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

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Summary

`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. It simulates phytoplankton cells as Lagrangian particles while nutrients are represented as Eulerian tracers taking the advantage of both types of models in one framework.

The model is used to elucidate temporal and spatial variations in phytoplankton cell density, stoichiometry, as well as growth and division behaviors induced by diel cycle and physical motions ranging from sub-mesoscale to large scale processes. The phytoplankton physiology model is 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).
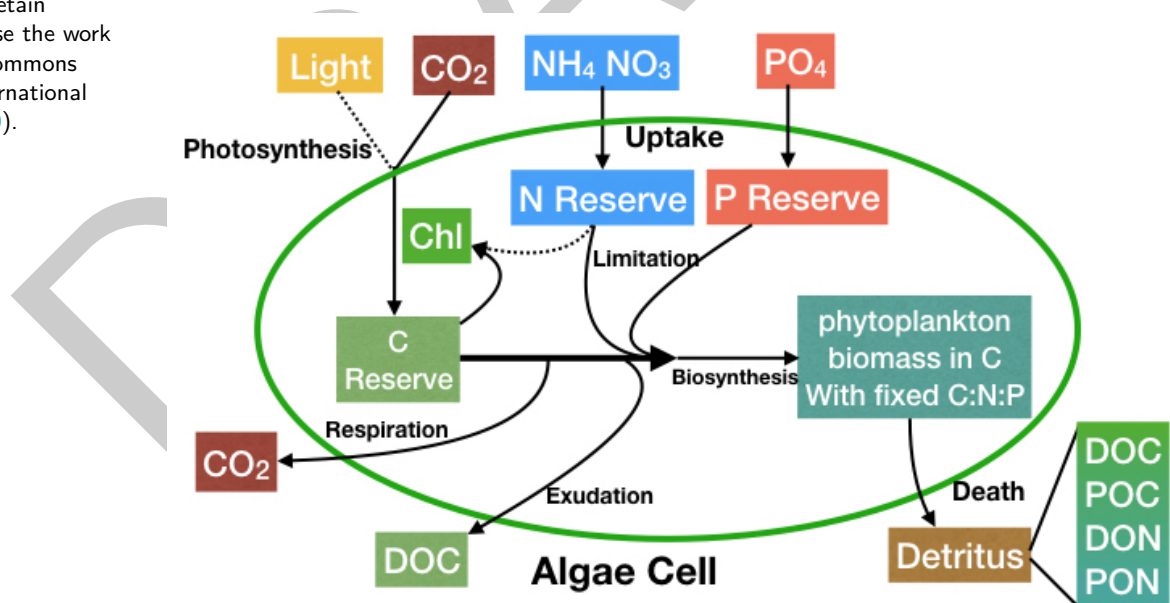
Figure 1: Schematic diagram of phytoplankton physiology described in PlanktonIndividuals.jl.

`PlanktonIndividuals.jl` can simulate multiple functional groups of phytoplankton with different growth and division strategies which will illustrate the interactions within and between functional groups. The individuals can be simulated not only in a zero-dimensional domain (like lab experiments) but also in one-, two-, or three-dimensional domains where individuals

21 can be advected by velocities provided by various models or observations (e.g. `MITgcm`, `Ocea`
22 `nanigans.jl`). The model outputs include time series of individual trajectories, cell density,
23 biomass, and vital rates such as cell division rates, photosynthesis rate, and nutrient uptake
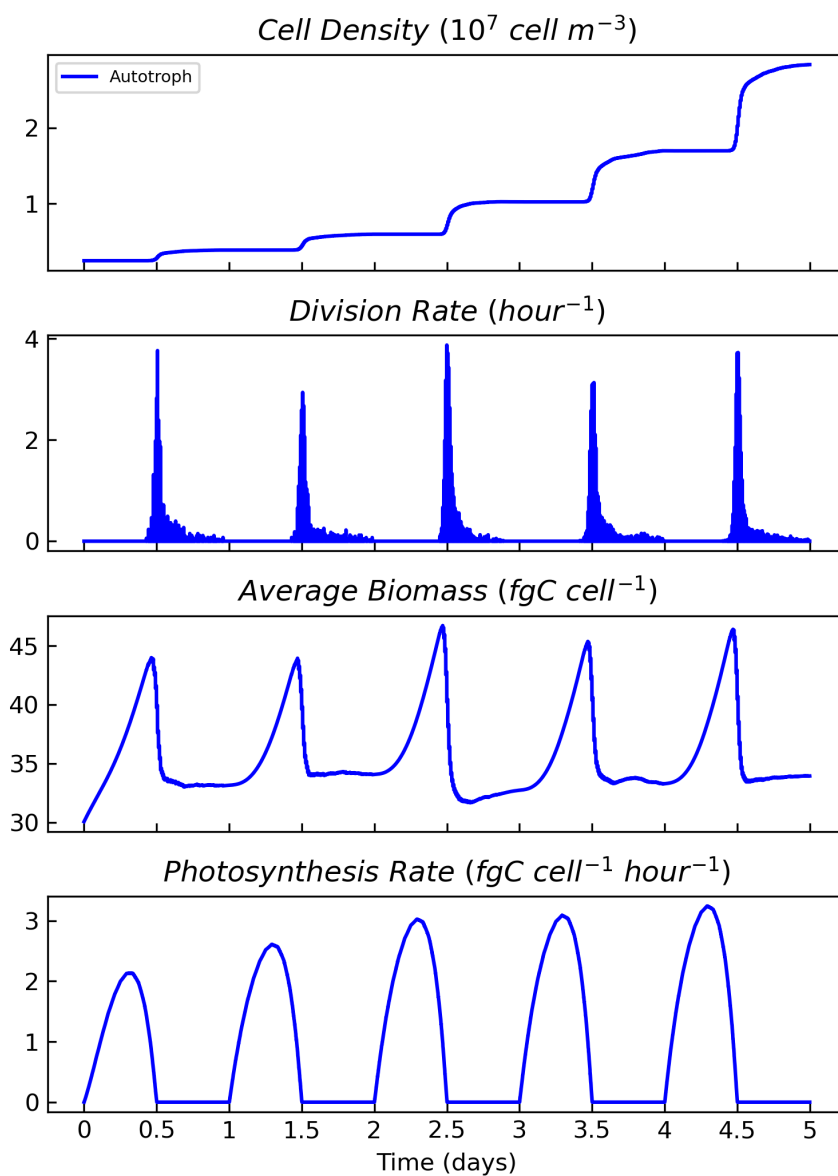24 rates (Figure 2).

