modules_complete

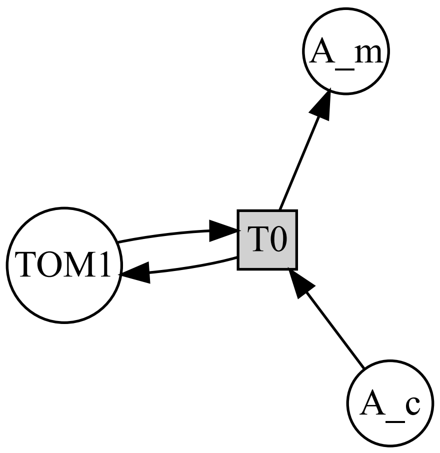
February 27, 2018

0.1 Advanced topic - Antimony modules!

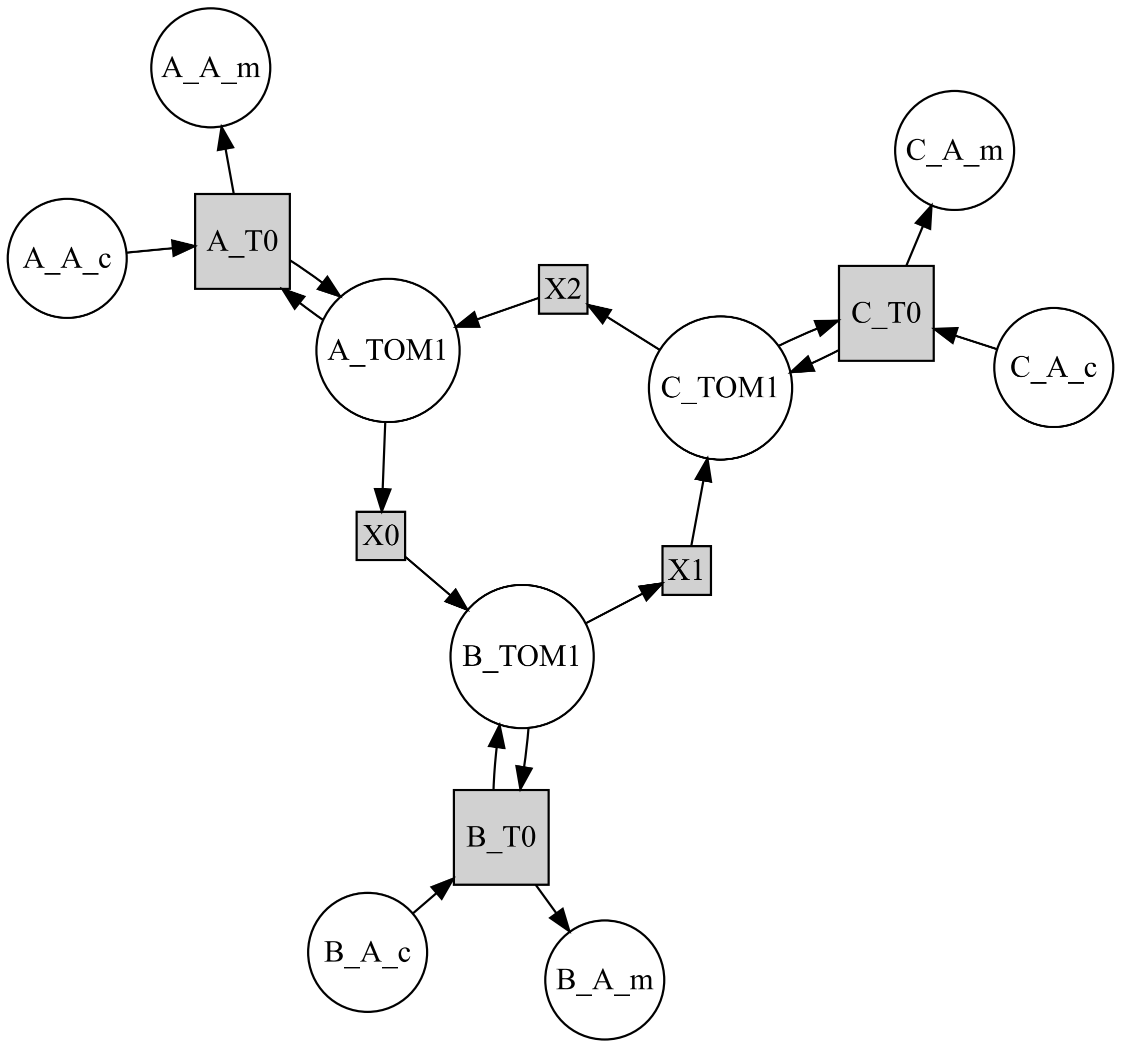
0.1.1 A minimal example:

```
In [1]: import tellurium as te;
        #import tellurium as te; te.setDefaultPlottingEngine('matplotlib')
        #import matplotlib.pyplot as plt
        #%matplotlib inline

        class Diagram(te.visualization.SBMLDiagram):
            def draw(self, layout='neato', file='graph.svg', **kwargs):
                """ Draw the graph.
                Optional layout=['neato'|'dot'|'twopi'|'circo'|'fdp'|'nop']
                will use specified graphviz layout method.
                :param layout: pygraphviz layout algorithm (default: 'neato')
                :type layout: str
                """
                self.g.write('test.dot')
                self.g.layout(prog=layout)
                self.g.draw(file)
                from IPython.display import SVG
                return SVG(file)


        r = te.loada('example.antimony')
        diagram = Diagram(r.getSBML())
        diagram.draw()
```

```
Out[1]:
```



```
In [121]: model_circle = '''
          import "example.antimony"

          model circle
              A: example()
              B: example()
              C: example()

              X0: A.TOM1 -> B.TOM1;
              X1: B.TOM1 -> C.TOM1;
              X2: C.TOM1 ->  A.TOM1;
          end

          '''

          circle = te.loada(model_circle)
          diagram = Diagram(circle.getSBML())
          diagram.draw()

Out[121]:
```



