Physics- and Chemistry-Informed Deep Learning to Advance Satellite-Derived $PM_{2.5}$ Data

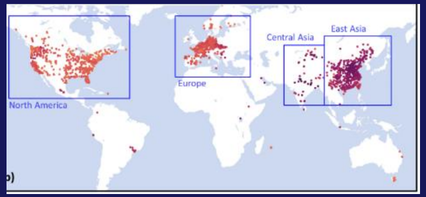
Randall Martin

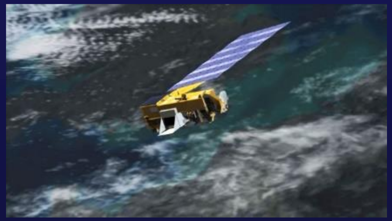
with contributions from

Nathan Jacobs, Chi Li, Siyuan Shen, Aaron van Donkelaar, Dandan Zhang

HAQAST Madison
May 13, 2026

Two Alternative Frameworks for Deep Learning





Deep learning

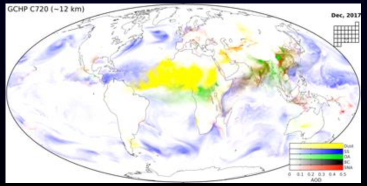
Direct $PM_{2.5}$ Estimates

Geophysical Satellite-Derived $PM_{2.5}$

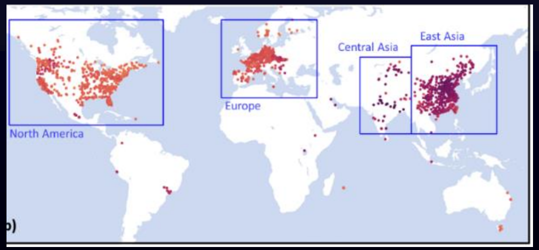
Process-Constrained $PM_{2.5}$ Estimates

Aerosol Optical Depth (AOD) from multiple satellite instruments and algorithms constrained with AERONET

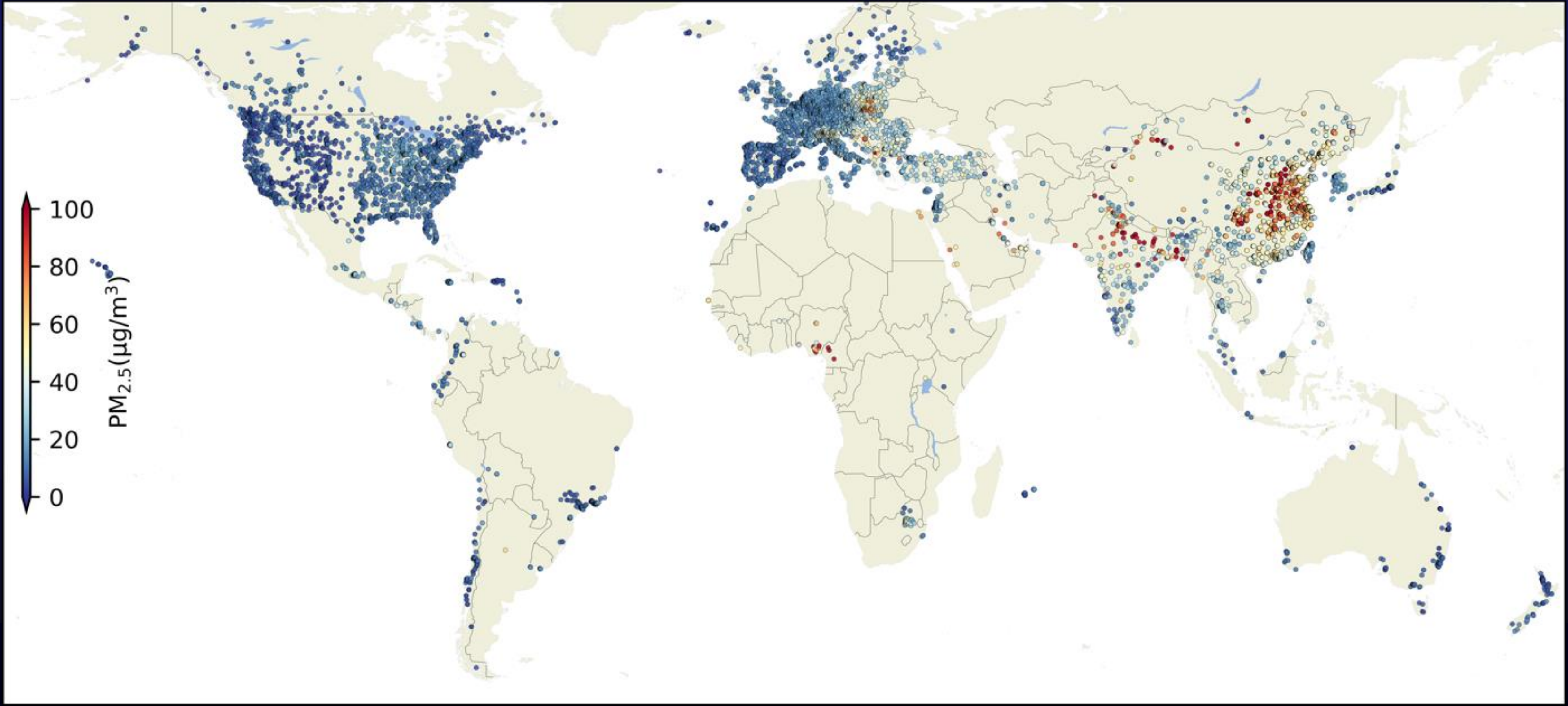
Apply Chemical Transport Model (GEOS-Chem) to Calculate coincident local solution to $PM_{2.5} = f(x,y,t,AOD)$



