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# Crafting the Future: Machine Learning for Ocean Forecasting

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**Abstract.** Artificial intelligence and machine learning are accelerating research in Earth system science, with huge potential for impact and challenges in ocean prediction. Such algorithms are being deployed on different aspects of the forecasting workflow with the aim of improving its speed and skill. They include pattern classification and anomaly detection, regression and diagnostics, state prediction from nowcasting to synoptic, sub-seasonal, and seasonal forecasting. This brief review emphasizes scientific machine learning methods that have the capacity to embed domain knowledge, to ensure interpretability through causal explanation, to be robust and reliable, to involve effectively high dimensional statistical methods, supporting multi-scale and multi-physics simulations aimed at improving parameterization, and to drive intelligent automation as well as decision support. An overview of recent numerical developments is discussed, highlighting the importance of fully data-driven ocean models for future expansion of ocean forecasting capabilities.

## 1 Introduction

Research into applications of artificial intelligence (AI) and machine learning (ML) in ocean, atmospheric and climate sciences has accelerated at a breathtaking pace over the last 5 years or so (e.g., Schneider et al., 2023; Eyring et al., 2024). With essentially all these applications concerned with ML, we will drop the more broadly defined "AI" term in most of the following, except when used by references cited. We will also take the perspective of scientific machine learning (SciML), defined in a 2019 U.S. Department of Energy report on "Basic Research Needs for Scientific Machine Learning" (Baker et al., 2019), which emphasizes five key elements of SciML algorithms: (i) ML approaches that incorporate domain knowledge, such as physical principles, symmetries, constraints, expert feedback, computational simulations, and formal uncertainties; (ii) ML approaches that are interpretable, such that user's confidence in ML-based model predictions may be bolstered by causal explanations based on a user's domain knowledge; (iii) ML approaches that are robust and reliable as a prerequisite to for making high-stakes, high-regret decisions; (iv) ML approaches that are data-intensive, i.e., that ingest high-dimensional, noisy, and uncertain input data which contain complex structures and which require statistical and probabilistic methods to deal with ill-conditioning, non-uniqueness, and over-fitting; (v) ML approaches that enhance modeling and simulation to support, e.g.,

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multi-scale, multi-physics simulations in terms of improved model parameterization or model acceleration; and (vi) ML approaches to support intelligent automation and decision support, which can range from quality control to application-oriented post-processing workflows. Arguably, all of these criteria are fundamental to the uses of ML in ocean prediction.

Next, following the review by Reichstein et al. (2019), it is useful to distinguish different categories of ML applications, (A) classification and anomaly detection, which is concerned with, e.g., finding extreme event patterns or the classification of important structures or regimes; (B) regression, which is concerned with state reconstruction of important state variables, parameters, or diagnostics (metrics) from available data; and (C) state prediction, ranging from nowcasting to operational forecasting, to sub-seasonal to seasonal prediction. A comprehensive collection of review articles on deep learning in Earth sciences is Camps-Valls et al. (2021), covering both algorithmic foundations as well as examples of all three categories.

Because the subject of this document is on ocean prediction, we will focus the following on the third category, state prediction.

## 2 State prediction

The workflow of operational ocean prediction largely follows that of numerical weather prediction (NWP). Its core engine is a data assimilation (DA) framework, consisting of a physical model, i.e., a complex algorithm for solving a set of partial differential equations (PDEs), a workflow for quality-controlling and ingesting diverse observational data streams into the DA system (ideally in near-real time), and an optimal estimation algorithm that combines models and data in a formal manner that produces statistically optimal forecasts (Park and Zupanski, 2022). As pointed out by S. Penny in a 2022 U.S. National Academy of Sciences workshop on Machine Learning and Artificial Intelligence to Advance Earth System Science (NASEM, 2022), ML approaches hold the prospect for accelerating various elements of the DA workflow. We briefly summarize ML approaches targeting the physical model as well as the DA algorithm. Opportunities in the application of ML for partial differential equation (PDE) based models fall into two main categories, one concerned with targeted insertion of ML within a physical model, sometimes termed "soft AI", the other with the complete replacement of the physical model by a surrogate model, termed "hard AI" (Chantry et al., 2021). In the former, certain elements or subcomponents of a physical model are replaced by a surrogate model (e.g., a neural network), whereas in the latter, the entire model is emulated.

