SED-ML part 2

- Brief introduction to L1V2
- Parameter estimation
- Qualitative models
- Simulation core library
- Potential feature requests

SED-ML L1V2

- Two main additions plus some tidying-up.
- Algorithm class proposal.
- Nested tasks proposal.

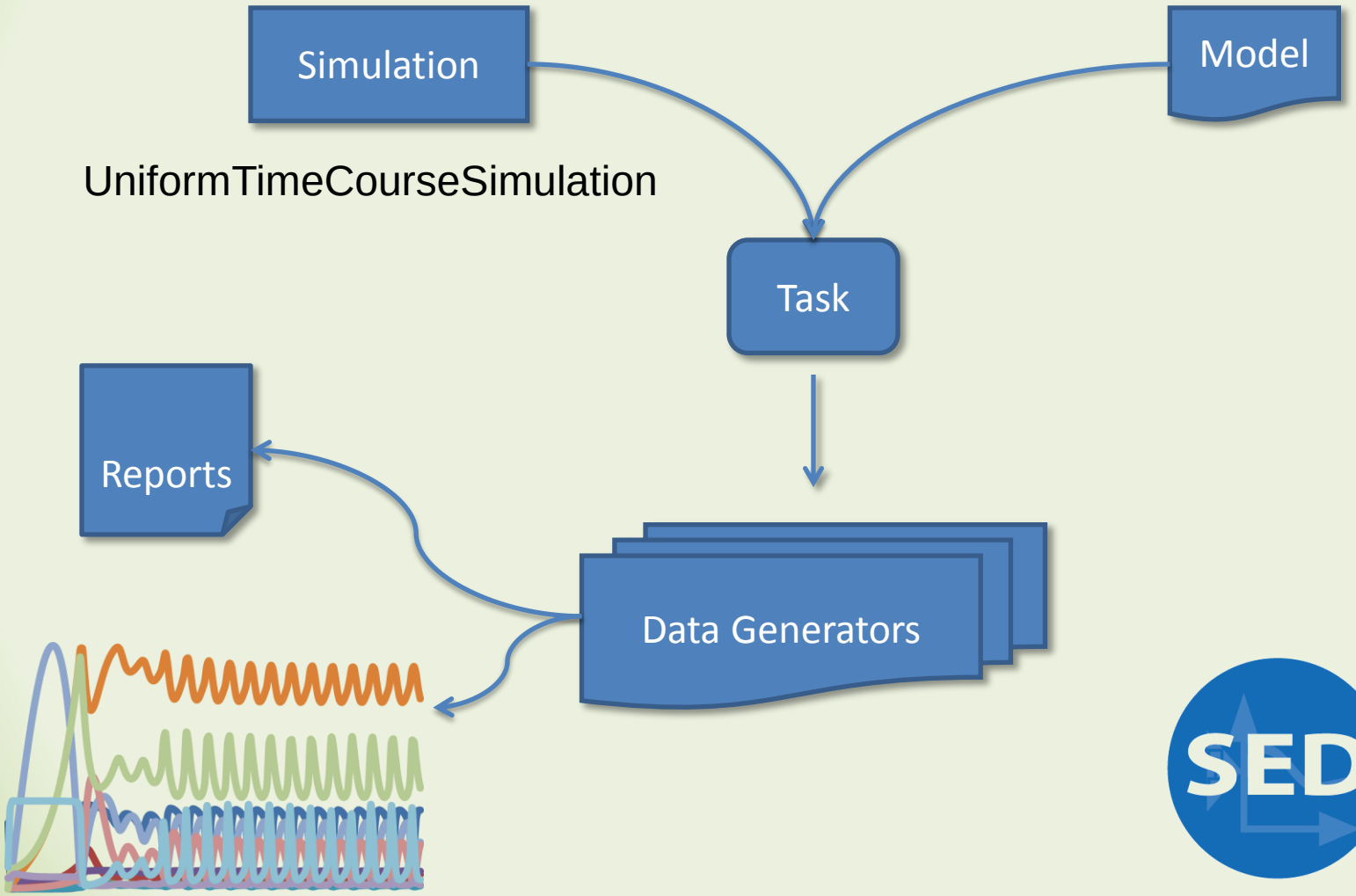
Algorithm class proposal

- Currently no mechanism to parameterize a particular simulation algorithm.
- Proposal: extend algorithm class to support parameterization.
- Adds a list of algorithm parameters which allows the author to encode values for the algorithm parameters defined in KiSAO.

```
<algorithm kisaoID="KISAO:0000032">
        <listOfAlgorithmParameters>
                <algorithmParameter kisaoID="KISAO:0000211" value="23"/>
        </listOfAlgorithmParameters>
</algorithm>
```

