Manuals for the Maximum Entropy Principle with Lagrange Multiplier method algorithm

This algorithm consists of two main programs for: (I) optimization of Elementary Mode Coefficients (EMCs) by MEPLM and (II) prediction of a flux distribution by Enzyme Control Flux (ECF).

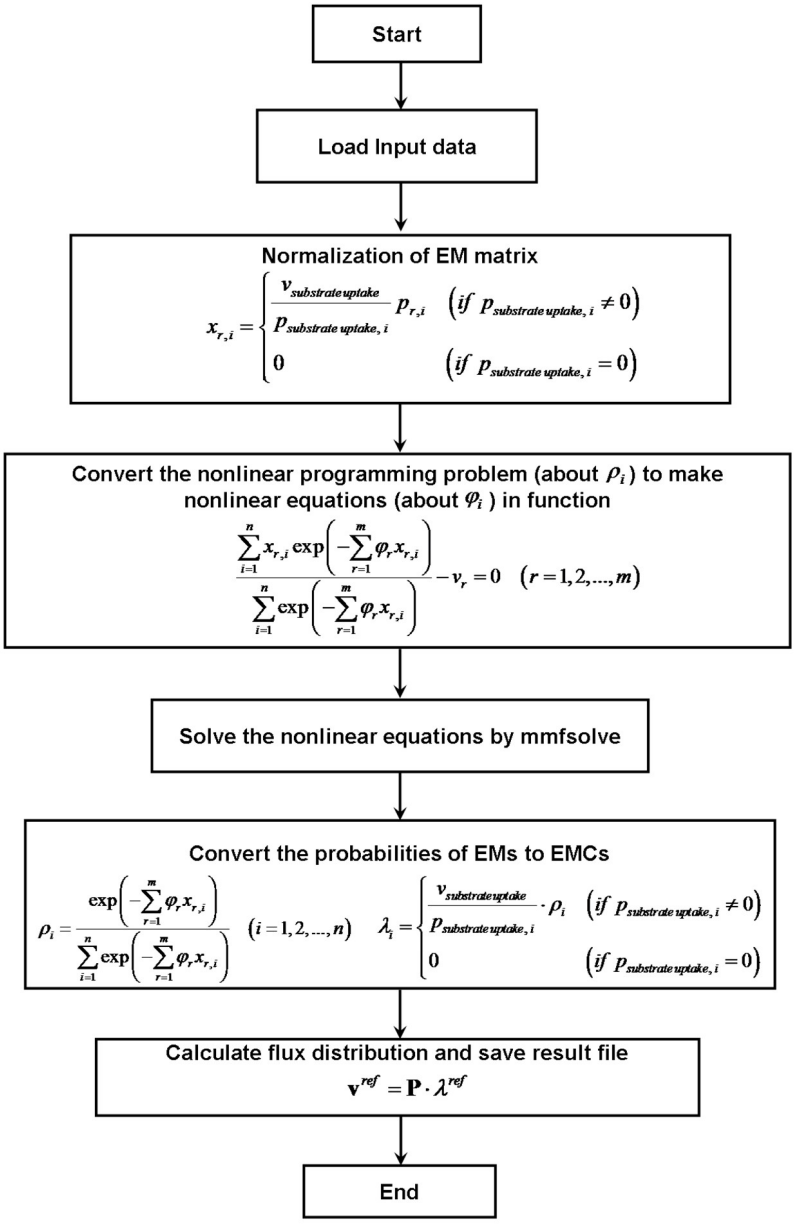

Figure S6. Schematic diagram of the MEPLM program

Program I: MEPLM_optimization.m

Input: MEPLM_optimization.mat

ems: whole matrix of elementary modes (reactions × elementary mode);

uptakeflux: flux for uptake reaction (1 × 1);

numuptake: the row in elementary mode matrix for uptake flux (1 × 1);

flux: flux for each reaction (1 × reactions);

Output: emc.mat

EMC: elementary mode coefficient (elementary mode × 1).

In matlab

>> MEPLM_optimization

ProgramII: ECFLM.m

Input: emm_flux_enzyme.mat, emc.mat

In emm_flux_enzyme.mat :

ems: whole matrix of elementary modes (reactions × elementary mode);

numuptake: the row in elementary mode matrix for uptake flux (1 × 1);

enzprofile: enzyme activity profile (reactions × 1);

In emc.mat:

EMC: the elementary mode coefficients optimized by MEPLM_optimization.m **(elementary mode × 1).**

Output: predictedflux.mat

predflux: predicted flux distribution (reactions × 1).

In matlab

>> ECFLM