Project Summary

Submesoscale-Resolving Large Eddy Simulations Using Reduced Biogeochemical Models

Improved understanding of biogeochemical tracer properties, evolution, and patchiness in the upper ocean requires a comprehensive look at the interactions between tracers and turbulence at submesoscales and smaller. The proposed project seeks to provide this understanding through cutting-edge simulations of two-way coupled turbulent and biogeochemical processes in the upper ocean. This project is motivated by the growing awareness of the influence of submesoscale physical processes (e.g., sub-km scale turbulent mixing) on the creation of tracer patchiness. Examining this problem from a computational standpoint, however, is enormously costly, and realistic biogeochemical models are currently too large for coupled integration with already demanding simulations of upper ocean physical processes. As a result, new reduced biogeochemical models, solved in novel ways, must be developed to perform large eddy simulations (LES) of coupled biogeochemistry and physical processes at submesoscales.

In the proposed project, techniques adapted from the field of combustion for the reduction of large chemical kinetics mechanisms will, for the first time, be used to reduce the size of large ocean biogeochemical models. The resulting reduced models will then be solved in a two-way, fully-coupled, yet computationally efficient, manner within high-fidelity, submesoscale-resolving LES of the ocean mixed layer. Solution of the reduced models will be performed on graphical processing units (GPUs) using a high-order Runge-Kutta-Chebyshev (RKC) time integration scheme. This project will culminate in the simulation of realistic ocean scenarios and comparisons will be made with observational data from the Drake Passage to determine the role of submesoscale processes in generating small-scale patchiness in the partial pressure of carbon dioxide. Ultimately, insights obtained from the LES will be used to develop a better understanding of the interactions between small-scale turbulence and biogeochemistry in the upper ocean, including the characteristics, dynamical origins, and effects of tracer patchiness.

Intellectual Merit: Integration of complex biogeochemical models within high-fidelity LES has previously been exceptionally difficult, but the proposed model reduction, as well as the use of GPUs and the high-order RKC integrator, will enable high-resolution studies of fully-coupled turbulent and biogeochemical processes at submesoscales. These improvements will be made possible by leveraging techniques from chemical kinetics modeling for combustion, where reduction and integration of large chemical mechanisms in high-fidelity simulations has been common for nearly a decade. The proposed simulation effort will provide insights into the effects of submesoscale turbulence, including wave-driven Langmuir turbulence, on the upper-ocean carbon cycle, and will inform the future development of improved Earth system models (ESMs). In particular, interactions between submesoscale turbulence and biogeochemical tracers are thought to be the cause of tracer patchiness and require substantial further study to develop more accurate subgrid-scale parameterizations for ESMs. Moreover, simulations of the Drake Passage will provide concrete insights and understanding of tracer patchiness for realistic conditions.

Broader Impacts: This interdisciplinary research effort will be undertaken by a collaborative team consisting of an expert in numerical simulations of both reacting and oceanographic flows, a biological oceanographer with extensive knowledge of ocean biogeochemistry, and an expert in chemical model reduction and solution. The biogeochemical modeling tools developed in this project will be made available to the broader oceanographic community, and involvement of interdisciplinary PhD students will expose a new generation to computational methods in oceanography and the Earth sciences. We will provide genuine research experience and mentorship to undergraduate students, particularly those under-represented in STEM, by designing projects derived from, and complementary to, the proposed research. Significant research findings, particularly those of direct relevance to anthropogenic climate change, will be communicated to the general public through social media, public presentations, press releases, and popular science websites. Ultimately, this project will benefit society through improvements to ESMs used to study climate, resulting in more accurate predictions of future climate impacts on human health, safety, and property. Dissemination of significant research findings also has the potential to influence policy and mitigation strategies related to climate change.

1 Problem Statement

The properties and evolution of reactive tracers in the upper ocean are critical for understanding the global carbon cycle and climate. Such tracers include phytoplankton, nutrients, and CO_2. Phytoplankton, confined to the upper ocean due to light penetration and the pycnocline, consume inorganic carbon and nutrients that diffuse across the air-sea interface or are entrained from depth. Similarly, CO_2 diffuses across the air-sea interface and transforms into carbonate and bicarbonate through chemical reactions.

Both phytoplankton and CO_2 are examples of reactive tracers that can be created and destroyed. These tracers are additionally mixed vertically and horizontally by turbulent processes, resulting in spatially non-uniform tracer distributions that exhibit spatial heterogeneity, or "patchiness", over a wide range of scales. Since concentrations of these reactive tracer species at mixed-layer boundaries can greatly affect exchange rates, it is crucial to include the coupling of this turbulent mixing in reactive-tracer subgrid-scale parameterizations for Earth system models (ESMs).

Recent research has shown the importance of submesoscale (SM; 1∼10 km) eddies on reactive tracers (see [1, 2] for reviews), but the effects of small-scale (1 m∼1 km) motions on the evolution and properties of realistic biogeochemical (BGC) tracers have yet to be examined. Small-scale turbulence includes both wave- (i.e., Langmuir) and shear- (i.e., wind) driven turbulence, and can affect reactive tracers since small-scale mixing times can be similar to reaction (e.g., chemical) time scales. Additionally, small-scale motions affect the depth of the mixed layer and near-surface flushing.

Research Questions: Improved understanding of BGC tracer properties, evolution, and patchiness in the upper ocean requires a comprehensive look at the interactions between tracers and turbulence at submesoscales and smaller. The proposed project seeks to provide this understanding, with an emphasis on addressing the following fundamental science questions:

- **Q1.** What are the effects of SM turbulent mixing on the evolution and patchiness of BGC tracers, particularly chlorophyll and dissolved inorganic carbon?
- **Q2.** How does small-scale tracer patchiness depend on other upper-ocean mixing processes, including wave-driven Langmuir turbulence and buoyancy-driven vertical convection?
- **Q3.** What are the spectral characteristics of tracer patchiness, and how do mixing processes occurring at different scales impact these characteristics?
- **Q4.** What are the effects of ocean biogeochemistry (e.g., changes to density and viscosity) on turbulence properties at submesoscales?
- **Q5.** How does tracer patchiness affect the supply of nutrients, primary production, the aggregation and sinking of particles, and the transfer of carbon at the air-sea interface?
- **Q6.** Is it necessary to account for SM turbulent processes in order to accurately predict real-world BGC tracer evolution?

These questions will be addressed using cutting-edge large eddy simulations (LES) of two-way coupled turbulent and BGC processes in the upper ocean. These computationally expensive simulations will be enabled by the development of reduced BGC models and the use of co-processor acceleration.

2 Project Overview

In the proposed project, techniques adapted from the field of combustion for the reduction of large chemical kinetics models will, for the first time, be used to reduce the size of large ocean BGC models. The resulting reduced models will then be solved in a fully coupled yet computationally efficient manner within high-fidelity, SM-resolving LES of the ocean mixed layer. Insights obtained from the LES will be used to develop a better understanding of the interactions between small-scale turbulence and biogeochemistry in the upper ocean, including the characteristics, dynamical origins, and effects of tracer patchiness.

