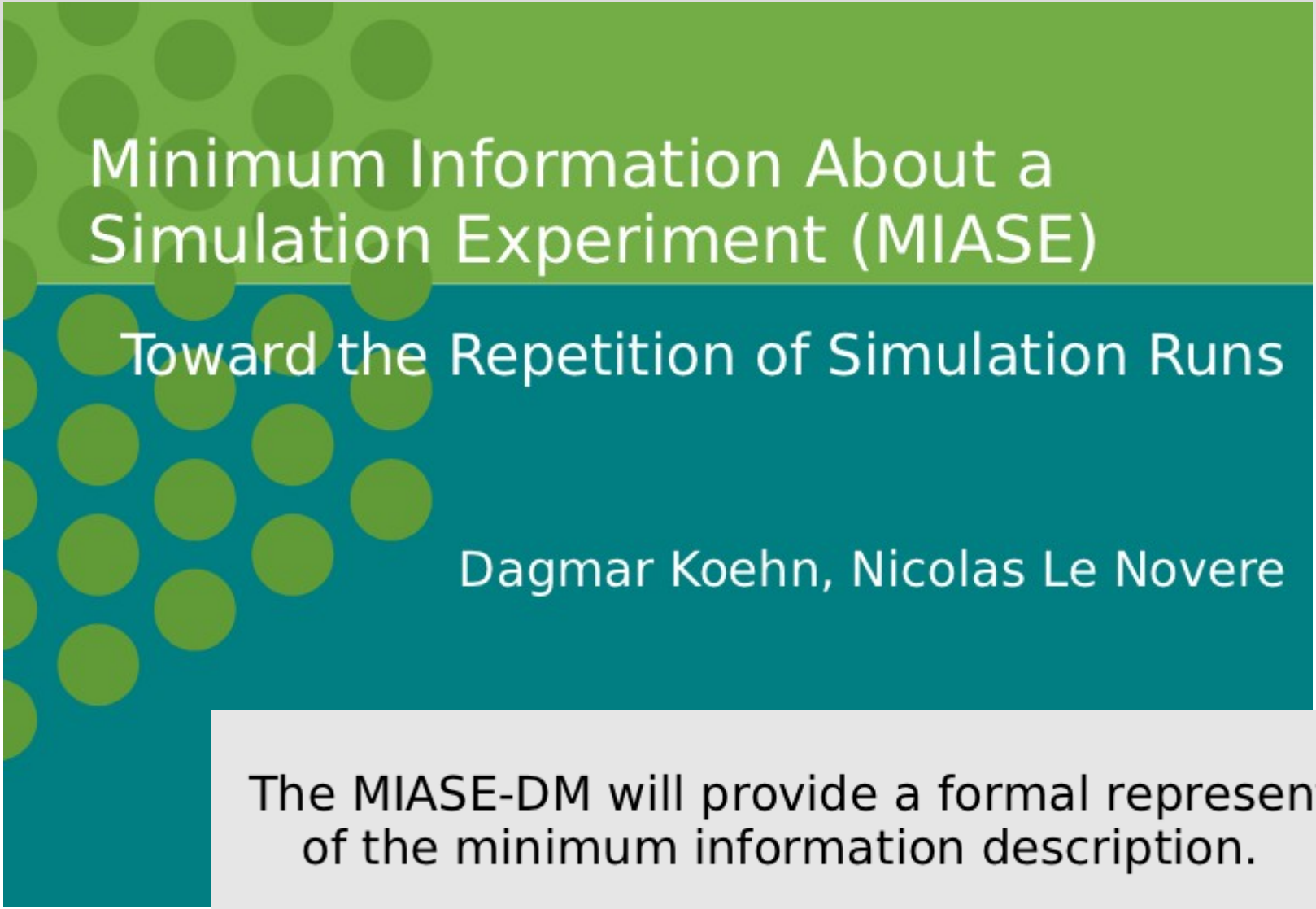
Reproducible simulation setups

How it all began



SBML Forum 2007 @ Long Beach

How it all began



