



## **HiSEA DELIVERABLE 4.4**

### **OPERATIONAL MODELLING PROCEDURES**

**WORK PACKAGE NUMBER: 4**

**WORK PACKAGE TITLE: SERVICE DESIGN AND CLOUD COMPUTING**



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## Executive Summary

This deliverable provides the guidelines to set up an operational service following the “digital twin” concept. Necessary actions to import model forecasts are defined, existing providers (e.g. Copernicus Service, GFS, etc.) identified. The required operational ‘chain’ of models to run in the platform (hydrodynamics, waves, oil dispersion) is also described as well as the storage process of data. This chain serves as a guideline for the implementation and execution of WP5.





# 1 Introduction

HiSea aims to provide a set of services focused on different coastal user's needs (navigation safety, ports operations, aquacultures, etc.) allowing to exploit the added value of integrated Earth Observation (EO) technologies (satellite, airborne and ground based), Copernicus Marine Service and ICT to deliver customized and ready to use information. These services will provide an easy way to get in-situ data, local high-resolution forecasts and products and services (e.g. meteo-oceanographic conditions at specific locations, identification of optimum or critical working windows, support to sea pollution response actions, etc.) to a broad range of different users.

Nowadays, managers try to get access to the best available information to evaluate the constraints and risks on the sites they operate and prevent and/or adapt to any event that may impact their activities. The fast increase in the amount of observations and forecast data, currently made available from different institutions, has enabled different stakeholders and users of the marine environment to make decisions based on objective information.

An effective way to get access to this useful information is through “operational services” or “digital twins” as how these services are being lately popularized. A digital twin is a virtual replica of an object, being, or system that can be continuously updated with data from its physical counterpart. Supported by an estimated 25 billion connected global sensors by 2021, digital twins will soon exist for millions of things. A jet engine, a human heart, even an entire city can all have a digital twin that mirrors the same physical and biological properties as the real thing. The implications are profound: real-time assessments and diagnostics much more precise than currently possible; repairs executed in the moment; and innovation that is faster, cheaper, and more radical.

In the case of the business cases addressed by HiSea, the existence of such digital twins also can provide a relevant contribution to better planning and operation, allowing to adopt proper informed preventive and corrective actions. The construction of a digital twin involves three important components:

- a model of the system,
- an evolving set of data relating to the system, and
- a means of dynamically updating or adjusting the model following the data.

This document addresses more in detail the third component: provide efficient means of dynamically updating or adjusting the model following the data.

The model(s) used in a digital twin does not need to be data-driven, but it should produce results that are directly equivalent to a measured quantity (so that the model updating process is data-driven). The model will likely take in other measured quantities as boundary conditions or material properties.

The use of evolving data means that a key strength of the digital twin approach is that it provides an accurate description of systems that change over time. A validated model can provide a snapshot of the behaviour of a system at a specific moment but using that model within a digital twin can extend the use of that model to timescales over which the system and its behaviour will change significantly (Wright & Davidson, 2020).







For most high value engineering applications, the grand vision into which the digital twin fits is of a digitally enabled supply chain that can feed supplier data, in-house testing results, and on-line and off-line measurement results into a digital twin of products to obtain rapid performance predictions based on the latest data. For other applications, the real-time aspect is less critical (or real-time means hours not seconds), but the ability to evolve the model as reality changes and to make predictions with a high level of confidence that the model is accurate is still of benefit (Wright & Davidson, 2020).

Digital twins can also be of benefit to fundamental science. Scientific equipment can have characteristics that affect the experimental results. These characteristics may change over time and may be difficult to evaluate directly. A digital twin approach can ensure that the uncertainty associated with the results of the experiment can include justifiable contributions from these characteristics. Reliable interpretation of scientific results requires an understanding of the uncertainties associated with experimental results, and use of a digital twin can provide accurate estimates of, these uncertainties and identify methods of minimising them. In general, a model for a digital twin should be (Wright & Davidson, 2020):

- sufficiently physics-based that updating parameters within the model based on measurement data is a meaningful thing to do,
- sufficiently accurate that the updated parameter values will be useful for the application of interest, and
- sufficiently quick to run that decisions about the application can be made within the required timescale.

A further complication is that the existence of uncertainty means that validation (comparison with reality) needs to be treated as a statistical process. All measurements require associated uncertainties to be meaningful. This requirement implies that model inputs, and hence model outputs, and validation data all have associated uncertainties. So comparison of data with model results should generate an estimate of the probability that the values are consistent.

Uncertainty evaluation also gives a better understanding of how much trust can be placed in the model results. This trust is particularly important for models that include parameters that cannot be determined independently. These models are precisely the cases when the digital twin concept is so useful: it allows you to estimate what cannot be measure directly and thus improve the model.

