4. Architecture of ocean monitoring and forecasting systems

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4.1. Modelling systems architecture

An OOFS, with a global to regional scale, is based on numerical modelling of the ocean dynamics, biogeochemistry, and wave and data assimilation schemes for blending observations into the model and for providing the most accurate initial condition for the forecast (Tonani et al. 2015). An OOFS at coastal scale may usually use information from global/ regional scales in terms of initial and boundary conditions to initialise and force its ocean model core in a very limited area in order to provide very accurate spatial-temporal solutions and may not necessarily use data assimilation methods.

In general, to produce a forecast we need to:

- 1. know what the ocean is doing now (initial condition);
- calculate how the ocean will change in future (forecast);
 use oceanographic expertise to validate and refine
- the output (products).

These three steps, represented in Figure 4.1, are based on a few basic components: observations, numerical model, and oceanographic expertise. Most of the systems rely on data assimilation techniques (see Section 4.4 for a general introduction and Section 5.5 for more details about numerical schemes) for blending observation and models; therefore, data assimilation can be considered as one of the essential components of the system. In the case of coastal forecasting systems, downscaling from global/regional scale is the preferred approach as described in Section 5.4.4.

Step 1 is the production of the most accurate initial condition about the variables the forecasting system is aiming to predict. This means that we need the best knowledge of the present status of each variable at every model grid point. This information is difficult to retrieve from observations because their spatial/temporal coverage is usually very sparse. Model simulations instead provide a uniform coverage in space and time and, thanks to data assimilation techniques observations, they can be blended into the model simulation, improving their accuracy. For data assimilation, it is common to use observations from multiple sources, maximising the data coverage and the type of variables measured by in situ and satellite instruments. The initial condition for the forecast is usually the result of a complex set of multiple simulations with data assimilation covering past hours or days. For global and regional oceanographic systems it is common to have a data assimilation cycle of the order of a few days. These simulations of the past provide not only the best knowledge for initialising the forecast of the present but also valuable information on the near present that can be included in the final product delivered to the users.



Figure 4.1. Scheme of steps and main components of a forecasting system and of its architecture.

The model usually needs some external forcing as input. The type of information needed at its boundaries (e.g. ocean/ atmosphere, lateral boundaries, along the coast, etc.) can vary from model to model. An ocean dynamical model usually needs an atmospheric forcing from a real time weather prediction system to resolve the processes at the ocean/atmosphere interface. A regional/coastal model requires river runoff data at the interface with the coast and input values for its variables at the lateral boundaries. In case of coupled models (see Chapter 5 and Chapter 10, for example), external forcing fields might not be needed.

Step 2 is the projection in the future, the production of the forecast that is done by running the numerical model for hours, days or months in the future. The forecast lead time can vary from hours to days. Many systems have a forecast lead time of 3-15 days. The same forcing fields described in Step 1 are needed also for the forecast. The forcing fields could be from another forecast like the atmospheric forcing, that usually is from a weather prediction system, or they can be provided by climatological values or persisting the last available value.

Once the model has produced the forecast, it is validated and its output post processed to a standard format for the delivery to the users (Step 3 in Figure 4.1). The validation of the forecast cannot be done via direct inter-comparison with observations but is based on the validation of its initial condition and on studies covering an extended period in the past of the model skills.

As explained before, observations are a key component but have to be made available in real time and in a standard format. Observations in real time are usually ready to be used within a few hours from their acquisition but sometimes they can have delays of more than 24 hours. Timing of data availability will influence the design of the production cycle that has to compromise between using the maximum number of the observations and reducing the delay in the forecast release. The choice to be made has also to consider the need to release a new forecast as soon as possible even if this could imply a degradation of its accuracy.

The timeliness of the forcing fields is another limiting factor in the design of the production chain. We can take as an example a wave forecasting system in which the accuracy of the predicted fields is strongly correlated with the accuracy of the winds. We have to wait until the latest and more accurate wind forecast is made available before starting our production. Different solutions can be implemented depending on the characteristics of each system. The computational time needed for running each of the three steps described is a very important aspect as, depending on the cost for running a specific system, it could be a limiting factor. Timeliness is of paramount importance for the users and the production time should be reasonably short to avoid delivering forecasts referring to the past. A rule of thumb is that the production time needs to be consistently less than the production frequency. It means that for a daily cycle (production of a forecast once a day) the production time should be of the order of a few hours.

Even if the information provided in this section is focused on a forecasting system, with few modifications it can be also applied to a multi-year production system to produce a reanalysis. The main difference is that in this case you are not projecting in the future but in the past. This implies that you can blend observations and model simulations at each time step. The model is continuously corrected by the observations, increasing the accuracy of the simulations. The atmospheric forcing usually is also more accurate because it is an analysis and not a forecast, and hence the observations have been subject to a more restrictive data quality control compared to the real time ones.

The multi-year production is composed only of Step 1 and Step 3. In this case, in Step 1 the model and data assimilation cover a few hours/days spans over multiple decades of years. As the multi-year products are not limited by the timeliness, usually their major constraints are the computational time that can be extremely expensive as well as the availability of homogenous sources of forcing. These differences with respect to other forecast products have to be taken into account in the design of the production cycle.

In the next subsections the architecture details at the basis of an OOFS will be introduced.

4.1.1. Step 1 processes

4.1.1.1. Data access and pre-processing

The data access and pre-processing component should make available all the needed dataset that will be used to perform the analysis, and then the forecast (Step 2). Automatic acquisition of the data is mandatory for an operational system. It could be quite demanding depending on the dataset, the centres (or data providers) involved in data production and treatment, and the available network to connect the centres. For most of the dataset used in OOFS, at least a daily update is needed.

For atmospheric forcing the volume of the dataset can be big, and an efficient connection to Operational Meteorological Centres in charge of operational production of atmospheric analysis and forecast is critical. For example, the volume of hourly surface forcing fields from the ECMWF at global scale is 34 GB per day. Then, data pre-processing is necessary to interpolate the atmospheric fields to the ocean grid, if there is inhomogeneity between frequency of available forcings during the length of the specific run, atmospheric datasets must also be interpolated temporally. When a regional ocean model is employed instead of a global model, the retreatment of the atmospheric dataset may substantially reduce the volume of the atmospheric dataset and reduce the overall storage cost.

In-situ ocean observations can be downloaded in real time using WMO GTS or from dedicated interface such as the service developed in the Copernicus Marine Service (Le Traon et al., 2019), in which in situ observations are made available, documented, quality controlled, and homogenised, all very important tasks to be performed before assimilating such dataset in an OOFS. Satellite observations need to be pre-processed by a dedicated centre before their assimilation in an ocean operational system. Satellite observations are processed at various levels ranging from Level 0 to Level 4 which need to be made available depending on the data type. For example, Copernicus Marine Service also provides a unique access point to download all the available satellite observations in real time.

4.1.1.2. Data assimilation: analysed fields

Ocean analysis is based on a model, observations, and data assimilation scheme to provide the initial state of the forecast on the basis of a minimum error principle, i.e. the data assimilation modelling system (Figure 4.1). This component is central processing unit (CPU) consuming and should be performed on a supercomputer. High performance computing power is one of the most important constraints to define the resolution of the analysis system, along with the number of observations that will be assimilated in the system and the frequency and length of the analysis cycle. In an operational framework, the analysis cycle should be performed in a range of a few minutes to a few hours (maximum), choosing the best compromise between performances, quality of the analysis, and robustness of the operational system. This component will provide the initial state for the ocean forecast. The resulting time series of analysed ocean state is defined as the best analysis time series.

To perform an ocean analysis, we need the initial state of the model, based on the prior state of the model at the end of the previous analysis cycle, in situ and satellite observations, and atmospheric forcing analysis fields, collected and formatted in the previous acquisition and pre-processing phase (including all the static files that are necessary for the data assimilation modelling system). Outputs of this component are 3D fields to update the best analysis time series and restart files to initialise the next ocean forecast. Other diagnostics, metrics or post-processing may be computed online directly during the analysis cycle to optimise the system, and used as additional products for dissemination and archiving. Such products are also used during the validation phase (e.g. the mixed layer depth, the collocation between model output and observations, transports, etc.).

Note that in some coastal forecasting systems there is no direct data assimilation. If the model domain is small, in some occasions there is simply no available data to be assimilated. In these cases, the system relies totally on the boundary conditions and initial 3D fields derived from a larger scale model (see Section 5.4.4 for downscaling examples).

4.1.2. Step 2 processes

4.1.2.1. Forecast

The ocean forecast at some range is based on the numerical model initialised by the ocean analysis and forced by the atmospheric forecast fields as provided by the operational atmospheric centre. In most cases, the same model is used for both the forecast component and the analysis component, even if differences in terms of resolution and physical parameterizations could be envisaged especially in the framework of an ensemble forecast. The same constraints mentioned above about high performance computing apply in order to perform forecasts that are usually updated at least every day. Forecast range will also depend on the computing resources and on the main processes that have to be forecasted with a reasonable skill (to be defined by the developer of the forecasting system). The forecasting cycle should be performed in a range of a few minutes to a few hours. Inputs of the forecasting cycle are the initial state produced by the data assimilation modelling system (e.g. ocean analysis), all the static files needed to integrate the model, and the atmospheric forcing for the full forecast length. The forecast output is updated every day and consists of 3D and 2D ocean fields; it may include diagnostics, metrics and other post-processed dataset that can be useful to assess the quality of the product, to highlight specific features of the forecasted ocean properties and for the final delivery to users.

4.1.3. Step 3 processes

4.1.3.1. Post-processing

The post processing phase is devoted to building all the products that will be delivered to the users. It consists of files or datasets that are provided according to a) standard file format (e.g. according to CF Conventions, O^{1}); b) on a specific grid; and c) with homogeneous variables and metadata. Such products may be then used to compute new products as ocean monitoring indicator (OMI), ensemble mean and standard deviation in the framework of ensemble forecast.

1. https://cfconventions.org/

This post processing should be performed on a supercomputer in which all datasets provided by the analysis and forecast components are stored in order to save resources in the computing centre. Computing cost of this stage could be really high (for example, due to the interpolation procedure in the case that the products are delivered on a specific grid) and would also include large data transfer and input/ output access. The inputs of the post-processing component are represented by all datasets produced during the analysis and forecast cycles, while the outputs are all the products that will be delivered for internal and external users.

4.1.3.2. Validation

The objective of the validation component is to provide information on the quality of the operational system. The quality of the analysis is compared to already known or expected results (based on literature or climatological datasets) or to available observations. Quality of the forecast is performed by computing forecast skill in comparison to the analysis with the observation in delayed mode. The final step is to provide all this information to forecasters and users. Input of this component are model products, diagnostics and metrics computed during previous steps and the output could be numerical fields, time series and/or interactive maps that allows, through web interfaces or other kinds of applications, direct querying, comparison of different periods, and validation of the production.

4.1.3.3. Dissemination

The goal of the dissemination phase is to make all the products available to users on a dedicated infrastructure. This phase may be complex and the associated cost is very dependent on objectives and user needs. If the dissemination of the model is only internal, outputs could be made available through an intranet, using in-place storage capacities. Other approaches are mandatory for a more complex system providing a very large dataset and long-time series and designed to be accessed by several thousands of users, including a catalogue of products continuously maintained and updated, dedicated services for viewing, extracting and downloading the data. Cloud storage facilities are now the best infrastructure to disseminate operational ocean products.

4.1.3.4. Monitoring

The monitoring component is an important part of an operational system as it allows operators and forecasters to monitor the performances along all the production phases, from data access to dissemination. KPIs should be monitored during this phase, including availability of inputs and outputs during each phase, timeliness, time of delivery and delay of each component, anomaly and/or errors identified during each phase. Monitoring phase should be used to provide information to the users and to decide on a go/no-go to disseminate the products externally. Monitoring phase should be presented on a dedicated dashboard.

4.2. Inputs required

To run an OOFS as part of Step 1, the following sources of information are needed:

- Observations of EOVs are extremely important for an OOFS as they are used for assimilation and validation purposes. The main sources of observations are:
 - In-situ observations:
 - **Buoys**. Typically used to measure directional waves, atmospheric parameters (wind, atmospheric pressure and air temperature), EOVs (currents, temperature and salinity) and, less frequently, biogeochemical parameters. Some stations measure only on the surface, while others extend their observations to the whole water column. These variables are used for all kinds of OOFS: Wave in-

formation is critical for validation and is occasionally used in assimilation; oceanographic data are widely used in circulation modelling and the scarse biogeochemical stations are critical to complement the existing climatological data;

• **Tide gauges**. Measuring sea level, tide gauges are extremely useful for the validation of storm surge and circulation models, sometimes also used in data assimilation. In recent times, with the increased frequency sampling of modern tide gauges their use to validate wave models in coastal regions has extended;

• Argo drifters. Typically measuring profiles of salinity and temperature. More recently, bio-geo-chemical parameters are also being incorporated.

