Gathering users and developers to shape together the next-generation ocean reanalyses

Ocean reanalyses workshop of the European Copernicus Marine Service

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What: Gather together ocean reanalyses users and producers to identify users' needs of ocean reanalyses and design the strategy to improve ocean reanalyses to fulfill users' needs

When: 10-12 October 2023

Where: Toulouse, France and online

Objectives of the workshop:

Ocean reanalyses are reconstructions of the past ocean state combining ocean numerical models and earth observations through data assimilation techniques. As a result of their temporal and spatial consistency and continuity compared to earth observations only, and their high accuracy and quality compared to pure numerical model simulations, ocean reanalysis data are widely used in the scientific community (e.g., ocean and climate process studies) and private sectors (e.g., operational

planning, shipping, and fisheries). For almost a decade, the Copernicus Marine Service has provided users with high-quality, regularly extended global and regional ocean reanalyses. The objective of this workshop was to gather the international community to (1) understand the users' needs for ocean reanalyses, (2) identify the strengths and weaknesses of current ocean reanalyses, and (3) establish the way forward toward the next generation of ocean reanalyses by improving different aspects of these products to meet users' needs and science ambitions (4) improve collaborations within the community.

The three-day workshop was held in Toulouse (France) and brought together ocean reanalysis users, producers from European Copernicus services and beyond, and scientific experts on different aspects (data assimilation, ocean models, and observations). The workshop's hybrid format (online and in person) enabled us to welcome around 60 people in person and 1400 registrations online, with 700 unique connections on day one, 350 on day two, and 250 on day three. The key findings of each objective are given in the following sections; the last section highlights the next steps the ocean reanalyses community will carry out.

Users' requirements for ocean reanalyses

To have a comprehensive picture of users' requirements for ocean reanalyses, we designed three steps to collect and analyze users' feedback:

- A user survey was launched before the workshop
- Selected users were invited to present their experiences and recommendations at the workshop
- A real-time (live) user survey was conducted during the workshop

Before the workshop, the Copernicus Marine Service conducted the following user survey to identify the users' needs for ocean reanalyses:

- What do you use reanalyses for?
- How would you define a consistent reanalysis?

- What are your main requirements?
- What major improvements do you expect?
- What potential applications would you like to use reanalyses for?

351 worldwide ocean reanalyses users from the Copernicus Marine Service users database, participated in the survey and the outcomes (Figure 1 and Figure 2) show that the main requirements are:

- uncertainty quantification and information on the accuracy of the data
- higher spatiotemporal resolution, longer time series, additional variables, and easier access
- enhanced data assimilation
- a good agreement between reanalyses and observations within their combined error bars

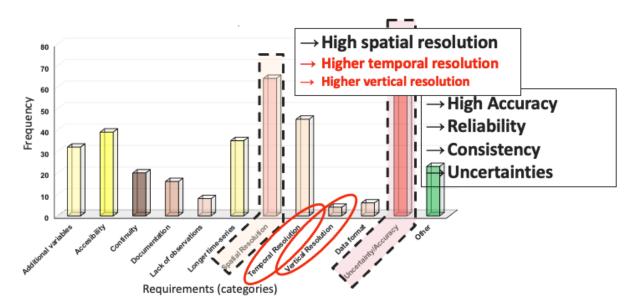


Figure 1 User (351 participants) survey of the users' needs for ocean reanalyses.
 The total number of users who voted for each requirement is shown in the bar plot as frequency.

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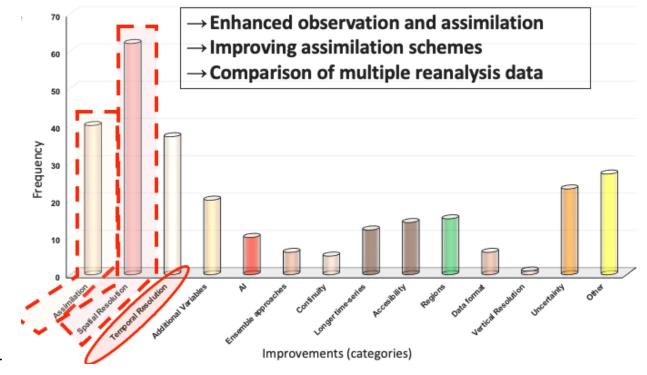


 Figure 2 User (351 participants) survey of the requirements on major improvements needed for ocean reanalyses. The total number of users who voted for each requirement is shown in the bar plot as frequency.