The digital twin concept adopted in HiSea is materialised in a service chain starting by the acquisition and treatment of data from different sources including (but not limited to) meteo-oceanographic and water quality forecasts, earth observation data from Copernicus program, local data from available in situ sensor networks (wave buoys, current meters, salinity, water temperature, etc.) and local forecasts from available models.

In the following paragraphs, a more detailed description of the procedures adopted in HiSea to set up these digital twins will be provided.







## 2 Setting up a service

The implementation of a service chain implies to set up a chain of procedures that can pick up data and models results from different providers, applying the necessary methods to make it available in readable formats and then implement analysing tools and filters to transform it into useful information capable of fulfilling the requirements of different user needs.

Along this process, it is of prime importance to guarantee the observation of quality assurance procedures in each step to avoid the dissemination of erroneous or low quality information.

### 2.1 Methods

The first link of the chain is to identify the available data sources and implement the appropriate data retrieving services. According to the HiSea approach, the implementation of the data importing services is done through the development of specific plugins for each of the available data sources. By this way, in presence of a different data source the process of including it in HiSea platform only needs the writing of a new plugin.

In this first stage a set of data sources covering different data formats and spatial and temporal resolution scales was selected to demonstrate the effectiveness of the selected approach.

### 2.2 Analysis and Querying

The next link in the chain deals with the fundamental aspects of how to store the data and the procedures to adopt to assure the data quality. Once these procedures are defined, it is also necessary to implement a set of procedures to apply filters to the data to move from data to information. These procedures must take in consideration both the possible extractable information and, of course, the user needs.

The adopted methods to solve these issues were described more in detail in D4.1: HiSea backend architecture guidelines.

### 2.3 Exploitation & Dissemination

The final link in the chain is the ability to deliver information to real users. This step involves for one side the perspective of the developers (in a sense they can try to make a proposal of the kind of information may be obtained from the available data) and the perspective of users (in a sense they will need to receive information in formats and in recipients that are adequate to their activity).

The first aspect is highly related to the experience of the developers, while the second highly depends on the user's feedback. This feedback may be obtained through the Advisory Board meetings and direct contact with different potential users. Most of the times, being those new products and services, it is necessary to perform this task several times as the perception of the benefits in using the services improve with the availability of practical examples.





### 3 Building a Service Chain

HiSea Operational Services are provided following a Service Oriented Computing (SOC) approach. Such services rely upon the use of several information elements that correspond to the parameters of the associated environmental models. The required information elements may stem from numerous information sources available in the web or privately managed networks, e.g. weather forecasts provided by open sites or privately operated sensor data and historical information data sources (Athanasopoulos et al., 2010).

All these needs, which includes the capability to deal with large volumes of exchanged information, decentralized control of service compositions, integration of distinct types of service and information sources, call for novel approaches that can facilitate the provision of adaptable service chains. In this document, it is outlined an approach supporting the adaptation and distributed execution of environmental service chains based on information collected from several sources.

Recent developments in Web service technologies and the semantic Web have shown promise for automatic discovery, access, and use of Web services to quickly and efficiently solve particular application problems. =An example of the application area is in the geospatial discipline, where Web services can significantly reduce the data volume and the required computing resources at the end-user side.

A key challenge in promoting widespread use of Web services in the geospatial applications is to automate the construction of a chain or process flow that involves multiple services and highly diversified and distributed data. This work presents an approach for automating geospatial Web service composition by employing geospatial semantics in the service-oriented architecture (SOA).

One of the objectives of HiSea is to define a set of Service Chains (technical solutions) necessary to transform data and methods in the information that is useful for different users. A Service Chain is the technical implementation of a pre-defined methodology that defines the data workflow and processing steps necessary to provide, water quality and quantity information fitted to the end-user needs. In the framework of HiSea it is intended to use geospatial semantics to include in a platform capable of providing automatic discovery, access, and chaining of geospatial Web services.

The implementation of such a concept implies to breakdown in unitary blocks the technical procedures needed to go from data to processed information useful to HiSea end-users. Each service chain will follow the generic workflow presented below:

- A set of procedures that cover all key processes;
- Monitoring processes to ensure they are effective and keeping adequate records. This requirement is related with Log module of the HiSea platform;
- Checking output for defects, with appropriate and corrective action where necessary. This requirement is related to the validation methodology to be developed to ensure quality Service Cases.





For each of the Service Cases, technical requirements need to be defined. At first, information and products useful for the HiSea end-users need to be identified. Then, since added value products need to be generated, the characteristics of the final products to be delivered by the HiSea platforms need to be identified. Those characteristics include:

- Formats;
- Spatial and temporal resolution;
- Accuracy of the products (reanalysis and forecasts);
- Actualization frequency;
- Exploitation requirements. The end-user may want a static product (table or an image) or something we can explore dynamically (e.g. zoom, overlap layers) or even do simple queries (e.g. configure alerts).