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 (population level) 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 waterbodys. Furthermore, individual-based models are able to introduce randomness in individuals which allows stochastic processes (e.g. cell division, grazing, death etc.) 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 Graphical Processing Units (GPUs) which were 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 for over 50 times compared with CPU simulations.

There are many software packages for individual-based modeling, both in Julia or other programming languages, aimed at different purposes. For example, `Netlogo` (Wilensky, 1999) and `Agents.jl` (Datseris et al., 2021) provide generic agent-based frameworks – with a focus on generality. In contrast, `oceanParcels` (Lange & Sebille, 2017) and `IndividualDisplacements.jl` (Forget, 2021) focus on the Lagrangian simulation of individual displacements in the ocean and climate system. However, we do not know of a framework that would provide the same features as `PlanktonIndividuals.jl`.

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 a two-way interactions with gridded nutrient fields (Eulerian) that are advected by the same flow fields (in 2D or 3D) in our package.

To illustrate advective processes, 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).
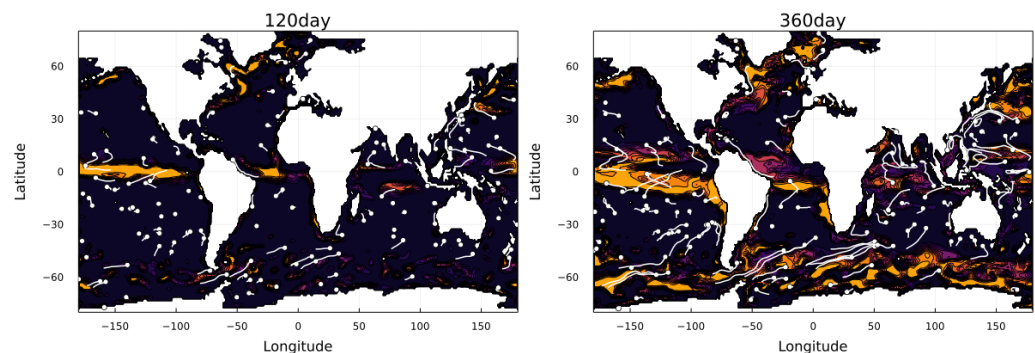
Figure 3: Model results of a 3-dimensional setup.

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

Acknowledgements

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. (2021). *Agents.jl: A performant and feature-full agent based modelling software of minimal code complexity*. https://doi.org/10.1177/00375497211068820

Droop, M. R. (1973). SOME THOUGHTS ON NUTRIENT LIMITATION IN ALGAE1. *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

94 Hellweger, F. L., Clegg, R. J., Clark, J. R., Plugge, C. M., & Kreft, J.-U. (2016). Advancing
95 microbial sciences by individual-based modelling. *Nature Reviews Microbiology*, *14*(7),
96 461–471. https://doi.org/10.1038/nrmicro.2016.62

97 Hellweger, F. L., Sebille, E. van, & Fredrick, N. D. (2014). Biogeographic patterns in
98 ocean microbes emerge in a neutral agent-based model. *Science*, *345*(6202), 1346–1349.
99 https://doi.org/10.1126/science.1254421

100 Inomura, K., Omta, A. W., Talmy, D., Bragg, J., Deutsch, C., & Follows, M. J. (2020). A
101 mechanistic model of macromolecular allocation, elemental stoichiometry, and growth rate
102 in phytoplankton. *Frontiers in Microbiology*, *11*, 86. https://doi.org/10.3389/fmicb.2020.
103 00086

104 Lange, M., & Sebille, E. van. (2017). Parcels v0.9: Prototyping a lagrangian ocean analysis
105 framework for the petascale age. *Geoscientific Model Development*, *10*(11), 4175–4186.
106 https://doi.org/10.5194/gmd-10-4175-2017

107 Wilensky, U. (1999). *NetLogo.* http://ccl.northwestern.edu/netlogo/

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