DARPA ACTM: Milestone 1 Report

AIBEDO: A hybrid AI framework to capture the effects of cloud properties on global circulation and regional climate patterns

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This milestone report expands on the model development details of hybrid model constituents: data-driven and physics based components, list of datasets to be used for training and validating the model, and an elaborate list of input and output variables to be extracted from the datasets.

Live documentation: https://aibedo.readthedocs.io/

Hybrid Model

Overall Model Development Update

1. We have identified the various hybrid model components: spatial, temporal and relevant physics constraints
2. We are exploring the components and variants of model architecture for different spatial and temporal resolution, computational trade-off, and interlinking of model parameters
3. We are developing an alpha version of the model to check data compatibility, model feasibility, and possible extensions

The hybrid model in AIBEDO consists of separate data-driven components for spatial and temporal dimensions and a set of physics-informed constraints that preserves the laws of physics and ensures generalizability across various scenarios. The data-driven components are carefully selected and tailored for AIBEDO: a spherical U-net model architecture to capture the earth system model variables, a multi-time scale LSTM network that can capture the decadal and seasonal trends in two different stages. These components, together with the physics constraints, would be a fully differentiable hybrid model that captures the relationships between the radiative effects of clouds, the atmosphere and ocean circulation, and regional temperature and precipitation.

Spherical U-Net Model Architecture

U-net is a specific form of convolutional neural network (CNN) architecture that consists of pairs of downsampling and upsampling convolutional layers with pooling operations (Figure 1) [1]. Unlike regular CNNs, the upsampling feature channels help the model learn the global location and context simultaneously. This technique has been proven extremely useful for biomedical applications and recently has been adopted in the earth sciences. While this is a more effective technique, one of the limitations of U-net architecture when applied to earth sciences is the inability to capture the spherical topology of data. Typically they are resolved by including boundary layer conditions/constraints. In our approach, we adopt a variant of U-net called "spherical U-net" for modeling the spatial component of AIBEDO, which is a *geodesy-aware* architecture and hence accounts for the spherical topology of Earth System data alleviating the need for external architectural constraints (as in [2]).

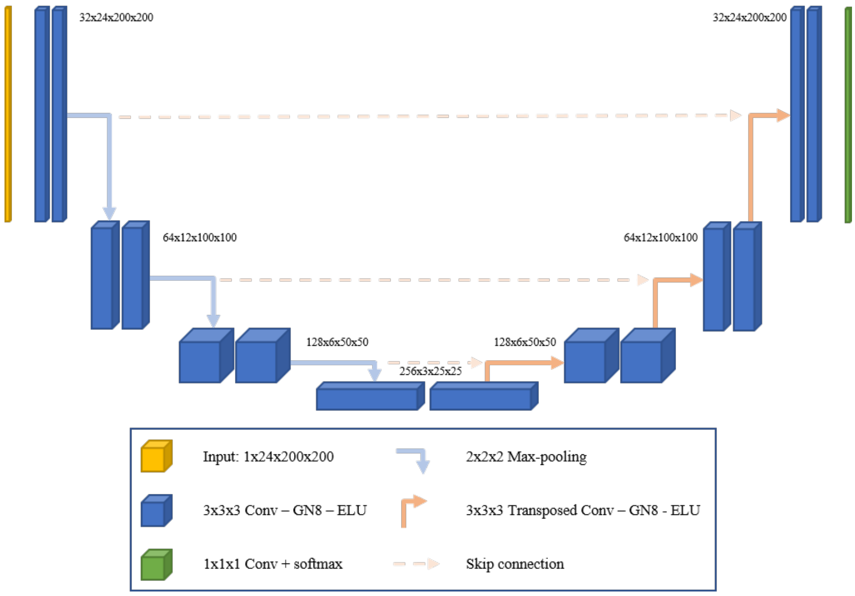

Figure 1: Standard U-Net Model Architecture [1]

The model uses special convolutional and pooling operations for representing spherical topology through Direct Neighbor (DiNe) convolution and spherical surface pooling operations (Figure 2). Also, the model takes input in the icosahedral surface for the better representation of the earth surface by resampling from the original 2-dimensional NetCDF grid data.