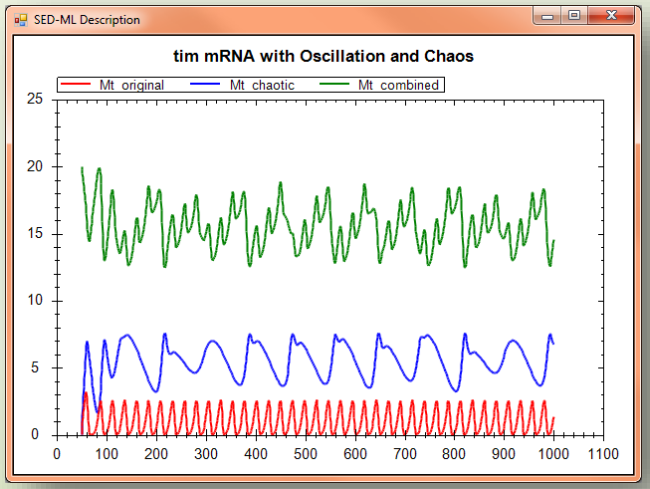
Nested tasks proposal

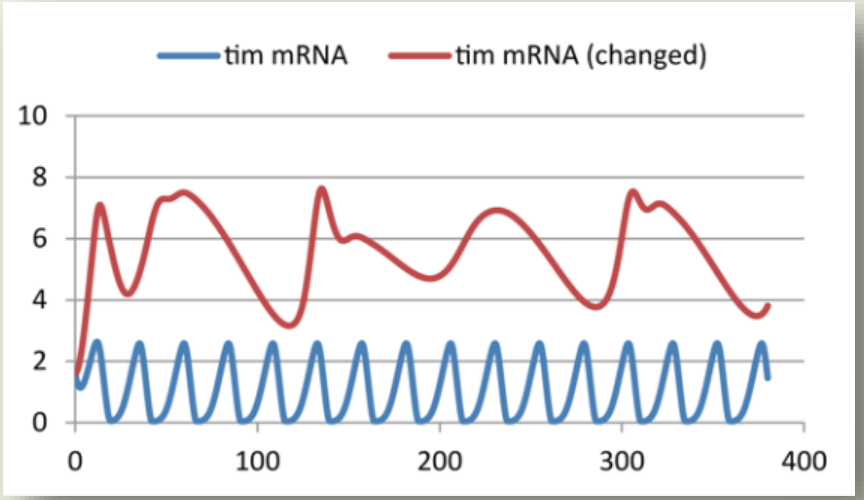
The Current State



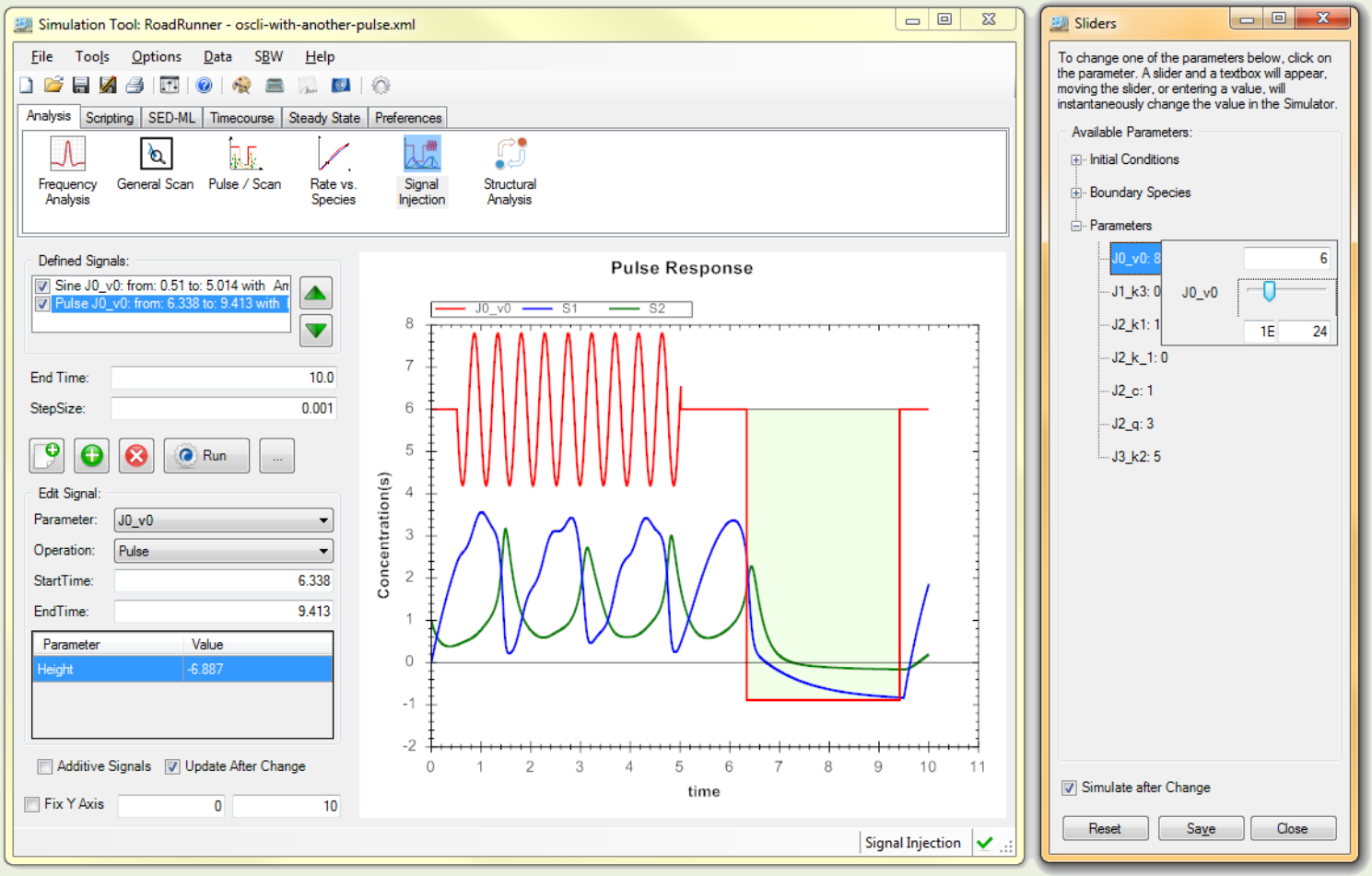
The Current State

- Carry out multiple time course simulations
- Collect results from these simulations
- Combine results from these simulations
- Report / Graph the results