Deep learning



Ground-based Measurements are Unevenly Distributed and Autocorrelated

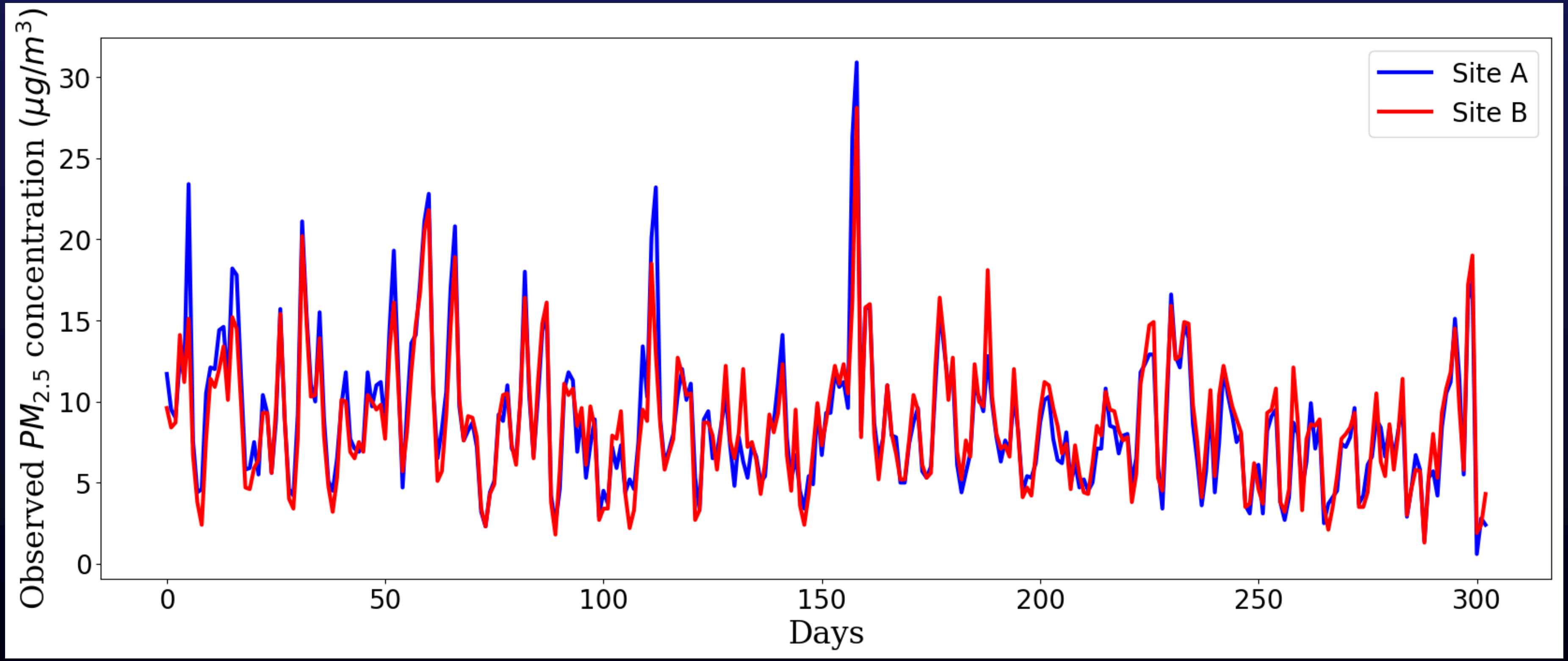


Shen et al., 2024

Nearby $PM_{2.5}$ Monitors Exhibit Autocorrelation

Withholding Adjacent Monitors in Traditional n-fold Cross Validation Overestimates True Model Performance

