3D PARTICLE-RESOLVED AEROSOL MODEL TO QUANTIFY AND REDUCE UNCERTAINTIES IN AEROSOL-ATMOSPHERE INTERACTIONS

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EXECUTIVE SUMMARY

This research addresses key uncertainties associated with aerosol-climate impacts. Aerosol particles influence the large-scale dynamics of the atmosphere and climate because they directly interact with solar radiation by scattering and absorbing light, and indirectly by acting as cloud condensation nuclei. Their sizes range from nanometers to micrometers, and a major source of difficulty in understanding the climate impact of aerosols is attributed to scale interactions. There is a high computational cost required for modeling those interactions. The particle-resolved 3D model WRF-PartMC-MOSAIC, which has the unique ability to track size and composition information on a per-particle level, was developed to address this problem while remaining computationally feasible. In combination with efficient algorithms, a resource with the capabilities of Blue Waters is essential to be able to address questions regarding the importance of aerosol composition for prediction of weather and climate at the regional scale.

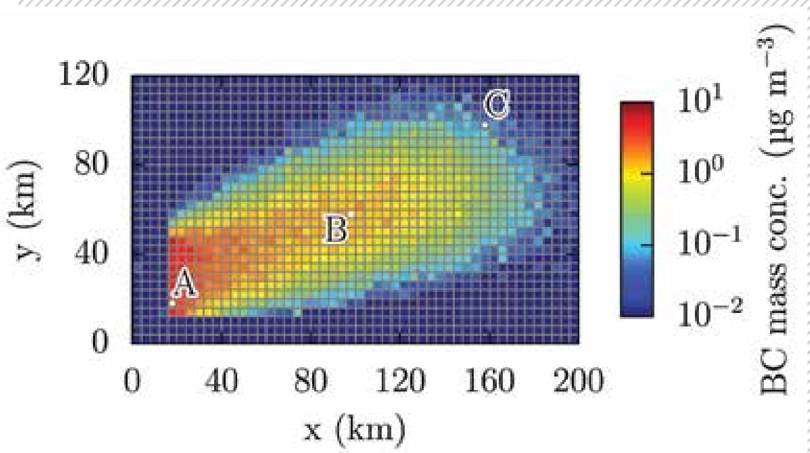

FIGURE 1: Black carbon mass concentration for an urban plume scenario where black carbon particles are emitted and transported by simulated wind fields. Location A is located near the emission source while Locations B and C are located downwind from the emission source.

INTRODUCTION

Many of the greatest challenges in atmospheric modeling and simulation involve the treatment of aerosol particles, ranging from the prediction of local effects on human health [1] to the understanding the global radiation budget via the aerosol indirect and direct effects [2]. Models provide important insights in the study of aerosols but experience a trade-off between the representation of physical detail and spatial resolution. Aerosol modeling has proven difficult because of the complex microscale physics of individual particles, which are not individually resolved in models largely due to computational constraints. Current methods of representing the high-dimensional and multi-scale nature of aerosol populations still make large simplifications. While this makes computation much cheaper, it introduces unknown errors into model calculations. This has far-reaching consequences for the estimation of climate-relevant aerosol quantities, such as the aerosols' ability to scatter and absorb sunlight as well as their ability to form clouds.

METHODS & RESULTS

To overcome the current limitations in representing aerosols and associated uncertainties, the particle-resolved model PartMC-MOSAIC [3] was coupled to the state-of-the-art 3D Weather Research and Forecast (WRF) model. The two models complement each other. PartMC-MOSAIC is a highly detailed aerosol model that tracks the size and complex composition of individual particles in the atmosphere but is unable to resolve spatial heterogeneities of aerosol populations. The 3D, regional WRF model is an advanced numerical weather model that captures the transport of chemical species in the atmosphere but assumes a simplified aerosol representation. The combined model has the advantages of both.