This project is motivated by the growing awareness of the influence of SM physical processes (e.g.,

sub-km-scale turbulent mixing) on the creation of tracer patchiness. Examining this problem from a computational standpoint, however, is enormously costly, and realistic BGC models, which currently include up to 60 biological and chemical species, are currently too large for coupled integration with already-demanding simulations of upper-ocean physical processes. For example, reacting flow simulations with roughly 50 species typically occupy 75–99 % of the total computational time in high fidelity simulations [3–5]. As a result, new reduced BGC models, solved in novel ways, must be developed to perform LES of coupled biogeochemistry and physical processes at submesoscales.

Using advanced techniques such as directed relation graph and computational singular perturbation methods, combustion scientists routinely reduce chemical-kinetic models with $\mathcal{O}(10^4)$ reactions and $\mathcal{O}(10^3)$ species down to models with $\mathcal{O}(10^2)$ reactions and $\mathcal{O}(10)$ species. Moreover, these reductions typically have little impact on predictions of quantities of interest (such as ignition delay time and burning rate). Such reduced models are critical when coupling reactions with finely resolved simulations of hydrodynamic processes, which themselves can require $\mathcal{O}(10^3$–$10^4)$ computational cores. Due to the considerable computational cost, even reduced kinetic models are increasingly being solved by combustion researchers on co-processors such as graphics processing units (GPUs).

In the proposed project, these reduction and solution techniques will be applied, for the first time, to widely-used BGC models such as those developed at the National Center for Atmospheric Research (NCAR) [6], the University of Bologna [7, 8], and the Geophysical Fluid Dynamics Laboratory (GFDL) [9]. Solution of the reduced models will be performed on GPUs using a high-order Runge–Kutta–Chebyshev (RKC) time integration scheme. Physical processes will be modeled by numerically solving the three-dimensional (3D), non-hydrostatic Boussinesq equations with and without wave forcing (the former leading to the creation of small-scale wave-driven Langmuir turbulence) for a range of different physical scenarios. The BGC and fluid flow equations will be solved in a fully-coupled fashion, thereby enabling a complete study of the interactions between small-scale turbulent mixing and biogeochemistry in the upper ocean. This project will culminate in the simulation of realistic ocean scenarios, and comparisons will be made with observational data from the Drake Passage Time-series Program to determine the role of SM processes in generating small-scale patchiness in the partial pressure of carbon dioxide (pCO_2).

2.1 Response to Review Comments

A previous version of this proposal was reviewed a year ago by the NSF Chemical Oceanography program and received generally positive reviews, with a final recommendation of "Very Good" from the panel. Although there were many positive comments, the most notable criticisms—which we have attempted to address in the present revised proposal—can be briefly summarized as:

- **Review 1 (VG):** "Few specific scientific hypotheses or questions have been posed . . . No plan has been proposed to involve undergraduate students in this work, or participate in outreach programs . . . With a combined budget of > \$700k, I would expect more effort to be made to engage with the broader community to build interest in the work."
- **Review 2 (VG):** "While there is a great deal of information on the more technical aspects of the proposed work, there is much less attention devoted to the methods that will be used to analyze and validate the simulations. . . The main weakness of the proposal is the broader impacts section."
- **Review 3 (VG/G):** "The proposal left me unclear as to which specific BGC questions or phenomena the investigators are ultimately interested in addressing. . . What is the current computational cost of running the BGC models in the LES framework? How much saving is necessary to make it viable for research? . . . What are the targeted scientific questions for application of the simulations? . . . Which tracers do you care about and why?"
- **Panel (VG):** "The proposal was too focused on the description of the methodology with the hypotheses solely focused on technical aspects of the approach. . . The connection between method-

ology and science application was too weak... PIs should include some external means of validating their modeling results... The broader impacts were relatively weak and could be enhanced."

In response, we have made many changes—both small and large—to the proposal, most notably:

- We refocused the proposal on scientific, rather than methodological, aspects. Most notably, a list of motivating scientific questions is provided at the beginning of the proposal, the previous methodology-focused objectives 1 and 2 have been combined into a single objective, and additional comments are provided in the work plan on the tracers that will be examined.
- We added a new objective 3 and corresponding work task focused on the real-world validation of the simulation results, with an emphasis on using the new LES capability to determine the impact of SM processes on pCO_2 tracer patchiness in the Drake Passage.
- We expanded and substantially strengthened the Broader Impacts. In particular, we now provide a more detailed description of how senior personnel will engage the broader scientific and educational communities, as well as communicate project findings to the public.
- The combined project budget has been substantially reduced to roughly $530k.

2.2 Intellectual Merit

Integration of complex BGC models within high-fidelity LES has previously been exceptionally difficult, but the proposed reduction of these models, as well as the use of GPUs with the high-order RKC integrator, will enable high-resolution studies of fully-coupled turbulent and BGC processes at submesoscales. These improvements will be made possible by leveraging techniques from chemical kinetics modeling for combustion, where reduction and integration of large chemical models in high-fidelity simulations has been common for nearly a decade. The proposed simulation effort will provide insights into the effects of SM turbulence, including wave-driven Langmuir turbulence, on the upper-ocean carbon cycle, and will inform the future development of improved ESMs. In particular, interactions between SM turbulence and BGC tracers are thought to cause tracer patchiness and require substantial further study to develop more accurate subgrid-scale parameterizations for ESMs. Ultimately, the proposed project will provide some of the most detailed and highest-fidelity information to date regarding the two-way coupled interactions between upper-ocean turbulent and BGC processes, and considering real-world scenarios in the Drake Passage will provide concrete insights and understanding of tracer patchiness for realistic conditions.

2.3 Broader Impacts

This highly interdisciplinary research effort will be undertaken by a collaborative team consisting of CU PI Hamlington, who has expertise in LES of both reacting and oceanographic flows, CU Co-PI Lovenduski, who is a biological oceanographer with extensive knowledge of ocean biogeochemistry, and OSU PI Niemeyer, who is an expert in the solution and reduction of chemical kinetic models. Through the proposed project, this team will impact a range of groups:

- **Oceanographic Community:** The biogeochemical modeling tools developed in this project will be made openly available to the broader oceanographic community, thereby permitting the study of other biogeochemical models for different physical scenarios.
- **Graduate Students:** Involvement of interdisciplinary (e.g., both engineering and natural sciences) PhD students will expose a new generation to computational methods in oceanography and the Earth sciences. The project personnel have a history of recruiting graduate students from traditionally underrepresented groups in science and engineering, including an Alaskan Native, Skyler Kern, who is currently supported by an NSF Graduate Research Fellowship in PI Hamlington's group and is working on modeling of marine hydrokinetic systems. Funds from this proposal will also support a female graduate student, Emily Klee, in PI Niemeyer's group.
- **Undergraduate Students:** The project personnel are strongly committed to moving diverse undergraduate STEM students forward into graduate programs by providing genuine research expe-

rience and mentorship to these students. In particular, PI Hamlington and Co-PI Lovenduski have served as mentors for the Summer Multicultural Access to Research Training (SMART) program at CU and the Significant Opportunities in Atmospheric Research and Science (SOARS) program at NCAR, and Co-PI Lovenduski has additionally participated in the Research Experiences in Solid Earth Sciences for Students (RESESS) program at UNAVCO. All of the SMART, SOARS, and RESESS students have achieved great success, receiving fellowships and awards, and all have gone on to pursue graduate school. At OSU, PI Niemeyer has mentored first- and second-year students through the Undergraduate Research, Scholarship, & the Arts (URSA) Engage program, some of whom continued to work in his group throughout their undergraduate program and are now pursuing graduate school; he has also recruited student researchers through the OSU Women & Minorities in Engineering program. We will continue to participate in the SMART, SOARS, RESESS, URSA Engage, and other undergraduate research programs by designing projects derived from, and complementary to, the proposed work described here.