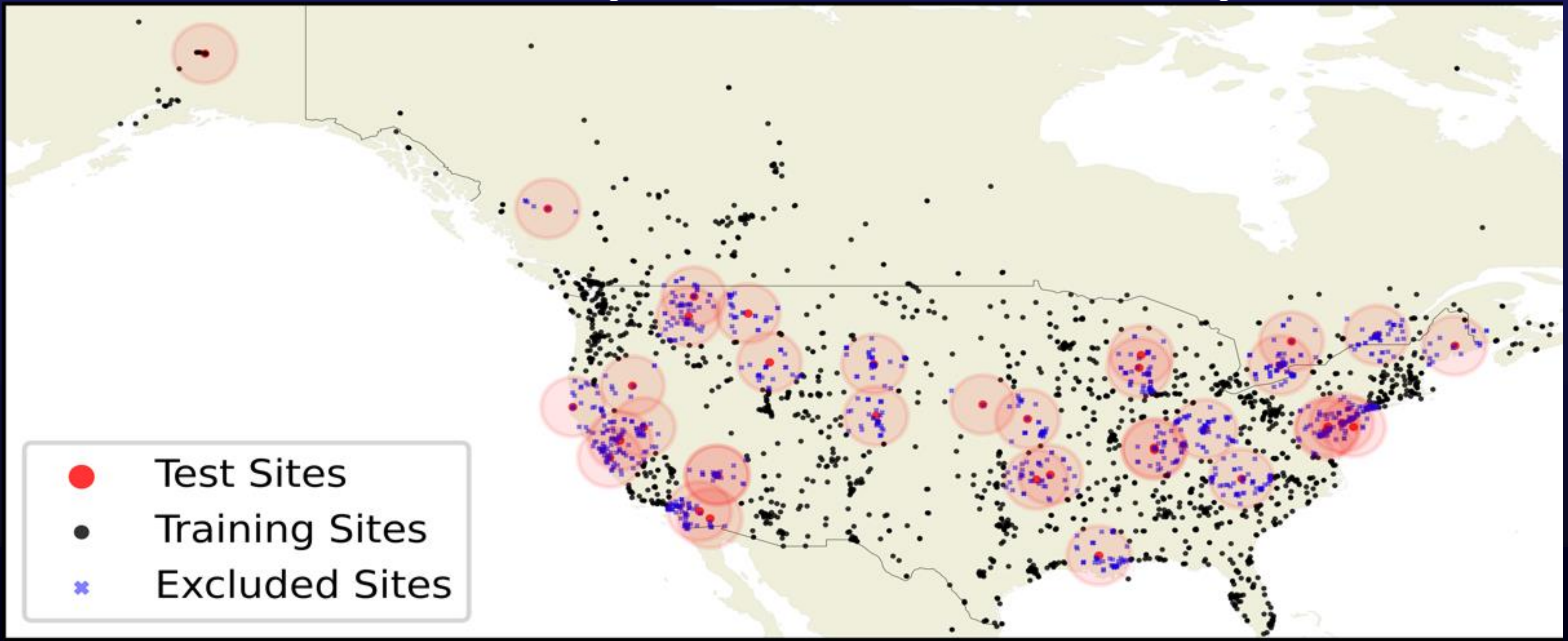
Timeseries of Two $PM_{2.5}$ Monitors 1km Apart