Based on this, it is possible to better define the necessary technical steps to generate a specific service used in a Service Case (e.g. wave conditions windows that are inadequate to ship operations). To assure the effectiveness of each of the available products, it is necessary to implement quality validation procedures and take efficient corrective actions if a problem is detected. The product quality validation may be achieved by means of implementation of unitary technical procedures in the different steps of the production chain, such as

- Download a file from ftp or similar action;
- Convert a file to a new format
- Read and write from a database;
- Interpolate from a grid to another;
- Prepare the input files of a numerical model;
- Run a numerical model;
- Write files;
- End-user uploading data;
- Etc.

The resulting service chain platform will be able to deliver a set of relevant products and services which will bring added value such as:

- supplying forecasting services with enhanced functionality at reduced costs and allowing improved access to historical data
- the standardisation and wider (potentially global) availability of data archives
- the incorporation of data collection and analysis services into projects offering data services to third parties
- incorporating measured or modelled data into model compositions via web services, in real time, if required
- offering project data analyses results as websites.





## 4 The architecture behind the service

### 4.1 The HiSea Platform

HiSea's versatility and powerful capabilities enable us to run an operational system presently managing a wide spectrum of services for different clients (ports, water and energy utilities, aquacultures and environmental authorities).

The HiSea server component allows storage and indexing of internally generated data (models) or through external links (Scada systems, FTP, Open DAP, Motu Web Service, etc.). Apart from this distributor role, it also allows scheduling of tasks such as running models, create a report, issue alerts, etc. and to connect to different front-ends (UIS). It uses a database backend to store persistent data. Hibernate is used as an ORM to abstract away from database specific design. All server side codes are developed in .NET. Functionalities are exposed as services (SOAP or REST).

The used technologies require a Windows compatible backend but accommodate the possibility of using cloud infrastructure (e.g. DIAS). The back end database is SQL Server or Postgres SQL.

HiSea clients (desktop, web or mobile) allows connection with the platform's server, to interpret and manage data and processes. This application allows the creation of a local data cache, thus allowing some options assessment evaluation, based on offline scenarios; nevertheless, the platform's most interesting potentialities are intimately connected with the system's exploration for operational scenarios.

The HiSea Server is divided into 5 main modules:

- Data Storage and indexing
- Data Acquisition
- Model Execution
- Reporting
- Publishing

#### 4.1.1 Data Storage and indexing

HiSea server needs to store or index data produced either by the Data Acquisition components or by Model Executions. Two main types of data are stored:

- Time series: data in a single point for a single property along time. For example, data from a temperature sensor on a weather station
- Grid data: data on a structure or unstructured grid (1D, 2D or 3D) that varies in time. For example, data from radar images or model results.
- Images: Images can be generated from GridData internally by the platform or from external sources





Time Series will be stored in a database. Grid and images will store metadata in the database and file on disk. All data is only stored for a limited interval in time. Automated backups/purges will be implemented.

#### 4.1.2 Data Acquisition

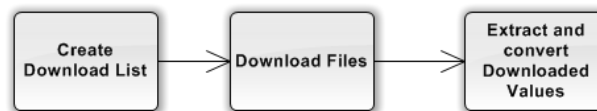
Data is available in multiple formats (egg: ascii, xls, etc. for Time Series or HDF5, NETCDF, GRIB for Grid Data). Multiple protocols can serve data, egg: FTP, http, OPEN DAP, Sensor Observation Service (SOS). Some types of data should be downloaded by the platform, while others should only be indexed.

The data acquisition module is responsible for:

- Downloading or rebuilding indexes to known data sources
- Transform between known formats and the HiSea platform uses for storage
- Indexing the new information in the HiSea platform data store

All these processes should occur in pre-defined intervals or on-demand.

Each data acquisition cycle is encapsulated in a “DataDownload Job”. This job is described by the following business diagram:



*Figure 1: Download job workflow*

Hereafter, an example of the data acquisition needed for the hydrodynamic model is provided. The modelling tool employed is the Delft3D-FM (DFM) modelling suite. DFM is a multi-dimensional i.e.; 1D, 2D and 3D hydrodynamic and transport simulation program. It calculates the unsteady flow and transport phenomenon that is resulted from tidal and meteorological forcing on unstructured, boundary fitted grids. DFM solves the Navier Stokes equation for an incompressible fluid. There are two computational schemes for heat transport in the model, namely complete heat flux model and excess temperature model. For the better representation of physical processes and for the accuracy the complete heat flux model was chosen. This scheme considers the effects of solar and atmospheric radiations, wind speed to calculate losses in heat due to back radiation, evaporation, and convection. For this scheme to be implemented, the model needs to be provided with atmospheric forcing data such as wind speed, solar radiation influx, air temperature, dew point temperature, and cloud cover. Those data are retrieved by means of the Climate Data Store Application Program Interface (CDSAPI), a service providing programmatic access to CDS data. A request example is shown in Figure 2 .

```
#!/usr/bin/env python
import cdsapi
c = cdsapi.Client()
c.retrieve("reanalysis-era5-pressure-levels",
    {
        "variable": "temperature",
        "pressure_level": "1000",
        "product_type": "reanalysis",
        "year": "2008",
        "month": "01",
        "day": "01",
        "time": "12:00",
        "format": "grib"
    }
)
```

