- **S**imulation **E**xperiment **D**escription **M**arkup **L**anguage
  https://sed-ml.github.io

- "The actual scholarship is the complete ... set of instructions (and data) which generated the figures."
- SED-ML is an XML-based format for encoding simulation setups, to ensure exchangeability and reproducibility of simulation experiments.

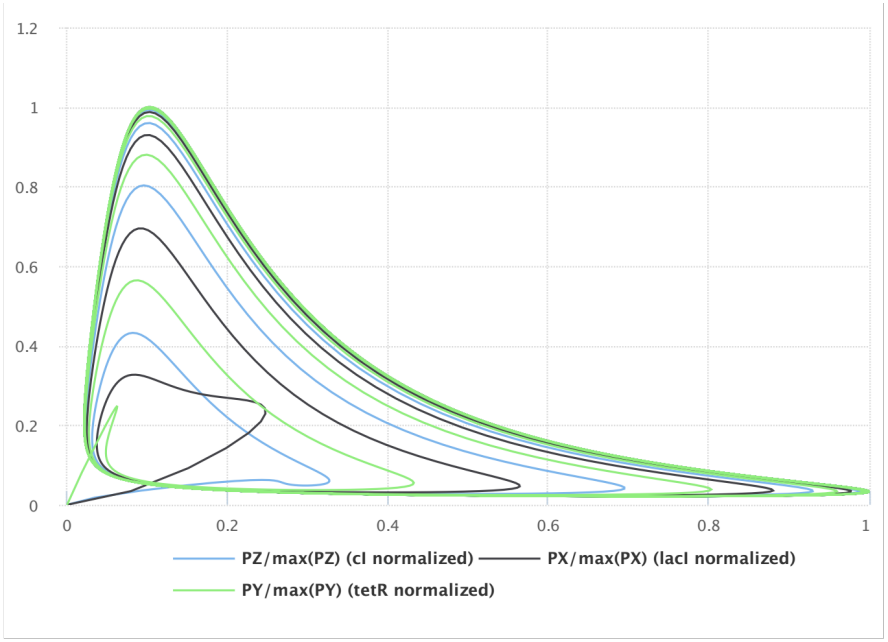


Figure 1.5: *Time-course simulation of the repressilator. Normalized* `lacI`, `tetR` *and* `cI` *in phase-plane. Simulation with SED-ML web tools [2].*

