Solution to Homework 4

```
clear; clc;
```

Load the model and answer the following questions: (1 point each)

```
load('../Data/e_coli_core.mat')
```

- How many metabolites and reactions are in the model?

```
disp(['Number of metabolites:' newline ...
    num2str(... % to display number using disp we have to convert it to string
    length(e_coli_core.mets)...
    )])
```

```
Number of metabolites:
72
```

```
disp(['Number of reactions:' newline num2str(...
    length(e_coli_core.rxns)...
    )])
```

```
Number of reactions:
95
```

- How many compartments are in the model? *Hint: use the compartment identifier in field .mets*

```
Compartments=unique(cellfun(... % applies a task on each cell in a cell array
    @(x) ... % x is specified as variable writing @(variable)
    x(end-1:end), ... % task we do for each x, take the last two entries
    e_coli_core.mets, ... % the actual data for which we do the task specified before
    'UniformOutput',false)); % ''If 'UniformOutput' is true, the outputs of the error handler m
                             % type as the outputs of FUN.'' not true here, so we set it to fal
disp(['Number of compartments:' newline num2str(...
    length(Compartments)...
    )])
```

```
Number of compartments:
2
```

- How many metabolites belong to each of the model compartments?

```
disp(['Number of metabolites in cytosol (c):' newline num2str(...
    sum(endsWith(e_coli_core.mets,Compartments(1))) ...
    )])
```

```
Number of metabolites in cytosol (c):
52
```

```
disp(['Number of metabolites in extracellular space (e):' newline num2str(...
    sum(endsWith(e_coli_core.mets,Compartments(2))) ...
    )])
```

```
Number of metabolites in extracellular space (e):
20
```

- What are the substrates and what are the products of citrate synthase reaction?

```
rxn_cs_idx = find(contains(e_coli_core.rxnNames,'Citrate synthase','IgnoreCase',true));

disp('Substrates of citrate synthase:'); ...
    disp(e_coli_core.metNames(e_coli_core.S(:,rxn_cs_idx)<0))
```

```
Substrates of citrate synthase:
    {'H2O H2O'     }
    {'Oxaloacetate'}
    {'Acetyl-CoA'  }
```

```
disp('Products of citrate synthase:'); ...
    disp(e_coli_core.metNames(e_coli_core.S(:,rxn_cs_idx)>0))
```

```
Products of citrate synthase:
    {'H+'        }
    {'Citrate'   }
    {'Coenzyme A'}
```

```

```

- How many reactions are reversible?

```
sum(e_coli_core.rev)
```

```
ans = 46
```

```
% or
sum(e_coli_core.lb<0 & e_coli_core.ub>0)
```

```
ans = 46
```

- Which reaction flux is optimized?

```
e_coli_core.rxnNames(e_coli_core.c~=0)
```

```
ans = 1×1 cell array
    {'Biomass Objective Function with GAM'}
```

Solving LP with Cobra Toolbox

- Use *optimizeCbModel* to calculate the value of maximum flux through the reaction you identified to be optimized in task f. (1 point)

```
Sol = optimizeCbModel(e_coli_core)
```

```
Sol = struct with fields:
         full: [95×1 double]
          obj: 0.8127
        rcost: [95×1 double]
         dual: [72×1 double]
```

```
        slack: [72×1 double]
       solver: 'pdco'
    algorithm: 'default'
         stat: 1
     origStat: 0
         time: 0.0320
        basis: []
            f: 0.8127
            x: [95×1 double]
            v: [95×1 double]
            w: [95×1 double]
            y: [72×1 double]
            s: [72×1 double]
```

- Is the underlying LP homogeneous, which field in the model struct defines/shows this? (1 point)

```
if all(e_coli_core.b==0)
    disp('The LP is a homogeneous system.')
else
    disp('The  LP is a non-homogeneous system.')
end
```

```
The LP is a homogeneous system.
```

As output from optimizeCbModel you not only get the optimal value of , but also one solution for v.

- What is the flux through fumarase at the optimal solution? (1 point)

```
disp(['The flux through fumarase at the optimal biomass is: ' newline ...
num2str(Sol.x(contains(e_coli_core.rxnNames,'fumarase','IgnoreCase',true))) ...
' mmol/gDW/h']) % this if
```

```
The flux through fumarase at the optimal biomass is:
5.3011 mmol/gDW/h
```

The model contains reversible reactions.

Change the model such that each reversible reaction is splitted into two irreversible reactions, **without** the use of a function like *convertToIrreversible()*. (3 points)

```
% We have to update fields
% .S
% .rxns and rxnNames
% .lb and .ub
% .c

e_coli_core_irrev = e_coli_core;

% for each reversible reaction append matrix with a column that have oposite sign
% such that substrates become products and the other way around
e_coli_core_irrev.S = [e_coli_core.S -e_coli_core.S(:,e_coli_core.rev==1)];

% we append the list of rxn names by the original name extended with '_rev'
% for the backward direction
e_coli_core_irrev.rxns(end+1:end+sum(e_coli_core.rev)) = cellstr(strcat(e_coli_core.rxns(e_coli
e_coli_core_irrev.rxnNames(end+1:end+sum(e_coli_core.rev)) = cellstr(strcat(e_coli_core.rxnName
```

```
e_coli_core_irrev.lb(end+1:end+sum(e_coli_core.rev)) = 0; % add lb for backward rxns
e_coli_core_irrev.lb(e_coli_core.rev==1) = 0; % set lb for foreward rxn to zero

e_coli_core_irrev.ub(end+1:end+sum(e_coli_core.rev)) = e_coli_core.lb((e_coli_core.rev==1))*-1;
% since the negative lower bound is not necessarily -1000 we take the
% previous lower bound*-1 as new upper bound for reversible rxns

e_coli_core_irrev.c(end+1:end+sum(e_coli_core.rev)) = 0; % add objective coefficients for backw
e_coli_core_irrev.rev = zeros(size(e_coli_core_irrev.S,2),1); % mark all rxns as irreversible

Sol_irrev=optimizeCbModel(e_coli_core_irrev)
```

```
Sol_irrev = struct with fields:
         full: [141×1 double]
          obj: 0.8141
        rcost: [141×1 double]
         dual: [72×1 double]
        slack: [72×1 double]
       solver: 'pdco'
    algorithm: 'default'
         stat: 1
     origStat: 0
         time: 0.0080
        basis: []
            f: 0.8141
            x: [141×1 double]
            v: [141×1 double]
            w: [141×1 double]
            y: [72×1 double]
            s: [72×1 double]
```

An exchange reaction (e.g. A -> or -> B) is a reaction that only consumes or only produce a metabolite.

- How many import reactions are in the model? How many export reactions are in the model?

Hint: you can use the model with splitted reversible reactions from the step before, otherwise be careful that A <-> would be counted as import and export reaction. (3 points)

```
Import_rxn = find(all(e_coli_core_irrev.S>=0));
disp('Number of import reactions:'); ...
    disp(length(Import_rxn))
```

```
Number of import reactions:
     7
```

```
Export_rxn = find(all(e_coli_core_irrev.S<=0));
disp('Number of export reactions:'); ...
    disp(length(Export_rxn))
```

```
Number of export reactions:
    20
```