



Climate Modelling User Group [CMUG]

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Interim progress report on WP5.4: Seasonal predictability of ocean biogeochemistry and potential benefits of ESA CCI data assimilation

Centres providing input: Met Office, Barcelona Supercomputing Center

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DMI
Danish Meteorological Institute



THE UNIVERSITY
of EDINBURGH



Deutsches Zentrum
für Luft- und Raumfahrt
German Aerospace Center



Barcelona
Supercomputing
Center
Centro Nacional de Supercomputación





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Interim progress report on WP5.4: Seasonal predictability of ocean biogeochemistry and potential benefits of ESA CCI data assimilation

1. Purpose and scope of this report

This document is an interim progress report on WP5.4 (“Seasonal predictability of ocean biogeochemistry and potential benefits of ESA CCI data assimilation”) of the CCI+ CMUG project.

WP5.4 aims to explore the potential benefits to our capacity to predict key ocean biogeochemical variables at seasonal time scales when ESA CCI products for physical fields (sea surface temperature, sea surface salinity, sea level, sea ice) and biogeochemical fields (ocean colour) are assimilated into state-of-the-art modelling systems. Two partners (Met Office and Barcelona Supercomputing Center) will separately perform sets of experiments assimilating different combinations of ESA CCI products into the ocean physical-biogeochemical reanalysis configurations of their respective global seasonal forecasting systems. The results of these experiments will be inter-compared and conclusions drawn as to the optimal assimilation strategy for initialising seasonal forecasts of ocean biogeochemical variables, and the relative importance of satellite observations of physical and biogeochemical fields.

This report sets out the motivation for the work, and describes the observational data and modelling systems used. Progress to date on setting up and running the experiments is summarised, together with planned next steps.



2. Introduction

Recent significant progress in Earth System Models (ESMs), which consist of global climate models that also represent chemical and biological processes, has resulted in comprehensive simulations of important aspects of the Earth System beyond just physical processes. The incorporation of biogeochemical components in ocean models has allowed for the representation of changes in marine biological primary productivity and its main nutrients, as well as the carbon cycle, enabling the use of ESMs for predicting changes in key biogeochemical variables at seasonal to decadal time scales. Such ESM-based predictions represent the variations of key ecosystem drivers (e.g., pH, oxygen, net primary production, chlorophyll), which have been shown to have close relationships with habitat distributions in marine ecosystems (e.g., Tommasi et al., 2017; Park et al., 2019). Successful predictions of variations of ecosystem drivers, in conjunction with marine ecosystem models, have the potential to be used for predicting variations in fish populations and yields and thus provide useful information to aquaculture, fishers and policy makers. Furthermore, they may play an important role in environmental monitoring and protection, for instance in relation to coral reefs and marine protected areas.

ESM-based predictions are commonly initialised from model reanalyses that assimilate observations. Such reanalyses typically assimilate physical oceanic variables that describe the ocean state (e.g., temperature and salinity). However, the potential benefits of additionally assimilating biogeochemical data, such as chlorophyll or phytoplankton carbon biomass, have not been thoroughly investigated. Here, we assess the representation of ocean biogeochemical fields in two ESM-based reanalysis systems assimilating different combinations of physical and biogeochemical CCI essential climate variable (ECV) data. From this we will draw conclusions about the optimal assimilation strategy for using CCI products to initialise seasonal predictions of ocean biogeochemistry.

We aim to address the following science questions:

- What is the value of assimilating physical and biogeochemical CCI ocean ECVs in generating initial conditions for seasonal predictions of ocean biogeochemistry?
- What is the dominant factor at initialisation (the physical or the biogeochemical state) in determining the ocean biogeochemistry predictive skill at global and regional scales?
- What is the best strategy for constraining initial conditions in order to achieve the highest prediction skill in ocean biogeochemistry?

WP5.4 will focus on reanalysis skill. Study OWP5.4 will then use a subset of the reconstructions produced in WP5.4 to initialise and run seasonal reforecasts, and assess their comparative skill in predicting key ocean biogeochemical variables.



3. Observations

Data from the following CCI ECVs is being used for assimilation and/or validation:

- Sea surface temperature (SST)
- Sea surface salinity (SSS)
- Sea level
 - Sea level anomaly (SLA)
- Sea ice
 - Sea ice concentration (SIC)
 - Sea ice thickness (SIT)
- Ocean colour (OC)
 - Chlorophyll concentration
 - Primary production (PP)
 - Phytoplankton carbon
 - Particulate organic carbon (POC)

The exact data used will be a mixture of CCI products and products from other sources which have been either derived from CCI data or produced by the same teams. Full details of the products used are given in Table 1.

