Physics-Informed Machine Learning Model for In-situ Life-Cycle Prediction of Condensation Trails

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Abstract

We develop the first end-to-end machine learning (ML) pipeline for prediction of the life cycle of condensation trails, i.e., starting with engine operating conditions leading to contrail formation, followed by cirrus cloud persistence. The few existing contrail models use simplified physics-based models, and therefore the predications deviate from the observations by extending the prediction horizon or in cases where the size of the contrail extends dramatically. Our pipeline is comprised of three stages: (i) given the flight and weather condition an auto-encoder-based regression predicts the profile of the initial phase of contrail formation of turbofan engines, i.e., double-jet mixing. (ii) A similar architecture then predicts the short-term horizon of formation, where the contrail substantially has evolved from its initial condition; (iii) a long-horizon LSTM is then rolled-out model with weather condition as exogenous forcing, using the output of the previous stage model as the first few time-steps of prediction. In our developed framework, high-fidelity physics-based simulations are used to generate the data for training. We only off-load the complicated physics of cloud microphysics to the ML models and retain the first-principal model of convection. At the inference, the model queries "an online" weather database to emulate an in-situ application of the model.

1 Introduction

While the aviation industry produces less than 2.5% of the CO2/NOx gases, it is estimated to be responsible for 3.5% of climate change. This disproportional contribution to effective radiative forcing can be traced to the effects of condensation trails (contrails) [1]. Regardless of the high uncertainty in the reported contribution, recent studies/attempts strive to schedule flight paths to lower the probability of contrail formation [2, 3], e.g., American Airlines "contrail avoidance" [4]. The effectiveness of such efforts remains, for the most part, unquantified [4] or at best, at the level of proof of concept [2]. This is mainly due to the lack of capability in predicting the long-term evolution of contrails, as many tools are based on simplified cloud thermodynamics with minimal contributions from microphysics, lacking enough fidelity to predict when and where a persistent contrail will form [5], and how that translates into radiative forcing. Although high fidelity resolution of the contrails by leveraging multi-physics solvers are possible over short-time horizons, the required wall-time and/or computational resource limits their usability in fleet or in-situ scenarios, where these predictions must practically be completed in a short wall-time or be updated with the constraint

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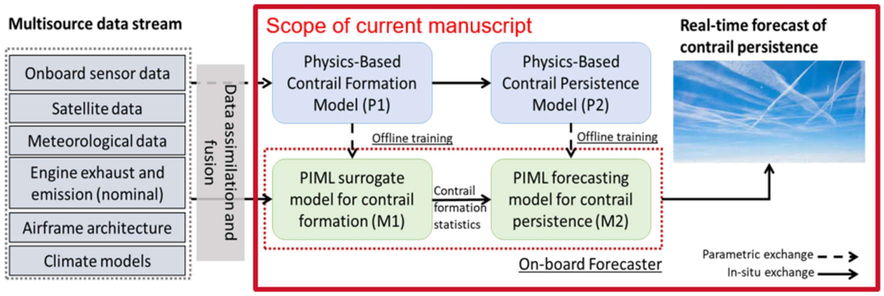

Figure 1: The CONtrail Forecasting through In-situ Reliable Multisourced Modeling and Sensing (CONFIRMMS)

of limited computational resources. Our contributions can be summarized as follows: i. the first end-to-end ML model of dynamics of contrail formation to formation of cirrus clouds (different than labeling the satellite images [6] or retrospect study of contrails, e.g., [7]), ii. which is trained on high-fidelity multi-physics simulations. We have built a Physics-Informed Machine Learning framework, cable of predicting the likelihood of persistent contrail formation with a lead time of up to 10 min at any point during the flight (CONtrail Forecasting through In-situ Reliable Multisourced Modeling and Sensing, i.e., CONFIRMMS, Figure 1). The scope of the current manuscript is the ML framework, which is designed to perform contrail prediction for any aircraft in the fleet, given the most recent update of the weather prediction or onboard sensors at any segment of the flight. The PIML is trained on high-fidelity multi-physics simulation data emulating the flight conditions over a range of seasons and weather conditions. The inference can be enhanced by including observation data from on-board sensors to detect visible contrail as well as satellite data for late-stage persistence.

