COBRA cheat sheet

Important information COBRA Toolbox is contained in matTFA
matTFA/ext/Cobra205_vDec2014

Thus, adding matTFA and its subfolders to the MATLAB-Path variable will allow you access to all COBRA functions.

Starting up MATLAB with COBRA and CPLEX:

Model variables (used / not used in exercises)

rxns	Reaction abbreviations
mets	Metabolite abbreviations
S	Stoichiometric matrix
rev	Reversibility
lb	Lower bound (reaction flux)
ub	Upper bound (reaction flux)
c	Objective function (reaction)
metCharge	Metabolite charges (at physiological pH)
rules	Rules how gene associate with reactions
genes	Genes associated with reactions
rxnGeneMat	
grRules	
subSystems	Metabolic subsystems present
confidenceScores	
rxnReferences	
rxnECNumbers	Enzyme Commission number of reaction
rxnNotes	
rxnNames	Full reaction names
metNames	Full metabolite names
metFormulas	Chemical formula of metabolites
metChEBIID	ChEBI identifier of metabolites
metKeggID	KEGG identifier of metabolites
metPubChemID	PubChem identifier of metabolites
metInchiString	Inchi string of metabolites
b	
description	

COBRA functions

changeRxnBounds	Change upper or lower bounds of a reaction or a set of reactions
optimizeCbModel	Solve a flux balance analysis problem
changeObjective	Changes the objective function of a constraint-based model
singleGeneDeletion	Performs single gene deletion analysis using FBA, MOMA or linearMOMA
fluxVariability	Performs flux variablity analysis

changeRxnBounds

changeRxnBounds Change upper or lower bounds of a reaction or a set of reactions

```
 model = changeRxnBounds(model,rxnNameList,value,boundType)

INPUTS
 model          COBRA model structure
 rxnNameList    List of reactions (cell array or string)
 value          Bound values
                Can either be a vector or a single scalar value if the same
                bound value is to be assinged to all reactions

OPTIONAL INPUT
 boundType      'u' - upper, 'l' - lower, 'b' - both (Default = 'b')
                Bound type can either be a cell array of strings or a
                string with as many letters as there are reactions in
                rxnNameList

OUTPUT
 model          COBRA model structure with modified reaction bounds

 Markus Herrgard 4/21/06
```

optimizeCbModel

optimizeCbModel Solve a flux balance analysis problem

```
 Solves LP problems of the form: max/min c'*v
                                 subject to S*v = b          : y
                                            lb <= v <= ub    : w
 FBAsolution = optimizeCbModel(model,osenseStr,minNormFlag)

INPUT
 model (the following fields are required - others can be supplied)
   S            Stoichiometric matrix
   b            Right hand side = dx/dt
   c            Objective coefficients
   lb           Lower bounds
   ub           Upper bounds

OPTIONAL INPUTS
 osenseStr      Maximize ('max')/minimize ('min') (opt, default = 'max')

 minNorm        {(0), 'one', > 0 , n x 1 vector}, where [m,n]=size(S);
                0      Default, normal LP
                'one'  Minimise the Taxicab Norm using LP.
                                 min |v|
                                   s.t. S*v = b
                                        c'v = f
                                        lb <= v <= ub
                -----
                The remaining options work only with a valid QP solver:
                -----
                > 0    Minimises the Euclidean Norm of internal fluxes.
                       Typically 1e-6 works well.
                                 min ||v||
                                   s.t. S*v = b
                                        c'v = f
```

```
                                    lb <= v <= ub
                n x 1   Forms the diagonal of positive definiate
                        matrix F in the quadratic program
                                min 0.5*v'*F*v
                                st. S*v = b
                                    c'*v = f
                                    lb <= v <= ub

  allowLoops    {0,(1)} If false,  then instead of a conventional FBA,
                the solver will run an MILP version which does not allow
                loops in the final solution.  Default is true.
                Runs much slower when set to false.
                See addLoopLawConstraints.m to for more info.

 OUTPUT
  FBAsolution
    f         Objective value
    x         Primal
    y         Dual
    w         Reduced costs
    s         Slacks
    stat      Solver status in standardized form
               1   Optimal solution
               2   Unbounded solution
               0   Infeasible
              -1  No solution reported (timelimit, numerical problem etc)
    origStat  Original status returned by the specific solver
```

changeObjective

changeObjective Changes the objective function of a constraint-based model

```
  model = changeObjective(model,rxnNameList,objectiveCoeff)

 INPUTS
  model             COBRA structure
  rxnNameList       List of reactions (cell array or string)

 OPTIONAL INPUT
  objectiveCoeff    Value of objective coefficient for each reaction
                    (Default = 1)

 OUTPUT
  model             COBRA model structure with new objective

  Monica Mo & Markus Herrgard - 8/21/06
```

singleGeneDeletion

singleGeneDeletion Performs single gene deletion analysis using FBA, MOMA or linearMOMA

```
  [grRatio,grRateKO,grRateWT,delRxns,hasEffect] =
singleGeneDeletion(model,method,geneList,verbFlag)

 INPUT
  model         COBRA model structure including gene-reaction associations
```

```
 OPTIONAL INPUT
  method         Either 'FBA', 'MOMA', or 'lMOMA' (Default = 'FBA')
  geneList       List of genes to be deleted (default = all genes)
  verbFlag       Verbose output (Default false)
  uniqueGene     Run unique gene deletion (default = 0).


 OUTPUTS
  grRatio        Computed growth rate ratio between deletion strain and wild
type
  grRateKO       Deletion strain growth rates (1/h)
  grRateWT       Wild type growth rate (1/h)
  hasEffect      Does a gene deletion affect anything (i.e. are any
reactions
                 removed from the model)
  delRxns        List of deleted reactions for each gene KO
  fluxSolution   FBA/MOMA/lMOMA fluxes for KO strains

  Markus Herrgard 8/7/06
  Aurich/Thiele 11/2015 unique gene deletion option (delete all alternate
transcripts and if solKO.stat not 1 or 5, grRateKO(i) = NaN;)
```

fluxVariability

```
 fluxVariability Performs flux variablity analysis

  [minFlux,maxFlux] =
fluxVariability(model,optPercentage,osenseStr,rxnNameList,verbFlag,
allowLoops)

 INPUT
  model              COBRA model structure

 OPTIONAL INPUTS
  optPercentage      Only consider solutions that give you at least a
certain
                     percentage of the optimal solution (Default = 100
                     or optimal solutions only)
  osenseStr          Objective sense ('min' or 'max') (Default = 'max')
  rxnNameList        List of reactions for which FVA is performed
                     (Default = all reactions in the model)
  verbFlag           Verbose output (opt, default false)
  allowLoops         Whether loops are allowed in solution. (Default = true)
                     See optimizeCbModel for description

 OUTPUT
  minFlux            Minimum flux for each reaction
  maxFlux            Maximum flux for each reaction

 OPTIONAL OUTPUT
  Vmin           Matrix of column flux vectors, where each column is a
                 separate minimization.
  Vmax           Matrix of column flux vectors, where each column is a
                 separate maximization.
```