ECV	Product	Assimilation	Validation
SST	CCI v3.0	Along-track L2P/L3U (MO) Daily L4 (BSC)	Daily and monthly L4
SSS	CCI v4.41	Along-track L2P (MO)	Weekly and monthly L4
Sea level	CMS L2 C3S L4 CMS L4	Along-track L2 (MO)	Daily and Monthly L4
Sea ice	CCI/OSI SAF v3.0 C3S SIT	Daily L4 SIC (MO)	Daily and monthly L4 SIC Daily and monthly L4 SIT
Ocean colour	CCI v6.0 BICEP/NCEO	Daily L3 chlorophyll (MO) Monthly L3 phytoplankton carbon (BSC)	Daily and monthly L3 chlorophyll Monthly L3 primary production Monthly L3 phytoplankton carbon Monthly L3 particulate organic carbon

Table 1. Use of CCI ECVs for assimilation and validation.

Additionally, EN4 in situ temperature and salinity data will be used for assimilation and validation. ESA OceanSODA satellite/in situ derived carbon (if found to be suitable), SOCAT in situ carbon, and GLODAP in situ carbon and nutrient data will be used for validation.



4. Modelling systems

Two different modelling and assimilation systems are used in WP5.4, the ocean-ice-biogeochemistry reanalysis components of the global seasonal forecasting and climate modelling systems used at the Met Office and Barcelona Supercomputing Center - Centro Nacional de Supercomputación (BSC). These are respectively described below.

4.1 Met Office

The physical ocean and sea ice models used are the GOSI9 configuration (Guiavarc'h et al., 2025) of NEMO v4.0.4 and SI³. As part of the Met Office's seamless modelling approach, GOSI9 forms the physical ocean-ice components of the next generation of coupled ocean-atmosphere numerical weather prediction, seasonal forecasting, and climate modelling systems. The new versions of the forecasting systems are scheduled to become operational in late 2025, while the new climate model versions will contribute to CMIP7.

For global ocean forecasting and reanalysis GOSI9 is coupled with a 3D-Var configuration of the NEMOVAR data assimilation scheme in the FOAM system, as described by Mignac et al. (2024). FOAM provides the ocean initial conditions of the GloSea seasonal forecasting system (MacLachlan et al., 2015), and is the basis of the ocean reanalysis used to initialise historical reforecasts used for bias correction.

The ocean biogeochemical model MEDUSA (Yool et al., 2013) is used in UKESM1 (Sellar et al., 2019) which contributed to CMIP6, and an updated version is under development for use in UKESM2 which will contribute to CMIP7. MEDUSA does not form part of the operational FOAM or GloSea systems, but the latest version has been coupled with GOSI9 and NEMOVAR as part of this work.

Using NEMOVAR, all ECVs listed in Section 3 can be assimilated into FOAM-MEDUSA. In the operational FOAM system, a multivariate assimilation of SST, SLA, and in situ temperature and salinity is performed with physical balance relationships providing cross-correlations as described in Waters et al. (2015). SIC is also assimilated. In research mode, SSS can be added to the multivariate assimilation as described by Martin et al. (2019). This capability has been further developed as part of ongoing work at the Met Office as part of the SSS-CCI CRG. Chlorophyll from ocean colour can be assimilated as described by Ford (2021), and the nitrogen balancing scheme of Hemmings et al. (2008) used to update the wider biogeochemical model state (Ford et al., 2012).

GOSI9 provides a hierarchy of resolutions: 1°, 1/4°, and 1/12°. In common with the GloSea reanalysis, 1/4° resolution is used in this work. Also in common with the GloSea reanalysis, atmospheric forcing is provided by the ERA5 reanalysis from ECMWF.



