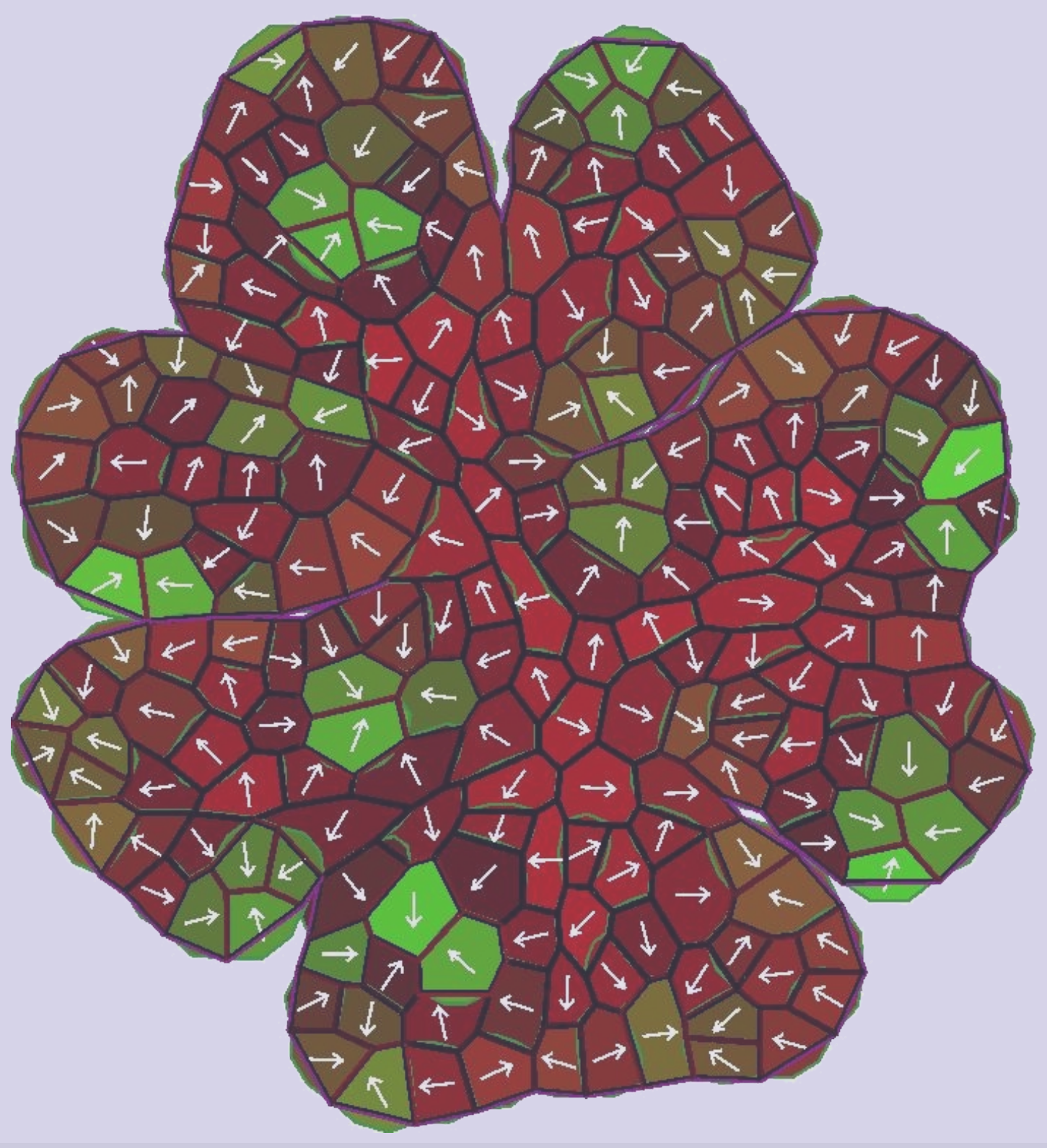

Towards a web-based simulation experiment description repository

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The Problem with Models

Modellers are producing more and more complex models. Unless these models are sufficiently characterised and made available to the research community their reuse will be minimal, and reproducing simulation experiments incorporating them will prove problematic. Consensus on the content and form of experiment recipes that combine models and simulations will encourage model sharing and facilitate reuse.

