Instructions for the parameter estimation code used in 'Quantifying nutrient throughput and DOM production by algae in continuous culture'

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Below, there are brief technical instructions for running the parameter estimation procedure used in 'Quantifying nutrient throughput and DOM production by algae in continuous culture' and viewing its output. Please send an e-mail to Anne Willem Omta (omta@mit.edu), in case you encounter any problems.

The procedure starts with a burn-in stage to approach the global optimum, followed by spinup stage to generate a first estimate of the means and standard deviations of the parameters. During these stages, the jump size is kept fixed. Subsequently, we take the jump size for each parameter equal to the standard deviation of that parameter as estimated during the spinup stage. This allows for a more effective exploration of the parameter space around the global optimum.

The model code and input have been compressed into the file MetroCode.tar.bz2. When working under Linux or Unix, this file can be unzipped into a directory named MetroCode through the commands bunzip2 MetroCode.tar.bz2 and tar -xvf MetroCode.tar. Within this directory MetroCode, the *.f files contain the FORTRAN code, whereas the *.txt files contain the chemostat 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_chemo_sim.f and rchemo_Solve_sim.f. Under Linux/Unix, the code may be compiled with

gfortran -o Metro Metropolis_chemo_sim.f rchemo_Solve_sim.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, with the 1st column being $y_{Ex,P,0}$, the 2nd column $y_{Ex,N,0}$, the 3rd column a_P, the 4th column a_N,

the 5th column $K_{P,i}$, the 6th column $K_{N,i}$, the 7th column $V_{m,P}$, the 8th column $V_{m,N}$, the 9th column $P_{m,C}$, the 10th column $K_{C,i}$, the 11th column $R_{C:P(DOP)}$, the 12th column $R_{C:N(DON)}$. Then, Matlab or a statistical package can be used to calculate the means and standard deviations for the various parameters. The code for the final stages is in the files Metropolis_chemo_res.f, rchemo_Solve_sim.f, and rchemo_Solve_wri.f. The parameter means and standard deviations calculated from the spinup stage have to be filled in as par(1) through par(12) and a(1) through a(12), respectively, in Metropolis_chemo_res.f, again in the order listed above. Under Linux/Unix, the code may be compiled with

gfortran -o Metro_wri Metropolis_chemo_res.f rchemo_Solve_sim.f rchemo_Solve_wri.f

and the executable Metro_wri is run as a background process with ./Metro_wri & The output file fort.52 will contain all the stored parameter sets of this last stage. Again, Matlab or a statistical package may be used to calculate the means and standard deviations for the various parameters and to plot the posterior distributions (histograms). The file fort.101 will contain the N:P, C:N, C:P, and residual phosphate concentrations and the file fort.102 will contain the N:P, C:N, C:P, and residual nitrate concentrations used to create Figure 3.