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A description of Validation Processes and Techniques for Ocean Forecasting

Marcos Garcia Sotillo[1], Marie Drevillon[2], Fabrice Hernandez[3]

[1]Nologin Oceanic Weather Systems, Santiago de Compostela, Spain
[2]Mercator Ocean International, Toulouse, France
[3]LEGOS, Institut de Recherche pour le Développement, Toulouse, France

Correspondence to: Marcos Garcia Sotillo (marcos.sotillo@nowsystems.eu)

Abstract. Operational forecasting systems architecture requires clear identification of best practices for assessing the quality of ocean products: it plays a key role not only for the qualification of predictions skill, but also for advancing in the scientific understanding of the ocean dynamics from global to coastal scales. The Authors discusses on the role of observing network for performing validation of ocean model outputs, identifying current gaps (i.e., different capacity in assessing physical essential ocean variables versus biogeochemical ones), but also emphasizing the need of new metrics (tailored for end-users comprehension and usages). An analysis on the level of maturity of validation processes from global to regional systems is provided. A rich variety of approaches exist, and the most we move towards the coast the higher is the complexity in calculating such metrics, due to increased resolution but also somehow limited by the lack of coastal observatories worldwide. It is provided as example how the Copernicus Marine Service currently organizes the product quality information from producers (with dedicated scientific documentation, properly planned and designed) to end-users (with publication of targeted estimated accuracy numbers for its whole product catalogue).

1 Introduction

Product quality assessment is a key issue for operational ocean forecasting systems (OOFS). There is a long tradition in scientific research related to model validation and, through coordinated community initiatives there have been in recent times important progress on this field related to operational oceanographic services (Hernandez, 2015; 2018).

Strong efforts to define operational oceanography's best practices have started; among others: the Ocean Best Practices (Pearlman, et al., 2019 and https://www.oceanbestpractices.org/) and the ETOOFS guide (Alvarez-Fanjul et al., 2022). In the latest ETOOFS guide, several sections are dedicated to model validation: i.e.: Section 4.5 on Validation and Verification, and sub-sections on Validation Strategies for ocean physical models (Section 5.7), Sea ice models (Section 6.2.6), storm surge (Section 7.2.6), wave models (Section 8.7) and biogeochemistry models (Sction 9.2.6) or the specific section (Section 12.9) on quality assessment for intermediate and end users.

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2 Observations for validation

The lack of observations is the primary, and obvious, difficulty to validate an OOFS on a specific site. In that sense, it is very difficult to overcome observational gaps and, if they exist, OOFS validation processes are seriously hindered by them.

While validation is a global necessity and challenge, an overview of the current European capacity in terms of operational modeling of marine and coastal systems presented by Capet et al. (2020) is instructive. It included contributions from 49 organizations around Europe, representing 104 operational model systems simulating mostly hydrodynamics, biogeochemistry and sea waves and it provides an updated mapping of the European capability in terms of OOFSs. Not being the characterization of the operational validation status of the European OOFSs among the primary objectives of the mapping performed, this contribution shows how, and to what extent, different observational data are used for model skill assessment. As shown in Figure 1, most of the validations systems are mainly using fixed platforms, satellite remote sensing and coastal tide gauges.