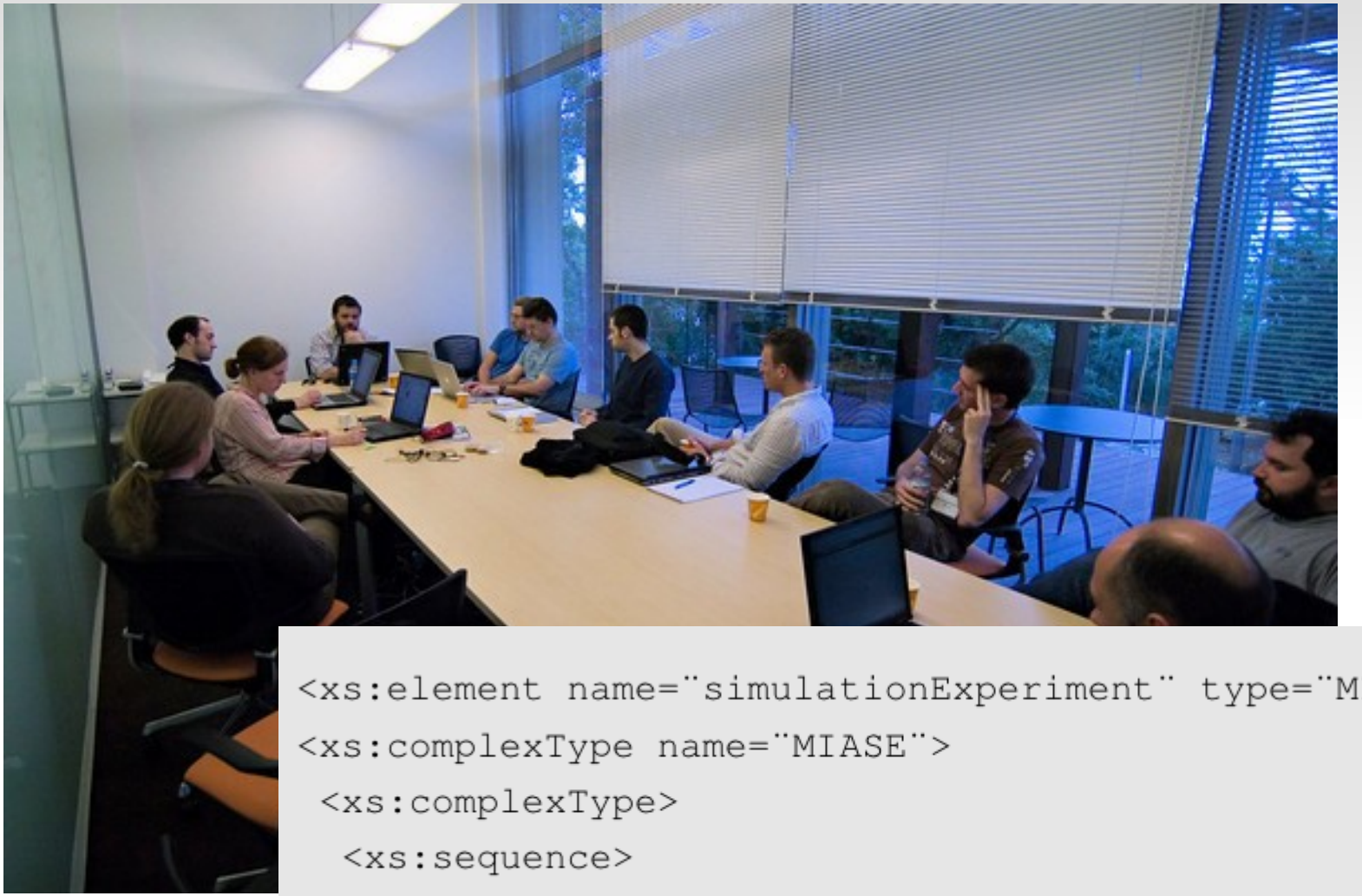
The MIASE-DM will provide a formal representation of the minimum information description.