### 2.1 "Soft AI" – enhancing forecast models with ML algorithms

A major source of model uncertainty is the parameterization of subgrid-scale (SGS) processes, both in terms of structural errors (formulation of functional representations of parameterizations) as well as parametric uncertainties (calibrating empirical parameters in the functional representations). Exciting efforts are underway to apply machine learning to replace conventional functional representations subgrid-scale turbulent oceanic processes with surrogate models that are based on machine learning (Bolton and Zanna, 2019; Zanna and Bolton, 2020, 2021; Frezat et al., 2021a, 2021b; Zhang et al., 2023; Sane et al., 2023, Perezhogin et al., 2023); a longer list of related efforts exists for numerical weather prediction and has been reviewed by Dueben et al. (2021) and Boualègue et al. (2024). These surrogates, mostly some form of neural networks, have been trained

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on (i.e., fit to) what are considered simulations of much higher fidelity where these processes are resolved (e.g., large eddy simulations). Related efforts aim at learning improved parameterizations from online bias correction or analysis increments incurred in sequential data assimilation (e.g., Gregory et al., 2023, 2024). Rapid progress is expected on this front in the coming years.

A second important application of "soft AI" is the desire to replace specific numerical algorithms within PDE-based models by surrogate models in order to accelerate the simulation's time-to-solution. Studies exist within the generic field of computational fluid dynamics (Kochkov et al. (2021) and atmospheric modelling (Kochkov et al., 2024), and with ocean-specific applications currently underway, all of which taking advantage of the concept of differentiable programming (Sapienza et al., 2024). For an overview of ideas of hybrid methods that integrate machine learning and physics-based modeling in Earth system modeling broadly, see Irrgang et al. (2021).

### 2.2 "Hard AI" – replacing numerical simulations with surrogate models

Over the last decade, with the acceleration of AI based solutions in other fields, a number of approaches to model the atmosphere and ocean using different hard AI have been developed. It is necessary to distinguish between three different conceptual approaches: (i) data driven, (ii) physics-informed, and (iii) neural network solvers for PDE.

The first approach would be the adaptation of neural networks that have been proven useful in other fields to reproduce the results of numerical model simulations (see Minuzzi and Farina (2023), Xie et al. (2023), Xu et al. (2023), Puscasu (2014), Gracia et al. (2021), Accarino et al. (2021)). The results of these AI-based solutions may produce meaningless output, as the training strategy of a neural network is to minimize a mathematical loss function, i.e., the mean squared error between the prediction and the original target. An evolution of this approach is to include some physical constraints in the loss function in order to force the ML algorithm to produce more consistent outputs, as the Navier-Stokes equation (Ma et al., 2022; Daw et al., 2021). This method is known as physical-informed neural networks (PINNs; but see Du et al., 2023, for a cautionary tale on extrapolation using PINNs). Recently, another approach, which tries to solve differential equations using neural networks, is under development. Although this method is mostly developed for other physics fields, the methodology and knowledge can be applied to ocean modeling (Zubov et al., 2021; Smets et al., 2023).

There are several neural network architectures that are actively being used for data driven or physical-informed networks: (i) Long Short-term Memory, (ii) Convolutional, (iii) Generative Adversarial Networks, and (iv) Reservoir Computing.

Long Short-term Memory networks use a special type of neuron that keeps track of previous inputs (short-term memory) and are especially useful for predicting time-series, as the current state of the ocean is constrained by the previous states. Convolutional networks use a mathematical operation called convolution to compress information, learning features or patterns in the input. This kind of network is useful for 3D input data, i.e. feeding a 3D grid with the spatial grid of the ocean and the depth (third dimension) provide different variables values for each grid node, like sea surface temperature, height or current speed and direction. The Generative Adversarial Network combines two different networks, one is a generator that tries to produce a solution from an input and the second network has to determine whether the input is real data or produced by an AI.

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These two networks compete one against the other (as adversaries), so when the generator network is good enough, the discriminator will not be able to determine if the image is real or fake. Finally, Reservoir Computing (RC), a method based on recurrent neural networks with a pool of interconnected neurons forming the "reservoir", is particularly well adapted to the emulation of time series (e.g., Penny et al., 2022, Platt et al., 2023).
These ML algorithms have been successful for the following applications: waves (James et al., 2018), sea surface temperature (Wolff et al., 2020), sea level (Nieves et al., 2021), dissolved oxygen (O'Donncha et al., 2022), ocean color (Chen et al., 2019), ocean surface circulation (Sinha and Abernathey, 2021), and sea ice drift (Andersson).

