



Improving Accuracy and providing Uncertainty Estimations: Ensemble Methodologies for Ocean Forecasting

Ibrahim Hoteit¹, Eric Chassignet², Mike Bell³

¹Physical Science and Engineering Division, King Abdullah University of Science and Technology (KAUST), Thuwal, Saudi Arabia

²Center for Ocean-Atmospheric Prediction Studies, Florida State University, United States

³MetOffice, Exeter, UK

Correspondence to: Ibrahim Hoteit (ibrahim.hoteit@kaust.edu.sa)

Abstract. Ensemble forecasting has emerged as an essential approach for addressing the uncertainties inherent in ocean prediction, offering a probabilistic framework that enhances accuracy of both short-term and long-range forecasts. By more effectively addressing the intrinsic chaotic nature of mesoscale and sub-mesoscale variability, ensemble methods offer critical insights into forecast errors and improve the reliability of predictions. This paper reviews the ensemble methodologies currently used in ocean forecasting, including techniques borrowed from weather prediction like virtual ensembles and Monte Carlo methods. It also explores the latest advancements in ensemble data assimilation, which have been successfully integrated into both ocean general circulation models and operational forecasting systems. These advancements enable more accurate representation of forecast uncertainties (error-of-the-day) by sampling perturbations conditioned on available observations. Despite the progress made, challenges remain in fully realizing the potential of ensemble forecasting, particularly in developing tools for analyzing results and incorporating them into decision-making processes. This paper highlights the crucial role of ensemble forecasting in improving ocean predictions and advocates for its wider adoption in operational systems.

