Instructions for using the parameter estimation software

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Below, there are brief technical instructions for using the parameter estimation software. An overview of the parameter estimation procedure is given in Appendix B of the article. Please send an e-mail to omta@mit.edu, in case you encounter any problems.

For the batch culture parameter estimation, there is first a spinup during which the Metropolis procedure with a root-mean-square jump size that is 5% of the initial-guess value for all the parameters. The code for this is in the files Metropolis_plankt.f and plaphy.f; necessary input files are Flynn_datC.txt, Flynn_datN.txt, Flynn_datChl.txt, Flynn_dat_time.txt. Under Unix, the code is compiled with

f95 -o Metro Metropolis_plankt.f plaphy.f

and the executable Metro is run as a background process with

./Metro &

The file fort.42 contains a write-out for each parameter at each 10th iteration; from this write-out, a standard deviation is calculated for each parameter which is used as the step size in the final part of the procedure. The file fort.43 contains a write-out for each parameter at the very last iteration which is used as input for the final part of the procedure. For that purpose, the name of the file needs to be changed: cp fort.43 fort.41.

For the final part of the procedure, the file Metropolis_plankt_res.f is used, with the standard deviations calculated from fort.42 filled in under a(1) through a(9). The code is compiled with

f95 -o Metro_res Metropolis_plankt_res.f plaphy.f

and the executable Metro_res is run as a background process with

./Metro_res &

This gives the output upon which Figs. 2 and 3 are based, as well as Table 1 and 2.

The chemostat parameter estimation works in the same fashion, with Metropolis_chemo_sim.f and rchemo_Solve_rev.f for the spinup and Metropolis_chemo_res.f and rchemo_Solve_rev.f for the final part of the procedure. The input files are d_Plim4AW.txt, CN_Plim4AW.txt, CP_Plim4AW.txt, and NP_Plim4AW.txt.