Computational Modeling of Phytoplankton Dynamics with Climatic and Ecological Ramifications

Phytoplankton encompass a broad range of aquatic, microscopic, photosynthetic species of viruses, bacteria, fungi, protists, animals, and archaea. They are responsible for about half of all global primary production, the production of nutritional organic matter from inorganic compounds via photosynthesis and other metabolic processes (Käse & Geuer, 2018). Phytoplankton are key to biogeochemical cycling, helping circulate nitrogen, phosphorus, silica, and other micronutrients (Sarker et al., 2023). They also absorb 30% of anthropogenic carbon emissions (Rohr et al., 2023). Beyond photosynthesis, carbon sequestration is also performed through exportation, a process where, after death, cellular matter sinks to the ocean floor, forming carbon sinks. Phytoplankton regulate climate not only through controlling carbon circulation, but also through light reflection. Certain functional groups produce dimethylsulfoniopropiothetin, a complex, sulfur-containing molecule. This compound decomposes into dimethylsulfide, which in turn decomposes into compounds that reflect solar radiation (Deppeler & Davidson, 2017). It is in fact believed that biochemical processes such as this one helped cause the first major ice ages on Earth (Käse & Geuer, 2018). Additionally, phytoplankton lie at the base of marine food chains, serving as prey for various species of zooplankton and fish (Käse & Geuer, 2018; Loschi et al., 2023). Therefore, phytoplankton are an integral part of the global climate and environmental systems, making the ability to understand how their operations and functionalities are to change because of global warming incredibly crucial.

Understanding The Impact of Global-Warming Induced Aquatic Changes on Phytoplankton

With that in mind, the impact global warming has had on oceanic conditions themselves must first be considered. Climate change has led oceans to becoming warmer, more acidic, anoxic, and stratified. Sea levels are rising, while salinity and micronutrient concentrations are losing uniformity. Moreover, ocean currents have begun to slow down (Berwyn, 2018). The thermohaline cycle involves the cycling of warmer, fresher, and less dense pelagic (surface) water with colder, denser, saltier benthic (deep-sea) water. This allows for the mixing of nutrients, the distribution of heat, and the regulation of climate. Analysis of past climate patterns reveals that a slower thermohaline cycle has been associated with more extreme climate patterns (Berwyn, 2018). However, it is important to note that changes in ocean conditions are not uniform, but rather, vary extensively by region (Winder & Sommer, 2012). That means environmental conditions, which impact the nature of phytoplankton populations, are not homogenous, adding a layer of complexity when determining the impacts they are to face.

Similarly, phytoplankton are undergoing some overarching changes. Common trends include shifting phenology, a change in preferences towards smaller, more buoyant cells, and poleward migration (Ratnarajah et al., 2023). However, under the surface, population modifications are far more complex. For example, certain groups are favored under eutrophic conditions, that is, conditions where there are excessive micronutrients, leading to an unhealthy amount of growth in algal blooms that deplete ecosystem resources, whereas others under fresher or darker conditions (Winder & Sommer, 2012). There are a voluminous amount of environmental factors (e.g., light, heat, nutrients, pH, salinity, etc.) that impact phytoplankton dynamics (Winder & Sommer, 2012). Moreover, each species operates under different sets of ideal conditions. This raises a dilemma. To illustrate this, consider two phytoplankton species living in the same area. Suppose that one species can tolerate a pH range of 5.9 to 6.5, whereas another one tolerates a range of 6.7 to 7.3. With ocean acidity changing heterogeneously, if one area of the ocean has a pH of 6, and another area a pH of 7, then each species would migrate to the area matching their respective preferences, heavily modifying taxonomic composition, biomass, exportation, and other dynamics. However, there are other influential environmental factors, making it important to consider how multiple factors simultaneously impact dynamics. Using the example given, would another factor, such as dissolved oxygen, have precedent over pH when it comes to these species seeking ideal conditions? Moreover, these migrations would leave predators bereft of a major source of food. How would that impact the entire ecosystem? What climatic shifts may result? The circumstances and questions raised by a scenario like this capture the essence of what this study aimed to address.