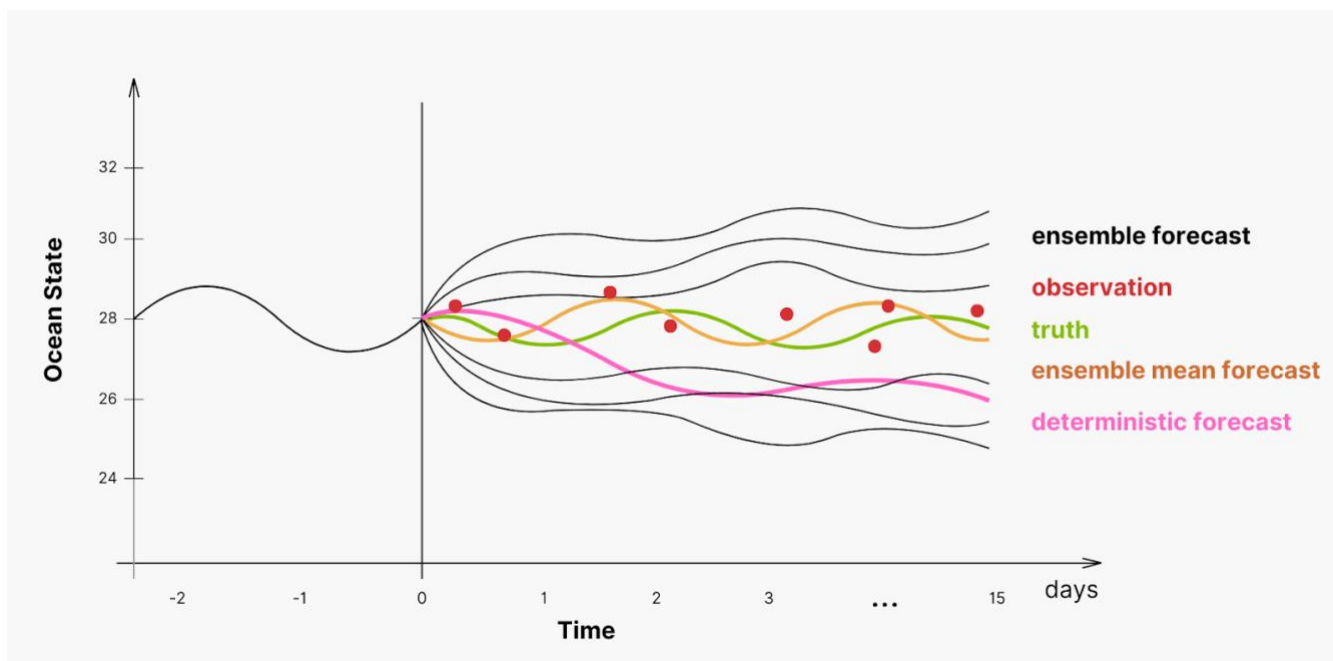
1 Introduction to Ensemble Forecasting

Forecasts of the ocean state generated by numerical models are inherently uncertain owing to the nonlinear chaotic nature and imperfect internal physics of the ocean models, and inevitable uncertainties in their inputs such as initial and boundary conditions, atmospheric forcing, bathymetry, etc. (e.g., Lorenz, 1996; Pinardi et al., 2008; Sandery et al., 2014; Vandenbulcke and Barth, 2015; Kwon et al., 2016; Sanikommu et al., 2020). Thus, the future ocean cannot be completely described by a single forecast model run, and is better described by a set, or ensemble, of forecasts that provides an indication of the range of possible future ocean states and that represents the uncertainty in the forecasts, also known as errors-of-the-day (Houtekamer and Zhang, 2016; Hoteit et al., 2018) (Figure 1).

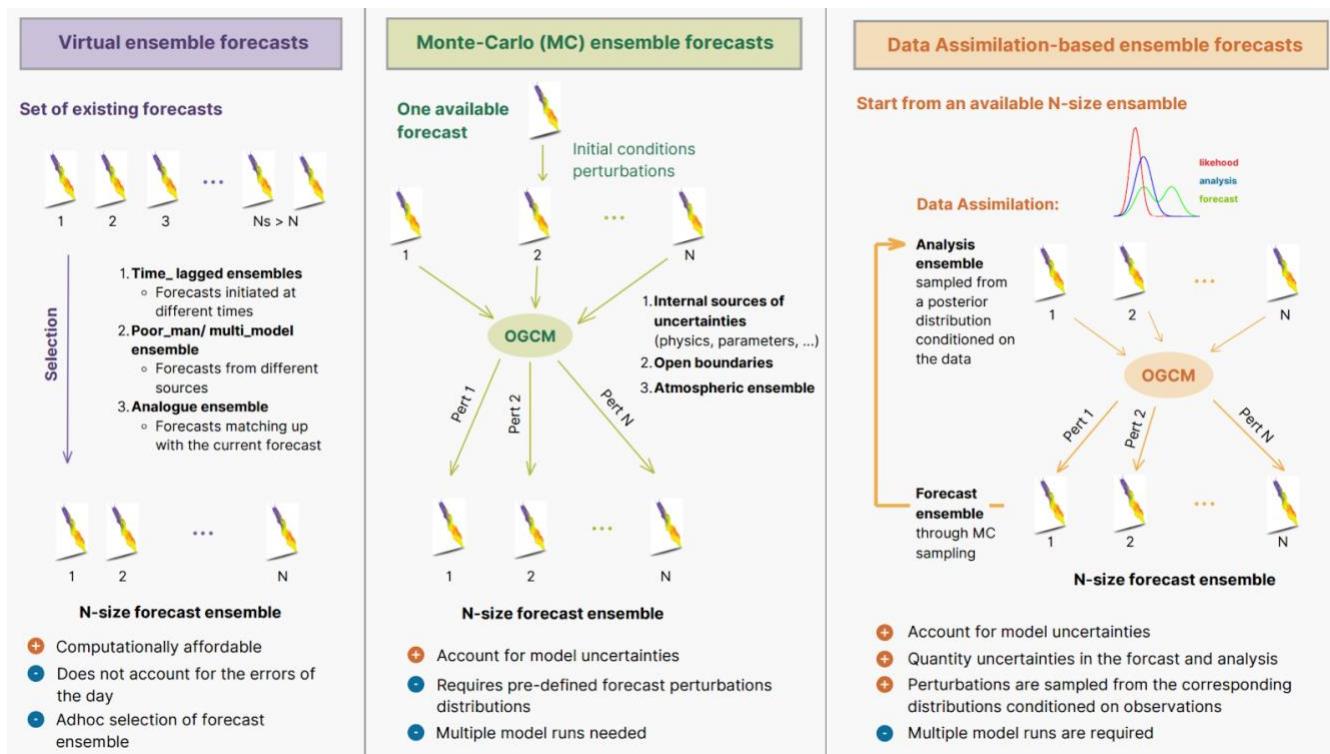
Ensemble forecasting has increasingly become a key aspect of weather and climate predictions – see Du et al. (2019) for a review – as it provides a basis to communicate forecasts confidence to end users for better decision. Similarly, it should become