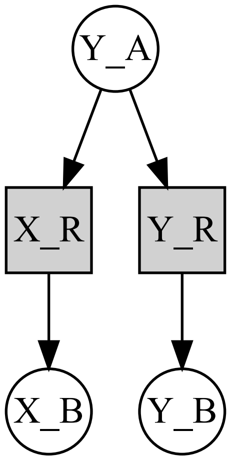
```
In [122]: circle = te.loada(model_circle)
          print(circle.getAntimony())

// Created by libAntimony v2.9.4
model *circle()

  // Compartments and Species:
  compartment A_cell, A_mitochondria, B_cell, B_mitochondria, C_cell, C_mitochondri
  species A_TOM1 in A_cell, A_A_c in A_cell, A_A_m in A_mitochondria, B_TOM1 in B_c
  species B_A_c in B_cell, B_A_m in B_mitochondria, C_TOM1 in C_cell, C_A_c in C_ce
  species C_A_m in C_mitochondria;

  // Assignment Rules:
  A_kineticLaw := A_k1*A_TOM1*(A_A_c - A_A_m)/A_I;
  B_kineticLaw := B_k1*B_TOM1*(B_A_c - B_A_m)/B_I;
  C_kineticLaw := C_k1*C_TOM1*(C_A_c - C_A_m)/C_I;

  // Reactions:
  A_T0: A_A_c + A_TOM1 -> 2 A_A_m + A_TOM1; A_kineticLaw;
  B_T0: B_A_c + B_TOM1 -> 2 B_A_m + B_TOM1; B_kineticLaw;
  C_T0: C_A_c + C_TOM1 -> 2 C_A_m + C_TOM1; C_kineticLaw;
  X0: A_TOM1 -> B_TOM1; ;
  X1: B_TOM1 -> C_TOM1; ;
  X2: C_TOM1 -> A_TOM1; ;

  // Species initializations:
  A_TOM1 = 10;
  A_A_c = 100;
  A_A_m = 1;
  B_TOM1 = 10;
  B_A_c = 100;
  B_A_m = 1;
  C_TOM1 = 10;
  C_A_c = 100;
  C_A_m = 1;

  // Compartment initializations:
  A_cell = 100;
  A_mitochondria = 10;
  B_cell = 100;
  B_mitochondria = 10;
  C_cell = 100;
  C_mitochondria = 10;

  // Variable initializations:
  A_I = 1;
  A_k1 = 0.01;
  B_I = 1;
  B_k1 = 0.01;
  C_I = 1;
  C_k1 = 0.01;

  // Other declarations:
  var A_kineticLaw, B_kineticLaw, C_kineticLaw;
  const A_cell, A_mitochondria, B_cell, B_mitochondria, C_cell, C_mitochondria;
  const A_I, A_k1, B_I, B_k1, C_I, C_k1;
end
```

```
In [168]: model_is = '''

          model simple
```

```
    R: A -> B; 0.1;
end

model reactions
    X: simple();
    Y: simple();

    X.A is Y.A;
end

'''

mapk = te.loada(model_is)
print(mapk.getAntimony())
diagram = Diagram(mapk.getSBML())

diagram.draw(layout='dot')
```

```
// Created by libAntimony v2.9.4
model *reactions()

  // Compartments and Species:
  species Y_A, X_B, Y_B;

  // Reactions:
  X_R: Y_A -> X_B; 0.1;
  Y_R: Y_A -> Y_B; 0.1;

  // Species initializations:
  Y_A = ;
  X_B = ;
  Y_B = ;
end
```

