AI-Automated Detection of Subgrid-scale Processes for Adaptivity Guidance

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Focal Area(s)

The proposed white paper focuses on focal areas 2 and 3, and intends to build a pipeline to automate the detection of unresolved processes based on model errors and assist subsequent modeling solutions.

Science Challenge

In Earth system science, many physical/biological and chemical phenomena happen at scales finer than the discretization of numerical models and are consequently unresolved at the grid scale. Unresolved processes create a major source of uncertainty and limit the predictability of Earth System Models (ESMs). The characterization and modeling of these fine-scale behaviors can improve the representation of the system mean, its ensemble spread and hence its predictability. This white paper targets unresolved processes within integrated water cycle components of ESMs. Our goal is two-fold: 1) the identification of local heterogeneities and anomalies that could be improved with finer resolutions or fully resolved subgrid-scale (SGS) models and, 2) the development of modeling strategies in regions of poor uncertainty. We propose an artificial intelligence (AI)-driven pipeline to automatically detect SGS water cycle processes to inform subsequent adaptive modeling. In particular, this framework applies to cloud dynamics, aerosol physics, soil micro-modeling, air-sea fluxes, and ocean or large lake circulation.

Rationale

Predictability of the integrated water cycle by ESMs is limited, in part, due to the inadequacy of representing the feedbacks of SGS and unresolved processes to grid scale and resolved phenomena. In the ocean, for example, the mixing that takes place when high-mode internal gravity waves break exerts a strong control on the large-scale stratification and overturning circulation. In the atmospheric water cycle, one of the largest uncertainties in climate simulations is due to model inefficiency in representing the SGS phenomena in cloud dynamics and microphysics. This is partly limited by model resolution which is too coarse to resolve turbulence and microphysical processes in clouds such as aerosol activation to droplets and to rain drops by collision and coalescence. In addition, variabilities of meteorological fields not resolved by the ESM grids influence aerosol generation, aerosol-cloud interactions and removal processes. On land, microtopography within the soil impacts water flows and storage, which affect soil biogeochemical cycles and other chemical and hydrological processes. Soils in ESMs, currently resolved at 25-50 km, do not allow microtopography changes on the scale of 0.1-1 m. Unresolved processes driven by microtopography can feedback to larger scales, though the mechanisms through which this occurs are

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not well understood. By improving our ability to detect SGS tendencies and their impact on the resolved scales of ESMs, we address the Associated Research Question 5 from the Integrated Water Cycle Scientific Grand Challenge of the CESD Strategic Plan. **Limited fine-scale information:** Fine-scale information from observational data or high-fidelity model outputs is rarely available over extended regions, limiting our understanding of fine-scale processes and hence their modeling. For instance, mesh sizes of ocean models in ESMs are coarse, and bathymetry and seabed features are sparse compared to the length scales of seabed elements. However, SGS seabed features such as abyssal hills or mega-ripples influence internal gravity waves and boundary layer turbulence, and hence affect ocean circulation and mixing. In the same vein, high-fidelity cloud microphysics and turbulence models such as direct numeric simulation simulate unresolved sub-grid processes in clouds. However, they are performed case-by-case, due to their computational expense---even on leadership-class supercomputers---over a large domain. **SGS parameterizations:** SGS parameterizations are often based on idealized theoretical or empirical models of the SGS process (e.g., interfacial stress and drag forces, and in-cloud liquid water content and updraft velocity). Often, the same SGS parameterization is used over different regions or model resolutions, leading to sub-optimal representations of SGS tendencies. Recently, stochastic models have been used to enhance the SGS variability (e.g., stochastic enhancement of air-sea fluxes; Bessac et al. 2019). Finally, refining meshes is limited by the lack of scale-aware SGS parameterizations. For instance, some of the microphysics parametrization for shallow clouds in the DOE's Energy Exascale Earth System Model (E3SM) (Golaz et al., 2019) needs to be re-tuned for high-resolution (~0.25 degree) configuration from standard resolution model (~1 degree). **Mesh refinement limitations:** Regions within ESMs can be targeted for mesh refinement to directly resolve flows, in particular for unstructured mesh models such as E3SM. For instance, recent studies have explored how to vary ocean mesh resolution based on physical characteristics (e.g., coastline complexity and topographic gradients) and posterior information (e.g., sea surface variability) (Hoch et al., 2020; Pringle et al., 2020). However, the influence of teleconnections (e.g., effects of distant ocean currents on coastal flows and vice-versa) and the complexity of coupled interactions within ESMs makes the generalization of even static mesh design extremely challenging. Finally, the specification of mesh resolution should consider simultaneously the employment of SGS parameterizations, especially in transition regions between high and low resolution meshes; but the implementation of SGS parameterizations in transition regions is often unclear.

