An Introduction to Operational Chains in Ocean Forecasting

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Abstract. Operating the ocean value chain requires implementation of steps that must work systematically and automatically to generate ocean predictions and delivers ocean data information in standard format. This task, that represent the backbone of operational forecasting systems, implies the design of robust workflows, that organize pre-processing of the upstream data, run of the core models and post-processing before the final delivery. Operational chains require dedicated computational resources to supply demanding modelling runs but also processing and analysis of big volume of data, in relation to the specific spatial scale and consistently for the forecast lead times. The monitoring of each step of the workflow through key performance metrics can support not only the timely delivery but also identifying problems and troubleshooting. The paper illustrates the main challenges foreseen by operational chains in integrating complex numerical frameworks from global to coastal scale and discusses on existing tools that facilitate orchestration of operational chain components, including examples of existing systems and their consolidated capacity in providing high quality and timely ocean forecasts.

1 Introduction

Operational ocean forecasting systems integrate advanced numerical modelling, aimed at resolving ocean dynamics and processes from global to coastal scale, and robust computational suites that are devoted to run models, orchestrating different data pre- and post-processing blocks, with the ultimate goal of providing high quality and reliable ocean forecasts to enhance decision-making, monitoring and planning for a sustainable use of ocean resources. In the last years, the number of ocean observations – from remote sensing (Gould et al., 2013) and in-situ (Le Traon et al., 2015) platforms – available for operational oceanography has increased in number, quality and timeliness, making possible to improve ocean models, to validate numerical ocean products and to support monitoring activities (Tonani et al., 2015; Davidson et al., 2019). Data-assimilation techniques, aimed at blending the observations into the model, have been evolved numerically to provide the most accurate description of the past and the best initial conditions for the forecast. As computing power has increased, numerical solvers have evolved towards high-resolution models that can capture small-scale features enabling global, regional and coastal simulations and predictions at higher resolution and over longer time spans. The numerical information

produced is then processed to make it usable by operational applications and services. Some recent ocean modelling examples in support of operational ocean and coastal services are compiled in Section 4.2. Therefore, as shown in Chapter 4

35   of Alvarez-Fanjul et al. (2022), the architecture of an operational ocean forecasting system includes pre-processing of ocean observations, quality control assessments, objective analysis, data assimilation, initial field generation, numerical forecasting, data post-processing, together with the generation and dissemination of products. All these steps have influenced the evolution of forecasting systems from a technological point of view, facing the need to harmoniously interconnect complex steps towards the final delivery to users. This chapter will give an overview of the technical characteristics of processing

40   suites that guarantee reliable operations and products provision.

2 Technical characteristics of an operational chain for ocean forecasting

The objective of an operational chain is to systematically and automatically perform a series of complex numerical steps to ensure the generation of ocean predictions and the delivery of related products to end-users. The main phases of its workflow are: pre-processing, modelling component(s) run, and post-processing. Figure 1 shows, as an example, the overall workflow

45   of the chain implemented for the Global Ocean Forecasting System operated by NMEFC (China). Here, the main steps, as designed for the specific operational system, include data pre-processing, data assimilation, numerical simulation, and production for final delivery.

Pre-processing consists of accessing and preparing upstream data (i.e., observations, atmospheric forcings, other model outputs to be used as boundary conditions, etc.) to be ingested by the modelling component. In the case of ocean

50   observations, it is responsible for the collection, transmission, analysis, and quality control. The time consumption of data assimilation depends on the amount of data used and on its complexity. Ocean models also need atmospheric forcing fields. Indeed, the performance of ocean operational forecasting systems is very sensitive to the type of atmospheric forcing used (Li et al., 2021), and different atmospheric forecasting fields are needed to be collected and interpolated into the ocean model grid to compute wind stress, surface heat fluxes or surface water exchanges. The timeliness for the preparation of the

55   atmospheric forcing, usually part of the first step of an operational suite, depends firstly on the (scheduled) atmospheric model forecast availability and secondly on the computational efficiency, and the time spent in having the atmospheric forcing data ready to be used by the ocean model.

