compare

November 12, 2017

1 Reproducibility between tools

The following scripts checks that solutions are reproducibile between tools. Reproducibility of the model simulations was tested by comparing the numerical SOA results between `sbmlutils` and `iBioSim` for models with unique solutions. Results were assumed as numerical identical if the absolute difference for every time point t_k for all dynamical FBA species c_k in the model was smaller than the tolerance $\epsilon = 1\text{E}{-3}$, i.e.,

$$abs(c_i(t_k)_{sbmlutils} - c_i(t_k)_{ibiosim}) \leq \epsilon \; \forall c_i, t_k$$

```
In [31]: """
         Helper class for comparing simulation results.
         """
         import pandas as pd
         from matplotlib import pyplot as plt
         from pprint import pprint
         import warnings

         class DataSetsComparison(object):
             """ Comparing two simulation results.
             Currently only supports comparison between two datasets.
             """
             eps = 1E-3  # tolerance for comparison

             def __init__(self, files, dfs, columns=None):
                 self.files = files
                 self.columns = columns
                 for df in dfs:
                     # check that identical number of timepoints
                     if len(df) != len(dfs[0]):
                         raise ValueError("DataFrames have different length: \
                                          {} != {}".format(len(df), len(dfs[0])))

                 if columns:
                     assert len(self.files) == len(self.columns)
                     for column in self.columns:
                         assert len(column) == len(self.columns[0])
```

```
        self.read_dfs(dfs)
        self.diff = self.df_diff()

    def read_dfs(self, dfs):
        """ Read the dataframes using the files and given column ids."""
        self.dfs = []

        for k, df in enumerate(dfs):
            file = self.files[k]
            if self.columns:
                cols = self.columns[k]
                try:
                    df1 = df[cols]
                except KeyError:
                    pprint(df.columns)
                    raise
                df1.columns = self.columns[0]  # unify columns
                self.dfs.append(df1)
            else:
                # no columns specified, necessary to figure out the mapping
                print("-"*40)
                print(file)
                print("-"*40)
                pprint(df.columns)

        return self.dfs

    def df_diff(self):
        """ DataFrame of all differences between the files."""
        return self.dfs[0]-self.dfs[1]

    def is_equal(self):
        """ Check if DataFrames are identical within numerical tolerance."""
        return abs(self.diff.abs().max().max()) <= DataSetsComparison.eps


    def info(self):
        pprint(self.files)
        pprint(self.columns)

    def print_diff(self):
        print("\n# Elements")
        print(self.diff.shape)

        print("\n# Maximum column difference")
        print(self.diff.abs().max())
```

```
            print("\n# Maximum element difference")
            print(self.diff.abs().max().max())

            print("\n# Datasets are equal (diff <= eps={})".format(self.eps))
            print(self.is_equal())
            if not (self.is_equal()):
                warnings.warn("Datasets are not equal !")


        def plot_diff(self):
            for cid in self.diff.columns:
                plt.plot(self.diff[cid], label=cid)
            plt.legend()
            plt.show()

        def report(self):
            print("*" * 80)
            self.info()
            self.print_diff()
            print("*" * 80)
            self.plot_diff()
            self.diff
```

1.1 toy_wholecell

```
In [32]: wholecell_version = 14
         files = [
                 "./toy_wholecell/toy_wholecell_mk_v14-sbmlutils_dt1.0_tend50.0.csv",
                 "./toy_wholecell/toy_wholecell_mk_v14-ibiosim_dt1.0_tend50.0.csv"
         ]
         wholecell_dsc = DataSetsComparison(
             files=files,
             dfs=[pd.read_csv(file) for file in files],
             columns = [
                 ["time", "[A]", "[C]", "[D]"],
                 ["time", "A", "C", "D"],
             ]
         )

         wholecell_dsc.report()
```