This is an essential source of information for large scale circulation modelling;

• **Ship-of-opportunity**. Usually measuring SST and SSS via thermosalinograph or releasing Expendable Bathythermograph to measure temperature throughout the water column. These data are usually employed for circulation modelling;

• **Gliders**. Gliders can provide a 3D field of ocean structures that can be highly valuable for validation of circulation modelling and assimilation in regional and coastal scales. Gliders can also provide valuable biogeochemical information;

• **HF radars**. The surface current fields are used for validation and data assimilation in circulation models. Additionally, the wave measurements can be used for validation in wave forecasting systems;

• Marine Mammals CTDs. As in the case of the gliders, this is an increasingly important source of information that allows us to gather detailed information on small-scale ocean and coastal features.

• Satellite observations provide information on the following variables:

• Sea level anomaly. These data are a critical variable for data assimilation in large scale circulation models;

• Sea surface temperature. As the previous, usually it is employed in data assimilation as well as in validation of ocean circulation forecast systems;

• Sea ice concentration. Used for both validation and data assimilation in ice models, coupled to circulation models;

• **Waves**. This variable is being used in large scale wave forecast systems for data assimilation and, on some occasions, for validation;

• Ocean colour. Mainly employed for assimilation and validation in biogeochemical models. Can also be used as a secondary source for validation in circulations, since sometimes coastal structures are evident.

 Bathymetric datasets. Bathymetry is at the base of every OOFS and, therefore, it is indispensable for all systems;

• Surface forcing. Provided by operational NWP systems. These data are used for describing air-sea-sea

ice interactions. Momentum, heat and freshwater fluxes are of paramount importance for all the processes at sea. Therefore this forcing is needed in almost any OOFS, with only a few exceptions (for example, some very high resolution wave propagation systems can operate without it, because the influence of forcing is already considered on other larger scales);

• Land forcing fields (i.e. discharge of water and nutrients from rivers). Mainly used in circulation and biogeochemical modelling. This source of data is very relevant to provide accurate solutions at the coastline. Unfortunately, on some occasions real time data are not available and the modellers must rely on climatologies;

 Ocean fields. They are provided by OOFS at larger scale to work as initial and boundary conditions (for example 3D temperature fields for downscaling applications in circulation modelling). When nesting, it is indispensable to have these fields. It is a frequent technique in all kinds of regional scale and coastal OOFS;

• Climatologies. Sometimes climatologies are employed for validation or initialization when no other data are available. These data sources are also employed in validation processes, to check that the models do not depart too much from real values in regions where measurements are not frequent.

The following sections contain first an introduction on how to deal with ocean data from the perspective of the data provider, and then a description of the above mentioned data sources, including a list of international providers.

4.2.1. Obtaining and preparing ocean data

The quality of OOFS products is highly dependent on the availability of in situ and satellite observations; these are used, through data-assimilation, to constrain the analysis and the forecasting systems, and validate their outputs. However, prior to use these observations, they need to be properly retrieved, efficiently organised, and carefully quality controlled (Le Traon et al., 2009). In the architecture of an OOFS, this is accomplished by the so-called DMS, the data management component. The ultimate goal of this system is to ease the use of oceanographic observations, providing consistent and harmonised products ready to be used for data assimilation and validation.

Figure 4.2 shows how data flow should be organised in a DMS. To get the most out of information, a DMS is responsible for gathering and organising the ocean observations (satellite and in-situ) in high-quality products and then to disseminate them in a timely fashion that meets the requirements of modelling and data assimilation centres. Once acquired,



Figure 4.2. Typical DMS data flow from upstream international networks for OOFS.

observation must be supplemented by uncertainty estimates and quality flags (part of the quality control process), which are key for validation and data assimilation. Then, they are prepared according to the specific file formats and distributed to users.

4.2.1.1. Data retrieval and characterization

First task of a DMS is to gather observations available from selected data providers (e.g. space agencies, international in-situ data networks, etc.). The choice of observations to be retrieved, processed and delivered depends on a previous analysis of the needs expressed by the prediction systems. In general, a tight coordination, upstream with data providers and downstream with prediction systems, is necessary to keep needs updated and ensure that the required observations are provided timely.

Ocean observations are made using several sensors, including in situ and remotely sensed ones, covering a broad range of spatial and temporal scales. Ocean observations made by remote sensing sensors usually include data for monitoring sea level, SST, salinity, surface wind and currents, sea ice, and ocean colour; these observations are acquired on a global basis and distributed at several different levels of processing, ranging from raw data to detected geophysical variables. Space Agencies (e.g. ESA, NASA, EUMETSAT, JAXA) are responsible for the provision of such observations.

In-situ observations are of paramount importance for OOFS because they provide information about the ocean interior that cannot be observed from space. In-situ observations can locally sample high-frequency and high-resolution ocean processes, in particular in the coastal zone, that are essential for model and satellite validation activities. In-situ observations are acquired through various network programs at both global and regional scale.

Data from a global prediction system, to be used to define boundary conditions of a nested regional one, or terrain/ atmospheric forcing in certain scenarios will be part of the data to be inputted in the prediction system.

Knowledge of the processes that have been undertaken to produce a given observation and its characteristics is of high importance, as it allows a user to decide upon the product's fitness for a particular application. To this end, it is important to ensure that metadata associated with each of the retrieved dataset contain the appropriate information (e.g. instrument/platform characteristics, tests performed and failed, origins of the data stream, data processing history, and information about the datasets).

4.2.1.2. Quality Control

In general, a Prediction System needs two types of input data. Initially NRT data are needed for hourly to weekly forecasting activities; at a later stage and for applications in which longterm stability is needed (e.g. reanalysis, climate monitoring, and seasonal forecasting), DM data comes into play. Due to their different utilisation, quality control procedures for the two types of data are applied in different ways and with different methodologies.

NRT input data, delivered within a few hours to maximum one week from acquisition, are usually automatically quality

Code	Meaning	Comment
0	No QC was performed	-
1	Good data	All real time QC tests passed.
2	Probably good data	These data should be used with caution.
3	Bad data that are potentially correctable	These data are not to be used without scientific correction.
4	Bad data	Data have failed one or more of the tests.
5	Value changed	Data may be recovered after transmission error.
6	Value below detection/quantification	The level of the measured phenomenon was too small to be detected/ quantified by the technique employed to measure it. The accompanying value is the detection/quantification limit for the technique or zero if that value is unknown.
7	Nominal value	-
8	Interpolated value	Missing data may be interpolated from neighbouring data in space or time.
9	Missing value	_

Table 4.1. Copernicus Marine quality control flags as applied to Global Ocean In-Situ Near-Real-Time Observations product (INSITU_GLO_NRT_OBSERVATIONS_013_030, \mathscr{O}^2).

controlled using a priori agreed upon procedures. For in-situ observations, quality control tests aim mainly at detecting outliers; these procedures check for inconsistencies in the measurements often using local statistics built from a long time series of similar data. Quality control of remotely sensed observations is performed by comparisons with in-situ observations when available, or by comparison to long-time series (i.e. climatologies) derived from the same product. These procedures aim at defining the accuracy of the product and detecting anomalous observations. As a result, for both in-situ and remotely sensed NRT products, quality flags are positioned to inform the users about the level of confidence and, where possible, the level of accuracy attached to the observations.

In-situ DM data are usually subject to an off-line quality control using statistical tests to check for spatial consistency and to a much more refined climatology test, usually with strong involvement of scientific experts in the quality-control process. Satellite observations delivered in DM usually benefit from improved ancillary data (e.g. more precise satellite ephemerides, meteorological reanalysis, etc.) used in the retrieval process, resulting in a more accurate product.

Besides the activities aimed at establishing the quality of the required observations, a DMS shall also monitor the performance of the different providers in terms of availability, possible degradation of their sampling, and timeliness. This additional information also needs to be regularly provided to prediction systems making use of these observations.

A DMS should also set up a procedure to gather, in form of reports, regular information on the data that have not been used by the prediction systems, because they were deemed to be of inadequate quality; this procedure, often called "Blacklisting", has significant value for improving automated procedures for data quality control.

Table 4.1 shows the standard quality control (QC) indexes assigned to Copernicus Marine Service in-situ and satellite data.

^{2.} https://doi.org/10.48670/moi-00036

4.2.1.3. Data Formats

Observations usually arrive at a DMS in a variety of formats, depending on the platform being used to acquire and broadcast them or on the software used to retrieve the variables of interest. For ease of use, a DMS will format all the incoming observations in data structures which satisfy the OOFS requirements. Data formats are usually defined during the development of the OOFS infrastructure in coordination with the prediction systems and detailed in dedicated documents. Besides a detailed description of the format in which the data or products will be stored, key subjects to be addressed in such documentation include:

- standards that will be used to build the data structures hosting the incoming observations (e.g. NetCDF format);
- semantics, provided by a recognized common convention (e.g., CF), which are then used to write metadata; and
- a description of the transformation algorithms for all data handling (e.g. transformation algorithms to/from standards).

To enhance interoperability and sharing of data, non-proprietary solutions commonly used by the community are favoured during the selection of data format.

4.2.1.4. Data Delivery

The ultimate task of a DMS is to deliver datasets required for assimilation and validation activities to prediction systems, including uncertainty estimates that are critical for the effective use of the data. For the best possible exploitation of this data, an easy-to-access and robust service to visualise and access present and past available observations and associated metadata must be deployed. Metadata include latency information on data availability as a key parameter in the data flow. It is important that new observations are made accessible to the prediction systems with the shortest possible delay.

Access to data can be achieved in different ways:

- "Pull services" enable users to request data according to their needs; this type of service should integrate tools that allow constraining the area of interest and time covered by the information;
- "Push Services" are often based on subscription, which literally push the data to users following prescribed specific requirements.

Beyond visual navigation of data, a dissemination service should also include utility tools allowing transformation (e.g. format conversion and coordinate transformation), aggregation, and integration of a given variable regardless of source.

Another aspect to be considered as key for a successful dissemination service is the ability to perform appropriate extractions according to different data geometries (e.g. gridded datasets, unstructured gridded data, vertical profiles etc.).

4.2.2. Description of existing in-situ observational oceanographic data

In the next sections, it will be introduced the main observational oceanographic data from in-situ platforms used by OOFS. Details about their usage in numerical modelling and validation, as well as providers, are described in Chapters 5 to 9.

4.2.2.1. Buoys

Operational drifting buoys are a primary source of data on ocean surface conditions. They are deployed and maintained by autonomous groups, subject to different intergovernmental agreements, under the coordination of the Data Buoy Cooperation Panel (DBCP, @³). The Global Drifter Program (GDP) works in collaboration with national meteorological/oceanic agencies to routinely deploy large quantities of drifting buoys in support of their research and operational programs. Maintaining drifting buoy density distribution is a major challenge, due to the difficulty of high latitude deployments and because Lagrangian drifting buoys follow ocean currents and tend to cluster together near convergence zones.

Moored buoys are anchored at fixed locations, reporting temperature and salinity profiles, and are concentrated mostly in the tropical oceans and the coastal regions of Brazil, Europe, India, and the United States (\mathcal{O} ⁴). The different programs/ agencies responsible for handling the tropical mooring networks are:

- the Tropical Atmosphere-Ocean/Triangle Trans-Ocean Buoy Network in the equatorial Pacific (TAO/TRITON) (McPhaden et al., 1998);
- the Prediction and Research Moored Array in the Tropical Atlantic (PIRATA) (Bourlès et al., 2008);
- the Research Moored Array for African-Asian-Australian Monsoon Analysis and Prediction (RAMA) in the Indian Ocean (McPhaden et al., 2009).

3. https://www.ocean-ops.org/board

4. https://www.ocean-ops.org/dbcp/platforms/types.html

The TAO/TRITON, PIRATA and RAMA moored arrays are part of the DBCP's moored buoy network through the Tropical Moored Buoy Implementation Panel (TIP).

Data from the DBCP GBN is transmitted through the GTS of the WMO and archived by the operational agencies. At present, the GBN has over 1,380 drifting buoys and 260 coastal/national moored buoys and 70 tropical arrays. While COVID-19 restrictions imposed stress on deployment opportunities, the drifting and moored buoy networks successfully maintained a healthy and resilient status in data quantity, quality, coverage and timeliness, due to the prolonged lifetime and improved performance of buoys (O^{5}).