an integral part of ocean forecasts. Ensemble forecasting was indeed proven to provide extended ocean prediction skills compared to deterministic forecasts, especially for extended time-scale predictions (Mullen and Buizza 2002; Ryan et al., 2015). This ensemble probabilistic framework is also needed for short-range forecasting to better describe the intrinsic chaotic nature of the mesoscale and sub-mesoscale variability resolved by the new generation high-resolution ocean models (Thoppil et al., 2021). Information about forecast uncertainty can be used in many ways. For instance, the probabilistic information that ensembles provide are particularly valuable for early warnings of hazardous conditions in the ocean and can be integrated into the decision-making process based on economic values (Richardson, 2000; Du and Deng, 2010). On short timescales, the probabilistic information is useful to trigger the deployment of environment protection measures in the event of an oil spill (Barker et al., 2020), to advise fishermen about the most probable regions of fishing zones, to help coast-guards on the probable areas to focus for search and rescue operations (Melsom et al., 2012), or to advise on path planning for autonomous marine vehicles (Yoo et al., 2021), etc. On climate time scales, ensemble forecasting is useful for providing probabilistic information on climate indices such as El Nino and the Indian Ocean Dipole (Schiller et al., 2020).



45 **Figure 1: Schematic illustration of deterministic hindcast (black line at the forecast date 0) and forecast (pink line after day 0), and ensemble forecasts (black lines after day 0) of the ocean state. The ensemble forecasts were driven by various sources of uncertainties (including initial conditions, atmospheric forcing, model physics, bathymetry, ...). The ensemble forecast mean and the unknown truth are respectively represented by the orange and green lines. Solid red dots denote SST observations.**



50 **Figure 2: Schematic diagram illustrating the steps involved in various ensemble forecasting methods. Characteristics of each method are also listed.**

1.1 Methods

Ensemble forecasts find their roots in weather forecasting and can be generated (i) as virtual ensembles whose members are selected from deterministic forecasts and/or historical runs, (Hoffman and Kalnay, 1983; Ebert, 2001; Du, 2004; Schwartz and Sobash, 2017), (ii) or by applying some form of Monte Carlo (MC) analysis in which a set of forecasts are produced by perturbing the model physics and/or inputs, as a way to account for their inherent uncertainties (Martin et al., 2015; Houtekamer and Zhang, 2016; Hoteit et al., 2018). Ensemble forecasts may also be generated following a multi-model approach as the forecasts of different ocean models, or from their combination with MC forecasts (Figure 4.5-2). Ideally, the actual future oceanic state should fall within the predicted ensemble range.

- 60 • Virtual ensemble forecasts. The lower-cost virtual ensembles can be used to quantitatively estimate forecast uncertainties based on existing forecasts through various techniques including for instance: (a) the time-lagged ensemble, which automatically creates a forecast ensemble by pulling multiple forecasts that have been initiated at different times, (b) the poor-man ensemble, which gathers single-model forecasts from different sources and is thus a multi-model ensemble from existing forecasts, and (c) the analogue ensemble, made of past forecasts matching up with the current forecast. These methods are straightforward but may result in restricted ensembles due to the limited



available sources of existing forecasts. They are also not designed to capture the flow-dependent error-of-the-day (Du et al., 2019).

