

vingnette

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1 SIMPLE SEDML VINGNETTE

This notebook provides examples of using `SimpleSBML`, a Python system for creating and validating Simulation Experiment Description Markup Language (SED-ML) descriptions of computational experiments for models written in the Systems Biology Markup Language (SBML) community standard.

Throughout, we use the term **display variable** to refer to a subset of variables in the model that the user wants to observe (e.g., floating species). A **parameter scan** variable is a parameter of the model that is being varied to see its effect on display variables.

SimpleSEDML provides APIs at two levels. The high level API is task oriented. Four tasks are considered. * Time course simulation for a single model. In this task, the user wants to see the interaction between display variables over time. * Time course simulation for multiple models. Here, the user wants to compare the time courses of the same display variable in different models. * Parameter scan for a single model. The user wants to see how display values are affected by changes in scan parameters. * Parameter scan for multiple models. The user wants to compare the effect on the same display variable in different models as a scan parameter is changed.

The above use cases are encapsulated into 4 different API calls with optional parameters related to the simulation and changing values of the parameters of the model. These API calls produce an object with the following methods: * `getSEDML` produces SED-ML for the experiment. * `getPhraSEDML` produces the PhraSED-ML for the experiment. * `execute` returns a `DataFrame` and a plot of the variables specified in the constructor. * `makeOMEXFile` creates an omex file

The low level API is essentially a python wrapper for PhraSED-ML, and is available from all objects produced in the high level API.

Below, we illustrate each one of the high level APIs.

2 Preliminaries

```
[1]: # Handle execution locally and in Colab
try:
    import SimpleSEDML as ss
except:
    !pip install SimpleSEDML
    import SimpleSEDML as ss
import pandas as pd
```

```

/Users/jlheller/home/Technical/repos/SimpleSEDLML/ssed/lib/python3.9/site-
packages/urllib3/__init__.py:35: NotOpenSSLWarning: urllib3 v2 only supports
OpenSSL 1.1.1+, currently the 'ssl' module is compiled with 'LibreSSL 2.8.3'.
See: https://github.com/urllib3/urllib3/issues/3020
    warnings.warn(

```

```
[2]: MODEL_ANT = '''
      model myModel
        J1: S1 -> S2; k1*S1
        J2: S2 -> S3; k2*S2

        S1 = 10
        S2 = 0
        k1 = 1
        k2 = 1

        S1 is "species1"
        S2 is "species2"
      end
      '''
```

```
[3]: MODEL2_ANT = '''
model myModel
    J1: S1 -> S2; k1*S1
    J2: S2 -> S3; k2*S2
    J3: S3 -> S1; k3*S3

    S1 = 10
    S2 = 0
    k1 = 1
    k2 = 1
    k3 = 0.1
end
'''
```

3 Use Case 1: Single module time course

3.1 Default parameters

```
[4]: ?ss.makeSingleModelTimeCourse
```

```
Init signature:
ss.makeSingleModelTimeCourse(
    model_ref: str,
    project_id: Optional[str] = None,
    ref_type: Optional[str] = None,
    simulation_type: str = 'uniform',
```

```

    project_dir: Optional[str] = None,
    display_variables: Optional[List[str]] = None,
    start: float = 0,
    end: float = 5,
    num_step: Optional[int] = None,
    num_point: Optional[int] = None,
    title: Optional[str] = None,
    algorithm: Optional[str] = None,
    is_plot: bool = True,
    model_parameter_dct: Optional[dict] = None,
)
Docstring:      Class to create a time course simulation for a single model
Init docstring:
Creates a time course simulation

Args:
    model_ref: reference to the model
    project_id: ID of the project, if None, uses the default project ID
    ref_type: type of the reference (e.g. "sbml_str", "ant_str", "sbml_file",
    ↪ "ant_file", "sbml_url")
    simulation_type: type of the simulation
                    (e.g., "uniform", "uniform_stochastic", "steadystate", "onestep")
    project_dir: directory to save the files
    display_variables: variables to be plotted and included the report
    start: start time
    end: end time
    num_step: number of steps
    num_point: number of points to be plotted
    algorithm: algorithm to use for the simulation
    title: title of the plot
    is_plot: if True, plot the results
    model_parameter_dct: dictionary of parameters whose values are changed

```

Returns:

```

    SingleModelTimeCourse: a time course simulation object
File:      ~/home/Technical/repos/SimpleSEDML/src/SimpleSEDML/
    ↪ single_model_time_course.py
Type:      type
Subclasses:

```

```
[5]: smtc = ss.makeSingleModelTimeCourse(MODEL_ANT, title="My Plot", num_point=100)
```

```
[6]: print(smtc.getPhraSEDML())
```

```

project_model = model
"/var/folders/02/1b248q1j50dch2pthzkvxmpr0000gn/T/tmpw6ssp34_/project_model.xml"
project_sim = simulate uniform(0, 5.0, 99)
project_sim.algorithm = CVODE

```

```
project_task = run project_sim on project_model
report time, S1, S2, S3
plot "My Plot" time vs S1, S2, S3
```

```
[7]: print(smtc.getSEDML())
```

```
<?xml version="1.0" encoding="UTF-8"?>
<!-- Created by phraSED-ML version v1.3.0 with libSBML version 5.19.5. -->
<sedML xmlns="http://sed-ml.org/sed-ml/level1/version4"
xmlns:sbml="http://www.sbml.org/sbml/level3/version2/core" level="1"
version="4">
  <listOfModels>
    <model id="project_model"
language="urn:sedml:language:sbml.level-3.version-2" source="/var/folders/02/lb2
48q1j50dch2pthzkvxmpr0000gn/T/tmpw6ssp34_/project_model.xml"/>
  </listOfModels>
  <listOfSimulations>
    <uniformTimeCourse id="project_sim" initialTime="0" outputStartTime="0"
outputEndTime="5" numberOfSteps="99">
      <algorithm name="CVODE" kisaoID="KISA0:0000019"/>
    </uniformTimeCourse>
  </listOfSimulations>
  <listOfTasks>
    <task id="project_task" modelReference="project_model"
simulationReference="project_sim"/>
  </listOfTasks>
  <listOfDataGenerators>
    <dataGenerator id="report_0_0_0" name="time">
      <math xmlns="http://www.w3.org/1998/Math/MathML">
        <ci> time </ci>
      </math>
      <listOfVariables>
        <variable id="time" symbol="urn:sedml:symbol:time"
taskReference="project_task" modelReference="project_model"/>
      </listOfVariables>
    </dataGenerator>
    <dataGenerator id="report_0_0_1" name="S1">
      <math xmlns="http://www.w3.org/1998/Math/MathML">
        <ci> S1 </ci>
      </math>
      <listOfVariables>
        <variable id="S1"
target="/sbml:sbml/sbml:model/sbml:listOfSpecies/sbml:species[@id='S1']"
taskReference="project_task" modelReference="project_model"/>
      </listOfVariables>
    </dataGenerator>
    <dataGenerator id="report_0_0_2" name="S2">
      <math xmlns="http://www.w3.org/1998/Math/MathML">
```

```

        <ci> S2 </ci>
    </math>
    <listOfVariables>
        <variable id="S2"
target="/sbml:sbml/sbml:model/sbml:listOfSpecies/sbml:species[@id='S2']"
taskReference="project_task" modelReference="project_model"/>
    </listOfVariables>
</dataGenerator>
<dataGenerator id="report_0_0_3" name="S3">
    <math xmlns="http://www.w3.org/1998/Math/MathML">
        <ci> S3 </ci>
    </math>
    <listOfVariables>
        <variable id="S3"
target="/sbml:sbml/sbml:model/sbml:listOfSpecies/sbml:species[@id='S3']"
taskReference="project_task" modelReference="project_model"/>
    </listOfVariables>
</dataGenerator>
</listOfDataGenerators>
<listOfOutputs>
    <report id="report_0">
        <listOfDataSets>
            <dataSet id="report_0_0_0_dataset" label="time"
dataReference="report_0_0_0"/>
            <dataSet id="report_0_0_1_dataset" label="S1"
dataReference="report_0_0_1"/>
            <dataSet id="report_0_0_2_dataset" label="S2"
dataReference="report_0_0_2"/>
            <dataSet id="report_0_0_3_dataset" label="S3"
dataReference="report_0_0_3"/>
        </listOfDataSets>
    </report>
    <plot2D id="plot_1" name="My Plot">
        <listOfCurves>
            <curve id="plot_1__report_0_0_0__report_0_0_1" logX="false"
xDataReference="report_0_0_0" logY="false" yDataReference="report_0_0_1"/>
            <curve id="plot_1__report_0_0_0__report_0_0_2" logX="false"
xDataReference="report_0_0_0" logY="false" yDataReference="report_0_0_2"/>
            <curve id="plot_1__report_0_0_0__report_0_0_3" logX="false"
xDataReference="report_0_0_0" logY="false" yDataReference="report_0_0_3"/>
        </listOfCurves>
    </plot2D>
</listOfOutputs>
</sedML>