How it all began

Picture: sbmlteam on smugmug

Superhackathon 2008 @ Okinawa

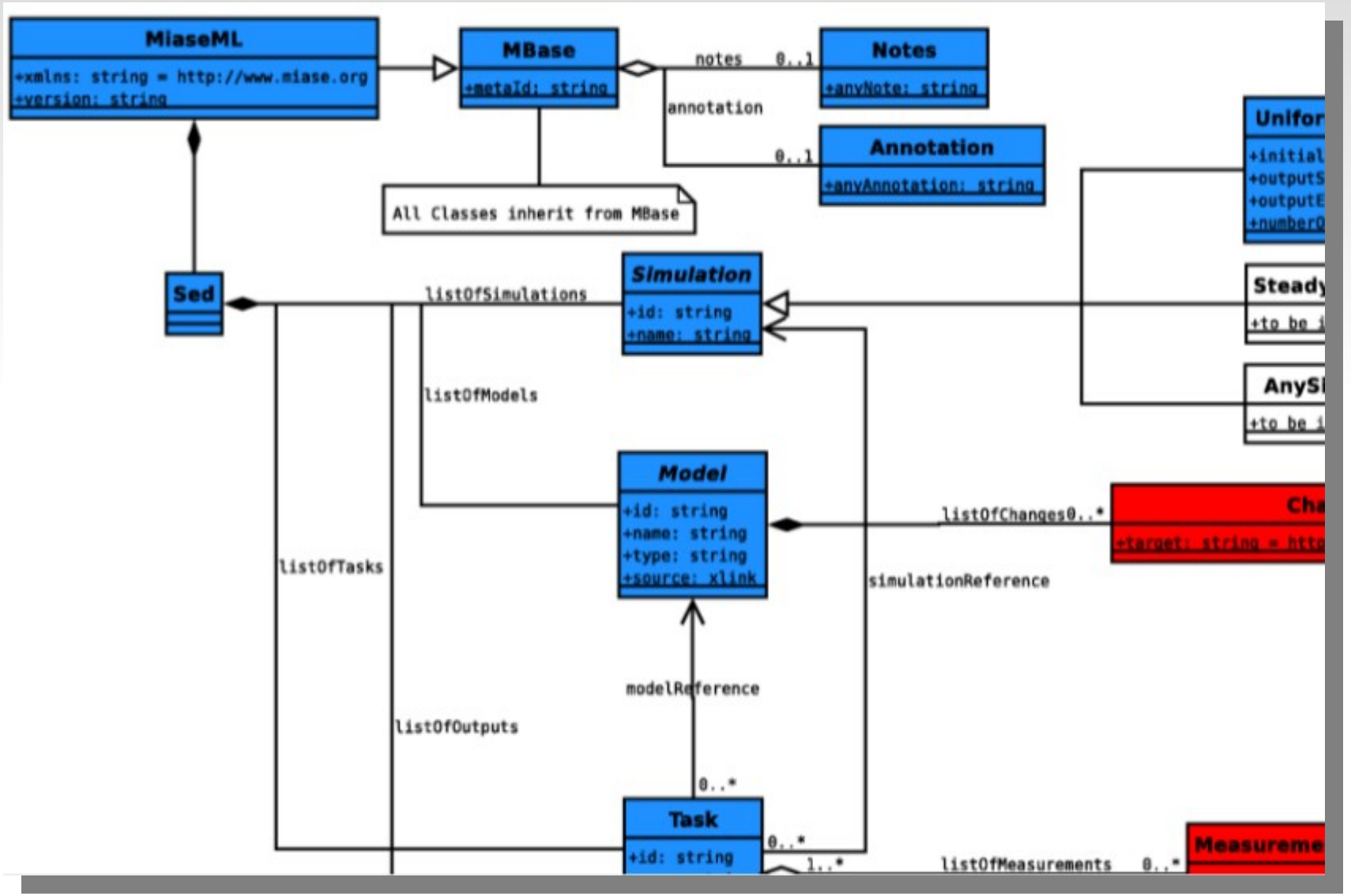
How it all began



```