Examples of Parametric Variability

Parameters that influence phytoplankton conditions are present at the molecular, genomic, cytological, and ecological level. Changes in their values can impact various important biological characteristics, including primary production and metabolic rates. For instance, biochemical processes like DNA methylation, whereby a methyl functional group is applied to the fifth carbon in the carbon ring of the nitrogenous base of cytosine, with warming ocean temperatures, has been found to inhibit amino acid metabolism, as well as respiration and photosynthesis in phytoplankton, while enhancing fatty acid metabolism (Wan et al., 2023). This means that there is a slower rate of primary production and carbon sequestration, inhibiting phytoplankton's role both as the base of marine food chains and as climate regulators. However, seeing as ocean temperature shall change heterogeneously, the extent to which this trend occurs shall vary.

Meanwhile, micronutrients also play a major role in influencing metabolic rates. For example, phosphorus is an integral component of all forms of metabolism, making phosphorus-containing compounds crucial for phytoplankton. However, as discussed above, varying levels of micronutrients, including these compounds, impact dynamics in different ways. It has been found that increased phosphorus levels has allowed for all metabolic processes to occur at faster rates, bolstering the ability of phytoplankton to sequester carbon and provide greater biomass for its predators. However, excessive phosphorus concentrations can be toxic and lead to eutrophication (Li et al., 2023). Moreover, toxicity and metabolic rates vary across different species.

Another example of significant environmental variability is water temperature. Different genera of phytoplankton exhibit different responses to warming ocean temperatures. For example, using a modified Eppley Curve, an exponential function that models the relationship between growth rates and water temperature, one analysis found that, while growth rates are expected to increase alongside temperature, the rate at which the growth rate increases for diatoms was greater than that of dinoflagellates, cyanobacteria, and coccolithophores (Anderson et al., 2023). Additionally, dissimilar thermal attributes are predicted to result in differential migration patterns among different functional groups.

In conjunction with the explanation offered in the previous section, these examples illustrate that for any environmental parameter, there is a great amount of nuance when it comes to the impact that phytoplankton face. This nuance only expands when multiple variables are considered in tandem. It is extremely difficult to perform an experiment that involves multiple independent variables, as confounding factors would easily arise. The alternative would be to perform an experiment using only one variable, which would fail to account for the multifactor interactions that occur. The results of such a procedure across different instances would also vary, failing to paint a solid picture of the impact of that one parameter (Chang et al., 2022).

Computational Modeling of Phytoplankton Dynamics: Progress and Current Limitations

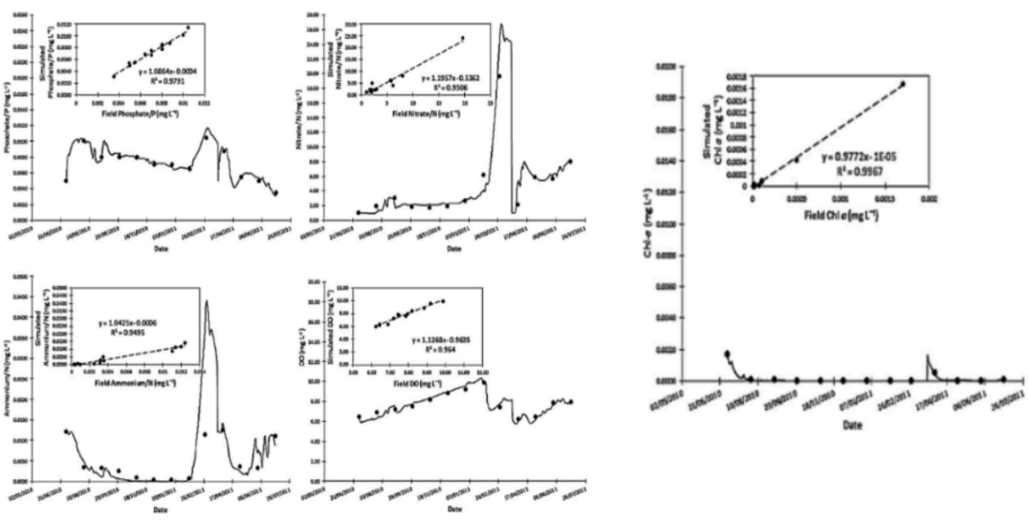
As a result, a computational modeling approach is imperative, as it can be used to capture the nuances of this situation, and provide greater insight into what the observed results signify. In essence, this is what the goal of this project is: to take the complex relationships in phytoplankton populations, and organize, synthesize, and contextualize them, delineating ramifications.