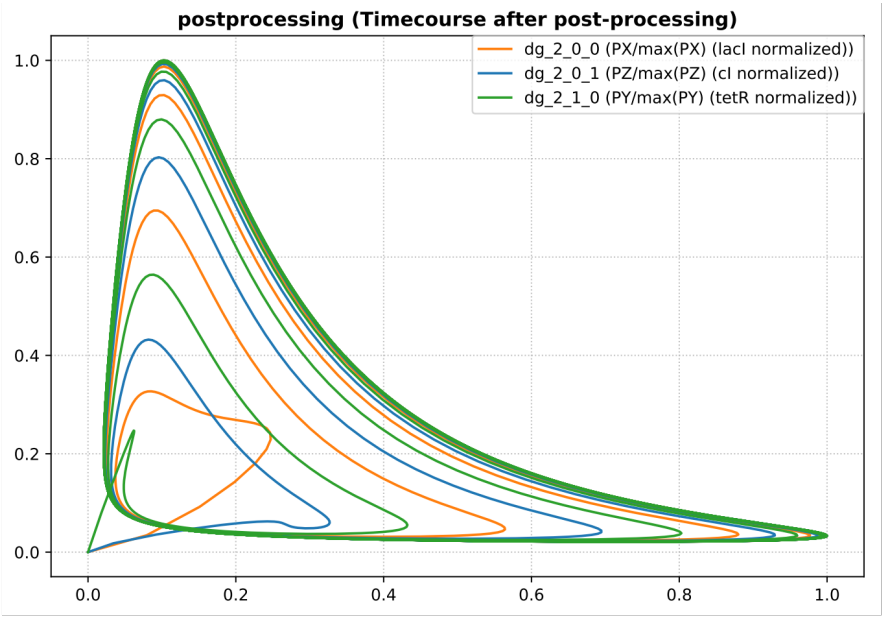
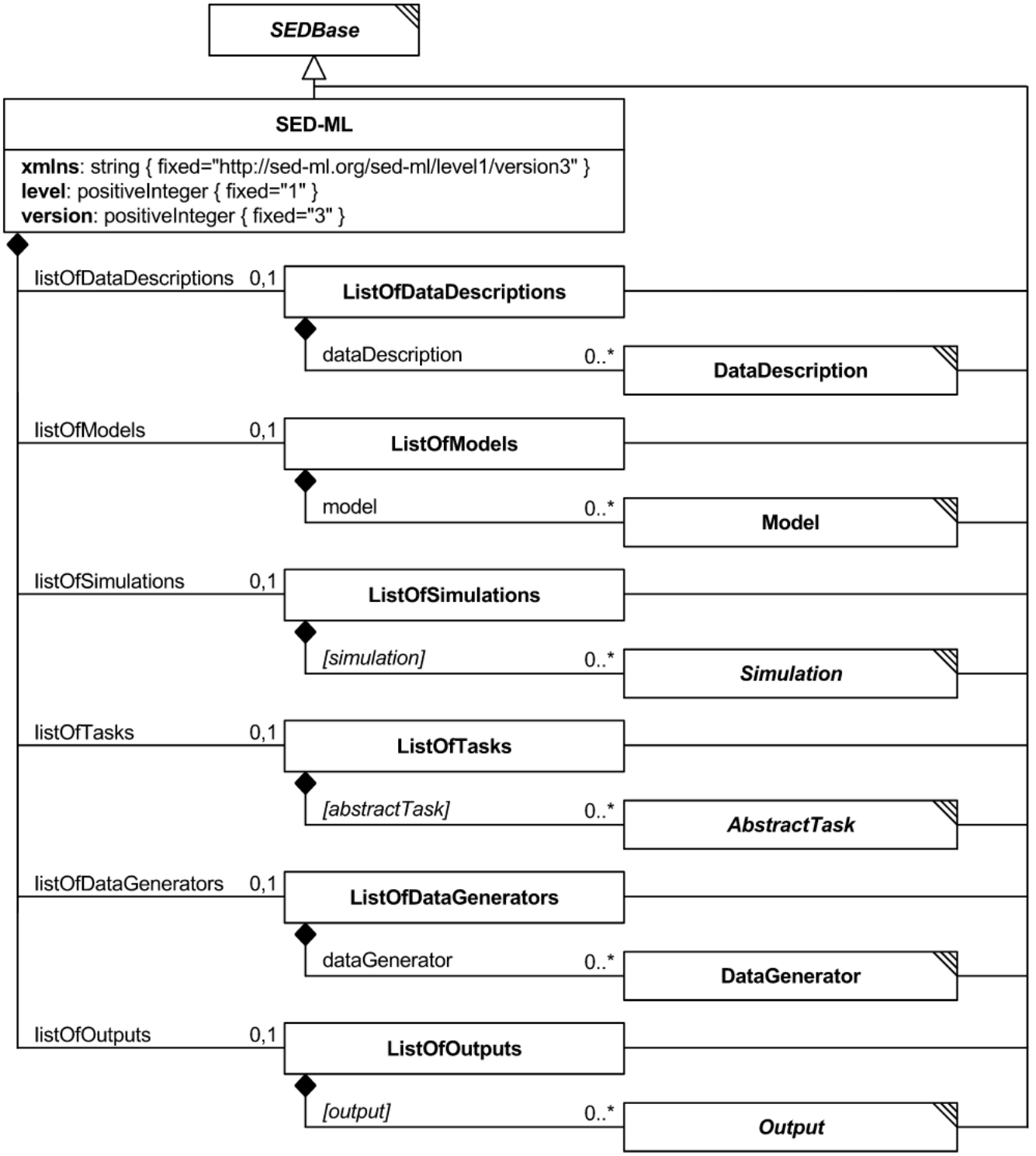


Figure 1.6: *Time-course simulation of the repressilator. Normalized* `lacI`, `tetR` *and* `cI` *in phase-plane. Simulation with tellurium [5].*