<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

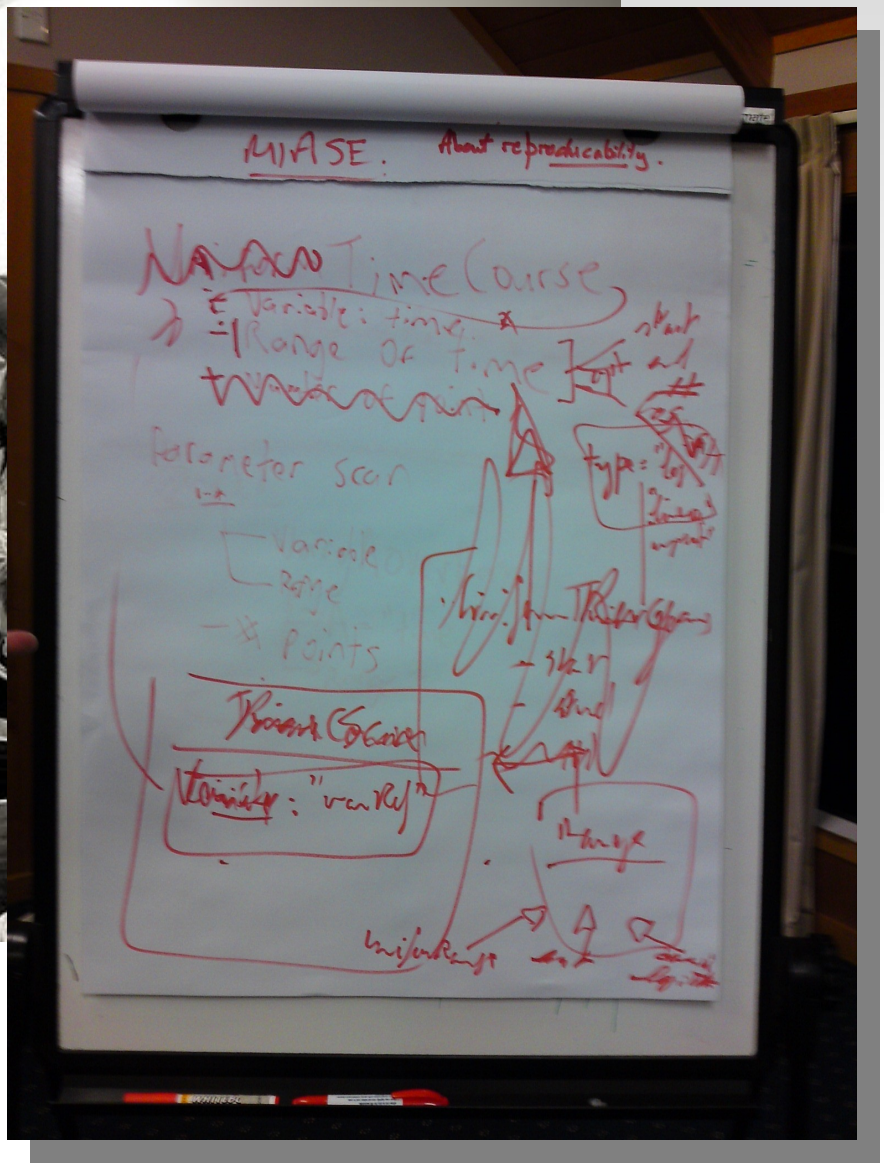


How it all began

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>
```