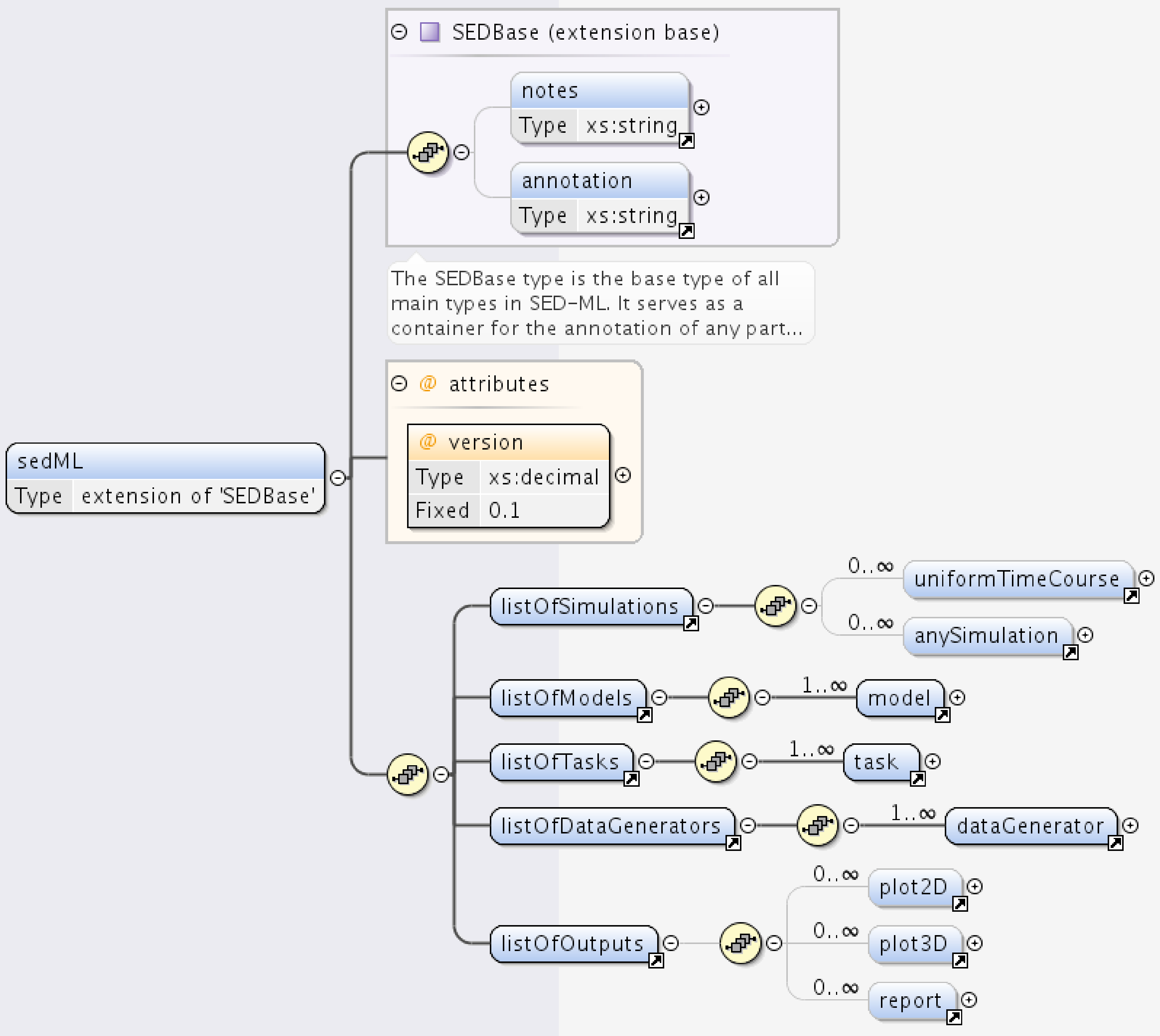
A set of guidelines specifying the *Minimum Information About a Simulation Experiment*(MIASE)[1] proposes a common set of information necessary to reproduce simulation experiments that incorporate quantitative models.

