BLUE WATERS
SUSTAINED PETASCALE COMPUTING

Allocation: Illinois/300 Knh

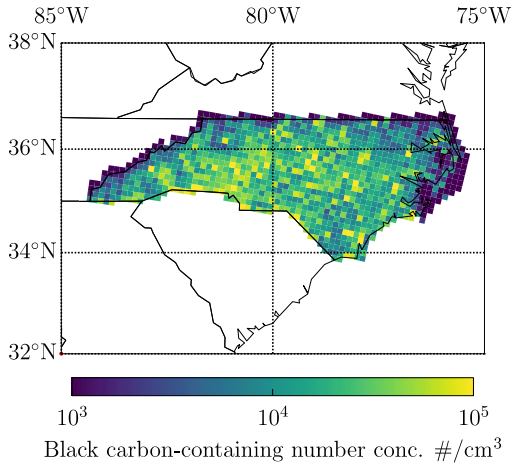
PI: Matthew West
University of Illinois at Urbana-Champaign

Geoscience

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

Research Challenge

- The treatment of aerosol particles provides challenges in atmospheric modeling and simulation.
- Current models provide important insights, but do not resolve individual particles and their microscale interactions.
- This makes computation much cheaper, but 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.



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

Methods & Codes

The particle-resolved model PartMC-MOSAIC was coupled to the state-of-the-art 3D Weather Research and Forecast (WRF) model. These complement each other with the box model PartMC-MOSAIC handling the highly detailed aerosol model and the 3D regional WRF model capturing the transport of chemical species in the atmosphere. This next-generation model captures complex aerosol composition that current-generation models are unable to simulate.

Results & Impacts

- This research provides the first-ever particle-resolved aerosol simulation for a realistic, spatially resolved three-dimensional domain.
- On the order of 100 billion computational particles were tracked in this simulation.
- Future studies may be able to use this research to quantify how much individual source categories contribute to the pollution at a certain location.

Why Blue Waters

Cutting edge model formulations push 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 computational challenges due to computationally intensive equations per particle and memory requirements to track high-dimensional particle composition. To simulate aerosols at both a high spatial and compositional resolution, tens of thousands of cores with fast interconnections among those cores, and sufficient memory per process are used.