- **K–12 Students:** We will engage K–12 students through summer research experiences for high school students and through short, age-appropriate presentations on climate science in the local school system. PI Hamlington has formerly mentored a local high student in his research group, and this student is now an undergraduate at CU.
- **General Public:** Significant research findings, particularly those of direct relevance to anthropogenic climate change, will be communicated to the general public through social media, public presentations, press releases, and popular science websites. PI Hamlington has previously given public lectures as part of the Café Scientifique and "CU on the Weekend" lecture series, both PIs have Twitter accounts where research findings are shared, and PI Niemeyer was formerly an Associate Science Writer at Ars Technica. Furthermore, PI Niemeyer maintains a research group blog where projects, findings, and activities are described for the public. We will continue and expand our scientific writing and communication efforts to disseminate findings of the proposed project to the broader public.
- **Society:** This research will benefit society through improvements to ESMs used to study climate, resulting in more accurate predictions of future climate impacts on human health, safety, and property. Dissemination of significant research findings also has the potential to influence policy and mitigation strategies related to climate change.

3 Project Objectives

The ultimate objective of the proposed project is to examine the coupled interactions between submesoscale turbulent processes and biogeochemistry in the upper ocean, with a specific focus on the origins of tracer patchiness. More specific objectives, including a brief description of the approaches used and relevant hypotheses, are provided in the following.

- **Objective 1:** Model upper-ocean biogeochemistry in a low-cost, high-fidelity manner through fully-coupled LES of turbulent and BGC processes, using co-processor acceleration.
  Approach: BGC flux models from NCAR, the University of Bologna [7, 8], and GFDL will be reduced to roughly 10 species using techniques developed in combustion research. The reduced models will be solved using a fourth-order RKC integrator on GPUs, concurrently with the solution of fluid flow equations in the NCAR LES model [10–13].
  Hypotheses: (*1.i*) Existing BGC models can be reduced in size by an order of magnitude with little loss of accuracy for relevant quantities of interest; (*1.ii*) Integration of BGC models can be performed efficiently and accurately on GPUs; (*1.iii*) GPUs will improve performance by at least an order of magnitude compared to simulations without GPU acceleration.
- **Objective 2:** Determine the effects of SM turbulent processes on upper-ocean biogeochemistry and tracer patchiness for *idealized* ocean conditions.

Approach: In this process study, reduced models will be integrated in parallel with the NCAR LES model using the RKC algorithm on GPUs to obtain the first predictions of BGC processes at submesoscales, including sub-km scales, for several idealized physical scenarios.
Hypotheses: (*2.i*) Langmuir (i.e., wave-driven) turbulence significantly impacts tracer properties, evolution, and patchiness; (*2.ii*) Changes to vertical convection by different surface heat fluxes impact small-scale BGC tracer patchiness; (*2.iii*) BGC tracers can substantially affect turbulence through changes to density, viscosity, and heat fluxes.

- **Objective 3:** Determine the effects of SM turbulent processes on upper-ocean biogeochemistry and tracer patchiness for *realistic* scenarios, including validation using real-world observations.
Approach: LES using fully-coupled reduced BGC models will be performed with initial and large-scale conditions obtained from the Drake Passage Time-series Program. Simulated evolution and spatial/spectral characteristics of pCO_2 patchiness will be compared with observations.
Hypotheses: (*3.i*) pCO_2 exhibits substantial patchiness at submesoscales, including spatial heterogeneity at scales smaller than are attainable observationally; (*3.ii*) SM turbulence provides a source of pCO_2 patchiness that gives good agreement with observations at larger scales.

4 Background

4.1 Submesoscale Turbulence

This project is specifically focused on the effects of SM turbulent processes from meter to kilometer scales on realistic ocean biogeochemistry and tracer patchiness. This scale range includes mixed-layer restratification due to coherent vertical motions of water masses by quasi-hydrostatic, quasi-geostrophic SM eddies and wind- and wave-influenced fronts, as well as vertical mixing by 3D shear- and wave- (i.e., Langmuir) driven turbulence. At best, ESMs can resolve mesoscale and larger SM processes, but smaller SM and small-scale boundary layer processes, such as Langmuir turbulence, are unresolved. Given that recent studies have demonstrated the importance of tracer transport on scales left unresolved within ESMs [1, 2], it is imperative that an improved understanding be obtained of the effects of these processes on tracer dynamics, including the creation of tracer patchiness. Knowledge gained from such studies can assist in the development of improved physically-accurate subgrid-scale tracer parameterizations.

Although SM eddies and Langmuir turbulence commonly involve similar horizontal velocities of $\mathcal{O}(0.1\,\mathrm{m/s})$, their typical vertical velocity scales, and hence their ability to transport tracers, differ substantially. The ratio of horizontal-to-vertical length scales is $\mathcal{O}(1)$ for Langmuir cells, so the largest horizontal distance between these cells tends to vary with mixed layer depth [14]. The corresponding ratio of horizontal-to-vertical velocities is also $\mathcal{O}(1)$ for Langmuir cells. SM eddies, by contrast, tend to occur on horizontal scales that are roughly ten to a hundred times wider than the mixed-layer depth under typical upper-ocean stratification, mixing, and frontal strength conditions [15–19]. Furthermore, geostrophic flows avoid horizontal convergence and are therefore associated with small vertical velocities, so weaker SM fronts and eddies (i.e., those with small Rossby numbers) have horizontal-to-vertical velocity ratios that are even greater [20].

4.2 Biogeochemically Reactive Tracers

The evolution and properties of mixed-layer tracers such as CO_2, phytoplankton, and nutrients are closely coupled to the dynamics of upper-ocean turbulence. The evolution of such tracers occurs primarily in the oceanic mixed layer where light is plentiful; air-sea exchanges of energy, momentum, gases, and freshwater occur (e.g., [21]); and various scales of turbulent motion actively transport tracers. Prior observational [22–28] and numerical [29–37] studies have shown that the coupling between BGC tracers and fluid processes results in patchy distributions of tracers at the ocean surface. The origins and characteristics of this patchiness are understood to have potential biological and physical origins, particularly at small (i.e., sub-kilometer) scales. However, these prior studies