2 Life-cycle of Contrails

For the sake of ML modeling, we have broken the life cycle of a contrail into two phases, (i) formation, and (ii) persistence. The governing forces, physics and timescale of these phases have motivated the design of separate ML models. In the initial steps engine exhaust mixing with the surrounding atmosphere, the engine/flight conditions are the governing factors, that can readily be available from the aircraft instrumentations. In the second phase, the mixture of engine exhaust and atmosphere disperses and is advected and goes through different weather conditions that are predicted using weather predictions, leading to aircraft-induced cirrus clouds.

2.1 Formation model

An axisymmetric steady-state double-jet fluid-flow model generates the fluid entrainment/mixing profiles for 150 m downstream of the engine exhaust (denoted by z). The thermodynamics of ice-particle formation are then incorporated to solve the number and size of ice participles, which then are represented by a visibility criterion, i.e., $\tau \propto N^2 d$; where N is number of activated ice particles, and d is the diameter of ice particles. This model is initialized with engine exhaust properties, estimated by a simplified model of turbofan engine given the flight and weather conditions. The entire $\tau(z)$ series as a function of the input parameters is predicted. This is a high dimensional prediction problem, since $\tau(z)$ is a series of dimensionality 150. The high dimensionality makes the prediction problem challenging. Hence, a dimensionality reduction is proposed using a fully connected autoencoder to reduce the $\tau(z)$ to a lower dimensional space of size 10 [7]. A neural network-based regression model is jointly trained with the autoencoder, which predicts the 10-dimensional latent space from the input parameter space (Figure 2).

2.2 Persistence model (Training)

Persistence model predicts the long-term evolution of the formed contrail states, i.e., visibility, cloud area, and ice diameter, at the location of the bounding box of a contrail given the weather forecast following the formation. This model ties with the formation model prediction. Our approach breaks

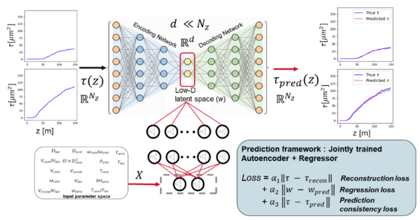

Figure 2: Joint dimensionality reduction and regression framework to predict optical thickness from input space of engine and atmopheric variables

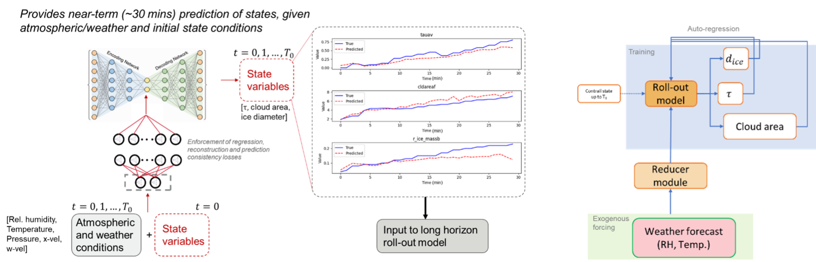

Figure 3: (Left) Joint dimensionality reduction and regression framework to predict optical thickness from input space, (right) Temporal predication of long horizon prediction of contrail states

down the persistence learning into two steps. Step 1: Transition model – predicts a short-term state of the contrail parameters given the initial condition from the formation model as well as the corresponding weather forecast for a pre-set length of time, here 20 minutes. Step 2: Long horizon roll-out model – auto-regressively evolves the state of the contrail for an arbitrary length of prediction, given the corresponding weather forecast, here 12 hours. The dataset for training of these models is sourced from weather forecasters (e.g., ECMWF) and the high-fidelity multi-physics simulations of the contrail.

2.2.1 Step 1: Transition to persistence model

We have trained an auto-encoder regression model to predict a fixed-time-horizon evolution of the contrail parameters (Figure 2). The initial condition of the state of the contrail as well as the near-term reduced statistics of a weather forecast are fed into the model. At the current stage of the development, the reduced weather statistics include relative humidity, and temperature at the center point of the bounding box of the contrail. The model returns a short-term prediction of contrail states which are then used to initialize the model of step 2.

