MI

BW

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

Allocation: Illinois/300 Knh
PI: Matthew West[1]
Co-PI: Nicole Riemer[1]

[1]University of Illinois at Urbana-Champaign

EXECUTIVE SUMMARY

This research aims at reducing key uncertainties in quantifying the impact of atmospheric aerosol particles on the Earth's climate. Aerosol particles can be brought into the atmosphere by a wide range of human activities or by natural sources. They profoundly impact the large-scale dynamics of the atmosphere because they interact with solar radiation, both directly by scattering and absorbing light and indirectly by forming cloud droplets. These impacts depend on the particles' sizes and their compositions, which continuously change in the atmosphere. The uncertainties in quantifying these impacts originate from scale interactions and the high computational cost required for modeling these. To tackle this problem, we developed the particle-resolved 3D model WRF-PartMC-MOSAIC, which has the unique ability to track size and composition information at a per-particle level. Particle-resolved simulations at the regional scale not only require efficient numerical algorithms but also a computational resource with the capabilities of Blue Waters. Together, these methods and the petascale resources allow for ultra-high-detail simulations that are needed to quantify the impact of aerosol particles on weather and climate at the regional scale.

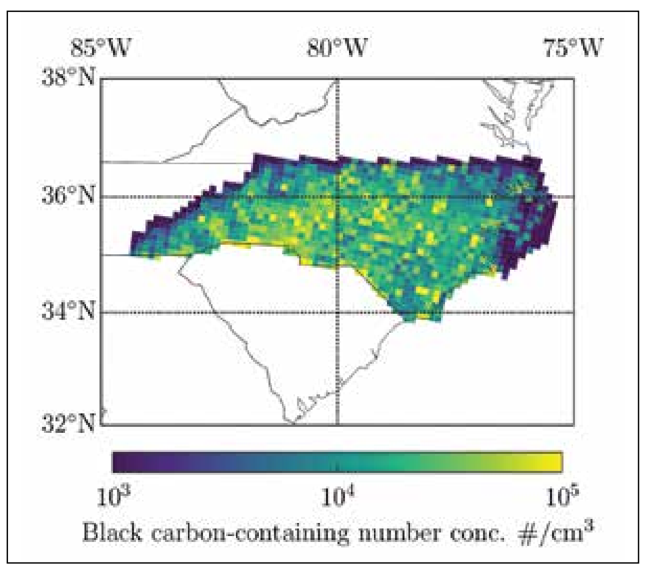

Figure 1: Horizontal distribution of simulated number concentration of black-carbon-containing particles near the surface.

RESEARCH CHALLENGE

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 of 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 representation of physical detail and spatial resolution. Due to computational constraints, models do not resolve individual particles and their microscale interactions. Instead, current methods of representing the high-dimensional and multiscale nature of aerosol populations apply 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 aerosols' ability to scatter and absorb sunlight as well as their ability to form clouds.

METHODS & CODES

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 [4]. Aspects of these two models complement each other. The box model 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 crudely simplified aerosol representation. The resulting WRF-PartMC-MOSAIC model uses a 3D Eulerian grid for the atmospheric flow, while explicitly resolving the evolution of individual aerosol particles per grid cell. This next-generation model captures complex aerosol composition that current-generation models are unable to simulate.

RESULTS & IMPACT

We present results from the first-ever particle-resolved aerosol simulation for a realistic, spatially resolved three-dimensional domain (North Carolina). Aerosol and trace gas emissions were taken from the 2005 National Emission Inventory [5], and the meteorology corresponded to January 24, 2000. On the order of 100 billion computational particles were tracked in this simulation, including their composition changes due to gas-to-particle conversion, and coagulation events.

Fig. 1 shows the modeling domain and the spatial distribution of black carbon-containing particle number concentrations near the surface after eight hours of simulation. Black carbon aerosol is of interest because of its adverse health impacts and because of its warming impact on climate. While this is a fundamental bulk quantity, common to any chemical transport model, the particle-resolved aerosol representation provides unprecedented detail of particle composition and source tracking. Fig. 2 (top) shows the originating sources of all particles within a given grid cell. This allows source attribution for any location within our domain. Fig. 2 (bottom) shows an example of the complex continuum of aerosol composition that exists within a single grid cell; particles of similar diameters can have very different chemical composition—information that is usually lost when using traditional aerosol models. The variations in particle composition are determined by their emission source characteristics, here with highway vehicles containing the largest black carbon mass fractions. During the simulation, aerosol composition evolves due to coagulation and condensation of secondary gas species, resulting in a complex continuum.