	Small scale $\tau_t \sim 10^2\,\mathrm{s}$	Submesoscale $\tau_t \sim 10^5\,\mathrm{s}$	Mesoscale $\tau_t \sim 10^7\,\mathrm{s}$	Large scale $\tau_t \sim 10^8\,\mathrm{s}$
Surface transfer of CO_2: $\tau \sim 1\,\mathrm{s}$	10^2	10^5	10^7	10^8
Hydration/hydroxylation: $\tau \sim 10\,\mathrm{s}$	$\mathbf{10^1}$	10^4	10^6	10^7
Protolysis/hydrolysis: $\tau \sim 10^{-7}\,\mathrm{s}$	10^9	10^{12}	10^{14}	10^{15}
Equilibration of CO_2: $\tau \sim 10^2\,\mathrm{s}$	$\mathbf{1}$	10^3	10^5	10^6
Nutrient uptake: $\tau \sim 10^5\,\mathrm{s}$	10^{-3}	$\mathbf{1}$	10^2	10^3
Phytoplankton growth: $\tau \sim 10^5\,\mathrm{s}$	10^{-3}	$\mathbf{1}$	10^2	10^3
Phytoplankton loss: $\tau \sim 10^5\,\mathrm{s}$	10^{-3}	$\mathbf{1}$	10^2	10^3
Zooplankton growth: $\tau \sim 10^5\,\mathrm{s}$	10^{-3}	$\mathbf{1}$	10^2	10^3
Zooplankton loss: $\tau \sim 10^6\,\mathrm{s}$	10^{-4}	$\mathbf{10^{-1}}$	$\mathbf{10^1}$	10^2
Zooplankton reaction: $\tau \sim 10\,\mathrm{s}$	$\mathbf{10^1}$	10^4	10^6	10^7

Table 1: Damköhler numbers, τ_t/τ, for various physical and biogeochemical [39, 49] processes in the upper ocean.

have also revealed a major unresolved difficulty in fully describing the origins of tracer heterogeneity: understanding and explaining the impacts of multiscale turbulent fluid processes on tracer evolution, and the "solubility" and "biological" carbon pumps in particular.

Ocean biogeochemistry is affected by fluid processes over an enormous range of scales, spanning large-scale (∼10,000 km) budgets to millimeter-scale flows where kinetic energy and tracer variance are dissipated [38, 39]. Many important fluid processes take place between these scales, and processes at widely disparate scales may also interact [40–42]. Recent studies have shown that physical transport by mesoscale and SM circulations can give rise to substantial tracer heterogeneity [22, 31, 32, 43–45]. In particular, prior studies [44, 46–48] have revealed that upwelling associated with mesoscale and SM fronts plays a key role in nutrient transport, phytoplankton production, and bloom timing and budgets. These upwelling motions produce $\mathcal{O}(1\,\mathrm{km})$ variations in tracer distributions at the surface, which are also affected by biological and chemical processes.

The most significant tracer-flow couplings are expected to occur when time scales of transport processes rival time scales of reactions. Table 1 shows Damköhler numbers for interactions between different fluid transport and BGC processes, where the Damköhler number is a non-dimensional parameter that relates the chemical or biological reaction rate to the transport rate. Similarities in time scales suggest potentially strong tracer-flow coupling effects, and Table 1 shows that there are generally strong interactions between small-scale turbulence and chemical processes, and between SM turbulence and biological processes. These $\mathcal{O}(1)$ Damköhler numbers specifically motivate further investigation of tracer-turbulence interactions at submesoscales.

Due to the multiscale nature of BGC tracer dynamics in the mixed layer, previous studies have often focused on increasing the complexity of BGC modeling while employing relatively simple background flows [e.g., 29, 37, 50–52]. By contrast, the proposed project is focused on modeling *realistic* BGC tracers in the presence of *realistic* SM turbulence. There are several, relatively large, BGC models available for this task, and three such models in particular will be studied here:

1. *BGC Elemental Cycling (BEC) Model* [6]: Includes 32 state variables and accounts for various phytoplankton functional groups, multiple nutrient types, one zooplankton type, and also carbonate chemical species.
2. *BGC Flux Model (BFM)* [8]: Includes 56 state variables and partitions species into living, non-living organic, and non-living inorganic functional groups, while exchange of matter occurs through units of carbon, nitrate, and phosphate.
3. *Carbon, Ocean Biogeochemistry and Lower Trophics (COBALT) Model* [9]: Includes 33 state variables and describes various elemental cycles, including nitrogen, carbon, phosphorous, and

iron, and includes three phytoplankton groups.

Each of these models are publicly available and will be reduced using techniques from combustion research described in the next section. The resulting reduced models will be made publicly available and will also be written in a format suitable for community BGC modeling projects such as the Marine Biogeochemistry Library (MARBL, led by M. Long at NCAR).

4.3 Kinetic Model Reduction and Integration

The need to study the combustion of petroleum-based fuels and biofuels has resulted in ever-growing chemical kinetic models describing fuel oxidation. These models contain hundreds to thousands of chemical species, and thousands to tens of thousands of elementary reactions. Due primarily to their large size and complexity, such detailed models cannot be used directly in high-fidelity simulations. Even when using moderately sized models (e.g., 50 species or less), the computations required for chemistry can occupy 75–99 % of the total computational time in multidimensional simulations [3–5]. This cost arises from the vast range of species time scales—on the order of nanoseconds to seconds [53]—which induces stiffness in the equations governing the rates of species production and consumption. Stiff differential equations typically require implicit integrators, the cost of which scale quadratically to cubically with the number of species in the model [53]. In response to these challenges, the combustion/chemical kinetics community has developed various methods to reduce the computational cost of using detailed kinetic models [53, 54]. These typically fall into three major categories: model size reduction/simplification, time-scale analysis, and integrator improvements.

Although numerous methods exist, in recent years model-size-reduction methods based on the directed relation graph (DRG) approach have enjoyed wide popularity due to their effectiveness and efficiency in eliminating large numbers of species and reactions [55–61]. These methods quantify species importance by analyzing interactions with other species, without requiring expert intuition. When applied to large models for liquid transportation fuels (e.g., greater than 1000 species), DRG methods typically produce reduced or "skeletal" models with 100–300 species remaining [62, 63].

Reduction methods based on analyzing species/reaction time scales typically eliminate stiffness rather than reduce model size, achieved by removing short time scales caused by rapidly depleting species and/or fast reversible reactions. Classically, these were treated using the quasi-steady state (QSS) [64, 65] and partial equilibrium [66, 67] assumptions, respectively, which replace differential equations with algebraic relations for some species. More systematic approaches for time-scale reduction analyze the chemical kinetics Jacobian matrix to identify QSS species and partial equilibrium reactions, such as the computational singular perturbation (CSP) method [68–72]

Integrator improvements attempt to reduce the cost of integrating the differential equations for any chemical kinetic model. Typical approaches integrate the stiff kinetics differential equations using high-order implicit solvers [73] that use multi-step backward differentiation formulas. These solvers have seen wide success in general modeling codes, but the high computational expense of numerical Jacobian matrix evaluation and factorization (scaling quadratically and cubically with number of species, respectively [53]) impedes their use in large-scale simulations. Alternatively, many reacting-flow simulations do not experience severe stiffness, and other methods offer better performance. PI Niemeyer has shown that explicit and stabilized explicit methods like RKC outperform implicit solvers—particularly when parallelized on GPUs—in situations with little or "moderate" stiffness [74]; this motivates the use of the RKC solver in this project.