Siyuan Shen

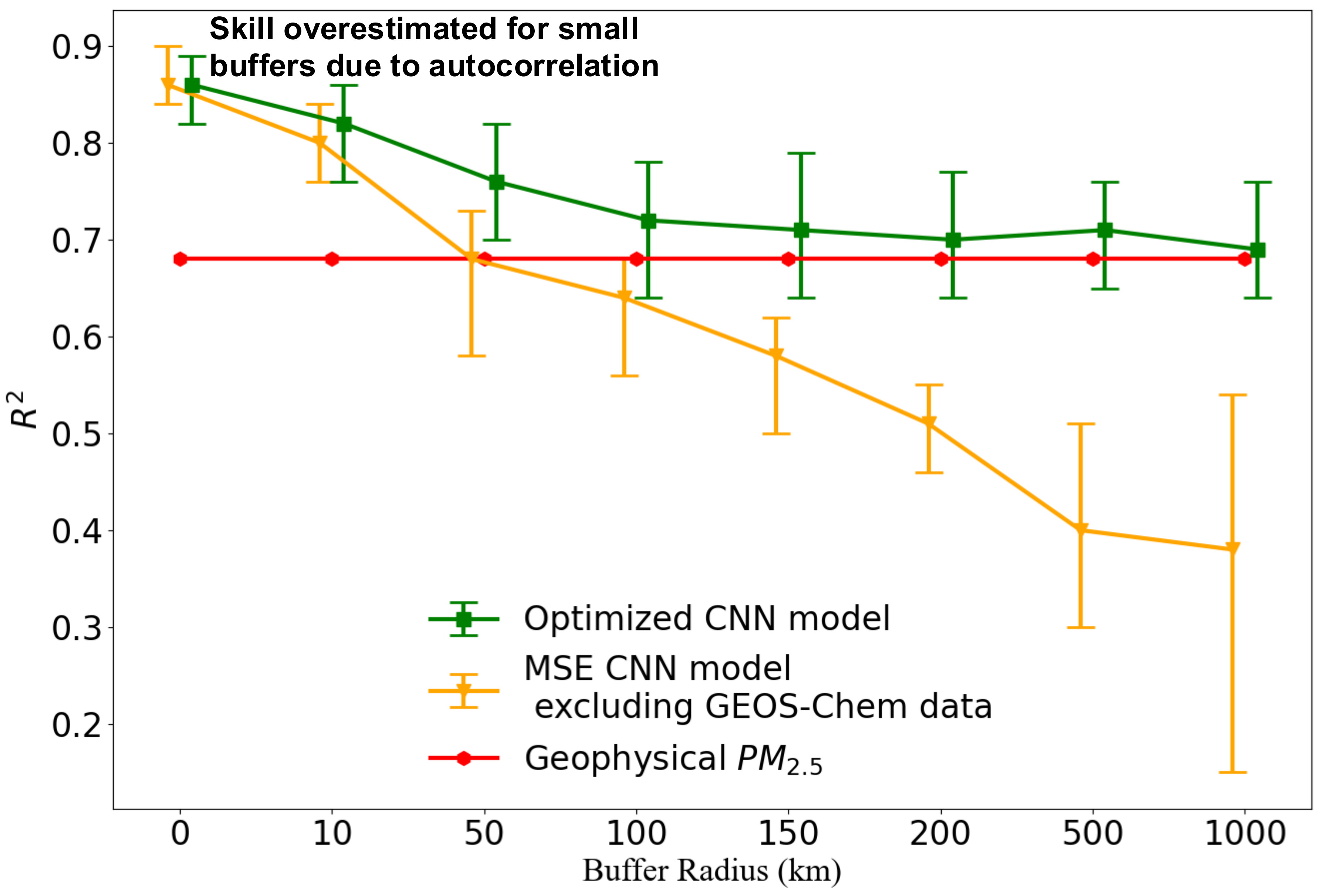
Strategy to Address Spatial Autocorrelation: Buffer Leave-One-Out Cross Validation

Exclude from training all sites within buffer surrounding test site



Shen et al., ES&T Air, 2024

Geophysical Constraints Aid Prediction in Sparsely-Monitored Regions
Value of Physics- and Chemistry-informed Deep Learning



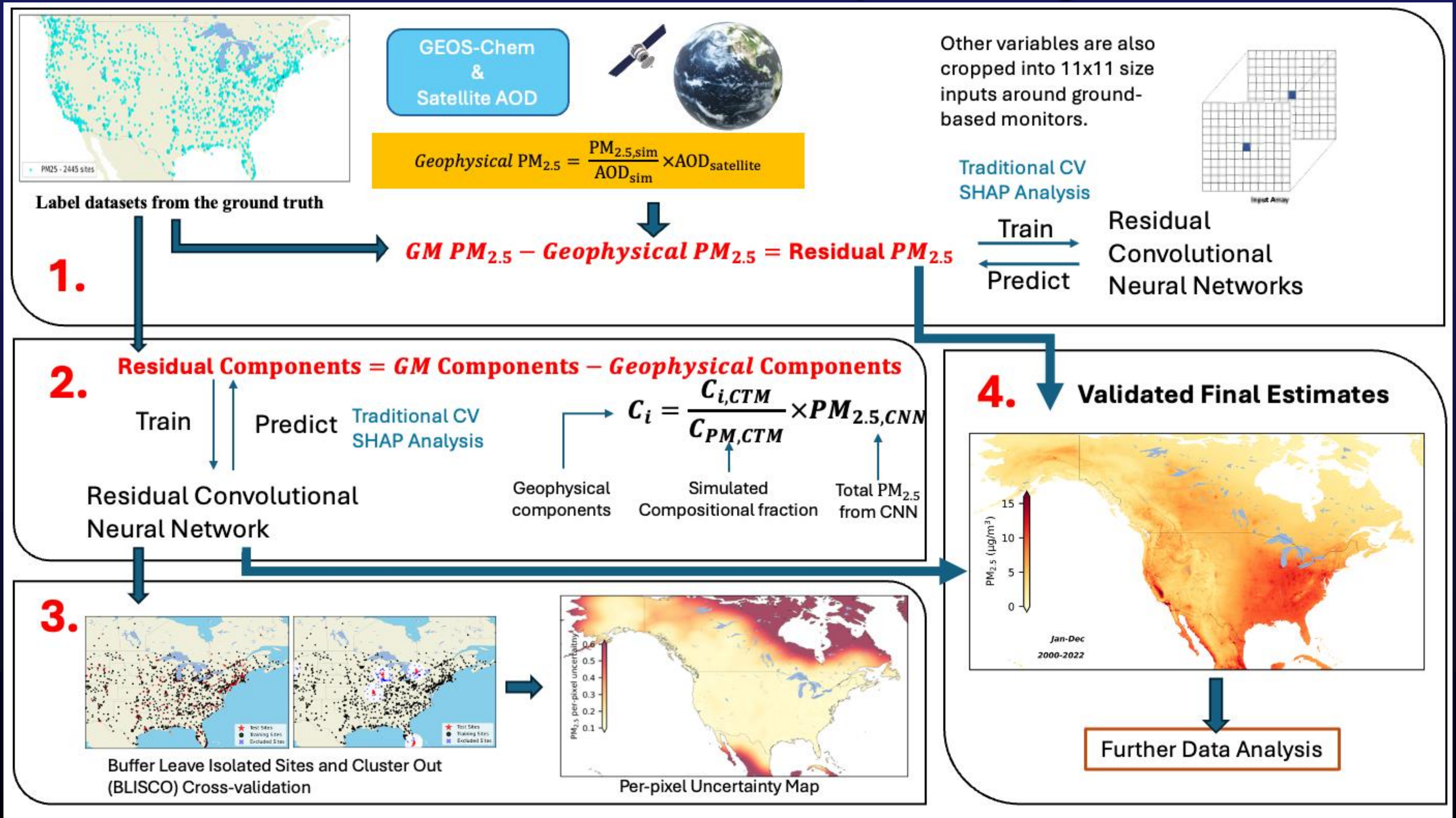
Optimized model relaxes to geophysical $PM_{2.5}$ with increasing distance from monitor

