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Simulating Plankton Evolution with Adaptive Dynamics in 3 spatial Dimensions (SPEAD-3D model)

User guide to compile, execute and modify the SPEAD-3D model

This user guide is designed to reproduce the results of the SPEAD-3D simulations presented in the paper called *"Oceanic circulation and resource limitation control the global patterns of phytoplankton diversity"* submitted to *Science* in September 2025.

This user guide is designed to be short. Feel free to ask any question.

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I/ Downloading the SPEAD-3D model

The SPEAD-3D model is a plankton eco-evolutionary model written in FORTRAN 77. It was developed by modifying the pre-existing ecosystem model of the MIT Darwin project (https://darwinproject.mit.edu/). As SPEAD-3D simulates the global ocean in 3 dimensions, and as advection and mixing by oceanic currents play a key role in plankton ecology, the SPEAD-3D model requires inputs of current speed and vertical diffusivity along all three spatial dimensions (longitude, latitude, depth), which are taken from simulation outputs of the MIT general circulation model (MITgcm). Inputs of photosynthetically active radiation, iron atmospheric deposition, and temperature (the latter from MITgcm) are also required. Finally the outputs, consisting of binary files (.data) and metadata (.meta), are read using a Matlab script.

The SPEAD-3D code (FORTRAN code, namelists and execution scripts) by itself is available on GitHub (https://github.com/oceanglobe/SPEAD-3D_default) and will be made available on Zenodo upon publication.

The Matlab script for output analysis and the physical input files are available on the webpage of the Ocean Globe Laboratory (http://oceanglobe.info/FORTRAN/MITgcm_SPEAD3D/SPEAD_3D_archives_zipped.zip)

Due to its computational cost, SPEAD-3D is not designed to run on a personal computer, but on a high performance cluster, using parallel computing.

II/ Architecture of the SPEAD-3D model

We called "SPEAD/" the master directory of the model.

The "SPEAD/MITgcm/" directory contains the standard version of MITgcm + Darwin-3. It is recommended not to change any file in this directory.

The "SPEAD/ECCOgcm/" directory contains the physics outputs (temperature, current speed and turbulent diffusivity) from a 1° x 1° MITgcm simulation, which we use as input for SPEAD-3D. In the GitHub repository, this directory is empty because the files are too heavy to be stored here. However, you can download the physical input files on the webpage of the Ocean Globe Laboratory (https://oceanglobe.org/contact/)

The “SPEAD/Matlab/” directory contains the Matlab analysis script and the Matlab functions required by the script.

The “SPEAD/SPEAD-merge/” directory contains all files specific to SPEAD-3D. It is called “merge” because the files it contain can also be used to run the model in a vertical 1D setting or with discrete ecotypes. However, the default version of SPEAD-3D is global, three-dimensional in space and based on a continuous-trait approach.

- The “SPEAD/SPEAD-merge/code/” subdirectory contains all the files of the FORTRAN code that differ from the standard version of MITgcm + Darwin-3. Any future development of the code should be done in this folder, not in the “MITgcm” folder.

- The “SPEAD/SPEAD-merge/data” subdirectory contains all the SPEAD-3D model parameters that can be changed without re-compiling, in the format of namelists.

- The “SPEAD/SPEAD-merge/input” subfolder contains some physical input files necessary to run the SPEAD-3D model, such as surface PAR and iron deposition.

- The SPEAD-3D model executable is built in the “SPEAD/SPEAD-merge/make” subfolder, producing an executable called “mitgcmuv”. In this subfolder, the compilation process also writes symbolic links to all the FORTRAN function files used to build the code. The address of these FORTRAN files may be in “SPEAD/MITgcm/” (standard MITgcm + Darwin-3) or in “SPEAD/SPEAD-merge/code/” (code specific to SPEAD-3D)

- The “SPEAD/SPEAD-merge/output/” subdirectory is where the SPEAD-3D model runs and where all its outputs are stored. Outputs take the form of binary files containing all the numerical values of the outputs at each grid point (“.data” files) and metadata files containing metadata such as the dimension of the grid or the number of tracers (“.meta” files). The names of the output files (for instance “TRAC_0000144000.data”) contain a time stamp (“0000144000” = last month of the 50^{th} year) and a tracer class (“TRAC” = state variables of SPEAD-3D)

- The “SPEAD/SPEAD-merge/run/” subdirectory is where the compilation and execution scripts are launched. These scripts then automatically write in “make/” and “output/” respectively. Once the SPEAD-3D moel is compiled, the executable file is also stored in the “run/” subdirectory.

III/ Compiling and executing the SPEAD-3D model (SPEAD/SPEAD-merge/run/)

To compile SPEAD-3D, go to the “SPEAD/SPEAD-merge/run” directory, and execute the Shell script called “compile_SPEAD_3D.sh”.

> ./compile_SPEAD_3D.sh

If the compilation works correctly, an executable called “mitgcmuv” should appear. This executable cannot be executed directly, but only through an execution script called “run_script_3D.sh”

> sbatch run_script_3D.sh

The scripts and the command to run them may have to be modified depending on the cluster.

