NAME

setfluxes − transfer (free) flux settings from FWDSIM, HDF5, or CSV to FluxML.

SYNOPSIS

setfluxes [*options*]

DESCRIPTION

Setfluxes is a tool for transferring settings of free fluxes from FWDSIM (XML), HDF5, or CSV documents to FluxML. Most common use cases are:

1. using **fitfluxes**(1), you generated optimized flux settings which are now available in a FWDSIM (XML) file. In order to do linearized statistics with **fwdsim**(1) you use **setfluxes** for transferring the flux settings to a FluxML document.
2. using **ssampler**(1), you generated thousands of random flux distributions in order to do a multi−start optimization with **fitfluxes**(1). You can now use **setfluxes**(1) to write the flux distributions, one after the other, to a FluxML document.
3. using the spreadsheet application of your choice, you created a CSV file containing a flux distribution for your network. Instead of manually editing the FluxML fail you can use **setfluxes** to automate this task.

COMMON OPTIONS

−h, −−help
Show a brief help for all command line options.

−i, −−in <FILE> [default: stdin]
The name of the FluxML (XML) input file. If omitted, the FluxML document is expected on standard input.

−o, −−out <FILE> [default: stdout]
The name of the FluxML output file. If omitted, the modified FluxML document is written to standard output.

−c, −−configure <CFG> [default: 'default']
Because FluxML documents may contain several **<configuration/>** elements this option allows to specify the configuration that should be used for the simulation. If this option is omitted it is assumed that the FluxML document contains a configuration with the name "default".

DATA SOURCE OPTIONS

−F, −−fwd <FILE>
Specify a FWDSIM (XML) file as data source, usually generated by either **fwdsim**(1) or **fitfluxes**. The layout of these files is documented in manual page **fwdsim**(5).

−H, −−hdf <FILE>
Use a HDF5 file as data source. The HDF5 file is expected to have the following layout:

- '/flux/names' should be a vector of strings containing the flux names with suffixes '.n' or '.x' for net and exchange fluxes
- '/flux/data' should be a matrix of double precision floating point numbers. The columns of the matrix are associated with the flux names in the elements of '/flux/names'

In case the line number (option **−l**) is omitted it is assumed that the first dataset in line 1 should be transferred.

−C, −−csv <FILE>
Use this parameter to specify a CSV file containing the flux distribution. The CSV file should have the following layout:

- a column heading (the first row) should list the flux names with suffixes '.n' or '.x' for net and exchange fluxes

- starting with the second row each row of the CSV file contains one complete flux setting

In case the line number (option **−l**) is omitted it is assumed that the first dataset in line 1 (row 2) should be transferred.

−l, −−line <LINENUM> [default: 1]
When using a HDF5 or CSV file as data source, specify the line number (row number) of the flux distribution which should be written to the generated FluxML document. If this parameter is omitted the first first flux distribution is selected.

SPECIAL OPTIONS

−f, −−force
Write all flux settings to the generated FluxML document without checking whether they existed in the input FluxML document. Use this option if your input FluxML document contained no settings for the free fluxes, or the choice of free fluxes in the input FluxML file does not match the choice in the data source. If this parameter is not specified **setfluxes** tries to detect non−matching combinations of data source and FluxML input document.

−D, −−data <PATH> [default: '/flux/data']
For a HDF5 data source, specify the path to the flux values. Use with care.

−N, −−names <PATH> [default: '/flux/names']
For a HDF5 data source, specify the path to the flux names. Use with care.

EXAMPLES

Transfer the flux distribution found in a FWDSIM document to a corresponding FluxML document network.fml (most simple case):

setfluxes −i network.fml −F network.fwd −o network_new.fml

Transfer the 123'rd flux distribution found in a HDF5 file samples.h5 to a corresponding FluxML document network.fml:

setfluxes −i network.fml −H samples.h5 −l 123 −o network_new.fml

Convert an old FTBL network specification to FluxML and replace the flux settings by the values contained in line 5 of a CSV file. Simulate the result using **fwdsim**(1):

ftbl2fml −i network.ftbl | setfluxes −C samples.csv −l 5 | fwdsim −o results.fwd

SEE ALSO

fwdsim(1), fitfluxes(1), ftbl2fml(1)

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