

Demo-Version 13CFLUX2 Web Service Description

Author: Birgit Stute,
Modeling and Simulation Group
IBG-1: Biotechnology
Forschungszentrum Jülich GmbH
Germany

Date: version 1.1, 1/ 2013

All rights reserved.



Installation Requirements for the Usage of the Python Scripts

Linux:

Python: Python package can be installed from the distribution repository

Setuptools: Setuptools is needed to install python-suds. Setuptools can be downloaded at <http://pypi.python.org/packages/source/s/setuptools/> or use the provided setuptools-0.6c11.tar.gz. You can install it by terminal with:

```
tar xfvz setuptools-0.6c11.tar.gz
cd setuptools-0.6c11
python setup.py install
(If python is not installed in /usr/local/lib than:
python setup.py install --prefix="path_to_the_lib
_directory_where_Python_is_located",
For example if python is saved in /usr/lib/python2.7 than you
have to use: python setup.py install --prefix=/usr/ )
```

Python-suds: Suds is a lightweight SOAP python client for consuming Web Services

Python-suds can be downloaded from <https://fedorahosted.org/suds/> or use the provided python-suds-0.4.tar.gz. You can install it by terminal with:

```
tar xfvz python-suds-0.4.tar.gz
cd python-suds-0.4/
python setup.py install
(If python is not installed in /usr/local/lib than see above at the
instruction for Setuptools)
```

Save the python_script.tar.gz on your linux machine.

Unpack it with the terminal command: `tar xfvz python_scripts.tar.gz`.

Navigate into python_script directory. You can start here the python scripts with “./”.

For example:

```
./fitfluxes.py -h
```

If you add the path to the python_scripts into the PATH-variable (by adding the line `export PATH=$PATH:"path_to_python_script"` to .bashrc) python scripts can be called from any directory.

For example:

```
fitfluxes.py -h
```

Windows

Python: *Python* can be downloaded from <http://www.python.org/getit/releases/2.7.3/> or you can use the provided python-2.7.3.msi.
Double-click on python-2.7.3.msi and just follow the instructions to install python on your windows machine.

Python-suds: You can use the provided suds-0.4-py2.6.zip.
Unzip the zip file. Copy the suds-0.4-py2.6/suds directory into the path_to_python/Python27/LIB/ directory.

Add the path to python directory in the PATH-variable:

Control Panel → System and Security → System → Advanced system settings → environment variable:

edit system variable PATH:

Add:"; path_to_python_directory"

Save and unzip the python_script.zip archive.

Open the command terminal.

Navigate to the directory python_script

```
cd "path_to_python_script_directory"
```

You can run the python scripts by entering the python-script-name with its arguments into the command line.

For example:

```
fitfluxes.py -h
```

Functionality of 13CFLUX2 Versions

The Demo Version of 13CFLUX2 includes the core functions of the 13CFLUX2 software. These are the following tools:

- fmllint*** - tool to control the syntax of the FluxML input files (FluxML - network model document format)
- fwdsim*** - forward simulation of the mathematical problem given by the stoichiometry, the atom transitions, the input substrate and the flux constraints of an isotope labeling network. This program simulates for given valid flux distributions the resulting isotopomer measurements.
- sscanner*** - tool to determine one valid flux distribution for the independent fluxes (free fluxes) of the network, which not violate the flux constraints. The *sscanner* determines the analytical center of the feasible flux space.
- ssampler*** - tool to determine several random valid flux distribution for the independent fluxes (free fluxes) of the network by sampling the feasible flux space.
- setfluxes*** - tool to transfer (free) flux settings from FWDSIM, HDF5, or CSV to FluxML.
- fitfluxes*** - tool to fit a flux distribution of a network by reproducing a set of isotope labeling measurements and minimizing the offset to the real measurements in an optimization process.

Note: The Demo Version has the following two limitations:

The use of the software in the demo version is restricted to models with less than **4 free fluxes** (independent fluxes) and less than **15 measurement data**.

Functionality of the Academic License

The **academic license** includes some additional functionality:

collectfitdata - tool for collecting together simulation results into a HDF5 file.

edopt - tool for substrate mixture optimization (experimental design)

edscanner - experimental design scanner (for statistical mixture quality).

multifwdsim - multi-processor frontend for *fwdsim*.

multifit - a multi-start, multi-processor frontend for *fitfluxes*.

multiperturb - multi-processor frontend for *perturb*.

perturb - tool for flux and measurement value perturbation

Web Service

The use of Web Services entails small differences in the use of 13CFLUX2 compared to the native installed software and leads to slightly different program output of the 13CFLUX2 programs.

The Web Service is accessed by python scripts. Each of the python scripts encapsulates a 13CFLUX2 program call:

```
fmllint    ->    fmllint.py
fwdsim     ->    fwdsim.py
sscanner   ->    ssacnner.py
ssampler   ->    ssampler.py
fitfluxes  ->    fitfluxes.py
```

Web Service specific features are:

1. For the tool *fwdsim* normally more than one output format can be chosen per call. In the Web Service-based Demo Version of 13CFLUX2 only one output format per call can be selected.
2. The man pages are not available. PDF versions of the man pages can be found in the folder “Man Pages (for 13CFLUX2 Demo WS)”.
3. Less important optional command line arguments of the 13CFLUX2 tools are not available in the Web Service solution. (Compare the help functions of the python scripts `[toolname].py -h` with the manuals of 13CFLUX2)
4. The Web Service solution provides no information on `stdout` except an error is produced. Usually 13CFLUX2 programs emit useful extra information on `stdout`. For example, for *fitfluxes* the progress of the residuum decay within the optimization procedure can be followed in the command window.