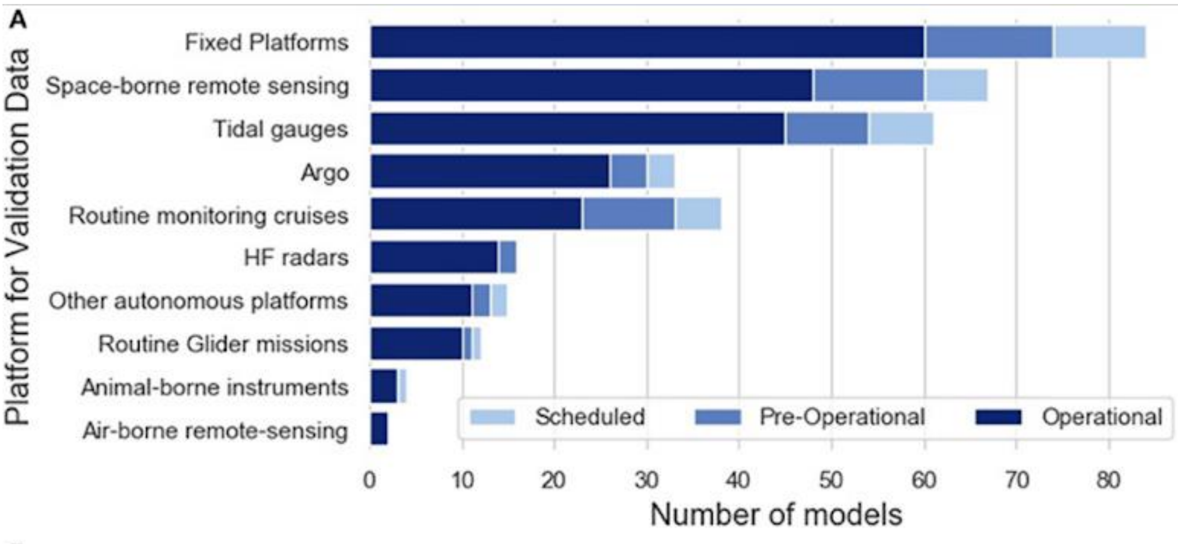

Figure 1: (from Capet et al. 2020). Observing platforms providing data used for model skill assessment and validation purposes; and number of models (from the EuroGOOS survey that use them).

It is important to note that the aggregate results of the study do not provide differences between basin/regional systems and the more coastal ones. Indeed, in this contribution most of the Copernicus Marine MFC NRT systems are included, making that some observational data sources not so coastal oriented (such as the Argo) will be used by a high number of European OOFSs. The same may happen with the use of space-borne remote sensing products, which is more limited in its use for validation OOFS as we move to more limited small coastal model domains.

Use of satellite products for OOFS validation is common in the case of global, basin and regional systems, but limited in the case of coastal ones (if used, mainly in those systems that present a bigger spatial geographical coverage, going beyond the shelf break). Furthermore, new incoming observational technologies (i.e., the new Sentinels missions, swath altimetry, HF

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Radars, BGC-Argo, etc.) and opportunities to use of new coastal observing systems (links with Member State networks and/or specific R&D projects) will enhance model validation capacities. New validation tools may also be developed for coordinated Observing System Experiments (OSEs) and Observing System Simulation Experiments (OSSEs) related to the optimization of these observation networks. Taking advantage of these OSSEs framework, AI emulated variables will be developed which will increase validation capacities. Increased awareness on the need for enhancing observing networks, bringing new initiatives and efforts to better integrate existing ocean observing systems with the OOFS validation processes is needed.

3 OOFS Validation: A matter of EOVs

The Copernicus Marine Service, a comprehensive multi-product service, dealing with more than 150 products and involving more than 60 EOVs for the blue, green and white ocean, can be useful to infer the different level of model validation performed depending on the targeted EOV. The Copernicus Marine PQ strategic Plan (Sotillo et al., 2021) points:

- The physic blue world versus the green component. The lack of biogeochemistry observations conditions not only at the biogeochemical model validation, but even the modelling itself. Due to the maturity of the physical OOFS, compared to the less numerous biogeochemical OOFS components, and the different level of observational availability, the assessment of physical parameters is more developed than the one for biogeochemistry parameters; The Copernicus Marine Service identifies the need of special efforts for biogeochemical model product validations. Due to the lack of in situ data, phenomena such as primary production and bloom of phytoplankton are most of the time assessed using Ocean Color satellite information, with the limitations that satellite observed chlorophyll values have especially on coastal areas. Furthermore, it is necessary to also assess in biogeochemical models the factors that cause these blooms (i.e., transport of nutrients). Carbon, oxygen, and ocean acidification are parameters of interest both at regional and global scales that need a better validation. BGC-argo floats can enhance the monitoring, but mostly off shelves and far from coastal areas. Finally mention that in the bio model validation, it is important to evaluate together the errors in the physical system, particularly vertical transport and mixing which strongly impact the coupled biogeochemical models. Thus, a monitoring of errors on key parameters of the physical forcing should help to characterize causes of errors of biogeochemical products.
- Sea ice concentration, due mainly to observation by satellite, is assessed and brings to sea ice extent, sea ice drift, sea ice thickness and sea ice edge validation. New validation metrics (some related to end-user needs) should be developed for sea ice temperature and icebergs concentration maps, and specific assessments on interannual time scales, multi-year sea ice parameters need to be specifically addressed.
- Sea surface temperature is the most used EOV, being the most monitored parameter, and usually assessed with (in-situ and remotely sensed) multi-product approaches, considering regional specificities (for high frequency products, particular attention should be paid to diurnal cycle and tidal mixing effects). Generally, validation on surface layers is privileged with respect to the rest of layers across the water column, existing a clear decreasing gradient towards

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deeper levels. Availability of in-situ observations has greatly improved since the 2000s with the Argo program. At depth, T/S data are the most used observations in Product Quality assessment. However, at synoptic scales, water mass distribution stays partially sampled in the upper ocean. There are significant regional differences, not always being the coastal areas the privileged ones (indeed, the autonomous Argo measure network changed the usual fact of coastal and on-shelf areas being traditionally the more sampled).

