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

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EXECUTIVE SUMMARY

This research aims to reduce key uncertainties in quantifying the impact of atmospheric aerosol particles on Earth's climate. Aerosol particles can be brought into the atmosphere by a wide range of either human activities or natural sources. Aerosols profoundly impact the large-scale dynamics of the atmosphere because they interact with solar radiation—both by scattering and absorbing light, and by forming clouds. These impacts depend on the particles' sizes and their compositions. The uncertainties in quantifying these impacts originate from scale interactions and the high computational cost required for modeling them. To tackle this problem, we developed the particle-resolved 3D model WRF–PartMC, with the unique ability to track size and composition information on a per-particle level. Particle-resolved simulations require efficient numerical algorithms and a computational resource with the capabilities of Blue Waters. Together, they allow for ultra-high-detail simulations needed to quantify the impact of aerosol particles on weather and climate at the regional scale.

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 understanding the global radiation budget via the indirect and direct effects of aerosols [2]. Models provide important insights but experience a trade-off between the representation of physical detail and spatial resolution. Due to computational constraints, current 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 how aerosol particles impact regional and global climate—a topic of great societal relevance.

METHODS & CODES

To overcome the current limitations in representing aerosols and associated uncertainties, we coupled the particle-resolved model PartMC–MOSAIC [3] 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 model uses a 3D Eulerian grid for the atmospheric flow while explicitly resolving the evolution of individual aerosol particles per grid cell.

RESULTS & IMPACT

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 innovation of the WRF–PartMC model consists of representing many of these microscale processes explicitly on a per-particle level, which allows for an improved process-level simulation of the key interactions among aerosols, clouds, and radiation. WRF–PartMC is the only model of its kind, and this work is changing the field of aerosol science because it provides the first benchmark for more approximate models commonly used in the field. It also provides a basis for rigorous coarse-graining to develop physically robust parameterizations for use in larger-scale models. By simulating at a much higher level of detail, particle-resolved models can help close the gap in understanding the effects of modeling choices in global models. Regional-scale particle-resolved simulations allow the quantification of the spatial heterogeneity that determines the conditions where highly detailed aerosol composition is necessary. This next-generation model captures the complex aerosol composition that current-generation models are unable to simulate.

We present results from a particle-resolved aerosol simulation for a realistic, spatially resolved three-dimensional domain in California. Aerosol and trace gas emissions were taken from the 2011 National Emission Inventory [5]. The meteorology corresponded to June 17, 2010, which coincides with the Carbonaceous Aerosol and Radiative Effects Study (CARES) field campaign conducted during May–June 2010. We tracked approximately 50 billion computational particles in this simulation, including their compositional changes due to gas-to-particle conversion, their coagulation events, and their transport by wind and turbulence. The simulation ran on 81 cores. Most of the compute time was spent on particle coagulation and dynamic gas-particle partitioning on a per-particle basis.

Fig. 1 shows the modeling domain and the spatial distribution of the aerosol number concentrations near the surface after 12 hours of simulation. High-number concentrations are present near major highways since traffic is a major particle source. While aerosol number concentration is a fundamental bulk quantity common to any chemical transport model, the particle-resolved aerosol representation provides unprecedented detail for particle composition and source tracking. Fig. 2 shows an example of the complex continuum of aerosol composition that exists within the single grid cell marked with a star in Fig. 1; 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, creating a high-dimensional composition space that only a particle-resolved model is able to resolve.

As the model tracks composition and source information of thousands of simulated particles per grid cell, individual particles may also be explored. For example, 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 sources such as agriculture and fossil fuel combustion. These capabilities will be useful in future studies for quantifying how much individual source categories contribute to pollution at a certain location.

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 as many as 100 billion tracked particles creates 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 requires tens of thousands of cores, fast interconnections between those cores, and sufficient memory per process.

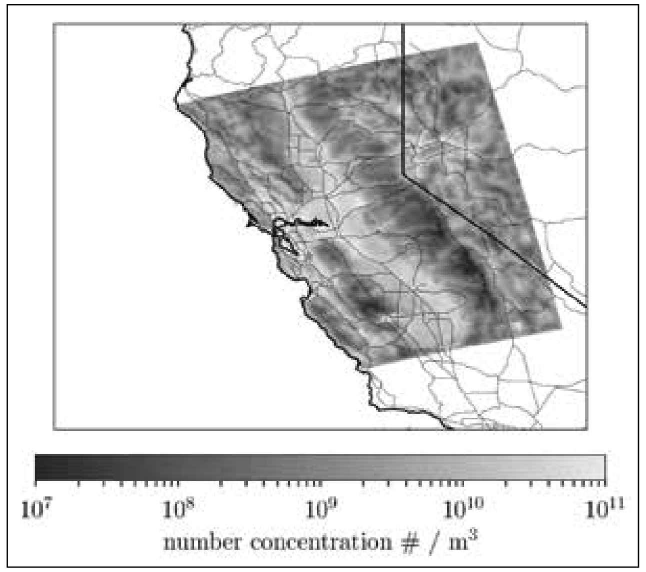

Figure 1: Horizontal distribution of particle number concentration located near the surface after 12 hours of simulation.

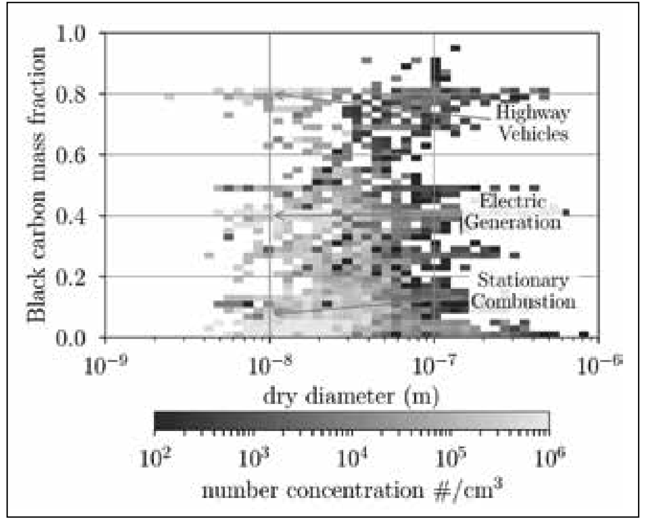

Figure 2: WRF–PartMC resolves population-level details. Two-dimensional number distribution as a function of particle dry diameter and black carbon mass fraction indicates the number concentration of particles within a range of diameters and a range of fractions of black carbon mass, for the grid cell denoted by a star in Fig. 1.