SHIMMER ReadMe, 6th May 2016

1. Hardware and Software Requirement

SHIMMER is written and can be executed in the free open source computing environment and programming language R, which is available for download on the web (http://www.r-project.org/). SHIMMER uses the adaptive time-step solver "lsoda" from the deSolve package (Soetaert et al., 2010) **which must also be installed**. On a standard desktop computer running R, the model usually takes less than 1 min to simulate 10 years of succession.

2. Download SHIMMER

A package named "SHIMMER", containing the source code of SHIMMER as well as example input and testing data is available at http://jamesbradleyweb.weebly.com/research.html under the sub-heading "SHIMMER" (click "**Download SHIMMER .zip package**").

The package contains one folder named "demo", containing 2 sub-folders:
1) demo_MAC (if you are running RStudio on a Mac)
2) demo_WIN (if you are running R on Windows)
The differences in the code are minor – mostly to do with plotting.

Within these two folders are further sub-folders:

- "SHIMMER": containing the model source code for a single run of SHIMMER.
- "input_data_Svalbard": containing the following time-series of forcings:
    - par.csv – solar radiation (already accounting for inhibition by snow)
    - temp.csv – soil temperature
    - snow.csv – snow depth
    - ICS1.csv – input (deposition) of C substrate (labile)
    - ICS2.csv – input (deposition) of (refractory)
    - IPON1.csv – input (deposition) of organic N (labile)
    - IPON2.csv – input (deposition) organic N (refractory)
    - IPOP1.csv – input (deposition) organic P (labile)
    - IPOP2.csv – input (deposition) organic P (refractory)
    - IDIN.csv – input (deposition) DIN
    - IDIP.csv – input (deposition) DIP
- "observations": field data.
    - "C_aut.dat": total autotrophic microbial biomass
    - "C_het.dat": total heterotrophic microbial biomass
    - "CS.dat": total organic carbon

The entire "demo" folder should be copied to a local computer such that the directory is: "C:/RFolder/model/demo/" (Windows) **or** "/Users/jamesbradley/Documents/RFolder/model/demo/" (Macintosh) **or** the folder paths contained in SHIMMER.R script should be modified (*path*, *path_root*, *pathdr* and *pathte*) according to where the "demo" folder is copied to.

3. Source Code Files Description

This section provides a brief description of all source code files present in the sub-folder "SHIMMER". This should be read alongside the SHIMMER (1.0) *Geoscientific Model Development* publication (Bradley et al., 2015) for clarity on variables, parameters, balance equations etc.

SHIMMER.R

- Specify length of model run here (nyears) (note: must be a positive integer).
- Execute this code (copy and paste into R Console window) to run the model.

Library > SHIMMER_set_parameter_values.R

- Specify parameter values here.
- The default settings of the model correspond to the Midtre Lovénbreen forefield, Svalbard (Bradley et al., 2016).
- See Bradley et al. (2015) for a description of parameters.

Library > SHIMMER_NEW_load_and_make_drivers.R

- Load the forcing data and replicate for duration of model run (nyears).
- Note: forcing data must be specified as daily values (as per examples).

Library > SHIMMER_set_start_values.R

- Specify initial conditions here (starting value for each state-variable).

Library > SHIMMER_NEW_model_definition.R

- Contains the equations which formulate the model.

Library > SHIMMER_compute_totals.R

- Derive rates from time-series of output variables.

Library > SHIMMER_construct_array.R

- Construct 3-D array from output variables.

Library > SHIMMER_basic_plots.R

- Examples of basic plots of model output.

4. Model Operation

In R, specify working directory to: "C:/RFolder/model/demo/demo_WIN/SHIMMER/" (if using Windows. For Mac, change path as appropriate).

Open SHIMMER.R script and execute in console (note: package "deSolve" (Soetaert et al., 2010) must be installed).

To run the model, copy and paste the *SHIMMER.R* script into the R Console window.

5. Output

Model output is created as variables within R (out, out2 and out_array). By default, they are not saved locally, however this can be done by using a command such as:

write.table(out,file=paste("out","model_run.csv",sep="_"),sep=",",row.names=FALSE)

The dataframe “out” is a 2-D time-series of output data comprised of columns for each output (variables, totals and rates), and rows for each day simulated. All units are in μg g^{-1} dry soil or equivalent.