Excluding process-based constraints from a CTM (GEOS-Chem) reduces performance away from monitors

CNN=Convolutional Neural Network

Shen et al., ES&T Air, 2024

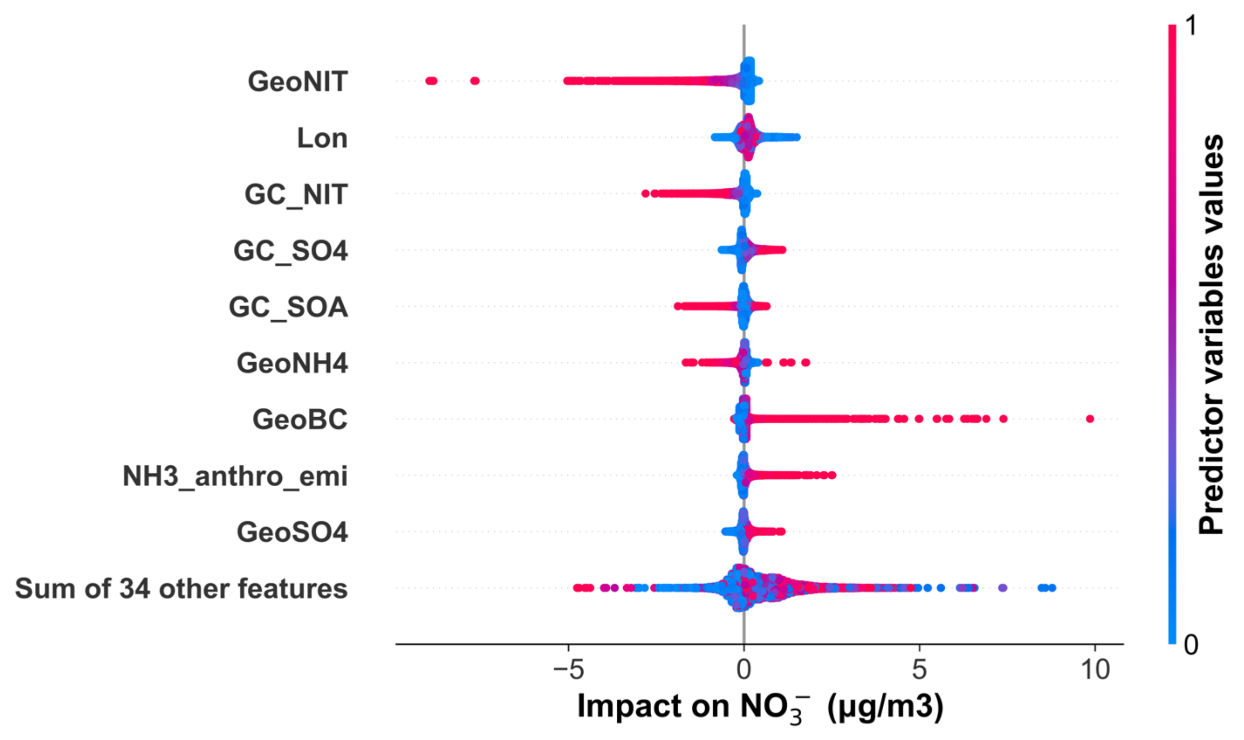
Enhancing Estimation of $PM_{2.5}$ Chemical Composition by Including Geophysical A Priori Information in Deep Learning