- In the case of salinity, in-situ measurements from fixed moorings, ARGO drifters or offshore, coastal profiles with CTD or XBT instruments, and surface transects with thermo-salinometer are the most common data sources used for OOFS model validation. Averaged maps of sea surface salinity derived from remotely sensed satellite data (such as the SMOS ones) can be used to validate models, especially far from coastal areas. The approach to regionally validate sea level model solutions is based on comparison to satellite altimetry, at the scales of interest, from open ocean to coastal dynamical responses. Enhancement of sea level validation in coastal and on-shelf areas is needed and preparation for the use of the new wide swath altimetry products should be done in following years. On the other hand, comparison of coastal OOFS model products with sea-level measurements from tide-gauges is quite common and external metrics linked to Storm Surge services (including total sea levels, tidal solution, residuals) are considered; for many coastal systems, especially for those with more limited spatial coverages, the comparison with local tide-gauge, usually installed in ports, is the only direct model-observation comparison feasible.
- Currents and associated transports, especially near surface, are parameters with strong impact in many applications and their assessment is usually done using independent observations (as most of today's systems do not assimilate this kind of observations). Both Eulerian and Lagrangian approaches need to be considered and in-situ observations from current meters at moorings, ADCPs, surface drifters or deep floats, as well as from coastal HF radar systems. Satellite altimetry can be used to assess geostrophic/non geostrophic properties of the ocean, and some derived estimation of currents from satellite SAR, or from SST/Ocean color images, can also be used on specific areas.

4 Operational Validation: status across different OOFSs

A discussion on the status of operational validation in the different existing OOFS systems is provided here. There are significant differences between the validation of global/basin/regional OOFSs and the very coastal OOFSs. This is addressed in the following sections: 1) on the operational validation performed within the Copernicus Marine service, a good example (and operational pushing key operational oceanographic player) of how operational validation of basin/regional OOFSs contributes to generate product quality (PQ) information on the service; and 2) on the more localized coastal OOFSs (here, a variety of approached is faced; some description of it, using for Europe inputs from EuroGoos coastal model capability mapping, and examples from systems all over the world (in North and South America, Africa and Asia).

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4.1 Validation of global/basin/regional model systems: The Copernicus Marine example

The Copernicus Marine Service (Marine Service or CMEMS, Le Traon et al., 2019), presented here as an example of state-of-the-art system in terms of validation at the regional scale, relies on a very complex system of systems framework which interconnects European OOFS (more than 14 model-based and/or observations production centers). It aims to deliver state-of-the-art, consistent, and reliable information, derived from space and in-situ observations and from models – including forecasts, analyses and reanalyses – on the physical and biogeochemical state over the global ocean and the European regional seas.

A scientifically sound and well communicated Product Quality assessment arises as one of the main cross-cutting functions of the Marine Service (see further details on its achievements along the first phase of the service in Sotillo et al., 2022), strongly linked to the operational production performed at individual OOFS level. This applies to most of the service phases, from the design to the operational delivery of products, including communication and training activities.

Individual OOFS, producers of the regional components of the Marine Service, daily verify the scientific quality of their model products (i.e., NRT forecast/analysis and MY reanalysis), using quantitative validation metrics, described in standard protocols and plans, and using extensively any available observational data sources, as referred in previous sections. Regular updates of a subset of the validation metrics assessed by the own producers (including Class2 validation of model products at mooring sites and Class4 regional validation metrics) is made available to end-users through a dedicated website: the Copernicus Marine Product Quality Dashboard (pqd.mercator-ocean.fr).

Furthermore, the Marine Service is responsible for informing end-users about relevant PQ information in a transparent way. To this aim, reference scientific PQ documentation is issued for each delivered product. These documents, stating the expected quality of a product by means of validation metrics computed along the qualification phase of the new model system, are updated for every quality change associated with any new operational release.