2.2.2 Step 2: Long horizon roll-out model

An auto-regressive model with exogenous forcing is trained to predict the long-term evolution of the contrail. The model returns τ, d_{ice}, and cloud area at each time step, given the d_{ice}, and cloud area at the previous time-step(s), i.e., auto-regressive, for an arbitrary length of the prediction horizon. A classic deep Long short-term memory (LSTM) is trained with a linear layer that maps the hidden layer to the output vector [9]. The number of previous time-steps used for the prediction at the next step (i.e., lookback window) is one of the hyper-parameters and is the key motivation of defining the transition model developed in step 1, as we want to restrict our persistence model only to the initial condition of the contrail. At the inference stage, the model is initialized with output of the transition model and then rolled out based on its own output to an arbitrary prediction horizon. Additionally, the weather forecast up to and including the prediction step is reduced to 1-dimensional statistics and is input of the model as an external forcing, making the model capable of handling exogenous forcings.

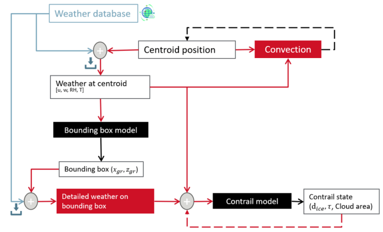

Figure 4: Roll out of the trained model at inference which combines physics-based convection with the ML model

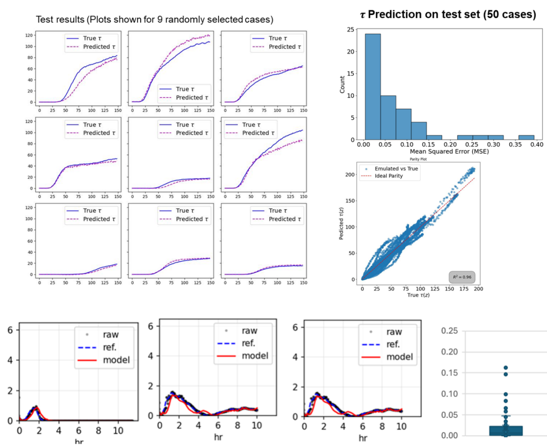

Figure 5: Direct prediction of $\tau(z)$ profiles from the input space. Left panel shows a qualitative comparison of the predicted and the true (CFD generated) profiles. The right panel shows the results – the MSE and the parity plot. Bottom panel shows, the $\tau(t)$ over long-time horizon of some cases, and boxplot of the MSE error of test cases

2.3 Persistence model (On-line inference)

In the previous steps, the transition and roll out models are trained using off-line weather data, i.e., the contrail path and bounding box are precalculated and all the weather data is extracted the path of bounding box of contrail. This approach assumes the weather at the location of the contrail as known, however, these variables directly depend on the location and size of the contrail, which should be inferred from the ML model. Accordingly, at the inference step, the path and limits of the bounding box are predicted independently. The path of the center of the contrail is predicted using a simple convection, additional models are trained to predict the limits of the bounding box. Note that the bounding box models can only have access to the weather data at the center of the box or detailed weather data of the previous time-steps. For other contrail state parameters, the weather details are then sampled from the bounding box and are fed into the contrail roll out model, as previously described. Figure 4 demonstrates the data pipeline at the inference step.

3 Experiments and results

To evaluate the prediction performance quantitatively, the mean squared error (MSE) of the predictions and the R^2 values are reported. The distribution of MSE in the test set is biased towards a low value (< 0.05), along with a high $R^2 = 0.96$, indicating high accuracy of the $\tau(z)$ predictions in the test set. This is particularly clear by evaluating the profiles (Figure 5). The output of formation model and an offline database of ECMWF predication is then passed to the inference model. The MSE error and the predicted visibility profiles of some of the test cases are plotted in Figure 5. Note that our model predicts location of the possible contrail, and querying the weather data predicts active contrail area, and the ice diameter given the humidity and temperature and history of contrail.

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