Facilitating better and faster simulations of aerosol-cloud interactions in Earth system models

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Focal Area(s):

1. Predictive modeling through the use of AI techniques and AI-derived model components; the use of AI and other tools to design a prediction system comprising a hierarchy of models.
2. Insight gleaned from complex data (both observed and simulated) using AI, big data analytics, and other advanced methods, including explainable AI and physics- or knowledge-guided AI.

Science Challenge

One major challenge that Earth system models (ESMs) face in providing credible prediction of the Earth system and its water cycle characteristics (e.g., mean state, variability, and extreme events) is to accurately simulate aerosol-cloud interactions (ACI). The physical, chemical, and dynamical processes affecting ACI are extremely complex and they range from nanoscale to planetary scale. In each model development cycle, scientists spend significant efforts investigating model deficiencies and uncertainties associated with aerosols (e.g., emissions, chemical processes, aerosol microphysics, and transport) and clouds (e.g., macrophysics, microphysics, turbulence, and large-scale circulation) in order to develop improved treatments. However, despite decades of active research, ACI is still a major source of uncertainty in climate projections, even though great progress has been made. Specific scientific challenges include: (i) Parameterizations are developed based on limited data; (ii) The complexity of a parameterization required for accurate predictions is not understood; (iii) Incomplete and unknown physics leads to errors in the fully coupled Earth system; and (iv) Complex physics is computationally too expensive to employ in ESMs.

Rationale

This whitepaper seeks to utilize novel artificial intelligence (AI) and machine learning (ML) techniques to facilitate better and faster representations of ACI in ESMs. We will use explainable AI (XAI) or interpretable AI (IAI) techniques, variational autoencoders (VAEs), and neural networks (NNs) to develop new understanding of ACI and their manifestation in the Earth system using ensemble simulations of DOE's E3SM, large-eddy simulations (LES), detailed process models, and observations. The new understanding will provide insights into E3SM's

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calibration and development needs, improving process representations as well as their interactions with the host model.

Narrative

Plenty of existing applications demonstrate how AI approaches provide better and faster processing of data. While many of these methods were previously considered black boxes, many methods now exist to open the black boxes and peer inside. IAI methods build AI approaches that are human-interpretable from the beginning, while XAI methods allow for post-hoc analysis of the decision-making process of the algorithm (*1*). In the past few years, multiple studies have highlighted the importance and usefulness of XAI and IAI in atmospheric science research (*2, 3*). Our team has utilized XAI and IAI techniques (*3*) (e.g., layerwise relevance propagation (LRP) and backward optimization (BO)) to identify indicator patterns of forced changes (*4*). Building on our previous success, the XAI and IAI techniques can be used to identify and compare indicator patterns or emergent properties of ACI from E3SM ensemble simulations (with perturbed physics (*5*), varying resolutions (*6*), or perturbed emissions (*7*)) and global observations (e.g., meteorological analysis, satellite data, etc.). The goal is to track down the impacts of parametric uncertainty, resolution, and emission uncertainty on ACI locally (through fast physics) and remotely (through circulation feedback). This research activity helps to address the first three science challenges and identifies the structural deficiencies of E3SM that requires development efforts.

Over the last few years, our team has used AI/ML approaches to emulate subgrid processes (*8, 9*) and to develop physically regularized NN-based emulators for ACI parameterizations (*10*). The application of XAI and IAI discussed above helps prioritize development of emulators so that model developers can target critical model deficiencies and develop improved treatments. The development of better emulators will be based on a large ensemble of LES (*11*) that cover a wide range of aerosol, cloud, and meteorological regimes, process models (*10*) for individual ACI processes, or observations (*12*) (ground-based measurements, aircraft measurements, or satellites that provide process-level information). The newly developed emulators will replace or supplement ACI parameterizations in ESMs. Moreover, because even a perfect NN-based emulator does not necessarily lead to improvements in process representation due to limitations in model formulation for describing the process (*13*), AI/ML techniques can be used to expose those limitations. The challenge is to determine the right level of complexity required for accurate simulation of ACI in different aerosol, cloud, and meteorological regimes. For example, how many moments does a cloud microphysics parameterization need to describe the droplet spectrum to properly capture ACI processes such as autoconversion and accretion? How many moments does a turbulence parameterization need to accurately capture the cloud-base updraft velocity characteristics for realistic simulation of aerosol activation? Does the needed complexity of parameterizations depend on model resolutions and regimes of aerosol, cloud, and meteorology? To address this challenge, the VAEs can be used to verify the reproducibility of the data by a parameterization (or an emulator), providing an objective assessment to determine the minimum level of parameterization complexity that is usable in ESMs. This research activity helps to address all four science challenges and ensures the generalizability of process representations.

Finally, we have also used AI/ML approaches to correct the model bias online (*14*) with respect to observations or a high-resolution model simulation. This approach ensures that the ESM produces a realistic climatology. In the meantime, analyzing the bias correction term can provide valuable information on the model uncertainty and limitations in space and time. Applying this approach to E3SM ensemble simulations (with perturbed physics, varying resolutions, or perturbed emissions) can further improve our understanding and direct parameterization improvements.

Expected outcome

This whitepaper expects to establish new practices in Earth system modeling that integrate AI/ML approaches to improve the understanding and predictability of ACI and their manifestation in the Earth system. As ESMs increase in resolution and employ more complex physics, understanding and improving those models becomes more challenging. The new practices are expected to facilitate this process so that better and faster parameterizations can be more easily developed. This whitepaper focuses on ACI, but similar approaches can be adopted to address other Earth system predictability challenges.

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