gEFM Algorithm

gEFM is a tool based on the Canonical Basis approach and uses Bit Pattern trees for computation. The implementation is in C++. The code is compiled and tested for linux. For windows, following modification is required in BitVector.h because u_int32_t is defined in linux.

```
typedef uint32_t u_int32_t;
typedef uint64_t u_int64_t;
```

Here are some constants that can be changed according to the requirements.

Header File	Constant	Default Value	Explanation
BitVector.h	MAX_REACTION_COUNT	448	Maximum number of reactions supported
BitPatternTreeNode.h	MAX_PATHWAYS	10	Maximum number of pathways stored in the leaf node of bit pattern tree
	MAX_BPT_TREE_NODES	20000	Maximum number of bit pattern tree nodes
GlobalData.h	ZERO	1e-5	Tolerance level for zero
Network.h	LINE_SIZE	102400	Size of buffer to store a single line in the network file
	TOKEN_SIZE	1024	Size of a single token in a line of the network file
Pathway.h	MAX_METABOLITES	200	Maximum number of metabolites in the network
PathwayPool.h	MAX_PATHWAY_POOL_SIZE	2000000	Maximum number of pathway that can be stored
ReversibleTreeNode.h	MAX_REVERSIBLE_TREE_NODES	20000	Maximum number of reversible tree nodes

Compiling

The code has been compiled and tested using gcc 4.8.2. The code also requires libstdc++. The code can be optimized using –O3 flag to improve performance.

Network File

The network file is a tab separated plain text file with the following format.

- First line is a tab separated list of reaction names. The first two entries should be empty (the line should start with two tabs).

- Second line is a tab separated list indicating if a reaction is reversible (1 represents a reversible reaction, 0 represents irreversible reaction). The first two entries should be empty (the line should start with two tabs).
- Subsequent lines correspond to metabolites. First entry in the line is metabolite name. Second entry is 1 if metabolite is external or 0 if metabolite is internal metabolite. Reset of the entries represents stoichiometric coefficients of the metabolite in reactions specified in the first line.

A sample network file is available under the file name Sample.txt.

Program Output

The program's output is also tab separated. It first computes elementary flux modes and then calculates the reaction coefficients.

Program Options

The program can accept an optional flag -noRevDup before the network file name. This flag suppresses printing of two EFMs consisting of same reversible reactions (one operating in the forward direction and other operating in the reverse direction). When this flag is specified, only one EFM is printed.