Cultivating Macroalgae for Biofuels: Visualizing the Chemistry

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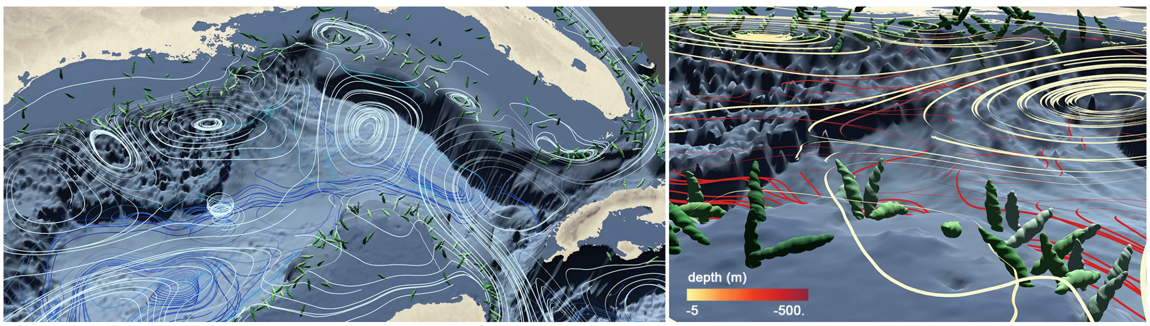

Fig. 1. Currents and chlorophyll locations in Gulf of Mexico, using the E3SM DOE simulation [4]. Left, streamlines of currents colored by depth. Right, streamlines colored by nitrate concentration levels. Visualization constructed using Artifact-Based Rendering [7].

ABSTRACT

Marine macroalgae in the Gulf of Mexico is an important potential source for biofuel. However, identifying locations with the correct biogeochemical and hydrodynamic conditions for cultivation on a large enough scale to meet the needs of the U.S. private energy sector is impossible from purely observational studies. Large-scale, HPC modeling of earth systems processes enables researchers to study complex physical relationships with high fidelity. Here, we present novel visualization techniques showing the results of a global run of the E3SM's MPAS-Ocean model data with biogeochemistry extensions to improve ongoing research in macroalgae cultivation.

CCS Concepts: • **Applied computing → Earth and atmospheric sciences**; • **Human-centered computing → Visualization techniques**.

Additional Key Words and Phrases: ocean biogeochemistry, macroalgae cultivation, scientific visualization, art and design, biofuel mariculture

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1 INTRODUCTION

Marine macroalgae is a diverse group of aquatic plants that grows globally near coastlines and occasionally in regions of the open ocean with ideal biogeochemical conditions. Global cultivation and farming of macroalgae has increased six-fold in recent decades [1]. In the United States, macroalgae is a source for food and fertilizer production [3, 8]. As research into economically-viable alternatives to fossil fuels has intensified [6, 9, 10], recent investigations through the DOE's Advanced Research Projects Agency-Energy Marine Research Inspiring Novel Energy Resources (U.S. ARPA-E MARINER) Program indicates that macroalgae may be a potent and abundant source for biofuel [12]. The MARINER Program [12] estimates that geographic conditions in the U.S. may harbor the potential to produce "roughly 10% of U.S. annual transportation energy demand." Successful deployments of large-scale marine macroalgae cultivation for biofuel production depend on numerous factors including fine-scale hydrodynamic conditions; biogeochemical processes; nutrient availability for long-term, sustained macroalgae growth; and macroalgae trajectories for free-floating capture systems. [11, 12] Further, macroalgae canopies and farm structures must be designed to handle the hydrodynamic load of macroalgae biomass in diverse regions.

In order to identify regions with both surplus growth and ideal conditions for cultivation and farming, researchers with the MARINER Project are turning to high-level, multi-scale, multi-resolution and coupled modeling techniques capable of simulating these complex, dynamic processes and variables in-situ. Coupled climate models enable scientists to study Earth systems in ways that are not possible via direct observation. By performing large-scale runs of its E3SM climate model, the Department of Energy produces datasets that can be shared across the open science community to study critical issues concerning climate and environmental change. Employing these models requires analogously high-level visualization techniques that allow researchers to analyze multivariate volumetric data in spatially co-located simulations. Such techniques require, in turn, both advanced mathematical transformations and sophisticated visual design methods to maximize practical data analysis [2]. Here, we present novel visualization techniques showing the results of a global run of the E3SM's MPAS-Ocean data with biogeochemistry extensions to identify potential locations for macroalgae cultivation for biofuel in the Gulf of Mexico. This is part of a larger effort within the Department of Energy to upscale biofuel production to meet the demands of the US energy sector. This work represents an explanatory submission of ongoing research.