Apart from this “static” information on model validation, disseminated through the Quality documentation, and focused on the assessment of daily operational products, the Copernicus model providers have their own on-line model validation processes. The Copernicus Marine service model production needs to be carefully monitored at each step, and then, quality of any upstream data used in the model runs shall be properly assessed (even if such upstream data is quality controlled by the data providers). Indeed, regular exchanges are organized between observations and model producers within the service to discuss data assimilation and validation issues. Scientific quality is one of the most important model performance indicators, and the producers report to the Service on quality monitoring activities quarterly (being any change that affects model solutions to be justified from a Product Quality point of view).

Consistency in the choice of model validation metrics and the way they are presented is important because it will make it easier for users to understand the Product Quality information provided and to browse in the product portfolio. Given the wide range of Copernicus Marine products and production methods, it is not always scientifically meaningful to provide the same type of information for all systems. The Product Quality cross-cutting strategy (Sotillo et al., 2021) therefore seeks a balance between the homogeneity of the information and its relevance. Indeed, the Copernicus Marine Service is a first achievement towards the interconnection of operational oceanography services at basin scale, and digital ocean platforms based on cloud technology will enable new validation capacities and will facilitate setting up dynamic uncertainty for most of the products. The frequency of the updates will also increase to better serve coastal OOFS, where short-term forecast and quality info should be delivered on daily (desirable) or weekly basis.

4.2 Validation of coastal OOFS: a world of variety

There is not a common operational validation approach in coastal OOFSs, and the degree of operationality for the OOFS' validation is highly dependent on the type of OOFS set-up (i.e. system with data assimilation scheme activated, generating analysis or on the other hand, OOFS based on a free forecast model system), the extension of the area of interest (being different for very limited coastal systems or going into a larger regional extent), the OOFS purpose (system targeted on a primary end-user with specific interests or needs, or if the OOFS delivers a general multi-parameter/purpose service) and finally in the availability, and degree of operational access, to local in-situ observational data sources.

Most of the OOFS have some system validation. Even those models used for research purposes or in the process of maturing their operationality (pre-operational state) have some kind of model validation, typically the early stages of the model set-up configuration, often running in hindcast mode on specific time periods to take benefit of existing observational data campaigns. In pre-operational systems, or in early stages of OOFS services, an operational validation system is not so common, while model providers are working on the configuration of operational processes for an automatic PQ model assessment, and meanwhile, maintaining some offline model validation (using available observations or focused on specific targeted periods when outstanding events occurred, or when observational campaigns are available).

It is worthy to note that Capet et al. (2020), concludes that only 20% of models provide a dynamic uncertainty together with the forecasted EOVs, which would be required for a real-time provision of confidence levels associated with the forecasts (e.g., as is usual for instance in weather forecasts). Usually, model providers perform operational and off-line validations, focusing mostly on the best estimate solution, and not so on the forecast skill assessment; scientific statistical metrics are computed using available in-situ observational data sources from their own networks or external observational data providers (using observational products from core services such as Copernicus, other national/regional/local public providers or from the industry, if available); in very coastal high resolution systems with quite limited geographical areas the use of satellite data is not so common for the model validation due to the lack of remotely sensed product coverages. This is the case of many OOFS all over the world. For instance, the South African ocean forecast system (SOMISANA-Sustainable Ocean Modelling Initiative: A South African Approach; https://somisana.ac.za/explore) delivers downscaling of global model products for specific coastal applications in key coastal areas. In these cases, scientific model validation is mostly done offline by model producers, comparing their best estimated hindcast solutions with the existing historic/operational in-situ observations from coastal moorings or tide-gauges. Currently, there is not a direct transfer of information about the product quality from the service to the OOFS users, neither computation of forecast skill assessment nor end-user-oriented metrics. However, some interesting initiatives, mostly linked with the engaging of stakeholder and product disseminations through end-user services

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platforms, are on-going and in the SOMISANA OOFS roadmap is included the implementation of an operational validation protocol, including forecast assessment.

The most common situation is that model validation is performed by the OOFS providers themselves. However, in some cases (usually targeted services) there may be options for some external validation, performed not by the provider itself, but directly by the targeted end-user(s). This is the case of the DREAMS service (Hirose et al., 2013; 2021) in the west Japan coast, where model solutions are validated directly by the end-users of the service: in this case, fisheries, through a program with fishing boats as ship of opportunity; Ito et al., 2021). As DREAMS model provider states: "The fishermen watch carefully the coastal ocean prediction to meet better catches. They are inevitably the serious users to claim the quality of prediction".