## 3 Enhancing data assimilation with ML algorithms

There is a strong conceptual correspondence between machine learning and data assimilation (e.g., Abarbanel et al., 2018). This provides various opportunities for embedding ML approaches within operational data assimilation workflows deployed in ocean prediction. Examples so far are largely restricted to "toy problems" (such as the "Lorenz 96 model") or reduced-order versions of Earth system models but targeting eventual applications for ocean prediction (Bocquet et al., 2020; Brajard et al., 2021; Penny et al., 2022).

### 3.1 "Hard AI" – replacing numerical simulations with surrogate models

The concept of digital twins (DTs) is rapidly gaining traction within the ocean science community and Earth system science more broadly (e.g., Bauer et al., 2021a, 2021b). Following the definition from NASEM (2022) (see also Niederer et al., 2021; National Academies of Sciences, Engineering, and Medicine, 2023), a DT is "a set of virtual information constructs that mimics the structure, context and behavior of an individual/unique physical asset, or a group of physical assets, is dynamically updated with data from its physical twin throughout its life cycle and informs decisions that realize value. A digital twin is highly dynamical, mimicking the time evolution of its physical asset (PA) via advanced simulation and emulation capabilities; it is updated by ingesting vast amounts of observational data of diverse types; and it enables WHAT-IF queries and multiple realizations to support prediction of responses of the PA to hypothetical perturbations with quantified uncertainties."
Virtually all aspects of ocean forecasting – and ML opportunities therein – may be viewed through the DT lens, from the need to generate high-fidelity simulations or digital representations, ingesting, i.e., assimilating large, heterogeneous data streams, the development of fast surrogates or emulators to either accelerate simulations or provide comprehensive uncertainty estimates, to the generation of diagnostic data that create value for (possibly rapid) decision support.

### 3.2 Challenges

Among the challenges of fully realizing the opportunities of ML approaches in ocean prediction is the fact that, in the absence of adequate, densely sampled observational data, most ML applications rely on the use of data obtained from high-fidelity model simulations as training data sets. These data sets are very expensive to generate, limited in the temporal ranges that they can represent, remain subject to unquantified structural and parametric model uncertainty, require vast amounts of storage (order of PetaBytes), and are thus challenging to query. Cloud-based solutions are the most promising approach for ubiquitous data access and analysis capabilities "close to the data" (Abernathey et al., 2020).

Within the realm of machine learning (ML) applications for ocean forecasting, progress has been somewhat limited. Recent developments, however, have marked a shift in this landscape, particularly with the introduction of Fourier Neural Operators (FNOs) for modeling oceanic processes, as suggested by Bire et al. (2023), Chattopadhyay et al. (2023), and Sun et al. (2024). These studies present fully data-driven ocean models that match the capabilities of traditional numerical ocean models in predicting high-resolution sea surface height (SSH) fields. FNOs, already established in the domain of weather forecasting (e.g., Bonev et al., 2023; Watt-Meyer et al., 2023), are attractive for their performance in learning complex, high-dimensional mappings and their ability to incorporate physical laws and constraints, which are prominently observable in the spectral domain. Concurrently, Wang et al. (2024) introduced a transformer-based model tailored for oceanic applications, demonstrating performance that rivals that of leading operational global ocean forecasting systems. Similar advances are being made in data-driven prediction of sea ice cover in the polar oceans (see Bertino and Heimbach, this issue). This body of work signifies the emergence of a promising research avenue in fully data-driven ocean modeling, despite it still lagging considerably behind the advancements seen in weather forecasting. We posit that the drive of Hard AI solutions in NWP by private sector companies is related to the prospect of high-stakes / high-reward applications. Such applications for ocean predictions should be better articulated to attract similar research efforts. Careful evaluation of skill, such as now being discussed more comprehensively in NWP (e.g., Charlton-Perez et al., 2024) will also be required for operational ocean prediction.

Another challenge presents the extension of ML applications to seasonal, inter-annual and multi-decadal (i.e., climate) time scales (see e.g., the discussion in Gentine et al. (2021) and Beucler et al. (2024)). Here, the increased need of models or invariant operators (physics-based or surrogates) to conserve fundamental properties (mass, energy, momentum, active tracers) puts severe demands on ML approaches. Arguably, as these approaches increasingly incorporate physical knowledge, they will converge to the realm of classical inverse methods (Willcox et al., 2021). In this context, the concepts of differentiable programming and "online learning" are rapidly gaining traction to bridge physics-based modeling with SciML (e.g., Gelbrecht et al., 2023; Shen et al., 2023; Zhang et al., 2023; Sane et al., 2023, Kochkov et al., 2024).

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## Competing interests

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

## Data and/or code availability

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

## Authors contribution

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