4.2.2.2.Tide gauges

Tide gauges are instruments on fixed platforms, located usually along the coastline, that measure water level with respect to a local height reference. Their primary objective is to support coastal zone monitoring and management, tide prediction, datum definition, harbour operations and navigation; additionally, they are used in sea level hazard warning systems, for climate monitoring, model validation and assimilation, and to detect errors and drifts in satellite altimetry. Tide gauge data complement the sea surface height data provided by the spatial altimeters, by providing higher temporal sampling (up to 1 min or less, allowing detection of higher resolution sea level phenomena) from in-situ data at the coast, where the quality of altimetry is lower.

The Global Sea Level Observing System (GLOSS; @⁶) is the main international program responsible for collection, quality-control and archiving of tide gauge observations. The following data centres contribute to GLOSS data services:

PSMSL (\$\nothermole\$^7\$), responsible for the global database of monthly and annual mean sea levels for long-term sea level change studies from tide gauges (\$\nothermole\$^8\$);

• UHSLC (𝔊), in which high-frequency tide gauge data (hourly and daily) can be found. Two datasets are provided, with different levels of quality control: research quality (updated annually) and Fast-Delivery (updated every 1-2 months);

- 6. http://www.gloss-sealevel.org
- 7. https://www.psmsl.org/
- 8. https://www.psmsl.org/
- 9. http://uhslc.soest.hawaii.edu

- IOC Sea Level Station Monitoring Facility (IOC/ SLSMF: Information State Sta
- SONEL (Image in) is the GLOSS data centre for GNSS time series at tide gauge locations, if available. This information is the source of vertical land movement at the site and provides an ellipsoidal height reference of the tide gauge.

Figure 4.3 shows the global distribution of tide gauges together with the total number of installed stations from 1800 to 2000s (Hamlington et al. 2016), collected by the PSMSL. It shows the sparse distribution of tide gauges stations in some areas, such as Africa and South America.

The EuroGOOS launched an initiative through its dedicated Tide Gauge Task Team (TGTT) working group (12) to capitalise the expertise, usage and further improvement of the tide gauges network in the continent. This working group has launched several actions to enhance the connection between GLOSS and European data portals such as EMODnet and Copernicus Marine Service. These data portals integrate tide gauge data with other in situ, satellite and model data, and provide a one-point access for most of the tide gauges data for operational and scientific activities.

4.2.2.3.Argo

Argo is a global array of approximately 4,000 free-drifting profiling floats, designed to measure the temperature and salinity of the upper 2,000m of the ocean. The array covers the global ocean reasonably well and is one of the main in-situ observation data sources for ocean data assimilation and validation.

Each standard float has a resting depth of 1000m for 9 days. Every 10 days it is programmed to descend to 2000 m and then ascend to the surface measuring temperature and salinity in the ocean column. Data is transmitted via satellite and distributed on the GTS in BUFR code. Similar real-time quality-controlled Argo profiles can be obtained from two Global Data Assembly Centres (GDACs) - based one in Monterey, USA, and the other in Brest, France - that were set up as part of the international GODAE. For their behind real-time analyses, some operational centres use real-time Argo floats from both the GTS and the two GDACs.

- 10. http://www.ioc-sealevelmonitoring.org
- 11. http://www.sonel.org
- 12. https://eurogoos.eu/tide-gauge-task-team/

^{5.} https://public.wmo.int/en/media/news/ocean-observing-system-report-card-2020



Figure 4.3. Top: global spatial distribution of the 1420 tide gauges in the PSMSL RLR dataset.Bottom: number of available tide gauges in the PSMSL RLR dataset through time (blue). Available gauges for the Northern Hemisphere (red) and Southern Hemisphere (black) are also shown for comparison (source: \textcircled{O}^{13}).

By 2020, Argo is collecting 12,000 data profiles each month (400 a day). The most updated picture of available operational Argo at global scale is shown in Figure 4.4. Further details are available at $@^{14}$. There was a slight 10% decrease in daily data flow in early January 2021, but overall spatial-temporal coverage has progressed since 2020 despite the challenges of the worldwide pandemic. Satellite-tracked surface drifting buoys are extremely cheap and useful to measure mixed layer currents, sea surface temperature, atmospheric pressure, winds, and salinity. They are part of the GDP and are able to reach a maximum 15 m depth. An updated map of operational surface drifters is shown in Figure 4.5. Further information is available at @¹⁵.

15. https://www.aoml.noaa.gov/phod/gdp/index.php.

^{13.} https://climatedataguide.ucar.edu/climate-data/tidegauge-sea-level-data

^{14.} https://argo.ucsd.edu



Figure 4.4. Global distribution of Argo network in January 2021 (source: 16).







4.2.2.4. Ship-of-opportunity program

Figure 4.6. The network status of global XBT lines provided from Ocean-OPS in December 2020. Purple indicates the XBT reference lines and red indicates deployment in 2020 (source: 18).

The SOOP, promoted by the JCOMM, is a network of merchant and research ships equipped with sophisticated tools and technology that allow scientists to explore ocean environments. The instrumentation usually used are:

• XBT @¹⁹, used to collect temperature observations of the upper 1 km of the ocean (Figure 4.6). Data from the XBT drop is automatically generated, transmitted by satellite and distributed on the Global Telecommunications System (GTS) in the Binary Universal Form for the Representation of meteorological data (BUFR) format. For operational use, these messages from around the globe are decoded and stored in real-time databases by each operational centre. Approximately 20,000 XBTs are deployed annually by the scientific and operational communities;

• CTD Ø²⁰, which detects how the conductivity and temperature of the water column changes relative to depth. Conductivity is a measure of how well a solution conducts electricity and it is directly related to salinity. By measuring the conductivity of seawater, the salinity can be derived from the temperature and pressure of the same water. The depth is then derived from the pressure measurement by calculating the density of water

- 16. https://www.ocean-ops.org/board
- 17. https://www.ocean-ops.org/board
- 18. https://www.ocean-ops.org/board
- 19. https://www.aoml.noaa.gov/phod/goos/xbt_network/
- 20. https://oceanexplorer.noaa.gov/facts/ctd.html

from the temperature and the salinity. CTD are attached to a much larger metal frame called a rosette, which may hold water-sampling bottles that are used to collect water at different depths, as well as other sensors that can measure additional physical or chemical properties;

- TSG ${}^{\otimes 21}$ are used for measuring sea surface temperature and sea surface salinity;
- ADCP @²² are able to measure how fast water is moving across an entire water column, using a principle of sound waves called the Doppler effect;
- Research vessels and voluntary observing ships participate in the SOOP ${}^{\otimes 23}$

The SOOP is directed primarily towards the continued operational maintenance and co-ordination of the XBT ship-of-opportunity network but other types of measurements, such as CTD probes, are also being made. The SOOP XBT program has been greatly impacted by the global COVID-19 pandemic. In early 2020, the program was temporarily suspended. However, almost half of lines resumed after June 2020, and by December 2020 there were 37 ships active on 25 lines (Figure 4.6), with 4266 profiles visible on GTS (source: \mathscr{O}^{24}).

4.2.2.5. Gliders

Ocean gliders are autonomous underwater vehicles that move through the water column, ascending and descending with changes in buoyancy. Observations from ocean gliders have recently become an important data source in regional ocean data assimilation systems. The gliders are reusable and can be remotely controlled, making them a relatively cost-effective method for collecting repeated subsurface ocean observations. They also allow data acquisition in severe weather conditions. Equipped with a variety of sensors, the gliders are designed to measure ocean temperature, salinity and current profiles. Furthermore, the unique design of the gliders enables them to move horizontally through the water while collecting vertical profiles.

The OceanGliders program coordinates 27 nations' efforts, including 76 national and institutional glider programs (Figure 4.7). Despite the difficult context of Covid-19 restrictions, the OceanGliders program was able to operate over 200 gliders

21. https://www.aoml.noaa.gov/phod/tsg/background.php

22. https://oceanexplorer.noaa.gov/technology/ acoust-doppler/acoust-doppler.html#:~:text=An%20acoustic%20Doppler%20current%20profiler,physical%20properties%20of%20the%20ocean.

23. https://www.ocean-ops.org/sot/soop/

24. https://public.wmo.int/en/media/news/ocean-observing-system-report-card-2020



Figure 4.7. Active gliders in 2020-2021 (source: *P*²⁵).

in 2020 (source: \mathscr{O}^{26}). Most of the glider groups share their real-time data via the GTS network.

4.2.2.6. HF radars

HF radar systems measure the speed and direction of ocean surface currents in real time in coastal areas. They utilise high frequency radio waves for performing such measurements: a pair of radar antennas are positioned on shore and can measure surface currents (over 1-2 m in the water column) up to 200 km offshore with a resolution spanning from 500 m to 6 km depending on the radar frequency (2027). Figure 4.8 shows a sketch (adapted from Mantovani et al., 2020) of mutual functioning of a pair of antennas - Radar A and Radar B: they measure the radial components (vector in blue from Radar A and vector in green from Radar B) that may

be used to compute total velocity inside each discrete cell (vector in orange). This technology is increasingly used in many applications to support downstream services for coast guard search and rescue activities, oil spill emergencies, water quality monitoring and marine navigation. Nevertheless, they are extremely useful for validating coastal models as well as assimilating OOFS at regional scale.

At international level, the GHFRN has been established as part of the GEO to promote high-frequency radar technology for scientific and operational activities along the coast. Roarty et al. (2019) include an updated list of countries and organisations providing surface current information to the GHFRN. Figure 4.9 shows the global distribution of HF radar stations organised within the three regions of the ITU.



25. https://www.oceangliders.org/

26. https://public.wmo.int/en/media/news/ocean-observing-system-report-card-2020

27. https://tidesandcurrents.noaa.gov/hfradar/



Figure 4.9. Global distribution of HFR stations: in green, stations that share their data with global data providers; in red, those that are private and do not share their data (Roarty et al., 2019).

An example of an operational HF radar network is provided by that one managed by Puertos del Estado, operating in Spain, to monitor coastal and harbour zones. Figure 4.10 shows on the left the current operational HF radar network: selecting one of the regions in the red boxes - for example the Ebro Delta, on the right - the user may visualise the animation of the measurements collected during the reference observing period. Data may be accessed through the EMODnet Physics webportal.



4.2.2.7. Marine Mammals CTDs

Marine mammal CTD data are very important for ocean modelling and sea ice verification in high latitudes, particularly in the marginal sea ice zone. Since 2004, several hundred thousand profiles of temperature and salinity have been collected by instrumented animals (Figure 4.11). The use of elephant

28. http://www.puertos.es/



Figure 4.11. Elephant seal with CTD tag ©JB Pons, in C. Guinet, 2018, CEBC/CNRS (available at $@^{29}$).

seals has been particularly effective to sample the Southern Ocean and the North Pacific. These hydrographic data have been assembled in quality controlled databases that can be accessed through the MEOP consortium (\bigcirc ³⁰).

Currently, the MEOP data portal distributes three different databases:

- the MEOP-CTD database: quality-controlled CTD profiles;
- the MEOP-SMS database: submesoscale-resolving high density CTD data;
- the MEOP-TDR database: high spatial density temperature/light data.

Real-time marine mammal CTD data are uploaded to the GTS as shown at \mathscr{D}^{31} .

4.2.2.8. Autonomous underwater vehicles

An AUV is a self-propelled, unmanned, untethered, underwater vehicle capable of carrying out simple activities with little or no human supervision. Reasons for employing AUV range from the ability to obtain superior data quality (for example, obtaining high-resolution maps of the deep seafloor) to establishing a pervasive ocean presence (for example, using many small AUV to observe oceanographic fields) (Bellingham, 2009).

4.2.2.9. List of most relevant international in-situ data providers

Providers of international in-situ observations to be used for assimilation/validation are listed in Table 4.2.