SEDBase
SED-ML
xmlns: string { fixed="http://sed-ml.org/sed-ml/level1/version3" }
level: positiveInteger { fixed="1" }
version: positiveInteger { fixed="3" }
listOfDataDescriptions 0,1
ListOfDataDescriptions
dataDescription 0..*
DataDescription
listOfModels 0,1
ListOfModels
model 0..*
Model
listOfSimulations 0,1
ListOfSimulations
[simulation] 0..*
Simulation
listOfTasks 0,1
ListOfTasks
[abstractTask] 0..*
AbstractTask
listOfDataGenerators 0,1
ListOfDataGenerators
dataGenerator 0..*
DataGenerator
listOfOutputs 0,1
ListOfOutputs
[output] 0..*
Output

1.2.2 Applying pre-processing

A common step in a simulation experiment is the adjustment of model parameters before simulation. When changing the parameter values for the protein copies per promoter `tps_repr` and the leakiness in protein copies per promoter `tps_active` like stated below, the system's behavior switches from sustained oscillations to damped oscillations. The simulation experiment leading to that behavior is described as:

1. Import the model as in Section 1.2.1 above.
2. Change the value of the parameter `tps_repr` from `0.0005` to `1.3e-05`.
3. Change the value of the parameter `tps_active` from `0.5` to `0.013`.
4. Select a deterministic method.
5. Run a uniform time course for the duration of 1000 min with an output interval of 1 min.
6. Plot the amount of `lacI`, `tetR` and `cI` against time in a 2D Plot.

Figure 1.3 on the following page and Figure 1.4 on the next page show the results of the simulation.

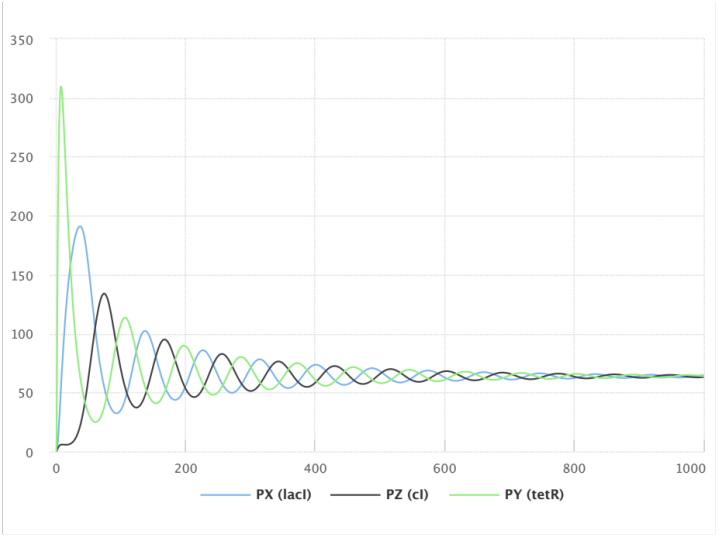


Figure 1.3: *Time-course simulation of the repressilator after changing parameters* `tps_repr` *and* `tps_active`*. Simulation with SED-ML web tools [2].*