5 Preliminary Results

5.1 Multiscale Simulations of Non-Reactive Tracers at Submesoscales

Using the NCAR LES model, the effects of multi-scale turbulence on non-reactive tracers have been examined over a spatial scale range from 20 km down to 5 m [75]. The simulations included the effects of both wave-driven Langmuir turbulence and SM eddies, and explored the evolution

and distribution of tracers with different initial and boundary conditions. The simulation domain included a Langmuir-only region, which contained only small-scale, 3D wind- and wave- driven boundary layer turbulence, and an SM-eddy region, which contained small-scale turbulence as well as larger SM features. Tracer properties were found to be highly dependent on the relative strengths of restratification by SM eddies and vertical mixing by Langmuir turbulence, and these dependencies were shown to have an effect on the vertical eddy diffusivity. Tracers released at different initial depths were shown to be transported differently depending on their proximity to SM eddies and the depth at which they were released. Vertical mixing of tracers with varying air-sea flux rates was found to depend on the ratio of the characteristic time scale associated with the flux rate and the dominant near-surface mixing process. A multi-scale analysis showed that tracer vertical transport was achieved by small-scale processes only in the Langmuir-only region, while in the SM eddy region, transport was achieved by both small- and large-scale processes.

Relevance to Present Project: The NCAR LES model can be used to model the evolution of an arbitrarily large number of tracers with a scale range that spans over three orders of magnitude. Substantial effects of SM turbulence on tracer transport and mixed layer structure were observed.

5.2 Effects of Langmuir Turbulence on Carbonate Chemistry

The effects of Langmuir turbulence on carbonate chemistry have been explored using the NCAR LES model and a second-order RKC integrator for an eight-species carbonate chemistry model [76]. Physical scenarios were the same for all simulations except for the applied strength of Langmuir turbulence, which was varied from no Langmuir turbulence up to a Langmuir number of 0.2. Three different chemistry models were also used: (*i*) an infinitely slow non-reactive model, (*ii*) a time-dependent model, and (*iii*) an infinitely fast equilibrium model. The presence of Langmuir turbulence was found to increase the surface flux rate of CO_2 by continually flushing out the surface layer of the domain, resulting in a greater air-sea gradient in CO_2. As the strength of Langmuir turbulence increased, the flux rate also increased. The choice of carbonate chemistry model was found to substantially affect the flux rate, with the infinitely fast chemistry increasing the rate the most through rapid conversion of CO_2 into bicarbonate and carbonate. The combination of both Langmuir turbulence and different carbonate chemistry models revealed that the two effects are not simply additive and are coupled in a complex manner.

Relevance to Present Project: Carbonate chemistry has been implemented in the NCAR LES model and solved using a low-order RKC scheme. This thus demonstrates that reactive tracers can be implemented in the NCAR LES model, efficiently solved using the RKC method, and that multi-scale simulations of reactive tracers using LES of the upper ocean are possible.

5.3 Reduced Order Modeling of Open Ocean Biogeochemistry

A reduced-order BGC model called BFM17 was developed from the full BFM [7, 8] using intuition and sensitivity analysis [77]. The full BFM defines all biological and chemical components (e.g., phytoplankton, zooplankton, dissolved organic matter) as vectors comprised of carbon, nitrogen, phosphate, and chlorophyll. This chemical functional family approach allows for non-Redfield internal composition ratios to occur, which is highly variable over the year [7, 78]. As in the present project, the motivation for reducing the full BFM was the need for a model accurate enough to reproduce real upper-ocean ecological dynamics, but that can also be integrated within a high-resolution LES at a reasonable computational cost. Since the aim of this study was to examine open-ocean regimes, BFM17 retains all components from the full BFM that are critical to open-ocean ecosystem dynamics, and eliminates those that are not. The new reduced-order model has been coupled to a 1D physical model to perform a parameter sensitivity study, and calibrated using open-ocean observational data from the Bermuda Atlantic Time-series Study (BATS) [79]. Initial results show that the BFM17 model agrees well with the BATS data, in contrast to models of lesser complexity, demonstrating

that a small increase in complexity and the inclusion of several key processes greatly increases the ability of the model to capture open-ocean ecological dynamics.

Relevance to Present Project: A reasonably accurate reduced BGC model has been developed from the full BFM using intuition and sensitivity analysis. However, more powerful reduction techniques, such as those proposed here, may result in smaller and more accurate models.

6 Research Tasks

The objectives in Section 3 will be achieved over three years by the three senior project personnel and two PhD students at CU and OSU. Relevant hypotheses (outlined in Section 3) are indicated after each subtask title (e.g., *h1.i* denotes hypothesis *1.i*).

It should be noted that the tracers of primary interest are those directly related to the ocean carbon cycle. In particular, the BGC model reduction in Task 1 and process studies in Task 2 will focus on the evolution and characteristics (both spatial and spectral) of chlorophyll and dissolved inorganic carbon, while the observational comparisons in Task 3 will focus primarily on pCO_2.

6.1 Task 1: BGC Model Solution in LES

Outcome: Fully coupled LES solver for upper ocean turbulence and biogeochemistry using realistic reduced BGC models and computational acceleration by GPU co-processors.

Subtask 1.1 Unit Problems for Model Reduction [*h1.i*]: Reduction of combustion models typically involves performing simulations of autoignition in a homogeneous, closed volume or extinction in a perfectly stirred reactor, to both generate relevant thermochemical data for the analysis and to assess error of a reduced model. These phenomena do not apply to the relatively slower chemical timescales of ocean biogeochemistry, however, and so different phenomena will be investigated to perform the reduction. In this project, four different "unit" problems, in order of increasing complexity, will be used for model reduction (metrics for comparison are also identified):

1. *Relaxation to steady state after step changes in concentration:* Ignoring the effects of turbulent advection and molecular diffusion, the 0D temporal evolution of BGC models will be examined by solving the system of ODEs comprising the model. The relaxation time of relevant state variables will be examined after a step change in concentration, where accuracy will be determined by comparing relaxation times from full and reduced models.
2. *Stochastic partially stirred reactors:* A system of notional fluid parcels within which "events" such as inflow, outflow, reaction, and mixing occur can be used to emulate a turbulent reacting flow by stochastically varying the timescale of each event [80–84]. Steady-state concentrations and equilibration times will be used to compare the accuracy of full and reduced models.
3. *One-dimensional mixing models:* Vertical mixing by turbulence can be represented using the 1D Princeton Ocean Model (POM) [85]. For the setup of this model, vertical profiles of temperature and salinity will be linearly interpolated in time from climatological monthly profiles. The model prognostically computes horizontal velocities and the turbulent viscosity and diffusivity using a surface climatological wind stress. Full and reduced BGC models will then be integrated over long times to obtain stable annual cycles of tracers. Spatial (i.e., depth) and temporal distributions of tracer concentrations from full and reduced models will be compared. A similar approach was used for the BFM17 model testing described in Section 5.3.
4. *Single-scale 3D LES:* The small-scale and SM simulations described in Task 2 are sufficiently small to integrate full BGC models with roughly 50 species or less, allowing direct comparison of full and reduced models in the presence of realistic 3D upper ocean turbulence. Statistics and spectra quantifying tracer patchiness will be compared between full and reduced models.

The first two unit problems resemble those widely used in combustion research, and the second two problems are closely connected to work that has already been performed for other biological and

chemical models, as described in Sections 5.3 and 5.2, respectively. Development of these unit problems will be led by Co-PI Lovenduski, whose extensive experience in upper-ocean biogeochemistry will allow selection of the most relevant physical and BGC scenarios for each problem. Simulations for the unit problems will be performed by PI Niemeyer and the OSU PhD student.

