

PlanktonIndividuals.jl: A GPU supported individual-based phytoplankton life cycle model.

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Software

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Summary

Marine phytoplankton contributes ~50% of the total primary production on Earth forming the basis of the food web in the oceans. Understanding the spatial distribution and temporal variations of the phytoplankton community is essential to the global carbon and nutrient cycles. PlanktonIndividuals.jl is a fast individual-based model that represents the phytoplankton life cycle in detail, is written in Julia, and runs on both CPU and GPU. The model is used to elucidate temporal and spatial variations in phytoplankton cell density and stoichiometry, as well as growth and division behaviors induced by diel cycle and physical motions ranging from sub-mesoscale to large scale processes.

PlanktonIndividuals.jl can simulate multiple functional groups of phytoplankton with different growth and division strategies. It can thus effectively represent the interactions within and between functional groups. It simulates phytoplankton cells as Lagrangian particles (moving frame) while nutrients are represented as Eulerian tracers (fixed frame). The model thus takes advantage of both frameworks – Eulerian simulations employ a fixed mesh to represent flow fields on a grid, while plankton individuals move following the velocity field interpolated to their locations.

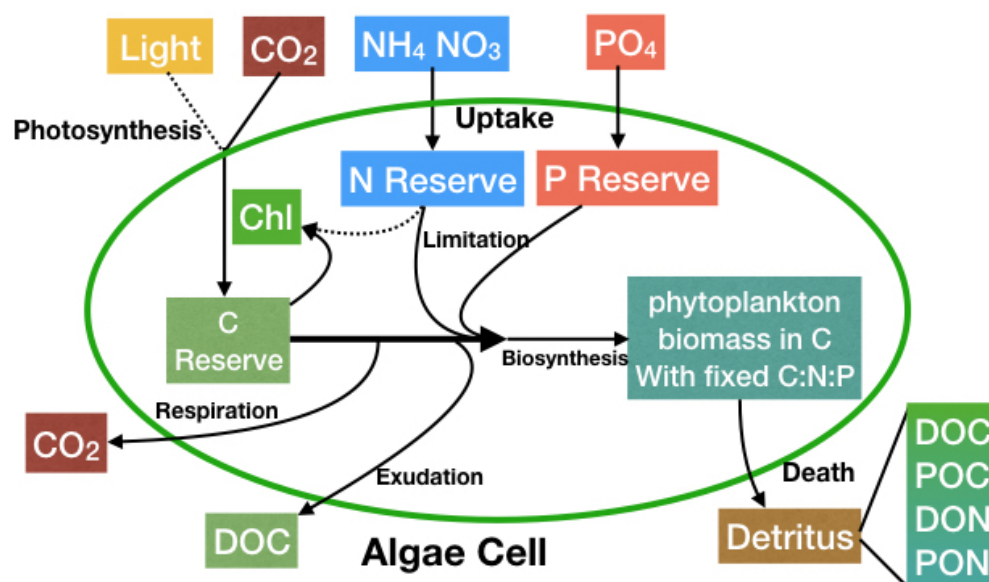


Figure 1: Schematic diagram of phytoplankton physiology described in PlanktonIndividuals.jl.

The equations included in PlanktonIndividuals.jl to describe phytoplankton physiology are

22 state of the art (Figure 1) with the widely-used Droop model (Droop, 1973) implemented for
23 nutrient uptakes. The photosynthesis formulation by Geider et al (Geider et al., 1997) is also
24 implemented for carbon fixation. Additionally, exudation and mixotrophy are also accounted
25 for in the model (Wu et al., 2021). Both simulated phytoplankton cells and nutrient tracers are
26 advected by the same velocity field provided externally. The growth rate and nutrient uptake
27 rates of each simulated cell are decided by the nutrient availability, light intensity, and ambient
28 temperature at the position of the cell. And in turn, the nutrient consumed or released by
29 phytoplankton cells are added to (or subtracted from) the nutrient fields at the grid point the
30 cells are in.

