BLUE WATERS
SUSTAINED PETASCALE COMPUTING

Allocation: Illinois/240 Knh

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Geoscience

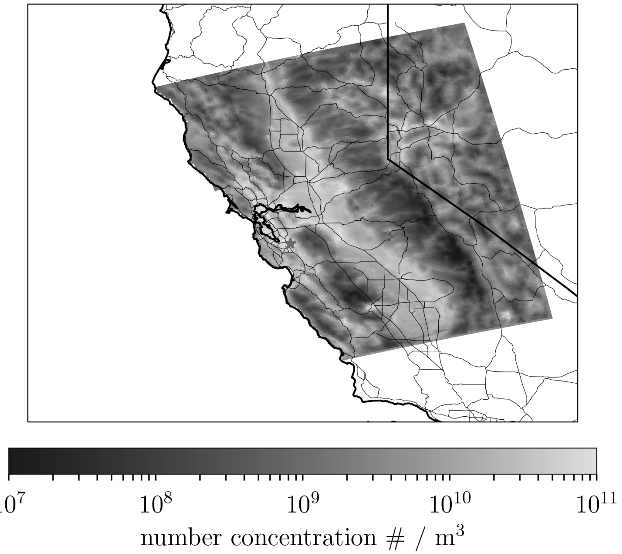

Figure: Horizontal distribution of particle number concentration located near the surface after 12 hours of simulation.

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

Research Challenge

This research aims to reduce key uncertainties in quantifying the impact of atmospheric aerosol particles on Earth's climate. 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. Due to computational constraints, current models do not resolve individual particles and their microscale interactions so methods representing the high-dimensional and multiscale nature of aerosol populations apply large simplifications which also introduces unknown errors.

Methods & Codes

To overcome the current limitations in representing aerosols and associated uncertainties, two models were combined.

- **PartMC–MOSAIC -** a detailed aerosol model that tracks the size and complex composition of individual particles in the atmosphere.
- **3D regional Weather Research and Forecast (WRF)** - an advanced numerical weather model that captures the transport of chemical species in the atmosphere.

Results & Impact

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 and captures the complex aerosol composition that current-generation models are unable to simulate. Results obtained from a particle-resolved aerosol simulation for a realistic, spatially resolved three-dimensional domain in California - 50 billion computational particles, including their compositional changes due to gas-to-particle conversion, their coagulation events, and their transport by wind and turbulence.

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.