29. https://www.cebc.cnrs.fr/wp-content/uploads/publipdf/2019/GC124006.pdf

- 30. http://www.meop.net/
- 31. http://www.meop.net/meop-portal/ctd-srdl-technology.html

Provider	Description	Website
WOD	World Ocean Database provides uniformly formatted, quality con- trolled, publicly available ocean profiles	Kustaal ceters for Environmental https://www.ncei.noaa.gov/products/ world-ocean-database
Argo	Argo provides data access to Global Data Assembly Centres in Brest (France) and in Monterey (USA)	https://argo.ucsd.edu/about/status/
Copernicus Marine Service	Copernicus Marine Service through the INS TAC for the operational pro- visioning of near real time and reprocessed datasets used by the MFCs for assimilation and validation	Copernicus Marine Service
SeaDataNet	SeaDataNet infrastructure, provides aggregated datasets (ODV collec- tions of all unrestricted SeaDataNet measurements of temperature and salinity by sea basins) and climatologies (regional gridded field products) based on the aggregated datasets and data from external data sources such as the CORA and the WOD for all the European sea basins and the Global Ocean	SeaDataNet
EMODnet	European Marine Observation and Data Network is a long-term, marine data initiative funded by the European Maritime and Fisheries Fund which, together with the Copernicus space programme and the Data Col- lection Framework for fisheries, implements the EU's Marine Knowledge 2020 strategy. EMODnet Physics provides a single point of access to vali- dated in-situ datasets, products and their physical parameter metadata of European Seas and global oceans. More specifically, time series and datasets are made available, as recorded by fixed platforms (moorings, tide gauges, HF radars, etc.), moving platforms (Argo, Lagrangian buoys, ferryboxes, etc.) and repeated observations (CTDs, etc.)	EMODnet https://www.emodnet.eu/ www.emodnet-physics.eu

Table 4.2. List of most relevant international in-situ data providers.

4.2.3. Description of satellite observational oceanographic data

Satellite altimetry is one of the most important techniques for operational oceanography. Figure 4.12, adapted from International Altimetry Team (2021), shows an overview of the radar altimetry constellation and timeline as available from early 90' and with a projection beyond 2030: it demonstrates how altimetry can be considered as a well-established Earth observation platform from space and its evolution contributes to scientific advances in ocean dynamics. Figure 4.12, in particular, reports the main international missions operational temporal framework: before 2020, we have a number of satellites that are not operational anymore (in orange) but that provide a huge and valuable source of historical observations. Then there are modern operational satellites for the provisioning of near real time altimetry data (in yellow): for some of them, the data provider is also able to report the degraded quality period. New missions (e.g., SWOT, Sentinel6) are planned to be launched starting from 2022. These missions should be able to provide very high quality and high resolution altimetry products (light yellow to green). Some of the operational satellite platforms are also part of the DUACS (in dark blue): these consist of a multi-mission merged dataset for measuring, in particular, ocean mesoscale dynamics (more details are also available at \emptyset ³²).

32. https://duacs.cls.fr/



Figure 4.12. Altimetry satellites timeline (adapted from International Altimetry Team, 2021).

Satellite altimetry has substantially advanced understanding of the oceans by providing unprecedented observations of the surface topography at scales larger than 200 km, thus increasing our knowledge of global ocean circulation from the role of mesoscale eddies in shaping ocean circulation to the global sea level rise. The following sections describe the variables measured by satellites.

4.2.3.1. Satellite sea surface temperature

The SST is another important data source for ocean data assimilation and monitoring oceanic conditions. Since the beginning of operational satellite SST observations in 1981, the number and diversity of sensors have increased dramatically and are still evolving (O'Carroll, et al. 2019). A combination of infrared - onboard both LEO and geostationary orbit platforms - and passive microwave (LEO only) radiometers provide a comprehensive global SST coverage to meet the minimum data specification to be used in operational ocean models (as defined by GODAE in Bell et al., 2009).

Most satellite SST observations assimilated into ocean prediction systems are processed in accordance with guidelines and formats specified by the GHRSST (Donlon et al., 2009); an example of a multi-product ensemble is shown in Figure 4.13.





Figure 4.13. Example of SST maps as provided by GHRSST multi-product ensemble (source: ${}^{\otimes}$ ³³)

33. https://www.ghrsst.org/latest-sst-map/

GHRSST formatted products supply SST data either in satellite swath coordinates level 2 preprocessed (L2P) or level 3 composite (L3) gridded netCDF4 format files. L2P and L3 data products provide satellite SST observations together with a measure of uncertainty for each observation in a common GHRSST netCDF format (GHRSST Science Team, 2012). Auxiliary fields are also provided for each pixel as dynamic flags to filter and help interpret the SST data. These data are ideal for data assimilation systems or as input to analysis systems. Gridding a single L2P file produces an "uncollated" L3 file (L3U). Multiple L2P files are gridded to produce either a "collated" L3 file (L3C) from a single sensor or a "super-collated" L3 file from multiple sensors (L3S) (source: \textcircled{O}^{34}).

There are a wide range of satellite SST products in L2P or L3 format provided by various GHRSST regional and data assembly centres. The following is a list of SST products from different satellite sensors that are common to many ocean prediction systems:

• Passive Microwave Radiometers on LEO polar-orbiting satellites provide low spatial resolution SST at around 1 mm depth, with global coverage of the Earth at the equator up to twice daily and more frequently at higher latitudes. SST products obtained from passive micro-wave radiometers are effective at detecting ocean front variability in regions at least 50 km from land, under either clear or cloudy conditions but not precipitation. Most ocean prediction systems assimilate SST observations at ~25 km spatial resolution from the AMSR2 aboard the JAXA polar-orbiting satellite. These data are made available via the JAXA EORC (𝔅 ³⁵) and Remote Sensing Systems (𝔅 ³⁶).

• Infrared radiometers on LEO satellites provide high spatial resolution SST at around 10 micrometer depth, with global coverage of the Earth under clear sky conditions up to twice daily at the equator and more frequently at higher latitudes. SST products commonly used are measured by the Advanced Very High-Resolution Radiometer (AVHRR) instrument flown by the Meteorological Operational satellite (MetOp) series of polar-orbiting environmental satellites launched by the ESA and operated by the EUMETSAT. Two types of AVHRR SST products used in ocean prediction systems are: 1) the 1.1 to ~4 km spatial resolution FRAC AVHRR L2P and 2) the 4.4 to ~18 km resolution GAC AVHRR L2P, produced by the OSI SAF within EUMETSAT (@³⁷), OSPO (@³⁸), and NAVOCEANO.

- 34. https://www.ghrsst.org/ghrsst-data-services/products/
- 35. https://www.eorc.jaxa.jp/en/
- 36. http://www.remss.com/missions/amsr/
- 37. http://www.osi-saf.org/?q=content/sst-products
- 38. https://www.ospo.noaa.gov/

The NAVOCEANO FRAC and GAC AVHRR L2P SST data are made available under the MISST (\bigcirc ³⁹) project sponsorship by the ONR and the PO.DAAC (\oslash ⁴⁰) operated by the NASA JPL. The newest NOAA JPSS satellites (Suomi-NPP and NOAA-20) are now equipped with the VIIRS sensors, that have a wide range of infrared channels, and provide SST at 0.75 km to 1.5 km resolution. In order to facilitate ingestion into real-time operational ocean systems, the VIIRS level 3 Uncollated (L3U) data are produced by the NOAA OSPO (\bigcirc ⁴¹), and publicly available from NOAA OceanWatch (\bigcirc ⁴²) and PO.DAAC.

 Infrared radiometers on geostationary satellites above the equator provide high spatial (2~5 km) and temporal (10~60 minute) resolution SST observations over a fixed geographic region. There are several GEO satellites distributed around the equator and operated by different agencies (i.e. ESA, ISRO, NOAA, JMA, JAXA, KMA and CMA); they provide high temporal resolution SST that can improve clear-sky masking by using temporal information to separate the effects of faster moving clouds and other atmospheric features from the slower evolving SST fields (O'Carroll et al., 2019). One example is the AHI sensor of the JMA geostationary satellite "Himawari-8", which allows relatively high-frequency measurement of SST (every 10 minutes with horizontal resolution ~2 km) in a wide area of the Western Pacific (Kurihara et al., 2016). Data are made available by JAXA (\mathscr{P}^{43}), NOAA (\mathscr{P}^{44}) and the Australian Bureau of Meteorology via the National Computational Infrastructure (@ 45).

Surface diurnal warming events occur in ocean regions of high solar radiation, clear skies, and calm seas. They are more common in the tropics (Zhang et al., 2016) but have also been observed at high latitudes (Eastwood et al., 2011). The warming events produce near-surface thermal gradients that create daytime near-surface or warm-layer temperatures up to 2-4°C warmer than nighttime (Donlon et al., 2002). Some operational centres exclude daytime satellite SST observations to reduce the diurnal warm bias and only use night-time satellite SST to assimilate into ocean analyses and forecast models. Most GHRSST L2P or L3U format SST data are cor-

39. https://www.nopp.org/projects/multi-sensor-improvedsea-surface-temperature-misst

- 40. https://podaac.jpl.nasa.gov/
- 41. https://www.ospo.noaa.gov/

42. https://coastwatch.noaa.gov/cw/satellite-data-prod-ucts/sea-surface-temperature.html

43. http://suzaku.eorc.jaxa.jp/GHRSST/

44. https://coastwatch.noaa.gov/cw/satellite-data-prod-ucts/sea-surface-temperature/acspo-ahi.html

45. https://nci.org.au/

rected for bias by subtracting the SSES bias value associated with each SST value (GHRSST Science Team, 2012), derived by data providers using recent matchups with SST observations from drifting buoys and tropical moorings (Petrenko et al., 2016) that produce SST estimates at around 0.2 m depth.

4.2.3.2. Satellite Altimeter

The main parameter that can be derived from satellite altimeters is SLA relative to a reference mean dynamic topography. SLA is fundamental for sea level monitoring and ocean data assimilation. Two freely available common data sources for real-time altimetry data retrieval are the RADS - which was developed by the DEOS and the NOAA Laboratory for Satellite Altimetry (Naeije et al., 2000; Scharroo, 2012) - and the Copernicus Marine Service (Figure 4.14).

The DEOS is building and developing the RADS database that incorporates validated and verified altimetry data products. The database is consistent in accuracy, correction, format and reference system parameters. The capability of such a database has attracted users with less satellite altimeter expertise. Currently, RADS enables users to extract the data from several present and past satellite altimeter missions like GEOSAT, ERS1, ERS2, ENVISAT, TOPEX/Poseidon (T/P), JASON1, JASON2, JASON3, CRYOSAT2, SENTINEL-3A, and SARAL @⁴⁶.

The Level 3 SLA product from Copernicus Marine Service is another open accessible data source for SLA. It shares many of the most useful features of the RADS service, including adaptation to changes in the available satellite fleet and



Figure 4.14. Global ocean along track sea level anomaly (source: \mathscr{O}^{47}).

46. http://rads.tudelft.nl/rads/data/authentication.cgi47. https://datastore.cls.fr/catalogues/global-ocean-along-track-sea-level-anomalies/

maintaining homogeneity. Although superficially RADS and Copernicus Marine Service seem providing the same type of SLA observation they are not identical and a detailed explanation of differences is non-trivial, as the RADS data includes many of the corrections used by Copernicus Marine Service, as well as the corrections applied in its own processing. Users are encouraged to explore the differences between these two data streams and choose the suitable satellite altimeter data source for their own data assimilation system.

4.2.3.3. Satellite Sea Surface Salinity

Measuring SSS from space is a relatively recent technique that relies on L-band radiometry (which has evolved to a point where useful information is provided every few days). Satellite SSS offers the advantages of global coverage and the ability to capture space and time scales not afforded by in-situ platforms such as vessels, moorings, and Argo profiling floats. Figure 4.15 shows a year of satellite SSS products from the ESA's SMOS and NASA Aquarius and SMAP missions. It is worth noting that regions of high variability of >0.2 psu - including coastal oceans, western boundary currents, the Indonesian Seas, and the Southern and Arctic Oceans - are either not sampled or poorly sampled by Argo (Vinogradova et al., 2019).



Figure 4.15. Variability in space-borne sea surface salinity during one year (colors) superimposed with locations of currently operational Argo floats (white dots) from Vinogradova et al. (2019).

Level 3 observations (L3 - provided on a grid but with no in-filling) with various temporal and spatial averaging from the SMOS, Aquarius, and SMAP satellites are available, as are level 2 data (L2; SSS values at the native swath resolution). For SMOS and Aquarius, L3 products are available daily, with separate files for the ascending and descending parts of the orbit. The products used are from the LOCEAN ($@^{48}$) and the JPL ($@^{49}$) respectively for SMOS and Aquarius. While there is

48. www.catds.fr

49. https://podaac.jpl.nasa.gov/

Northern Hemisphere, May 25, 2022





a daily L3 SMAP product, it is based on observations from an 8-day period that would require a complicated observation operator in the data assimilation.

The availability of SSS from SMOS, Aquarius and SMAP has enabled ocean forecast validation (e.g., Vinogradova et al., 2014; Martin, 2016). In recent years, efforts have been put into assimilating satellite SSS data, which is challenging for several reasons. Largely, these are related to the magnitude of errors in the data, particularly in the SSS products needed for operational-style forecasting systems that are required at high temporal resolution (Martin et al., 2019). Quality control of satellite SSS has proved to be a very important process for ocean data assimilation.