2 VISUALIZATION TECHNIQUES

2.1 3D modeling/visualization for mariculture

The ocean is a complex, three-dimensional system. Aspects of ocean systems that occur **below** the mariculture zone affect the mariculture zone itself. To understand the complex physical properties of the ocean's biogeochemistry more fully, we must visualize these hydrodynamic processes in three dimensions.

Our investigation of the Gulf's biogeochemistry begins with a pre-computed run of MPAS-O/BGC model on a global unstructured grid. The global dataset consisted of 12 monthly timesteps of 1.445 million hexagonal surface cells, 2.9 million points, and 70 layers, with 12 scalar and 1 vector variables, for a timestep size of 13.77 GB. After converting to a triangulated surface and 'stacking' the layers to create triangular prisms, we have over 28 million cells and 14.5 million points. We excised the Gulf of Mexico region, reducing the grid size to 915K cells and 487.5K cells, with a timestep size of 112 MB. We note that this proof of concept is well short of the desired resolution for decision making at the mariculture farm scale.

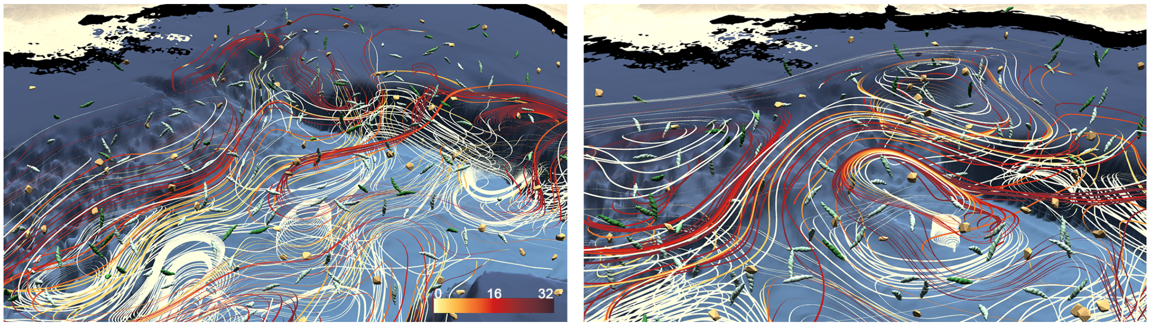

Fig. 2. In the Gulf of Mexico, 3D current streamlines are encoded by nitrate concentrations, January, left; and May, right.

2.2 Data, the Pre-Processing Pipeline

Our data pre-processing consists of two steps: a geographic clip of the global data to the region of interest, and the re-representation of the data in a form suitable for visual analysis. While we could simply transform each timestep of the data to a VTK representation and then use VTK tools to perform the geographic clip, we instead choose to do so in one step so that we read the global grid information once, cull the Gulf of Mexico region to form a base visual analysis grid, then iteratively read the time-varying data, assign as necessary to a copy of the base grid, and write individual time steps in VTK form.

2.3 Biogeochemistry Representation

The MPAS-O/BGC model produces properties on an implicit 3D grid defined by a set of two-dimensional hexahedral cells that are stratified vertically by a set of per-cell layer thicknesses. The implicit 3D grid is therefore composed of the hexahedral prisms that result from extruding the 2D hex cells in the vertical dimension by the varying layer thicknesses. Properties are defined at the vertices of the hex prisms, the centers of the extruded hexagonal prisms, or (rarely) at the centers of the horizontal faces of the 3D cells.