- Monte Carlo (MC) ensemble forecasts. This kind can be generated by perturbing the ocean model physics and/or inputs (Du et al., 2019). Uncertainties in the ocean model could be accounted for by perturbing its internal sources of uncertainties which could come from the missing physics, parameterization schemes, and numerical errors. Different approaches were suggested such as (a) the multi-physics approach which uses a different parameterization scheme for each ensemble member, (b) the perturbed parameters approach of a selected parameterization scheme, and (c) the stochastic parameterizations approach which injects stochastic perturbations into the physical parameterization schemes. Alternatively, given that the short-term predictability of the atmosphere and the ocean is dominated by their initial conditions (ICs), various methods to perturb the initial model state have been proposed to generate ensembles. These include (i) random perturbations sampled from some available error statistics, (ii) the singular vectors and their variants designed to represent the perturbations with the fastest error growth, and (iii) the vector breeding approach, which computes the initial perturbations as the differences between a pair of past concurrent forecasts. Different approaches were also suggested to perturb the open boundaries and the atmospheric forcing, but ensembles of atmospheric and oceanic forecasts are now available from the global operational prediction centers and can be readily used to generate ocean forecasts ensembles.

Virtual ensemble forecasts were traditionally more common for operational purposes as they do not require major extra computations, although their large ensemble spread (measure of uncertainty) was deemed as a disadvantage. The multi-model approach involves the tedious task of running and maintaining different ocean general circulation models (OGCMs), though this could be handily done by combining the forecasts from different operational centers. Until recently, ensemble forecasts generated by a MC approach were widely used for research purposes but started to make their way into more operational use. Despite their demonstrated skills, these produce adequate forecasts only when the ensemble is a representative sample of the probability distribution of the underlying dynamical system (Leith, 1974). Setting the ranges, or more generally, the probability distributions of the perturbations and varying them in time for those dynamical variables remains a challenge. The tremendous advances in ensemble data assimilation (EnDA) approaches and their successful implementations with ocean general circulation models (OGCMs), and also operationally, now provide another framework to represent the error-of-the-day, not only for the initial conditions but also for the inputs and parameters, by offering the possibility of sampling the perturbations from their actual, albeit approximate, distributions conditioned on available observations (Hoteit et al., 2018; Carrassi et al., 2022).

95 **1.2 Probabilistic assessment**

Forecast ensembles are evaluated through their sample statistics, mainly their mean, which can be directly compared with the observations, once available, and their spread – the standard deviation with respect to the ensemble mean, which is an important indicator of the confidence in the prediction; a small/large spread indicates low/high uncertainty in the forecast. High-order



moments, such as skewness and Kurtosis, are also analyzed for more information about the shape of the ensemble distribution.

100 Probabilistic validation and verification methods, including reliability, resolution, sharpness and rank histograms, are also used to evaluate ensemble forecasts (Johnson and Bowler, 2009). An ensemble is reliable when its sampled probability of a predicted event gives an estimate of the expected frequency of the event occurring. Resolution is defined as the degree to which the forecast deviates from the climatological event frequency. For a reliable ensemble, increasing this deviation enhances the usefulness of the forecast. In the same context, sharpness measures the ability of an ensemble forecast to spread away from

105 the climatological average. Ideally, an ensemble forecast needs to be reliable, with as many forecasts as possible away from the climatological average. Rank histograms are also used to determine the reliability of ensemble forecasts and for diagnosing errors in their mean and spread [Hamill, 2000]. These are generated by repeatedly tallying the rank of the observations relative to corresponding ensemble values sorted in increasing order.

1.1.1 Current status of ensemble forecasts in OOFSS

110 Despite the early establishment of ensemble methods for ocean data assimilation and forecasting (Evensen, 1994), ensemble forecasts only recently found their ways to the operational centers. This is mostly because the centers prioritized using the available computational resources to increase the resolution of ocean models. This was due to the need to resolve the mesoscale to sub-mesoscales processes to better describe the energy cascade in the ocean (e.g. D'addezio et al., 2019; Davidson et al., 2021). Recent developments in ocean ensemble forecasting followed the improved coverage in ocean observations that

115 provided increased information to accurately constrain the initial ocean state for extended forecast horizons the better coordination between ocean forecasting groups, the ease of access to atmospheric ensembles, and the ever-increasing availability of computational power (Metzger et al., 2010; Smith et al., 2011). Ocean ensemble forecasts are now routinely generated at several operational ocean centers on both global and regional scales to cater to different needs as summarized in Table 1.