As the model tracks composition and source information of thousands of computational particles per grid cell, individual particles may also be explored. For example, a single particle with a particular size and black carbon mass fraction may be examined, marked with a red dot in Fig. 2. By tracking mass of constituent species (not shown), we can determine that the selected particle has grown considerably due to the condensation of nitrate. Additionally, by tracking source history (not shown), the contributing aerosol emissions sources can be determined where this selected particle has undergone multiple coagulation events with particles from different emission sources such as agriculture and fossil fuel combustion. These capabilities will be useful in future studies for quantifying how much individual source categories are contributing to the pollution at a certain location.

Aerosol modeling is challenging because of the multiscale nature of the problem—the macroscale aerosol impact on climate is determined by microscale processes on the particle scale. The WRF-PartMC-MOSAIC model provides a tool that represents many of these microscale processes explicitly, which allows for an improved process-level simulation of the key interactions among aerosols, clouds, and radiation. This model framework therefore serves as the first benchmark for more approximate models, and provides a basis for rigorous coarse-graining to develop physically robust parameterizations for use in larger scale models.

WHY BLUE WATERS

Access to Blue Waters allows for a cutting edge model formulation 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 with on the order of 100 billion tracked particles creates many computational challenges due to computationally intensive equations per particle and memory requirements to track high-dimensional particle composition. To enable simulations of aerosols at both a high spatial and compositional resolution, there is a need for tens of thousands of cores, fast interconnections among those cores, and sufficient memory per process.

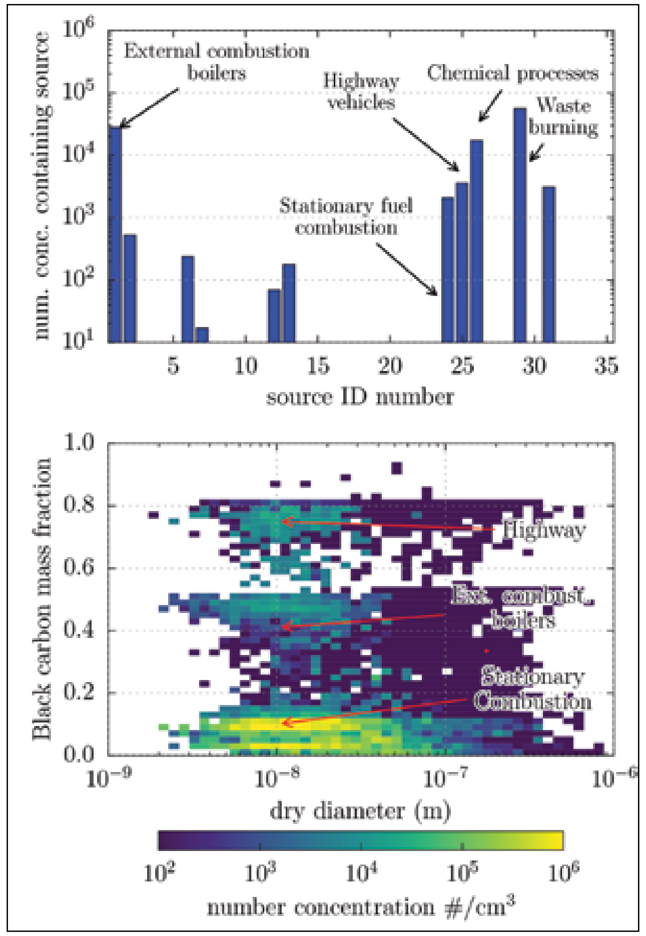

Figure 2: WRF-PartMC-MOSAIC resolves population-level details. (Top) Emission source information is tracked for each grid cell. (Bottom) Two-dimensional number distribution as a function of particle dry diameter and black carbon mass fraction indicates the amount of particles within a range of diameters and a range of fractions of black carbon mass.

PUBLICATIONS AND DATA SETS

PartMC particle-resolved aerosol simulation code, version 2.4.0, released February 2, 2017.