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	*Rostock University, Germany*
Nicolas Le Novère	*European Bioinformatics Institute, UK*
Frank T. Bergmann	*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

The logo question

Logos:Susanne.biermann@uni-rostock.de

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

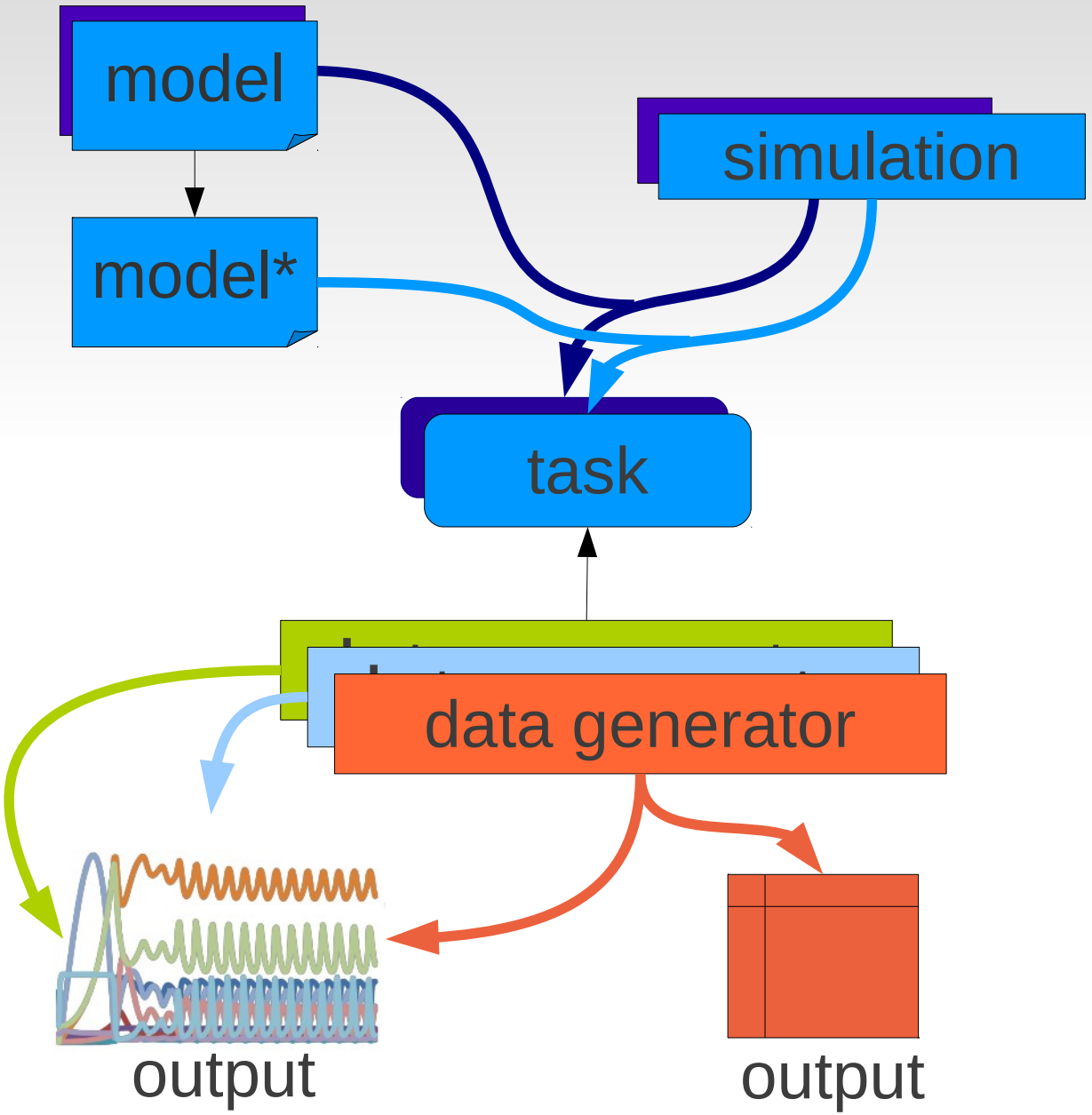
Editors

Dagmar Waltemath	*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*

- Election of editorial board

sed-ml-editors@lists.sourceforge.net

Language overview

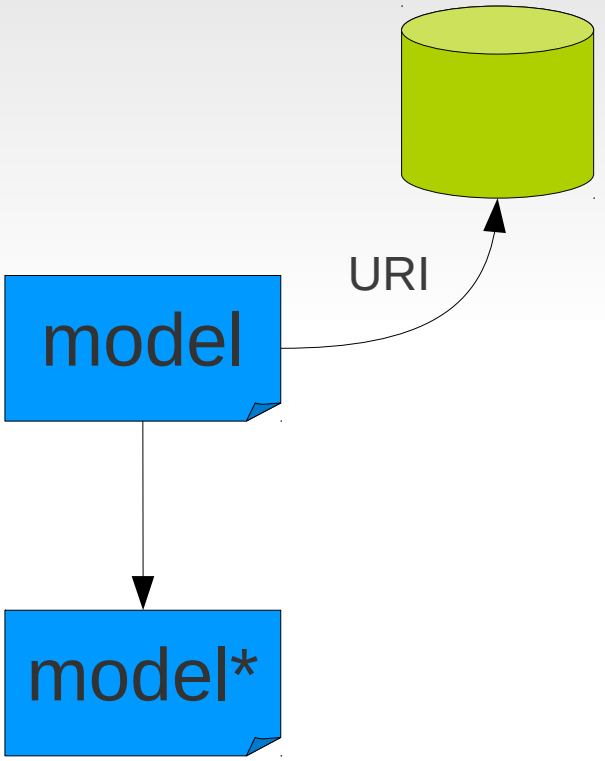


- **Model Class**
  References models used during the experiment
- **Simulation Class**
  Defines simulation settings and steps
- **Output Class**
  Specifies the result output