Subtask 1.2 Reduction of BGC Models [*h1.i*]: To obtain models able to capture realistic BGC processes, particularly in the presence of unsteady SM turbulence, the BEC [6], BFM [7, 8], and COBALT [9] models outlined in Section 4.2 will be reduced using formal methods originally developed to reduce extremely large chemical kinetic models in combustion. Unit problems 1–3 described in Subtask 1.1 will be used to generate relevant state data (e.g., temperature, species concentrations, diffusivities) for the reduction process, and all four unit problems will be used to quantify the performance of candidate reduced models (i.e., by comparing the predictions between the reduced and original models). Two steps will be used to reduce the detailed BGC models:

1. *Directed relation graph with error propagation (DRGEP):* First, we will apply the DRGEP method [58, 60, 86, 87] to the BGC models to obtain initial "skeletal" models. The DRGEP method identifies unimportant species to remove from a model by mapping species to nodes of a directed graph. The weights of directed edges between nodes quantify how much accurately calculating one species' production and consumption depends on the presence of another species in the model. Then, a graph search quantifies the importance of all species to certain target species by calculating their overall "distance." Species with importance values below a cutoff threshold can be removed, along with any reactions in which they participate.
2. *Quasi-steady state approximation:* Next, we will identify candidate QSS species using computational singular perturbation (CSP) analysis [63, 68–70]; the differential equations for these species can be replaced with algebraic equations, reducing stiffness and allowing solutions to be obtained more easily. We will identify QSS species as those which contribute little to slow modes in the dynamics (practically, obtained from the CSP analysis) [63, 88, 89]. We will then construct the reduced model by generating an analytical solution for the QSS species' concentrations that couples with the remaining differential equations for the non-QSS species [63, 89].

The reduced models will be made available in multiple formats and shared openly with the community. PI Niemeyer and the OSU PhD student will lead the model reduction given their extensive experience in this area [60, 63, 84, 86, 87, 90, 91]. Identification of further models to be reduced (beyond BEC, BFM, and COBALT) will be advised by Co-PI Lovenduski.

Subtask 1.3 BGC Model Solver Using GPUs [*h1.ii*]: Preliminary results by the PIs (see Section 5.2) show that a second-order RKC solver reduces the computational cost of integrating carbonate chemistry with the NCAR LES model. Prior work by PI Niemeyer showed that this solver, when implemented on a GPU, outperforms traditional implicit, stiff solvers [74]. However, the relatively low order of the method may introduce unwanted numerical error. Thus, we will develop a fourth-order RKC solver for the reduced BGC models from Subtask 1.2 that is designed for concurrent GPU-based evolution of the BGC species alongside the fluid-flow equations.

The fourth-order RKC solver will derive from literature methods [92, 93], but be tailored for efficient GPU execution. Design of the GPU-based RKC algorithm will involve analysis of integrator waste [94] to identify components that cause poor GPU-parallel performance. Solver accuracy will be assessed through comparisons with results (e.g., for unit problem 1 in Subtask 1.1) from the second-order RKC solver and classical RK solvers. Speed will be compared by performing identical integrations using the fourth-order RKC solver on traditional CPUs and GPUs.

PI Niemeyer and the OSU PhD student will lead this task, which complements—but does not overlap—an ongoing effort investigating stiff solvers for combustion using co-processors [84, 94–97].

Subtask 1.4 Coupling of RKC Solver with NCAR LES [*h1.iii*]: Initially, the RKC solver will be coupled with NCAR LES in a one-way fashion, whereby information is transferred in one direction from the fluid-flow solver (e.g., temperature, pressure, fluid velocities, salinity) to the BGC solver on the GPU. This will involve careful synchronization of information transfer. The ultimate objective of this subtask, however, is full two-way coupling between the biogeochemistry and turbulent fluid flow. This introduces new computational challenges, addressed here, and new modeling demands, addressed in Task 2 (Section 6.2). It should be noted, however, that such two-way coupling is not, in itself, a problem and is *always* included in combustion simulations where heat release from reactions changes the density, viscosity, and other fluid properties.

Within the field of combustion, operator-splitting techniques are by far the most common approaches for modeling two-way coupled tracer and fluid-flow problems, where the tracers are considered "active". Operator splitting, also known as time-step splitting and the fractional-step method [98–104], evaluates separately the rates of change of the physical processes (e.g., diffusion, convection, chemical kinetics) and combines them to obtain the overall change. These processes occur simultaneously, but this approach approximates the correct change for small time-step sizes and matches exactly as the time-step approaches zero.

Here we will compare three forms of operator splitting to couple the fluid flow and tracer evolution: Strang splitting, balanced splitting, and a semi-implicit midpoint method [104]. These will be compared in terms of numerical efficiency and accuracy, the latter using a typical Strang splitting with extremely low time-step sizes to emulate the "true" solution. The most efficient and accurate method will then be used for the two-way coupling with NCAR LES. This subtask will be led by PIs Hamlington and Niemeyer, as well as both PhD students.

6.2 Task 2: Process Study of Turbulence and BGC Coupling at Submesoscales

Outcome: Characterization of coupled turbulent and biogeochemical processes, including the properties and origins of tracer patchiness, at submesoscales for idealized physical scenarios. Research questions 1–5 identified in Section 1 will be addressed in this task.

Numerical Formulation: Reactive tracer equations have already been implemented in the NCAR LES model [12, 76, 105–109]. The fluid dynamic equations that will be solved are the wave-averaged Boussinesq (WAB) equations, with an equation of state that includes both temperature and salinity. The WAB equations differ from the standard Boussinesq equations by the presence of the Lagrangian velocity, $\boldsymbol{u}_L$, in the advective and modified pressure terms. The Stokes drift velocity required to obtain $\boldsymbol{u}_L$ is taken from the empirical Donelan spectrum [110, 111] and decays super-exponentially from the surface. Each of the reactive tracers are described by a transport equation [112, 113] that includes contributions from molecular diffusion, chemical reactions, and subgrid-scale (SGS) turbulent transport. For all reactive tracers, source terms will be given by the reduced models obtained from Task 1. A detailed description of numerical methods used in the NCAR LES model, including the treatment of SGS terms, is provided in Refs. [11, 105, 106].

Biogeochemistry will be simulated using two-way coupling with turbulence. We will explore three sources of coupling: (*i*) Density will be made to depend on the local fluid composition, accounting for the presence of phytoplankton and other non-neutrally buoyant material. This dependence can be accomplished through changes to the equation of state and will result in modified vertical motions due to local variations in density. (*ii*) Concentrations of certain BGC species (e.g., phytoplankton) will be used to moderate the heat flux such that the temperature field becomes coupled to tracer characteristics, thereby altering thermal vertical mixing. (*iii*) To account for effects of surface-confined BGC tracers on wave properties and surface roughness, the Strokes drift velocity and wind shear stress will be made to depend on the concentration of certain tracers. Determining the most physically consistent coupling will be led by PI Hamlington and Co-PI Lovenduski.