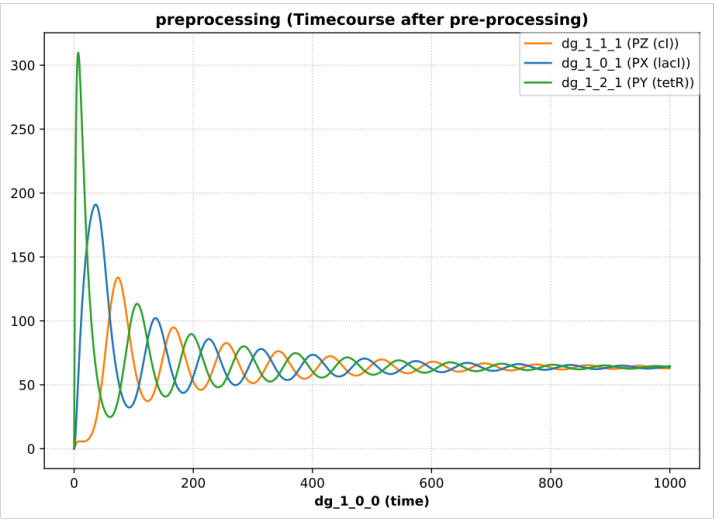
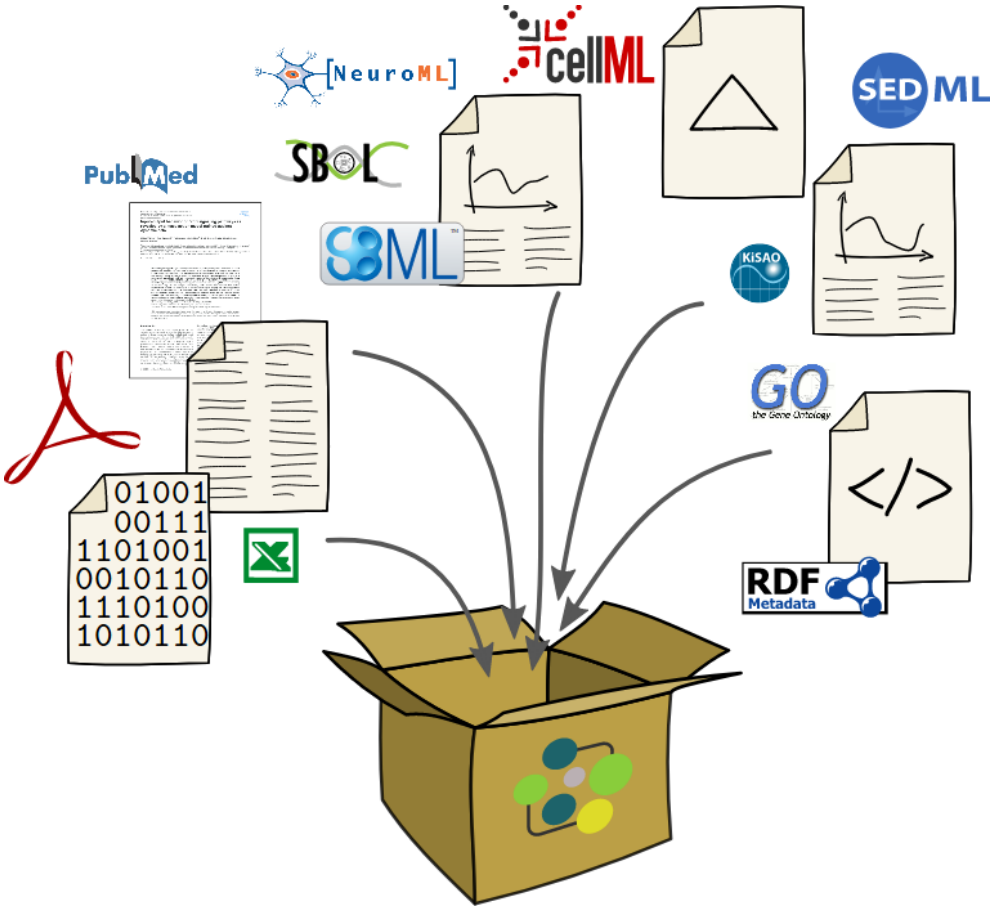


Figure 1.4: *Time-course simulation of the repressilator after changing parameters* `tps_repr` *and* `tps_active`*. Simulation with tellurium [5].*

SED-ML + COMBINE archive

- A COMBINE archive is a single file bundling the various documents necessary for a modeling and simulation project, and all relevant information
- Allows to bundle
  - Data
  - Models (SBML & CellML)
  - Simulation Descriptions (SED-ML)
  - Annotations
  - Results
  - ...



SED ML @ COMBINE2018

- Breakouts
  - Day 2 (Tuesday, October 9): 15.30 – 17.00
  - Day 3 (Wednesday, October 10): 13.30 – 15:00
- Agenda: Finishing the L1V4 specification
  - Plotting extension
  - Better specify use of ata
  - Bug fixes
  - Updating the schema document
  - Parameter fitting ?!
- https://sed-ml.github.io/

Lucian Smith

Matthias König