Presently, there are many limitations with computational models of phytoplankton dynamics. One major limitation is the misunderstanding of the role zooplankton play in the modeling process. Different models have made different assumptions about how zooplankton interact in ecological systems, leading to divergent predictions in climate and food web scenarios (Rohr et al., 2023). Indeed, it has been found that more robust data collection methods and raw data on zooplankton is necessary (Ratnarajah et al., 2023). It is a dearth in overall data that limits the predictive power of these computer models. There is a particular lack of data from the Southern hemisphere (Deppeler & Davidson, 2017).

That is not to say that accurate models have not been developed. In fact, there have been models developed for small bodies of water, such as the Tucuruí reservoir in Pará, Brazil (Deus et al., 2013). This computer model was based off of field data on chlorophyll a, dissolved oxygen, ammonia. Through linear regression analysis including R^2, root mean square error, and the slope of regression lines comparing computer predictions to actual results, it was determined that the model was in fact accurate. Figure 1 (Deus et al., 2013) depicts the linear regression between the predicted and field values of these parameters. With extremely high R^2 values, the model was deemed fit to perform other functions within study. This provides a strong example for how the accuracy in computer model predictions can be assessed, allowing for model results and ramifications to be validated. Indeed, validation relies on some form of statistical analysis, which varies from model to model.

Figure 1

An Example of Computational Model Validation Techniques: Tucuruí Reservoir as a Case Study



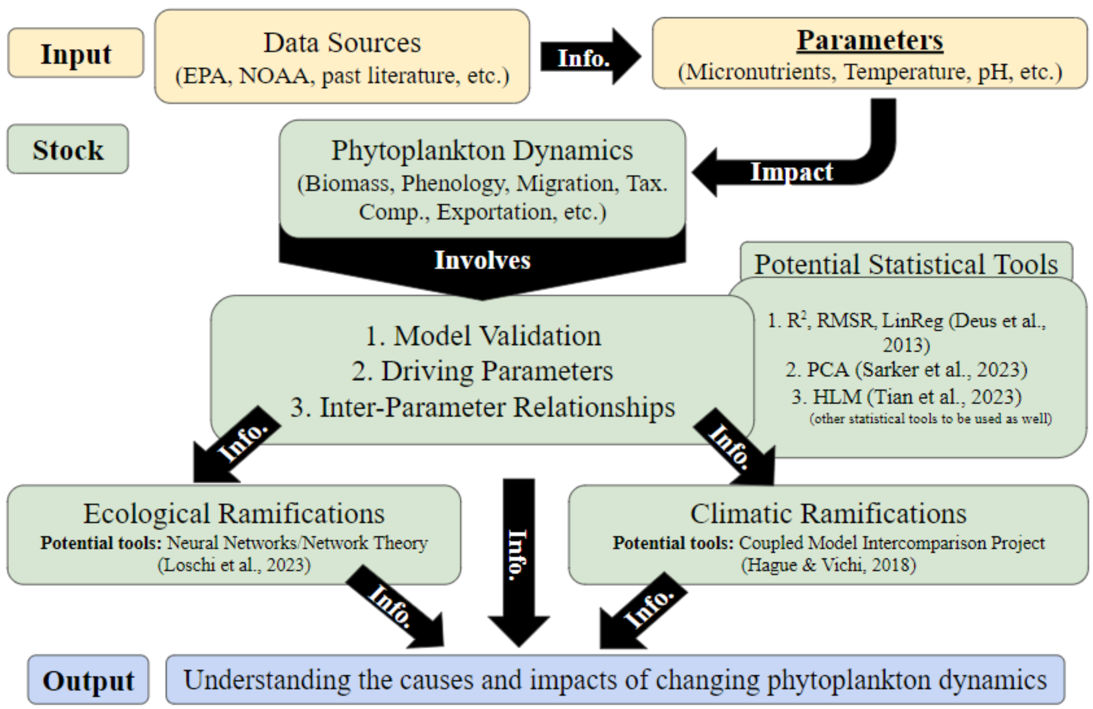
Note. Each parameter contains a larger graph depicting the raw comparison between field data and computer predictions. From lop left to bottom right, the parameters shown are phosphate, nitrate, ammonia, dissolved oxygen and chlorophyll a. Embedded within are the linear regressions that compare the computer model predictions against the actual field data. Therein lie the R^2 values which serve to evaluate model accuracy. The R2 values for phosphate, nitrate, ammonia, dissolved oxygen, and chlorophyll a were 0.9791, 0.9506, 0.9495, 0.964, and 0.9967, respectively.