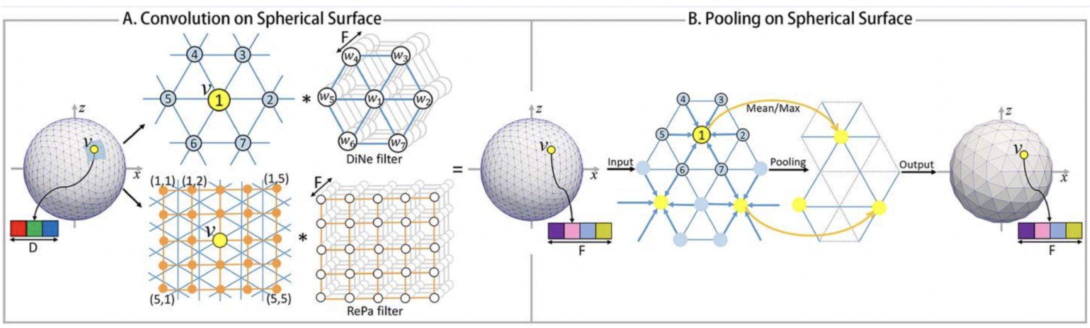

Figure 2: Convolution and Pooling Operations in Spherical U-Net Architecture (Source: Zhao et al. [3])

> **Ongoing Work:** PARC team is currently exploring and developing variants of CNN, U-net and Spherical U-Net model architectures using a subsample of Earth System Model output data. We are documenting the model accuracy, computational complexity and bottlenecks of each model architecture. We are exploring the feasibility of graph-based sampling for the spherical network model (such as the DeepSphere architecture [4]). We will continue to expand the data points in model training as and when we receive the preprocessed data from the University of Victoria team.

Multi-timescale Long Short-Term Memory (LSTM) Networks

While the spatial model maps cloud properties with circulation and regional climate variables for a given step, the temporal component aims to predict the output for the next time step for a set of input conditions. Our goal to model temporal component is to initially understand how the circulation, precipitation, and temperature could change over time and subsequently observe if there are any patterns of climate tipping points. The tipping point characterization in our model does not intend to model the dynamics of nonlinear feedback loops in the earth system, but we would look at the large-scale trends over time at the decadal scale first, and then narrow down to any changing trends in seasonal scale to identify "early-onset" of tipping points.

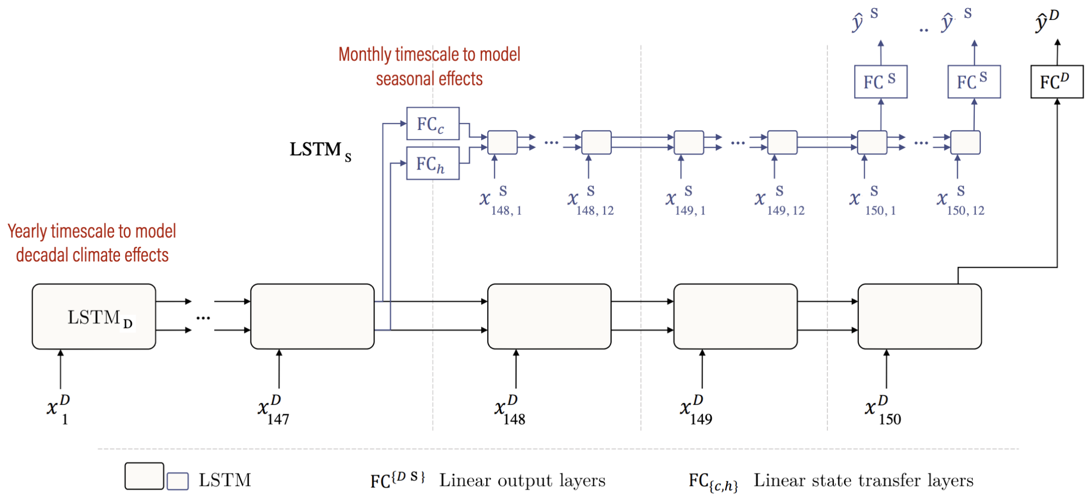

Figure 3: Components of Multi-Timescale LSTM Model (Adapted from Gauch et al. [5])

We use two distinctive LSTM networks to implement this functionality: one for modeling long-term climate impacts at the decadal scale ($LSTM_d$) and another for modeling shorter-term seasonal changes ($LSTM_s$). We will run the decadal-scale model $LSTM_d$ first, where we will make yearly predictions. The hidden states of $LSTM_d$ at every year will then be used by $LSTM_s$as initial states to make monthly predictions. Since the two LSTM branches may have different hidden sizes, we will feed the states through a linear state transfer layer. Figure 3 shows an illustration of a multi-time scale LSTM network.

