Building an AI-enhanced modeling framework to address multiscale predictability challenges

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Focal Area(s)

Build an AI-enhanced modeling framework that integrates the three focus areas in the solicitation.

Science Challenge

The 4M-2N complexities (Multiscale, Multiphysics, Multibody, Multidimension, Non-linearitiy, and Non-Gaussianality) of atmospheric aerosol-cloud-precipitation-turbulence-radiation system poses physical and computational challenges to further advance predictive models; We plan to address the challenges by developing an AI-enhanced modeling framework that facilitates automated calibration and improvement of subgrid parameterizations, enhance data assimilation of measurements to improve initial and boundary conditions used to drive the physical model, and optimally blends data-driven and physics-based forecasting models.

Rationale

Accurate prediction of water cycle depends heavily on representations (parameterizations) of still poorly understood subgrid processes occurring in the the aerosol-cloud-precipitation-turbulence-radiation system, which represents an extreme example of 4M-2N complexities. The system involves micrphysical processes over a wide range of scales from the smallest turbulent eddies (~ 1 mm) to convection (~ km) to global scales in terms of air motion, and from nano-sized aerosol particles to cloud droplets of micrometers to precipitation of millimeter. The system is further riddled with convoluted nonlinearities (e.g., turbulence cascade and microphysical processes) and sensitive thresholds controlling phase changes and cloud-precipitation conversion (Liu, 2019). Understanding such complex processes and upscaling them to adequate representation in climate models present daunting scientific challenges. BER has taken up the challenges, together with other agencies, through modeling programs such as Energy Exascale Earth System Model (E3SM) and observational programs such as the Atmospheric Radiation Measurement (ARM) facility. However, significant knowledge gaps remain at scales smaller than typical grid sizes of cloud-resolving models (CRM) (e.g., 1 km) and large eddy simulation (LES) models (e.g., 100 m), including cloud microphysics, turbulence-microphysics interactions, and turbulent entrainment-mixing between clouds and environmental air, and their complicated interactions with radiative transfer. These processes are either represented in very rudimentary ways or not represented at all in climate models; the problem will become more acute with the future E3SM reaching CRM/LES resolution over the global domain. Another challenge to improve water cycle predictability lies in the need of accurate and consistent initial (and boundary conditions for limited area models) used

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to drive the models. Data assimilation has proven to be essential for the progress of numerical weather prediction, but success in climate and high-resolution models is limited due to computational cost and/or lacking high-resolution measurements. Furthermore, virtually all parameterizations contain empirical parameters that have been tuned manually against measurements, making parameter generalization and identification of parameterization structural biases questionable. Further model development calls for an organic framework that can be used to conduct dynamic model evaluation with the capabilities of automatic parameter calibration and identification of structure biases. The framework also needs to be "smart" in terms of optimally balancing measurements used for data assimilation and those for model evaluation/calibration, and "flexible" to fix identified model deficiencies. Last but not the least, addressing these physical challenges poses additional challenges in computational, algorithmic and big data sciences.

With the advancements in physical modeling, observations, artificial intelligence (AI), machine learning (ML), and high performance computers (HPC), now is the time to develop a cross cutting AI/ML/HPC-enhanced modeling framework to address the above-mentioned challenges, by forming an interdisciplinary team from the Environmental and Climate Sciences Department and Computational Sciences Initiative of the Brookhaven National Laboratory (BNL). This new cross-cutting framework targets CRM/LES models with the domain size over which BER maintains high-resolution measurements (e.g., ARM) and the spatiotemporal resolution of future global climate models, consisting of three closely related components detailed below.

Narrative

1) Automated model calibration system with data assimilation

A fundamental deficiency of climate models lies in the existence of empirical parameters and structural biases in subgrid parameterizations due to incomplete process understanding/knowledge and/or inadequate approximations. The empirical parameters have been largely tuned manually with measurements collected under specific conditions. Such manual tuning is tedious and the parameters lack generalizability to other conditions on which the parameters likely depend. Model evaluation is more based on individual variables such as temperature, less on emerging relationships (Eyring, et al., 2019) and still less on causal networks (Runge et al., 2015). Furthermore, determining structural biases is more challenging than determining the parameter values. Another fundamental deficiency lies in the fact that the initial and boundary conditions used to drive the model are inaccurate and/or inconsistent with the physical model. Optimal assimilation of measurements into the physical model (data assimilation) is a primary way to deal with this deficiency, and has proven to be instrumental in improving weather predictability. However, data assimilation has been largely limited to NWP and to state variables such as temperature. There are growing needs for high resolution and multiscale data assimilation (CRM/LES scales), and the concurrent optimization of state variables and model parameters (Anderson et al., 2009).