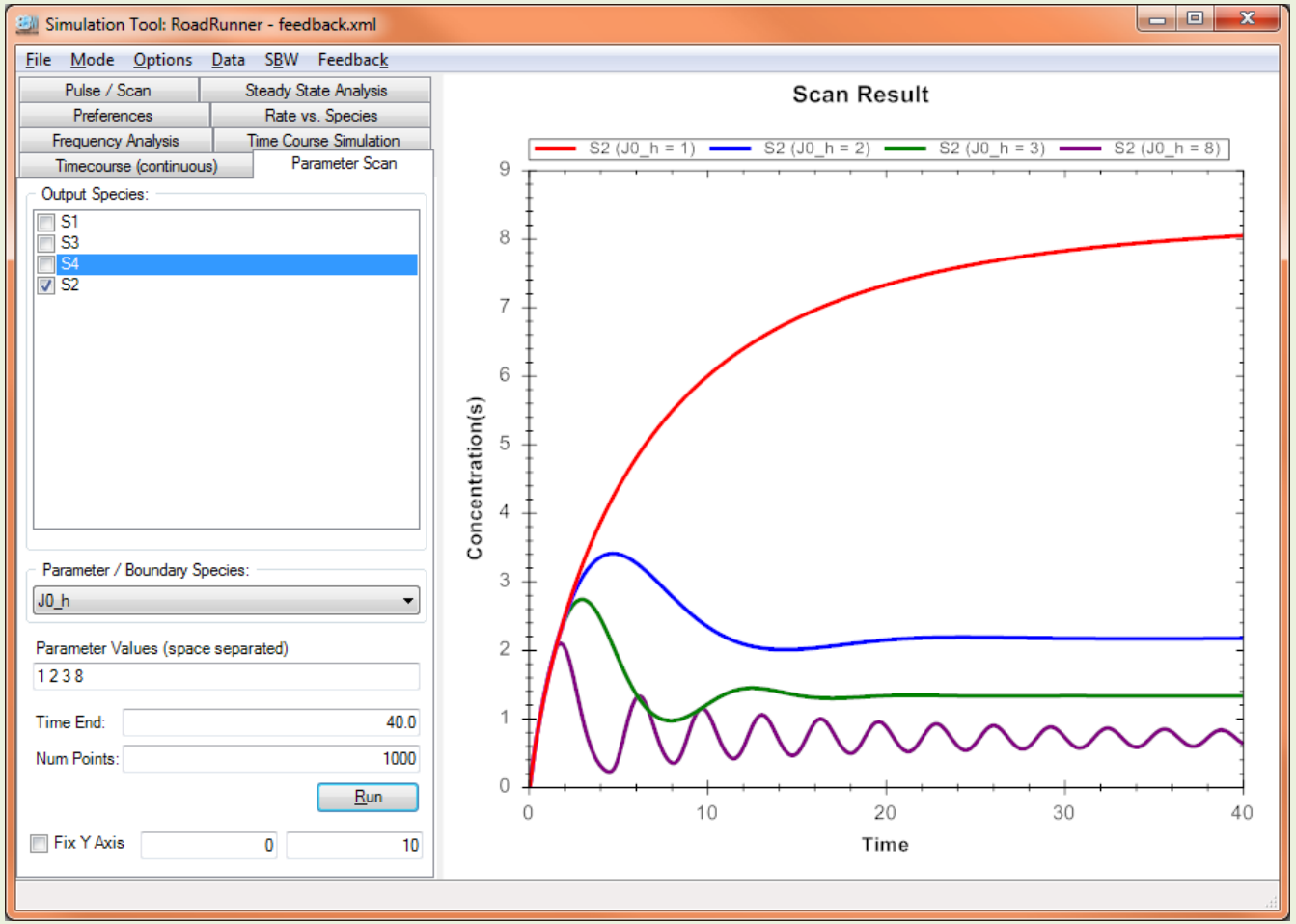




What it does not cover



Parameter Scans



Motivation

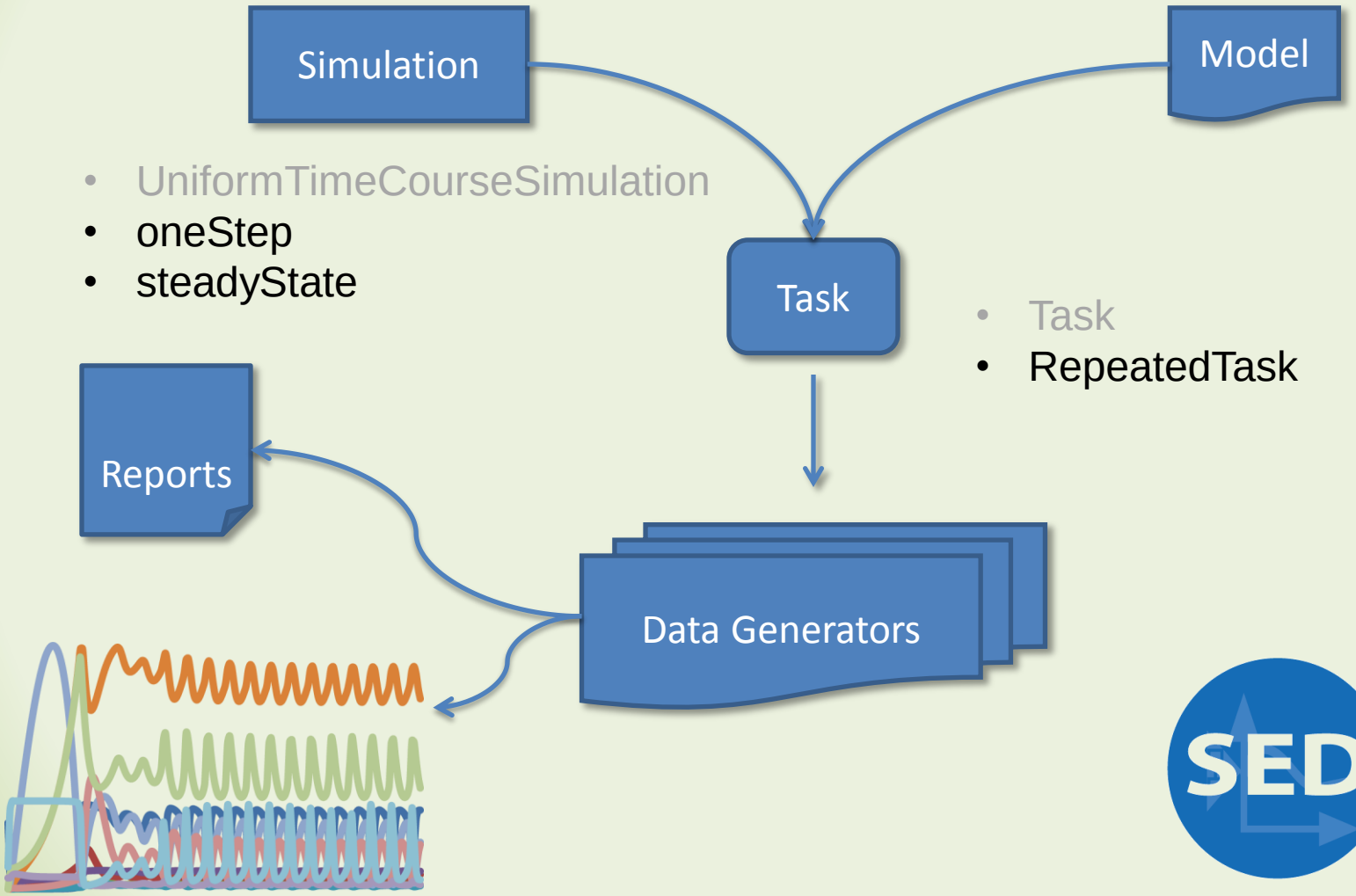
- Of course there are more simulations to be captured. But the extensions ought to happen in an orthogonal way, so that we can cover more of what people want to do, by adding additional:
  - Simulation Classes
  - Task Classes
  - DataGenerator Classes
  - Output Classes