> **Ongoing Work:** PARC team is implementing the temporal model using two training schemes:
>
> - *Teacher forcing strategy*: we are designing the both LSTM approaches as feed-forward networks, where the ground truth from a prior time step will be used as input
> - *Curriculum learning strategy*: we will increment the task difficulty by gradually increasing the rate of using predicted value from current time step by feeding to the input of next time step prediction
>
> In addition, we are also exploring pros and cons of structurally combining the spatial and temporal components effectively.

Physics informed constraints

Training a machine learning model is often times stochastic and involves learning the input-output mapping, successfully. In complex physical systems such as cloud-atmosphere interactions, there might be situations where this mapping is unique and a machine learning model may learn non-unique solutions as it has no previous underlying knowledge of the dynamics and may even overfit to the training data. This causes the model's generalizability to unseen conditions and future predictions to suffer. To hedge against this risk, often times physics-informed constraints, applied to model learning, can be useful [6, 2]. This is a critical step in building a model that is generalizable, and produces bounded and physically consistent results.

For the hybrid model, we will impose two major physics-based constraints:

- The energetics-based radiative forcing budget, and
- The energetics-based local precipitation budget.

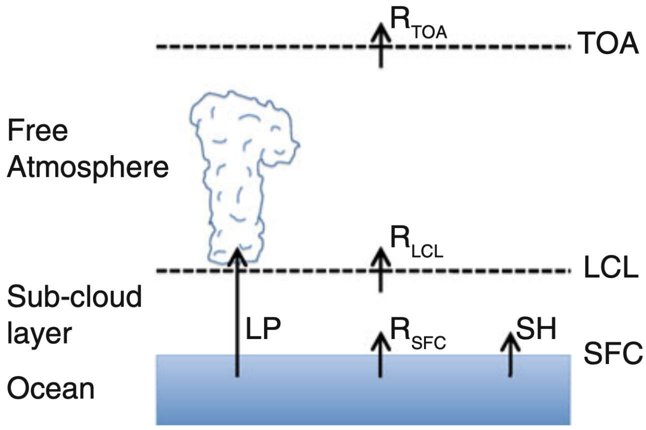

Figure 4: A schematic of the typical energy budget. Adapted from Takahashi (2009) [7]

Energetics-based radiative forcing budget

The response to any radiative forcing is constrained by energetics. Roe at al. [8] show that in response to a forcing, the local energy budget equilibrates via (1) climate feedbacks that modify the top-of-atmosphere (TOA) radiative fluxes, and (2) changes in horizontal energy transport (by the atmosphere and ocean) and energy storage (by the ocean). Previous studies [8] indicate that response of the TOA fluxes and moist static energy transports can provide a leading order estimate of the temperature response. It is well understood that climate feedbacks to perturbations (as in changes in clouds or radiative forcing) impacts climate variables both locally, and remotely [9, 7, 10]. Functionally, the climate response due to an imposed cloud radiative forcing can be described as

$$R_{cl} = \lambda \Delta T - \nabla \cdot (\Delta F_{atm}) - \nabla \cdot (\Delta F_{ocn}) - \Delta OHU \tag{1}$$

where R_{cl} is the term that accounts for the contributions from the radiative forcing due to clouds, $\lambda \Delta T$ incorporates the effect from radiative feedbacks λ, OHU is the ocean heat uptake, ΔF_{ocn} is the change in the ocean heat transport, and ΔF_{atm} is the change in the atmospheric moist static energy transport.

Local precipitation budget

In response to any climate perturbation, the local precipitation response can be diagnosed through the changing energy budget of the column, which includes top-of-atmosphere and surface flux constraints and horizontal dry static energy divergence [11]. Mathematically, this can be represented as

$$L\delta P = \delta Q + \delta H \tag{2}$$

where P is the precipitation rate/flux, L is the latent heat of condensation, H is the change in the vertical flux integral of the dry static energy, and $Q = R_{TOA} - R_{SFC} - SH$ (where the R_{TOA} are the top-of-atmosphere fluxes, R_{SFC} are the surface radiative fluxes, and SH is the surface sensible heat flux), and δ denotes the difference between the two climate states.