In the case of the Brazilian REMO service (Lima et al., 2013; Franz et al., 2021), the validation is done in the house only for the targeted end-users; either by the Navy or by the PETROBRAS oil company teams. On the PETROBRAS side, they have several current meters sites where they compare in situ measurements with not only the REMO forecast, but also from all the other available Ocean Forecasting Systems that deliver forecasts on that given day. At the Navy side, they do several validations that include the thermohaline structure, the Taylor Diagrams for few properties as well as the transport for the Brazil Current and the tidal analysis of both level and currents where they have data available. Furthermore, there can be very high-resolution coastal OOFSs that can be implemented for specific purposes and only for specific periods of time, to provide model data as input for instance during the design and construction time phases of big infrastructures. In this case, the implementation of this specific model solution goes together with the monitoring of the area by the company in charge of the project, and model validation during the construction life, and after the operations are developed. In this kind of services, model and validation is usually done in the house, not always publicly disseminated products or results.

There are coastal systems, that have big domains (going into regional) and that may include DA schemes, or pure forecast local coastal systems (run by providers of regional/basin systems in which the local systems are nested) that tend to have operational validation systems (taking benefit of the extensive use of the observational data sources done for assimilation purposes). There are examples of OOFSs supported by state agencies, such as the Canadian Government CONCEPTS (Canadian Operational Network for Coupled Environmental Prediction Systems) that develops and operates a hierarchy of OOFS. These include the whole downscaling approach: going in this Canadian case from the Global Ice Ocean Prediction System (GIOPS; Smith et al., 2016) used to initialize coupled deterministic medium range predictions (Smith et al., 2018), as well as ensemble predictions (Peterson et al., 2022). The global system provides boundary conditions to the Regional Ice-Ocean Prediction System (RIOPS; Smith et al., 2021), which in turn provides boundary conditions and nudging fields for a Coastal Ice Ocean Prediction System (CIOPS; Paquin et al., 2023). Recently, six port-scale prediction systems have also been put in place. CONCEPTS also develops and operates deterministic and ensemble wave and storm surge prediction systems. Proposed changes to these systems must follow a set of formalized verification standards. Evaluation of forecast skill as a function of lead time is also made. Monitoring systems are also in place to ensure the quality of real-time analyses. Forecasts are evaluated in near real-time as part of the OceanPredict Class4 intercomparison activity (Ryan et al., 2015), and evaluations are predominately made against available observations, but also include comparison to analyses for the longer-range coupled

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forecasts. These include assimilated satellite (sea level anomaly, sea surface temperature, sea ice concentration) and in situ observations (Argo, buoys, moorings, gliders, field campaigns, …). Additional independent evaluations are made against tide gauges, ADCP, HF Radar, drifters, ice beacons (Chikhar et al., 2019) and estimates of sea ice and snow thickness. Evaluations are also made of transports across reference sections and of surface fluxes (both against observations as well as in terms of budgets; e.g., Roy et al. (2015) and Dupont et al. (2015)). Finally, user-relevant verification is made in terms of sea ice (e.g. probability of ice, ice formation and melt dates) and ocean (e.g. eddy identification and properties) features (Smith and Fortin, 2022). An ongoing effort is underway to quantify unconstrained variability in the systems and to provide uncertainty estimates to users.

There are also coastal OOFSs delivered by national agencies or organisms that run their own observational networks. In these cases, usually they take advantage of synergies of the combination of high-resolution model solutions and operational observational data sources (being the in-situ operational observational capacity developed by running operational networks or through the sustained periodic measurement at fixed stations) progressing towards more operational validation procedures. This is the case in Spain of ocean model systems from different state and regional government agencies: i.e., Puertos del Estado (SAMOA; Sotillo et al., 2020), SOCIB (WMOP; Mourre et al., 2021), MeteoGalicia (MG; Costa et al., 2012) or the case of the Marine Institute ocean forecasting systems for Ireland (Nagy et al., 2020) with coastal systems focused on very limited -highly sensored- bay areas. Even in these optimal cases, operational validation is mainly limited to model best estimate solutions, and generation of end-user metrics or uncertainty estimation is still missing, but in the long-term evolution roadmaps.

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The contact author has declared that none of the authors has any competing interests.

Data and/or code availability

This can also be included at a later stage, so no problem to define it for the first submission.

Authors contribution

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