Original figure: Frank Bergmann

Model definition

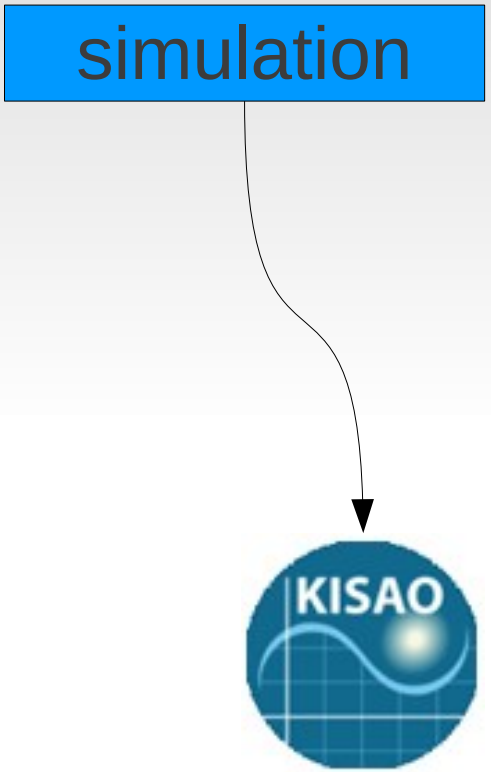
- Link to model code
  - in standard format
  - using unambiguous reference (e.g. MIRIAM identifiers)
- Encoding language
  - using SED-ML language URNs
- Model pre-processing (e.g. update in model parametrisation or structure)



Simulation definition

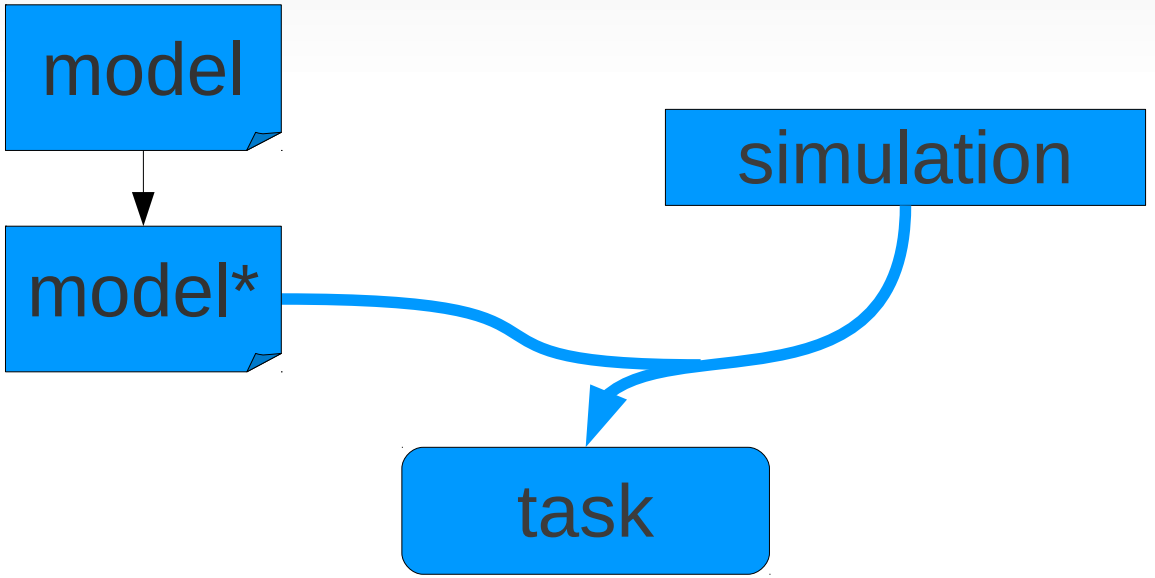
- Simulation setup
- Experiment type
  - Currently: time course simulations
- Algorithm
  - KiSAO