Figure 2: Data acquisition: ERA5 request example. Image from: <https://cds.climate.copernicus.eu/api-how-to>

Because the number and format of files are unknown the “Create Download List” and “Extract and convert downloaded values” will be abstracted by three interfaces `IDownloadEnumerator` and `ITimeSeriesConverter` and `IGridFilesConverter`. Each unique download source can use any combination of these interfaces to create a successful download.



Figure 3: Downloader components

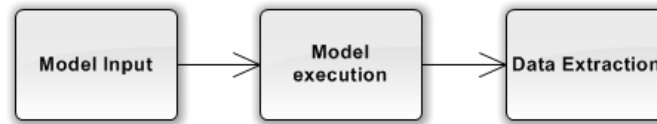
### 4.1.3 Model Execution

AQUASAFE, DELFT-FEWS platform can execute mathematical models on user demand or pre-defined intervals. The work cycle for a model execution is assumed as:

- Data Preparation or input
  - Boundary conditions
  - Initial conditions
- Model Executions



- Data extraction



*Figure 4: Model execution workflow*

The data preparation step will create the necessary boundary and initial condition files. Boundary conditions will force the model execution throughout the model run. Initial conditions set the start values for model properties and can be obtained from different data acquired by different sources, as described in the previous section. Those data are processed to be compatible with the model requirements (spatial interpolation of data, format transformation, etc.). As an example, ERA5 retrieved data are gridded and stored as NETCDF (Figure 5).

```
'grid': [1.0, 1.0], # latitude/longitude grid:
#east-west (longitude) and north-south resolution (latitude).
#default: 0.25 x 0.25 - option not available through the
#Climate Data Store (CDS) web interface
'format': 'netcdf'
},
'era5_u10_%s.nc'%(year))
```

*Figure 5: Extract and convert files to formats used by the model and the HiSea platform.*

Sometimes initial conditions are obtained from the results of previous executions. This will be referred to as “Hotstart”, in opposed do “Coldstart”, when initial conditions are set from other sources or default values.

This work cycle is controlled by a “Model Job”. The exact implementation of each of the steps in the work cycle is abstracted by two interfaces:

- IModelHandler interface:
  - Create input files compatible with the respective model from the formats know by the AMOS Server
  - Create files compatible with AMOS server from model result files
  - Change model input files (eg: model start date and end date, Hotstart, etc...)
- IModelEngine interface:
  - Execute the model (batch files, windows processes, etc)
  - Check if model execution was successful or not
  - Manage model Log Errors.

Each model implemented in the platform must implement these two interfaces. This allows the platform to be expanded to other models any time required.





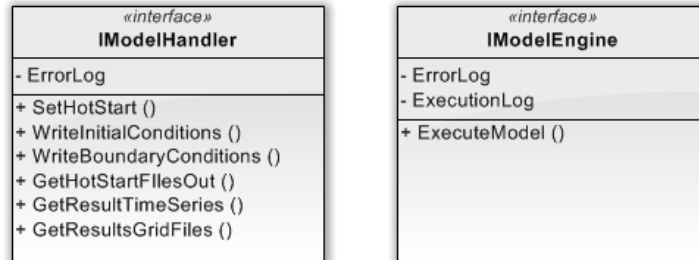


Figure 6: Model job interfaces

#### 4.1.4 Reporting

Reports created by the platform can contain Time Series and images. Images can be created from grid files or Time Series indexed in the database, creating charts or maps. Reports can also contain raw Time Series values in the form of tables. An example is shown in the figure below.