```

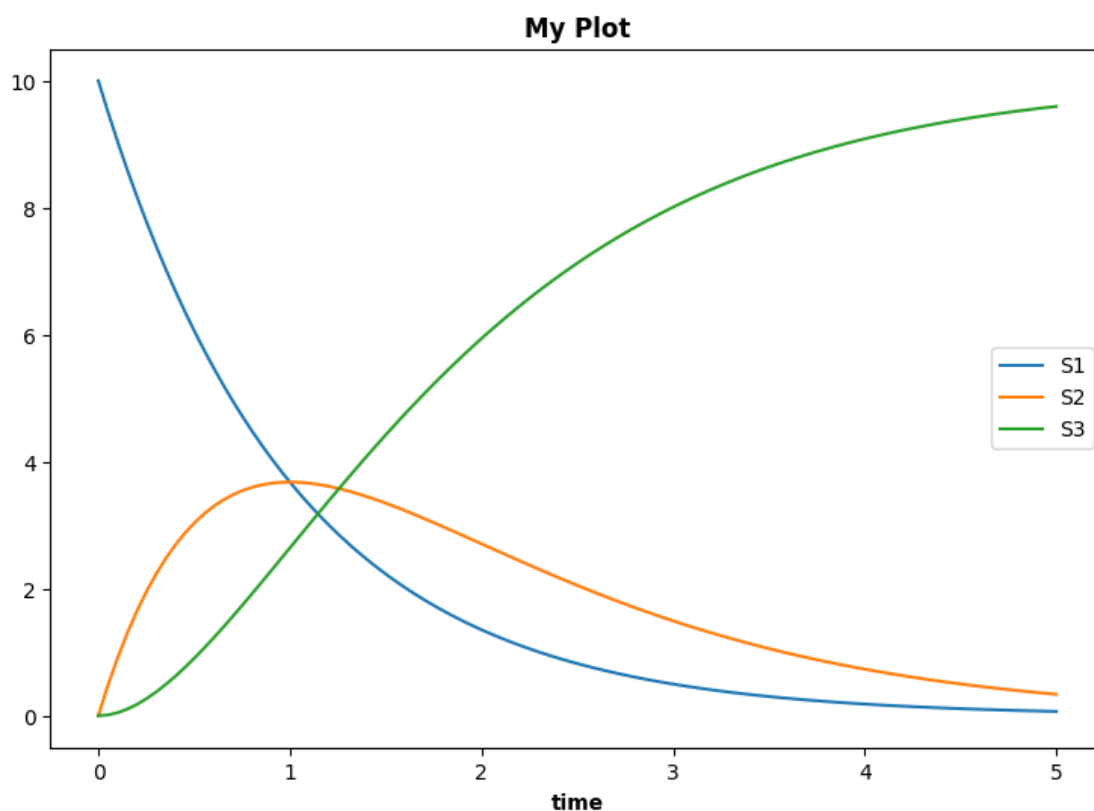
We can also look at the PhraSED-ML that gets generated by changing the object that gets returned.

```
[8]: print(smtc.getPhraSEDML())
```

```
project_model = model
"/var/folders/02/lb248q1j50dch2pthzkvxmpr0000gn/T/tmpw6ssp34_/project_model.xml"
project_sim = simulate uniform(0, 5.0, 99)
project_sim.algorithm = CVODE
project_task = run project_sim on project_model
report time, S1, S2, S3
plot "My Plot" time vs S1, S2, S3
```

And we can execute the SEDML, getting both a plot and a DataFrame of time course values.

```
[9]: df = smtc.execute()
```



```
[10]: df.head()
```

```
[10]:
```

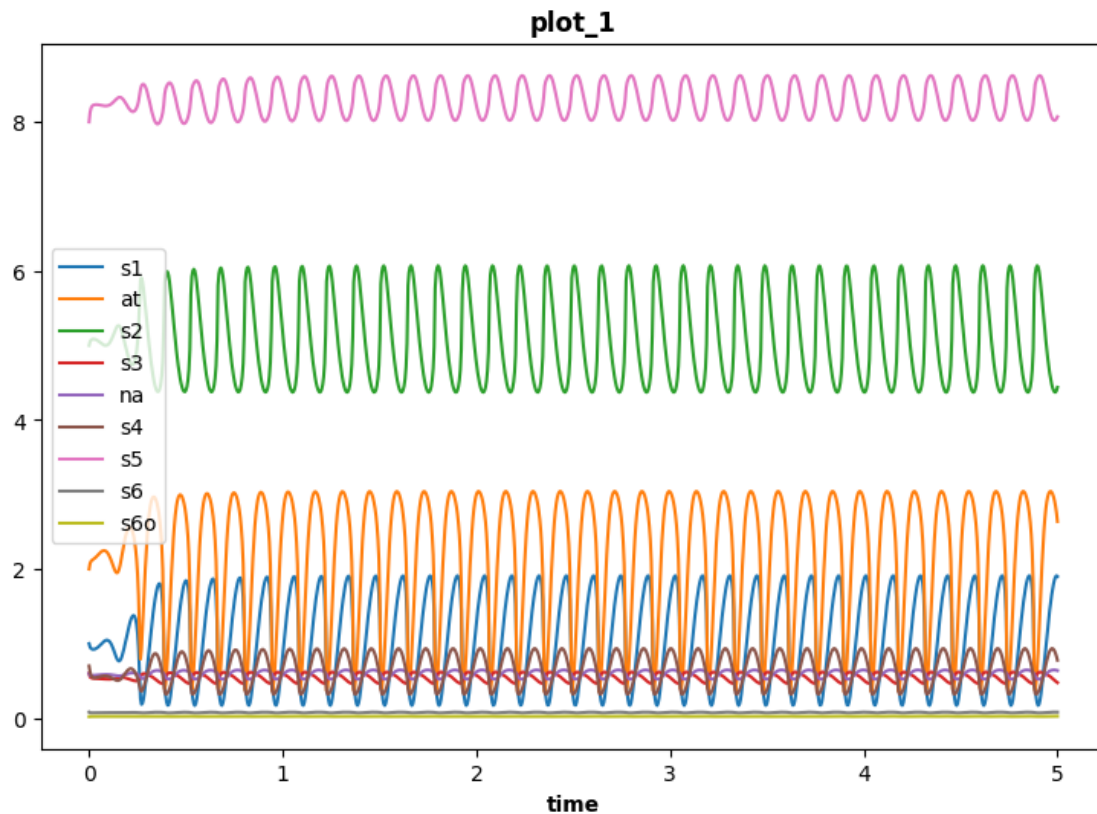
	time	S1	S2	S3
0	0.000000	10.000000	0.000000	0.000000
1	0.050505	9.507491	0.480176	0.012332
2	0.101010	9.039239	0.913054	0.047707
3	0.151515	8.594049	1.302129	0.103823
4	0.202020	8.170784	1.650664	0.178552

```
[11]: # Eliminate the temporary files
      smtc.cleanUp()
```

3.2 Non-default arguments

```
[12]: WOLF_URL = "https://www.ebi.ac.uk/biomodels/services/download/get-files/
      ↪MODEL3352181362/3/BIOMD0000000206_url.xml"
```

```
[13]: smtc = ss.makeSingleModelTimeCourse(WOLF_URL, num_point=1000)
      _ = smtc.execute()
```