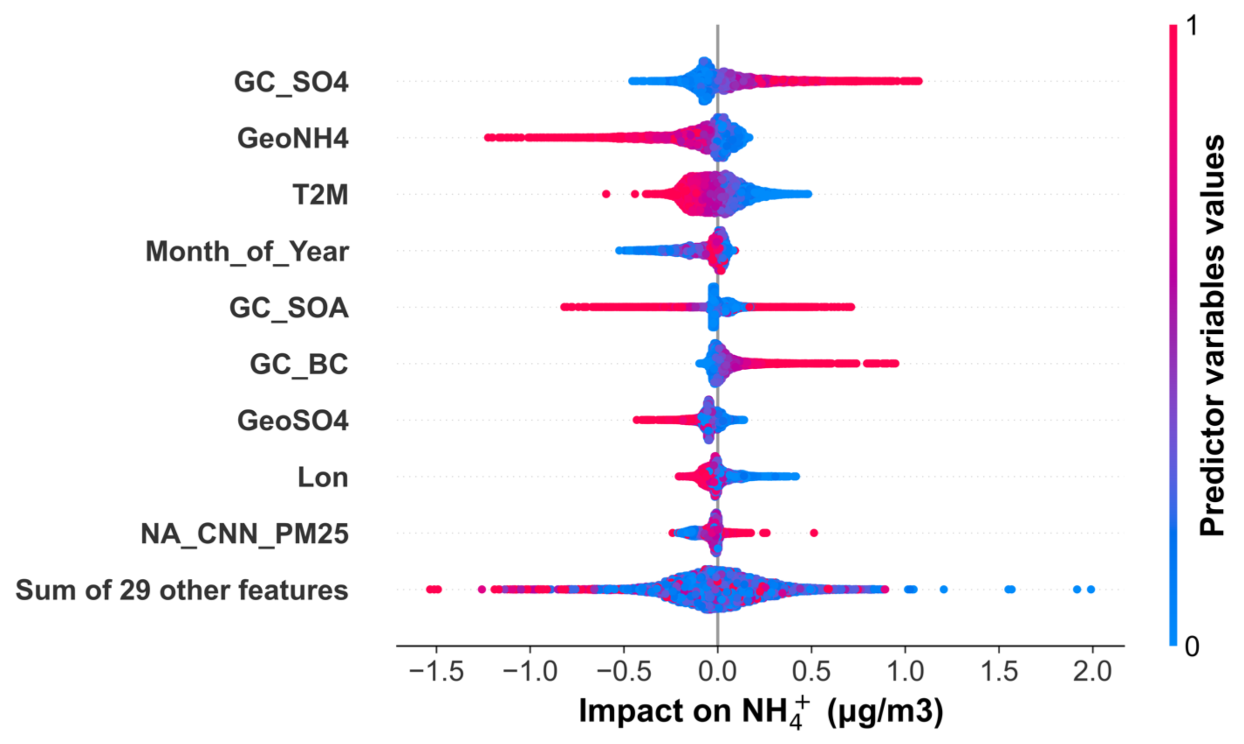


Shen et al., ES&T Air, 2026

Results from Shapley additive Explanations (SHAP) Analysis: Geophysical Predictors Based on GEOS-Chem Physical and Chemical Constraints Are Most Important