31 The simulations can be set up not only in a zero-dimensional domain (like lab experiments) but
32 also in one-, two-, or three-dimensional domains. The external inputs required by the package
33 include velocity fields, temperature fields, and surface photosynthetically active radiation
34 (PAR) fields. Our package is able to use velocity and temperature fields provided by different
35 fluid dynamic models (e.g. Oceananigans.jl, MITgcm, etc.) and observations. Two default
36 parameter sets are included in the package, biogeochemical parameters of nutrient tracers, and
37 phytoplankton physiological parameters for individual phytoplankton cells. These parameters
38 can be varied to simulate different phytoplankton species and biogeochemistry. The outputs of
39 PlanktonIndividuals.jl include time series of individual trajectories, cell density, biomass,
40 and vital rates such as cell division rates, photosynthesis rate, and nutrient uptake rates
41 (Figure 2).

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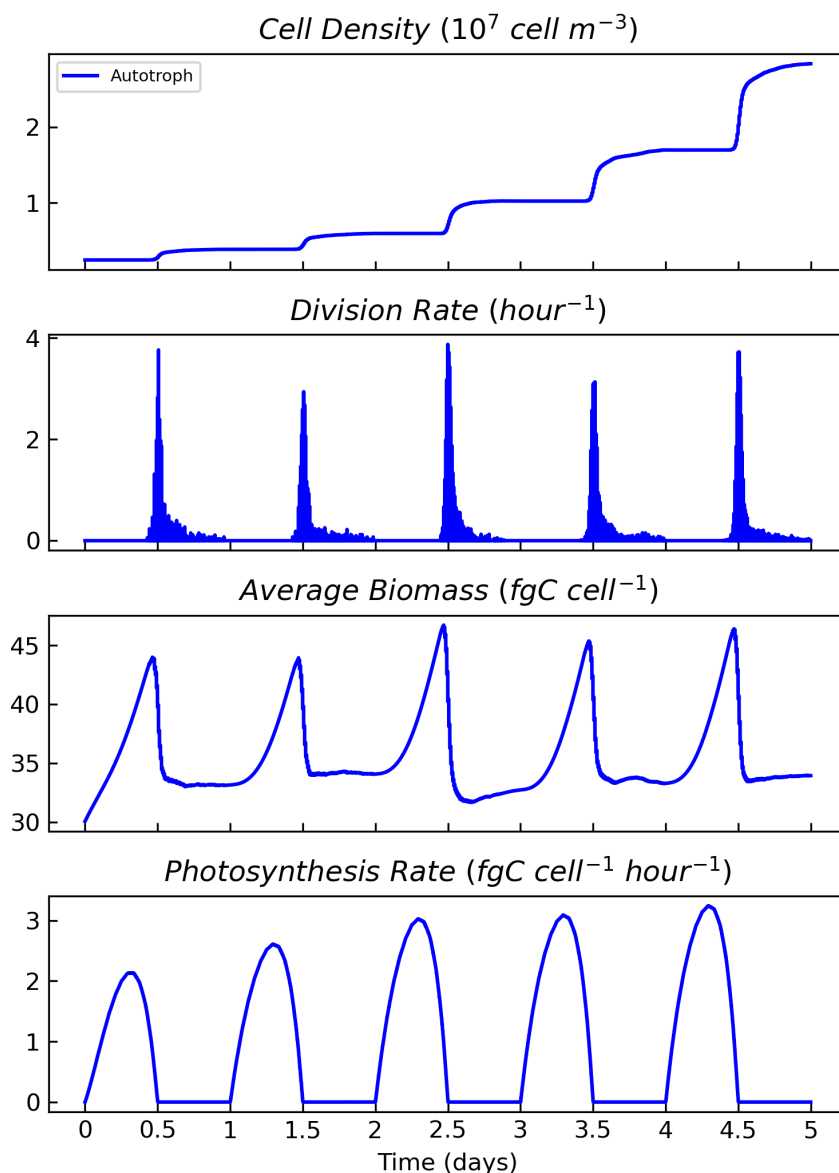


Figure 2: Model results of a 0-dimensional setup.

Statement of need

Phytoplankton models, like those incorporated in ecological and biogeochemical models, are essential tools to explore and understand phytoplankton life cycles, interactions between species, population dynamics, and community structures in various water bodies (e.g. lakes, coastal waters, and open ocean) (Follows et al., 2007; Geider et al., 1997). Individual-based / Lagrangian models differ from Eulerian models in the way they represent heterogeneous populations like cells of different sizes, nutrient quotas, and life cycle stages (Clark et al., 2011;

49 [Hellweger et al., 2014, 2016](#)).