4.2.3.4. Satellite sea ice

The sea ice concentrations from Nimbus-7 SMMR sensor and DMSP SSM/I passive microwave data, are accessible from the NASA NSIDC DAAC (@⁵¹) (Figure 4.16). This sea ice concentration dataset is generated from brightness tem-

^{50.} https://earth.gsfc.nasa.gov/cryo/data/current-state-sea-ice-cover

^{51.} https://doi.org/10.5067/8GQ8LZQVL0VL

perature data and is designed to provide a consistent time series of sea ice concentrations spanning the coverage of several passive microwave instruments. The data are provided in the polar stereographic projection at a grid cell size of 25 x 25 km. This is then interpolated to 10 km resolution, level 3 composite of SSMIS level 2 data, on a polar stereographic grid (O⁵²). Daily files are available within 24-48 hours after last satellite acquisition.

The same satellite sea ice concentration data originating from NSDIS SSM/I aboard the DMSP series of polar-orbiting sun-synchronous satellites, are provided by the OSI SAF (@⁵³). The global daily sea ice concentration is processed by OSI SAF at 10 km resolution as level 3 composites of SSMIS level 2 data on a Polar Stereographic grid. Northern Hemisphere and Southern Hemisphere daily files are available within 6 hours after last satellite acquisition.

4.2.3.5. Ocean Colour

Ocean colour measurement consists of detecting spectral variations in the water-leaving radiance (or reflectance), which is the sunlight backscattered out of the ocean after interaction with water and its constituents (Groom et al., 2019). This is a very significant measurement for the monitoring of ocean water quality, ocean acidification, or to understand the global carbon cycle, apart from using it for assimilation

and validation. In the open ocean, the signal is largely influenced by the presence of phytoplankton and dissolved organic matter; in coastal waters, it is also influenced by resuspended particulate matter and river runoff that transports other kinds of anthropogenic particulate. In the framework of the Copernicus Marine Service, two types of products are delivered by the OC TAC (\bigotimes ⁵⁴):

• CHL is the phytoplankton chlorophyll concentration. For the global and regional seas, OC TAC selected the state-of-the-art product algorithm on the basis of optical characteristics of the basin and round robin procedure. For the regional seas, daily chlorophyll fields are produced by applying two different algorithms for open ocean (Case I) and coastal waters (Case II). The data are then merged into a single chlorophyll field providing a regional product with an improved accuracy of estimates in coastal waters.

• The OPTICS product includes all other variables retrieved from ocean colour sensors: IOP, such as absorption and scattering, the diffuse attenuation coefficient of light at 490 nm (Kd490), Secchi depth (transparency of water), spectral Rrs, PAR, CDOM, and the SPM.

Figure 4.17 shows an example of chlorophyll concentration at global scale from the MODIS Aqua satellite.



Figure 4.17. MODIS Aqua chlor_a seasonal composite for Spring 2014 (source: 🖉 55).

53. http://www.osi-saf.org/?q=content/sea-ice-products

54. https://marine.copernicus.eu/about/producers/oc-tac

55. https://oceancolor.gsfc.nasa.gov/atbd/chlor_a/

^{52.} https://nsidc.org/data/nsidc-0081



swh - S3A L2P WAVE Product - Cycle 43 [Qualified Data]

Figure 4.18. Sentinel-3 SRAL significant wave height Level-2 global map (source: 6/56).

4.2.3.6. Significant Wave Height

The SWH (or Hs) is the average wave height (from trough to crest) of the highest third (33.33%) of the waves in a given sample period. The Sentinel-3 mission is able to monitor wave heights from 0 to 20 m. The marine sea state SWH product is a critical product for all maritime safety and rescue operations (from ${}^{\circ}\!\!{}^{57}$).

Figure 4.18 shows an example of SWH for the global ocean from Sentinel-3A measurements.

4.2.3.7. Providers of satellite data

Providers of satellite observations to be used for assimilation/validation are listed in Table 4.3.

4.2.4. Bathymetry

The term "bathymetry" refers to the ocean's depth relative to the sea level. It is an important element in any ocean model, since it allows us to represent the geographical and topographical peculiarities of the sea floor. It has a strong influence on the circulation, notably its barotropic and depth-integrated features, in particular (but not only) at sills and straits,

56. https://www.eumetsat.int/new-S3-sral-wave-products 57. https://sentinels.copernicus.eu/web/sentinel/user-guides/sentinel-3-altimetry/overview/geophysical-measurements/significant-wave-height



An example of a bathymetric dataset: Figure 4.19. the EMODnet bathymetry (source: @⁵⁸).

on coastal and in shelf seas. For this reason, its accuracy may determine the goodness of the ocean model, although there are issues of smoothing and grid mislocation that need to be considered and solved by using ad hoc spatial analysis.

58. https://www.emodnet-bathymetry.eu

Provider	Description	Website
Copernicus Marine Service	Copernicus Mawrine Service through the SL, SST, OC, WAVE TACs for the operational provisioning of near real time and reprocessed datasets used by the Monitoring and Forecasting Centres (MFCs) for assimilation and validation	Copernicus Marine Service
GHRSST	The Group for High-Resolution Sea Surface Temperature (SST) (GHRSST) provides a new generation of global high-resolution (<10km) SST products to the operational oceanographic, meteoro- logical, climate and general scientific community	GHRSST
AVISO++	AVISO++ provides altimeter data	AVISO+ https://www.aviso.altimetry.fr/en/ home.html
EUMETSAT	EUMETSAT is the European operational satellite agency for monitoring weather, climate and the environment from space. In particular, it provides SST and altimeter data	EUMETSAT
NOAA NSIDC	NOAA National Snow and Ice Data Centre provides sea ice concen- tration in the polar region	NSIDC https://nsidc.org/

Table 4.3. List of most relevant international satellite data providers.

A bathymetric dataset needs to be interpolated onto the model's grid. Pre-processing of the bathymetric fields should be necessary for numerical reasons: since bathymetry datasets are usually finer than the model grid, they may need to be smoothed before inserted on the model grid. Effective resolution and vertical coordinates of the ocean model could also constrain the smoothness of the bathymetry.

Figure 4.19 shows an example of a bathymetric dataset as provided by EMODnet bathymetry.

Table 4.4 includes a list of public providers of bathymetric datasets (Marks and Smith, 2006).

4.2.5. Atmospheric forcing

Typically, NWP systems provide atmospheric surface forcing fields to OOFS in order to compute water, heat, and momentum fluxes. Such fields may be also supplemented by real-time or near real-time observations and other averaged datasets including climatology. Certainly, in a more complex modelling framework, an ad hoc atmospheric model can be developed at the same resolution of the ocean model in order to provide high resolution atmospheric fields (coupled systems, see Chapter 10 for further details).

In general, typical surface data input required by an OOFS that is provided by an NWP model includes:

- Sea ice coverage;
- Downward surface longwave radiation;
- Upward surface longwave radiation;
- Downward surface shortwave radiation;
- Upward surface shortwave radiation;
- Dewpoint depression at 2 m;
- Surface latent heat;
- Mean sea level pressure;
- Surface sensible heat;
- Specific humidity at 2 m;
- Air temperature at 2 m;
- Cumulative precipitation rates;
- Zonal and meridional wind components and wind speed at 10 m (or surface wind stresses);
- Short-wave radiation heat flux penetrating through ice;

Product	Description	Provider
DBDB2	Digital Bathymetric DataBase at 2 min by 2 min uniform grid global bathymetry and topography data developed for the ocean model. It was developed by the Naval Research Laboratory	https://www7320.nrlssc.navy.mil/ DBDB2_WWW/
ETOPO1	1 arc-minute global relief model of Earth's surface that integrates land topography and ocean bathymetry. It was built from numerous global and regional data sets. Historic ETOPO2v2 and ETOPO5 global relief grids are depreciated but still available	National Centers for Environmental Information http://www.ngdc.noaa.gov/mgg/ global/
GEBCO	Gridded Bathymetry Data for the World's oceans at 15 arc-second resolution. It operates under the joint auspices of the IHO and the UNESCO IOC	CEBCO https://www.gebco.net/
SRTM+	Global bathymetry and topography. SRTM15+ is the last version at 15 arc-second resolution, built upon the latest compilation of ship- board sounding and satellite-derived predicted depths. V2.0 is part of the last release of GEBCO_2020 (Tozer et al., 2019)	http://topex.ucsd.edu/marine_topo/
EMODnet Bathymetry	It is part of the EMODnet project, funded by the European Commis- sion, which brings together marine data into interoperable, contin- uous and publicly available bathymetric dataset for all the maritime basins in European waters and for the global ocean	EMODnet

Table 4.4. Bathymetric dataset products and providers.

- Ice freezing/melting heat flux;
- Zonal and meridional ice stress on ocean;
- Sea-Ice basal salt flux.

The above list is not exhaustive and inputs can vary based on the needs of the OOFS. For example, it can be used SST from the OOFS along with the air temperatures at 2 m to calculate sensible heat flux instead of using that provided by NWP. More details on thermodynamic and momentum forcing of the ocean can be found in Barnier (1998), Barnier et. al. (1995), Josey et al. (1999).

Figure 4.20 shows an example of surface forcing atmospheric fields from the ECMWF IFS.

A list of global NWP systems is provided in Table 4.5.







Dataset	Description	Provider
GFS	Global Forecast System, produced by the National Centers for Envi- ronmental Prediction (NCEP), provides analysis and forecast atmo- spheric fields for the global ocean at the resolution of about 28 km	https://www.ncdc.noaa.gov/ data-access/model-data/ model-datasets/global- forcast-system-gfs
NAVGEM	Navy Global Environmental Model runs by the United States Navy's Fleet Numerical Meteorology and Oceanography Center (FNMOC)	https://www.usno.navy. mil/FNMOC/meteorology- products-1m
ECMWF IFS and ERA5	European Center for Medium range Weather Forecasting that pro- vides reanalysis, analysis and forecast atmospheric fields at medi- um, extended, and long range	ECMWF https://www.ecmwf.int/
Met Office UK	United Kingdom Meteorological Office that produces the Unified Model, a numerical model of the atmosphere used for both weather and climate applications	Met Office https://www.metoffice.gov.uk/
GEM	Global Environmental Multiscale model, an integrated forecasting and data assimilation system developed in the Recherche en Prévi- sion Numérique (RPN), Meteorological Research Branch (MRB), and the Canadian Meteorological Centre (CMC)	https://collaboration.cmc.ec.gc.ca/
Table 4.5.	Atmospheric forcing products and providers.	

59. https://www.ecmwf.int/







Figure 4.22. An example of river runoff discharge (monthly data) time series from GRDC related to Ceatal Izmail station (Romania) that monitors the Danube basin (source: 🔊 1).

60. https://www.bafg.de/GRDC/EN/Home/homepage_node.html

61. https://www.bafg.de/GRDC/EN/Home/homepage_node.html

Dataset	Description	Provider
GRDC	Global Runoff Data Base, built on an initial dataset collected in the early 1980s from the responses to a WMO request to its member countries to provide global hydrological information	https://www.bafg.de/GRDC/EN/01_ GRDC/13_dtbse/database_node.html
Dai and Trenberth	Dai and Trenberth Global River Flow and Continental Discharge Dataset contains time series of all available monthly river flow rates observed at the farthest downstream station for the world's largest 925 rivers, plus long-term mean river flow rates and continental dis- charge into the individual and global oceans, produced originally by Dai and Trenberth (2002) and Dai et al. (2009) and Dai (2021)	MCAR & UCAR
EFAS	European Flood Awareness System developed and operational with- in the Copernicus Emergency Management Service. It provides grid- ded modelled daily hydrological time series forced by meteorologi- cal observations. It includes river discharge, soil moisture for three soil layers and snow water equivalent	Emergency Management https://www.efas.eu/
GLOFAS	Global Flood Awareness System, operational within the Copernicus Emergency Management Service. It couples state-of-the art weather forecasts with a hydrological model and with its continental scale set-up, providing downstream countries with information on up- stream river conditions as well as continental and global overviews	Emergency Management https://www.globalfloods.eu/
EMODnet Physics	EMODnet Physics gathers, harmonises and makes available near real time river runoff and in-situ river runoff trends (monthly and annual means), accessible through the website with MapViewer controllers	EMODnet https://map.emodnet-physics.eu/

Table 4.6. River data providers.