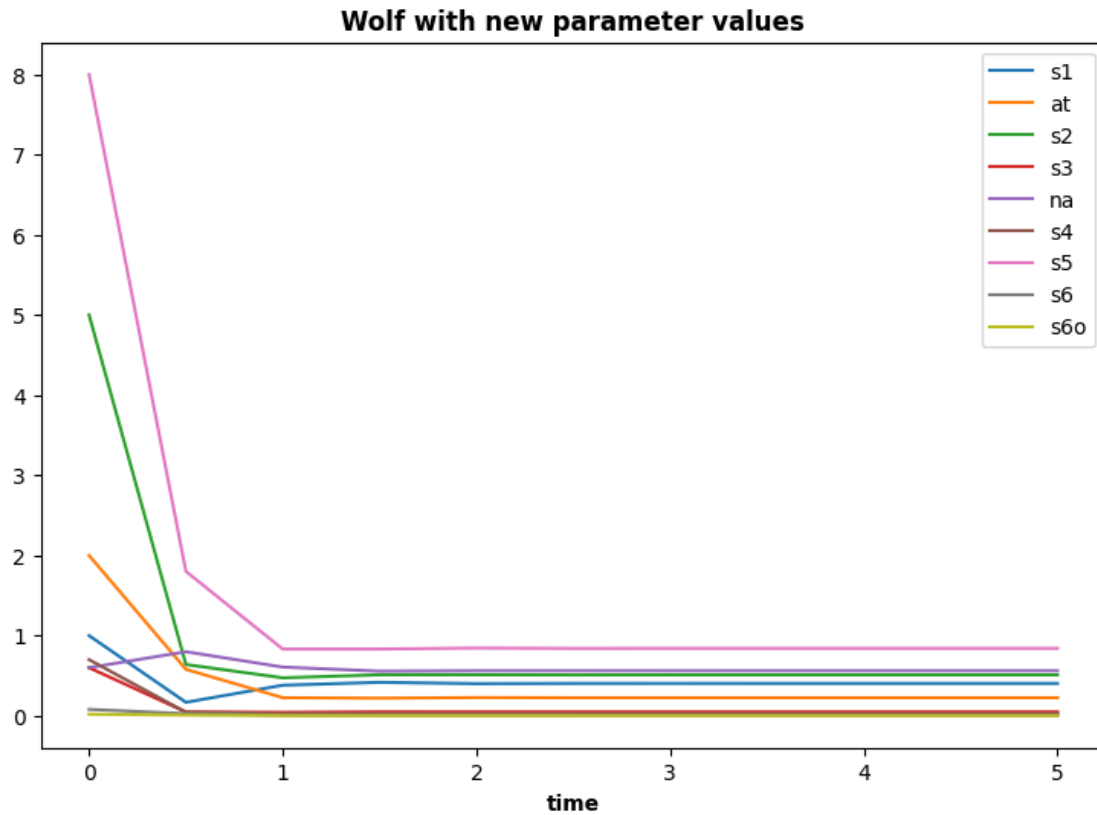


```
[14]: ss.getModelInformation(WOLF_URL)
```

```
[14]: Model: Wolf2000_Glycolytic_Oscillations
Parameters: {'k0': 50.0, 'k1': 550.0, 'k2': 9.8, 'k31': 323.8, 'k33': 57823.1,
            'k32': 76411.1, 'k34': 23.7, 'k4': 80.0, 'k5': 9.7, 'k6': 2000.0, 'k7': 28.0,
            'k8': 85.7, 'k9': 80.0, 'k10': 375.0, 'atot': 4.0, 'ntot': 1.0, 'n': 4.0, 'ki':
            1.0}
Floating Species: {'s1': 1.0, 'at': 2.0, 's2': 5.0, 's3': 0.6, 'na': 0.6, 's4':
            0.7, 's5': 8.0, 's6': 0.08, 's6o': 0.02}
```

Boundary Species: {}
 Number of Reactions: 11
 Number of Species: 9

```
[15]: smtc = ss.makeSingleModelTimeCourse(WOLF_URL, model_parameter_dct=dict(k0=5,
    ↪k1=55),
      title="Wolf with new parameter values")
df = smtc.execute()
```



```
[16]: df.head()
```

```
[16]:
```

	time	s1	at	s2	s3	na	s4	s5	\
0	0.0	1.000000	2.000000	5.000000	0.600000	0.600000	0.700000	8.000000	
1	0.5	0.167970	0.579162	0.639675	0.047800	0.799205	0.043673	1.801447	
2	1.0	0.381272	0.225642	0.473636	0.042924	0.607620	0.025901	0.832152	
3	1.5	0.417602	0.220384	0.511794	0.049333	0.556435	0.026954	0.832856	
4	2.0	0.400847	0.227533	0.511717	0.049070	0.561399	0.027128	0.845115	

	s6	s6o
0	0.080000	0.020000
1	0.026906	0.008861


```

2  0.007774  0.002500
3  0.007070  0.002255
4  0.007238  0.002310

```

```
[17]: smtc.cleanUp()
```

4 Use Case 2: Multiple Models Time Course

When comparing the time course simulation of multiple models, we want to compare selected **display variables** from the models, either in plots or in a DataFrame. This is done with the `MultipleModelTimeCourse` object.

```
[18]: mmtc = ss.makeMultipleModelTimeCourse([MODEL_ANT, MODEL2_ANT],
      ↪model_parameter_dct=dict(k1=10), num_point=100)
```

```
[19]: print(mmtc.getSEDML())
```

```

<?xml version="1.0" encoding="UTF-8"?>
<!-- Created by phraSED-ML version v1.3.0 with libSBML version 5.19.5. -->
<sedML xmlns="http://sed-ml.org/sed-ml/level1/version4"
xmlns:sbml="http://www.sbml.org/sbml/level3/version2/core" level="1"
version="4">
  <listOfModels>
    <model id="model0" language="urn:sedml:language:sbml:level-3.version-2" source="/var/folders/02/1b248q1j50dch2pthzkvxmpr0000gn/T/tmp5r3m1cv3/model0.xml">
      <listOfChanges>
        <changeAttribute target="/sbml:sbml/sbml:model/sbml:listOfParameters/sbml:parameter[@id='k1']/@value" newValue="10"/>
      </listOfChanges>
    </model>
    <model id="model1" language="urn:sedml:language:sbml:level-3.version-2" source="/var/folders/02/1b248q1j50dch2pthzkvxmpr0000gn/T/tmp5r3m1cv3/model1.xml">
      <listOfChanges>
        <changeAttribute target="/sbml:sbml/sbml:model/sbml:listOfParameters/sbml:parameter[@id='k1']/@value" newValue="10"/>
      </listOfChanges>
    </model>
  </listOfModels>
  <listOfSimulations>
    <uniformTimeCourse id="mmtc_sim1" initialTime="0" outputStartTime="0" outputEndTime="5" numberOfSteps="99">
      <algorithm name="CVODE" kisaoID="KISAO:0000019"/>
    </uniformTimeCourse>
  </listOfSimulations>
  <listOfTasks>
    <task id="tmodel0" modelReference="model0" simulationReference="mmtc_sim1"/>
    <task id="tmodel1" modelReference="model1" simulationReference="mmtc_sim1"/>
  </listOfTasks>
</sedML>

