Implementation of Ocean Biogeochemical Modeling and Ocean Color Data Assimilation within NOAA/NCEP's Next-Generation Global Ocean Data Assimilation System (NG-GODAS)

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Ocean biogeochemical and ecological forecasts provide early warning of ecosystem changes and their impacts on water quality, human health, and/or regional economies, allowing for sufficient lead time to develop mitigation strategies and take corrective actions. Ocean biogeochemical and ecological processes also provide important geophysical feedback to weather and climate systems, through complex ocean biophysical and ocean-atmosphere interactions. The inability to represent ocean biogeochemical and ecological processes and their feedback to oceanic and atmospheric physics in the current generation of operational forecast systems, as well as our limited understanding of the underlying mechanisms of past extreme weather and ecological events, reduces our capability to predict critical weather conditions and ecological "tipping points" and affects management effectiveness at both global and regional scales. Through a project funded by the JPSS Proving Ground and Risk Reduction (PGRR) program, we developed and evaluated ocean biogeochemical modeling and data assimilation tools as well as the required infrastructure at EMC, in support of NOAA/NCEP's operational weather, subseasonal-to-seasonal (S2S), and ecological predictions. This document provides an overview of key milestones of the implementation of an ocean biogeochemical model and the assimilation of satellite-based ocean color observations within NOAA/NCEP's Next-generation Global Ocean Data Assimilation System (NG-GODAS).

1. Ocean biogeochemical modeling

The biogeochemistry model implemented in NG-GODAS is adapted from NOAA/GFDL's BLING model (Biogeochemistry with Light, Iron, Nutrients and Gas version 2, or BLINGv2; Dunne *et al.*, 2020), and is coupled to the Modular Ocean Model version 6 (MOM6; Adcroft *et al.*, 2019) currently being implemented in the Unified Forecast System (UFS). BLINGv2 states are treated essentially as generic tracers in MOM6, and so are subject to advective and diffusive transports, as well as source and sink terms from boundary fluxes (e.g., atmospheric deposition, riverine inputs) and biogeochemical processes (e.g., burial, denitrification). The coupled MOM6-BLINGv2 model has been successfully tested at horizontal resolutions of 1° and 0.25° using NG-GODAS. Preliminary results suggest that upper-ocean physics (e.g., SST) are moderately sensitive to ocean biogeochemical (e.g., Chl-a) variability with a response of up to 1°C in some regions (Figure 1).



c) Δ SST (°C; MOM-BLING - MOM6-only) 2011 November



Figure 1. a) SeaWiFS Chl-a climatology (Nov.) used to calculate short-wave radiation penetration in the MOM6 physics-only run; b) MOM6-BLING simulated Chl-a averaged over November 2011; and c) difference in sea surface temperature (SST) between the two experiments, suggesting that upper-ocean physics, such as SST, are sensitive to Chl-a variability.

2. Ocean color data assimilation

NG-GODAS employs the sea-ice ocean and coupled assimilation (SOCA), based on the Joint Effort for Data Assimilation Integration (JEDI). The JEDI project is the backbone for performing data assimilation across the variety of UFS applications. We further developed SOCA to allow the integration of near real-time satellite ocean color products into MOM6-BLINGv2 simulations.

2.1 Ocean color observations

Level-2 data streams have been established from NESDIS into NCEP for NOAA-20/VIIRS and S-NPP/VIIRS historical and near real-time ocean color observations (i.e., chlorophyll concentration, or Chla, and particulate organic carbon, or POC), specifically from NOAA CoastWatch and NASA OB.DAAC to NOAA's Research and Development High-Performance Computing System (RDHPCS). The required software to preprocess VIIRS Level-2 ocean color products for basic quality control and ingestion by the JEDI system were developed. Specifically, these observations are converted into a unified data format (i.e., IODA compatible) that can be ingested by any model employing the JEDI system for data assimilation.

2.2. Chl-a and POC analysis

To assimilate Chl-a and POC, the corresponding biogeochemical states saved in the model restart file are updated during each data assimilation cycle (i.e., 24 hrs) based on increments calculated in JEDI/SOCA. Other key states, such as phosphate concentration, are updated by solving BLING internal equations for phytoplankton growth and nutrient limitation based on chl-a or POC increments. The background error covariance ("B") matrix for the ocean color observations will be computed using the "Background error on Unstructured Meshgrid" (BUMP) in the SABER package of JEDI, and is assumed to be diagonal. For each grid-point, the observational error variance will be set to be proportional to the observed values (e.g., observational error = 30% for Chl-a; Tsiaras *et al.*, 2017). The UFOs will estimate "ocean color" properties from the biogeochemical model as the corresponding variables averaged over the first optical depth at each grid-point. Figure 2 shows a preliminary Chl-a daily analysis using the 3-dimensional variational (3DVAR) scheme.



Figure 2. (upper panels) Simulated "background" Chl-a in MOM6-BLING and Level-2 Chl-a derived from NOAA-20/VIIRS imagery on 2018/04/15, used for Chl-a assimilation; (lower panels) Chl-a increments calculated based on the 3DVAR scheme in

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