Modeling Noise: Paths toward AI-Enabled Stochastic Earth System Models and Parameterizations

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Focal Area: The use of AI to design an earth system prediction framework comprising of a hierarchy of modeling approaches

Science Challenge: Accurate probabilistic prediction of extreme events with an improved degree of confidence

Rationale

Some of the key challenges in Earth system prediction arise from an uncertain representation of unpredictable natural variability, across time and space scales. This variability, hereafter referred to as noise, represents the quantity against which the strength of a signal of interest is measured to assess predictability. Underestimating or overestimating this noise in Earth system models can lead to issues ranging between overconfidence in an erroneous prediction and a lack thereof in an otherwise accurate one. Noise is part of the physical processes in the Earth system and can amplify or damp a signal of interest in a complex manner that is not systematically characterized. Specifically, while there has been significant progress in our understanding of multiscale interactions among known modes of variability (potentially predictable signals), how these are impacted by the noise is not clear. Recent effort toward stochastic parametrization schemes that provide a representation of noise due to uncertain sub-grid processes in climate models (Berner et al., 2017 and references therein) has shown promise not only in reducing biases and improving probabilistic prediction but also in improving the representation of natural variability in the model toward what is observed. However, today's standard schemes for stochastic parametrization are still simplistic as they do not take the state of the atmosphere into account (other than by the use of multiplicative noise for model tendencies). Furthermore they require hand-tuning and trial-and-error testing for the magnitude of the added noise, which is difficult in a chaotic system that is as complex as the Earth system. Machine learning (ML) and artificial intelligence (AI) are promising new approaches: Deep learning

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methods can allow models to directly learn not only the signal or errors but also the uncertainty in data from systems as complex as weather and climate models. Therefore, ML and AI area promising to be useful tools to develop more accurate stochastic parameterizations (Gagne et al., 2020, Beucler et al., 2020) to efficiently mimic realistic sub-grid-scale variability that arises from processes such as the lifecycles of clouds (Hagos et al., 2020; Mooers et al., 2020), boundary layer gustiness (Bessac et al, 2020), turbulence in the ocean mixed layer, etc.

Such an undertaking requires an efficient hierarchy of AI-enabled models that correctly propagate signals and noise across scales. Some of such models can then serve as stochastics parameterizations that enable accurate representation of generation and propagation of noise into and out of the sub-grid scale of dynamical Earth system models. In this white paper, we propose the development of an AI-enabled hierarchy of stochastic Earth system models and discuss how some of them can be used as parameterizations of cumulus convection as well as air-sea and land-atmosphere coupling processes in dynamical Earth system models.

Narrative: Reduced dimension surrogate models

There are a few roadblocks to the development of AI-enabled climate models that mimic dynamical models that at the same time are amenable to an efficient investigation of the propagation of noise and errors across scales and components. The key among them is dimensionality. The number of degrees of freedom required to represent the Earth system is very large and its upper limit is difficult to estimate. That means it is hard to distinguish whether or not the relationships a given ML algorithm is supposed to capture are valid over the entire high dimensional hyperspace. Then there is the issue of availability of ground truth, as even observations include errors and quantifying these errors is a challenge. In this white paper we propose the development of a class of stochastic surrogate models that can help address the above discussed scientific and technical challenges.

(a) The stochastic surrogate models

In order to develop a hierarchy of AI-enabled Earth system models that is easy to run, analyze and interpret, and ultimately facilitate the development of stochastic parameterizations for dynamical Earth system models, one must reduce the dimensionality. There are several strategies for doing that. One is identifying a set of basis functions that represent a spatial structure of the climate state and extract the temporally varying coefficients. Then one can develop an AI-enabled model of the temporally varying coefficients. There are different ways to accomplish this. One way is to exploit the analogy to the development of a spectral model where the basis vectors represent the spatial structure, and a numerical model represents the variability in the amplitude for each harmonic. Another way is to use principal component analysis (PCA) to separate spatial patterns (hereafter represented by vector **X**) from temporal variability (represented by vector **S**) and develop a model for the latter. In any case, the outcome is to represent the climate state by vector **S,** whose elements are random functions of time representing the variability at the range of scales of interest. A third approach is a Linear Inverse Modeling framework (Newman et al., 2003; Martinez-Villalobos et al., 2017), where the predictive modes are represented as covariance functions in a reduced space (e.g., functions of PCAs). We can also model the system with reduced complexity and represent higher complexity processes as AI-driven stochastic processes (Chattopadhyay et al., 2020; Crommelin and Edeling, 2020; Alcala and Timofeyev, 2020; Leinonen et al., 2020). To characterize noise relevant for predicting high-frequency signals, convection-resolving simulations such as the DYAMOND ensemble (Stevens et al., 2019) provide comprehensive data coverage to characterize variability in small-scale processes (Christensen, 2020). Such datasets can be combined with ultra-high-resolution satellite imagery (available as global, daily 3-5m resolution data, e.g. from planet.com) using a transfer learning approach.