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To initiate a direct discussion with users, we invited representative ocean reanalysis users from different sectors (e.g. downstream services, ocean biology, ocean and climate monitoring [Dayan et al, 2023], and training of AI-based ocean forecast systems) to present their experiences of using reanalyses, further needs, and the improvements they expect. The main outcome of the presentations confirms that ocean reanalysis can be a useful database for research and downstream applications, as well as for preparing the future evolution of prediction systems with AI-based methods. Additionally, users called for additional analysis into the consistency between regional and global reanalyses, as well as improvements in the quality of reanalyses at the global and regional levels.

During the workshop, we conducted an on-site survey with online participants to gather users' feedback. In addition to improvement in the documentation of reanalyses, the outcome of this on-site survey confirmed the previous survey of users' needs as summarized above (shown in Figure 1 and Figure 2).

Current ocean reanalysis products and plans

To identify the gaps in ocean reanalyses, we convened an overview (e.g. the strengths and weaknesses, and plans for the next generation) of current ocean reanalysis products, covering both global and regional (e.g. Arctic and regional seas) products, from:

- Blue ocean (physical and waves)
- Green Ocean (biogeochemistry and higher trophic levels)
- White ocean (sea ice)

Blue Ocean

Several global reanalysis teams presented the status of their reanalyses: the Simple Ocean Data Assimilation reanalysis (SODA) [Carton et al., 2018], the Estimating the Circulation and Climate of the Ocean reanalysis (ECCO)[Forget et al., 2015], the Japanese Meteorology Agency reanalysis (JMA) [Fujii et al. 2023], the Mercator Ocean GLORYS reanalysis [Lellouche et al., 2021]. Most products are available at a spatial resolution of 0.25°, with one of the Copernicus Marine Service reanalyses (GLORYS12) at a higher resolution of 0.083° (i.e., 1/12°), and ECCO data at a lower resolution of 1°.

According to users' needs, higher spatial resolution ocean reanalyses are in high demand, particularly in coastal regions. To meet users' needs, data producers are already acting to increase the resolution of their products; for example, the ECCO team is preparing the next generation of ocean reanalyses at 0.25° and 0.1°. To alleviate the high cost of computing power to produce high-resolution global reanalyses, an alternative way to serve users' preferences is to provide regional ocean reanalyses at higher spatial resolution. For example, the SODA group has a regional ocean reanalysis

available in the Arctic region at a horizontal resolution of 0.1° [Carton et al., 2023] and the JMA has regional ocean reanalyses around the region of Japan at a resolution of 2 km [Hirose et al. 2019]. The Copernicus Marine Service also provides users with ocean reanalyses for six regions: the Mediterranean Sea and the Black Sea (Escudier et al., 2021; Lima et al., 2021); the Baltic Sea; Northwestern Shelves of the North Atlantic; Ireland Biscay Iberian; and the Arctic[Xie et al., 2017].

Longer time series of ocean reanalyses are also one of the main requests of users. Currently, most global reanalyses start from 1993 when satellite altimetry data are available to be assimilated into the system. The underlying computational complexity prevents data producers from providing high-resolution and long-period reanalysis records simultaneously. Alternatively, different data streams could meet users' needs. For instance, reanalysis producers outlined plans to provide a longer series (back to the 1950s) at a low spatial resolution (e.g.0.25°) and also downscaled to a higher resolution(e.g. 0.08°) for a more recent period (from the 1990s).

Another priority that emerged from the workshop was the need to have strong coupled ocean waves and physics in Blue Ocean reanalyses. Extreme wave events can have significant socio-economic and environmental impacts [Casas-Prat et al. 2024]. The provision of wave reanalyses is essential for understanding the historical variability and long-term changes in wave conditions and for many downstream applications (Hemer et al. 2011). The Copernicus Marine Service offers users both global and regional wave reanalyses with different periods and resolutions depending on the system. At the international level, an ensemble of global wave reanalyses and hindcast products is available to users [Morim et al., 2019, Morim et al. 2022,] as the outcome of the Coordinated Ocean Wave Climate Project (COWCLIP). A coordinated effort and collaboration is needed between Copernicus Marine Service and COWCLIP to provide better wave reanalyses to worldwide users.