Other forcing data sources, such as freshwater inputs from river discharges, are progressively being included in ocean forecast models. In regional, rather than global, ocean models, this pre-processing block must include the preparation of the

60   necessary data (usually from a global or basin model) that will be imposed as boundary conditions along the open boundaries of the limited domain.

Incorporating observations (both from satellites and in situ platforms) into an ocean model via data assimilation is crucial for operational forecasting (and reanalysis) systems to obtain accurate estimates of the ocean state (Tonani et al., 2015) and initial condition for the forecast. Complex methodologies are developed and implemented in ocean forecasting chain that are

65   strongly link to the ocean model used, to the model resolution and to the observation assimilated using different class of data
      assimilation (cimmings et al, 2009)

      Running of the ocean model is the most complex and demanding part of the operational chain. Numerical models include
      physical parameterization and solvers for the numerical integration of the Navier-Stokes equations. This complexity can be
      computationally demanding, so by employing parallel computing, we can distribute this workload across multiple cores. This

70   allows us to run high-resolution ocean models faster. Hence, the use of multiple cores and parallelization is crucial in state-
      of-the-art ocean modelling.

      Once the model run is complete, the resulting data must be post-processed by interpolating the numerical outputs (if needed)
      onto specific regular spatial grids and by applying procedures aimed at transforming the raw model data into a standardized
      format (e.g., CF compliant[1]). Such post-processing can be executed afterwards as an independent process or in parallel while

75   the model is running.

      Finally, the ocean forecast products are released directly to users through different specific dissemination mechanisms
      (among others, FTP, THREDDS, web services and API, cloud-based solutions, etc.).

      From a computational point of view, the execution of an operational chain can require significant computing resources,
      including the use of a number of cores to produce the numerical solution that can be released in accordance with the correct

80   forecast lead time: they can therefore be executed in dedicated clusters, benefitting from heterogeneous computing
      capabilities, by using CPU or GPU resources.
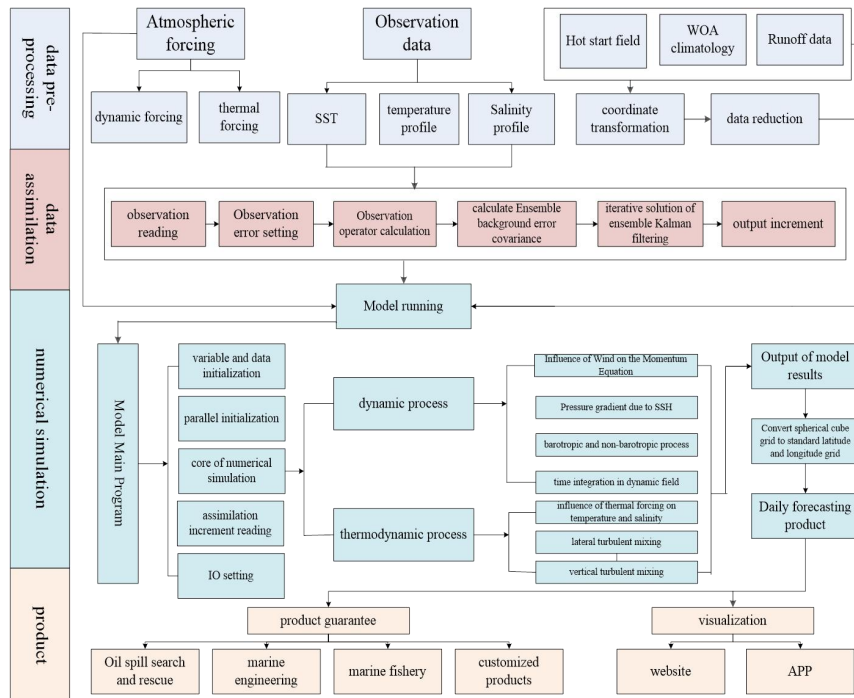
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[1] https://cfconventions.org

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Figure 1: Operational chain of Ocean Forecasting System (example of global system in NMEFC, China).

