A Grand Challenge "Uncertainty Project" to Accelerate Advances in Earth System Predictability: AI-Enabled Concepts and Applications

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Focal Areas

The proposed grand challenge project is AI-enabled via application of machine learning (ML) to climate model and observational data streams (focal area 3), and applications include AI-guided observing system design and model/component/parameterization selection (areas 1 and 2). The project is structurally agnostic as to whether model or observing system components use AI approaches or not, but uncertainties must be estimated and propagatable in both.

Science Challenge

Global model intercomparison projects (MIPs) have often sought to inform the uncertainty in earth system model (ESM) predictions of societally relevant quantities such as equilibrium climate sensitivity (ECS) by a range or probability density function (PDF) over contributed simulations. However, the assessment of uncertainty in any given ESM's predictions has been essentially limited to a small ensemble over random internal variability, which is generally dwarfed by any given model's uncertainty associated with physics parameterization choices.

Here we propose an "uncertainty project" that will deliver a PDF of predicted quantities from every participating ESM, wherein prediction spread will furthermore be traceable to the uncertainty of underlying parameter choices, and spanning multiple models will span structural choices—yielding a simple yet paradigm-shifting methodological advance. The framework will simultaneously enable multi-ESM climate observing system simulation experiments (COSSEs), and provide a systematic assessment of the key knowledge gaps that require additional laboratory, field, and process study to reduce uncertainties in societally relevant predictions.

Rationale

This proposal is emerging from GISS ModelE3 ESM development in the area of cloud physics, so we begin with an example of research needs/gaps from that work. Here, some of our greatest development concerns arise where we lack fundamental process-level understanding, as in ice formation. Namely, it is currently unclear what is the main *process* that is forming the majority of ice crystals in commonly occurring convection, apparently via secondary ice production at warm temperatures. We are keenly awaiting laboratory data for candidate mechanisms, which is not yet in hand to crucially establish their efficiency. Our progress is also hampered by a lack of uncertainty characterization in currently available measurements of ice crystal number size distributions. Furthermore, the same multiplication process may be responsible for a majority of ice crystals in many extratropical mixed-phase clouds, whose variable representation in CMIP6 ESMs may be a leading cause of differences in cloud phase feedback and ECS. Yet we have been required to deliver an ESM with the cloud physics knowledge at hand.

For CMIP6 the GISS team devised an AI-enabled means of addressing such sources of uncertainty by preparing a small *physics* ensemble rather than a single ESM configuration. To our knowledge this is the first explicit such effort to be submitted to CMIP. As briefly described below, we also used human intelligence to deliberately span a wide range of diagnostic primary ice production (as a proxy for uncertain secondary mechanisms) during final winnowing of physics parameter sets. Here we propose that this recently completed GISS effort demonstrates the success of an AI-driven foundation that can be much further exploited to supply a full PDF of targeted predictions such as ECS.

DOI: https://doi.org/10.2172/1769643
DOE BER, AI4ESP 2021 #AI4ESP1046 (https://www.ai4esp.org)

Inherent to the GISS approach is the use of global data sets with prescribed uncertainty characteristics to select "equally good" physics parameter sets. Adding a synthetic data set at this point would lead to a COSSE suitable to guide observing system design. For instance, a reanalysis-based data set could be added to consider designs for the Planetary Boundary Layer mission that is currently in NASA's Incubation program. Systematic use of COSSEs could remove a great deal of guesswork from such major national investments, and would directly engage ESM development centers in such decisions. COSSE results that demonstrate outstanding value (via reduction of uncertainty in high-value predictables) could furthermore quantitatively support marginal increases in mission cost and risk where they are warranted for societal benefit. Such a COSSE-like approach could be similarly used to guide investments in ground-based long-term measurements to reduce leading uncertainties (e.g., of ice nucleating particles and aerosol properties).

To estimate uncertainties in ESM cloud physics parameters, the GISS team relied partly on case studies that had been used for ModelE3's development in single-column model (SCM) mode, compared with large-eddy simulations (LES). Any level of microphysics model detail may be used in such LES case studies (two-moment, size-resolved bin, or Lagrangian particle-based), allowing a highly flexible connection to the process-level knowledge gaps that underlie many ESM cloud physics parameterization uncertainties. It has furthermore been demonstrated that an SCM's behavior is highly predictive of its parent ESM skill in global simulations, offering a concise "physics fingerprint" of that ESM. LES intercomparison case studies (many based on DOE data) have become widely used in process studies and model development. The French modeling community recently proposed international file format conventions for LES/SCM case studies arising from their use spanning weather and ESM development. Such LES cases have also recently been used to directly estimate cloud-climate feedback parameters as a function of cloud type. Here we propose establishing an LES/SCM case study library associated with this "uncertainty project" that will serve as an efficient foundation for testing ESM sensitivity to parameter combinations in SCM mode, identifying key knowledge gaps in physical processes (against field observations), and integrating parameterization advances based on new laboratory data.

We have introduced motivating uncertainties in ice formation, but the GISS development process considered uncertainties in many other processes. In the brief narrative below, we describe how our AI-enabled development process arrived at a small physics ensemble for submission to CMIP6, so we know that the first proposed steps are achievable for a multi-ESM effort.