50 The unique power of individual-based modeling lies in the ability to track the position, biomass,
51 and physiological state of individual cells or plankton patches, as they move through space over
52 time. Eulerian models in turn can only track the density of plankton biomass in “well-mixed”
53 grids of simulated water bodies. Furthermore, individual-based models are able to introduce
54 randomness in individuals which allows stochastic processes (e.g. cell division, grazing, death
55 etc.) to reproduce the diversity found in real ecosystems.

56 Due to computational limitations, previous microbial individual-based models could only
57 simulate a limited number of individuals, with each individual representing cell populations
58 rather than individual cells ([Hellweger et al., 2016](#)). In order to overcome this obstacle,
59 `PlanktonIndividuals.jl` exploits the power of Graphical Processing Units (GPUs) which
60 were first developed for video rendering but now offer extremely efficient, highly parallelized
61 computing power. With GPU support, the simulations in `PlanktonIndividuals.jl` are sped
62 up over 50 times compared with CPU simulations.

63 There are many software packages for individual-based modeling, both in Julia or other
64 programming languages, aimed at different purposes. For example, `NetLogo` ([Wilensky, 1999](#))
65 and `Agents.jl` ([Datseris et al., 2021](#)) provide generic agent-based frameworks – with
66 a focus on generality but lack of physical and biogeochemical equations, which are the
67 core of `PlanktonIndividuals.jl`. In contrast, `oceanParcels` ([Lange & Seville, 2017](#)) and
68 `IndividualDisplacements.jl` ([Forget, 2021](#)) focus on the Lagrangian simulation of individual
69 displacements in the ocean and climate system. However, these packages mainly focus on
70 simulation of passive particles that do not feed back on gridded variables. In addition, they do
71 not include detailed equations of phytoplankton physiology and biochemistry.

72 Our package is unique in the way that it is tailored to the analysis of marine ecosystems across
73 a wide range of scales using HPC systems. To this end, `PlanktonIndividuals.jl` provides a
74 comprehensive description of phytoplankton physiology and biogeochemistry, written in a fast
75 language, Julia, and with GPU support. It further innovates in combining the Eulerian and
76 Lagrangian perspectives. Plankton individuals (Lagrangian) indeed have a two-way interactions
77 with gridded nutrient fields (Eulerian) that are advected by the same flow fields (in 1D, 2D or
78 3D) in our package.

79 To illustrate the two representations of advective processes in the model (Eulerian + Lagrangian),
80 we performed a one-year simulation of a passive tracer, initialized to a concentration of 1
81 below 50m depth and 0 above 50m depth, along with 512 particles moving in three dimensions
82 ([Figure 3](#)).

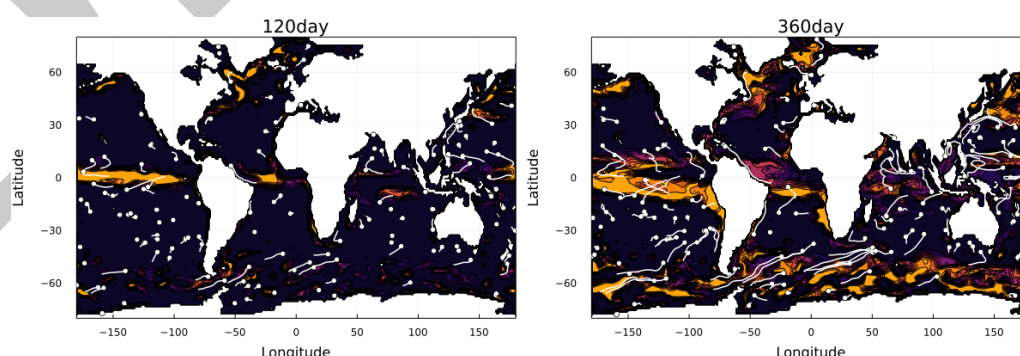


Figure 3: Model results of a 3-dimensional setup. The map shows the concentration of a passive tracer. White dots represent the individuals with their trajectories shown in white liens.

83 Further development plans include implementation of macro-molecular model ([Inomura et al., 2020](#))
84 and support for distributed parallelism with CUDA-aware MPI.

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