The operational chain is then required to orchestrate a complex sequence of tasks in flexible and efficient way, allowing

85   lifecycle monitoring and troubleshooting. When designing an operational chain, it is important to decide which programming language is most appropriate for coding each task belonging to each of the main steps: this choice depends on the characteristics of the numerical procedure to be adopted for solving a specific task. For example, for acquisition of upstream data from various external databases or datastore, the forecaster can adopt:

- Bash/Shell scripting that offers functions like wget or curl for accessing files made available by a provider, and cron
90   for scheduling its execution.
- Python codes for accessing data through web APIs (for example, like the Copernicus Marine Toolbox that is a Python-based tool for accessing the Copernicus Marine Data Store) and performing some initial basic manipulation (i.e., subsetting in space and time, interpolation to target grid, etc.).

The ocean model couple to data assimilation scheme is technically much more complex to run and there are also some

95   compilation and performance requirements to be met. The operational chain is then instructed to launch a task that submits each model run to be executed directly on the dedicated core(s) or to a job scheduler that verify resources availability. In addition, the ocean model itself is usually coded in a pre-defined programming language (such as Fortran or C/C++, or others) and can be executed in parallel mode using MPI/OpenMP,or GPU-based parallel paradigms (i.e., CUDA, OpenCL, OpenACC, etc.).

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100   Data post-processing, product generation, and product delivery can usually be done in parallel during the model run time, as independent tasks from the overall workflow: again, it can adopt procedures coded in Bash/Shell, Python, or Julia or other interpreted languages that can guarantee flexibility, simplicity and preliminary data analysis tasks.

The operational chain workflow engine can be ad-hoc coded to organize sequentially the tasks to be executed. A basic approach can be determined by the implementation of a software package that includes:

105   • A main script, designed to collect the specific tasks and subtasks as requested by the operational chain.

• A list of scripts, each representing the task to execute.

• One or more specific scripts that are supposed to track the status of the operational chain execution by creating logs to further support monitoring.

The evolution of this approach towards systematic monitoring of the overall lifecycle and automatic detection of issues is
110   represented by the adoption of a workflow manager. It is a tool that assists the forecaster in orchestrating complex sequences of tasks, including detection of anomalies during the execution and supporting the seamless processing of information. Workflow manager adopted by the Earth Science community include:

• ECFLOW[2], developed by ECMWF.

• Cylc[3].

115   Others, extensively used by industry but progressively chosen also by forecasting centers, are:

• Apache Airflow[4].

• Prefect[5].

3 Key Performance Metrics

To ensure that an operational ocean forecasting system delivers accurate and timely products, it is necessary to identify
120   metrics that can be implemented for measuring performances and that can support the resolution of potential anomalies and issues.

Based on the analysis performed in Ciliberti et al. (2023), the main properties of an operational forecasting system that can be used to monitor its performance are:

• Quality: it certifies that the delivered product/service consistently performs well and provides useful results. This
125   can be measured by providing relevant metrics aimed at measuring the degree to which the forecast product matches the observation (through validation exercises).

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[2] https://confluence.ecmwf.int/display/ECFLOW
[3] https://cylc.github.io/
[4] https://airflow.apache.org
[5] https://www.prefect.io/

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- Reliability: it refers to whether the user can rely on the forecast product to make decisions. As shown by the World Climate Service[6], it is a measure of the quality of a probability forecast that varies between 0% (i.e. the a posteriori observation is never in the forecast range) to 100% (i.e. the a posteriori observation is always in the forecast range).

130 - Timeliness: it is a measure of the time between the expectation that the information will be available and the time when it is actually available for use. To save time, it is usual to execute in parallel two or three parts of the operational chain. However, not all parts can run in parallel. Pre-processing and data assimilation should be finished before the ocean model starts running. In contrast, post-processing, product generation, and release can be done in parallel with model running. Timeliness management depends on characteristics of different cases or different user

135 needs. With coupled and ensemble models development, it is difficult to have a strict time control.

- Accessibility: it refers to the capacity for a user to get access to forecast product, including authentication and authorization (if needed).

- Usability: the adoption of standards for data and metadata ensures the product can be used well and is self-describing. Data with a defined file format, adequate documentation and high quality can be used and reused. This

140 metric can be measured through users' surveys.