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



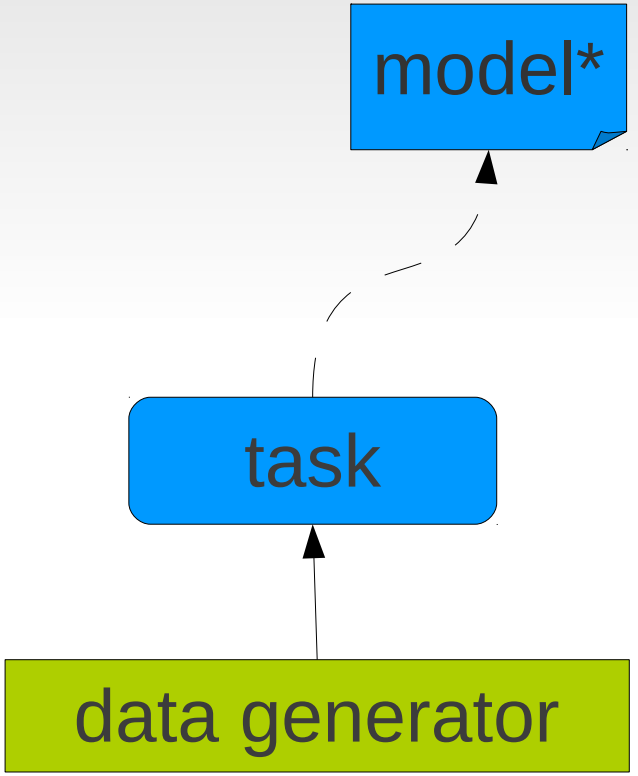
Task definition

- Link model and simulation



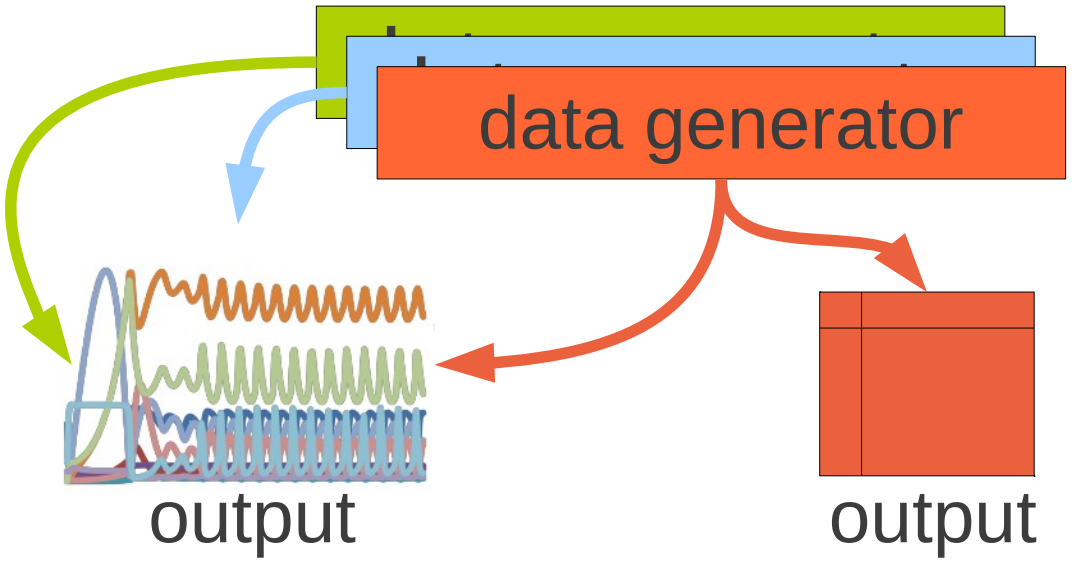
Data generator definition

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



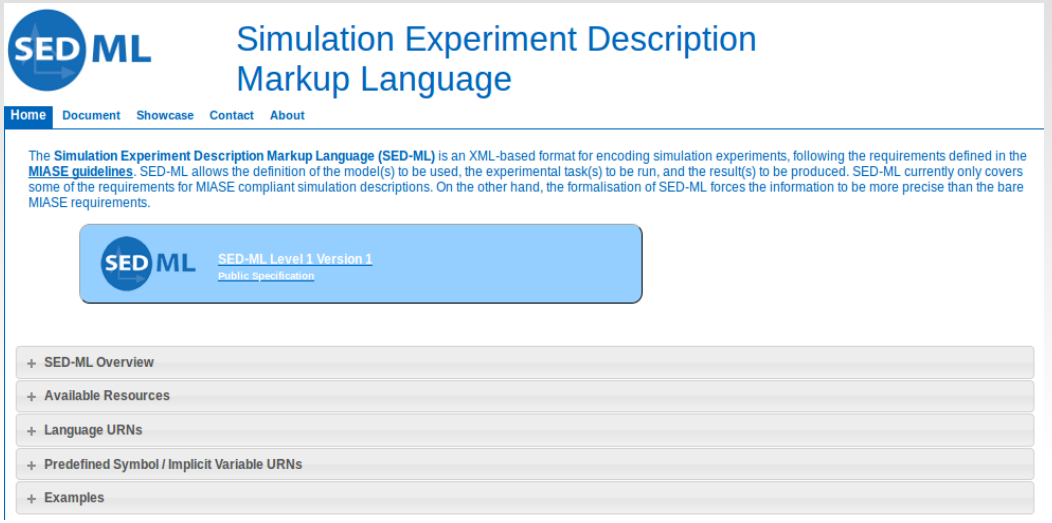
Output definition

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

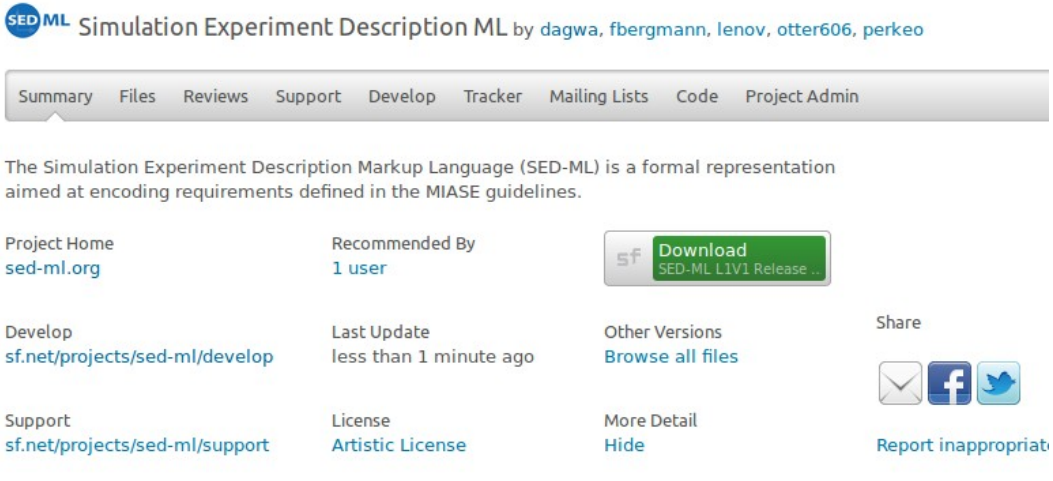