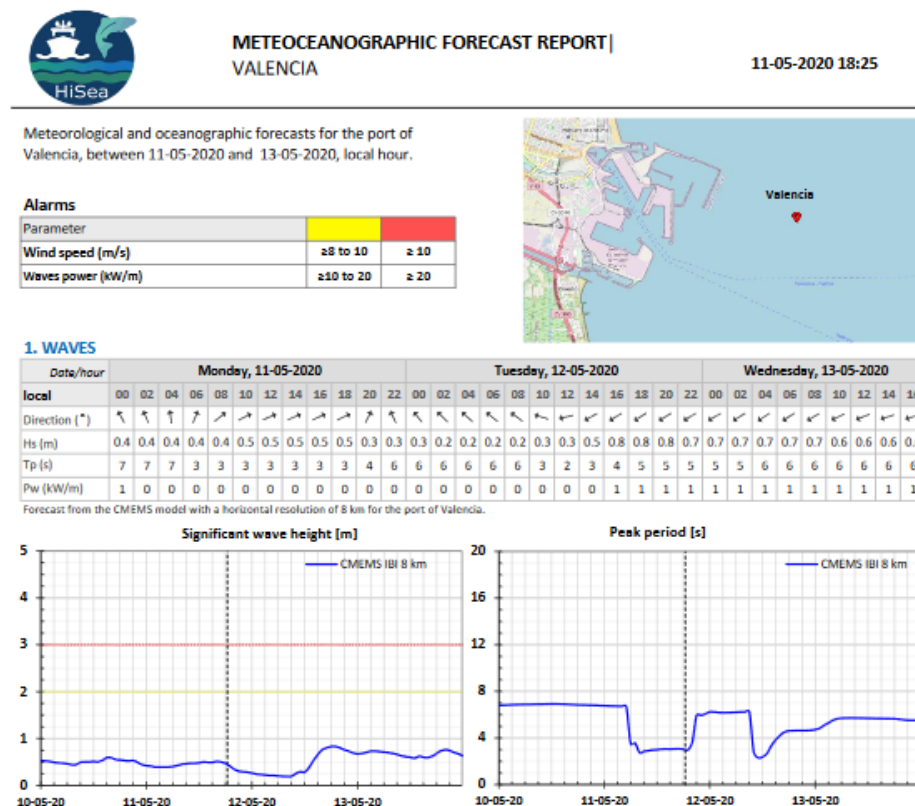


Figure 7: An example of the automatically generated HiSea report





Reports can be created in office compatible formats (Open XML), pdf, xml or simple ASCII. Other formats can be incorporated in the future since the design general base structure is flexibly based on interfaces. A report is described by a report class:

Report
+ Name : Uml.String + Description : Uml.String + TimeSeries : vector<ReportTimeSeries> + Images : vector<ReportImages> + Template : MetaFile + ReportCreatorAssembly : AssemblyDescription

*Figure 8: Report class*

The report class contains the assembly that will use to create the report (“ReportCreatorAssembly”, the platform can expand in the future to different report formats). “ReportTimeSeries” and “ReportImages” are classes containing the elements that can be placed in the report. Each contains a “ReportMarker” identifier so the report creator can correctly position it.

The class also contains a template file that is used by the report creator assembly. Report creation is triggered either by a Publishing job, Model Job or on user demand.

#### 4.1.5 Publishing

Publishing is used to disseminate reports or alerts to a list of users. Publishing can occur by:

- E-mail
- SMS
- Http
- FTP
- Local file share





Publishing is represented by the Publication class:

Publication
+ Description : Uml.String + PublisherAssembly : AssemblyDescription + PublisherConfiguration : Uml.String + ReportList : vector<Report> + DistributionList : vector<Distribution>

*Figure 9: Publication class*

The publisher assembly is responsible for the dissemination protocol (sms, email, et). Configuration for each protocol is serialized in xml in the “PublisherConfiguration” property. The “DistributionList” property groups the target users and “ReportList” the reports to disseminate.

#### 4.1.6 Services building

Provided services are supported by a complex data flow that includes downloads of external data, executions of internal models and distribution reports (forecasts, alerts, execution logs, etc.). The management of information is made via different roles:

- **Datacenter:** the system main data base responsible for getting data from external and internal sources, transform it and make it available for the production and distribution systems;
- **Production:** the part of the system that manages the models runs. These runs may be executed in different external machines including supercomputers;
- **Distribution:** the part of the system that manages the delivery of services to users.

Service Cases are built using joining a set of Chains that, in turn, assembly some individual Building Blocks that corresponds to the elementary pieces of the chain of value.



## 5 Required operational infrastructure

An operational system requires a proper infrastructure capable of assuring reliable service. This service has three main components that include critical issues which must be observed:

- Storage
- Communications
- Computational power

### 5.1 Storage

Data storage capacity represents one of the biggest challenges of our days. The capability of producing data in growing amounts is leading to a situation in which every day, hundreds of Gigabytes are being produced. No matter how fast the storage capacity is increasing (and the price per Gigabyte is decreasing) there will always be needed for more storage space. In the end, the central question is how to properly manage the storage requirements and keep well balanced options between the real needs and the wish to store all the produced data (will I need this data in the future?).

Until now, HiSea is storing one solution per day of each of the models that are running in order to keep a historical record that may be later used for local meteo-oceanographic characterization. This already represents a large number of Terabytes of stored data that is kept in external disks.

The most obvious solution in the future is to move all this storage to the cloud but, for the moment, this solution is not yet competitive.

### 5.2 Communications

Communications represent another challenge for keeping the service running. The operational chain implies daily downloads and uploads of several gigabytes of data, and this means access to large bandwidth connections.