Variables are Ordered By Importance



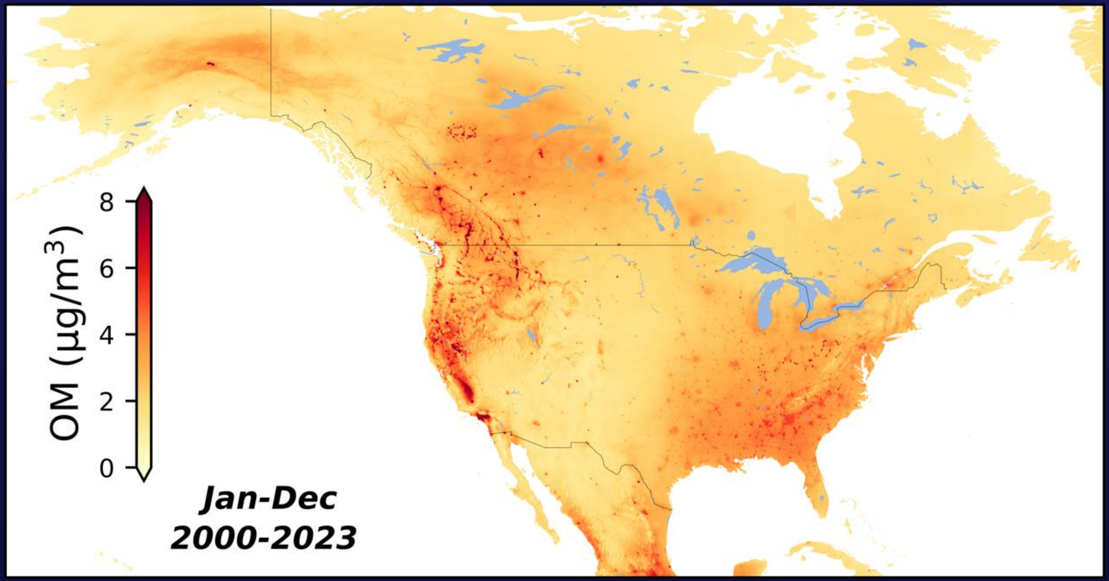


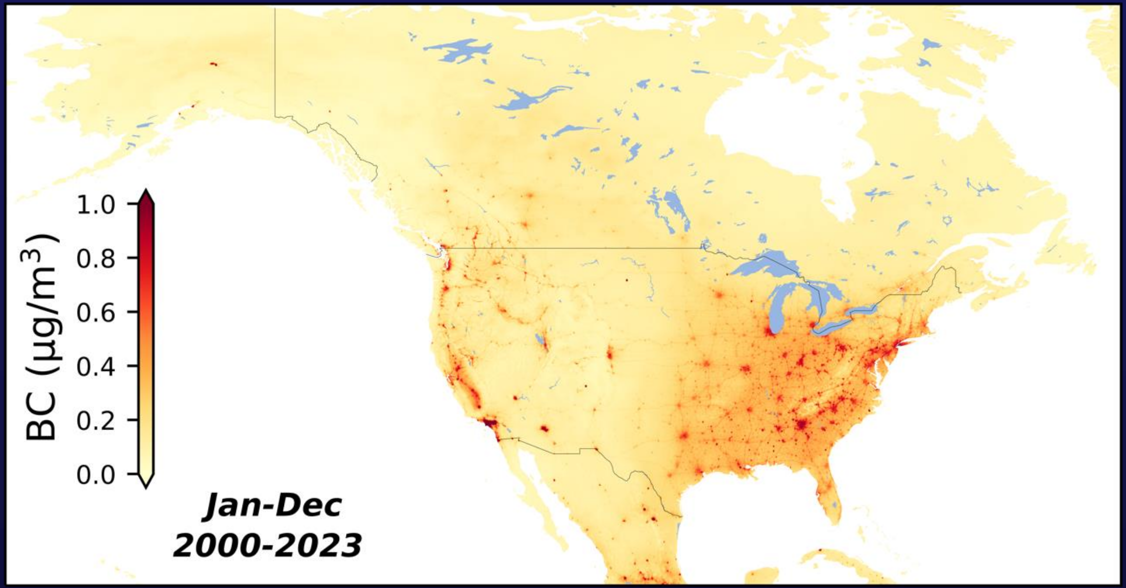
Geo indicates geophysical a priori constrained by GEOS-Chem output
GC indicates GEOS-Chem

Shen et al., ES&T Air, 2026

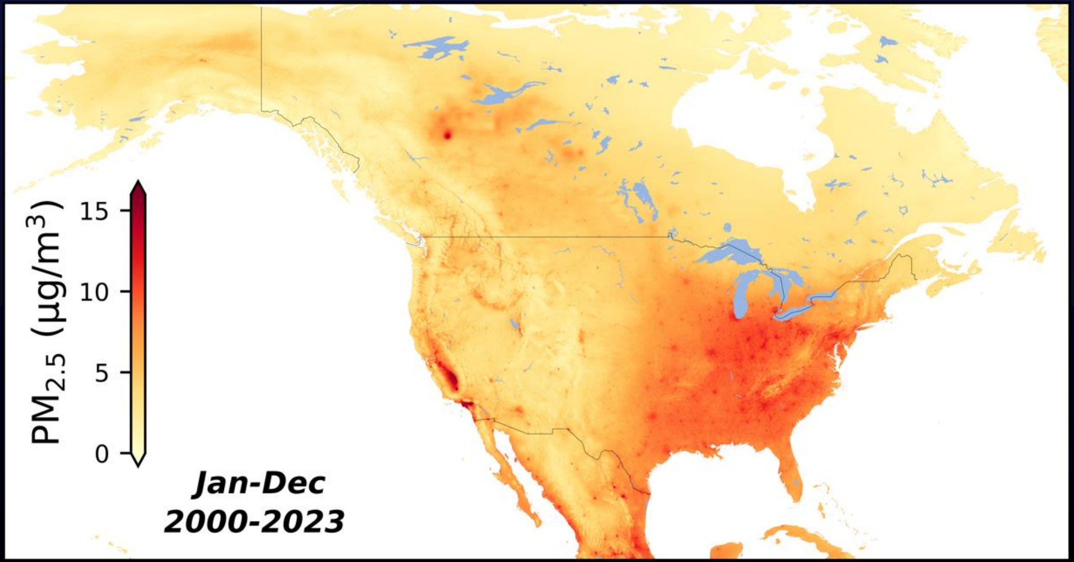
GEOS-Chem Process Information Enhances Skill of Deep Learning