```

```

</listOfTasks>
<listOfDataGenerators>
  <dataGenerator id="report_0_0_0" name="time">
    <math xmlns="http://www.w3.org/1998/Math/MathML">
      <ci> tmodel0_____time </ci>
    </math>
    <listOfVariables>
      <variable id="tmodel0_____time" symbol="urn:sedml:symbol:time"
taskReference="tmodel0" modelReference="model0"/>
    </listOfVariables>
  </dataGenerator>
  <dataGenerator id="report_0_0_1" name="species1">
    <math xmlns="http://www.w3.org/1998/Math/MathML">
      <ci> tmodel0_____S1 </ci>
    </math>
    <listOfVariables>
      <variable id="tmodel0_____S1"
target="/sbml:sbml/sbml:model/sbml:listOfSpecies/sbml:species[@id='S1']"
taskReference="tmodel0" modelReference="model0"/>
    </listOfVariables>
  </dataGenerator>
  <dataGenerator id="report_0_0_2" name="species1">
    <math xmlns="http://www.w3.org/1998/Math/MathML">
      <ci> tmodel1_____S1 </ci>
    </math>
    <listOfVariables>
      <variable id="tmodel1_____S1"
target="/sbml:sbml/sbml:model/sbml:listOfSpecies/sbml:species[@id='S1']"
taskReference="tmodel1" modelReference="model1"/>
    </listOfVariables>
  </dataGenerator>
  <dataGenerator id="report_0_0_3" name="species2">
    <math xmlns="http://www.w3.org/1998/Math/MathML">
      <ci> tmodel0_____S2 </ci>
    </math>
    <listOfVariables>
      <variable id="tmodel0_____S2"
target="/sbml:sbml/sbml:model/sbml:listOfSpecies/sbml:species[@id='S2']"
taskReference="tmodel0" modelReference="model0"/>
    </listOfVariables>
  </dataGenerator>
  <dataGenerator id="report_0_0_4" name="species2">
    <math xmlns="http://www.w3.org/1998/Math/MathML">
      <ci> tmodel1_____S2 </ci>
    </math>
    <listOfVariables>
      <variable id="tmodel1_____S2"
target="/sbml:sbml/sbml:model/sbml:listOfSpecies/sbml:species[@id='S2']"

```

```

taskReference="tmodel1" modelReference="model1"/>
  </listOfVariables>
</dataGenerator>
<dataGenerator id="report_0_0_5" name="S3">
  <math xmlns="http://www.w3.org/1998/Math/MathML">
    <ci> tmodel0_____S3 </ci>
  </math>
  <listOfVariables>
    <variable id="tmodel0_____S3"
target="/sbml:sbml/sbml:model/sbml:listOfSpecies/sbml:species[@id='S3']"
taskReference="tmodel0" modelReference="model0"/>
  </listOfVariables>
</dataGenerator>
<dataGenerator id="report_0_0_6" name="S3">
  <math xmlns="http://www.w3.org/1998/Math/MathML">
    <ci> tmodel1_____S3 </ci>
  </math>
  <listOfVariables>
    <variable id="tmodel1_____S3"
target="/sbml:sbml/sbml:model/sbml:listOfSpecies/sbml:species[@id='S3']"
taskReference="tmodel1" modelReference="model1"/>
  </listOfVariables>
</dataGenerator>
</listOfDataGenerators>
<listOfOutputs>
  <report id="report_0">
    <listOfDataSets>
      <dataSet id="report_0_0_0_dataset" label="tmodel0.time"
dataReference="report_0_0_0"/>
      <dataSet id="report_0_0_1_dataset" label="tmodel0.S1"
dataReference="report_0_0_1"/>
      <dataSet id="report_0_0_2_dataset" label="tmodel1.S1"
dataReference="report_0_0_2"/>
      <dataSet id="report_0_0_3_dataset" label="tmodel0.S2"
dataReference="report_0_0_3"/>
      <dataSet id="report_0_0_4_dataset" label="tmodel1.S2"
dataReference="report_0_0_4"/>
      <dataSet id="report_0_0_5_dataset" label="tmodel0.S3"
dataReference="report_0_0_5"/>
      <dataSet id="report_0_0_6_dataset" label="tmodel1.S3"
dataReference="report_0_0_6"/>
    </listOfDataSets>
  </report>
  <plot2D id="plot_1" name="species1">
    <listOfCurves>
      <curve id="plot_1__report_0_0_0__report_0_0_1" logX="false"
xDataReference="report_0_0_0" logY="false" yDataReference="report_0_0_1"/>
      <curve id="plot_1__report_0_0_0__report_0_0_2" logX="false"

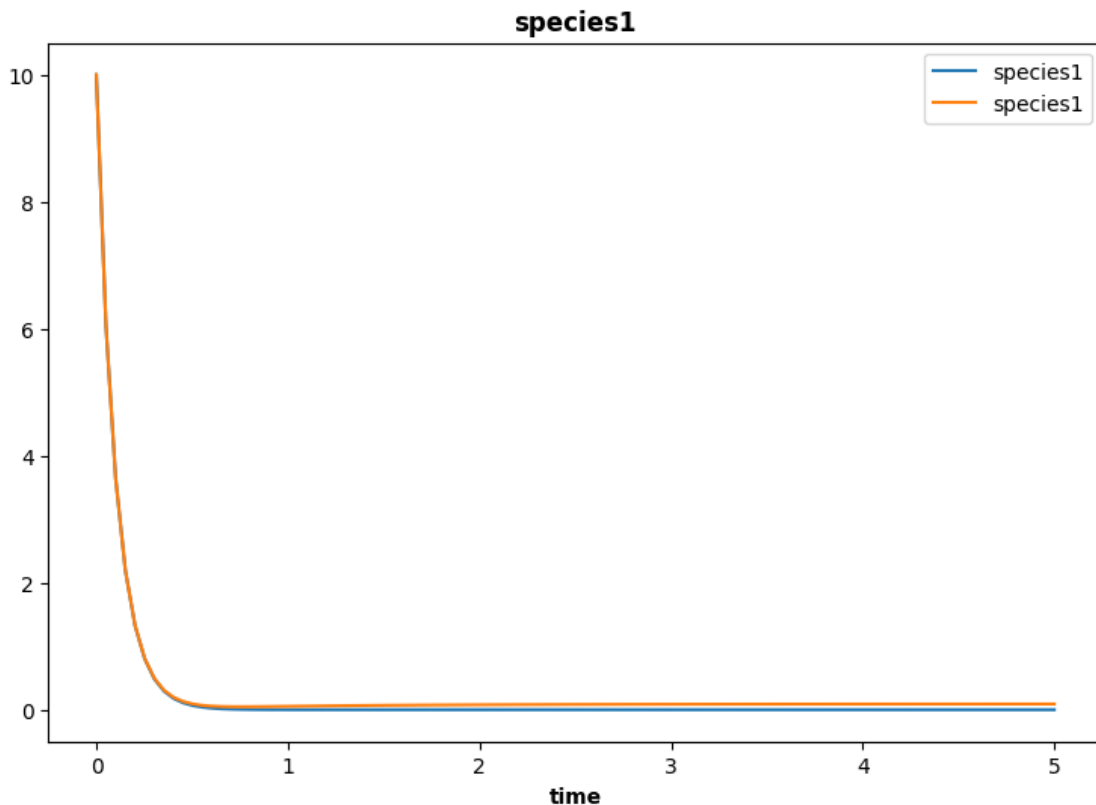
```