4.2.6. Land forcing

Rivers represent the natural element connecting land and ocean through the coastline. They impact both coastal and basin-wide circulation and dynamics through net freshwater flux; additionally, they are responsible for biotic diversity and eutrophication, particularly in coastal waters.

Water discharges, nutrients, and organic materials represent sources of freshwater and biogeochemical fluxes for an OOFS, and we have to account for them once we set a numerical model. This kind of data may come from observations or from other models (hydrological or biogeochemical models). In particular, information about discharge, and possibly also salinity and temperature if available, should be provided for the river mouth at given coordinates. As an example, in Figure 4.21 is shown the distribution at global scale of stations that operated/are operating in a certain temporal period contributing to the GRDC. Once the user selects one of the stations, the web service returns the water discharge timeseries (Figure 4.22) allowing to download and integrate it as an input dataset in the ocean model setup.

Table 4.6 provides a list of international databases for river data.

Below are listed some other initiatives for handling freshwater inputs with focus on icebergs and R&D project:

• Altiberg is a database for small icebergs (< 3km in length), detected by altimeters using the high-resolution waveforms (Tournadre et al., 2016), \mathscr{O}^{62} ;

62. http://cersat.ifremer.fr/user-community/news/ item/473-altiberg-a-database-for-small-icebergs • BRONCO stands for "Benefits of dynamically modelled river discharge input for ocean and coupled atmosphere-land-ocean systems": it is a Service Evolution Project run in the framework of Copernicus Marine Service to improve and standardise input of river discharge into global, regional and coastal models, @⁶³;

• LAMBDA stands for Land-Marine Boundary Development & Analysis: it is another Service Evolution Project run in the framework of Copernicus Marine Service. It aims at improving the Copernicus Marine Service MFCs thermohaline circulation in coastal areas by better characterization of the land-marine boundary conditions, @⁶⁴.

4.2.7. OOFS fields as input for downscaling

An OOFS may be set also using information from other OOFSs: this is the case of the so-called nesting models (for major details see Section 5.4.4). For example, the GLO-PHY - herein referred to as parent model - provides lateral open boundary conditions to the Mediterranean Sea Forecasting System (MedFS) - herein referred to as child model. Both systems are part of the Copernicus Marine Service catalogue. Figure 4.23 shows a typical ocean field at global scale from GLO-PHY - in this case, we display sea surface temperature forecast product. The parent model provides temperature, salinity, sea surface height, zonal and meridional velocity components to the Mediterranean Sea through 3 open boundaries located in the Atlantic Ocean. Ocean fields from the parent model are spatially and temporally interpolated over the open boundary sections and provided to the ocean circulation model of the child domain. Figure 4.24 shows as example the Mediterranean Sea surface currents forecast product after integrating the numerical model accounting for the GLO-PHY ocean fields as lateral open boundary conditions.

For major details about the setup of both systems, please refer to the Copernicus Marine Service web pages dedicated to each product.

4.2.8. Climatology from observations

To describe the general oceanographic conditions at different time scales and spatial resolutions, climatological fields computed from observations can be used. They are defined as mean values of a certain variable in a certain period (e.g. month, season, etc.). They may be used for creating initial and/or boundary conditions for an ocean model, as well as validating numerical results and performing data assimilation.

Since observations are irregularly distributed in space, an objective analysis (Chang et al. 2009) is needed in order to

- 63. https://www.mercator-ocean.fr/en/portfolio/bronco-2
- 64. http://www.cmems-lambda.eu/







Figure 4.24. The MedFS sea surface currents on 26 May 2022 (source: \mathscr{O}^{6} through the Ocean Viewer \mathscr{O}^{68}).

produce spatially gridded dataset that can be easily used by a numerical model. Numerical model results, being gridded, can be easily aggregated in time to produce a climatological field to be used as initial or boundary condition.

Climatologies may be also computed from NWP products to modify or to formulate ocean surface fluxes using mean momentum conditions from a reanalysis product (e.g., ECMWF ERA5, etc.) superposed with variability from the NWP fields. Additionally, observations such SSS and SST may be adopted for supplementing climatological data for surface flux relaxation to control model drifts. Finally, climatologies may be computed also from other ocean models to provide lateral open boundary conditions (numerics and methods will be presented in Chapter 5).

Figure 4.25 provides as an example of climatology the annual sea surface temperature computed over the period 1955-2017 for the global ocean by the WOA.

Table 4.7 provides a list of international atlases.

- 65. https://marine.copernicus.eu/
- 66. https://myocean.marine.copernicus.eu/
- 67. https://marine.copernicus.eu/
- 68. https://myocean.marine.copernicus.eu/



Annual temperature [°C] at the surface (quarter-degree grid)

Figure 4.25.	An example of climatology: temperature field from World Ocean Atlas Climatology ((source: 🔗 👳).
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Dataset	Description	Provider
WOA	World Ocean Atlas (Boyer et al., 2019) provides climatological tem- perature (ºC), salinity (unitless), density (kg/m3), mixed layer depth (m) and other biogeochemical parameters (for the latter, major de- tails are provided in Chapter 9)	National Centers for Environmental Information https://www.ncei.noaa.gov/products/ world-ocean-atlas
WOD	World Ocean Database (Boyer et al., 2019), is a continuation of the Climatological Atlas of the World Ocean (Levitus, 1982) and at pres- ent represents one of the world's largest collection of uniformly for- matted, quality controlled, and publicly available ocean profiles data	National Centers for Environmental Information https://www.ncei.noaa.gov/products/ world-ocean-database
SeaDataNet	SeaDataNet is a distributed Marine Data Infrastructure for the man- agement of large and diverse sets of data deriving from in situ of the seas and oceans. It provides an online access to data on regional cli- matologies products – gridded fields of sea temperature and salinity - for the European seas (Arctic Sea, Baltic Sea, Black Sea, Mediterra- nean Sea, North Sea, North Atlantic Ocean) and for the global ocean	SeaDataNet https://www.seadatanet.org/ Products/Climatologies

Table 4.7.Climatology products and providers.

69. https://www.ncei.noaa.gov/

4.3. Data Assimilation

Through data assimilation, OOFS combines observations and the numerical model solution with the scope of producing the best reconstruction of the ocean state to be used as initial condition of the forecasting cycle. According to Moore et al. (2019) and considering Figure 4.27, we can assume that a priori state estimate of the ocean computed from the numerical model (blue line in Figure 4.26) together with a priori direct but incomplete state estimate from ocean observations (black dots in Figure 4.26) produce a posteriori state estimate which "combines" all available information considering uncertainties in both model and observations (green line in Figure 4.26).



Figure 4.26. Data assimilation models (green) are helped by observations to produce more realistic forecasts, closer to real observations (source: MEDCLIC project, SOCIB-La Caixa Foundation).

Ocean data assimilation is then defined mathematically through a rigorous process that combines ocean observation statistics with statistics of ocean model behaviour to extract the most useful information, possibly from sparse observations of time-varying ocean circulation (Cummings et al., 2009). Broadening Step 1 in Figure 4.1, the main characteristics of the data assimilation modelling system can be presented as in Figure 4.27, which shows the major components of the data assimilation modelling system, which are defined by:

- access to observations;
- data quality control;
- data assimilation scheme.

Access to observations, quality, providers as well as examples have been presented in Section 4.2. Data quality control is performed by an automatic procedure, native in the assimilation scheme or performed in offline mode at the submission of the analysis cycle, which selects the best observational dataset from the one accessed. To do such selection, the procedure takes as input the quality flag value associated with each specific observation (see Figure 4.3): usually, observations with QC flag = 1 and/or 2 are selected and make eligible to be used by the data assimilation scheme.

Depending on the specific characteristics of the basin on which the system is working, the data quality control may include further checks to reject data which are not sufficiently good to be assimilated. Such criterion may be implemented in offline mode as pre-processing steps of the data access and management. This is the case, for example, of the Mediterranean Forecasting System (MedFS) delivered in the framework of Copernicus Marine Service: the system performs additional checks for Argo and SLA observations rejection based on specific criteria, which are listed in Table 4.8.

Data assimilation scheme is really the core of the system since it performs the mathematical work of combining model state and observations. Existing data assimilation methods are classified in 2 major groups (Bouttier and Courtier, 2002):

- sequential method, which considers past observations until the time of analysis: this is the case of NRT products (analysis);
- non-sequential method, which uses "future" observation: this is the case of the multi-year products (e.g., reanalysis).

Another distinction can be made between continuous and intermittent assimilation in time:

- continuous assimilation: for a given period of time the observations are collected and the correction to the analysed state is smoothed over a specific assimilation window;
- intermittent assimilation: for a given period of time, the observations are collected within a specific assimilation window to compute a correction.





Carrassi et al. (2018) and De Mey (1997) detail more the nature of the assimilation schemes used in physical, biogeochemical, ice and wave forecasting systems, describing the formulation of the problem and numerical approximation. These concepts are detailed in the theoretical chapters from 5 to 9, which are dedicated to show how such methods are used for setting up an OOFS.

From the scheme in Figure 4.27, we can derive some key definitions at the basis of the assimilation cycle: the innovation, defined as the difference between the first guess (or forecast) and the observation. The data assimilation method tries to estimate with less uncertainty than either the model prediction or observation: it deals with the computation of the increment, defined as the analysis minus the model first guess. The data assimilation system itself has been used to monitor observations and data quality control (Hollingsworth et al., 1986) by computing statistics involving observations, such as observation increments used to setup the blacklisting; this is a list of observations that the data assimilation has rejected and represents valuable information to be shared also with data providers in order to fix potential issues or bugs in the observational datasets.

ARGO QC1	Check on the date and location quality flags: only the profiles with both flags equal to 1 are taken into account
ARGO QC2	Out of the Mediterranean Sea region
ARGO QC3	Retain only ascending profiles (descending are rejected)
ARGO QC4	Check on the values of the quality flags of pressure, temperature and salinity for each depth: if one of the flags is not equal to 1, the layer is deleted
ARGO QC5	Check on the values of the temperature and salinity, data outside the following ranges are rejected: 0 <t<35; 0<s<45<="" th=""></t<35;>
ARGO QC6	Check on the thermocline: if distance between two subsequent measurements of temperature and salin- ity in the first 300 meters is larger than 40 m, the profile is rejected
ARGO QC7	Measurement between 0 and 2 m are rejected
SLA QC1	Check on the values of date, latitude, longitude, sea level anomaly and DAC: if one of these values is equal to missing value the measurement of sea level anomaly is rejected. Check on the quality flag of sea level anomaly: if the flag is not equal to 1 the measurement of sea level anomaly is rejected

Table 4.8. Quality control criteria adopted by the Mediterranean Analysis and Forecasting System (MedFS, \mathcal{O}^{70}) for in-situ (Argo) and SLA.

4.4. Numerical Ocean models

4.4.1. Definition and types of models

Ocean numerical models are the very core of the OOFS (see Figure 4.1). A numerical ocean model is a computational tool used to understand and predict oceanic variables (Griffies, 2006). A set of equations governing the dynamics and thermodynamics of the ocean are solved numerically to obtain a three dimensional dataset of simulated variables, which typically consist of EOV such as wave fields, velocity components, temperature, salinity and sea level, at any instant of time.

Depending on the problem and variables to be treated, different numerical models are employed:

- Temperature, salinity and currents fields are solved by means of ocean circulation models (see also Chapter 5);
- Ice models (see also Chapter 6);
- Sea level uses ocean circulation models, although typically are running under simplified equations (see also Chapter 7);

 Growth, propagation and decay of waves due to winds are calculated by wave models (see also Chapter 8).
 The rate of change of the wave spectrum is governed by transfer of energy from wind, wave-wave interaction and dissipation. Interaction with ocean bottom is critical at high resolution coastal processes; different models, with different physics, are available to solve this scale (mild-slope, Boussinesq, etc.);

• Biogeochemical processes in the ocean can be represented by biogeochemical models (see also Chapter 9), using coupled differential equations. Examples of such processes include cycles of carbon, nitrogen, iron, etc. Additional equations are used for time evolution of phytoplankton, zooplankton, etc., at varying levels of complexity. The chemistry and ecosystem equations are combined with the physical OGCM for the time-dependent estimation of variables.

70. https://medfs.cmcc.it/

4.4.2. Coupled models

Various dynamical components of the Earth system, such as NWP systems, OOFS, Sea Ice forecast systems, wave forecast systems, Land/Hydrological forecast systems, etc., can be coupled together (see also Chapter 10). The coupling is facilitated by using a common framework - like the ESMF which allows the various dynamical components to exchange forcing data with other components. Couplers are then designed to provide appropriate output/input information on model grids at every time step, as required. This provides a much more "tight" exchange of forcing data, which otherwise would be prohibitively expensive to provide using traditional file I/O. Different couplers allow for data exchange at different time scales. For example, atmosphere and sea ice can be coupled at smaller time intervals while ocean and sea-ice exchange information at much slower time intervals in the same coupled environment.

