Metatool SBW Module

Sri Paladugu

Sri_Rama_Krishna_Paladugu@kgi.edu
Systems Biology Workbench Development Group
Keck Graduate Institute
535 Watson Drive, Claremont, CA 91107, USA
http://www.sys-bio.org

Principal Investigators: Herbert M Sauro

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1 METATOOL

METATOOL is a C program developed from 1998 to 2000 by Thomas Pfeiffer (Berlin) in cooperation with Stefan Schuster and Ferdinand Moldenhauer (Berlin) and Juan Carlos Nuno (Madrid). It serves to derive conclusions about the pathway structure of metabolic networks from the stoichiometric reaction equations and information about reversibility and irreversibility of enzymes.

The SBW interface for metatool provides various functions to extract information from the output file generated by the metatool executable (meta4.3_double.exe).

1.1 Metatool Service – mt

Method Descriptions:

string getVersion()

Input Parameters: None
Output: Returns the String containing the version information for executable (meta4.3_double.exe).

int setMetaToolPath(string)

Input Parameters: Fullpath of metatool executable meta4.3_double.exe.
Output: Returns an integer value of 0 if the executable is present and 1 if the executable is not present at the input path.

Description: By default is the path isn't specified, SBWMetatool will search for the metatool executable in the current directory.

void runMetatool(string)

Input Parameters: Fullpath of metatool input file.
Output: None.

Description: Runs the metatool executable meta4.3_double.exe with the given metatool input file and generates the metatool output file. If the input file name is empty then the routine uses the default input metatool file name.

void runMetatoolWithSBML(string)

Input Parameters: SBML in the form of a string.
Output: None

Description: Runs the metatool executable meta4.3_double.exe with the input SBML string and generates the metatool output file.

void runMetatoolFromNOM()

Input Parameters: None
Output: None

Description: Runs the metatool executable meta4.3_double.exe with the SBML loaded in NOM(Network Object Model) and generates the metatool output file.

int getNumReactions()

Input Parameters: None
Output: Number of Reactions

Description: Returns the number of reactions from the metatool output file.

int getNumInternalSpecies()

Input Parameters: None
Output: Number of Internal Species

Description: Returns the number of floating species from the metatool output file.

int getNumExternalSpecies()

Input Parameters: None
Output: Number of ExternalSpecies

Description: Returns the number of boundary species from the metatool output file.

double[][] getStoichiometryMatrix()

Input Parameters: None Output: Stoichiometry Matrix

Description: Returns the Stoichiometry Matrix from the metatool output file.

double[][] getElementaryModes()

Input Parameters: None
Output: Elementary Modes Matrix

Description: Returns the Elementary Modes Matrix from the metatool output file.

double[][] getNullSpaceVectors()

Input Parameters: None
Output: NullSpaceVectors Matrix

Description: Returns the NullSpaceVectors Matrix from the metatool output file.

double[][] getConservationVectors()

Input Parameters: None
Output: ConservationVectors Matrix

Description: Returns the ConservationVectors Matrix from the metatool output file.

{} **getInternalList()**

Input Parameters: None
Output: List of Floating Species

Description: Returns the list of floating species from the metatool input file.

{} **getExternalList()**

Input Parameters: None
Output: list of Boundary Species

Description: Returns the list of boundary species from the metatool input file.

{} **getReactionNameList()**

Input Parameters: None
Output: list of Reaction Names

Description: Returns the list of reaction names from the metatool input file.

1.2 biospiceAnalyze Service – biospiceAnalyze

For descriptions of the biospiceAnalyze methods, please refer to BioSPICE documentation available at www.biospice.opg.

Method Descriptions for BioSPICE specific functions:

int initialize()

This method will be called by the BioSPICE dashboard if specific initializations are required.

string getName()

The Dashboard will call this to get the name of the module.

string getDisplayName()

Display Name used by the Dashboard.

{} **getInputTypes()**

Returns a list of input types for the module.