The solution for this requirement was to acquire data warehousing services, located in France and Germany (OVH and Hetzner), which provide machines with that type of internet connections at reasonable prices.

Also here, future lies on deploying all services on a cloud provider such as Azure but the costs, although converging, are still high. Maybe in 2-3 years, the situation is different.

### 5.3 Computation

The maintenance of a service based on running a good number of models daily requires the availability of proper computational power. As with communications, the present solution lies in several machines rented to the above referred providers. Presently a top level machine including last generation Xeon processors including 12 to 24 threads with 12 to 24 Gb of Ram may cost around 150 Euros/month (including already the large bandwidth communications).





Another option that is being actively tested is to use available resources in supercomputers which are also available for reasonable prices. HIDROMOD has been running tests in a Galician supercomputer, and it is likely that the high performance computing offer will increase a lot in the near future with the corresponding dropping in costs.





## 6 Fulfilling the Service needs

### 6.1 The hydrodynamic products

A local high resolution hydrodynamic model (powered by MOHID, DELFT3D, or equivalent) provides through its operational forecast system, a 7 days hydrodynamic forecast (+ 1 day hindcast) including the scales that characterize regional marine processes (e.g., tidal forcing, low frequency ocean dynamics, atmospheric forcing etc.). The forecasting system is based on a downscaling methodology based on the high resolution simulations or those provided by CMEMS. The available products are the result of these modelling results and data collected from current meters, tidal gauges, Argos buoys, Satellite Sea Surface Temperature (SST) images, Satellite Sea Level Anomalies (SLA) data. They consist essentially of the most common hydrodynamic parameters (water levels, currents, water temperature, salinity). Figure 10 depicts the Delft3D FM model results over the entire spatial domain used for simulation. The figure depicts seawater temperature for March and August as a representative month for winter and summer respectively.

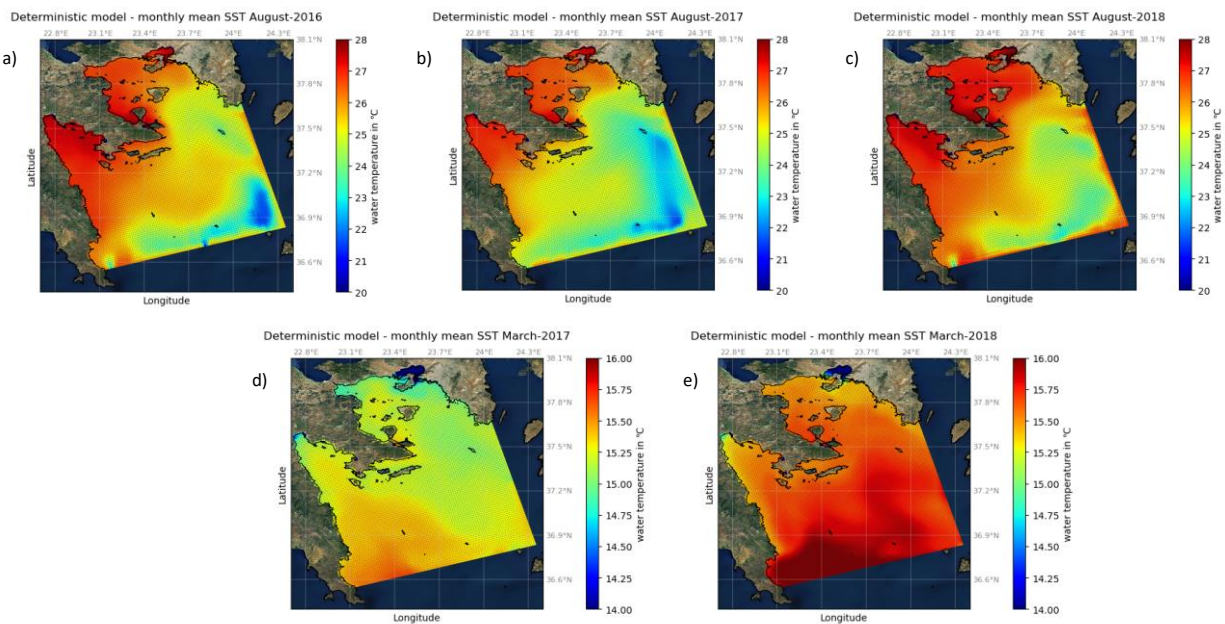


Figure 10: Deterministic model – monthly mean SWT a) August 2016 b) August 2017 c) August 2018 d) March 2017 and e) March 2018

### 6.2 The wave products

The operational wave modelling system provides a 7 days forecast for Portugal mainland, Azores and Madeira regions. The available products results from the simulations made with WWIII and SWAN models and data collected from wave buoys, ADCP's, satellite and radar. The map information consists essentially of the most common wave parameters





(significant wave height, maximum wave height, mean and peak period, wave power, wave direction, wave spectrum), it allows a good spatial visualization of the incoming waves and also a first assessment of the areas in danger.