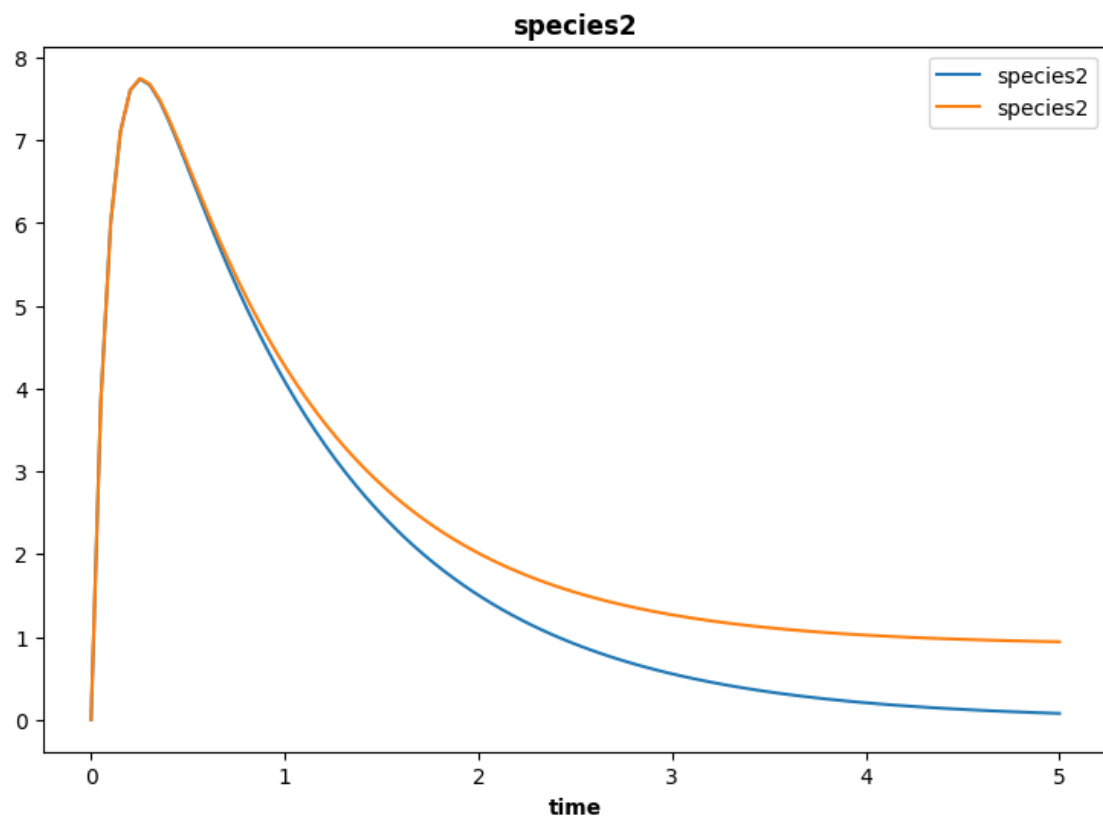
```

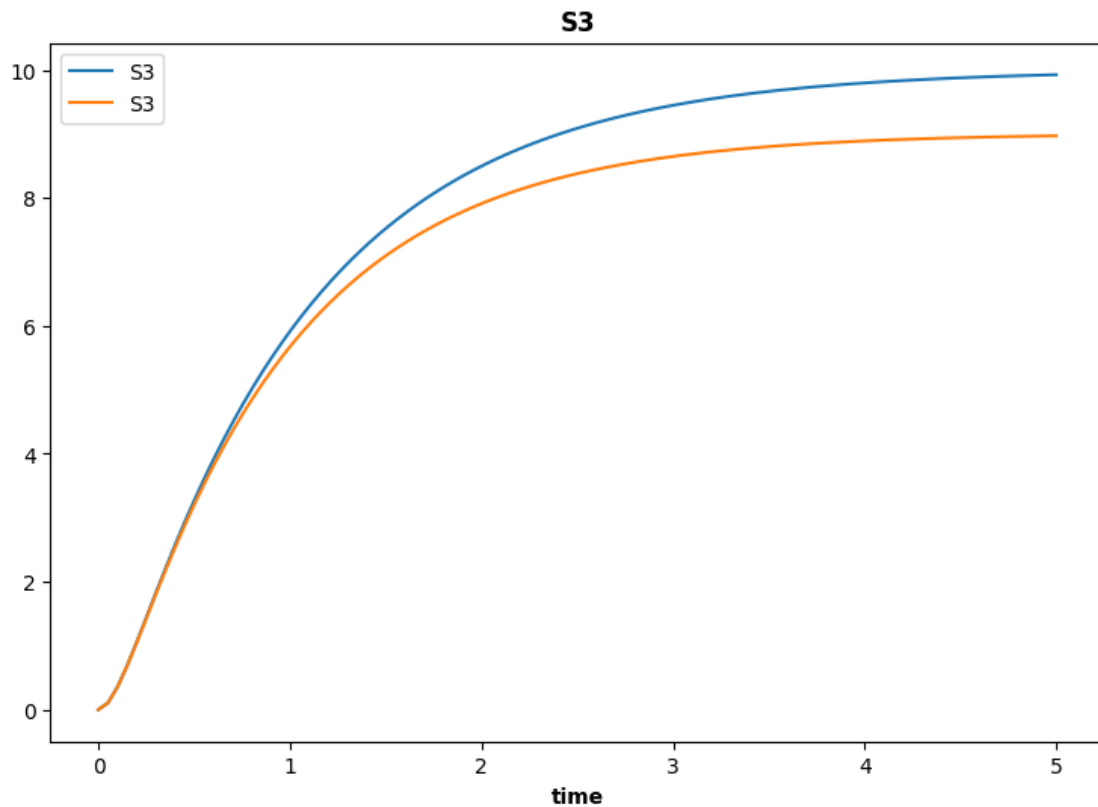
xDataReference="report_0_0_0" logY="false" yDataReference="report_0_0_2"/>
  </listOfCurves>
</plot2D>
<plot2D id="plot_2" name="species2">
  <listOfCurves>
    <curve id="plot_2__report_0_0_0__report_0_0_3" logX="false"
xDataReference="report_0_0_0" logY="false" yDataReference="report_0_0_3"/>
    <curve id="plot_2__report_0_0_0__report_0_0_4" logX="false"
xDataReference="report_0_0_0" logY="false" yDataReference="report_0_0_4"/>
  </listOfCurves>
</plot2D>
<plot2D id="plot_3" name="S3">
  <listOfCurves>
    <curve id="plot_3__report_0_0_0__report_0_0_5" logX="false"
xDataReference="report_0_0_0" logY="false" yDataReference="report_0_0_5"/>
    <curve id="plot_3__report_0_0_0__report_0_0_6" logX="false"
xDataReference="report_0_0_0" logY="false" yDataReference="report_0_0_6"/>
  </listOfCurves>
</plot2D>
</listOfOutputs>
</sedML>

```

[20]: `mmtc.execute()`







```
[20]:      tmodel0.time    tmodel0.S1  tmodel1.S1  tmodel0.S2  tmodel1.S2  \
0      0.000000  1.000000e+01  10.000000   0.000000   0.000000
1      0.050505  6.034751e+00   6.034912   3.858601   3.858627
2      0.101010  3.641824e+00   3.642859   5.997128   5.997406
3      0.151515  2.197752e+00   2.200499   7.106996   7.108161
4      0.202020  1.326293e+00   1.331475   7.604990   7.608033
..      ...
95     4.797980 -6.086515e-14   0.089539   0.091627   0.950471
96     4.848485  2.622485e-14   0.089569   0.087114   0.947766
97     4.898990  5.909949e-14   0.089597   0.082824   0.945208
98     4.949495  7.401011e-14   0.089624   0.078745   0.942790
99     5.000000  4.876985e-14   0.089650   0.074866   0.940504

      tmodel0.S3  tmodel1.S3
0      0.000000   0.000000
1      0.106649   0.106461
2      0.361048   0.359735
3      0.695252   0.691340
4      1.068717   1.060492
..      ...
95     9.908373   8.959990
```

96	9.912886	8.962665
97	9.917176	8.965194
98	9.921255	8.967585
99	9.925133	8.969846