Narrative

An AI workflow is proposed to improve fine-scale modeling of water cycle processes. The pipeline comprises: 1) unifying representation of model outputs and available observations to extract reliable errors and biases; 2) detecting features (e.g. regions or compound processes) leading to unresolved processes; 3) deciding on the best adaptation strategy, such as adaptive mesh refinement (AMR) or SGS models; and 4) incorporating the best adaptation strategy to improve model errors. The pipeline automates and assists identification of SGS processes and adaptive optimal modeling solutions, hence bringing together DOE's observational capabilities, exascale high performance computing (e.g., Aurora and Frontier), and E3SM model developments to improve the Earth system predictability. 1**. Augmented model outputs:** Model errors and biases will be calculated using climate simulation ensembles and where available, observations. These ensembles include previously completed model simulations (existing results from the Coupled Model Intercomparison Project) along with new simulations of different regional refinement and physics configurations or local high-fidelity simulation outputs (Schneider et al. 2017). Observational data are typically sparse and will be augmented by ML techniques (Fukami et al. 2020). Available data are, for instance, DOE's Atmospheric Radiation Measurement observatories, which provide detailed observations of atmospheric properties for the last several decades. By merging partial sources of information, the resulting model-model or model-observation augmentation lowers the use of computational resources over extended areas and/or model configurations. This augmentation serves as an enriched basis to estimate model errors along with resolution information and physics specifications. **2. Detection of unresolved processes:** The detection of features (processes and their compounds) and/or regions leading to unresolved quantities will be automated and rely on metrics that quantify the remaining SGS content (Maulik et al., 2019). These metrics will be resolution-dependent statistics or proxies, which machine learning (ML) techniques will map out from the augmented model outputs. The detection of features or regions will be automated through ML techniques such as semi-supervised learning guided by existing knowledge about unresolved processes. This setup further allows to identify transition regimes between high and low resolution in which scale-aware SGS parameterization is needed as a standalone or to accompany mesh refinement. **3. AI-assisted decisions for model improvement:** Having detected SGS features and their sensitivity to resolution and mesh configurations, an AI-decision tool will employ the best strategy for AMR or SGS models automatically or guide a user towards model improvement. For instance, non-obvious relationships between model resolution and cross-component coupled interactions will inform the development of accurate mesh configurations for a given computational cost. **4. SGS solutions:** Scale-aware SGS parameterizations will be developed to complement mesh refinement, or as a standalone model component (Bessac et al., 2020). ML techniques will be combined with a stochastic framework and available physics knowledge. By implementing stochastic SGS parameterizations into ESMs and running large numbers of ensembles, AI techniques can map SGS sensitivities to observable quantities. This motivates increased efforts in stochastic forms of SGS parametrization that reveal information that cannot be retrieved from deterministic processes, which rely on inputs of fluid flow and data at the resolved scale. **5. Adaptive mesh refinement:** Our proposed workflow for unresolved SGS processes creates a path to incorporate SGS parameterizations and AMR into E3SM components. AMR is especially challenging in the context of coupled climate models, where the coupler must deal with the independent time evolution of each component's mesh in order to exchange fields in a conservative manner. While indicators for adaptivity traditionally act locally at each cell, opportunities for ML-aided techniques exist in form of extraction of non-local couplings (Fidkowski & Chen, 2021), where AI helps detect wider-ranging interactions that induce refinement due to teleconnections. AI-based prediction of adaptivity can aide parallel load balancing of meshes by reducing communication. Current AMR approaches insufficiently mark cells for refinement due to cross-component interactions; new AI-based refinement criteria, could incorporate learned mesh resolution requirements from coupled interactions within ESMs.

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Suggested Partners/Experts (Optional)

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