### 6.3 The meteorological products

The operational meteorological system provides 7 days forecast for Portugal mainland, Azores and Madeira regions. The available products results, for the moment, from forecasts provided by external providers such as NOAA (GFS), Meteogalicia and Aveiro University (WRF) and data collected from meteorological stations, radar and satellite resumed in the form of maps and time series of the most common meteorological parameters (wind, temperature, visibility, humidity, pressure, etc...).

### 6.4 The water quality products

A local high resolution hydrodynamic model (powered by MOHID, DELFT3D, or equivalent) provides through its operational forecast system, a 7 days water quality forecast (+ 1 day hindcast). Model outcomes include, among others, the concentration of oxygen, chlorophyll-a, nitrate and phosphate. The forecasting system is based on ensemble prediction, therefore mean and other statistical parameters are also provided to characterize the forecast. Forecast are provided both as map and timeseries, as shown in Figure 11.

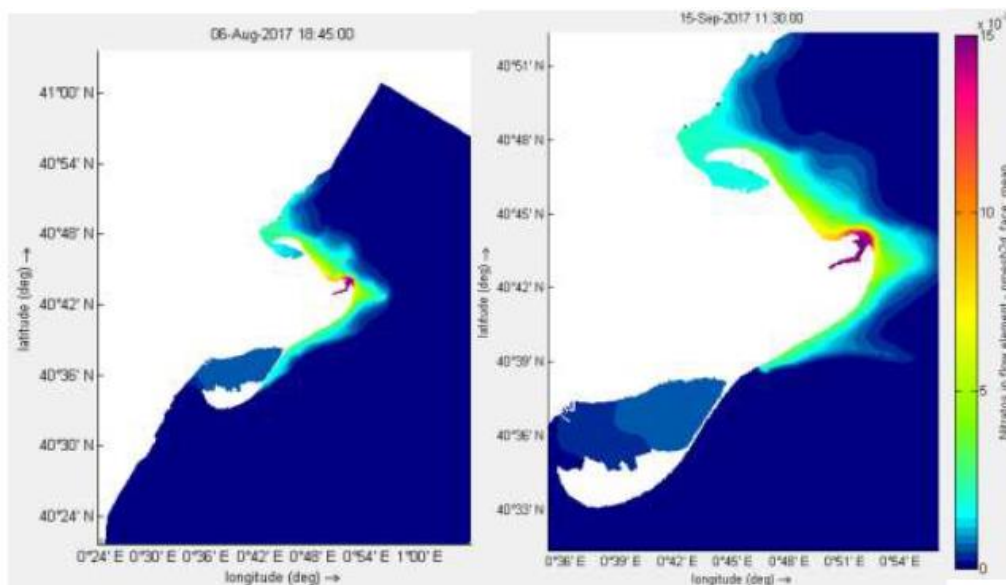


Figure 11: Nitrate dispersion from the Ebro river on 06 August and 15 September, 2017.





## 6.5 The large scale / regional services

The models available in the forecast system implemented throughout HiSea for the large-scale and regional/coastal scale. The large scale/regional models rely on the data provided by external providers such as the Global Forecast System (GFS) for the meteorological forcing and by CMEMS for the low frequency ocean dynamics. The tide forcing is using the global solution of FES 204. A schematic view representing the data flows associated to these global/regional processes is presented in Figure 12. These regional models are the used to feed the local high resolution models with necessary initial and boundary conditions.

## 6.6 The local services

High resolution forecasting services are implemented throughout HiSea for local areas providing spatial resolutions of the order of tens of meters. These services are based on different models for hydrodynamics, water quality and waves.