[100 rows x 7 columns]

```
[21]: mmtc.model_dct
```

```
[21]: {'model0': <SimpleSEDML.model.Model at 0x14ece9f10>,
      'model1': <SimpleSEDML.model.Model at 0x14e9c7d00>,
      'model2': <SimpleSEDML.model.Model at 0x14ed5c7c0>,
      'model3': <SimpleSEDML.model.Model at 0x14e9c7ac0>,
      'model4': <SimpleSEDML.model.Model at 0x14ea11400>,
      'model5': <SimpleSEDML.model.Model at 0x14ed0c2b0>}
```

```
[22]: print(mmtc.getPhraSEDML())
```

```
model0 = model
"/var/folders/02/lb248q1j50dch2pthzkvxmpr0000gn/T/tmp5r3m1cv3/model0.xml" with
k1 = 10
model1 = model
"/var/folders/02/lb248q1j50dch2pthzkvxmpr0000gn/T/tmp5r3m1cv3/model1.xml" with
k1 = 10
model2 = model
"/var/folders/02/lb248q1j50dch2pthzkvxmpr0000gn/T/tmp5r3m1cv3/model2.xml" with
k1 = 10
model3 = model
"/var/folders/02/lb248q1j50dch2pthzkvxmpr0000gn/T/tmp5r3m1cv3/model3.xml" with
k1 = 10
model4 = model
"/var/folders/02/lb248q1j50dch2pthzkvxmpr0000gn/T/tmp5r3m1cv3/model4.xml" with
k1 = 10
model5 = model
"/var/folders/02/lb248q1j50dch2pthzkvxmpr0000gn/T/tmp5r3m1cv3/model5.xml" with
k1 = 10
model6 = model
"/var/folders/02/lb248q1j50dch2pthzkvxmpr0000gn/T/tmp5r3m1cv3/model6.xml" with
k1 = 10
model7 = model
"/var/folders/02/lb248q1j50dch2pthzkvxmpr0000gn/T/tmp5r3m1cv3/model7.xml" with
k1 = 10
mmtc_sim1 = simulate uniform(0.0, 5.0, 99)
mmtc_sim1.algorithm = CVODE
tmodel0 = run mmtc_sim1 on model0
tmodel1 = run mmtc_sim1 on model1
tmodel2 = run mmtc_sim1 on model2
```

```

tmodel3 = run mmtc_sim1 on model3
tmodel4 = run mmtc_sim1 on model4
tmodel5 = run mmtc_sim1 on model5
tmodel6 = run mmtc_sim1 on model6
tmodel7 = run mmtc_sim1 on model7
report tmodel0.time, tmodel0.S1, tmodel1.S1, tmodel0.S2, tmodel1.S2, tmodel0.S3,
tmodel1.S3
plot "species1" tmodel0.time vs tmodel0.S1, tmodel1.S1
plot "species2" tmodel0.time vs tmodel0.S2, tmodel1.S2
plot "S3" tmodel0.time vs tmodel0.S3, tmodel1.S3

```

4.1 Creating an OMEX file

We can create an OMEX file for this experiment.

```
[23]: omex_path, _ = mmtc.makeOMEXFile()
      omex_path
```

```
[23]: '/Users/jlheller/home/Technical/repos/SimpleSEDML/examples/project.omex'
```

```
[24]: # We can examine the content of the OMEX file.
      !unzip -l project.omex
```

```

Archive:  project.omex
  Length      Date    Time    Name
-----
  1096  06-02-2025  17:41  metadata.rdf
  2262  06-02-2025  17:41  model0.xml
  2845  06-02-2025  17:41  model1.xml
  2262  06-02-2025  17:41  model2.xml
  2845  06-02-2025  17:41  model3.xml
  2262  06-02-2025  17:41  model4.xml
  2845  06-02-2025  17:41  model5.xml
  2262  06-02-2025  17:41  model6.xml
  2845  06-02-2025  17:41  model7.xml
  2262  06-02-2025  17:41  model8.xml
  2845  06-02-2025  17:41  model9.xml
  8831  06-02-2025  17:41  project.sedml
  1464  06-02-2025  17:41  manifest.xml
-----
 36926                                13 files

```

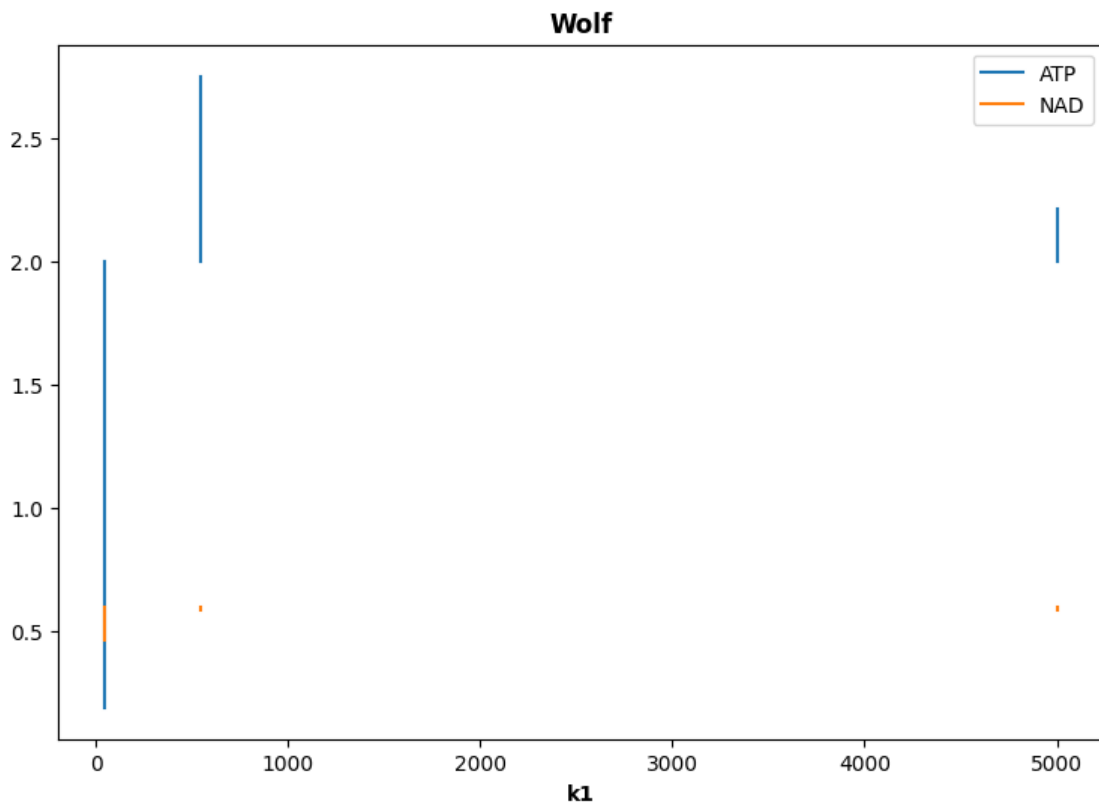
```
[25]: mmtc.cleanUp()
```


5 Use Case 3: Single Model Parameter Scan

```
[26]: smps = ss.makeSingleModelParameterScan(WOLF_URL, simulation_type="onestep",
                                             project_id="Wolf", title="Wolf",
                                             time_interval=10, display_variables=["at", "na"],
                                             scan_parameter_dct=dict(k1=[50, 550, 5000]))
print(smps.getPhraSEDML())
_ = smps.execute()
```

```
md_Wolf = model
"/var/folders/02/lb248q1j50dch2pthzkvxmpr0000gn/T/tmpf7299ulr/md_Wolf.xml"
si_Wolf = simulate onestep(10)
st_Wolf = run si_Wolf on md_Wolf
repeated_taskWolf = repeat st_Wolf for k1 in [50, 550, 5000], reset=true
report repeated_taskWolf.k1, repeated_taskWolf.at, repeated_taskWolf.na
plot "Wolf" repeated_taskWolf.k1 vs repeated_taskWolf.at, repeated_taskWolf.na
/Users/jlheller/home/Technical/repos/SimpleSEDML/src/SimpleSEDML/simple_sedml.py
:386: UserWarning:
```

Reports only generate data for the last repeated task.

