

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

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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.

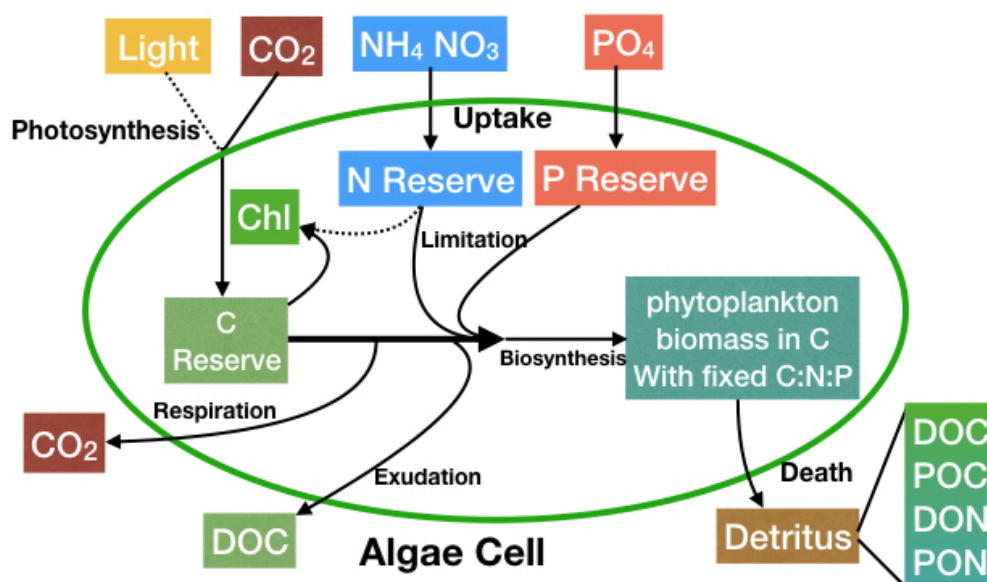


Figure 1: Schematic diagram of phytoplankton physiology described in PlanktonIndividuals.jl.

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

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

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

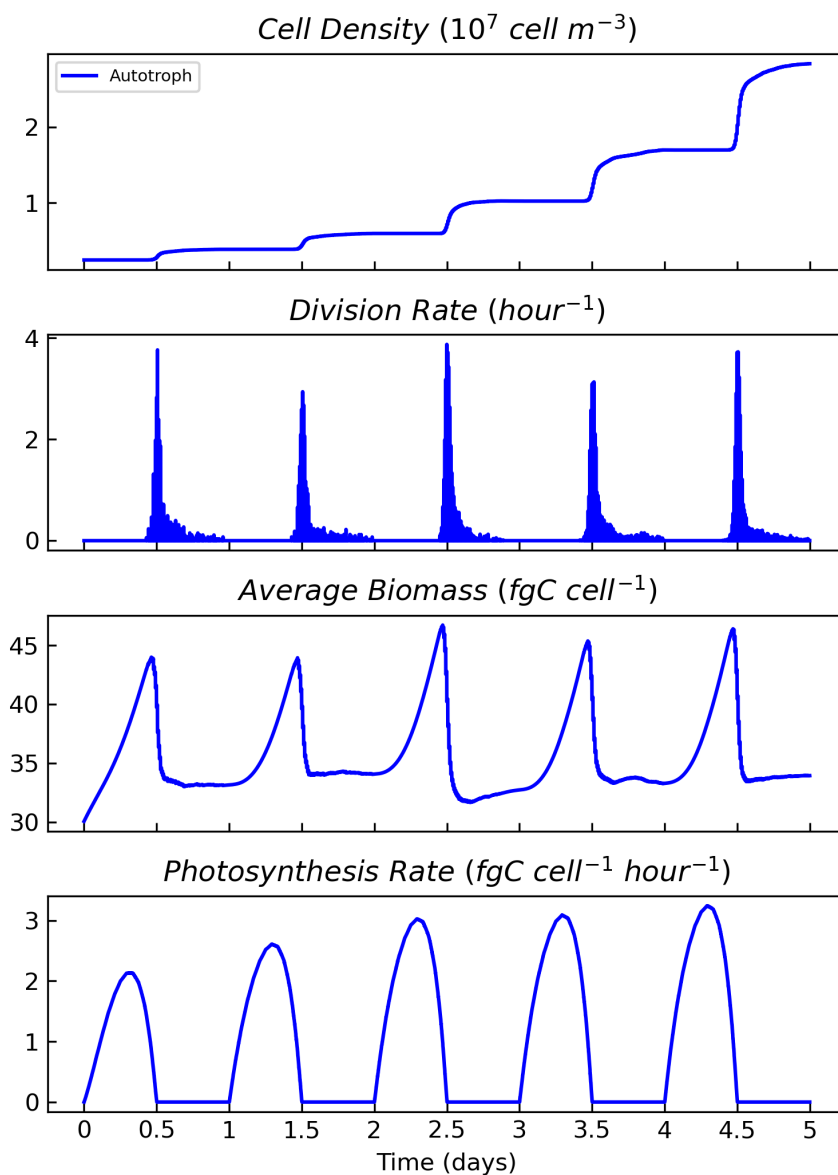


Figure 2: Model results of a zero-dimensional setup.