Figure 1 shows the spatial distribution of black carbon mass concentrations near the surface for a scenario simulated on Blue Waters. While this is a bulk quantity common to any chemical transport model, the particle-resolved aerosol representation provides greater detail of particle composition. Figure 2 shows the aerosol mixing state of black carbon at three highlighted locations in the domain shown in Figure 1. At each of these locations, a complex continuum of mixing states is present where particles of similar diameters can have very different chemical composition. Particles are emitted with particular fractions of black carbon determined by their source characteristics, and composition evolves due to coagulation and condensation of secondary gas species. Location A shows the presence of freshly emitted black carbon-containing particles, which consists of high black carbon mass fractions. Location B, located downwind from the emission source, has particles that have undergone aging, which decreased the black carbon mass fraction by adding mass from condensation of secondary gasses. Meanwhile, very little black carbon emissions have been transported to Location C. By using the physical process-level particle-resolved modeling, this phenomenon is accurately captured, allowing for the **most accurate** simulations aerosol impacts on climate to date.

WHY BLUE WATERS

Blue Waters allows for a **cutting-edge** model that pushes both science and computing by combining the large-scale features of state-of-the-art 3D models with the process level physical representation of box models. Modeling 3D domains on the order of 100 billion tracked particles creates many challenges due to computationally intensive equations per particle and memory requirements to track complex particle composition. Blue Waters provides the tens of thousands of cores, fast interconnections between those cores, and sufficient memory per process required for the simulation of aerosols at high spatial and compositional resolution.

NEXT GENERATION WORK

The next-generation Track-1 systems will allow future particle-resolved simulations at higher spatial resolution, for larger regions, and with a greater number of tracked particles to provide greater accuracy. These simulations will target regions where single particle measurements are made available from field campaigns such as the Carbonaceous Aerosols and Radiative Effects Study (CARES) [4] and future upcoming aerosol studies.

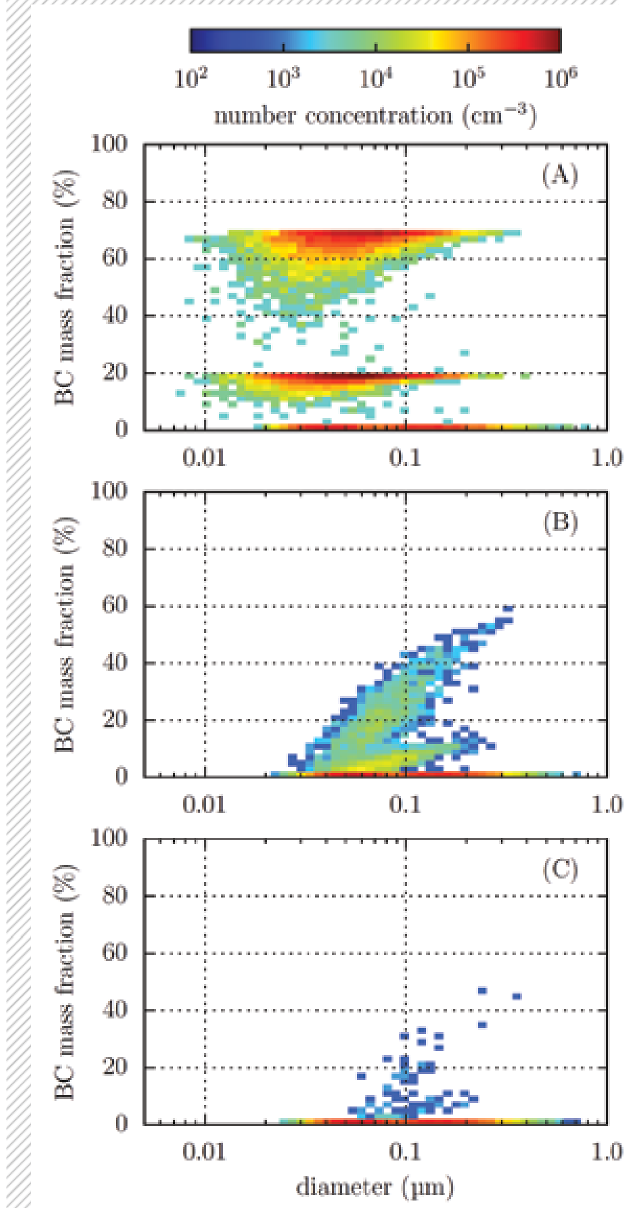

FIGURE 2: Two-dimensional number distributions as a function of particle dry diameter and black carbon mass fraction for locations shown in Figure 1. The number distribution indicates the amount of particles within a range of diameters and a range of fractions of black carbon mass.