Green Ocean

Biogeochemical reanalyses provide a wide range of variables essential to understanding processes such as primary production, acidification, de-oxygenation, and eutrophication, and to link to high trophic level ecosystem components. The demand for biogeochemical variables is increasing due to the growing threat of climate change on marine ecosystems, especially related to extreme events. To this end, all CMEMS model variables including biogeochemical nutrients should be available for users, including organic nutrient pools. In addition, global reanalyses for low and mid-trophic levels are becoming available to users for studying marine ecosystems in more detail. Besides CMEMS, other data producer centers (incl. SODA and ECCO) are planning to provide users with reanalyses of ocean biogeochemistry and marine ecosystems in the coming years.

Data assimilation for the Green Ocean is at a less mature stage than for the Blue Ocean. The variables provided by biogeochemical reanalyses have higher model uncertainty and are less well constrained by observations. As a result, the use case for many of these products is still being explored by the broader community.

White Ocean

The important and considerable impacts of sea ice melt [Hoag 2008; Cohen et al., 2021] in the Arctic Ocean call for improved White Ocean reanalyses. Such products allow us to monitor ocean and sea ice changes and enable downstream applications (e.g. shipping routes). Sea ice reanalyses are provided as the sea ice component of the global ocean reanalyses (ocean and sea ice coupled) and regional ocean reanalyses (Arctic and Southern Ocean). Previous intercomparison studies have shown that there is general agreement between different datasets for sea ice concentration and extent, but sea ice thickness and volume involve large uncertainties [Chevallier et al., 2017; Uotila et al., 2019]. Despite the large uncertainty, Uotila et al., 2019 shows that the ensemble mean of the ocean state in the polar regions is better represented than single reanalysis, indicating the usefulness of ocean reanalysis ensemble mean. Ongoing efforts to develop new sea ice models, increase the number of sea ice observations,

and assimilate sea ice thickness are expected to increase the quality of White Ocean reanalyses in the following years.

Coupling ocean components

Even though we have separated the ocean reanalyses in terms of Blue, Green, and White Ocean, the spatiotemporal evolution of the ocean depends on the interaction of all three domains. Indeed, increased coupling is viewed as an important goal for future ocean reanalysis development. The reanalysis community is working in this direction; for instance, in the last decade, the ocean reanalyses provided in the Copernicus Marine Service have progressed from uncoupled, to offline coupled, to online coupled systems. Other producers are planning to provide coupled ocean-atmosphere reanalyses in the coming years. However, most ocean reanalysis and data assimilation efforts are expected to continue running with atmospheric reanalyses as surface boundary conditions, and thus produce forced ocean reanalyses. This allows for higher resolution, more explicitly resolved processes, and higher accuracy at the mesoscale, high priorities for many users. The best compromise between complexity, resolution, and duration of ocean reanalyses may vary depending on each ocean reanalysis's targeted applications and user groups.

Ocean Reanalyses Uncertainty

Another priority for users is to have uncertainty quantification and quality information of ocean reanalyses. To further understand the skill of current ocean reanalyses, we invited speakers to review available uncertainty information about ocean reanalyses and possible methods to reduce uncertainty. Uncertainties in the Blue Ocean come from boundary conditions (e.g. atmospheric forcing, freshwater river inputs, open boundary conditions for regional reanalysis), initial conditions, observations assimilated, and model physics. Performing a large ensemble (32 members) of ocean reanalyses, Storto and Yang (2024) show that at the regional scale, observation-induced uncertainty is dominant and at the global scale atmospheric forcing-induced uncertainty becomes important. In a system like ECCO, on the other hand, it has been shown that uncertainties in parameterized subgrid-scale physics and atmospheric forcing fields

predominate (Forget et al 2015). Emerging neural network-based methods for model error correction could be used to reduce systematic errors in reanalyses, along with already established parameter optimization techniques (e.g., Forget, Ferreira, and Liang, 2015).

Uncertainty in global and regional wave reanalyses arises from atmospheric forcing fields, numerical wave modeling approaches, bias correction methods, and assimilation techniques (wave observations) [Morim et al. 2019; Morim et al. 2023]. The uncertainty in global wave reanalysis exceeds the climate change signal over many ocean and coastal areas primarily due to differences in atmospheric forcing fields [Morim et al. 2023]. Ensemble wave reanalyses are needed to better understand extreme wave events and their frequency and direction. Regionally downscaled wave reanalysis products based on high-resolution atmospheric forcing are needed to better resolve extreme events (such as tropical cyclone-generated waves) and wave characteristics within nearshore regions.

