EMBL-EBI

Towards SED-ML L1 V1: Simulation Experiment Description Language

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SED-ML is …

Simulation Experiment Description Markup Language

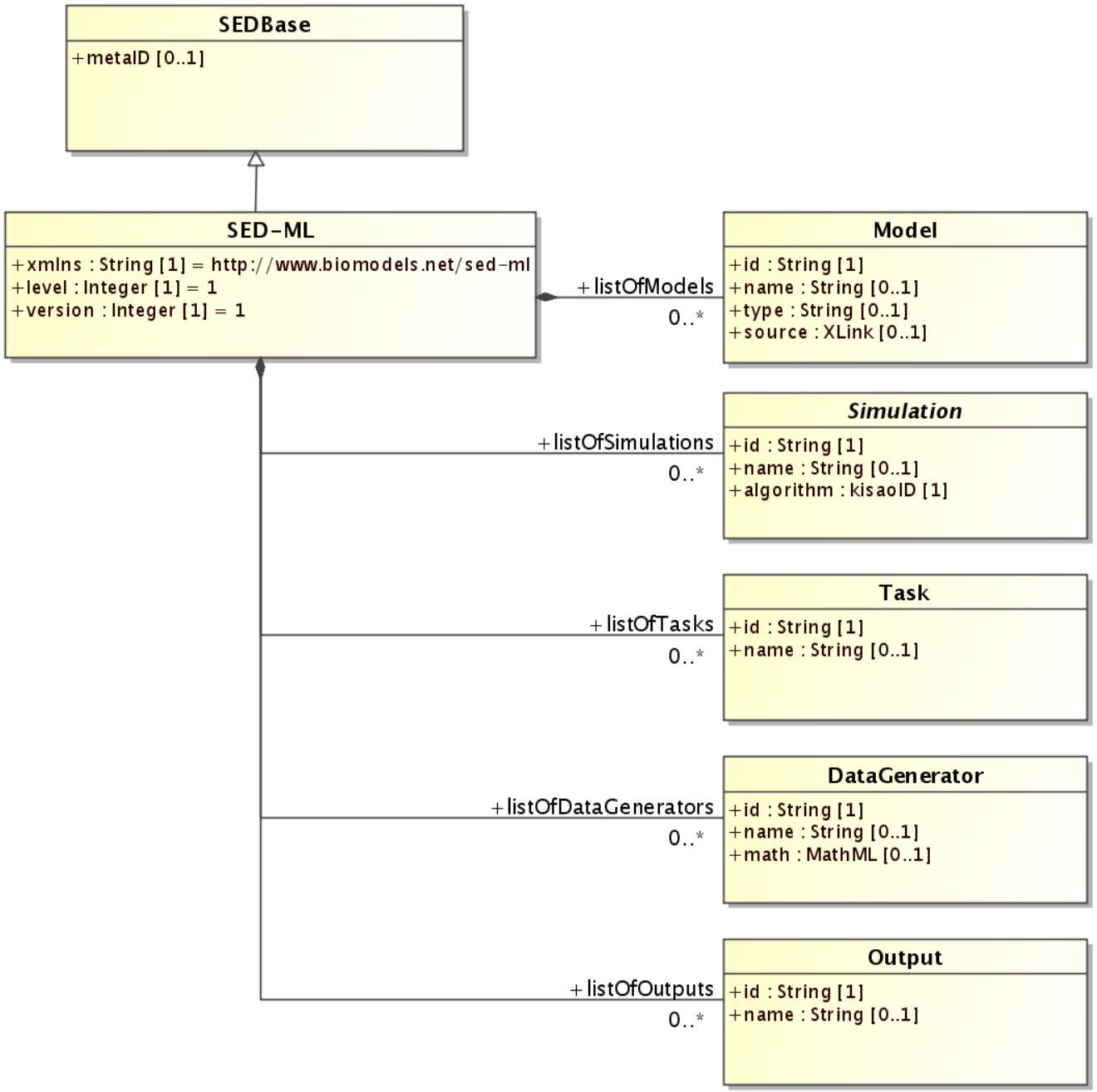
- … an XML format for encoding simulation experiments (**XML Schema**)
- … also available as a **UML model**
- … a community effort
- … part of biomodels.net
- … "MIASE-compliant" [MIASE paper submitted]
- … independent of the underlying model encoding format

http://www.biomodels.net/sed-ml

SED-ML can be used for ...