Column Name	Description	Column Name	Description
time	Day of simulation	*cum_I_Sub*	Cumulative C substrate input
A1	A1 biomass	*cum_G_X*	Cumulative C substrate from losses (G) and exudates (X)
A2	A2 biomass	*years*	Year of simulation
A3	A3 biomass	*A_total*	Total autotrophic biomass
H1	H1 biomass	*H_total*	Total heterotrophic biomass
H2	H2 biomass	*S_total*	Total C substrate
H3	H3 biomass	*Cmic_total*	Total microbial biomass
S1	C substrate (labile)	*PON_total*	Total organic nitrogen
S2	C substrate (refractory)	*POP_total*	Total organic phophorus
DIN	Dissolved Inorganic Nitrogen	*cum_A*	Cumulative growth (production) of autotrophs
DIP	Dissolved Inorganic Phosphorus	*cum_H*	Cumulative growth (production) of heterotrophs
PON1	Organic Nitrogen (labile)	*rate_A1*	Daily A1 growth rate
PON2	Organic Nitrogen (refractory)	*rate_A2*	Daily A2 growth rate
POP1	Organic Phosphorus (labile)	*rate_A3*	Daily A3 growth rate
POP2	Organic Phosphorus (refractory)	*rate_H1*	Daily H1 growth rate
cum_A1	Cumulative growth (production) of A1	*rate_H2*	Daily H2 growth rate
cum_A2	Cumulative growth (production) of A2	*rate_H3*	Daily H3 growth rate
cum_A3	Cumulative growth (production) of A3	*rate_DIC_A*	Daily DIC from autotrophs
cum_H1	Cumulative growth (production) of H1	*rate_DIC_H*	Daily DIC from heterotrophs
cum_H2	Cumulative growth (production) of H2	*rate_DIN*	Daily DIN assimilation
cum_H3	Cumulative growth (production) of H3	*rate_nf*	Daily nitrogen fixation
cum_DIC_A	Cumulative DIC from autotrophs	*rate_A*	Daily autotrophic growth (production)
cum_DIC_H	Cumulative DIC from heterotrophs	*rate_H*	Daily heterotrophic growth (production)
cum_DIN	Cumulative DIN assimilated into biomass	*rate_I_Sub*	Daily C substrate input

cum_nf	Cumulative nitrogen fixed	*rate_G_X*	Daily loss (*G*) and exudate (X) input
		rate_G	Daily loss (*G*) (necromass) input
		rate_X	Daily exudate (*X*) input

The dataframe "out2" is a 2-D time-series of annual totals (or rates), comprised of columns for each output, and rows for each year simulated. All units are in µg g^{-1} dry soil or equivalent.

Column Name	Description	Column Name	Description
year	Year of simulation	*annual_DIC_A*	Total annual DIC efflux from autotrophs
annual_A1	Total annual A1 production (biomass growth)	*annual_DIC_H*	Total annual DIC efflux from heterotrophs
annual_A2	Total annual A2 production	*annual_DIN*	Total annual DIN assimilated from soil
annual_A3	Total annual A3 production	*annual_nf*	Total annual nitrogen fixed from air
annual_H1	Total annual H1 production	*annual_A*	Total annual autotrophic production
annual_H2	Total annual H2 production	*annual_H*	Total annual heterotrophic production
annual_H3	Total annual H3 production		

The array "out_array" is a 3-D array of data from "out". The columns (x- axis) represent each output variable, total and rate, the rows (y-axis) represent each day of the year (1-365), and the depth (z-axis) represents each year. For example, out_array[2,5,3] is the biomass of A1 (the 2nd column in out) for the 5th day of the 3rd year. All units are in µg g^{-1} dry soil or equivalent. The purpose of the array is that it is simpler to average and sum data across specific time-intervals.

References

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BRADLEY, J. A., ARNDT, S., ŠABACKÁ, M., BENNING, L. G., BARKER, G. L., BLACKER, J. J., YALLOP, M. L., WRIGHT, K. E., BELLAS, C. M., TELLING, J., TRANTER, M. & ANESIO, A. 2016. Microbial dynamics in a High-Arctic glacier forefield: a combined field, laboratory, and modelling approach. Biogeosciences Discuss., 2016**,** 1-34.

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