2.4 Re-representing the data for Analysis

To visualize this using VTK data structures, we convert this implicit hex-prism grid into an explicit triangle-prism grid using conventional VTK-WEDGE cells. We begin by converting the 2D hex cell mesh to its triangular dual form by joining hex-cell centers. We then transfer these vertically to the centers of hex-grid cells using a combination of above- and below-layer thicknesses. We extend this grid vertically to the ocean surface and floor by adding half-thickness layers.

Next, we transfer properties as necessary from their locations in the input grid to the vertices of the triangle-wedge output grid. Cell-centered values in the input grid move directly to corresponding vertices of the output grid, while vertex-positioned (or face-centered) properties in the input grid must be interpolated. This leaves properties for the top- and bottom-most vertices of the output grid unassigned; rather than extrapolate values, we simply duplicate properties from the neighboring layers. Our output grid therefore does not vary vertically in the topmost and bottom-most layers.

2.5 Visualization

The science questions undergirding this work center on the relationships between physical properties contained in the data as they evolve over time. Generally, these properties are common ocean-modeling scalar and vector valued

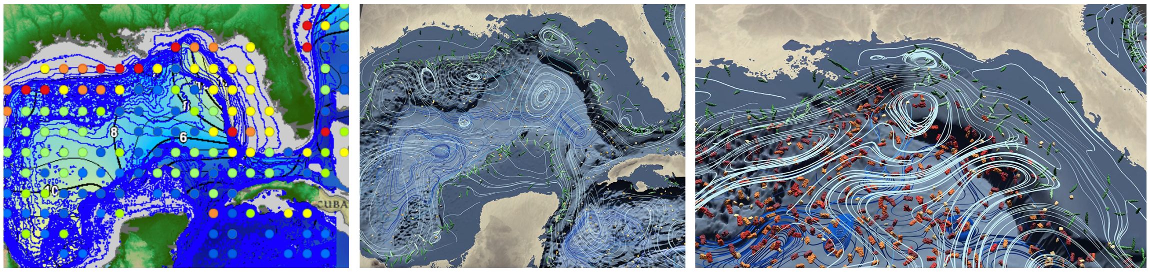

Fig. 3. Left: A NOAA visualization of the same data used in our visualizations—nitrate concentrations and phytoplankton. Center and Right: Our visualization of Gulf of Mexico bathymetry, chlorophyll, and depth-spanning ocean currents, shown as streamlines colored by depth.

properties such as flow, salinity, and temperature, in addition to various biogeochemical properties. As successful cultivation of macroalgae requires suitable levels of several such properties in the same location, we are interested in the understanding the simultaneous physical distribution of these properties. Common visualization techniques to show scalar properties in isolation - notably iso-surfacing and volume rendering - are poorly suited to this task: opaque derived surfaces obscure one another, and overlapping translucency gives rise to confusing combinations of color and density.

In our case, however, the precise location of property values and derived boundaries is less interesting than in the general distribution of the many properties. Here, we utilize statistical sampling to identify the relative density of underlying properties by the distribution of proportionate numbers of samples: where many samples per unit volume lie, the corresponding property is high, while where few samples exist, the corresponding values is low. By annotating samples of different properties using different glyphs, we can more easily parse the distribution of properties - even when co-located in overlapping regions.

3 ARTIFACT-BASED RENDERING

Visualizing multiple variables in the same three-dimensional space requires a sophisticated design structure in order to maintain fidelity of visual discrimination, as well as ease of interpretation and intuitive communication. Specifically, glyph forms, surface textures, and colormaps must be keenly balanced in order to direct attention where necessary, provide background context for foregrounded data groupings, and encode multiple variables without overwhelming the visual field or increasing the cognitive load beyond what is necessary. Here, we use the Sculpting Vis Collaborative's Artifact-Based Rendering application (ABR) to accomplish these ends [5, 7].

The Sculpting Vis Collaborative is a multidisciplinary, cross-institutional team creating tools that bring artists, designers, and others outside of the sciences directly into the visualization process.

Artifact-Based Rendering is a technical foundation and the input channel for the Sculpting Visualization Collective's project to enrich the visual vocabulary of scientific visualization through hand-crafted or naturally occurring objects.