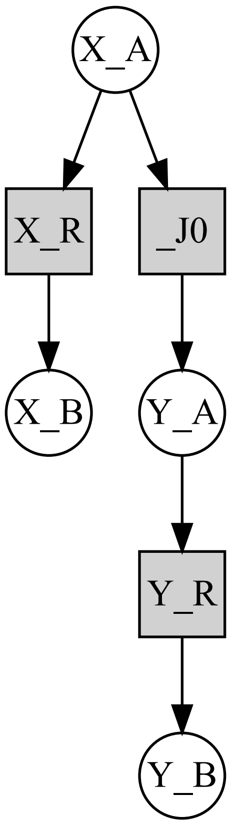
Out[168]:



```
In [176]: model_is = '''

          model simple
              R: A -> B; 0.1;
          end

          model reactions
              X: simple();
              Y: simple();

              X.A -> Y.A; ;
          end

          '''

          mapk = te.loada(model_is)
          print(mapk.getAntimony())
          diagram = Diagram(mapk.getSBML())

          diagram.draw(layout='dot')
```

```
// Created by libAntimony v2.9.4
model *reactions()

  // Compartments and Species:
  species X_A, X_B, Y_A, Y_B;

  // Reactions:
  X_R: X_A -> X_B; 0.1;
  Y_R: Y_A -> Y_B; 0.1;
  _J0: X_A -> Y_A; ;
  // Species initializations:
  X_A = ;
  X_B = ;
  Y_A = ;
  Y_B = ;
end
```

Out[176]:



0.2 Arrays of model instances?

```
In [172]: multi_comp = '''

          model cell
          #some stuff
          end

          model mitochondria
```

```
#some stuff
end

model nucleus
#some stuff
end

c0: cell();
n0: nucleus();
m0: mitchondria();
m1: mitchondria();
m2: mitchondria();
m3: mitchondria();
m4: mitchondria();
m5: mitchondria();

m1, m2, m3, m4, m5 in c0.cytosol;
nucleus in c0.cytosol;

'''
```

Consider an antimony model 'multi_comp' within Python you could do this:

```
In [174]: for i in range(6):
              multi_comp = multi_comp + "m%s: mitchondria();\n" % (i)

In [175]: print(multi_comp)



model cell
#some stuff
end

model mitochondria
#some stuff
end

model nucleus
#some stuff
end

c0: cell();
n0: nucleus();
m0: mitchondria();
m1: mitchondria();
m2: mitchondria();
m3: mitchondria();
m4: mitchondria();
```

```
m5: mitchondria();

m1, m2, m3, m4, m5 in c0.cytosol;
nucleus in c0.cytosol;

m0: mitchondria();
m1: mitchondria();
m2: mitchondria();
m3: mitchondria();
m4: mitchondria();
m5: mitchondria();
```

0.3 Deletions: delete species in submodels

```
In [125]: model_circle = '''
          import "example.antimony"

          model circle
              A: example()
              B: example()
              C: example()

              X0: A.TOM1 -> B.TOM1;
              X1: B.TOM1 -> C.TOM1;
              X2: C.TOM1 ->  A.TOM1;

              delete C.A_m
              C.kineticLaw := 0.1;

          end

          '''

          circle = te.loada(model_circle)
          print(circle.getAntimony())
```

```
// Created by libAntimony v2.9.4
model *circle()

  // Compartments and Species:
  compartment A_cell, A_mitochondria, B_cell, B_mitochondria, C_cell, C_mitochondri
  species A_TOM1 in A_cell, A_A_c in A_cell, A_A_m in A_mitochondria, B_TOM1 in B_c
  species B_A_c in B_cell, B_A_m in B_mitochondria, C_TOM1 in C_cell, C_A_c in C_ce

  // Assignment Rules:
  A_kineticLaw := A_k1*A_TOM1*(A_A_c - A_A_m)/A_I;
  B_kineticLaw := B_k1*B_TOM1*(B_A_c - B_A_m)/B_I;
  C_kineticLaw := 0.1;

  // Reactions:
  A_T0: A_A_c + A_TOM1 -> 2 A_A_m + A_TOM1; A_kineticLaw;
  B_T0: B_A_c + B_TOM1 -> 2 B_A_m + B_TOM1; B_kineticLaw;
  C_T0: C_A_c + C_TOM1 -> C_TOM1; ;
  X0: A_TOM1 -> B_TOM1; ;
  X1: B_TOM1 -> C_TOM1; ;
  X2: C_TOM1 -> A_TOM1; ;

  // Species initializations:
  A_TOM1 = 10;
  A_A_c = 100;
  A_A_m = 1;
  B_TOM1 = 10;
  B_A_c = 100;
  B_A_m = 1;
  C_TOM1 = 10;
  C_A_c = 100;

  // Compartment initializations:
  A_cell = 100;
  A_mitochondria = 10;
  B_cell = 100;
  B_mitochondria = 10;
  C_cell = 100;
  C_mitochondria = 10;

  // Variable initializations:
  A_I = 1;
  A_k1 = 0.01;
  B_I = 1;
  B_k1 = 0.01;
  C_I = 1;
  C_k1 = 0.01;

  // Other declarations:
  var A_kineticLaw, B_kineticLaw, C_kineticLaw;
  const A_cell, A_mitochondria, B_cell, B_mitochondria, C_cell, C_mitochondria;
  const A_I, A_k1, B_I, B_k1, C_I, C_k1;
end
```