Motivation

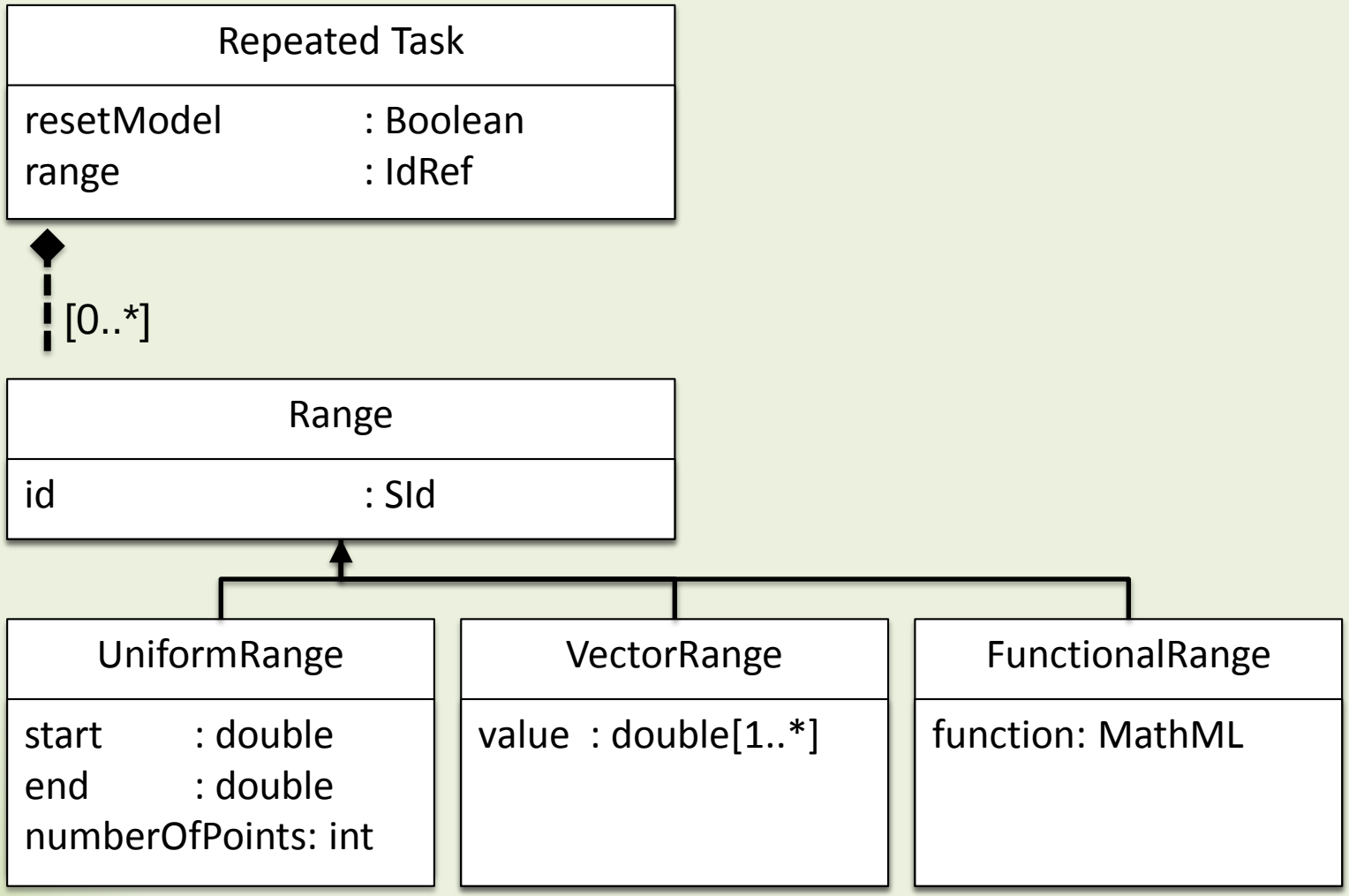
- Expand SED-ML, in a natural, compatible way, that allows software tools to carry out interconnected simulation tasks.

➔ Proposal of a new Task Class: The RepeatedTask, that allows multiple simulation tasks to be invoked while changing model variables.

