SIMULATING AEROSOL IMPACTS ON CLIMATE, ONE PARTICLE AT A TIME: A REGIONAL-SCALE, 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 the Earth's climate. Aerosol particles can be brought into the atmosphere by a wide range of anthropogenic activities (resulting from the influence of human beings on nature) or by natural sources. They profoundly impact the large-scale dynamics of the atmosphere because they interact with solar radiation by scattering and absorbing light and by forming clouds. These impacts depend on the composition and size of the particles.

The uncertainties in quantifying these impacts originate from scale interactions and the high computational cost of modeling them. To tackle this problem, the research team developed the particle-resolved 3D model WRF–PartMC, which has the unique ability to track size and composition information at 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 the ultrahigh-detail simulations needed to quantify the impact of aerosol particles on weather and climate at the regional scale.

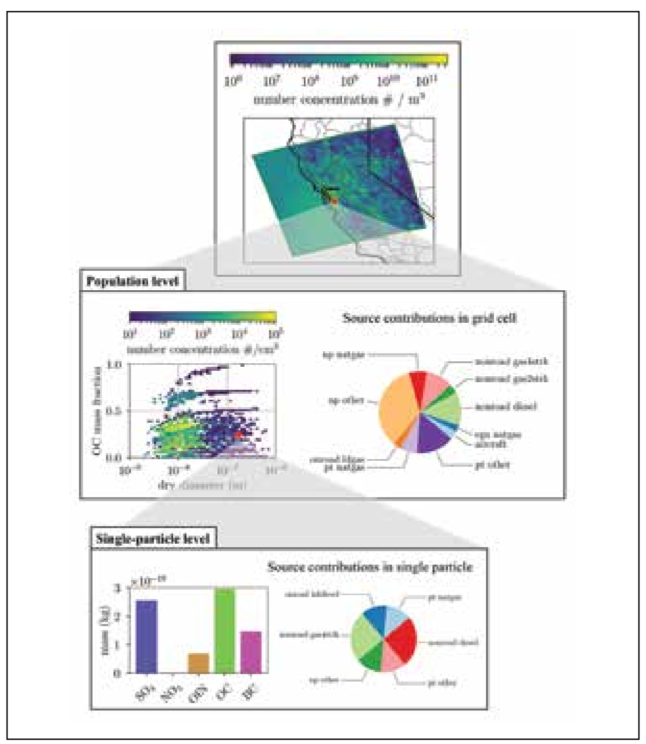

Figure 1: High-level detail obtained by WRF–PartMC: For any given simulated particle, the researchers store its chemical composition and the contributing sources. For each grid cell in the model domain, it is then possible to construct the full mixing state of the aerosol population as well as the full source apportionment profile.

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 their 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. 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, 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 model uses a 3D Eulerian grid for the atmospheric flow, while explicitly resolving the evolution of individual aerosol particles per grid cell.

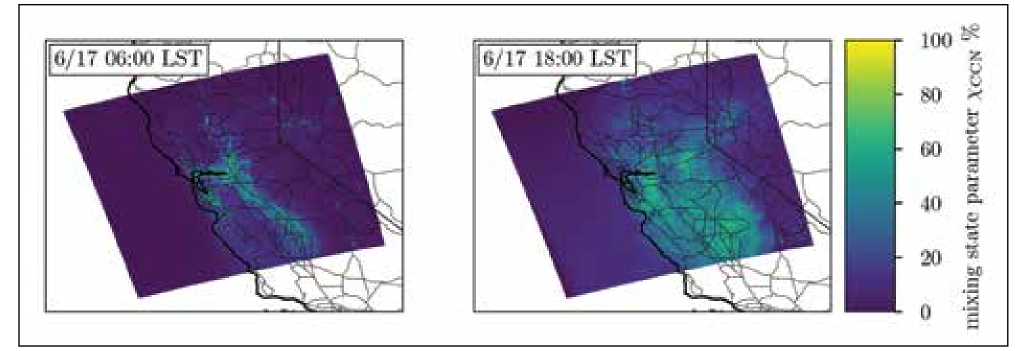

Figure 2: Horizontal distribution of mixing state parameter: A value of 100% indicates particles are fully internally mixed while 0% indicates fully externally mixed, two commonly applied assumptions in traditional models. WRF–PartMC is uniquely able to simulate a complex mixing state that varies both spatially and temporally.

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 research 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.

The research team produced findings from a particle-resolved aerosol simulation for a realistic, spatially resolved three-dimensional domain in California, U.S.A. Aerosol and trace gas emissions were taken from the 2011 National Emission Inventory [5], and the meteorology corresponded to June 17, 2010, which coincides with the Carbonaceous Aerosol and Radiative Effects Study field campaign conducted during May–June 2010. On the order of 50 billion computational particles were tracked in this simulation, including their compositional changes owing to gas-to-particle conversion, their coagulation events, and their transport by both the wind and turbulence. The simulation was run on 6,636 cores. Most of the compute time was spent on particle coagulation and dynamic gas-particle partitioning on a per-particle basis.

Fig. 1 shows an example of the level of detail that can be obtained by WRF–PartMC for a simulation for California. In such a model run, the team is simulating the complex aerosol dynamics and chemistry for about five billion individual particles. For any given particle in the simulation, its chemical composition and the sources of the constituent particles that it is composed of (particles aggregate because they coagulate with each other during transport) are stored. Next, the full mixing state of the aerosol population as well as the full source apportionment profile can be constructed for each grid cell in the model domain.

The full aerosol particle state allows for investigation of the spatial and temporal distribution of the mixing state parameter [6]. Fig. 2 shows the mixing state parameter χ_{CCN} at 06:00 LST (Local Standard Time) and 18:00 LST on June 17, 2010. The mixing state parameter χ_{CCN} represents the extent that hydrophobic (tending to fail to mix with water) and hydrophilic (tending to mix with water) species are internally mixed. At 06:00 LST, these components remain mostly externally mixed with exceptions in the vicinity of urban areas and roadways. At 18:00 LST, χ_{CCN} increased and is more spatially homogeneous. This indicates that the hydrophobic and hydrophilic material is becoming more internally mixed over the course of the day. The WRF–PartMC model allows for the full evolution of the aerosol mixing state, unlike traditional models. WRF–PartMC model results have been used to benchmark these more simplified models and evaluate the error incurred in models owing to simplifying assumptions.

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 on the order of 100 billion tracked particles creates computational challenges owing 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.

Access to the Blue Waters staff was essential for addressing issues regarding the I/O challenge of outputting billions of particles, their chemical composition, and physical properties. Discussion and suggestions of how to change the model output code led to a two-orders-of-magnitude reduction in the time required to generate output. This removed output as a bottleneck to code performance.