To save time, it is usual to execute in parallel two or three parts of the operational chain. However, not all parts can run in parallel. Pre-processing and analysis based data assimilation should be finished before the ocean model starts running to produce the forecast. In contrast, post-processing, product production, and release is usually done in parallel with model running.

145 Timeliness management depends on characteristics of different cases or different user needs. With coupled and ensemble models development, it is difficult to have a strict time control (Liu et al., 2018).

The adoption of a workflow engine facilitates the monitoring phase of the operational chain lifecycle. Figure 2 illustrates an example of how an operational forecasting service needs to monitor all the components of a specific operational suite to generate the proper KPIs (Key Performance Indicators) that later should be managed by the service to ensure a timely service.

150 The example shows how all the elements previously discussed, such as pre-processing, model execution, post-processing of raw model outputs, together with some time dedicated to the data push to catalogues and later storage, are included in this operational monitoring performed by the Copernicus Marine Iberia-Biscay-Irish Monitoring and Forecasting Center (IBI-MFC) for its operational suites. This control of the different components is recommended and helps operators to identify issues in the operational suites and in the environment that could potentially lead to incidents. Likewise, this monitoring by

155 component helps to manage the delays in the service related to different types of incidents. The operational KPIs on service timeliness that usually are used to verify that the service is meeting the timeliness requirements stated in its proposed Service Level Agreement (SLA), are computed using the time statistics daily provided by these time control monitoring processes.

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[6] https://www.worldclimateservice.com/2020/07/06/what-is-forecast-reliability/

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This monitoring is also important to identify and manage temporary incidents or continuous problems that may result in service delays or product outages.
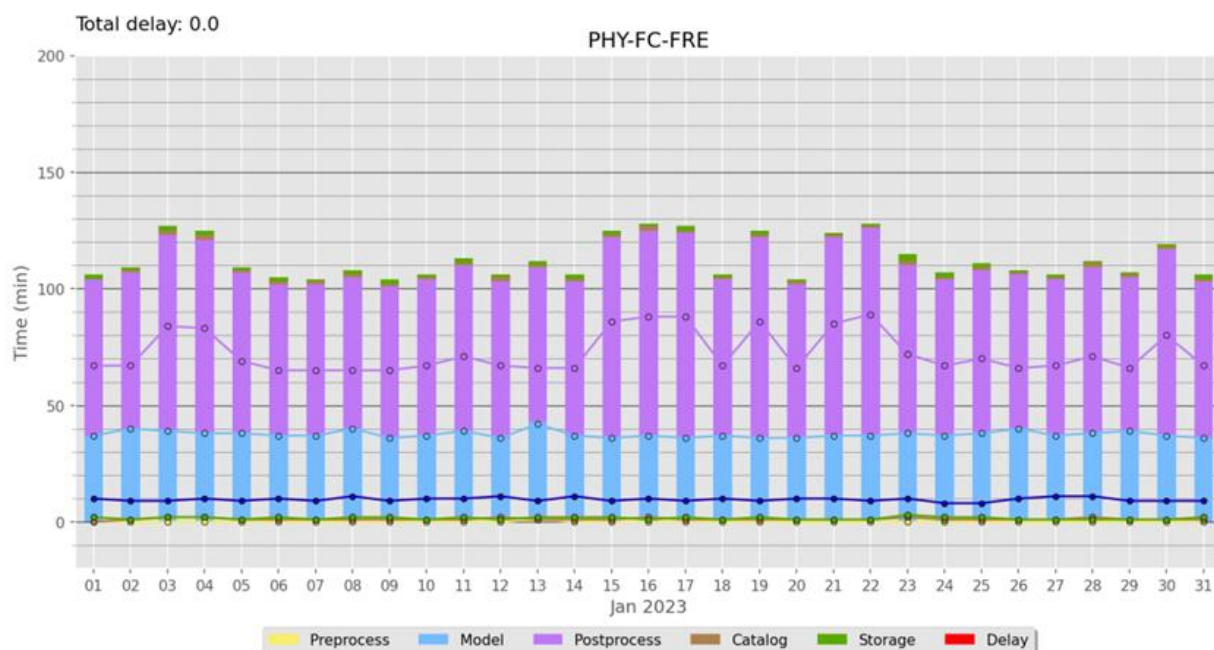
Figure 2: Example from the Copernicus Marine IBI-MFC Service Monitoring. Monthly summary statistics (for January 2023) from the time control monitoring performed for the IBI physical forecast operational suite. Monitoring of all the operational suite components (i.e. input data preprocessing, model execution, post processing of raw model outputs, and processes to push products into the catalogues and later storage) is included.