We have instantiated these guidelines in a web-based content management system. With our system you can create Simulation and Experiment Descriptions, enrich them with experimental data and annotate them with domain meta-information to facilitate classification, searching and cross referencing - all with the goal of reusing your models and reproducing your experimental results.

Simulation & Experiment Description Markup Language

One instantiation of the MIASE guidelines is SED-ML[2–4] - an XML schema, instances of which are recipes describing the combination of models and simulations into reproducible experiments. In particular, SED-ML describes five components essential to compose a simulation experiment description, i.e.:

- **simulations** – a description of the simulations' method, type and algorithm (KiSAO)[5]
- **models** – a description of the models' location, language and modifications
- **tasks** – the glue that combine models and simulations into experiments
- **data generators** – how to present the simulations' results, e.g. 2D graph
- **outputs** – how to transform raw simulation output into numerical or graphical results

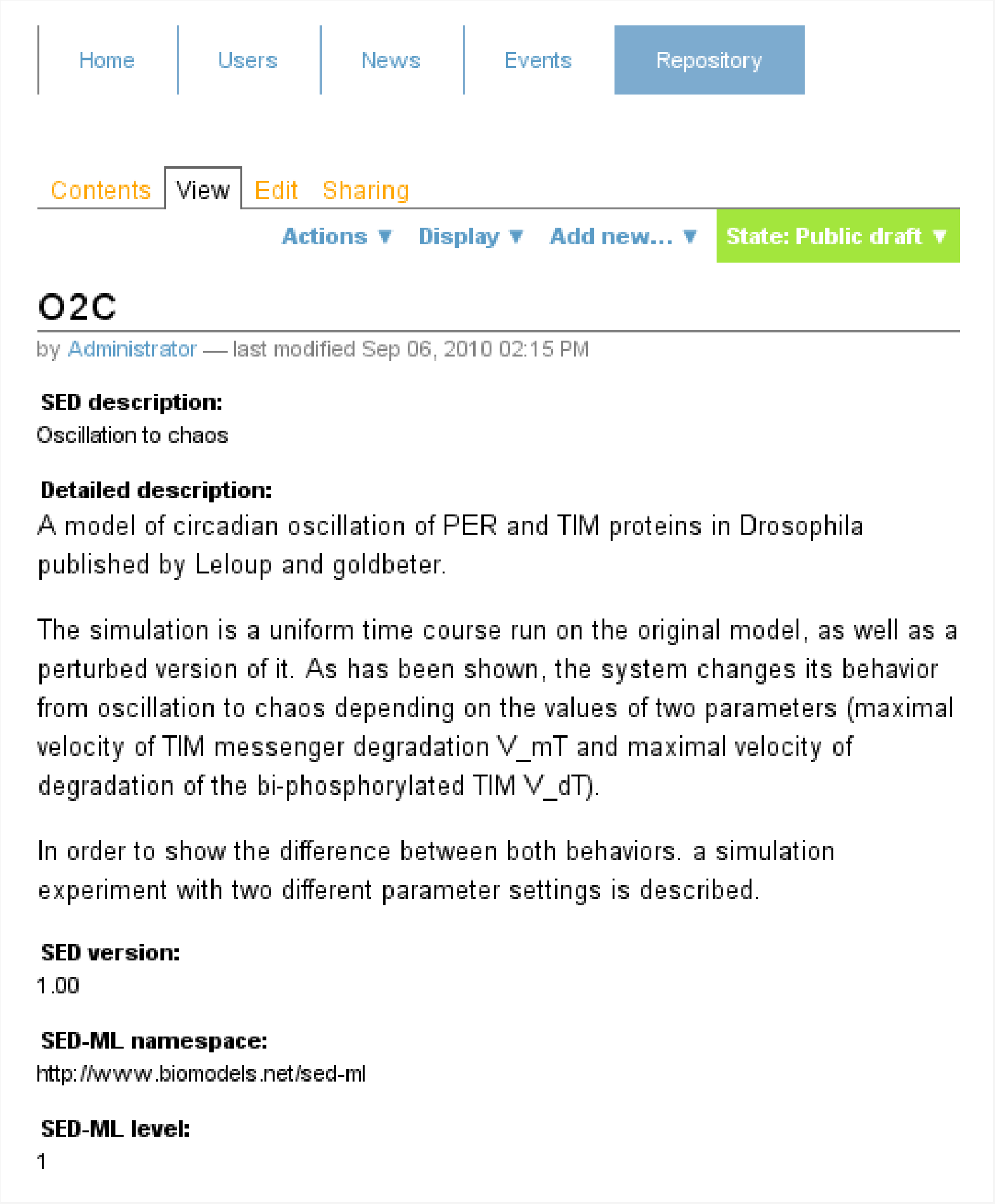


Insuring Experiment Results are Reproducible

The Simulation & Experiment Description Meta Language (SED-ML) is a means – like a recipe – to describe the combination of simulations and models in reproducible experiments. We have built a web-based simulation & experiment description repository based on SED-ML. Implemented as an add-on product to the open-source content management system named Plone™, our repository allows researchers to:

- **create** simulation & experiment descriptions (SEDs) compliant with SED-ML
- **annotate** simulations & experiments with domain meta-information from various ontologies
- **search** for simulations & experiments based on a variety of criteria, e.g. algorithm type
- **collaborate** with colleagues by allowing them to modify your simulations & experiments
- **curate** simulations & experiments to build a collection of verified and approved SEDs
- **export** simulations & experiments in SED-ML compliant XML

In contrast to EBI's existing BioModels database, which hosts only biochemical models written in SBML, our repository will uniquely record any simulation experiment, including those written in C++, thus making the tool generally applicable to the types of simulation models used within the NCSB.



O2C

by Administrator — last modified Sep 06, 2010 02:15 PM

SED description:
Oscillation to chaos

Detailed description:
A model of circadian oscillation of PER and TIM proteins in Drosophila published by Leloup and goldbeter.

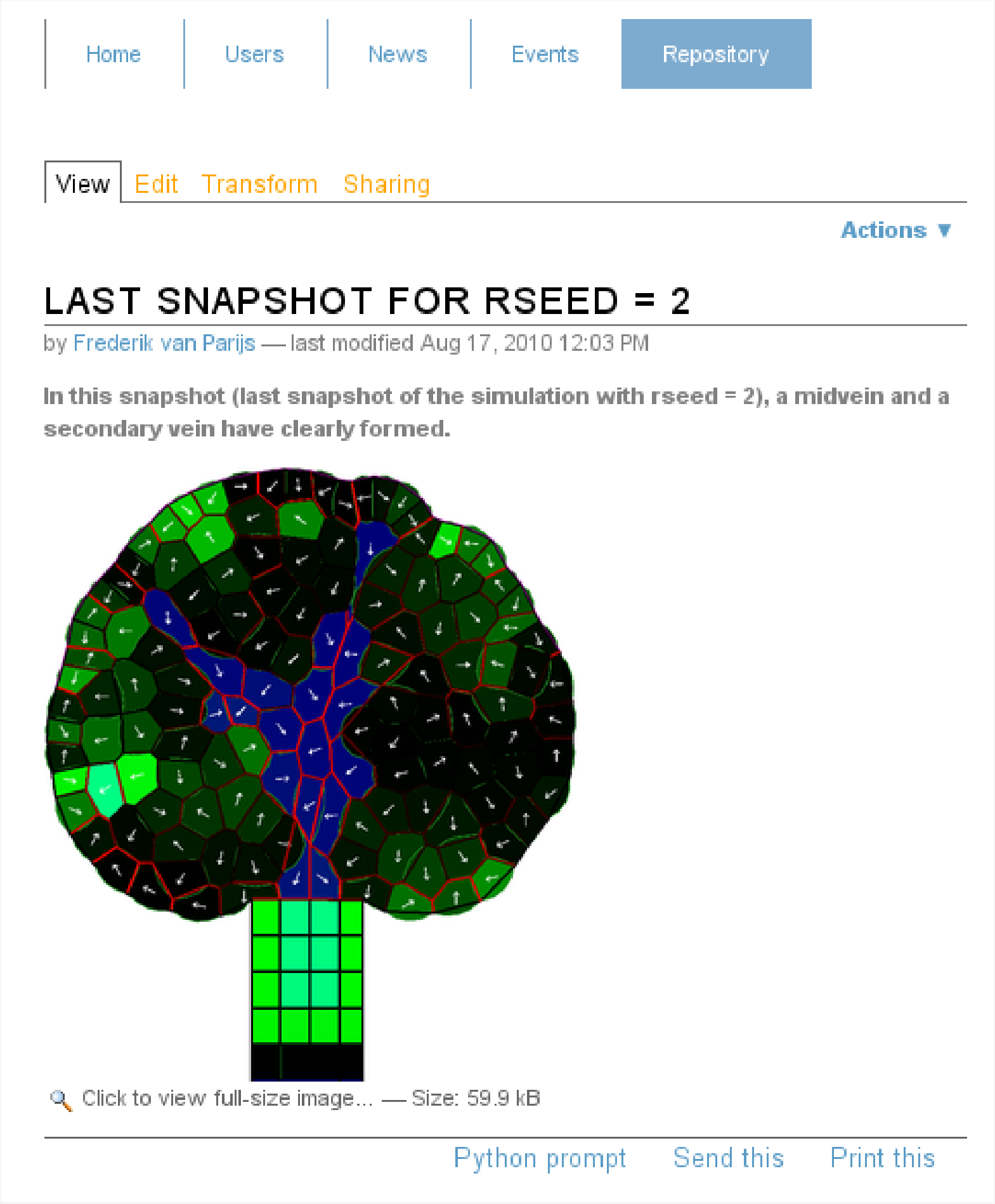
The simulation is a uniform time course run on the original model, as well as a perturbed version of it. As has been shown, the system changes its behavior from oscillation to chaos depending on the values of two parameters (maximal velocity of TIM messenger degradation V_mT and maximal velocity of degradation of the bi-phosphorylated TIM V_dT).