4.2 BSC

The BSC will use the ocean and sea ice components of the ESM EC-Earth for the impact assessment study. The EC-Earth model is a state-of-the-art coupled climate model developed and used for climate predictions, projections and biogeochemical studies by a European consortium of more than 20 operation and research institutions (Döscher et al., 2022). Its design is based on modules representing different Earth system components (atmosphere, ocean, sea ice, land surface, dynamic vegetation, atmospheric composition, and ocean biogeochemistry), which can be coupled in various model configurations (Fig. 1). The latest version, EC-Earth4.1.1, incorporates the Integrated Forecast System (IFS) from the European Center for Medium-Range Weather Forecasts (ECMWF) cycle 48r1 coupled with the general ocean circulation model Nucleus for European Modelling of the Ocean (NEMO version 4.2.2; Madec, 2015). The Tracer Model 5 (TM5) allows for the interactive simulation of atmospheric aerosols and reactive gas species (Van Noije et al., 2021), and PISCES (Aumont et al., 2015), as part of the NEMO system, represents marine biogeochemistry. EC-Earth3 contributed to the CMIP6 and has been extensively used with different configurations to produce climate predictions and projections. EC-Earth4 will be similarly used for CMIP7. The BSC team worked on developing a carbon cycle version of EC-Earth3 called EC-Earth3-CC, which for the ocean runs at a horizontal resolution of $1 \times 1^\circ$ and with 75 vertical levels. This has been transitioned to become EC-Earth4-ESM.

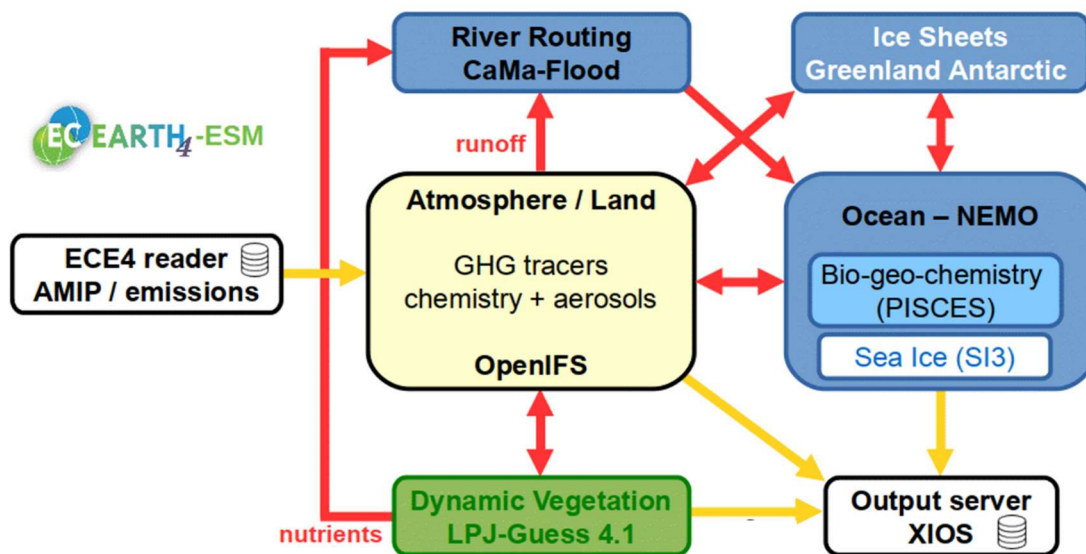


Figure 1. Schematic of EC-Earth4-ESM and its components. Taken from <https://ec-earth.org/ec-earth/ec-earth4/>.

The ocean biogeochemical model PISCES simulates the lower trophic levels of marine ecosystems (phytoplankton, microzooplankton, and mesozooplankton) and the biogeochemical cycles of carbon and the main nutrients (Phosphate, Nitrogen, Iron and Silicate). It includes 24 prognostic variables (tracers) including two phytoplankton compartments (diatoms and nanophytoplankton), and two zooplankton size classes (microzooplankton and mesozooplankton). The BSC team has recently developed an assimilation method to nudge



phytoplankton carbon tracers in PISCES with satellite-based estimates of surface POC and Carbon phytoplankton (C_Phyto). This method can be used in consonance with the nudging towards NEMO's physical variables such as SST.

5. Experiments

A series of ocean reanalysis experiments is being carried out with each of the modelling systems, testing different settings and combinations of ECVs in the assimilation. These are described below.

5.1 Met Office

Experiments will build on those performed separately with a physics-only version of the system as part of the SSS-CCI CRG. In that work, two reanalyses were run for 2016-2020, following a 5.5-month spinup with initial conditions taken from a previous GloSea reanalysis. One reanalysis assimilated SST, SLA, SIC, and temperature and salinity profiles; the standard version of the system as described in Mignac et al. (2024). The second reanalysis added assimilation of SSS-CCI data. ECV product versions were the same as those described in Section 3.

