Instructions for running the macromolecular model and the parameter estimation code

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Below, there are brief technical instructions for running the macromolecular model and the parameter estimation procedure. Please send an e-mail to Anne Willem Omta (omta@mit.edu), in case you encounter any problems.

The model code and input have been compressed into the file DalitDanielCode.tar.bz2. When working under Linux or Unix, this file can be unzipped into a directory named DalitDanielCode through the commands bunzip2 DalitDanielCode.tar.bz2 and tar -xvf DalitDanielCode.tar. Within this directory DalitDanielCode, the *.f files contain the FORTRAN code, whereas the *.txt files contain the batch culture data that are used as input of the parameter estimation procedure. The code for the burn-in and spinup stages is in the files Metropolis_Dalit.f and plaphy.f. Under Linux/Unix, the code may be compiled with

gfortran -o Metro Metropolis_Dalit.f plaphy.f plaphy_write.f

and the executable Metro is run as a background process with ./Metro &

The output file fort.42 will contain all the stored parameter sets. Then, Matlab or a statistical package can be used to calculate the means and standard deviations for the various parameters. The file fort.101 will contain 100 simulations with parameter sets accepted by the Metropolis algorithm, with time (days) in the 1st column, cell density (cells/ml) in the 2nd column, protein (ng/l) in the 3rd column, RNA (ng/l) in the 4th column, storage N (ng/l) in the 5th column, DIN (nM) in the 6th column, Chl (ng/l) in the 7th volumn, DNA (ng/l) in the 8th column, and carbohydrates+lipids (ng/l) in the 9th column.