	Small-Scale		**Submesoscale**	**Multiscale**	
Simulation identifier	SS	SN	LN	MS	MN
Stokes drift forcing	Stokes	–	–	Stokes	–
Equation set	WAB	B	B	WAB	B
Horizontal size (km), $L_x = L_y$	0.4	0.4	20	20	20
Depth (km), L_z	−200	−200	−200	−200	−200
Langmuir number, La_T	0.2–0.5	–	–	0.2–0.5	–
Characteristic timescale (s), τ_t	10^2	10^2	10^5	10^2–10^5	10^2–10^5
Horizontal grid size, $N_x = N_y$	256	256	256	4096	4096
Vertical grid size, N_z	256	256	256	256	256
Horiz. resolution (m), $\Delta_x = \Delta_y$	1.6	1.6	78	4.9	4.9
Vertical resolution (m), Δ_z	0.8	0.8	0.8	0.8	0.8
Simulation duration (virtual days)	5	5	30	30	30
Initialization	uniform	uniform	SD/GSJ	SD/GSJ	SD/GSJ
Initial mixed layer (m), H_{ML}	50	50	50–100	50–100	50–100
Thermal forcing	heat/cool	heat/cool	dirunal	dirunal	dirunal
Max number of tracers	30–50	30–50	30–50	10–20	10–20
Full BGC models implemented	3	3	3	–	–
Reduced BGC models implemented	3	3	3	2	2
Approx. number of simulations	144	36	24	8	8
Storage/variable/snapshot (GB)	0.125	0.125	0.125	32	32
Approximate CPUs required	256	256	256	2048	2048
Estimated core hours/simulation	20k	20k	20k	1M	1M
Estimated total core hours	2.9M	0.72M	0.48M	8M	8M

Table 2: Summary of the five ocean configurations to be examined in this project. 'WAB' denotes the Wave-averaged Boussinesq equations and 'B' denotes the Boussinesq equations. 'SD' denotes the temperature filament spindown configuration [40, 75] and 'GSJ' denotes the Gulf Stream Jet configuration [114–116].

Three sets of simulations will be performed in this task, as described in the following subtask descriptions and summarized in Table 2. All simulations will be led and performed by PI Hamlington and the CU PhD student, with substantial input from other project personnel.

Subtask 2.1 Small-Scale Simulations (SS and SN in Table 2) [*h2.ii*, *h2.iii*]: The evolution of coupled biogeochemistry and turbulence will be examined at small scales using LES in domains of size 400 m×400 m×−200 m with grids of size 256^3. Due to the relatively low cost of these simulations, it is anticipated that roughly 50 biogeochemically reactive tracers with different source terms and boundary conditions can be modeled. This will thus allow direct comparisons of full and reduced versions of the three BGC models outlined in Section 4.2 within the context of realistic 3D upper ocean turbulence. Horizontally uniform initial fields will be used for temperature, velocities, and reactive tracers, with initial vertical profiles obtained from 1D POM simulations. The LES will be performed for a range of physical conditions, corresponding to different strengths of wave driving (i.e., no driving and Langmuir numbers from 0.5 to 0.2), to different surface heat fluxes (i.e., cooling, heating, and adiabatic), and to different initializations from POM (e.g., from the BATS and other observational sites). Each simulation will be carried out for up to five virtual days, without diurnal forcing to achieve steady state conditions. Roughly 180 small-scale simulations will be performed.

Subtask 2.2 Submesoscale Simulations (LN in Table 2) [*h2.i*]: Coupled interactions between BGC tracers and SM eddies will be examined using LES in domains of size 20 km×20 km×−200 m with a coarse grid of size 256^3. Since small-scale turbulence is not resolved in these simulations, the Stokes drift term is set to zero and the simulations thus solve the Boussinesq equations. Once again,

due to the low cost of these simulations, a large number of reactive tracers can be included, thereby allowing direct comparison of full and reduced versions of all three BGC models. Due to the slower evolution of SM eddies, these simulations will be performed for up to 30 days using diurnal forcing through variations in the surface heat flux, at two different times of the year (i.e., fall and spring). Two physical scenarios will be examined in these simulations: (*i*) The spindown of a mesoscale temperature filament in the presence of a uniform velocity field (denoted 'SD' in Table 2). This case has been studied extensively by PI Hamlington in prior work, with details of the setup described in [40, 75]. (*ii*) The generation of SM structure by a Gulf Stream Jet (denoted 'GSJ' in Table 2). This classical case is described in [114–116] and leads to the formation of SM structure through gradients in velocity as opposed to temperature (as in the spindown case). Roughly 24 SM simulations will be performed over the course of the three-year project.

Subtask 2.3 Multiscale Simulations (MS and MN in Table 2) [*h2.i*, *h2.ii*, *h2.iii*]: The culmination of these process study simulations will be a series of multi-scale LES that include both small-scale wind- and wave-driven turbulence as well as larger SM features. The physical domain size in these simulations will be $20\,\text{km} \times 20\,\text{km} \times -200\,\text{m}$, but the resolution will extend down to the 1–10 m range to capture the effects of small-scale shear and Langmuir turbulence. Achieving this resolution will require grids of size $4096 \times 4096 \times 256$. Once again, the SD and GSJ physical scenarios will be simulated, and comparisons with the SM simulations in Subtask 3.2 will allow the effects of small-scale turbulence to be identified. Simulations will be performed for each scenario with and without Stokes drift forcing. Due to the high cost of these simulations, it will only be feasible to use reduced BGC models, and it is anticipated that only one or two reduced models will be examined. Each simulation will be performed over roughly 30 virtual days, again in the presence of diurnal forcing, for two different times of the year (e.g., fall and spring). A total of roughly 16 multiscale simulations will be performed over the course of the three-year project.

Analysis of Simulation Results: Data from the simulations will be analyzed qualitatively through visualizations of velocity, vorticity, temperature, and tracer fields. Quantitative insights will be obtained using second-order diagnostics such as variances and correlations, as well as marginal, joint, and conditional probability density functions (pdfs). Spectral diagnostics will be used to characterize tracer patchiness at different scales; less patchy distributions are characterized by steeper spectra [117, 118]. Spectra can be calculated by a number of methods [117, 119–121] and, in each case, patchiness is parameterized by the value of a wavenumber or length-scale scaling exponent. Spectral decompositions will also be used to understand multiscale interactions between tracers and turbulent processes; e.g., vertical transport of tracers by large- and small-scale vertical velocities.

To determine the dynamical origins of tracer patchiness, different terms in the tracer transport equations will be computed and compared for different conditions. This will allow the relative contributions of reactions, turbulent advection, and diffusion on the creation of tracer patchiness to be quantified. Moreover, by considering the spectral dynamical equations for the tracer fields, it will be possible to isolate the specific origins of tracer variability at different scales. We will also examine the effects of tracer patchiness on the supply of nutrients, primary production, particle aggregation/sinking, and the export of carbon, all of which can be quantified in the simulations.

6.3 Task 3: Turbulence and BGC Coupling in the Drake Passage

Outcome: Characterization of coupled turbulent and BGC processes, including the properties and origins of tracer patchiness, at submesoscales for a real-world scenario. Research questions 1, 3, 5, and 6 identified in Section 1 will be addressed in this task.