Resources

- SED-ML homepage
  http://sed-ml.org
- Specification



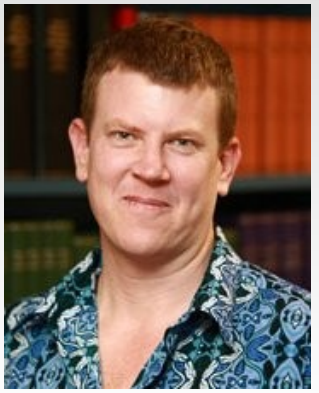
- SED-ML development
  https://sourceforge.net/projects/sed-ml/
  - bug tracker
  - mailing list

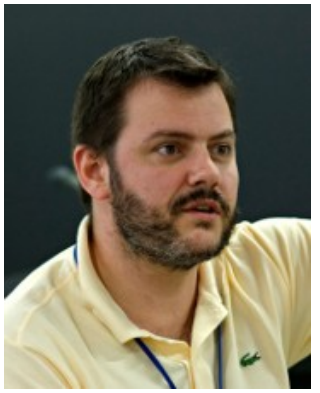


Thank you!

- Fellow SED-ML editors
  - Richard Adams
  - Frank Bergmann
  - David Nickerson
  - Andrew Miller
  - Nicolas Le Novere







- sed-ml-discuss members