In order to show the difference between both behaviors. a simulation experiment with two different parameter settings is described.

SED version:
1.00

SED-ML namespace:
http://www.biomodels.net/sed-ml

SED-ML level:
1



LAST SNAPSHOT FOR RSEED = 2

by Frederik van Parijs — last modified Aug 17, 2010 12:03 PM

In this snapshot (last snapshot of the simulation with rseed = 2), a midvein and a secondary vein have clearly formed.

Click to view full-size image... — Size: 59.9 kB

We have extended the SED-ML standard to accommodate source-code models, and enriched the output types with descriptive text, images and animations – which makes the repository useful as a laboratory notebook.

Results

- We can easily realise almost any collaboration scheme imaginable, e.g. research groups can have their own repositories where only curated and approved simulations & experiments are visible to the public, while works in progress are accessible to group members, and colleagues can collaborate on individual simulations & experiments.
- We can annotate simulations & experiments with domain meta-information, e.g. species name or algorithm type. In addition, any number of user defined tags can be applied to your simulations & experiments, all of which serve as search criteria to help you find and correlate information quickly and efficiently.
- We believe the synergy achieved by paring SED-ML precise standard with Plone's superior content management functionality will help foster and improve model reuse within the NCSB.

References

[1] D. Waltemath *et al.Minimum information about a simulation experiment (miase)* (unpublished,2010). biomodels.net/miase/.
[2] D. Köhn and N. Le Novère, in *Computational Methods in Systems Biology*, edited by M. Heiner and A. Uhrmacher , number 5307 in Lecture Notes in Computer Science (Springer Berlin / Heidelberg), p. 176-190. 10.1007/978-3-540-88562-7_15.
[3] D. Waltemath, N. Novère, and F. T. Bergmann *Simulation Experiment Description Markup Language (SED-ML): Level 1 Version 1 (Draft).* (2010).
[4] F. T. Bergmann, *A simple nested simulation for sed-ml* (2010). CellML SBGN SBO BioPAX MIASE Workshop.
[5] D. Köhn and N. Le Novère, *The kinetic simulation algorithm ontology (kisao) - a proposal for the classification of simulation algorithms in systems biology* (2008).

Future Work

- Add the ability to import SEDs from external SED-ML files.
- Develop tools to automatically reproduce experiments expressed in SED-ML.
- Improve the user interface by displaying related information simultaneously.
- Distribute our repository as an open-source Plone add-on product.

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