However, different models have been synthesized for different purposes. For example, some models have focused on the identification of driving parameters in phytoplankton dynamics. Using Principal Component Analysis (PCA), whereby the impact of parameters is measured using vectors, one study of coastal Bangladesh found that salinity, followed by micronutrient concentrations, turbidity, and water temperature played the most significant roles in regulating abundance and spatial variability in phytoplankton (Sarker et al., 2023). Other models have focused on inter-parameter relationships. One study of several lakes in Wuhan, China used a hierarchical linear model. After sorting the parameters into different levels and identifying statistically significant relationships, the one major inter-parameter relationship identified was a negative one between grasslands and water temperature (Tian et al., 2023). From an ecological lens, neural networks have been developed to model the changing flow caused by changing phytoplankton conditions. At a broad level, these networks take in various rates related to energy and matter transfer as parameters, the values of which can be modified to simulate different scenarios. Boit et al. 2012 suggests the gradual implementation of these factors through a series of successive neural networks. When applying this approach to Lake Constance, the fit of the model to predict observed dynamics was maximized, providing a format through which food webs of other systems can be created (Boit et al., 2012). Other studies, such as one of the Venice Lagoon, have been able to identify keystone species (Loschi et al., 2023). From a climatic lens, a focus has been placed on the accuracy of climate models in predicting bloom phenology, as well as other characteristics. The Coupled Model Intercomparison Project (CMIP), with its large scope, has been a particular area of focus. For example, one study found that bloom phenology in the Southern ocean is not accurately predicted as the sea ice concentration levels used in the model were not reflective of on-site levels (Hague & Vichi, 2018). Overall, there exists ample literature describing a myriad of empirical relationships and computational models of the various aspects of the changing characteristics of phytoplankton as well as those ramifications. What is lacking, however, is a unified apparatus to unite these models.

Given the background information and limitations presented, this paper seeked to create a series of computational models bound together as one entire system whereby parametric information on phytoplankton populations could be introduced and results for their populations, and in turn, the environment and climate could be produced. Figure 2 visualizes this overarching computational framework. This study applied this basic framework to data from the National Oceanic and Atmospheric Administration (NOAA)'s comprehensive 2018 World Ocean Database (WOD18). Specifically, the most spatiotemporally cosmopolitan dataset, the Ocean Station Dataset (OSD), was analyzed. These data include millions of casts, spanning multiple centuries and covering virtually the entire ocean (Boyer et al., 2018). Given this impressive scope, this allows the study to take a holistic approach to analysis, partially helping to address the lack of data in computational models. Within the OSD, total oceanic chlorophyll was used as an indicator for primary production. Factors tested include oxygen, micronutrients, pH, salinity, temperature, pressure, and alkalinity. To assess potential forecasting capabilities and overall model strength, a time series of all parameters (including the stated indicator), was created mainly using sinusoidal regression. Subsequently, the relationship of each factor with the indicator was observed using linear regression. Lastly, driving parameters were identified using Principal Component Analysis (PCA).

Figure 2

Proposed Overarching Computational Framework for Modeling of Changing Phytoplankton Dynamics



Note. This model takes the form of a systems diagram wherein an input is provided for the system stock, operations are performed, and an output is provided. This study proposes that parametric data act as the input, that computational and statistical methods act as the operations within the stock, and that the insights provided on phytoplankton, that is, the study goal, to act as the output. All potential tools proposed above, while useful for achieving their respective ends, however, not all techniques were utilized within this paper.

This apparatus could serve as a viable streamlined process for experts studying phytoplankton populations and their role in the environment and climate. Moreover, it has the potential to serve as a tool for policy makers with regards to water body management. For example, Tian et al. 2023 used results from a multi-agent based model to recommend a controlled increase in micronutrient concentrations and fish that feed exclusively on zooplankton (Tian et al., 2023). As a whole, this study has provided a potentially potent framework whereby the causes and impacts of phytoplankton conditions can be effectively observed.