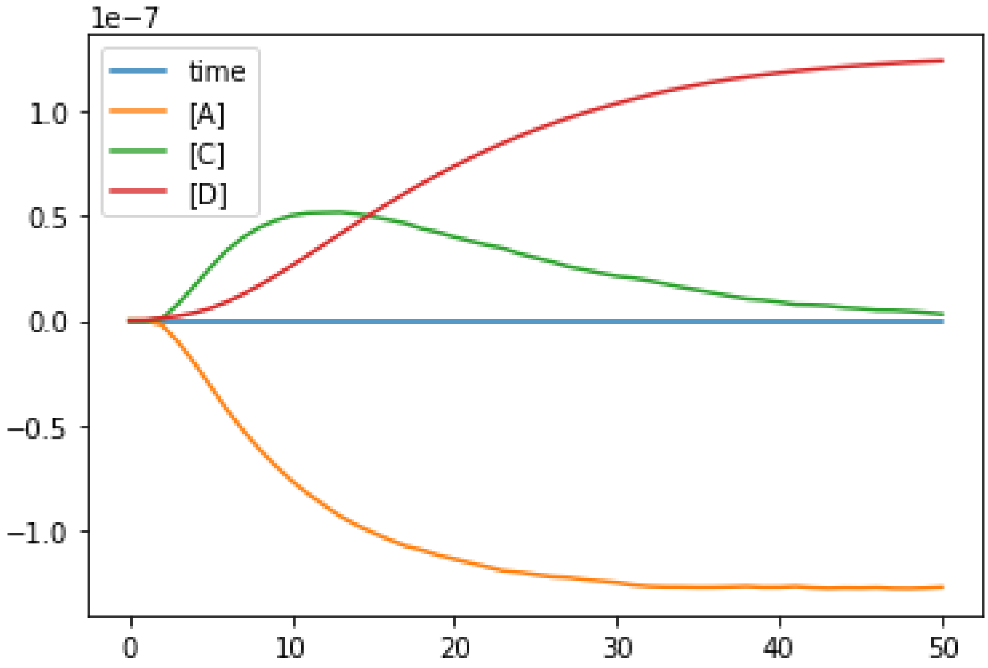
```
********************************************************************************
['./toy_wholecell/toy_wholecell_mk_v14-sbmlutils_dt1.0_tend50.0.csv',
 './toy_wholecell/toy_wholecell_mk_v14-ibiosim_dt1.0_tend50.0.csv']
[['time', '[A]', '[C]', '[D]'], ['time', 'A', 'C', 'D']]

# Elements
(51, 4)
```

```
# Maximum column difference
time    0.000000e+00
[A]     1.280189e-07
[C]     5.191503e-08
[D]     1.242827e-07
dtype: float64

# Maximum element difference
1.28018868395e-07

# Datasets are equal (diff <= eps=0.001)
True
********************************************************************************
```



1.2 toy_atp

```
In [33]: files = [
             "./toy_atp/toy_atp_mk_v12-sbmlutils_dt0.1_tend15.csv",
             "./toy_atp/toy_atp_mk_v12-ibiosim_dt0.1_tend15.csv"
         ]
         atp_dsc = DataSetsComparison(
             files=files,
             dfs = [
            pd.read_csv(files[0], sep="\t"),
            pd.read_csv(files[1])
        ],
        columns = [
            ["time", "[adp]", "[atp]", "[pyr]", "[glc]"],
            ["time", "adp", "atp", "pyr", "glc"],
        ]
    )

    atp_dsc.report()
```

```
    ---------------------------------------------------------------------------

    ValueError                                Traceback (most recent call last)

    <ipython-input-33-e7957bbc5a3f> in <module>()
     11     columns = [
     12         ["time", "[adp]", "[atp]", "[pyr]", "[glc]"],
---> 13         ["time", "adp", "atp", "pyr", "glc"],
     14     ]
     15 )


    <ipython-input-31-afecd26f9d49> in __init__(self, files, dfs, columns)
     19             # check that identical number of timepoints
     20             if len(df) != len(dfs[0]):
---> 21                 raise ValueError("DataFrames have different length:
     22
     23         if columns:


    ValueError: DataFrames have different length:                                        16 != 151
```