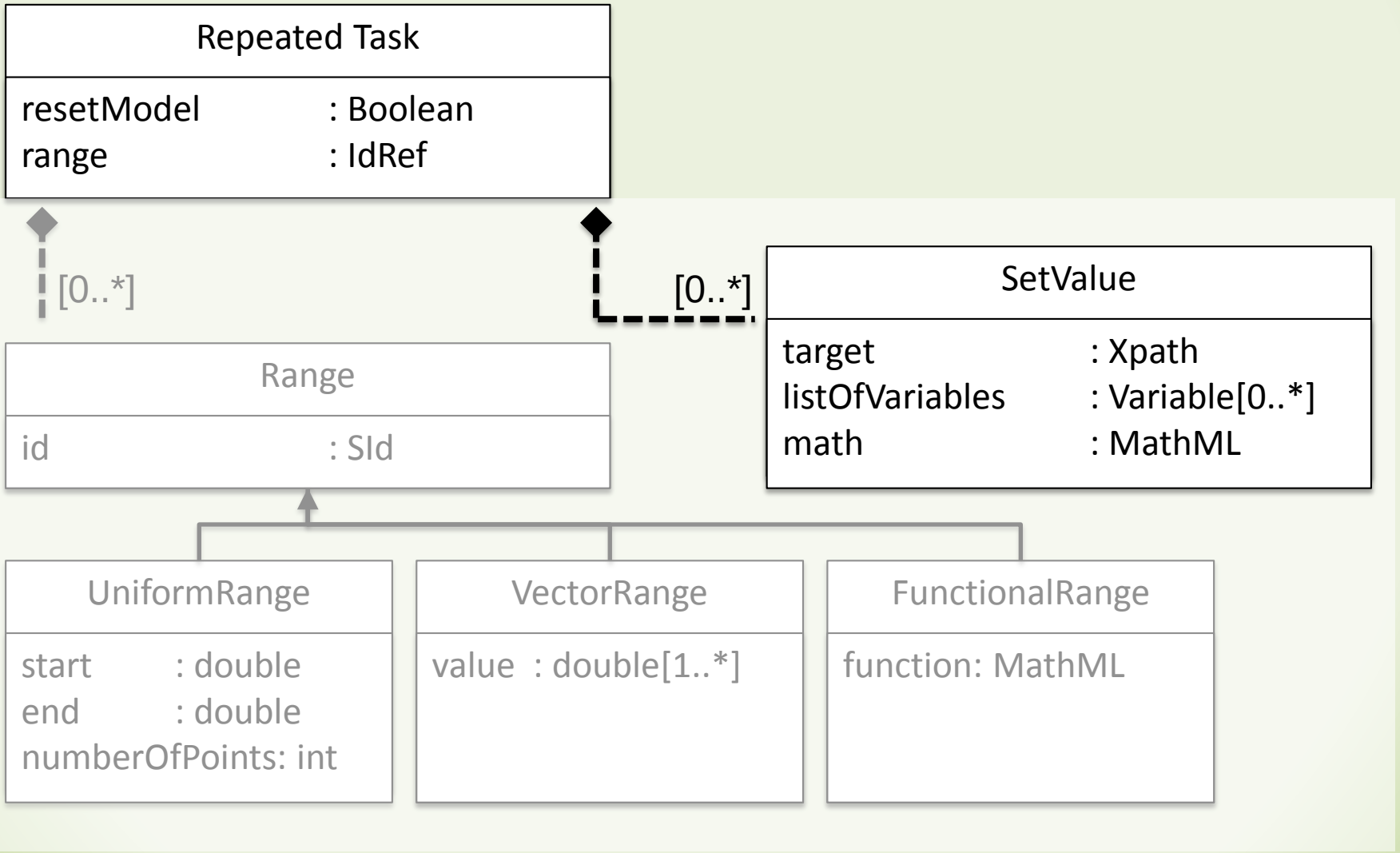
The Proposal



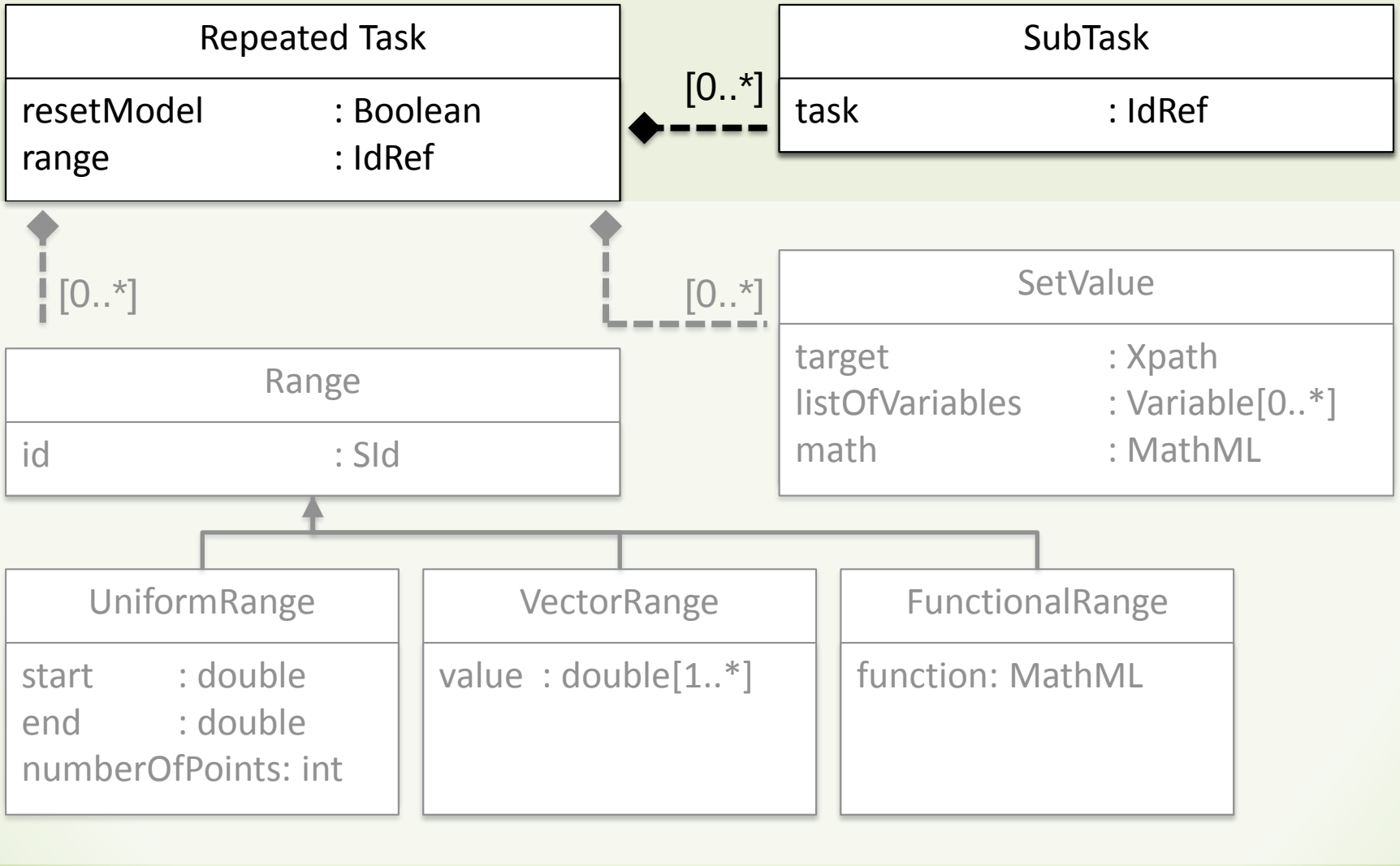
Repeated Task



Repeated Task



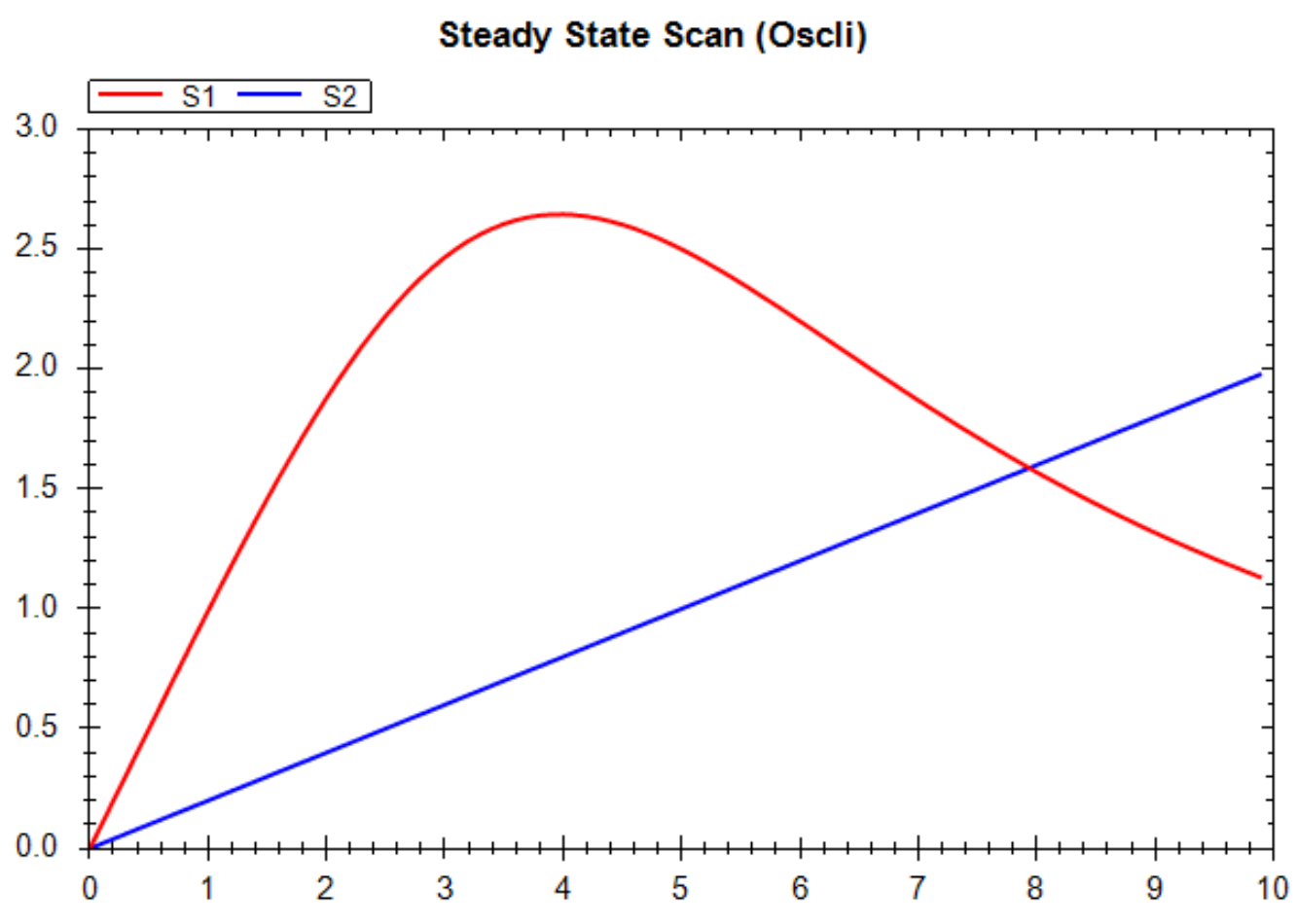