Deep Learning Enhances Accuracy and Resolution





Use of GEOS-Chem process information increases R^2 vs monitors by 20%-30%

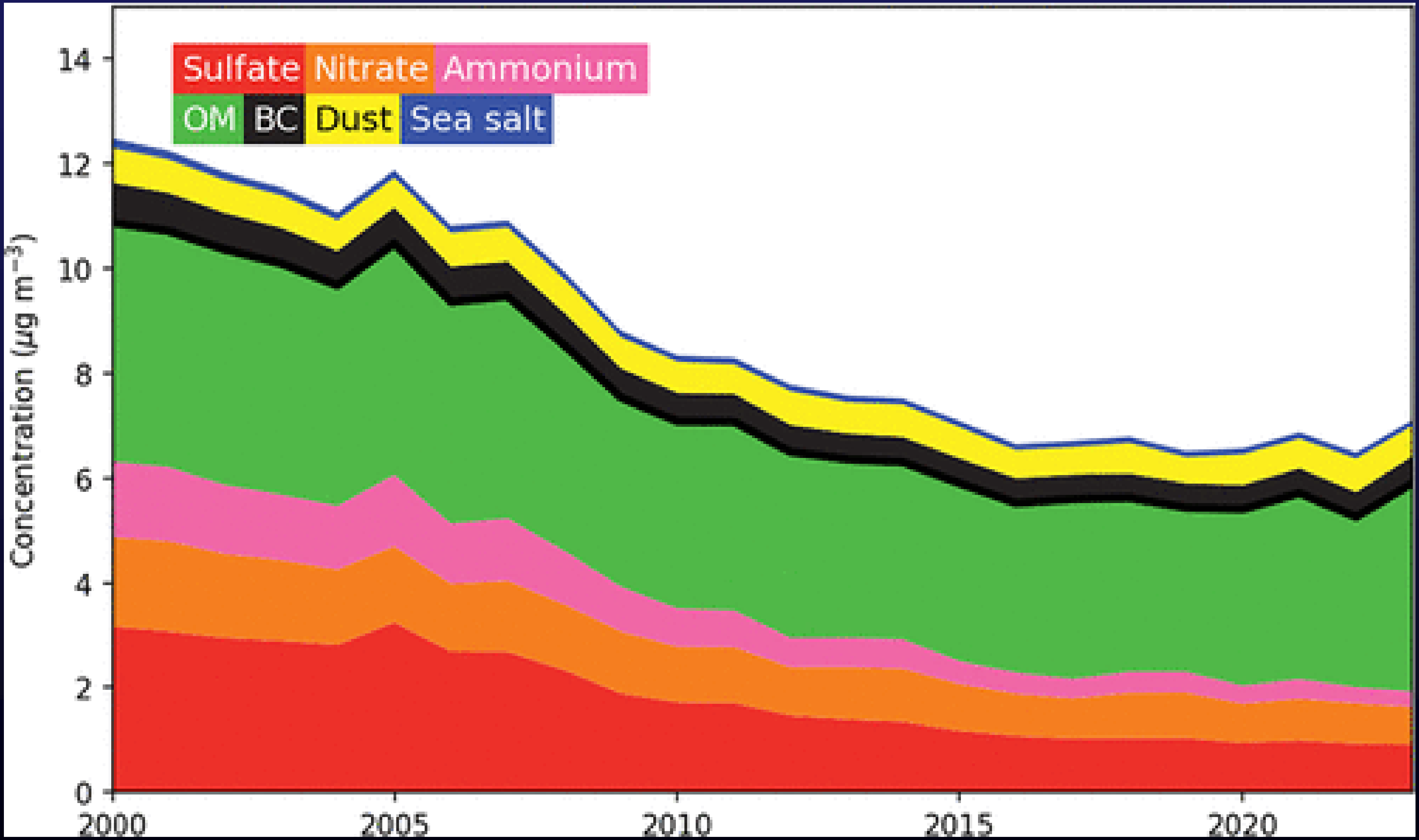


Deep learning increases R^2 vs monitors by 20%-40%, compared with pure geophysical approach

Data freely available: satpm.org

Shen et al., ES&T Air, 2026

Pronounced Reduction in $PM_{2.5}$ Exposure from Sulfate: Future Efforts at $PM_{2.5}$ Control Will Benefit from Increased Attention to Other Components



Data freely available: satpm.org

Determined from monthly data 1 km resolution

Shen et al., ES&T Air, 2026

Conclusions

- Growing confidence in inference of ground-level air quality from satellite remote sensing, chemical transport modeling, and deep learning when constrained with measurements

- Synergy of physical and chemical information from a chemical transport (e.g., GEOS-Chem) with data-driven machine learning approaches

- Numerous opportunities to apply these capabilities to inform air quality management in the context of societal and environmental change