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](#);

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

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

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

There are many software packages for individual-based modeling, both in Julia and other programming languages, aimed at different purposes. For example, `NetLogo` ([Wilensky, 1999](#)) and `Agents.jl` ([Datseris et al., 2022](#); [Vahdati, 2019](#)) provide generic agent-based frameworks – with a focus on generality but lack of physical and biogeochemical equations, which are the core of `PlanktonIndividuals.jl`. In contrast, `oceanParcels` ([Lange & Seville, 2017](#)) and `IndividualDisplacements.jl` ([Forget, 2021](#)) focus on the Lagrangian simulation of individual displacements in the ocean and climate system. However, these packages mainly focus on simulation of passive particles that do not feed back on gridded variables. In addition, they do not include detailed equations of phytoplankton physiology and biochemistry.

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

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

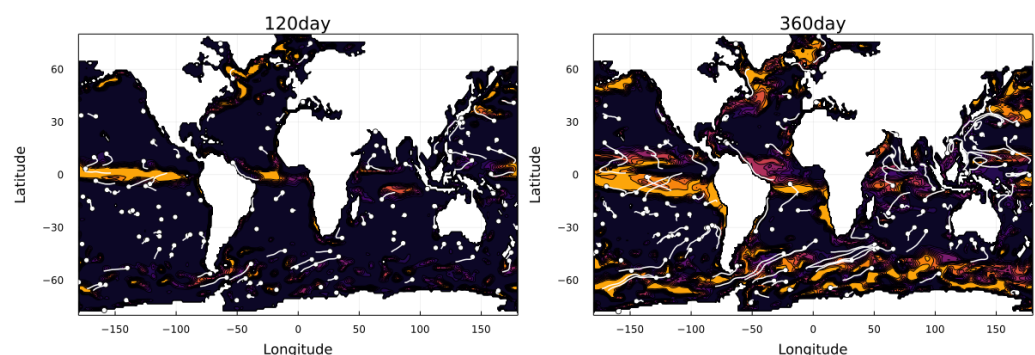


Figure 3: Model results of a three-dimensional setup. The map shows the concentration of a passive tracer. White dots represent the individuals with their trajectories shown in white lines.

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

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References

- Clark, J. R., Daines, S. J., Lenton, T. M., Watson, A. J., & Williams, H. T. (2011). Individual-based modelling of adaptation in marine microbial populations using genetically defined physiological parameters. *Ecological Modelling*, 222(23-24), 3823–3837. <https://doi.org/10.1016/j.ecolmodel.2011.10.001>
- Datseris, G., Vahdati, A. R., & DuBois, T. C. (2022). Agents.jl: A performant and feature-full agent-based modeling software of minimal code complexity. *SIMULATION*, 0(0), 0037549721106888. <https://doi.org/10.1177/003754972110688820>
- Droop, M. R. (1973). Some thoughts on nutrient limitation in algae. *Journal of Phycology*, 9(3), 264–272. <https://doi.org/10.1111/j.1529-8817.1973.tb04092.x>
- Follows, M. J., Dutkiewicz, S., Grant, S., & Chisholm, S. W. (2007). Emergent biogeography of microbial communities in a model ocean. *Science*, 315(5820), 1843–1846. <https://doi.org/10.1126/science.1138544>
- Forget, G. (2021). IndividualDisplacements.jl: A julia package to simulate and study particle displacements within the climate system. *Journal of Open Source Software*, 6(60), 2813. <https://doi.org/10.21105/joss.02813>
- Geider, R., MacIntyre, H., & Kana, T. (1997). Dynamic model of phytoplankton growth and acclimation: Responses of the balanced growth rate and the chlorophyll a: Carbon ratio to light, nutrient-limitation and temperature. *Marine Ecology Progress Series*, 148, 187–200. <https://doi.org/10.3354/meps148187>
- Hellweger, F. L., Clegg, R. J., Clark, J. R., Plugge, C. M., & Kreft, J.-U. (2016). Advancing microbial sciences by individual-based modelling. *Nature Reviews Microbiology*, 14(7), 461–471. <https://doi.org/10.1038/nrmicro.2016.62>
- Hellweger, F. L., Sebille, E. van, & Fredrick, N. D. (2014). Biogeographic patterns in ocean microbes emerge in a neutral agent-based model. *Science*, 345(6202), 1346–1349. <https://doi.org/10.1126/science.1254421>
- Inomura, K., Omta, A. W., Talmy, D., Bragg, J., Deutsch, C., & Follows, M. J. (2020). A mechanistic model of macromolecular allocation, elemental stoichiometry, and growth rate in phytoplankton. *Frontiers in Microbiology*, 11, 86. <https://doi.org/10.3389/fmicb.2020.00086>
- Lange, M., & Sebille, E. van. (2017). Parcels v0.9: Prototyping a lagrangian ocean analysis framework for the petascale age. *Geoscientific Model Development*, 10(11), 4175–4186. <https://doi.org/10.5194/gmd-10-4175-2017>
- Vahdati, A. R. (2019). Agents.jl: Agent-based modeling framework in julia. *Journal of Open Source Software*, 4(42), 1611. <https://doi.org/10.21105/joss.01611>
- Wilensky, U. (1999). *NetLogo*. <http://ccl.northwestern.edu/netlogo/>

Wu, Z., Dutkiewicz, S., Jahn, O., Sher, D., White, A., & Follows, M. J. (2021). Modeling photosynthesis and exudation in subtropical oceans. *Global Biogeochemical Cycles*, 35(9), e2021GB006941. <https://doi.org/10.1029/2021gb006941>