Uncertainty in the Green Ocean biogeochemical reanalyses is ascribed to several sources [Fennel et al., 2019]. Improving physical reanalyses has a positive impact on the transport processes, such as vertical mixing and injection of nutrients in the euphotic layer. However, in equatorial regions, data assimilation of physical variables can have detrimental effects on the biogeochemical solution [Gasparin, 2021; Park 2018]. Uncertainty also originates from the model formulation and parameter uncertainty (e.g. a better description of how light is absorbed and scattered in the water could improve phytoplankton growth and deep chlorophyll maximum dynamics). Biogeochemical data assimilation (e.g. an enhanced data assimilation scheme and additional variables and types of observations other than ocean color) could both constrain the state variables and be used to estimate model parameters.

For White Ocean sea ice reanalyses, atmospheric forcing, the sea ice model, and sea ice assimilation (observations assimilated) all induce non-negligible uncertainty.

However, implementing a multi-category sea ice model setup, improvement of data

assimilation, and assimilation of "new" types of observations such as sea ice thickness could reduce sea ice uncertainty.

Ocean reanalyses priorities from the Climate Community

In the climate community, ocean reanalyses have been used as initial conditions in seasonal forecasts and decadal predictions and as a benchmark for comparison in the Climate Model Intercomparison Project (CMIP)[Waliser et al., 2020]. A main requirement from the CMIP community is to use the same data format which specifies variable, dimension, coordinate, metadata, and file naming conventions. To improve accessibility, reanalysis data should be shareable and accessible by users. Reanalysis data should also be fully documented, including publications, Digital Object Identifiers (DOIs), and licenses such that users are permitted to share datasets across the community.

In terms of seasonal and decadal predictions, it is well known that the initial condition of the ocean plays a significant role in determining the predictability of the climate system [Balmaseda and Anderson, 2009; Stammer et al., 2016]. To help the decadal prediction and seasonal forecast community, improvements in reanalyses are needed for the following aspects: (1) time series extended further back in time (e.g., back to the 1950s) (2) global coverage (3) near real-time production (4) large ensembles of ocean reanalyses (5) temporal consistency.

Improvements in ocean reanalyses

During the workshop, data providers and users identified weaknesses in current ocean reanalyses. As a result, improvements in ocean reanalyses need to be carried out to reduce bias and uncertainty and to enhance quality. In particular, ocean reanalyses can be improved upon in four key areas.

Boundary Conditions

We started the session by reviewing the status of atmospheric reanalyses used as boundary conditions. For example, the NOAA-CIRES-DOE 20th-Century Reanalysis

(20CRv3) [Slivinski et al., 2021, 2019; Compo et al., 2011] covers almost 200 years which provides the opportunity to extend the ocean reanalyses back in time. However, changes in the observation network present major challenges in producing these long-time series of atmospheric reanalyses that ocean reanalyses will also face. 20CRv3 handles this challenge by only assimilating surface pressure observations, to avoid spurious signals from changes in upper-air and satellite observation networks. The ERA5 reanalysis [Hersbach et al., 2020] produced by ECMWF has been extended back to 1940 and is updated close to real-time. To understand better the use of atmospheric reanalyses as boundary conditions we need close collaboration and interaction (e.g. a complementary workshop) between these two communities as suggested by the survey. The river discharge values used in most ocean reanalyses are still climatological. Newly developed discharge datasets (e.g. GloFAS 4.0, EFAS v5.0, ECFAS) from the Copernicus Emergency Service could contribute to the improvement of ocean reanalyses. A time-resolved forcing dataset for nutrient loads from rivers is still lacking.

Numerical Models

Another key component of ocean reanalyses is the choice of numerical model and its optimisation in order to minimize biases. Key aspects are: (1) representation of the mixed layer, turbulent transport, and boundary layer processes (2) improvement of effective horizontal resolution (numerical scheme) (3) low-order representation of ocean dynamics, (4) avoiding unphysical energy transfer or cascades, (5) improved numerical schemes and optimized parameterizations and (6) representation of primary production and processes (e.g., light description, horizontal and vertical supply of nutrients).