The WP5.4 experiments will use this setup, but couple in MEDUSA, explore different combinations of ECV assimilation, and use the new Met Office supercomputer which is currently in the User Acceptance Testing phase. MEDUSA initial conditions will be taken from a CMIP6 OMIP run, and a short spinup performed as with the physics.

The following experiments are planned:

- 1) A free run with no data assimilation.
- 2) A run assimilating SST, SLA, SIC, and temperature and salinity profiles.
- 3) A run adding SSS assimilation to the above.
- 4) A run further adding OC assimilation to the above.
- 5) Tests with different assimilation settings.

1) will provide a baseline against which to assess the impact of the data assimilation. This is important given that older versions of the system have demonstrated negative impacts of physics assimilation on biogeochemical fields: see Ford et al. (2018) and Ford (2020) for discussion. 2) will replicate the standard FOAM/GloSea reanalysis setup for physics. 3) will show the impact of assimilating SSS, which is the one ocean ECV not previously assimilated into physical-biogeochemical ocean reanalyses. 4) will show the impact of adding biogeochemical data assimilation, as per the outlined in the science questions. 5) will depend in design on the results of the other runs, but in the event that some ECV assimilation has a negative impact on the biogeochemical state, there are changes to the assimilation options which can be explored in order to maximise biogeochemical skill.



5.2 BSC

Modelling experiments at the BSC will focus on evaluating the improvement of ocean biogeochemical reconstructions when nudging them towards SST and Carbon phytoplankton satellite data. The evaluation will be done comparing four different experiments (Fig. 2):

1. CONTROL RUN

This simulation is designed as both spin-up (starting in 1700) and reference simulation with free evolving ocean and biogeochemistry (no nudging).

2. ORAS5 RUN

A simulation running from 1980 to 2022 where the ocean dynamics (NEMO) is nudged toward ORAS5 reanalysis, as commonly done in EC-Earth4 simulations.

3. ESA-CCI SST RUN

A simulation equivalent to ORAS5 RUN but using the ESA-CCI product for Sea Surface Temperature (SST). Comparing this simulation with the previous one will allow quantifying the improvements associated with the exploitation of state of the art SST ESA products.

4. ESA-CCI SST+C_Phyto RUN

A simulation using two ESA-CCI databases: SST and C_Phyto. The former will nudge NEMO physics while the latter will nudge the phytoplankton Carbon concentration to bring PISCES closer to observations. Comparing this simulation with the previous one will allow quantification of the improvements associated with incorporating ocean biogeochemical fields to nudge EC-Earth4-ESM. Comparing it with configuration 2 will allow quantification of the total improvement of nudging both SST and C_Phyto.

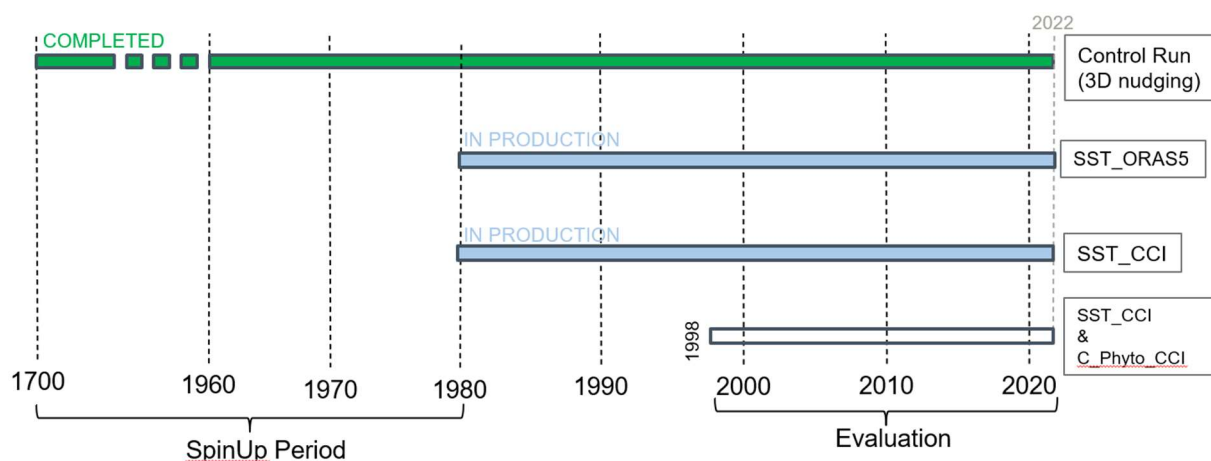


Figure 2. Time diagram of the four different experiments planned at the BSC.