Repeated Task



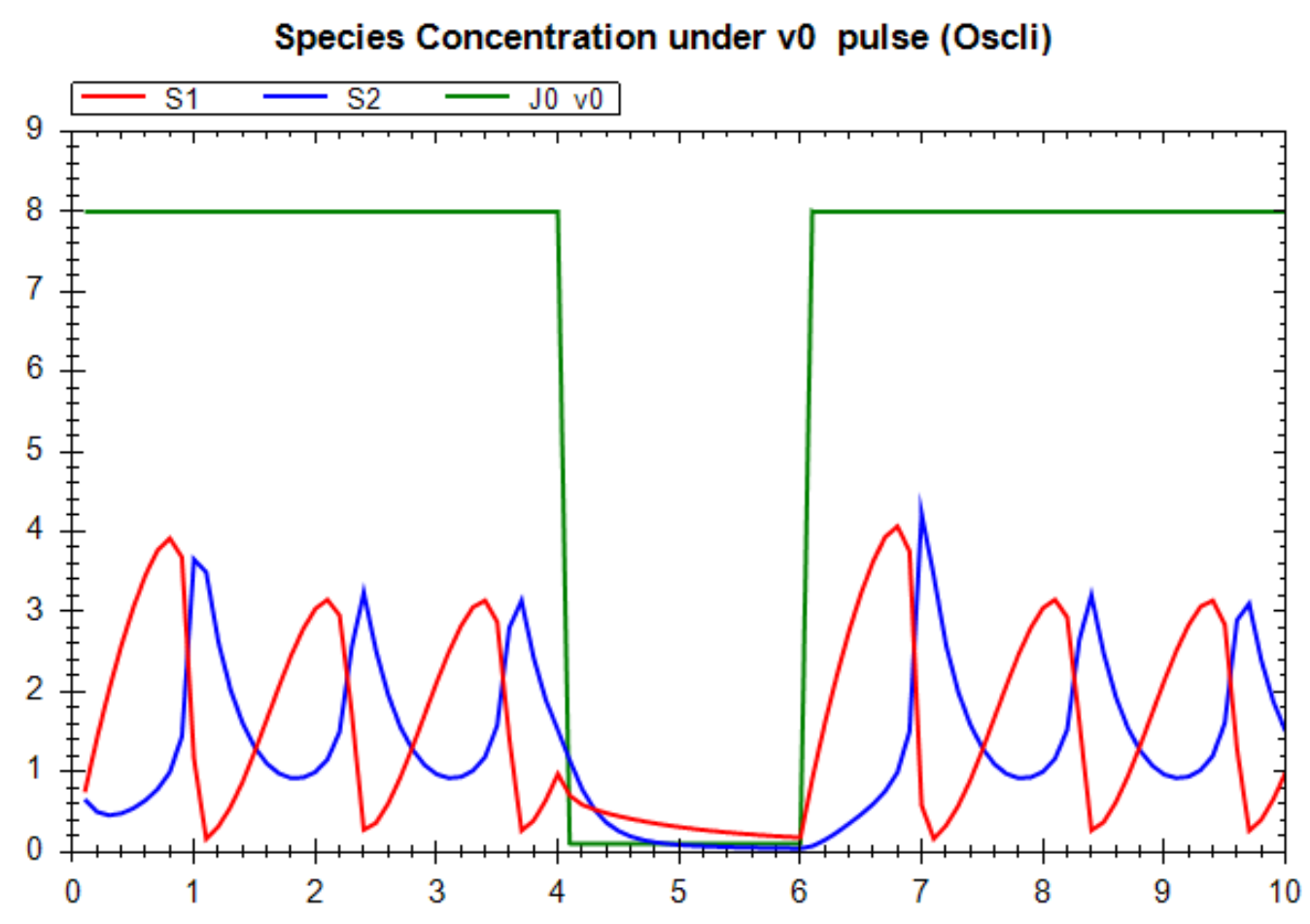
Features

- Carry out simulations,
- continue with other simulations
- Modify model variables during simulation runs