1.3 diauxic

```
In [34]: files = [
             "./diauxic_growth/diauxic_growth_lw_v4-sbmlutils_dt0.01_tend15.0.csv",
             "./diauxic_growth/diauxic_growth_lw_v4-ibiosim_dt0.01_tend15.0.csv",
         ]
         diauxic_dsc = DataSetsComparison(
             files=files,
             dfs = [
                 pd.read_csv(files[0]),
                 pd.read_csv(files[1])
             ],
             columns = [
        ["time", "[Ac]", "[Glcxt]", "[O2]", "[X]"],
        ["time", "Ac", "Glcxt", "O2", "X"],
    ]
)

diauxic_dsc.report()
```

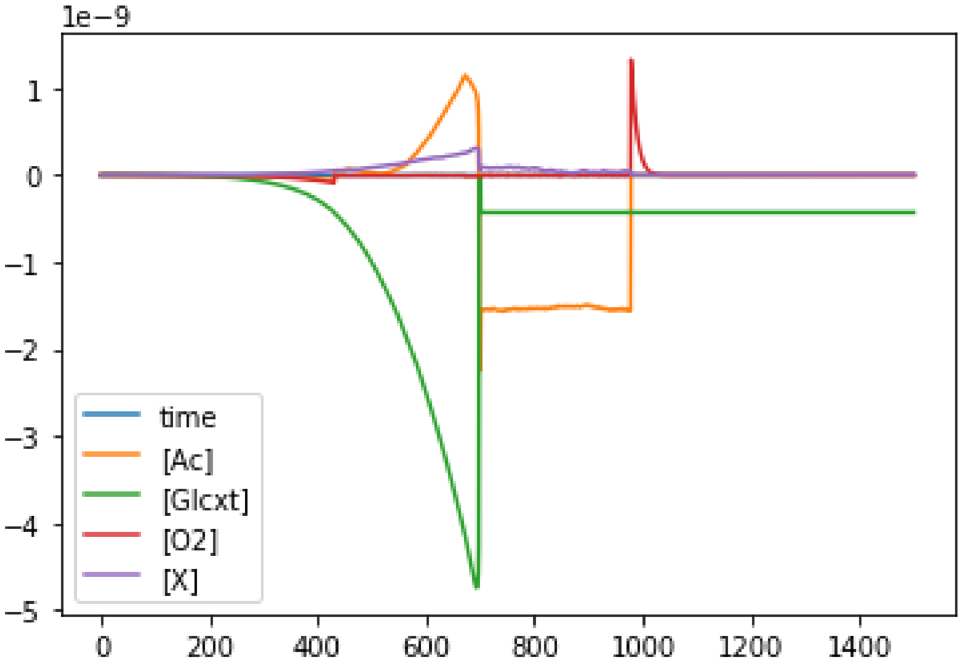
```
********************************************************************************
['./diauxic_growth/diauxic_growth_lw_v4-sbmlutils_dt0.01_tend15.0.csv',
 './diauxic_growth/diauxic_growth_lw_v4-ibiosim_dt0.01_tend15.0.csv']
[['time', '[Ac]', '[Glcxt]', '[O2]', '[X]'], ['time', 'Ac', 'Glcxt', 'O2', 'X']]

# Elements
(1501, 5)

# Maximum column difference
time       3.552714e-15
[Ac]       2.245718e-09
[Glcxt]    4.743860e-09
[O2]       1.326935e-09
[X]        3.114851e-10
dtype: float64

# Maximum element difference
4.74386013805e-09

# Datasets are equal (diff <= eps=0.001)
True
********************************************************************************
```



```
In [ ]:
```