Here, we consider the visualization of our raw data in two parts: the geometric processing of data to produce geometric entities: surfaces, pathlines, and samples; and the annotation of those geometric entities with visual properties to produce images that optimize communication. Paraview, a well-known visualization application that is well-suited to the former geometric computations, is paired with ABR to annotate its geometric results with natural forms to create evocative imagery and to render the results at interactive rates.

Our system therefore consists of two separate processes running in concert: Paraview, running in close proximity to the voluminous raw data, receiving the raw data and converting if to significantly smaller derived geometric entities, and passing the results to ABR, which runs asynchronously in proximity to the user, where rendering can be accomplished in real time. The connection between Paraview and ABR is a socket, enabling the user-facing ABR rendering process to be remote from the data-facing Paraview process.

4 MODEL OBSERVATIONS AND RESEARCH QUESTIONS

Our visualization of the E3SM biogeochemistry model demonstrates the model's correspondence with contemporary theories based on observational data. We see significant concentrations of nitrate around the Mississippi river delta in the first 0-200 meters of ocean depth. By tracking the direction of ocean currents in the model, we can show how these nitrates disperse across the continental shelf. The edge of the shelf supports the growth of plant life, including many types of macroalgae. Nitrate levels near the surface are higher and chlorophyll is correspondingly abundant (see Figure 1). Research investigating the precise levels of nitrate and other nutrients that are necessary to support macroalgae growth, along with many other interdependent conditions, is nascent and ongoing, particularly concerning data acquisition platforms. Visualizations that focus on clearly illustrating intravariate relationships are therefore essential to the advancement of this work.

Macroalgal growth conditions evolve with the seasons. Gulf ocean temperatures change throughout the year, shifting nutrient concentrations, which in turn influences major Gulf currents. These currents respond by shifting direction and velocity. We show the relationship between these conditions using streamlines (tracking current flow direction) encoded with a colormap that ramps from dark red to light yellow by nitrate concentration (see Figure 2). These streamlines are depth-spanning and time-varying by month, enabling us to reveal changes to both variables over the course of the seasons. Scientists with the MARINER project are investigating these regions to understand whether they might support large-scale mariculture farms. Despite the excess of nutrients populating the waters of the Mississippi River Delta, much greater quantities are needed to meet the demands of the U.S. energy sector.

Our visualization shows much higher concentrations of nitrate in the deepwaters of the central Gulf, corresponding with much cooler water temperatures. Scientists are considering the use of specialized equipment to bring these nitrates within 200 meters of the surface, where sufficient sunlight is present to allow macroalgae to photosynthesize. This could provide enough nourishment to free-floating macroalgae canopies in the open ocean, allowing farmers to produce much larger and more sustainable volumes of biofuel. Specific locations under consideration for the deployment of this equipment are large, stable eddies flowing counterclockwise (see Figure 3). These eddies naturally upwell some deepwater nutrients, and could prevent canopies placed near the centers of these eddies from drifting beyond desired boundaries with strong currents. Our visualization demonstrates how nitrates may be pulled up by these eddies, showing both depth and directionality of the currents and nitrate concentrations as sampled points mapped to hand-made glyph-forms.

Implementing these ideas at scale is extremely challenging in practice. A multitude of contingencies must be considered, along with threats posed by local weather and the effects of a warming climate. While observational studies investigating the viability of large-scale infrastructure for alternative energy systems can be prohibitively costly and impractical, HPC modeling provides a cost-effective alternative, allowing researchers to investigate complex science questions through iterative scenario testing. Visualization techniques that leverage art and design while enabling users to analyze these data co-located in true three-dimensional space prompt new, more productive research questions and better public-facing communication. Further, we argue that this work demonstrates a prototype for future visualization efforts focused on in-situ use for mariculture farmers in the field. These users will need to assess complex hydrodynamic and biogeochemical conditions on a daily basis in order to maintain mariculture structures over months and years at sea. This work lays the foundation for practical field visualization, and for a future of carbon-neutral energy sources.

5 CONCLUSION

As data and computing power continue to grow in complexity and scale, we must leverage advanced visualization techniques to keep pace. Here, we have demonstrated the value of visualizing environmental data both in three dimensions and by integrating arts and design methodologies. The combined approach produces a visualization that is intuitive to parse and easy to analyze at a glance, revealing latent intravariate relationships that are essential to the science behind this data.

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