4 Other operational chain relevant aspects

It is important to outline and summarize some general characteristics a user needs to consider in the setup of numerical ocean models for ocean forecasting:

- Infrastructure aspects.
  - o It is highly desirable that a model performs well on most of the most powerful HPCs available. In practice, this requires that the code is parallelised (using domain decomposition with MPI and/or OpenMP), is not excessively memory bound (particularly on CPU machines), and supports the low-level parallel processing required by GPUs. This requires analysis of the scalability and portability of the code as well as the restartability and reproducibility of the numerical ocean model solution.
  - o Workflow tools can support proper monitoring of the computing process lifecycle and facilitate troubleshooting as well as scalability of the operational configuration.

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- o the network is an essential element in the infrastructure of an operational chain, it must allow an effective link between the distribution centres upstream and downstream of the production centres.
  - o Storage must be linked to the HPC centre to ensure effective back-up of production and enable production to be restarted if necessary.

180 - Interfaces. In order to properly address the spatio-temporal scale of the ocean process to reproduce, it is needed to:
  - o Select a proper state-of-the-art option for subgrid scale parameterization: if the option is incompatible, the model should be able to generate an error message and stop.
  - o Use state-of-the-art bathymetries for the setup of new configurations. The user should also be able to use and specify smoothing techniques that can be applied to avoid model instabilities, whereas taking into
185   account the topographical peculiarities that can play a fundamental role especially in coastal models.
  - o Specify time-varying river inflows (i.e., discharges, nutrients) as inputs, generated from climatologies or from real-time data (e.g., from observations).
  - o Specify surface fluxes of momentum, heat, and freshwater and ancillary data such as surface temperatures and surface wave fields.
190 - o Couple the model to models of other physical systems (e.g., atmospheric, sea-ice or wave models) through one or more of the standard coupling systems (e.g., OASIS, US system, etc.); in some cases (like with waves and sea-ice) alternative or ad-hoc coupling approaches should be provided.
  - o Run biogeochemical (BGC) models as part of the overall integration (on-line coupling) or generate data to run the BGC model in off-line mode.
195 - o Interface the ocean model with data assimilation systems.
  - o Generate re-start and diagnostic files in a flexible manner.
- Design and documentation. To meet quality assurance requirements, it is highly desirable that the model:
  - o Has a clear design.
  - o Has a well-chosen modularity.
200 - o Is easily readable.
  - o Is written in a familiar language (such as Fortran90 or Python).
  - o Has a users' guide and a developers' guide.
  - o Can be further developed without excessive effort.
- Sustained support. The model needs to be sustainably supported by a lead agency, a consortium of agencies, a
205 committed user community or a combination of the above. This support should aim to ensure that:
  - o The model's formulation is improved as the state of the art evolves.
  - o Novel improvements are documented in peer reviewed publications.
  - o The code documentation is openly available and kept up to date.

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- o The code is openly accessible or made available subject to "legal" agreement (which might include, e.g., a commitment by a new user to contribute to further developments and testing of source code).
- o New users are supported by instructions for setting up relatively simple configurations which can easily be compiled, run and outputs checked.
- o New releases of the code are properly version controlled.
- o The methods by which the code is verified are described in its documentation.

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- o The results from standard test cases are made publicly available (an aspiration at this stage).

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Competing interests

None

Data and/or code availability

The data and code are available from the websites which all mentioned in the paper, others from all the authors.

Authors contribution

All the co-authors shared the common authority and contribution.

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