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Predicting the Optical Properties of Arbitrarily Shaped Black Carbon Aerosols with Graph Neural Networks

Kara D. Lamb and Pierre Gentine
Columbia University, Earth and Environmental Engineering, United States of America

Aerosols sourced from combustion such as black carbon (BC) are important short-lived climate forcers whose direct radiative forcing and atmospheric lifetime depend on their morphology. These aerosols are typically fractal aggregates consisting of ~20-80 nm spheres. This complex morphology makes modeling their optical properties difficult, contributing to uncertainty in both their direct and indirect climate effects. Accurate and fast calculations of BC optical properties are needed for remote sensing inversions and for radiative forcing calculations in atmospheric models, but current methods to accurately calculate the optical properties of these aerosols such as the multi-sphere T-matrix method or generalized multiple-particle Mie Theory are computationally expensive and must be compiled in extensive data-bases off-line and then used as a look-up table. Recent advances in machine learning approaches have applied the graph convolutional neural network (GCN) to various physical science applications, demonstrating skill in generalizing beyond initial training data by exploiting and learning internal properties and interactions inherent to the larger system. Here we demonstrate for the first time that a GCN trained to predict the optical properties of numerically-generated BC fractal aggregates can accurately generalize to arbitrarily shaped aerosol particles, even over much larger aggregates than in the training dataset, providing a fast and accurate method to calculate aerosol optical properties in atmospheric models and for observational retrievals. This approach could be integrated into atmospheric models or remote sensing inversions to more realistically predict the physical properties of arbitrarily-shaped aerosol and cloud particles. In addition, GCN's can be used to gain physical intuition on the relationship between large-scale properties (here of the radiative properties of aerosols) and small-scale interactions (here of the spheres' positions and their interactions).