Introducing CREDIT-chem: A Hybrid Physics–Machine Learning Framework for Modeling Atmospheric Aerosol Chemistry

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Background

The Importance of Atmospheric Chemistry

Atmospheric aerosols are **central** to both **regional air quality** and **global climate forcings**. To create accurate earth systems projections, **models** must **simulate their life cycles** and **chemical reactions**, including radiative effects, cloud microphysics, and aerosol aging.

The Challenges & CREDIT-chem's advancements

- **Physical Solvers:** Trapped between **either high accuracy** (extremely expensive) **or fast approximations** (physical oversimplifications)
- **Existing Machine Learning (ML):** **Very fast**, but **not physically conservative** and **doesn't scale well** with more chemical species or higher resolution
- **CREDIT-chem:** Our framework aims to use **ML's speed advantages**, while maintaining **accuracy, scalability, and physical conservation**

Input and Target Data Setup

CAM6-chem Target Dataset

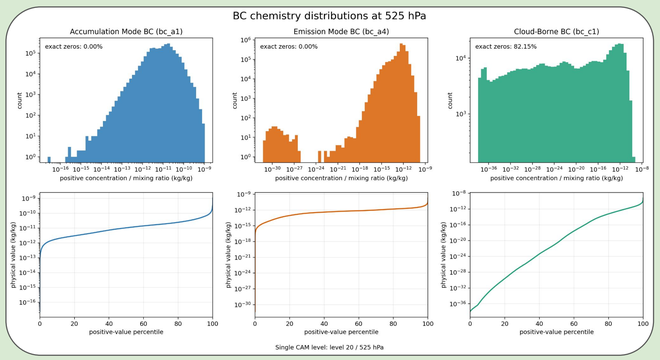
- **Data Resolution:** ~1° global resolution, 32 vertical levels, 1-hour time-step
- **Target Species:** **Emphasis on Black Carbon (BC)**; includes simulations for primary organic matter **(POM)**, secondary organic aerosols **(SOA)**, and **sulfates**; with given **meteorological inputs**

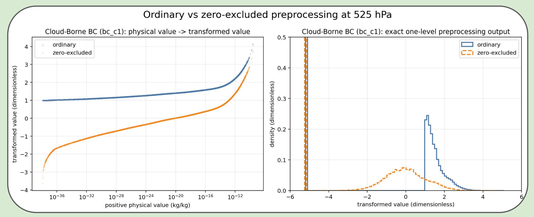
Quantile Transform – Zero Exclusion method

Chemical aerosol concentrations are **heavily non-normal**, **span multiple orders of magnitude**, and have **heavy zero-inflation**. Standard ML models **require normally distributed inputs** centered near 0 ($\mu \approx 0$, $\sigma^2 \approx 1$). To combat this, we developed the following transform method:

1. Empirically **fit a CDF** to exclusively all **non-zero aerosol concentrations**
2. Apply a **Logit transform to the CDF**, bounded to [-5, 5], to transform from a uniform distribution to a **normal distribution**
3. Exact **0 inputs** are **encoded as -5.25**; **outputs <-5.0** are **decoded to 0**

Methods - Data Distributions





Methods – Model Architecture

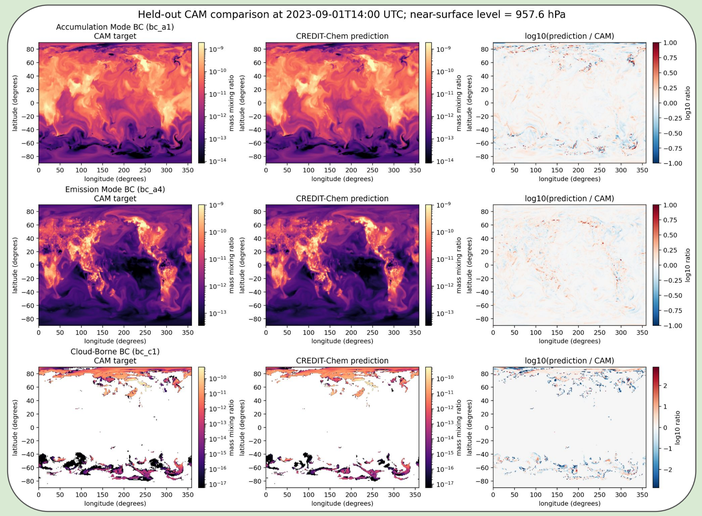
Hybrid Physical Transport–Columnar ML Prediction Scheme

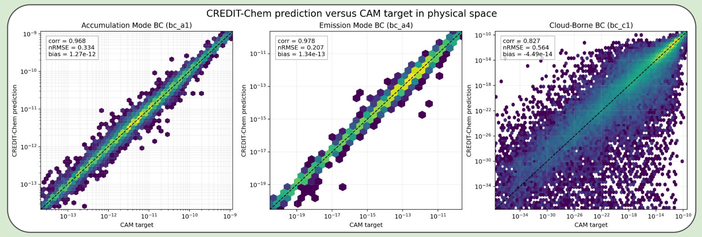
- **State Variables Update:** Initial **aerosol concentrations** and **meteorological variables** are **processed by a meteorological model** to yield updated state variables for the next time step
- **Physical Transport:** **Aerosol tracers** are **physically transported** across the global grid using a advection/convection scheme
- **Columnar ML Emulation:** The transported aerosols and updated state variables are **passed into the ML model,** which evaluates **each vertical column independently and in parallel** to predict local chemistry.

Why Columnar Predictions

- **Physical Constraints:** **Decoupling** aerosol transport with chemical processes allows for **explicit physical constraints**
- **Scalability:** Increasing grid resolution scales **inference time linearly**, while the **per column compute remains constant**
- **Model Capacity:** Processing a single column at a time allows for scaling to **much higher capacity models** while staying **fast at inference time**
- **Sample Richness:** Treating each column as a separate forecast allows for **much better generalization** compared to global models

Results





Conclusions

CREDIT-chem's Key Advantages

- **High Accuracy & Speed:** **Matches CAM6-chem outputs** with high correlation while **accelerating inference time** by multiple orders of magnitude.
- **Long-Term Stability:** Preliminary multi-step rollouts demonstrate **strong stability over extended time horizons**, validating its use for both short-term forecasting and long-term climate runs.

Limitations/Future Work

- **Comparative Performance:** Fully end-to-end ML models (e.g. CREDIT-chem cubed) **outperform the hybrid setup** under specific conditions, though they remain **bound by spatial resolution** scaling constraints.
- **High-Resolution Testing:** While the column-wise design is **theoretically built to scale**, testing accuracy and performance at sub-degree global resolutions **remains ongoing work.**
- **Transport Bottlenecks:** Framework runtime remains tightly **bounded by the efficiency of the physical transport** solver, especially at higher resolutions

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