0.3.1 Usually, deletion of a species is overkill.

0.3.2 Instead, overwrite assignments or kinetics!

```
In [126]: model_circle = '''
          import "example.antimony"

          model circle
              A: example()
              B: example()
              C: example()

              X0: A.TOM1 -> B.TOM1;
              X1: B.TOM1 -> C.TOM1;
              X2: C.TOM1 ->  A.TOM1;

              # Assignment rule-> ODE:
              C.kineticLaw := ;
              C.kineticLaw '= 0.1;
              C.kineticLaw = 0.1;

              # Delete reaction:
              #delete A.T0

              # Overwrite reaction
              A_TO: A.A_c -> A.A_m; 0.1; # Note, the Underline, Submodels are flatt
          end

          '''

          circle = te.loada(model_circle)
          print(circle.getAntimony())
```

```
// Created by libAntimony v2.9.4
model *circle()

  // Compartments and Species:
  compartment A_cell, A_mitochondria, B_cell, B_mitochondria, C_cell, C_mitochondri
  species A_TOM1 in A_cell, A_A_c in A_cell, A_A_m in A_mitochondria, B_TOM1 in B_c
  species B_A_c in B_cell, B_A_m in B_mitochondria, C_TOM1 in C_cell, C_A_c in C_ce
  species C_A_m in C_mitochondria;

  // Assignment Rules:
  A_kineticLaw := A_k1*A_TOM1*(A_A_c - A_A_m)/A_I;
  B_kineticLaw := B_k1*B_TOM1*(B_A_c - B_A_m)/B_I;

  // Rate Rules:
  C_kineticLaw' = 0.1;
  // Reactions:
  A_T0: A_A_c + A_TOM1 -> 2 A_A_m + A_TOM1; A_kineticLaw;
  B_T0: B_A_c + B_TOM1 -> 2 B_A_m + B_TOM1; B_kineticLaw;
  C_T0: C_A_c + C_TOM1 -> 2 C_A_m + C_TOM1; C_kineticLaw;
  X0: A_TOM1 -> B_TOM1; ;
  X1: B_TOM1 -> C_TOM1; ;
  X2: C_TOM1 -> A_TOM1; ;
  A_TO: A_A_c -> A_A_m; 0.1;

  // Species initializations:
  A_TOM1 = 10;
  A_A_c = 100;
  A_A_m = 1;
  B_TOM1 = 10;
  B_A_c = 100;
  B_A_m = 1;
  C_TOM1 = 10;
  C_A_c = 100;
  C_A_m = 1;

  // Compartment initializations:
  A_cell = 100;
  A_mitochondria = 10;
  B_cell = 100;
  B_mitochondria = 10;
  C_cell = 100;
  C_mitochondria = 10;

  // Variable initializations:
  A_I = 1;
  A_k1 = 0.01;
  B_I = 1;
  B_k1 = 0.01;
  C_I = 1;
  C_kineticLaw = 0.1;
  C_k1 = 0.01;

  // Other declarations:
  var A_kineticLaw, B_kineticLaw, C_kineticLaw;
  const A_cell, A_mitochondria, B_cell, B_mitochondria, C_cell, C_mitochondria;
  const A_I, A_k1, B_I, B_k1, C_I, C_k1;
end
```