Ongoing Work:
We are implementing the above as soft constraints in the loss function of the hybrid model as a Lagrangian multiplier, a form of regularization for the model and is based on previous studies for modeling non-linear dynamical systems [6, 2]. The formulations from literature are carefully chosen such that they are applied to constraining the top of the atmosphere and surface fluxes, thereby reducing the computational challenge and further simplifying the model development.

Datasets

We will be using output from several Earth System Models (ESMs) from the Coupled Model Intercomparison Project (CMIP) for training the hybrid model, and observational reanalysis data for validation and finetuning.

Training

Historical and future CMIP5/6 model output, focusing on seven state-of-the art ESMs with the highest quality metrics:

1. CESM1 (Community Earth System Model 1)
2. CESM2 (Community Earth System Model 2)
3. CESM2-WACCM (Whole Atmosphere Community Climate Model)
4. UK-ESM1 (The UK Earth System Modelling project)
5. E3SM-1-0 (Energy Exascale Earth System Model)
6. MPI-ESM (Max-Planck-Institut für Meteorologie)
7. MIROC6 (Model for Interdisciplinary Research on Climate)

Validation

To reduce biases present in the Earth System Model output, we will validate with state-of-the-art observational reanalysis data:

1. ERA5 (the latest European Centre for Medium-Range Weather Forecasts Reanalysis)
2. MERRA2 (The Modern-Era Retrospective analysis for Research and Applications)
3. NCEP (from the National Centers for Environmental Prediction)
4. JRA-55 (the Japanese 55-year Reanalysis)

All the observational reanalysis data listed above are available from hourly to daily timescales, which are finegrained enough to validate the model at both LSTM timescales.

Model variables

We will process all variables such that the seasonal cycle and forced trends from GHGs/aerosols are removed and all are re-gridded to a standard grid ($1^\circ \times 1^\circ$).

The **input variables** that will be included in the model are:

1. Cloud top temperature, which accounts for height of the cloud top and affects the top-of-atmosphere (TOA) emissions of the cloud
2. Optical depth, which accounts for the liquid water content and cloud condensation nucleus number of the cloud
3. Planetary albedo (reflectivity), which includes both the impacts of clouds and the impacts of clearsky albedo anomalies due to water vapor
4. Cloud radiative forcing, which is computed as all-sky net TOA flux minus the clear-sky net TOA flux

The **output variables** which the model will be trained on are:

1. Sea level pressure, which is a proxy for the lower tropospheric circulation
2. Surface skin temperature and/or surface air temperature
3. Precipitation
4. Ocean heat content, using the weighted vertical integral of 3-D ocean temperature
5. Global ocean overturning streamfunction and/or barotropic streamfunction

In addition to the above, we have identified the following **variables that are needed for formulating energy constraints**:

1. 3-D air temperature to compute the top-of-atmosphere radiative change due to the temperature feedback
2. 3-D specific humidity to compute the top-of-atmosphere radiative change due to the water vapor feedback
3. 3-D ocean temperature which we will use to compute the 2-D ocean heat storage
4. Surface albedo for computing the top-of-atmosphere radiative change due to the surface albedo feedback
5. Top-of-atmosphere and surface clearsky/allsky fluxes for computing (a) the cloud feedback and (b) for computing energy transports

Spatial and temporal resolution

- **Spatial resolution:** all variables re-gridded to 1°, as this is the typical resolution of CMIP6-class ESMs.
- **Temporal resolution:** monthly, in order to capture inter-seasonal time scales of adjustment just beyond typical meteorological time scales (days to 1-2 weeks); time scale of forward mapping will be up to 10 years, to capture the longest time scales of adjustment in the coupled atmosphere, sea ice, and ocean mixed layer; note that deep ocean time scales are beyond the scope of the current work, as they may be >1000 years.

Preprocessing steps

We are currently developing the 'datacube' of Earth System Model output that has dimensions of [latitude, longitude, month, variable]. The preprocessing steps include the following:

- Remove the annual mean climatology (ascertained through a moving 20-year window), seasonal cycle, and trends
- Re-grid to a standardized latitude-longitude grid (for example, 180×320)
- 3-D cloud fields will need to be vertically integrated to produce 2-D fields (such as cloud water content output as a 2D field in CMIP)

> **Ongoing Work:**
> The University of Victoria team is setting up a pipeline to access and preprocess the model training datasets (the ESM output data described above) to set up the datacube for hybrid model development. The team will be releasing the data to the PARC team continually. In addition, the subject matter experts from the University of Victoria team are guiding the PARC team on appropriate physics constraints to be included in the model.

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