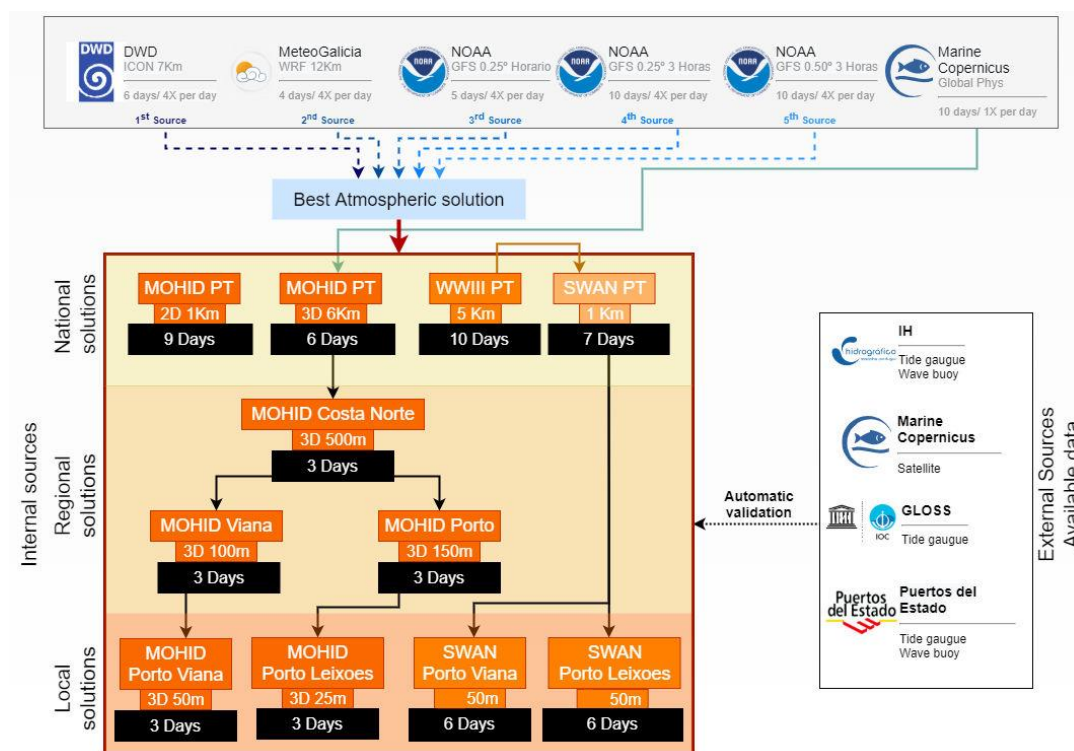


Figure 12: Example of the service chain supporting Leixões and Viana do Castelo harbours operational service

## 6.7 Products format

For the required areas the service can provide two main categories of products (see Figure 13):



- Maps for the entire area;
- Time series for a local station.

Maps products correspond to an average of the entire area, and time series corresponds to temporal variability for a specific monitoring station. Both could include a tabulation of the measured parameter (real-time acquisition) or predicted variables (forecasts provided by models).

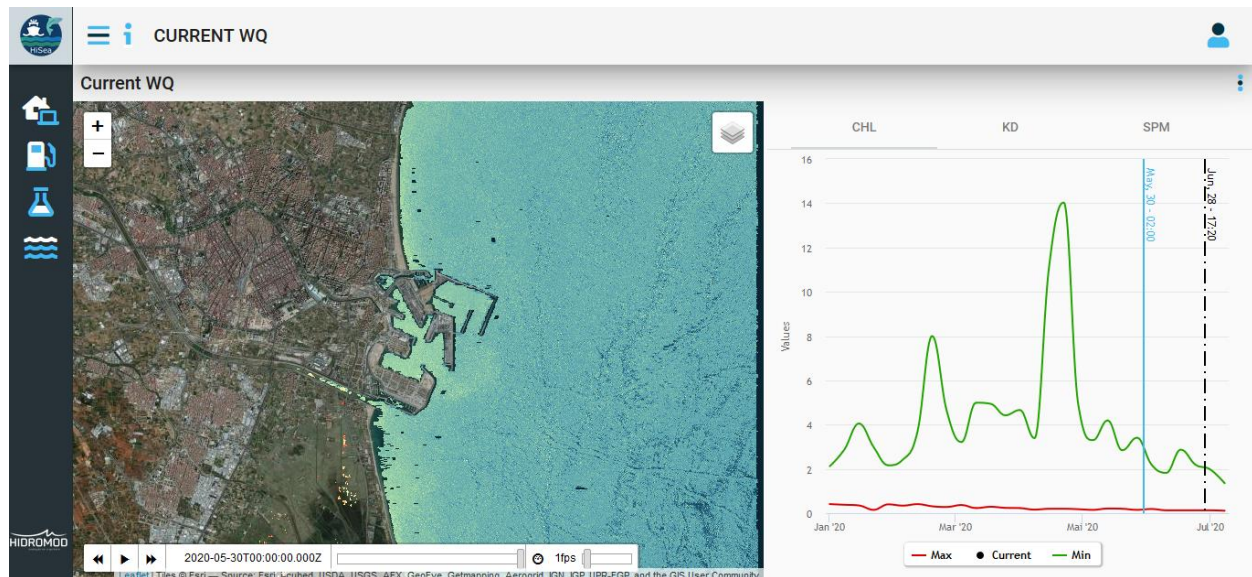


Figure 13: Chlorophyll-a concentration delivered both as a map for the entire area (left) and time series for a given location (right).



## 7 References

Wright L. & Davidson S., 2020, *How to tell the difference between a model and a digital twin*. Adv. Model. and Simul. in Eng. Sci. 7, 13 (2020). <https://doi.org/10.1186/s40323-020-00147-4>

