Towards SED-ML L1 V1: Simulation Experiment Description Language

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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
• 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)
• DataGenerator Class
  - Specifies the data needed in the output through reference to model entities and post-processing
    
    \textit{e.g. variable reference in model, normalisation of a result data set before output}

• Output Class
  - Define output type
    
    \textit{e.g. 2D plot, table …}

  - Define output plots using “data generators“
    (\textit{\rightarrow} DataGenerator Class)

    \textit{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 Any Simulation Class
  - desired: Parameter Scans, Optimisations ...

- SED-ML level 1, version 1 Specification:
  Plans for finalisation during biomodels.net meeting
  Seattle, April 2010 [http://biomodels.net/events.html](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)
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Fedor Kolpakov (BioUML)
Nicolas Le Novère
Ion Moraru (Virtual Cell)
Sven Sahle (COPASI)
Henning Schmidt (SB Toolbox)
Dagmar Waltemath

... and you.

http://www.biomodels.net/sed-ml
sed-ml-discuss@lists.sourceforge.net