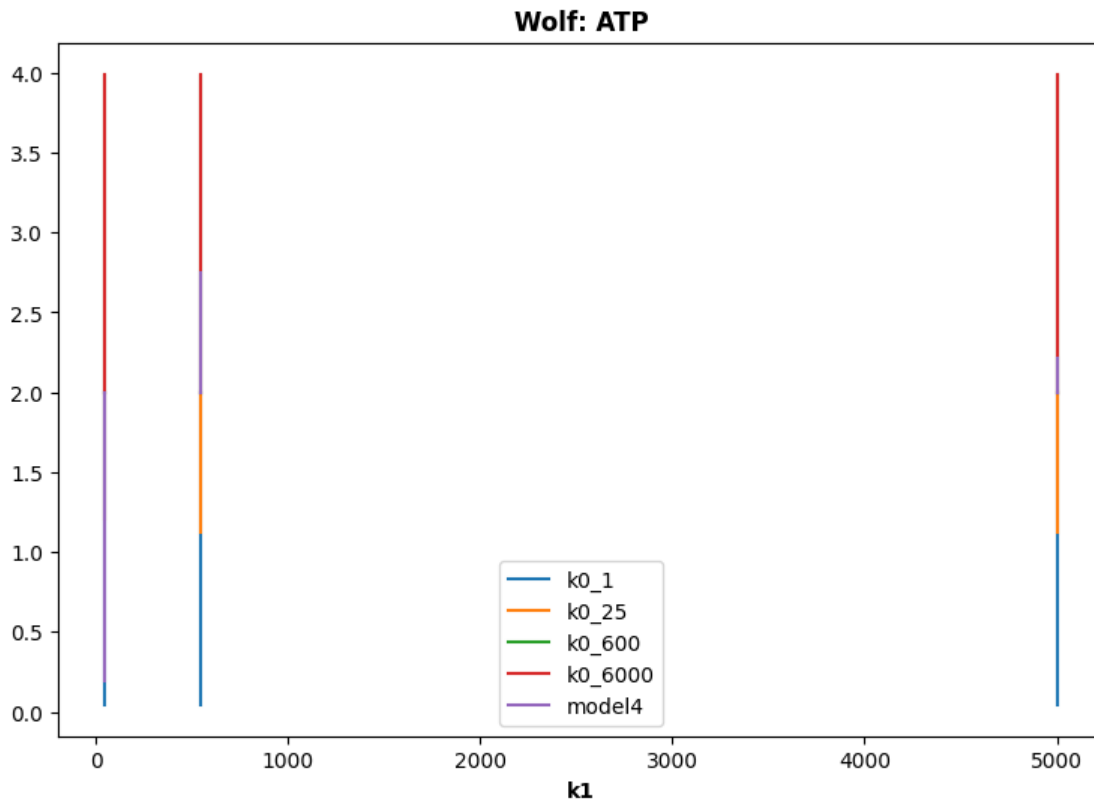


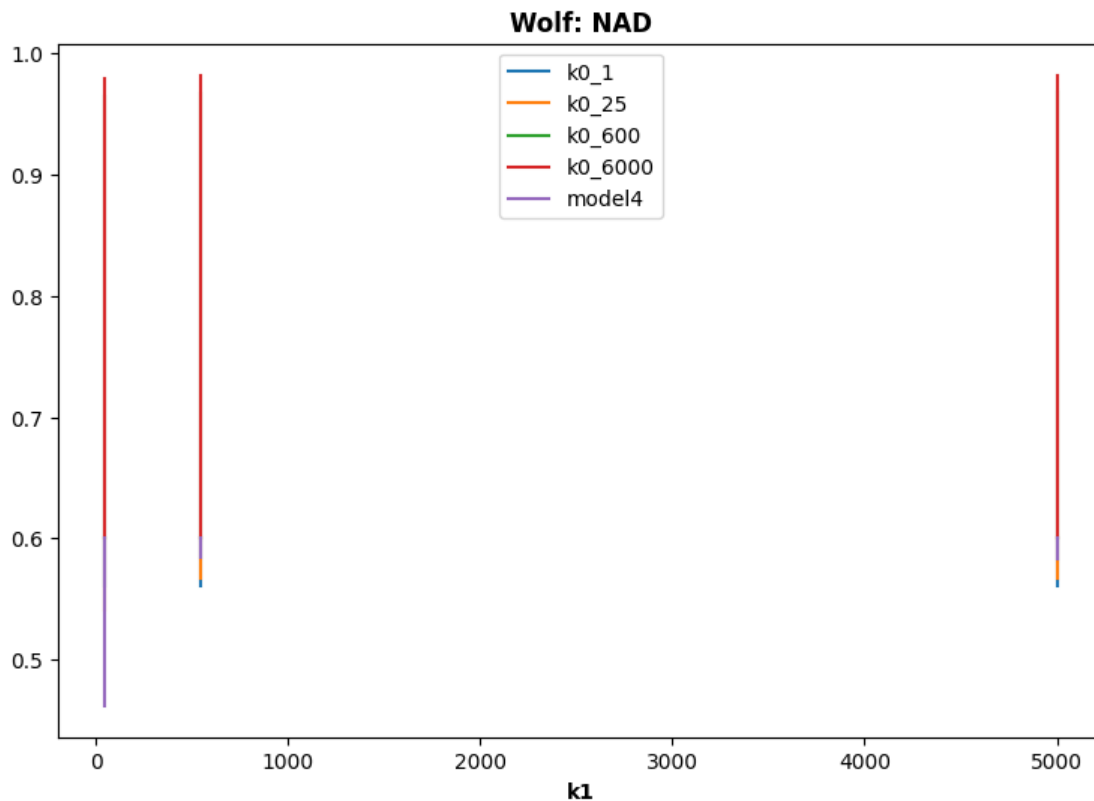
6 Use Case 4: Multiple Model Parameter Scan

```
[35]: mmps = ss.makeMultipleModelParameterScan([WOLF_URL], simulation_type="onestep",  
                                              project_id="Wolf", title="Wolf",  
                                              time_interval=10, display_variables=['at', 'na'], scan_parameter_df=pd.  
↳ DataFrame(dict(k1=[50, 550, 5000])))
```

```
[36]: # We create additional models and they will be included in the simulations,   
↳ plots and reports  
_ = mmps.addModel("k0_1", WOLF_URL, parameter_dct=dict(k0=1))  
_ = mmps.addModel("k0_25", WOLF_URL, parameter_dct=dict(k0=25))  
_ = mmps.addModel("k0_600", WOLF_URL, parameter_dct=dict(k0=600))  
_ = mmps.addModel("k0_6000", WOLF_URL, parameter_dct=dict(k0=6000))
```

```
[37]: #print(smeps.getPhraSEDML())  
_ = mmps.execute()
```





7 Low Level API

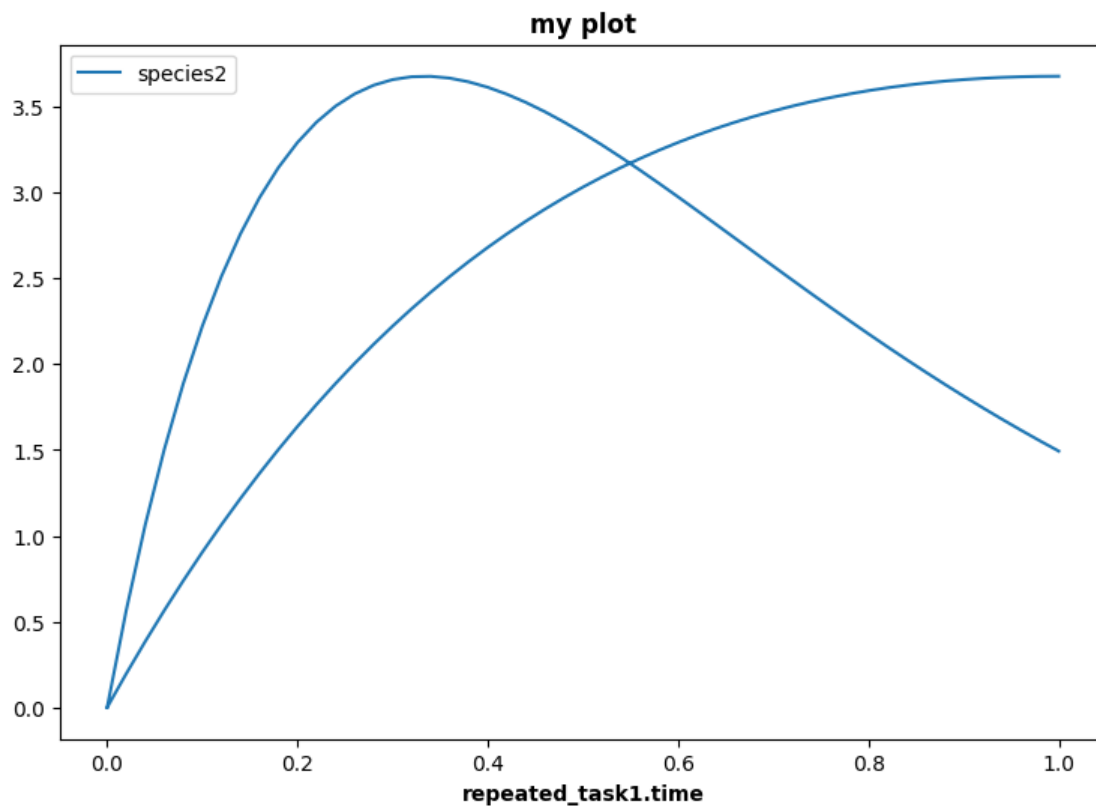
Below, we illustrate use of the low level API in isolation.

```
[30]: # Make DataFrame of changes to model parameters
parameter_df = pd.DataFrame(dict(k1=[1, 3], k2=[1, 3]))
```

```
[31]: ssed = ss.SimpleSEDML()
ssed.addModel("model1", MODEL_ANT, parameter_dct=dict(k1=3),
             ref_type="ant_str", is_overwrite=True)
ssed.addSimulation("sim1", "uniform", start=0, end=1, num_step=50)
ssed.addTask("task1", "model1", "sim1")
ssed.addRepeatedTask("repeated_task1", "task1", parameter_df=parameter_df)
ssed.addReport("task1.time", "task1.S1", "task1.S2", "task1.S3")
ssed.addPlot("repeated_task1.time", "repeated_task1.S2", title="my plot")
result_df = ssed.execute()
```

```
/Users/jlheller/home/Technical/repos/SimpleSEDML/src/SimpleSEDML/simple_sedml.py
:386: UserWarning:
```

