NAME

sscanner − generate an initial flux distribution for a metabolic network

SYNOPSIS

sscanner [*options*]

DESCRIPTION

The program **sscanner** is used to generate an initial flux distribution for a metabolic network. In order to perform this task **sscanner** reads a FluxML document (see also **fluxml**(1)), chooses some free fluxes and reinitializes the flux values with the analytical center of the specified constraints.

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 output FluxML file. If this option is omitted the resulting 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".

−L, −−list
Specifying this option results in a list of allowed configuration names for the specified FluxML document. The program exits immediately after emitting the list.

−l, −−log DEST
Specify the destination for the internal logging. In the most simple case **DEST** is a file name of a log file. In case the file exists new log messages are appended. Apart from log files it is possible to publish log messages to file descriptors, UNIX domain sockets, UDP and SCTP ports, and a small graphical user interface.

A file descriptor is specified by **fd:[num]**, where **[num]** is the number of the file descriptor.

A unix domain socket in the local file system is specified by **unix:[name]**, where **[name]** is the name of the socket file

A UDP or (connectionless) SCTP port is specified by **[proto]:[host]:[port]**, where **[proto]** is either "udp" or "sctp" and **[host]** is the name of the destination host and **[port]** is a UDP or SCTP port number on the destination host. Please note that the length of log messages is bounded by the minimum safe UDP packet size − log messages containing more than 548 characters will be truncated.

Finally, log messages can also be sent to a small GUI by specifying the destination **@gui@**. The GUI requires a working Perl/Tk installation and a running X server.

In order to capture all log messages concerning the command line processing this option should be specified in front of all other options.

−v, −−verbose 0..10 [default: 5]
Specify the verbosity 0, 1, ..., 10 of generated / emitted log messages. The meaning of the different log levels is as follows:

- **0 (QUIET)** do not emit log messages at all.

- **1 (ERROR)** only emit severe error messages.
- **2 (WARNING)** only report severe errors and warnings.
- **3 (NOTICE)** report all errors and warnings including important informal messages.
- **4 (INFO)** report all errors, warnings and all informal messages.
- **5 (THROW)** in case of an exception, try to give a diagnosis of the error; sometimes even gives a backtrace of the current function stack.
- **6 (DEBUG0)** emit the more important debugging messages.
- **7 (DEBUG1)** emit the less important debugging messages
- **8 (DEBUG2)** emit the superfluous debugging messages
- **9 (DEBUG3)** emit annoying debugging messages.
- **10 (DEBUG4)** don't dare to use it!

SPECIAL OPTIONS

−B, −−bounds
Determine the lower and upper bounds for the settings of the free fluxes by using an LP solver. The program exits immediately after emitting the list.

−C, −−constraints
This option causes a list of user defined and automatically inferred equality and inequality constraints to be generated. The program exits immediately after emitting the list.

−m, −−montecarlo <NUM>
Determine the setting of the free fluxes from the centroid of point cloud generated using Gibbs sampling, a Markov Chain Monte Carlo technique. This parameter requires the number of Monte Carlo samples to be specified.

−r, −−resample <n,x,nx> [default: nx]
This option is used to specify what to resample. Possible values are 'n', 'x', and 'nx' − for sampling only net fluxes, only exchange fluxes, or both net and exchange fluxes. The default is to resample both net and exchange fluxes.

−b, −−bound−net <VALUE> [default: 100]
The bound for the magnitude of unbounded net fluxes. Defaults to 100.

−p, −−bound−xch <VALUE> [default: 100]
The bound for unbounded exchange fluxes. Defaults to 100.

EXAMPLES

Generate a new flux distribution for the network in FluxML file network.fml representing the analytical center of the specified stoichiometric constraints. In case the stoichiometry of network.fml is unbounded a default bound of 100 is used for all unbounded net and exchange fluxes. The resulting flux distribution is written to another FluxML file.

sscanner −i network.fml −o new_network.fml

The same as above, however, the free fluxes are initialized to represent the centroid of a cloud of 100 uniformly distributed points. If 1 instead of 100 points are used this allows a random initialization of the stoichiometry (see also ssampler(1)):

sscanner −m 100 −i network.fml −o new_network.fml

Compute the lower and upper bounds of the free net and exchange fluxes. The result is written to standard output:

sscanner −i network.fml −B

SEE ALSO

fwdsim(1), fitfluxes(1), ssampler(1)

AUTHOR

Michael Weitzel

This manpage was written by Michael Weitzel <mich@el−weitzel.de>.