IV/ Modifying the SPEAD-3D model (SPEAD/SPEAD-merge/code/ and SPEAD/SPEAD-merge/data)

The SPEAD-3D model can be modified in two different ways:

- Parameter values (for instance the half-saturation of phytoplankton for iron) can be directly modified in a namelist in the "SPEAD/SPEAD-merge/data" directory, without re-compiling. Relevant examples include the following:

  - The number of time steps (nIter0), the duration in s of each time step (deltaTtracer) or the size of model boxes (delX in °, delY in °, delZ in m) are set in "data".

  - The addresses of the input files from the MITgcm physics simulation are written in "data.off".

  - In "data.diagnostics", the SPEAD-3D model variables that must be written in output files are specified.
    For each output file various fields must be defined:
    - The name of the files ("filename"), for instance "TRAC", "FPP" or "TRENDS".
    - The frequency of outputs in s ("frequency"). By default: 1 month.
    - The time of the first output ("timephase"). This can be used for instance to produce output files for the last year of simulation only.
    - The depth levels of outputs ("levels"). By default: the 9 first levels, that is, 0-265m.
    - The short name of each output variable ("fields"). All potential output variables and their short names are listed in "SPEAD/SPEAD-merge/run/available_diagnostics.log"

  - The "data.ptracers" file contains the number of tracers ("PTRACERS_numInUse") used in the model, the advection and diffusion schemes used for each tracer, the units of each tracer ("ptracers_units"), the initial conditions ("PTRACERS_initialFile" and "ptracers_ref") and the names ("PTRACERS_names") of each tracer.

  - The ecological parameters of SPEAD-3D, including the parameters presented in Le Gland et al. (2025), can be modified in "data.darwin".

- More substantial changes in how the code works (for instance, replacing the Michaelis-Menten nutrient uptake function by another function) require changes in the FORTRAN code itself, in the "SPEAD/SPEAD-merge/code" directory, and re-compilation. Here we briefly define the most important of these files:

  - SIZE.h: Physical dimensions

  - PTRACERS_SIZE.h: Number of biogeochemical tracers ("PTRACERS_num"), including both non-living (nutrients and organic matter) and living tracers.

  - DARWIN_SIZE.h: Number of living tracers (nTrac) and other key numbers of the ecological moel.

  - DARWIN_OPTIONS.h: Compilation options can be defined (#define) or undefined (#undef) here. Most compilation options add or remove a physical or biological process (for instance selective grazing on the most abundant ecotypes), or change the way a process is simulated (e.g. discrete or continuous approach to phytoplankton diversity).

- darwin_generate_constant.F: Set the values of biogeochemical constants, including some plankton traits. Called at the beginning of the simulation.

- darwin_generate_allometric.F: Same as above, but called at each time step for each grid box. Sets all the constants that depend on the trait distribution.

- darwin_plankton.F: Master function for all biogeochemical and ecological processes

- darwin_spead_phyto.F: Phytoplankton nutrient uptake, photosynthesis and growth.

- darwin_spead_remin.F: Remineralization of organic matter. Bacterial growth is computed here if bacteria are activated (not the case by default in SPEAD-3D).

- darwin_grazing.F: Grazing by zooplankton and mortality of all plankton types.

• SPEAD-3D can also be run using the more classical but more expansive discrete approach, where the phytoplankton state variables are the biomasses of discrete ecotypes with fixed ecophysiological traits.
Switching approaches requires changes in “data.diagnostics”, “data.ptracers” related to the number and names of tracers, and also to undefine two compilation keys (#undef SPEAD_CONTINUOUS_TRAIT / #undef SPEAD_CONTINUOUS_VARIANCE) in DARWIN_OPTIONS.h.

  SPEAD-3D can also be downgraded to a vertical 1D setting, with physics forcings from BATS station in the Sargasso Sea.
  Reducing the dimension of SPEAD requires changes in the files “data”, “data.off”, “data.diagnostics”, “data.ptracers”, “data.darwin” and “SIZE.h”,

  The script “spead_mode.sh” is designed to make all the required changes automatically, although none of these alternatives modes is necessary to reproduce the results of Le Gland et al. (2025).

V/ Analysing model results (Matlab script)

All the figures shown in Le Gland et al. (2025) were plotted using a post-processing script written in Matlab (version R2023b) and named “SPEAD-3D_ReadFortranOutputs”. All the functions called by this script are present in the “SPEAD/Matlab/” directory.

The analysis can be performed on any computer, not necessarily on the computationcluster. The output files defined in “SPEAD/SPEAD-merge/data/data.diagnostics” and stored in “SPEAD/ SPEAD-3D/output” must first be downloaded from the cluster.

Final Disclaimer: Absolute paths

In some files the absolute paths (starting by “/home/SPEAD/”) to some other files are written. This is the case for instance in “data”, “data.off”, “data.darwin”, “data.ptracers”, “run_script_3D.sh” and “spead_mode.sh”. These absolute paths will have to be adapted to the file system architecture of the computer where the SPEAD-3D model is executed.