A significant application of such "tight" coupling is for windwaves. Feedback from wave models in terms of radiation stress can be used to modify drag coefficients for calculating wind stresses. These can be particularly useful for complex seas driven by hurricanes.

4.5. Validation and Verification

Operational ocean services provide routine marine products to an ever-widening community of users and stakeholders. Some of the products delivered are generated by means of ocean models (i.e. forecasts, analyses, or reanalyses). Ocean models are powerful computational tools able to produce useful information in the absence of (or in between) ground truth information. The reliability of this information depends on the realism of the model itself, but also on the accuracy of its initial and boundary conditions, as well as on the capacity to constrain this model with contemporaneous high-quality observations. This information on models' quality and performance is almost more crucial for the end-users than the model solutions themselves. Thus, the reliability of model solutions must be assessed, and the MPQ must be quantified at the analysis, forecast, and reanalysis stages; it has also to be properly documented for end-users.

The purpose of this section is to give a general overview of the commonly used methodology and processes applied by existing operational ocean services to validate and verify their ocean model products. In particular, standard validation metrics and protocols were designed for oceanography model analyses and forecasts, and agreed among the community of OceanPredict forecasters (Hernandez et al, 2015, 2018). This section is focused on describing these validation methodologies and standards for model products. Specific details on the thematic (process oriented) validation for each kind of model use in the OO community (i.e., waves, storm surge, ocean circulation, biogeochemical, etc.), along with examples, illustrations and use cases, can be found in Chapters 5 to 9.

4.5.1. Basis statistical tools for time series validation

Several metrics can be computed for a quantitative analysis of the model-data time series validation: bias, maximum error MaxErr, RMSE, Pearson correlation coefficient (R) or Scatter Index (SI) are some of the most common examples and are obtained as:

$$bias = \sum_{i=1}^{N} (O_i - P_i)$$
(4.1)

$$MaxErr = O_i - P_i \tag{4.2}$$

$$bias = \sum_{i=1}^{N} (O_i - P_i)$$
 (4.1)

$$RMSE = \sqrt{\frac{\sum_{i=1}^{N} (P_i - O_i)^2}{N}}$$
(4.3)

$$R = \frac{\sum_{i=1}^{N} (P_i - \bar{P})(O_i - \bar{O})}{\sqrt{\sum_{i=1}^{N} (P_i - \bar{P})^2} \sqrt{\sum_{i=1}^{N} (O_i - \bar{O})^2}}$$
(4.4)

$$SI = \sqrt{\frac{\sum_{i=1}^{N} [(P_i - \bar{P}) - (O_i - \bar{O})]^2}{\sum_{i=1}^{N} O_i^2}}$$
(4.5)

where P_i and O_i refer to the forecasted and observed signals respectively, N is the number of time records, and ($\overline{}$) is the mean operator. Other type of skill scores can be used, such as the Coefficient of Efficiency (*COE*) (Legates and McCabe, 1999, 2013) obtained as:

$$COE = 1 - \frac{\sum_{i=1}^{N} |O_i - P_i|}{\sum_{i=1}^{N} |O_i - \bar{O}|}$$
(4.6)

A perfect model has a COE = 1.0, COE = 0.0: this implies that the model is no more able to predict the measured values than the measured mean; a negative COE value would indicate that the computed signal performs worse than the measured mean.

4.5.2. Ocean forecasting standard metrics for validation and intercomparison

There are different types of model products (i.e. forecast, analysis, reanalysis) and different types of model evaluation methodologies, which are mostly based on the comparison with reference values, aiming at building performance and skill scores. Among others, some of the most applied methods to assess OO models are:

1. Analysis (or forecast at various forecast lengths) versus contemporaneous observations (in situ, but also satellite) in the observations' space. This type of comparison to observations is also performed by the data assimilation system, so it is usually extensively used in operational oceanography. Since ocean in-situ observations are sparse and unevenly distributed, representativeness issues are frequent. Depending on the observation's coverage, the comparisons are either local (at one given observation location) or the statistics of the differences between model solutions and the observations are computed over rather large areas or long periods of time.

2. Model forecast versus model analysis (or observation only). In this case, the model forecast for a specific day is compared to the analysis of the same day, assuming that the analysis is the best available estimate of the ocean state for that day; this methodology can be applied only in delayed mode, when the analysis is available. The forecast can also be compared with gridded observations (an analysis of observations only, for instance satellite L4 observations).

3. Forecast versus persistence. Model fields at various forecast lengths are compared to their initial condition. The forecast is compared with the persistence of the last analysis available (or observations), in other words it is compared to what would have been the best estimate of the ocean state of that day if no model forecast were available. This comparison is performed expect-

ing that the model forecast is more accurate than persistence and allows to quantify the skill of the forecast.

4. Analysis (or forecast) versus climatology or versus literature estimates for less observed quantities. This approach is commonly used with currents or transports.

5. Observed versus modelled feature structure. In this case, the structure (location or intensity) of an observed feature (such as an ocean front or eddy) is compared to its modelled counterpart. Categorical scores can be defined from this type of model validation, possibly introducing space and/or time lags.

The results of these comparisons between model outputs and reference values can be combined in different ways to derive MPQ monitoring scores or metrics. In the numerical weather prediction community, there is a long tradition in model forecast verification methods with vigorous progresses related to the advent of probabilistic methods into operational numerical weather prediction (Jolliffe and Stephenson, 2003; Nurmi, 2003). On the other hand, the OO forecasting community, conditioned by the limited number of oceanic observations and their uneven distribution (mostly of them, surface ones), has shown that quality assessment



Figure 4.28. Classes of metrics currently used in the OceanPredict community to monitor the quality of ocean analyses and forecasts: a complete range of statistics and comparisons in space and time are necessary to assess the consistency, representativeness, accuracy, performance, and robustness of ocean model outputs.

must include four types of metrics to properly assess the consistency, representativeness, accuracy, performance, and robustness of ocean model outputs (Crosnier and Le Provost, 2007; Hernandez et al., 2009). These four classes of metrics (Figure 4.28) were adopted by GODAE OceanPredict and they have been extensively used in different OO initiatives. For instance, these four classes (with specific computation methods and definition of reference geographical areas) have allowed regular intercomparison exercises between global and regional ocean forecasts (see Ryan et al. (2015) for a global ocean forecasts intercomparison). A last type of metrics, defined from user feedback and called "user oriented" (such as categorical scores point 5), is also instrumental for the quantification of uncertainties dedicated to specific applications (Maksymczuk et al., 2016). Categorical scores using space and time lags or specific case studies, can also help considering the double penalty effect that can lower statistical performance while comparing high resolution model outputs with observations, as pointed out by Crocker, et al. (2020).

4.5.3. Qualification, validation and verification processes in support of operational ocean models' production

Qualification, validation and verification are terms commonly used in the quality control of OO model products. Usually, qualification refers to model quality assessment at the development stage, during which model parameters are optimised. In OO services, such as the Copernicus Marine Service, the qualification phase refers to a comprehensive scientific assessment of any new/updated operational ocean model application, which is performed before the entry into service of the proposed system (Sotillo et al., 2021). This qualification phase is often used to quantify the added value of the updated model system with respect to its previous existing version, comparing the performances of both system versions (V_{n+1} versus V_n) against a well-defined list of metrics, and using the same referential observational data. On the other hand, validation refers to the operational ocean analyses and forecast performance assessment, while in operation. Finally, verification is defined by Hernandez et al. (2015) as the a posteriori quantification of operational ocean forecast skill, preferentially based on independent data, which means observational products not used to constrain the model products; for instance, by means of any kind of data assimilation.

Achieving the best possible MPQ is a major objective for OO centres, and a MPQ itself is a key performance indicator for any OO service. Several model quality assessment stages can be defined along the life of an OO model product. Figure 4.29 illustrates the typical MPQ assurance loop adopted by OO services to ensure and quantify the quality of their model products. This approach is becoming popular across OO services to deal with MPQ at each major stage of development of an operational oceanography model (i.e. development, transition into operations, operational routine, and "after sales service" including delayed mode validation and expertise), using dedicated model assessment processes, and it counts with a long tradition in the operational meteorological and climate community.



Figure 4.29. Schematic view of different Model Product Quality assessment processes applied along the life of an Operational Oceanography (OO) service product in the development and dissemination stages. All processes rely on the use of the standard metrics (Figure 4.28) to compare the model product with observations as well as with other model solutions.

As shown in Figure 4.29, six main steps or phases can be distinguished within the MPQ assurance process. The first one, focused on research and development activities, supports the implementation/update of new/existing model products to be operationally delivered. At this research and development phase, relevant scientific quality information is developed - and that can also later published in peer reviewed publications - mostly ensuring that the ocean model application is state-of-the-art and based as much as possible on cutting-edge science. Both model versus observations (model-obs) comparisons and intercomparisons with other available model solutions (model-model intercomparisons) can be performed in support of this forecasting system development phase, and they are the basis for the evaluation of model sensitivity tests and scenarios. User oriented metrics, such as categorical scores or Lagrangian drift evaluations, (Drévillon et al, 2013) can be used in specific case studies to quantify the impact of changes in the model system, either during the system development phase or to prepare specific OSEs and OSSEs.

When the new model set-up application is scientifically tested and before the model system is scheduled for entry into service, there is a pre-operational qualification stage, along which the expected (reference) products' quality is established. In the qualification phase, it is critical that the model solution tested is generated in a pre-operational environment that ensures analogous conditions (i.e. same model applications, same type of forcing data, and analogous observational data sources to be assimilated) to the ones that are later applied in operations. It is also important to compare the quality of the product with its previous versions to ensure that there is no regression in terms of MPQ. The stability in time of the performance of the model is also assessed, using a data record of at least one year. Finally, as an outcome from this phase, the OO services can issue the "static" reference documentation on the quality of the product using the different assessment metrics computed. The document can be later delivered to end-users together with the product itself; for instance, see the QUID delivered together with any Copernicus Marine Service ocean product.

Once the model system is in operation, the OO centres perform the scientific validation and verification of the model products delivered on a routine online near-real-time basis, together with the control of the operational production. This on-line validation usually includes forecast model assessments with the available observational data sources (specially from NRT operational products) or with other model solutions (more recent available analysis or, in the case of regional models, comparisons with the parent solution in which are nested). This first on-line validation process is later completed with an extra assessment done in delayed mode. This delayed-mode validation, performed typically monthly, allows to generate more complete and robust validation metrics, extending the obs-model comparisons using observational information from extra data sources or more quality-controlled ones and more complete series of analyses and forecast cycles.

Finally, user feedback focused on specific processes, areas or events, as well as extra model product assessments performed by the producers themselves or by producers in collaborative frameworks (such as scientific research projects or other initiatives with targeted end-users) can significantly enhance the knowledge of the model products.

OO services are continuously progressing towards the regular delivery of up-to-date quality information, although there are remaining gaps in operational capacities to assess model solutions, mostly linked to shortcoming in the availability of ocean observations, and specially in NRT. Observational data used for model skill assessment and validation are mainly originating from drifting profilers, fixed mooring platforms, tide gauges, and remote sensing data. In their review on the operational modelling capacity in the European Seas, Capet et al. (2020), point out that only 20% of operational model services provide a dynamic uncertainty together with the forecast products. This uncertainty would be required for a real-time provision of confidence levels associated with the forecasts as, for instance, is usual in weather forecasts. This lack of uncertainty information, associated with a lack of observations, affects also the data assimilation capacity (Capet et al. (2020) noted that data assimilation is only implemented for 23% of the surveyed models, remaining exceptional in biogeochemical systems). The development of ensemble forecasting and that of probabilistic uncertainty information may help to fill this gap in the future. Peng et al. (2021) stressed the need for findability, accessibility, interoperability and reusability (FAIR data principles) of the information in earth science datasets. This confirms that pertinent product quality information has to be developed further as part of OO services.

4.6. Output preparation

4.6.1. Introduction

The OOFSs aim at delivering, by means of numerical ocean models, essential information on the ocean state to a wide community of stakeholders and users.

To meet users' requirements, the variables to be supplied must be carefully selected among the large amount of data produced by the OOFSs. In addition, spatial and temporal resolution at which these variables are obtained must also be well defined. Furthermore to these specifications, the efficient storage and delivery of the information supplied by the OOFS is of paramount importance to allow later manipulation. For this purpose, the outputs obtained from the modelling systems should be saved in standard formats that enable their easy use, treatment, and exchange.

