# Using COBRA Toolbox to read AraGEM sbml

### COBRA Toolbox

COBRA Toolbox is a set of Matlab scripts for constraint-based modeling that are run from within the MATLAB environment. We have evaluated version 2.0 obtained from SourceForge: <http://opencobra.sourceforge.net/openCOBRA/Welcome.html>.

They provide everythijng needed to get started, including libSBML (version 4.2.0), the SBMLToolbox (3.1.2), and the glpk\_mex interface to the GNU Linear Programming Kit and the COBRA Toolbox for Mac OS X 10.6 (64-bit), GNU/Linux Ubuntu 10.0 (64-bit), and Microsoft Windows 7 (64-bit).

It is recommended replacing the free glpk LP solver with a commercial solver. If working in an academic environment, it is currently possible to obtain a free academic license for MOSEK (<http://www.mosek.com/>).

In order to get started, you need to

1. Add the path to any commercial solver from within Matlab using addpath, e.g.

>> addpath 'c:\Program Files\mosek\6\toolbox\r2009b'

1. From the install directory of the COBRA Toolbox, run the initialisation routine

>> initCobraToolbox

This will add paths to all the Toolbox files and choose a solver. NB: if using a commercial solver, you may need to change order of solvers in the initCobraToolbox to make certain it picks the one you want.

### AraGEM sbml

The AraGEM COBRA zip file contains the files needed to simulate flux distribution during photosynthesis, namely the SBML file (AraGEM.xml) and three constraint files: objectiveFunction.txt; reactionConstraints.txt; boundarySpecies.txt.

In Matlab, go to the folder where the zip file was extracted to and load the model

>> model = readCbModel('AraGEM.xml')

model =

rxns: {1599x1 cell}

mets: {1733x1 cell}

S: [1733x1599 double]

rev: [1599x1 double]

lb: [1599x1 double]

ub: [1599x1 double]

c: [1599x1 double]

metCharge: []

rules: {1599x1 cell}

genes: {1399x1 cell}

rxnGeneMat: [1599x1399 double]

grRules: {1599x1 cell}

subSystems: {1599x1 cell}

confidenceScores: {1599x1 cell}

rxnReferences: {1599x1 cell}

rxnECNumbers: {1599x1 cell}

rxnNotes: {1599x1 cell}

rxnNames: {1599x1 cell}

metNames: {1733x1 cell}

metFormulas: {1733x1 cell}

metChEBIID: {1733x1 cell}

metKEGGID: {1733x1 cell}

metPubChemID: {1733x1 cell}

metInChIString: {1733x1 cell}

b: [1733x1 double]

description: 'AraGEM.xml'

The optimal solution (here minimum photons required to meet specified biomass synthesis) can be determined using

>> solution = optimizeCbModel(model,'min',0, 1)

solution =

x: [1599x1 double]

f: 0.2308

y: [1733x1 double]

w: [1599x1 double]

stat: 1

origStat: 5

solver: 'glpk'

time: 0.0470

and the solution can be printed out using

>> printFluxVector(model, solution.x)