120 **Table 1: Summary of operational ensemble forecasting systems operating across the globe.**

| Institution | Forecasting System | Domain | Ensemble Perturbations (Size) | Type of Forecast | Reference |
|----------------|--------------------|--------|--------------------------------|---------------------------------|------------------------------|
| Met Office, UK | FOAM | Global | Observations + Atmosphere (36) | Short-range ocean state | Lea et al., (2022) |
| NRL, USA | Navy-ESPC | Global | Observations (16) | Days to subseasonal ocean state | Barton et al., (2020) |



| | | | | | |
|----------------------------------|----------------------------|---------------------------|---------------------------------------|--------------------------------------|------------------------------------|
| Bluelink, Australia | OceanMAPS | Global | Time-lagged (3) | Short-range ocean state | Schiller et al., (2021) |
| NERSC, Norway | TOPAZ4 | North Atlantic and Arctic | Atmosphere (100) | Short-range ocean state | Nakanowatari et al., (2022) |
| BSH, Germany | Multiple-models | North Sea and Baltic Sea | Multi-model (13) | Short-range ocean state | CMEMS portal |
| KAUST, Saudi Arabia | MITgcm | Red Sea | Atmosphere + Internal physics (50) | Short-range ocean state | Sanikommu et al., (2020) |
| MET-Norway | Barotropic version of ROMS | Norway | Atmosphere (51) | Short-range storm surge | Kristensen et al., (2022) |
| ECMWF | IFS | Global | Internal physics (51) | Short-range waves | Browne et al., (2019) |
| NCEP | GWES | Global | Wind (30) | Short-range waves | Penny et al., (2015) |
| Bureau of Meteorology, Australia | ACCESS-S | Global | Internal physics + Time-lagged (30) | Multi-week to seasonal ElNino/IOD | Hudson et al., (2017) |
| CMA, China | CMMEv1 | Global | Multi-model + Initial conditions (90) | Multi-week to seasonal ElNino/IOD | Ren et al., (2019) |

2 Role of ensemble forecasts in next generation OOFSS

Recognizing the importance of representing uncertainties in ocean forecasts to meet the need of future demands in probabilistic predictions, ensemble forecasts are expected to become a standard output of any operational ocean product. The lack of high-density ocean observations further leaves the mesoscales and sub-mesoscales poorly unconstrained by the ocean analysis



125 systems. Uncertainties from the unconstrained scales might lead to larger forecast errors due to growing dynamical instabilities
(Sandery et al., 2017), which limits the forecasting skills of high-resolution ocean models (e.g., Thoppil et al., 2021). Ensemble
forecasting has been proven efficient to extend ocean forecasting horizons when model uncertainties in the initial conditions,
inputs, and physics are accounted for (Mullen and Buizza 2002; Ryan et al., 2015; Sanikommu et al., 2020). Ensemble forecasts
are also needed to provide errors statistics for the ocean analysis systems to better exploit the high-density observations to
130 come in the future from satellite missions such as Surface Water Ocean Topography (SWOT) (Fu and Ubelmann, 2014). Long
delayed by the desire of the community to increase the resolution of the ocean models to improve their realism, the ever-
increasing computing resources will provide more and more power to integrate these within ensemble forecasting frameworks.
Ocean forecasts are now produced by data assimilation (DA) systems. Ensemble forecasts could be generated from
deterministic DA systems, which produce one single-forecast, by simply perturbing the observations (or other parameters of
135 the assimilation system), or during the forecasting step using an ensemble forecasting method. Ensemble DA methods, on the
other hand, readily produce ensemble ocean perturbations that (approximately) represent the error-of-the-day and can be
directly used to generate ensemble forecasts. These could be also combined with standard ensemble forecasting methods to
further represent the missing information about the error growth in the computationally restricted DA ensembles. To fully
exploit the benefits from ocean ensemble forecasts, new tools to analyze and visualize, and also integrate these probabilistic
140 products in decision making and management of ocean services need to be developed and made available for the end users.

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Competing interests

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

260 **Data and/or code availability**

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

Authors contribution

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

Acknowledgements

- 265 The authors greatly acknowledge the contributions of Dr. Siva Reddy and Dr. Naila Raboudi to this article and for their invaluable insights and support throughout the writing process.