The purpose of this section is to provide information and recommendations on the characteristics of the outputs to be delivered in the frame of OOFSs, to maximise their utility and ensure that they meet the requirements demanded by the users.

4.6.2. Products and datasets

The data related to forecast systems are provided through products and datasets.

A "product" is a usable set of data (or one or more datasets) with its descriptive information (metadata). A product is the association of one or several datasets with some static and/ or dynamic metadata.

A "dataset" is the aggregation of analysis and forecast with the same geospatial structure or feature type: profiles, point series, trajectories, points, grids, grid series, etc. A dataset is composed of one or several data files. The aggregation is done so that the content of the dataset is predictable for the user (list of variables, predefined geographical bounding box) and expandable when the product is updated (time axis). A dataset can be accessed through an "Access service". A dataset is gridded when the data are stored in raster data files (e.g. in NetCDF format), and each file of the dataset contains some variables on the same geographical coverage. The difference between two files composing a gridded dataset shall be the time coverage of the variable(s).

4.6.3. Variables

The EOVs identified by the GOOS Expert Panels as fundamental measurements needed to address the current scientific and societal ocean-related issues, can play an overriding role as guidelines to incorporate the most relevant ocean information in the final OOFS output products and their inclusion is thus strongly encouraged.

These variables provide an optimal global representation of the state of the ocean (Lindstrom et al., 2012) and the affordable and technically feasible to generate information they give is particularly relevant for main ocean themes such as ocean health or climate.

Among these EOVs, the most important ones regarding ocean physics are mainly surface and subsurface temperature, salinity, currents, sea surface height, sea ice, and surface stress. In biogeochemistry, some of the most relevant are nutrients, oxygen, dissolved organic carbon, and particulate matter, whereas phytoplankton, zooplankton, and algal cover stand for major variables for biology and ecosystems.

4.6.4. Spatial resolution

Ocean modelling systems deliver outputs over discretized grids at specific horizontal and vertical resolutions. Usually, the most used horizontal grids are structured Arakawa B or C, which avoid the existence of a singularity point in the computational domain by locating north mesh poles on land instead. This particularity entails that those models generate data in non-regular meshes that can be more complex to handle. Other models can also produce unstructured data gridded in irregular patterns composed by simple shapes such as triangles or tetrahedra that allow the mesh to adjust to more complex geographical areas. Likewise, spatial resolution can be increased in specific regions presenting features or events of particular interest (e.g. coastal areas) by way of nesting techniques that allow the dynamic exchange of information between model parent and child domains.

Three dimensional grids of ocean circulation models are vertically discretized following different vertical coordinate systems. These coordinate systems are based on different ways of discretizing, such as the cartesian depth-following z-coordinate, the isopycnal ρ -coordinate, the terrain-following σ -coordinate, or the pressure p-coordinate. Their choice

is especially important since each of them has advantages and disadvantages in accurately representing the different ocean layers features.

To slightly simplify the managing of outputs for the model users, some later horizontal interpolation can be performed to generate final outputs in easier regular user-defined coordinate systems, although this must be achieved always ensuring that the information loss is minimised and the highest possible product quality is reached.

4.6.5. Time resolution

Final model outputs are typically distributed as time-averaged means or instantaneous values encompassing a wide range of time frequencies. The selected frequencies may depend on the variability of each variable and on the scope of the study for which the outputs would be employed, but hourly, daily, or monthly means are the most demanded outputs. Anyway, this feature is configurable in the models and hence can be modified as needed; for consistency, increases in spatial resolution usually should go hand in hand with rises of temporal resolution and therefore also higher-frequency outputs. In any case, later procedures can be applied to organize the final outputs as wished, splitting, or gathering the produced variables in different datasets, or computing averages for specific time periods.

4.6.6. Data format

Outputs formats constitute an essential aspect of the OOFS production. Formats highly depend on the models employed to generate outputs. In that sense, the utilisation of standard formats is especially significant to ease the data reading or processing with specific software or to improve the exchange between different systems, since they structure data in setups easily interpretable according to well-defined rules.

Among these formats, the most recommended is certainly the Network Common Data Form (NetCDF), a set of free software libraries and data interfaces widely applied in meteorology, oceanography, and earth sciences, and specifically designed for creating, accessing, and sharing array-oriented scientific data (\mathcal{O}^{71}).

NetCDF format features are:

- Self-Describing: netCDF files show information (metadata) on the contained data;
- Appendable: Data may be added to an already existing netCDF file without altering its structure;

- Scalable: Datasets from netCDF files can be easily subset through interfaces;
- Portable: netCDF files can be effectively retrieved from computing machines with different architectures;
- Shareable: netCDF files allow simultaneous access;
- Archivable: The access to earlier forms of netCDF data is possible with newer versions.

NetCDF also includes data access libraries for, among other programming languages, Fortran, Java, C, C++, as well as utility programs to open and manipulate the data files.

Metadata contained in the netCDF files are a key component since they supply major information on the data characteristics. To promote the sharing of such files, there are conventions specifically designed for defining common climate and forecast metadata, such as the COARDS CF conventions. These conventions allow the NetCDF files to accurately describe each variable data, as well as define their spatial and temporal properties. Thus, they simplify the process of comparing quantities between different sources and enhance the design of specific applications.

In particular, the CF metadata convention is an extension of the COARDS conventions especially intended for model-generated data. According to this convention, specific attributes provide a general explanation of the netCDF file contents, whereas others deliver associated descriptions of each variable included in the file. Furthermore, when following the CF convention, a special treatment is given to the essential model outputs coordinates (latitude, longitude, vertical and time). More information on CF conventions can be found at \bigcirc^{72} .

4.6.7. Display and analysis tools

Numerous tools are available for displaying, analysing, and handling ocean modelling output data, particularly when data are structured according to common formats such as NetCDF. Its libraries include helpful command lines such as "ncdump" that allows to quickly view a text representation of data and metadata information included in the file. Another command, "ncgen", is used to generate a netCDF file or the C/Fortran programs needed to create it from a description of the netCDF file previously obtained in a small language known as Compiler Description Language (CDL).

Aside from the previously mentioned netCDF libraries commands, many well-known packages and programming languages can open, manipulate (e.g. for modifying information, calculating arithmetic operations, computing statistics, etc.), or visualize netCDF files.

71. https://www.unidata.ucar.edu/software/netcdf/

72. https://www.unidata.ucar.edu/software/netcdf/

Among them, the most popular are:

- Ferret (https://www.unidata.ucar.edu/software/netcdf/),
- NCO (http://nco.sourceforge.net),
- CDO (https://code.mpimet.mpg.de/projects/cdo),
- Python (https://www.python.org/),
- Matlab (https://www.mathworks.com/),
- GrADS (http://cola.gmu.edu/grads),
- IDL (ttps://www.harrisgeospatial.com/Software-Technology/IDL),
- IDV (https://www.unidata.ucar.edu/software/idv),
- Panoply (https://www.giss.nasa.gov/tools/panoply),
- NCL (http://www.ncl.ucar.edu),
- ncview (ttp://cirrus.ucsd.edu/ncview),
- ncBrowse (https://www.pmel.noaa.gov/epic/java/ ncBrowse).

4.6.8. Output dissemination

The OOFSs require an accessible and reliable service to effectively distribute the data generated. This service must implement interfaces interoperable with the oceanography community (NetCDF outputs following CF convention, quality control procedures, etc.), and use common tools and protocols (e.g. Thredds-OpenDAP) for accessing the data.

The service mentioned should be based on systems that have been effectively serving users for years, ensuring that the outputs are provided considering the user requirements. In addition, all service components should be properly managed and maintained.

The model outputs should be archived in easy-to-access services from where users may obtain them, either requesting them through dedicated interfaces (pull service) or, for subscribed users, receiving the files via any well-known protocol such as ftp, ssh, etc. These services should also allow the users to subset the requested data from the original outputs.

4.7. User management and outreach

A marine service is the provision of marine information to assist decision making. The service must respond to user needs, must be based on scientifically credible information and expertise, and requires appropriate engagement between users and providers. It should be an integrated service gathering all ocean products into a single catalogue sustained on the long term.

The first mandatory step is to define the service to be provided and answer the following questions:

- What is the target audience of the service? It can include one or all the following users: national/local public environmental agencies, scientists and academia, citizens, private companies, etc.
- Which data policy is applied to the service? It can be an open service (open to all users with or without registration) or a restricted access service. It can also be a free of charge or a paid service.
- Which operational commitments and service level agreement are available to users? To engage through a

transparent and trust relationship with users, service commitments should be made publicly available.

Depending on the answers to the 3 above questions, the service will develop a patchwork of the following assets:

- Communication assets (both on and offline), ocean literacy tools, and societal awareness can for example include the activities below. These are designed to deliver the operational oceanography service expertise to a wider audience through the translation from scientific language and findings for different target audiences, and to distribute the tools to drive uptake.
 - Digital website, digital tools, social media (Twitter, Linkedin, Youtube, etc.);
 - Editorial (News, Events web section, etc.) and press relations (Newsletters, etc.);
 - Ocean Literacy and Outreach activities (outreach events, partner initiatives, museum exhibitions, etc.).

• An ocean data portal including the catalogue of ocean products should be made available online to download and visualise marine data.

 A searchable online catalogue of products should be made available including product metadata description and search parameters such as: free text, geographical areas, marine parameters, models or observations (satellite or in situ), resolution (spatial and temporal), coverage (spatial and temporal), update frequency, etc. It should also allow the user to download the selected data product (with or without registration, and with or without charges, depending on the definition of the service). The online catalogue should be compliant with the highest standards of usability and interoperability.

• Another major asset includes viewing tools to visually explore the different ocean products. Such tools can include the ability to create 2D maps, cross sections, select regions, and generate graphs with selected variables. Layering and superimposing layers with different opacities can be made possible allowing users to compare multiple datasets. In addition, the selected maps and time frames can be exported as videos, images or embedded elsewhere.

• Such ocean data portal encompasses product management activities to carefully and closely manage the product portfolio and each product life cycle. Product management allows to carefully track all product changes impacting users along with product metadata updates and homogenisation, which in turn need to be carefully communicated to the users.

• The user support desk is the point of contact for all questions and comments from users and its objective is to optimise user experience throughout the service. Various means can be used to initiate or conduct exchanges with users (e.g. chat box, e-mail address, online forms, phone, video-conferencing, etc.). The user support desk is also responsible for informing users of operational issues on products and services, such as incidents, maintenance, and improvements. In addition, it also provides an internal link between users and scientific and technical experts. Finally, it is also very involved in the training activity described below and participates in all such events. A client-oriented approach for specific users can be developed if needed for specific major accounts.

• User learning services or training activities allow to strengthen user uptake: its objective is to train, answer questions, facilitate user experience, share knowledge, and collect requirements. Training workshops are designed to train existing, new or beginner users. The target audience needs to be clearly defined and the training resources need to be developed accordingly. For example, participants can learn about products and services and their possible applications across a wide range of subjects during plenary and practical training sessions. Participants should be enabled to share their experiences as well as express their needs and requirements for future new products to be included in the portfolio. Finally, tutorial videos and jupyter notebooks (i.e. open-source web application that allows experts to create practical exercises and share codes) can be shared with participants to help them for their own code programming and understanding of how to use products.

• A service monitoring activity: the service should be monitored through key performance indicators (KPIs), reported quarterly and annually. Such KPIs assess the service reliability against operational commitments and service level agreement (timeliness, robustness, etc.). The service monitoring activity encompasses many KPIs to steer the service and its uptake, and for example provides figures about the product portfolio evolution, variation in the number of subscribers and their detailed characteristics, as well as monitoring of the service availability and product timeliness.

• User feedback and user satisfaction should be measured, monitored, analysed, and injected back into the service through the implementation of new or updated products and services to better fit user's demand.

• User engagement and market expansion activities can be developed to foster uptake of marine products, develop market intelligence, and seek novel opportunities for data use in new communities. Such activities include targeting developing blue markets, explaining the marine offer to new audiences, showcasing the use of data through use cases, launching marketing campaigns, organising or participating in events advocating the marine services and liaising with new partners and communities. Barnier, B., Siefridt, L., and Marchesiello, P. (1995). Thermal forcing for a global ocean circulation model using a three-year climatology of ECMWF analyses. Journal of Marine Systems, 6(4), 363-380, https://doi.org/10.1016/0924-7963(94)00034-9

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