Observations

The advantage of ocean reanalyses compared to unconstrained numerical model simulations is the assimilation of observations. To have a comprehensive observations database for ocean reanalyses is critical. The Global Ocean Observing System (GOOS) (https://www.goosocean.org/) is structured to assess observational needs, design a system to meet these needs and provide data dissemination for essential ocean variables. Additionally, the Copernicus Marine Service provides reprocessed L3 and L4

satellite observations and dedicated quality-controlled in-situ observation datasets close to real-time which support the production of reanalyses as part of the value chain from ocean observations to ocean prediction. Part of the satellite records are not yet assimilated in all reanalyses, such as gravimetry observations, which could improve long term trends, or sea surface salinity which could reduce large scale biases. Another way forward is the continuous improvement of historical databases towards an increased number of Findable, Accessible, Interoperable, and Reusable (FAIR) datasets. The ongoing effort in the biogeochemical observations will also help the Green Ocean community to further improve the quality of reanalyses by assimilating the multivariate observations. Meanwhile, the ocean reanalyses could provide feedback to the observation community to evaluate and optimize the observation network as discussed in Storto et al., 2019. Close interaction between the ocean reanalyses and observations network is crucial to benefit both communities.

Data Assimilation

Data assimilation is the tool to reduce ocean model errors by ingesting observations. Improved representation of error covariances in the assimilation process could help improve ocean reanalyses. Joint physical and biogeochemical data assimilation could improve biogeochemical ocean reanalyses. Emerging methods, for instance, approaches leveraging machine learning/deep learning, could lead to breakthroughs in the quality of ocean reanalyses, either through the improvement of components of existing frameworks (e.g., model correction, model parameterization, observation operator) [Farchi, et al., 2021; 2023] or through end-to-end data-driven approaches [Fablet et al., 2021; Boudier et al., 2023]. Differential programming, which enables adjoint modeling, and Bayesian inference also are good examples of model parameter optimization (Forget al 2015, Forget, Ferreira, and Liang, 2015). These methodological and technological developments will require dedicated research efforts at the crossroads of applied math, AI, and operational oceanography, including shared and open intercomparison frameworks.

Concluding remarks

It is the first time, to our knowledge, that reanalysis producers and users have gathered together to discuss the developments needed within the next generation of ocean reanalyses. Users' long-term priorities (e.g. longer period, higher resolution, uncertainty quantification, and quality, specific formats to serve more communities of users) are clear as stated in the user survey and invited presentations. The review of current ocean reanalyses and plans indicates that producers are progressing in the right direction to fulfill users' needs by increasing the horizontal resolution or extending the time series. However, to compensate for the high cost of computing power, multistreams of ocean reanalyses are needed to meet users' preferences further. Several weaknesses of ocean reanalyses have been identified; biases and uncertainty in the ocean reanalyses should be estimated and reduced, with several specific examples provided in the previous sections. Finally, to improve ocean reanalyses, we need to work closely with different communities (atmospheric reanalyses, ocean modeling, data assimilation, and observations) to identify the best approach. The emerging needs (e.g., digital twins of the ocean) and new technologies (e.g., Artificial Intelligence) provide the ocean reanalysis community with challenges and opportunities for future development.

Planned activities for the ocean reanalysis community

Based on the feedback from users and producers, an immediate action for the ocean reanalysis community is to initialize a new intercomparison project on ocean reanalyses (the on-site survey shows that 95% of participants agree).

In 2011 the ORA-IP project started as a CLIVAR-GSOP/GODAE-IV-TT joint initiative and continued after 2014 with the support of the "Evaluation of Ocean Synthesis" COST action. The activities were carried out based on key variables [Balmaseda et al., 2015] and the outcome of the ORA-IP shows consistency and discrepancy of ocean reanalyses for different variables and at different regions. For example, the intercomparison of AMOC by Karspeck et al., 2017 shows large uncertainty in the ocean reanalyses, but the later work by Jackson et al. 2019 demonstrates good agreement in AMOC variability and generally with observations in the Atlantic. Recently a few studies were carried out to intercompare high-resolution reanalyses in near-shore

waters (Amaya et al., 2023; Castillo-Trujillo et al., 2023; Russo et al., 2022). These contrasting intercomparison results highlight the continued improvement of ocean reanalyses and the need for periodic intercomparison activities to measure the progress being made in ocean reanalyses.

Therefore, after more than 10 years of development and improvement of ocean reanalyses, now is the moment to initialize a new intercomparison of ocean reanalyses to understand:

- The quality (uncertainty and accuracy) of current ocean reanalyses at global and regional scales, including green ocean reanalyses
- The strengths and weaknesses of existing ocean reanalyses for different applications and scientific studies
- The opportunities and challenges the ocean reanalysis community will face in the coming era

For the medium/long term, the European Copernicus Marine Service will use the outcomes of this workshop to define the strategy for future developments of ocean reanalyses to meet users' needs.

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