Narrative

We first describe the four basic steps taken during ModelE3 development:

1. **Identify uncertain ESM parameters and estimate uncertainty ranges.** We first identified ~40 parameters in the convective and stratiform cloud schemes that impact process rates (e.g., warm and cold rain formation, entrainment and detrainment) and cloud properties, including microphysics (e.g., ice crystal fall speeds) and macrophysics.
2. **Perform a perturbed parameter ensemble (PPE) with Latin hypercube subsampling over the multidimensional parameter space, and report diagnostics for comparison with observational data sets.** We used 1-year fixed-SST runs at a resolution lower than operational, and predicted diagnostics for apples-to-apples comparison with roughly 20 satellite data streams.
3. **Apply an AI-enabled emulator approach to predict the same diagnostics over the full parameter space.** Numerous neural network (NN) candidates with varying hyperparameter choices were trained on the PPE to emulate the model response of observable quantities to parameter perturbations, and a subset of highest-fidelity NNs (as judged by a separate validation PPE) were selected for use in the next step.

4. **Evaluate a cost function describing biases over the full parameter space against the satellite data streams within their defined uncertainties.** Parameter probability given observational constraint was estimated via Bayes' theorem by sampling the parameters using a Markov Chain Monte Carlo algorithm. Briefly, a modified random walk was performed in the 45-dimensional parameter space, at each point comparing the NN emulator's predictions to the constraining observations, resulting in a probabilistic map across the multiparameter space.

With these results and human intelligence at the fore, we then selected a small ensemble with deliberately diverse physics parameters. Here we propose that adding another sampling step and another emulation step would more fully realize the information content obtained by step 4:

5. **For a more complete ESM scenario (e.g., taking a slab ocean approach to estimate ECS and cloud feedbacks), perform an ensemble over diverse physics configurations selected based on the results of step 4.** Run relevant predictive simulations (versus 1-year in step 2) with equally rated but diverse physics parameter sets that also offer close agreement with radiative balance.
6. **Apply an AI-enabled emulator approach, trained on the results of step 5, to predict ESM scenario outcomes over a wider range of highly rated physics parameter sets.** Steps 5 and 6 parallel steps 2 and 3, except that the predictions of interest are now societally relevant model predictions (rather than outputs for comparison with global data sets).

The results of steps 5 and 6 could yield an AI-enabled estimate of ECS PDF over the uncertainties selected in step 1 for any given ESM, for instance. Alternate ML algorithms could readily be considered at steps 3 and 5, such as Gaussian process models, which naturally include a measure of emulator uncertainty. Comparison with global and long-term data sets could also incorporate instrument simulators and explicit observational targets such as the interannual variability of low cloud cover.

We note that this AI-enabled process operates on one structural baseline ESM configuration (parameters must be smoothly variable), but future efforts could optimize an approach to span structural modifications (on/off switches or scheme swaps). An initial exercise could also be more limited in scope, such as targeting stratiform warm and cold rain process uncertainties that have been identified as likely causes of CMIP6 ECS spread. ESM teams need not agree on schemes or parameter ranges, as these could be independently selected. The project requires ESM PPEs, and would benefit greatly from an SCM case study library over which physics parameter sets could be systematically tested. The project requires global observational constraints (thus organically integrating satellite data), but ESM teams need not agree on which are included or how in steps 3 and 4, and the project would benefit greatly from more detailed ancillary data. For instance, GISS is currently preparing DOE ARM long-term data and a forward simulator approach to evaluate precipitation processes that are not as well observed from space.

Why an ESM development community project? By fitting multiple ESMs with ML algorithms, directly comparable "uncertainty fingerprints" would be efficiently contained and shareable, as in a MIP archive. Such an overall "uncertainty project" (UP) would enable acceleration around the cycle of identifying knowledge gaps and filling them in a way that does not currently exist in the MIP framework. This project relies in equal parts on maturation of uncertainty estimation in both observations and models. Introducing traceability of uncertainties in ESM *predictions* to uncertainties in *parameters* overcomes a profound barrier to progress generally encountered in mining the data collected by MIPs: there is currently no direct way to understand how ESM parameterization uncertainties contribute, much less what are the additive and offsetting contributions that likely exist. Since this approach has never been tried, decisions would need to be made at a project level as has been demonstrated for MIP design. However, the most essential step is to decide that this route—a laser focus on uncertainties and their observational constraints across ESMs—could be transformational and is worthy of pursuit.

Suggested Partners/Experts

We suggest that the following experts across relevant areas may be able to present a related webinar or plenary presentation at a workshop (not all contacted; deferred to workshop planning):

- Jim Mather, DOE ARM — Role of MIPs in the current ARM Science Plan, historical and current context, future plans.
- Frédéric Hourdin, LMD/CNRS/UPMC — Overview of the pan-French DEPHY project for weather/ESM development using SCM/LES case studies, including use of ML for optimal parameter estimation.
- Israel Silber, Pennsylvania State University, and Scott Collis and Robert Jackson, DOE and Northwestern University — Development of the EMC2 open source ground-based lidar/radar simulator for evaluating ESMs, potential for “uncertainty-aware” applications to ESM outputs and observational data sets at fixed sites
- Daniel Knopf, Stony Brook University, and Nicole Riemer, University of Illinois — Role of closure studies in narrowing uncertainty in ESM ice nucleation schemes, potential for modular inclusion in the context of an ESM “uncertainty project”.
- Derek Posselt, NASA/JPL — Potential for the COSSE approach in NASA Earth observing system design.