{} **getOutputTypes()**

Returns a list if output types for the modules.

{} **getConfigurationParams()**

Sri - I need to complete this description.

{} **analyze({})**

Input Parameters: A list containing a SBML string.
Output: list containing - a list of column identifiers (reaction names) for elementary modes and a two dimensional elementary matrix.

Description: Accepts a list containing SBML string and invokes runMetatoolWithSBML method which in turn generates a metatool output file. Then the getElementaryModes( ) method is called which extracts the two dimensional elementary modes matrix from the metatool output file.

1.3 Use-case for Biospice Dashboard:-

To use this module in the BioSPICE dashboard, select a module capable of generating SBML output in the form of string and feed the output from it to Metatool module. Metatool then generates a list containing a list of labels representing the column names for elementary modes and a two dimensional elementary modes matrix. You can feed the output from Metatool to a Tableviewer capable of displaying a two dimensional matrix.

Simple Example (under windows because it requires JDesigner) :-

Pre-requisites:

1. You need to have SBW (Systems Biology Workbench installed on your system). Please uninstall any older versions of SBW from your system and download the new SBW installer from:-

`http://public.kgi.edu/~spaladug/one.html`

[or]

`http://www.sf.net/projects/jdesigner`

2. Download and install Biospice Dashboard. You can obtain Dashboard from

`http://www.biospice.org`

3. Download and install SBWBiospiceAnalyzers.exe. You can obtain the installer from:

`http://public.kgi.edu/~spaladug/one.html`

1.4 Instructions to use Biospice Dashboard:

0. Open JDesigner from Start Menu (Systems Biology Workbench → JDesigner).

1. Double-click on Dashboard shortcut. This should bring up Biospice Dashboard window.

2. A window containing various Analyzers should now appear on the left side of the screen.

3. Click on JDesigner Icon and then drag and drop it into the work flow editor on the right.

4. Click on Metatool Icon and then drag and drop it into the work flow editor on the right.

5. Click on Tableview Icon and then drag and drop it into the work flow editor on the right.

6. Now connect JDesigner to Metatool. (To do this click on arrow head that appears infront of JDesigner and draw a line connecting the arrow head of JDesigner to the tail of Metatool.)

7. Connect Metatool to Tableview as you did in the previous step. Your workflow editor should now appear as below:-

JDesigner ⟶ Metatool ⟶ TableView

8. Now click on Workflow button on the right hand corner of Workflow editor window. Select "Start" from the drop downlist that appears.

9. Goto JDesigner Window and open the SBML file using Open button.

10. Then Click on Biospice button on the top right hand corner.

11. This brings up a Table containing the elementary modes. The column headers of this table indicates the names of reactions given in sbml input file. Each row of the table indicates a separate elementary mode. The values in each cell indicates the relative fluxes that are carried along the branch. A zero in a cell indicates that the corresponding reaction is not visited along the path.

1.5 Special instructions to Linux Users:

Linux users needs to follow the below steps to install and use Metatool.

1. You need to have SBW (Systems Biology Workbench) installed on your system). You can obtain linux version from:

`http://public.kgi.edu/~spaladug/one.html`

2. Download SBW-NOM (Network Object Model's SBW Interface) from:

`http://public.kgi.edu/~spaladug/one.html`

3. Download Metatool (Metatool's SBW Interface) from:

`http://public.kgi.edu/~spaladug/one.html`

4. Start SBW Broker, by typing in the following command at shell prompt:

[Full Path of C++Broker Directory]/bin/Broker &

5. Register SBW-NOM with SBW Broker, by typing in the following commands at shell prompt:

[Full Path of SBW-NOM Directory]/bin/NOMModule -sbwregister

[Full Path of SBW-NOM Directory]/bin/NOMModule -sbwregister -unique

6. Register Metatool with SBW Broker, by typing in the following commands at shell prompt:

[Full Path of Metatool Directory]/bin/metatoolSBW -sbwregister -unique