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PNNL-36805

Expanding the representation of aerosol, cloud, and precipitation processes with graph network-based simulators

October 2024

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Abstract

We explored a novel framework for simulating the small-scale processes that drive the evolution of aerosol, cloud, and precipitation particles, which are a critical gap in the predictive understanding of weather and climate. Particle-based methods have emerged as an effective tool for modeling aerosol-cloud-precipitation interactions, but existing particle-based models are computationally too expensive to simulate the large domains relevant for the atmosphere or to represent the full suite of relevant processes. The lack of a comprehensive and efficient reference model is a critical bottleneck in our understanding of cloud and precipitation processes and our ability to parameterize these processes for regional- and global-scale simulations. To address this need, we explored an approach to accelerate and expand particle-based models using a new machine learning approach, graph network-based simulators (GNS). Rather than modeling the evolution of the system by numerically integrating continuity equations, the GNS represents dynamics through learned message passing. Our aim was to develop fast and accurate surrogate models for particle-based simulations. We explored applying GNS to simulate cloud droplet transport, growth, and evaporation under turbulent conditions, but we found the GNS over-smoothed the simulations. We then applied the GNS to simulate aerosol dynamics through gas condensation and found the GNS was able to reproduce the benchmark, physics-based simulation with high accuracy.

Summary

We trained Graph Neural Network-based Simulators (GNS) to learn simulation dynamics in particle-based simulations. The GNS was unable to capture the small-scale turbulent fluctuations that influence droplet transport, growth, and evaporation, but the GNS was well suited to learn the dynamics governing the evolution of aerosol size-composition distributions.

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Acronyms and Abbreviations

GNN	Graph Neural Network
GNS	Graph Network-based Simulator
PartMC	Particle Monte Carlo
MOSAIC	Model for Simulating Aerosol Interactions and Chemistry
DNS	Direct Numerical Simulation

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1.0 Introduction

Small-scale processes that drive the evolution of aerosol, cloud, and precipitation particles are a large source of uncertainty in numerical weather forecasts and climate projections (Seinfeld et al., 2016; Carslaw et al., 2018; Morrison et al., 2020a). Condensational growth, evaporation, melting, and collisions — referred to collectively as microphysics — govern the characteristics of cloud particle populations and the formation of precipitation. Microphysics is also critical for quantifying perturbations in cloud radiative properties and lifetime from human emissions of aerosol particles, which is a key uncertainty in assessing anthropogenic climate change (IPCC 2021). Though critical to our understanding of weather and climate, the representation of microphysics remains a major challenge for atmospheric models.

The most detailed representation of turbulence and droplet microphysics is direct numerical simulation (DNS), which tracks individual aerosol, cloud, and precipitation particles in a small volume of air while also resolving small-scale heterogeneity in environmental properties (e.g. Wang et al., 2009; MacMillan et al., 2022). However, tracking individual particles is computationally expensive, so DNS is currently limited to volumes of ~1 m^3, which is much smaller than even a single small cloud. To represent microphysics in cloud-scale, regional-scale, or global-scale atmospheric models, populations of aerosol, cloud, and precipitation particles must be simplified. Cloud-scale simulations have been developed that include bin representations that track a discretized representation of particle size distributions (e.g. Khain et al., 2015 and references therein) and super-droplet representations that track weighted Lagrangian particles (e.g. Shima et al., 2009). However, these schemes are computationally expensive, while also limited in their representation of processes. Importantly, these schemes neglect interactions between microphysical processes and small-scale turbulent fluctuations in environmental properties, and most schemes neglect in-cloud chemistry. Most weather and climate models use even simpler approaches that track the mass and number of each particle type, while assuming the distribution shape (e.g. Chen and Liu, 2004; Morrison et al., 2005). Recent efforts have focused on emulating detailed microphysics schemes to improve the accuracy of the simplified schemes used in large-scale models (e.g. Cotton et al., 2003; Morrison et al., 2020b), but training emulators has been limited because there is no reference model that resolves particle-to-particle interactions with the full suite of relevant processes. The lack of a reference model critically limits our understanding of cloud processes and is a major hurdle in efforts to evaluate and improve reduced microphysics schemes for large-scale models.

2.0 Accelerating Particle-based models with GNS

While particle-based methods are well suited for microphysics simulations, existing approaches are computationally too expensive to represent the full suite of relevant processes or to operate on large domains. Our approach is to replace expensive particle-based models with a combination of efficient GNS models. Under this framework, particles are represented as nodes on a graph, and dynamics are represented by learned message-passing along graph edges.

To provide a more complete representation of processes, we attempted to use two different types of particle-based models to train and evaluate graph network-based simulators (GNS). We will first trained a GNS of cloud-precipitation microphysics using DNS performed on a small domain of ~1 m^3 (MacMillan et al., 2022). We then trained GNS to represent aerosol-cloud chemistry using the Particle Monte Carlo Model for Simulating Aerosol Interactions and Chemistry (PartMC-MOSAIC; Riemer et al., 2009; Zaveri et al., 2008), which operates on a domain of a few cubic centimeters.

2.1 GNS of turbulent transport and microphysics

We first attempted to train a GNS using DNS runs from MacMillan et al., 2022. These simulations represent a series of cloud chamber experiments that were performed in the Pi Chamber at MTU. The DNS model represents the evolution of the air velocity, temperature, pressure, and water vapor mixing ratio while explicitly resolving all scales of turbulent motion. This fluid dynamics model is coupled to a particle-based microphysics model that tracks the position, velocity, diameter, and temperature of Lagrangian particles as they are transported within the chamber. To perform simulations in even this small domain, they restricted the Rayleigh number of the fluid by setting the gravitational constant to 0.043 m s^{-2}, and they did not represent in-cloud chemistry. We attempted to use these small domain direct numerical simulations to train a GNS of turbulent microphysics, but we found the GNS was unable to capture the small-scale fluctuations in environmental properties and the resulting evolution of the droplet size distribution.

2.2 GNS of aerosol dynamics

We then explored applying the GNS in a truly novel way, to simulate aerosol dynamics. Rather than simulating particle transport, as has been done in previous GNS applications, we trained a GNS to approximate the evolution of aerosol particle size and composition. We used the Particle Monte Carlo Model for Simulating Aerosol Interactions and Chemistry (PartMC-MOSAIC; Riemer et al., 2009; Zaveri et al., 2008) to train and evaluate this new GNS. Whereas other aerosol schemes simplify the representation of particle size distributions and composition, PartMC-MOSAIC tracks the composition of thousands of Monte Carlo particles to represent the full dimensionality of aerosol size-composition distributions. In this case, the nodes of the GNS will represent the mass of constituent species and local concentrations of trace gases. Rather than simulating the gas-aerosol chemistry directly, chemical interactions between gases and particles are represented by message-passing along graph edges.

We found the GNS represents the aerosol dynamics simulated by PartMC-MOSAIC with high accuracy. These findings are described in Ferracina et al, 2024.

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