A suite of the community Weather Research and Forecast (WRF) models with different configurations and setups has been used in related studies, including the standard configuration of nested WRF, high-resolution Large Eddy Simulation (LES) version of WRF-LES (Endo et al., 2015; Lin et al., 2015), and Single Column Model (SCM) version (SWRF). We plan to further to agument the WRF suite by developing an automated calibration framework that capitalizes on AI/ML/HPC advances. For example, ML models are computationally much faster than full physics-based simulations once trained, which makes it possible to accelerate the optimization in model calibration and data assimilation (Xu et al., 2018). ML can be used to develop superresolution emulators to further improve downscaling and physical understanding by training low resolution WRF simulations with high resolution simulations (Dong et al., 2016; Wang et al., 2019; Stengel et al., 2020; Leinonen et al., 2020). In particular, ML models can be applied to quantify functional uncertainties in the model structure, such as missing or approximated terms in parameterizations or moving from constant to state-dependent parameters (Ramadhan et al., 2020; Dandekar et al., 2020; Melland et al., 2020). The ability of deep ML algorithms (e.g., variational autoencoders) to learn reduced latent feature spaces raises the possibility that data assimilation can take place largely within a low-dimensional dynamical subspace at substantially reduced computational expense.

2) Development of new theories/parameterizations, and benchmarking models

A related but more challenging task is developing new parameterizations that fix existing model deficiencies. Two general directions merit investigation. The first focuses on building a general framework that encompasses existing parameterizations as special cases. Take cloud microphysics as an example. The current state of the art microphysics parameterization tracks two-moments of the particle size distribution (e.g., number concentration and mass concentration), a generalized parameterization will need to predict more than two moments so that the effect of the spectral shape of particle distributions can be addressed (Liu et al., 2007; Morrison et al., 2020). The second focuses on developing ML emulators (e.g., neural mixture models, stochastic recurrent neural networks, and spatiotemporal versions of attention-based models) of more detailed models as parameterizations including microphysics, shallow convection, PBL processes, and 3D radiative transfer (Schneider et al. 2017). Such ML emulator parameterizations hold the potential to explore and fix structural biases and consider process couppling. It is also possible to apply Bayesian versions of emulators to quantify model structural uncertainties within parameterizations. Obviously, both foci further call for developing new theories and/or more detailed models that can be used to either inform the parameterization development or directly as (parts) of new parameterizations. Particularly needed is a particle-resolved direct numerical simulation (DNS) model that can serve as a benchmarking microphysical model and fills many knowledge gaps (Gao et al., 2018).

3) Data-driven forecast models and model integration

An approach complementary to developing more accurate physics-based models is to learn more accurate ML models empirically from datasets (data-driven models). We expect that over short forecast lead times (e.g., less than an hour), data-driven ML models outperform physics-based models while the reverse true for longer lead times (Haupt et al., 2020). Thus, the optimal strategy for forecasting seeks to seamlessly unite these two approaches into a single closed system for forecasting over a wide range of space-time scales, and related to the data assimilation involved. One potential blending approach is to consider physical constraints from numerical models as a kind of Bayesian prior imposed on the predictions of data-driven models (Jonko et al., 2018), which can also be considered a form of transfer learning from physical to ML models (Ham et al., 2019).

It is noted that all the three efforts involve exploring integration of AI/ML models, physics-based models, and measurements, utilizing DOE frontier HPCs, and following the FAIR (Findable, Accessible, Interoperable, Reusable) principles. See the companion white paper entitled *"Black-Box Neural System Identification and Differentiable Programming to Improve Earth System Model Predictions*" by Urban et al. for more on the general AI/ML development.