- Simulation experiment encoding and model parametrization/perturbations
- Simulations using more than one model
- Simulations using models from different formalisms
  e.g. simulations using an SBML model and a CellML model
- Experiments with different simulation methods applied
  e.g. stochastic and deterministic simulation of a system
- Sequential Experiments [future version]
  e.g. *steady state analysis → simulation with parameter values*

SED-ML Main Structure



Model Class

References models used during the experiment

Simulation Class

Defines simulation settings and – steps

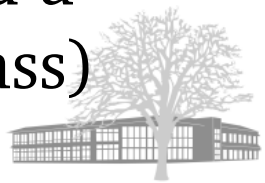
Output Class

Specifies the result output

SED-ML Top-Level Classes (1)

- Model Class
  - Unambiguous and stable references to models

    e.g. a MIRIAM URN
  - Changes necessary on the model before simulation
    → Change Classes *Change*{*Attribute*|*XML*|*Math*}
- Simulation Class
  - Simulation procedure, including the simulation steps, simulation duration, and algorithm used
    e.g. a KiSAO ID www.ebi.ac.uk/compneur-srv/kisao
- Task Class
  - Combine a defined model (→ Model Class) and a defined simulation setting (→ Simulation Class)



SED-ML Top-Level Classes (2)

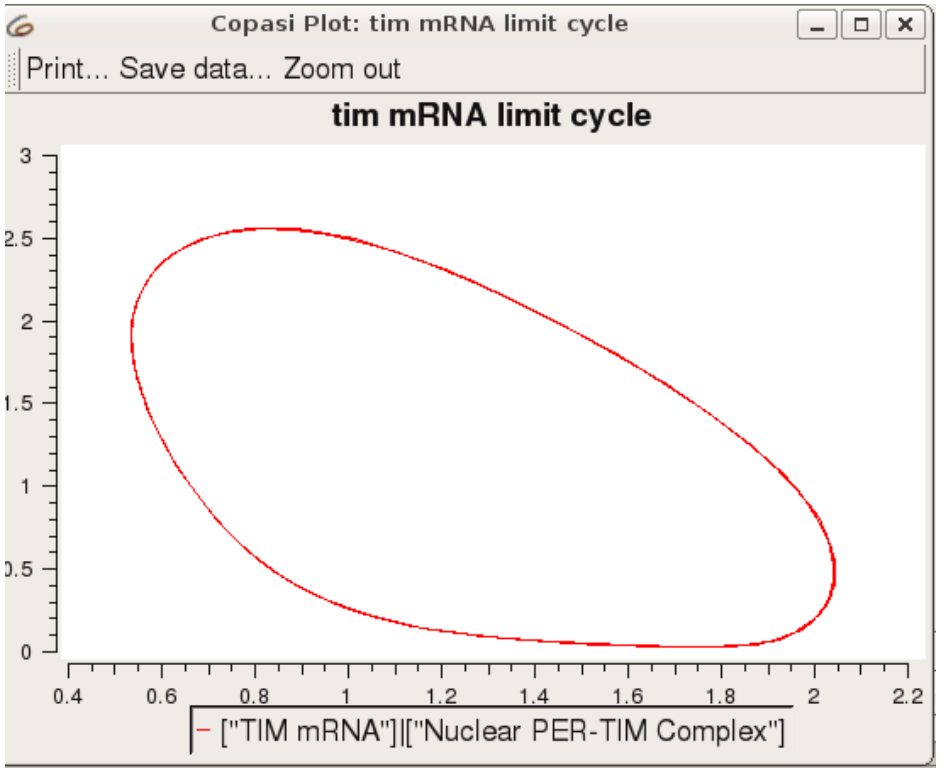
- DataGenerator Class
  - Specifies the data needed in the output through reference to model entities and post-processing