6. Summary of progress and next steps



Progress so far has mostly involved technical setup of the modelling and assimilation systems and preparing the observation data and experiments.

At the Met Office, work has focussed on coupling the latest version of MEDUSA with the latest version of the FOAM/GloSea reanalysis system, including the biogeochemical observation operator and data assimilation code. The observation operator changes take advantage of recent developments to the system (Mignac et al., 2024), which make the NEMO observation operator interface more generic and therefore more robust to add biogeochemical variables. The biogeochemical assimilation changes include the use of the nitrogen balancing scheme of Hemmings et al. (2008). The scheme was developed for the simpler HadOCC model (Palmer and Totterdell, 2001), and not used in a previous biogeochemical assimilation study with MEDUSA (Ford, 2021), but is designed to update the entire biogeochemical model state based on ocean colour data, which is likely to be important for maximising the skill of seasonal predictions of biogeochemistry. Its use has been expanded to be able to be used with the more complex MEDUSA. Furthermore, the systems are being ported to the new Met Office supercomputer. Final technical setup is being completed, and experiments will be set running shortly.

At BSC, the control simulation has been completed (see Fig. 2) and the CCI_SST downloaded and converted to the same grid as the one used in EC-Earth4-ESM. The second and third experiments (ORAS5 and SST_CCI runs) are now running and expected to finish in mid-March.

Additionally, plans and progress have been presented in various forums. Within CCI, this has included a poster and presentation at the 2024 Integration/Colocation meeting, and presentations at other CMUG meetings. Further afield, a poster was presented at the OceanPredict '24 Symposium in Paris in November 2024, and plans were presented at an OceanPredict Marine Ecosystem Analysis and Prediction Task Team meeting in Plymouth in July 2024.

Over the next few months, the remaining experiments will be run, and thorough validation and analysis of results performed. Initially, the Met Office and BSC experiments will be assessed independently, and then the two sets of results will be intercompared in order to draw common conclusions. Recommendations will be reported to ECV teams, and a final report submitted in summer 2025. The aim is for this to be followed by one or more journal publications, possibly including results from the optional study OWP5.4, which will follow immediately on from WP5.4 and run seasonal reforecasts with the Met Office system.

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8. Glossary

Acronyms	
(A)ATSR	(Advanced) Along Track Scanning Radiometer
AVHRR	Advanced Very High Resolution Radiometer
BGC	Biogeochemical or Biogeochemistry
BICEP	Biological Pump and Carbon Exchange Processes
BSC	Barcelona Supercomputing Center – Centro Nacional de Supercomputación
C3S	Copernicus Climate Change Service
CCI	Climate Change Initiative
CMIP	Climate Model Intercomparison Project
CMS	Copernicus Marine Service
CMUG	Climate Modelling Users Group
CRG	Climate Research Group
ECV	Essential Climate Variable

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ERA5	ECMWF Reanalysis 5
ESA	European Space Agency
ESM	Earth System Model
FOAM	Forecasting Ocean Assimilation Model
GLODAP	Global Ocean Data Analysis Project
GloSea	Met Office Global Seasonal Forecasting System
GOSI9	UK Global Ocean and Sea Ice configuration version 9
IPCC	International Panel for Climate Change
L2	Level 2
L2P	Level 2 Pre-processed
L3	Level 3
L3U	Level 3 Uncollated
L4	Level 4
MEDUSA	Model of Ecosystem Dynamics, nutrient Utilisation, Sequestration and Acidification
MO	Met Office
NCEO	National Centre for Earth Observation
NEMO	Nucleus for European Modelling of the Ocean
OC	Ocean Colour
OMIP	Ocean Model Intercomparison Project
OSI SAF	Ocean and Sea Ice Satellite Application Facility
OSTIA	Operational Sea Surface Temperature and Sea Ice Analysis
PISCES	Pelagic Interactions Scheme for Carbon and Ecosystem Studies
POC	Particulate Organic Carbon
PP	Primary Production
SI ³	Sea Ice modelling Integrated Initiative
SIC	Sea Ice Concentration
SLA	Sea Level Anomaly
SOCAT	Surface Ocean CO ₂ Atlas
SSM/I	Special Sensor Microwave Imager
SSS	Sea Surface Salinity
SST	Sea Surface Temperature
UKESM	United Kingdom Earth System Model