Reports only generate data for the last repeated task.



```
[32]: print(ssed.getSEDML())
```

```
<?xml version="1.0" encoding="UTF-8"?>
<!-- Created by phraSED-ML version v1.3.0 with libSBML version 5.19.5. -->
<sedML xmlns="http://sed-ml.org/sed-ml/level1/version4"
xmlns:sbml="http://www.sbml.org/sbml/level3/version2/core" level="1"
version="4">
  <listOfModels>
    <model id="model1" language="urn:sedml:language:sbml.level-3.version-2" source="/var/folders/02/lb248q1j50dch2pthzkvxmpr0000gn/T/tmp84qqrlw4/model1.xml">
      <listOfChanges>
        <changeAttribute target="/sbml:sbml/sbml:model/sbml:listOfParameters/sbml:parameter[@id='k1']/@value" newValue="3"/>
      </listOfChanges>
    </model>
  </listOfModels>
  <listOfSimulations>
    <uniformTimeCourse id="sim1" initialTime="0" outputStartTime="0" outputEndTime="1" numberOfSteps="50">
      <algorithm name="CVODE" kisaoID="KISA0:0000019"/>
    </uniformTimeCourse>
  </listOfSimulations>
</sedML>
```

```

    </uniformTimeCourse>
</listOfSimulations>
<listOfTasks>
  <task id="task1" modelReference="model1" simulationReference="sim1"/>
  <repeatedTask id="repeated_task1" range="vector_for_k2" resetModel="true">
    <listOfRanges>
      <vectorRange id="vector_for_k1">
        <value> 1 </value>
        <value> 3 </value>
      </vectorRange>
      <vectorRange id="vector_for_k2">
        <value> 1 </value>
        <value> 3 </value>
      </vectorRange>
    </listOfRanges>
    <listOfChanges>
      <setValue modelReference="model1"
target="/sbml:sbml/sbml:model/sbml:listOfParameters/sbml:parameter[@id='k1']"
range="vector_for_k1">
        <math xmlns="http://www.w3.org/1998/Math/MathML">
          <ci> vector_for_k1 </ci>
        </math>
      </setValue>
      <setValue modelReference="model1"
target="/sbml:sbml/sbml:model/sbml:listOfParameters/sbml:parameter[@id='k2']"
range="vector_for_k2">
        <math xmlns="http://www.w3.org/1998/Math/MathML">
          <ci> vector_for_k2 </ci>
        </math>
      </setValue>
    </listOfChanges>
    <listOfSubTasks>
      <subTask order="0" task="task1"/>
    </listOfSubTasks>
  </repeatedTask>
</listOfTasks>
<listOfDataGenerators>
  <dataGenerator id="report_0_0_0" name="task1.time">
    <math xmlns="http://www.w3.org/1998/Math/MathML">
      <ci> task1_____time </ci>
    </math>
    <listOfVariables>
      <variable id="task1_____time" symbol="urn:sedml:symbol:time"
taskReference="task1" modelReference="model1"/>
    </listOfVariables>
  </dataGenerator>
  <dataGenerator id="report_0_0_1" name="species1">
    <math xmlns="http://www.w3.org/1998/Math/MathML">

```

```

        <ci> task1_____S1 </ci>
    </math>
    <listOfVariables>
        <variable id="task1_____S1"
target="/sbml:sbml/sbml:model/sbml:listOfSpecies/sbml:species[@id='S1']"
taskReference="task1" modelReference="model1"/>
    </listOfVariables>
</dataGenerator>
<dataGenerator id="report_0_0_2" name="species2">
    <math xmlns="http://www.w3.org/1998/Math/MathML">
        <ci> task1_____S2 </ci>
    </math>
    <listOfVariables>
        <variable id="task1_____S2"
target="/sbml:sbml/sbml:model/sbml:listOfSpecies/sbml:species[@id='S2']"
taskReference="task1" modelReference="model1"/>
    </listOfVariables>
</dataGenerator>
<dataGenerator id="report_0_0_3" name="S3">
    <math xmlns="http://www.w3.org/1998/Math/MathML">
        <ci> task1_____S3 </ci>
    </math>
    <listOfVariables>
        <variable id="task1_____S3"
target="/sbml:sbml/sbml:model/sbml:listOfSpecies/sbml:species[@id='S3']"
taskReference="task1" modelReference="model1"/>
    </listOfVariables>
</dataGenerator>
<dataGenerator id="plot_1_0_0" name="repeated_task1.time">
    <math xmlns="http://www.w3.org/1998/Math/MathML">
        <ci> repeated_task1_____time </ci>
    </math>
    <listOfVariables>
        <variable id="repeated_task1_____time" symbol="urn:sedml:symbol:time"
taskReference="repeated_task1" modelReference="model1"/>
    </listOfVariables>
</dataGenerator>
<dataGenerator id="plot_1_0_1" name="species2">
    <math xmlns="http://www.w3.org/1998/Math/MathML">
        <ci> repeated_task1_____S2 </ci>
    </math>
    <listOfVariables>
        <variable id="repeated_task1_____S2"
target="/sbml:sbml/sbml:model/sbml:listOfSpecies/sbml:species[@id='S2']"
taskReference="repeated_task1" modelReference="model1"/>
    </listOfVariables>
</dataGenerator>
</listOfDataGenerators>

```

```

<listOfOutputs>
  <report id="report_0">
    <listOfDataSets>
      <dataSet id="report_0_0_0_dataset" label="task1.time"
dataReference="report_0_0_0"/>
      <dataSet id="report_0_0_1_dataset" label="task1.S1"
dataReference="report_0_0_1"/>
      <dataSet id="report_0_0_2_dataset" label="task1.S2"
dataReference="report_0_0_2"/>
      <dataSet id="report_0_0_3_dataset" label="task1.S3"
dataReference="report_0_0_3"/>
    </listOfDataSets>
  </report>
  <plot2D id="plot_1" name="my plot">
    <listOfCurves>
      <curve id="plot_1__plot_1_0_0__plot_1_0_1" logX="false"
xDataReference="plot_1_0_0" logY="false" yDataReference="plot_1_0_1"/>
    </listOfCurves>
  </plot2D>
</listOfOutputs>
</sedML>

```

```
[33]: ssed.cleanUp()
```

8 Cleanup

```

[34]: import os
EXAMPLE_REMOVE_FILES = ["simple_sedml_plot.png", "project.omex", "project.omex"]
example_dir = os.getcwd()
remove_files = [os.path.join(example_dir, f) for f in EXAMPLE_REMOVE_FILES]
for ffile in remove_files:
    if os.path.isfile(ffile):
        os.remove(ffile)

```