Observations: The Drake Passage Time-series Program (DPTP) has collected nearly 20 years of observations of surface pCO_2 from an underway sensor on the ARSV L.M. Gould as it crosses the Southern Ocean from the southern tip of South America to the northern tip of the Antarctic

Peninsula approximately 20 times per year [122–124]. The observations are collected every 160 s as the ship traverses the dynamic Antarctic Circumpolar Current, giving an unprecedented look at highly-resolved spatial BGC features, such as pCO_2 patchiness. As an example of this heterogeneity, during a summertime cruise last year, the Drake Passage underway system recorded surface ocean pCO_2 values ranging from as low as 107 µatm to as high as 478 µatm across a distance of 178 m. This pCO_2 heterogeneity has the potential to bias point-source measurements from surfacing floats that sample the surface only once every 10 days (e.g., [124–126]), and thus characterizing and understanding this patchiness is an important scientific question in its own right. Further, questions remain about whether the patchiness is more prominent in summer or in winter, and the DPTP is notable for its wintertime sampling (rare in the Southern Ocean due to rough sea conditions). Interpretation of the observational data will be led by PI Lovenduski [122, 123].

Subtask 3.1 Multiscale Simulations of the Drake Passage [*h3.i*]: We will investigate the role of submesoscale turbulence in pCO_2 patchiness across two seasons: (a) summer, when biological activity and physical turbulence both likely play a role in surface ocean pCO_2 patchiness; and (b) winter, when physical turbulence interacts with background tracer gradients. Available observations from the DPTP will be used to initialize and force (using well-established spectral-nudging approaches at large scales [127–131]) the NCAR LES model, and the reduced BGC models will be solved in parallel on GPUs. These simulations will provide the most realistic data to date regarding the interactions between SM turbulence and BGC tracers in the upper ocean, with a particular focus on the evolution and characteristics of pCO_2 at small scales. Since the simulations will be forced at large scales using observations, the simulations can be run for much longer than is possible using the idealized configurations described in Task 2. This will allow examination of effects such as entrainment of nutrients due to mixed-layer deepening; phytoplankton bloom timing, intensity, patchiness, and subduction; and carbon export from the surface ocean. Results from these simulations will be compared to other similar coarse-resolution SM simulations that use simpler BGC models [18, 45, 132]. These simulations will again be performed with and without wave driving to determine the impacts of Langmuir turbulence on BGC tracer evolution. The simulations will be jointly performed by PIs Hamlington and Niemeyer, as well as both PhD students.

Subtask 3.2 Data Analysis and Comparison [*h3.ii*]:Comparisons will be made between simulation results and available observational data. Using the resulting simulation data, spectral diagnostics will be employed to understand pCO_2 patchiness at different scales; less patchy distributions are characterized by steeper spectra [117, 118]. Spectral diagnostics of patchiness can be calculated by a number of methods [117, 119–121]. In each case, patchiness is parameterized by the value of a wavenumber or length-scale scaling exponent. Spectral decompositions and filters will also be used to understand multiscale interactions between tracers and turbulent processes; vertical transport of tracers by large- and small-scale vertical velocities, for example, can be measured through a decomposition of the velocity field. Once again, the effects of patchiness on the supply of nutrients, primary production, particle aggregation/sinking, and the export of carbon will be examined. This subtask will be led by PI Hamlington and the CU PhD student, with input from Co-PI Lovenduski.

7 Work and Management Plan

All research tasks will be completed according to the three-year plan on the next page. Completion dates of objectives in Section 3 are denoted "Obj1", "Obj2", and "Obj3".

Resource Requirements: The majority of the proposed simulations will be performed on the Summit supercomputer at CU and the Cheyenne supercomputer operated by NCAR. The NCAR LES model has already been run on Summit and Cheyenne by PI Hamlington, and the code has demonstrated good performance in carrying out the simulations described in Section 5. These supercomputers incorporate GPU co-processors on many of the nodes, thereby supporting the GPU

Task	Year 1				Year 2				Year 3			
	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4
Task 1: BGC Model Solution in LES												
Subtask 1.1: Unit problems for model reduction (OSU/CU)												
Subtask 1.2: Reduction of BGC Models (OSU/CU)												
Subtask 1.3: BGC Model Solver Using GPUs (OSU)												
Subtask 1.4: Coupling of RKC solver with NCAR LES (OSU/CU)							Obj1					
Task 2: Process Study of Turbulence and BGC Coupling at Submesoscales												
Subtask 2.1: Small-scale simulations (CU)												
Subtask 2.2: Submesoscale simulations (CU/OSU)												
Subtask 2.3: Multiscale simulations (CU/OSU)									Obj2			
Task 3: Turbulence and BGC Coupling in the Drake Passage												
Subtask 3.1: Multiscale Simulations of the Drake Passage (CU/OSU)												
Subtask 3.2: Data Analysis and Comparison (CU)												Obj3

acceleration efforts described in Section 6.1. Compilation of the code requires Fortran and MPI libraries, but the code has proven to be easily portable across multiple platforms. It has been shown for other problems [108] that NCAR LES has nearly ideal scaling to large numbers of processors.

Based on the size of the simulations summarized in Table 2, each of the five-day, 256^3 small-scale cases will require approximately 20,000 core-hours. A similar cost is anticipated for the submesoscale simulations. Each of the 30-day, $4096 \times 4096 \times 256$ multi-scale simulations, which will include 10–20 biogeochemical species, is expected to require approximately 1,000,000 core-hours. The Drake Passage LES described in Task 3 is expected to be of similar cost to the multi-scale simulations, and four such simulations are anticipated. Overall, successful completion of this project would thus require roughly 24 million core-hours over a three-year period, which is reasonable given the increasing availability of petascale supercomputers such as Cheyenne. This resource requirement will be supported by existing and new allocations on Cheyenne and other supercomputers (e.g., those available through NSF XSEDE and the Department of Energy).

8 Results from Prior NSF Support

OCE-1258995: Collaborative Research: Reacting Tracers in a Turbulent Mixed Layer; **PI:** Hamlington, **Co-PI:** Lovenduski; **Total award amount**: $401,386; **Duration**: 6/1/13–5/31/18.
IM: This project uses LES to examine the evolution of simple and generic reactive tracers in the presence of realistic small-scale turbulence produced at upper ocean submesoscales. **BI**: Insights from this project are directly relevant to gas and carbon budgets at the interface between the atmosphere and ocean, as well as to biological dynamics in the upper ocean. **Publications**: Five peer-reviewed journal papers have been produced [40, 75, 76, 133, 134], as well as numerous conference presentations and several conference posters. **Research products:** Software and simulation data produced as a result of this project will be made openly available on a web server at CU.

ACI-1535065: SI2-SSE: Collaborative Research: An Intelligent and Adaptive Parallel CPU/GPU Co-Processing Software Library for Accelerating Reactive-Flow Simulations; **PI:** Niemeyer; **Total award amount:** $299,887; **Duration:** 9/1/15–8/31/19 (NCE).
IM: A software library is being created to accelerate the solution of chemical kinetics equations in reactive-flow simulations on hybrid computing hardware. **BI:** Software tools will be provided for next-generation clean and efficient engine design, and for the study of difficult problems in combustion. **Publications:** Nine published journal papers [76, 84, 94, 95, 97, 135–138], multiple conference papers, and three software packages [96, 139, 140]. **Research products:** Journal articles are published in open-access journals or available as preprints, and software is shared on GitHub.

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