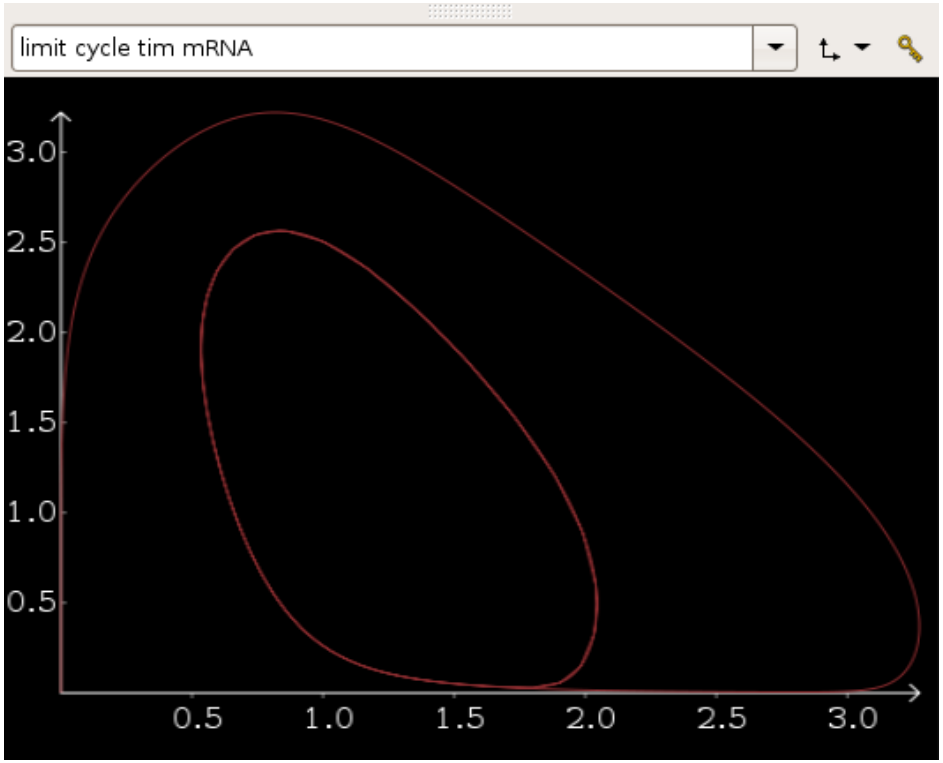
    e.g. variable reference in model, normalisation of a result data set before output
- Output Class
  - Define output type

    e.g. 2D plot, table …
  - Define output plots using “data generators“ (→ DataGenerator Class)

    e.g. data generators d1 on x-axis, d2 on y-axis

Simulation examples on Sourceforge





left: BIOM12 in COPASI, right: Leloup1999 in PCEnv

http://sed-ml.svn.sourceforge.net/viewvc/sed-ml/sed-ml/examples/

What's happening at the moment?

- Support more simulation types (no changes since 2009)
  - existing: UniformTimeCourse Class, generic AnySimulation Class
  - desired: Parameter Scans, Optimisations …

- SED-ML level 1, version1 Specification:
  Plans for finalisation during biomodels.net meeting Seattle, April 2010 http://biomodels.net/events.html

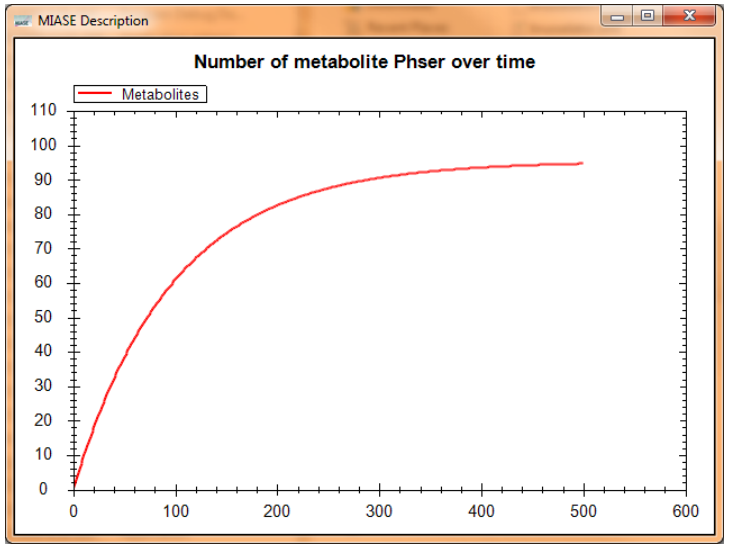
What is available?

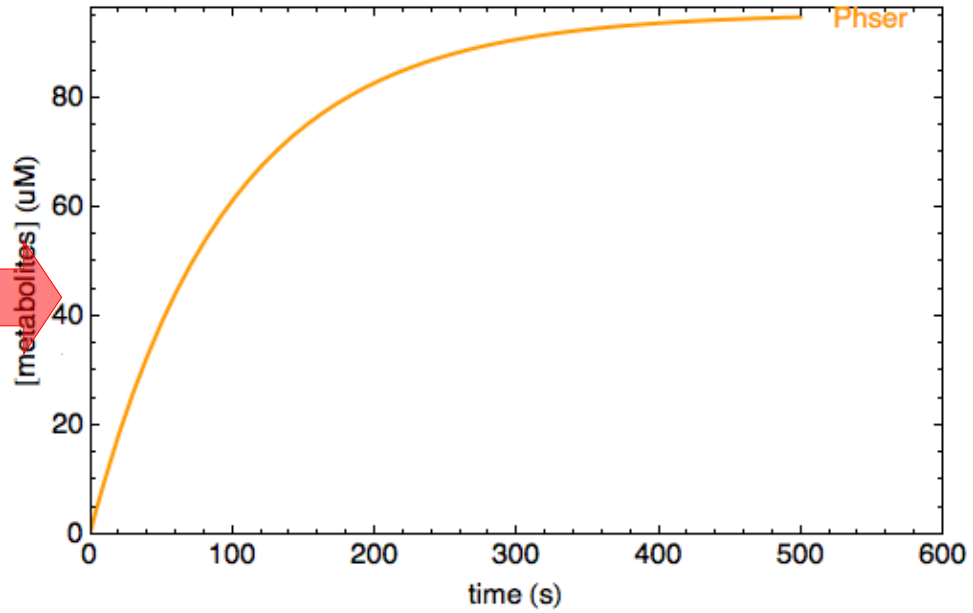
- SED-ML homepage:
  http://www.biomodels.net/sed-ml
- SED-ML at Sourceforge:
  https://sourceforge.net/projects/sed-ml
- SED-ML mailing list:
  sed-ml-discuss@lists.sourceforge.net