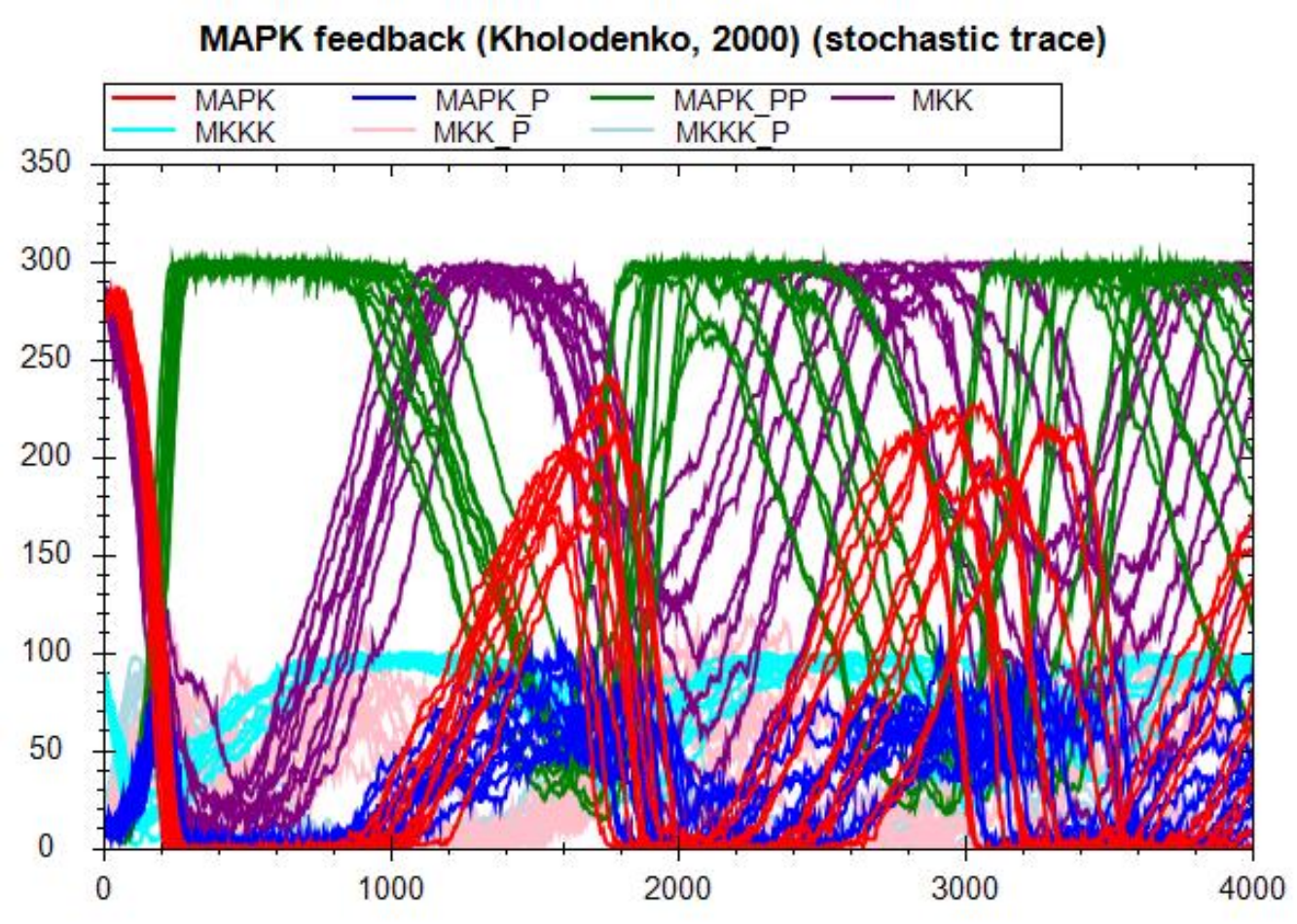
Parameter Scan



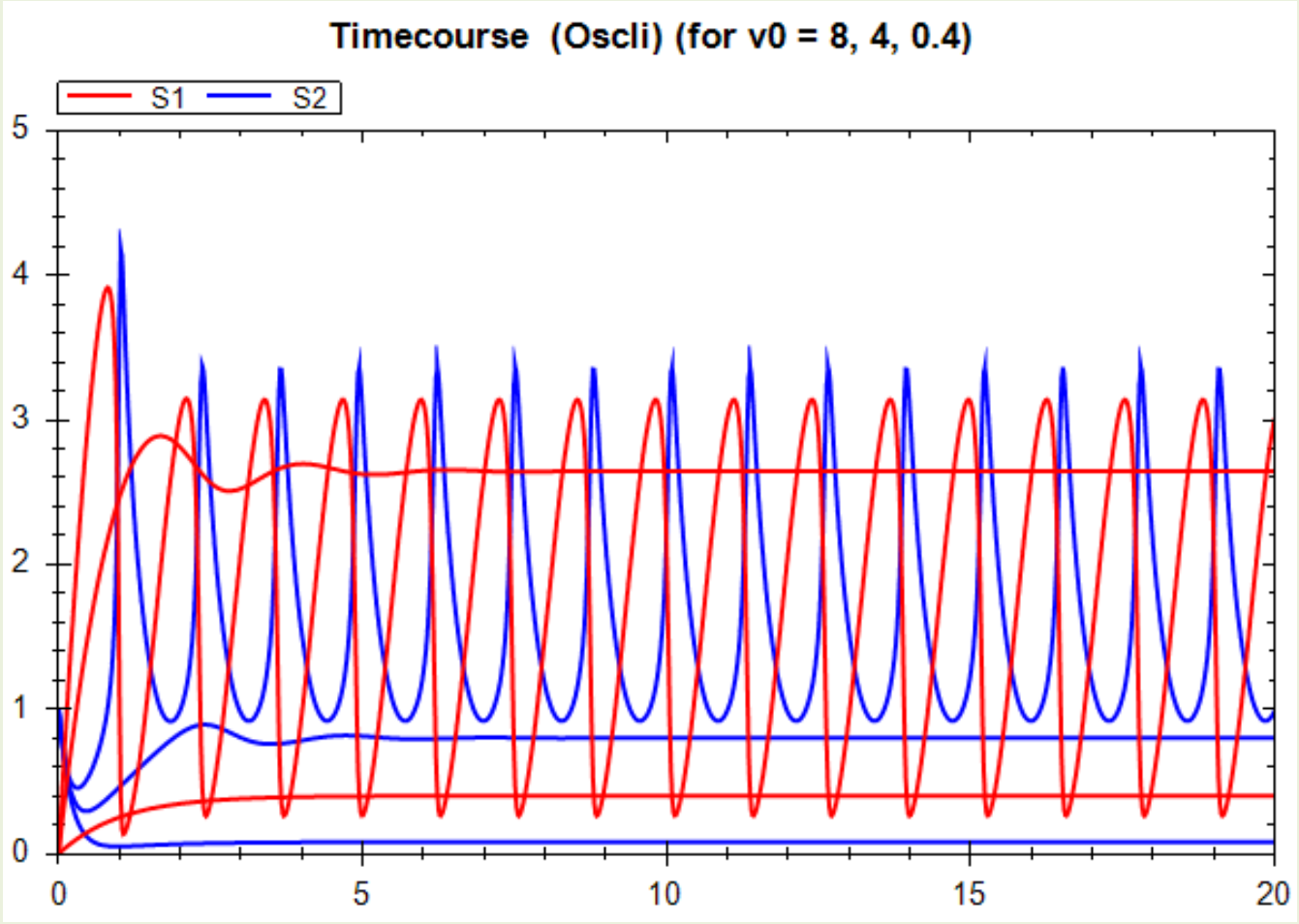
Pulse Experiments



Repeated Stochastic Traces



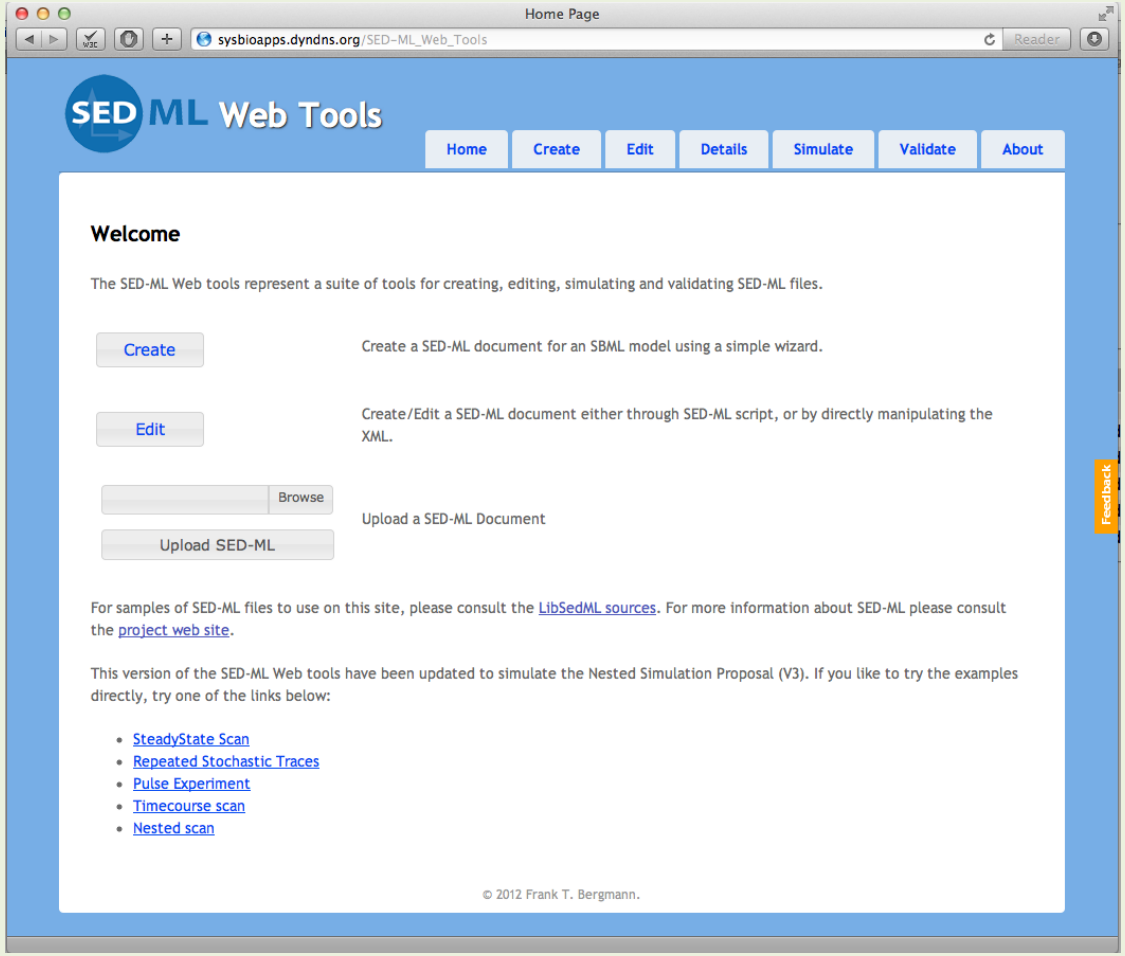
Time Course Parameter Scan



Place For Orthogonal Extensions…

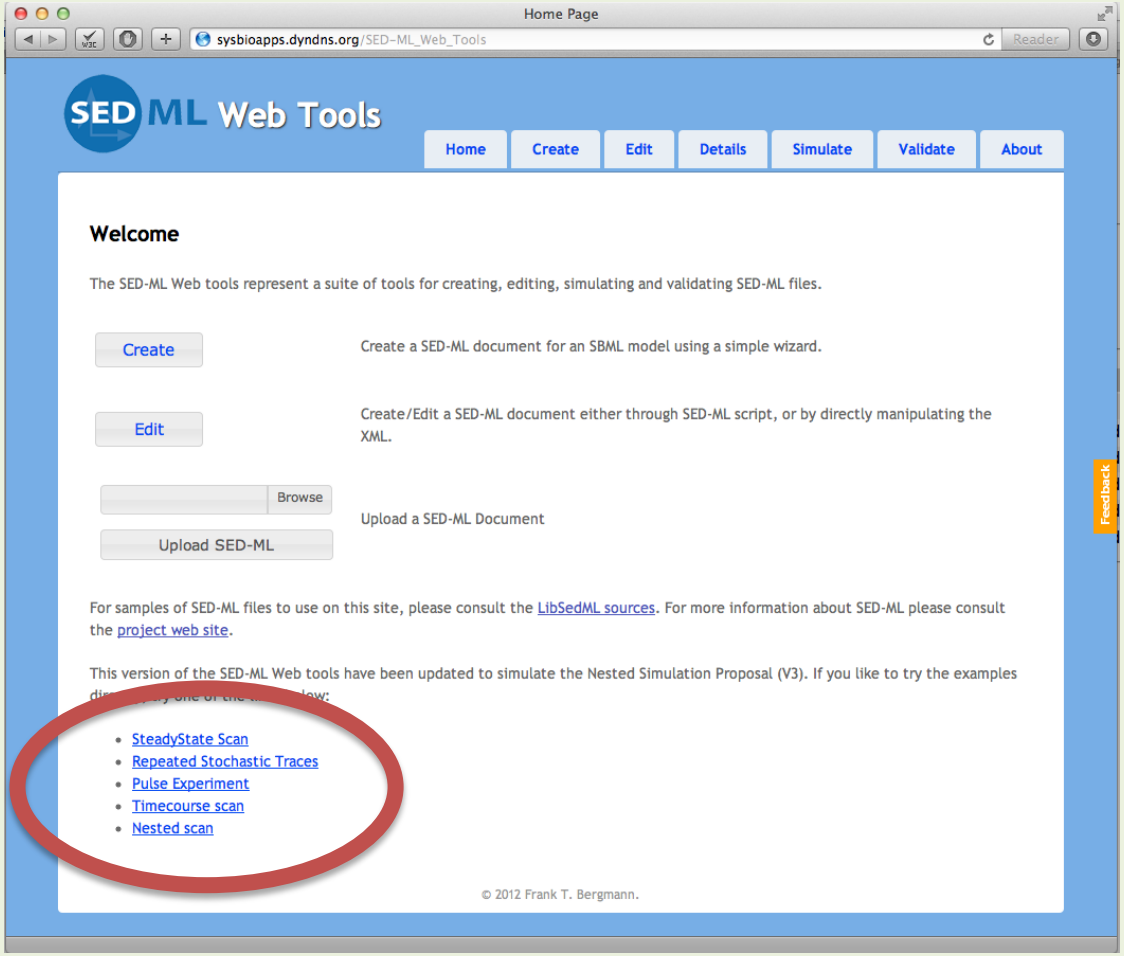
- Parameterizable Simulation Classes
- Storing the last state of a task as a new model
- Introduction of new Variables (for accessing implied variables)
- Advanced Post-processing in Data Generators
- Access of external data

Available Online



http://sysbioapps.dyndns.org/SED-ML_Web_Tools

Available Online



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