phytoParEffects.R (non-interactive R script)

Craig Snortheim

April 21, 2014

Directory Configuration

The script requires a *bin, sim, R,* and *results* folder on the same level within a directory. The *bin* folder contains glm32 and glm64 DLL files; *sim* folder contains the folders for each simulation; *R* folder contains the required R functions; *results* folder is folder in which results will be organized by this program.

Required Functions

The following functions (.R files) are required in the R folder mentioned above. These functions are sourced by the script:

GLMnetCDF.R	(Jordan Read & Luke Winslow)
GLM.nc.R	(Jordan Read & Luke Winslow)
getVarGLMnc.R	(Jordan Read & Luke Winslow; modified by Craig Snortheim)
phytoNMLedit.R	(Craig Snortheim)

Required Packages

rGLM

ncdf4

These two packages cannot be installed using the install.packages() function in R- follow the directions at the following site to first install ncdf4 and then rGLM:
https://github.com/GLEON/rGLM

Explanation of Settings Variables

basewd [character string]= base working directory- path to simulation folder of interest

simName [character string]= simulation name- name for the simulation; used to name the main results folder (along with the date-time of the run)

GLMncFile [character string]= GLM NetCDF file- name of the output file from GLM ("output.nc" by default)

exeName [character string]= executable name- name of the executable batch file to call to complete a run; make sure that the plotting functionality is turned off (ex. "glm_noplot.bat")

phytoFile [character string]= phytoplankton parameters file- name of the phytoplankton parameters file ("aed_phytoplankton_pars.nml" by default)

phytoList [character vector]= phytoplankton group list- a list of the names of the groups of phytoplankton of interest (as written in the phytoplankton parameters file)

parsList [character vector]= parameter list- a list of the names (symbols) of the parameters of interest, as written in the column headings of the parameter value table in the phytoplankton parameters file

parsInit [numeric vector]= initial parameter values- a vector of the initial/default parameter value in the order such that it corresponds to a parameter list loop nested inside a phytoplankton group list loop

Example:
```
phytoList<- c("micro", "chloro", "diatom")     #microcystis, chlorophytes, diatoms
parsList<- c("Pmax", "vT")        #max growth rate (/day); temperature scaling coef
parsInit<- c(0.5, 1.08, 0.5, 1.08, 1.25, 1.08)
```

Here, the first value of parsInit corresponds to the Pmax for micro; the second corresponds to the vT for micro; third corresponds to the Pmax for chloro; fourth corresponds to the vT for chloro; and so on. The order of the parameter values in parsInit is the parameters list embedded within the phytoplankton list.

sample.depth [numeric value]= sample depth- depth from surface (meters) at which to read the phytoplankton concentration from the GLM output

loop.counter [logical]= loop counter- if set to TRUE, the status of a the script (current loop/ total number of loops to be completed) will be printed to the console after each loop is completed

valueList [list object]= list of parameter values- each element valueList[[i]] corresponds to a vector of parameter values to be run for parameter parsList[i]

Example:
```
valueList<- list()
valueList[[1]]<- seq(from= 0.5, to= 1.6 , by= 0.1) #Pmax
valueList[[2]]<- seq(from= 1.05, to 1.10, by= 0.005) #vT
```

Following the previous example for parsInit, this valueList would run a simulation for each Pmax value from 0.5 to 1.6 in increments of 0.1 for each phytoplankton group in phytoList, and for each vT value from 1.05 to 1.10 in increments of 0.005 for each phytoplankton group in phytoList.

Script Output

All of the output from the script is written to a folder within the *results* folder. The main folder is named as the simName (set by user) followed by the date-time of the run in the format MMDDYYYY_HHMM. An example for a main folder name could be "Mendota07272014_1531".

Within this main folder, there are folders created for each run containing a time series CSV file for all phytoplankton species, including total phytoplankton (sum of all groups listed in phytoList). The units in these files are the default output from GLM, which is mmol-C/m^3. There is also a summary folder created for each phytoplankton group/parameter combination, which contains plots and CSV files of the following three items:

- Mean summer phytoplankton concentration
- Peak summer phytoplankton concentration
- Timing of peak summer phytoplankton concentration

"Summer" corresponds to June through August. There is one value for each phytoplankton group and parameter combination in the CSV files. The plots display only the phytoplankton group that is being

manipulated. Units in the CSV files are the default GLM units of mmol-C/m^3. Units on the plots are mg-C/m^3, since these units are usually more easily interpreted.

Running phytoParEffects.R

Run the script by simply clicking the "Source" button in R after editing the user settings in the script and saving the file.

Alternatively, one can use a batch file to run the script without R open. There are some complications with running R scripts from batch files in Windows, however. Below is a possible starting point for the batch file, but adjustments reflecting the user's operating system requirements and directory structure are necessary:

```
PATH C:\Program Files\R\R-3.0.2\bin\R
cd ..\..\R
Rscript phytoParEffects.R
Pause
```

The text following "PATH" should be the path to the R application on the user's computer. The text following "cd" should be the path to the phytoParEffects.R file. The third and fourth lines identify the R script to be run, and hold the command line window open to view any potential errors. The problem in Windows arises with the Rscript command not being recognized without edits to default system settings.

Cautionary Notes

- The text editing function phytoNMLedit.R is sensitive to changes in the structure of the phytoplankton parameters file, especially the data table at the bottom. When manually editing this file, be sure to preserve the original format. Tabs and spacing the data table should not be an issue, however, so long as the comma separator exists.
- There appears to be times when phytoplankton groups die out or grow to too high of a concentration, causing the FABM part of the model to crash. This leads to NA values in the output, and may cause an error in the phytoParEffects script if there are too many NA values (there will necessarily be an error if there are no non-NA values in the June-August time range). If this happens, try adjusting the parameter value ranges in the valueList variable to more realistic (or less extreme) values.