- Sed-ML online validator (Richard Adams, CSBE)
- Jlibsedml development (Richard Adams, Sourceforge)

What is available?

- Prototype implementations for SED-ML import/export
  - Roadrunner test implementation (Frank Bergmann)
  - Work with JWS Online Simulator (Jacky Snoep)



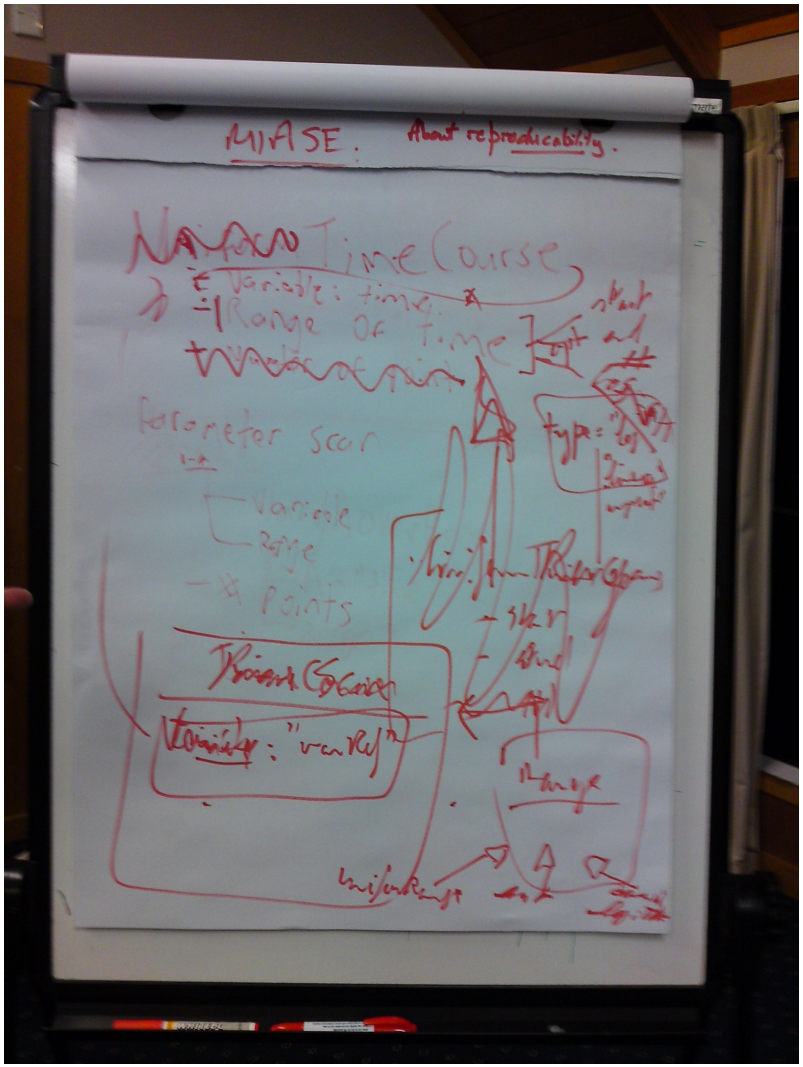


  - *on CellML side?*

Thanks to ...

Richard Adams (JlibSED-ML)
Frank Bergmann (roadrunner)
Mike Hucka
Fedor Kolpakov (BioUML)
Nicolas Le Novère
Ion Moraru (Virtual Cell)
Sven Sahle (COPASI)
Henning Schmidt (SB Toolbox)
Dagmar Waltemath

... and you.



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