Once the dimensionality is reduced, the next step is to develop the stochastic model that predicts the probability (**P**) of the system being in the state $\boldsymbol{S}_{t+1}$ given all previous states, i.e.;

$$\boldsymbol{P} = \boldsymbol{P}(\boldsymbol{S}_{t+1} = \boldsymbol{s} | \boldsymbol{S}_t = \boldsymbol{s}_t, \boldsymbol{S}_{t-1} = \boldsymbol{s}_{t-2}, \ldots, \boldsymbol{S}_0 = \boldsymbol{s}_0) \quad (1)$$

Several simplifications can be made to **P** based on the specific process of interest or the desired level of complexity. Among them is the level of memory the system would have. The simplest being approximating it by a Markovian model where the next state depends only on the present state, i.e.,

$$\boldsymbol{P} = \boldsymbol{P}(\boldsymbol{S}_{t+1} = \boldsymbol{s} | \boldsymbol{S}_t = \boldsymbol{s}_t) \quad (2)$$

AI techniques we can apply to achieve this include Bayesian neural networks, variational autoencoders, and generative adversarial networks. This stochastic Earth system model can be trained by both long-term observations as well as dynamical Earth system models or their hybrid. For example, if the training dynamical model has a bias in El Niño Southern Oscillation (ENSO) and the Madden-Julian Oscillation (MJO), the elements of $\boldsymbol{P}$ corresponding to the particular mode of variability can be corrected by introducing observations at the specific scale to obtain observationally informed posterior probability. From which the directionality of propagation of noise (and errors) can be systematically assessed. The key feature of such models is they can be used to examine the causality of processes and enable tracing of the propagation of signals, noises, and errors across scales. As noted above, the proposed hierarchy of stochastic earth system models can cover a broad range of scales depending on the specific application. On the one end, they could be used as weather models, where a specific range of high frequency variability is predicted while the low frequency components of the state vector **S** are kept constant as the "background state". On the other end, they can be used as parameterization of sub-grid scale variability as part of a traditional dynamical model as will be discussed below.

b) Application as parameterizations in dynamical Earth system models

In order to attain a detailed and accurate stochastic representation of Earth system processes while retaining our existing physical knowledge, an AI-trained stochastic surrogate model can be used to introduce probabilistic tendencies to dynamical Earth system models (Pathak et al., 2018; Piccolo et al., 2019; Watson, 2019, Brenowitz et al., 2020). Sampling from the probabilistic predictions then gives a stochastic parameterization that will give more realistic simulations when applied to the free-running model. Techniques to interpret complex AI models can then be applied to understand the resulting stochastic parameterization, and the insights gained can also be used to develop better human-designed parameterization schemes. Finally, the effect of stochasticity in the Earth system can also be diagnosed by comparing simulations using the AI stochastic parameterization with those using a deterministic counterpart.

Expected Activities and Outcomes

In this white paper, we propose the development of a hierarchy of stochastic Earth system models for characterization of noise and predictability, and ultimately improving the representation of generation and propagation of noise in dynamical Earth system models. As detailed above, the strategy involves:

1. Design of physically and mathematically justified dimension reductions of the state of the Earth system,
2. Development of probabilistic machine learning models that propagate the reduced dimension state vector forward in time,
3. Training and validation the models using observations and dynamical models while accounting for observational uncertainties,
4. Coupling of the AI-enabled models into a dynamical Earth system model as a parameterization of generation of noise, and
5. Analyzing generation and propagation of noise and their impact on the overall performance of the Earth system model.

Suggested Partners

David John Gagne (NCAR, Machine Learning expert)
Tim Palmer (Univ. of Oxford, ensemble prediction and stochastic modeling expert)

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