Title: Scaling a 3D particle-resolved aerosol model to address uncertainties in aerosol-atmosphere interactions

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1 Executive summary

This research aims to address key uncertainties associated with aerosol-climate impacts. Aerosol particles influence the large-scale dynamics of the atmosphere and climate because they interact with solar radiation, both directly by scattering and absorbing light and indirectly by acting as cloud condensation nuclei. Their sizes range from nanometers to micrometers, and a major source of difficulty in understanding the climate impact of aerosols is due to scale interactions and modeling those interactions due to computational cost. The particle-resolved 3D model WRF-PartMC-MOSAIC was developed, which has the unique ability to track size and composition information on a per-particle level, to address this problem while remaining computationally feasible. In combination with efficient algorithms, a resource with the capabilities of Blue Waters is essential. This allocation has taken the significant step of taking WRF-PartMC-MOSAIC from the small scale development stage to the stage where regional simulations may be conducted in future allocations.

2 Research activities and results

Particle-resolved modeling provides insights into uncertainties regarding aerosol and aerosol-cloud interactions which are crucial in climate prediction. 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 (Dockery and Pope, 1996) to the understanding the global radiation budget via the aerosol indirect and direct effects (Stocker et al., 2013). Aerosol modeling has proved difficult because of the complex microscale physics of individual particles, which are not individually resolved in models — largely due to computational constraints. Current methods of representing the high-dimensional and multi-scale nature of aerosol populations still make 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 optical properties and cloud condensation nuclei (CCN) activation properties.

To overcome the current limitations in aerosol modeling, the particle-resolved aerosol model PartMC-MOSAIC (Riemer et al., 2009) was developed. This model stores the composition of many individual particles directly within a well-mixed computational volume. PartMC-MOSAIC was coupled with the Weather and Research Forecast (WRF) model, a state-of-the-art, publicly available fluid dynamics code for numerical weather prediction. The resulting WRF-PartMC-MOSAIC model uses a 3D Eulerian grid for the atmospheric fluid 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.

Why particle-resolved modeling at the regional scale matters? The work of this allocation focused on the computational feasibility of the model to be run at the large-scale on Blue Waters so that a general allocation could be achieved to then address the science questions regarding aerosol-climate interactions. This particle-level understanding is essential to accurately understand and predict crucial aggregate quantities such as optical properties and cloud condensation nuclei activity. With the general allocation, quantification of errors in climate-relevant quantities such as CCN concentrations and optical properties will be possible. In addition to quantify errors, model results will be useful for benchmarking more simplistic aerosol models.

Blue Waters is essential as particle-resolved 3D atmospheric modeling is both compute-intensive and memory-intensive. A petascale resource with the capabilities of Blue Waters allows for a cutting edge model that pushes 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. 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 between those cores, and sufficient memory per process. Given our problem size and the decomposed subdomain being as small as 1×1 in the horizontal, future general allocations on Blue Waters will be necessary to achieve our scientific goals in the future.

This allocation was to explore the ability of the WRF-PartMC-MOSAIC code to scale up to the Blue Waters scale and to secure future general allocations. Previous model development and testing was performed on small department clusters, consisting of up to 84 cores. However to conduct regional scale simulations, the model will be required to scale up to tens of thousands of cores. This purpose of this allocation was to test the ability of the model at more realistic problem sizes than previously done. Figure 1 displays the results of testing on Blue Waters. Figure 1 shows the weak and strong scaling properties of WRF-PartMC-MOSAIC. As a result of this scaling and performance testing, this project will be continued with the general Blue Waters allocation in “3D particle-resolved aerosol model to address uncertainties in aerosol-atmosphere interactions”.

In addition to scaling results, a few longer time period simulations were performed to examine computational performance over the course of entire simulations rather than short scaling simulations. Figure 2 shows the results of black carbon concentrations for a simulation conducted on a North Carolina domain. This simulation was for a 12 hour period and required $\approx$ 9 wall clock hours using 3551 cores. A simulation of this scale involved over 2 billion simulated particles.

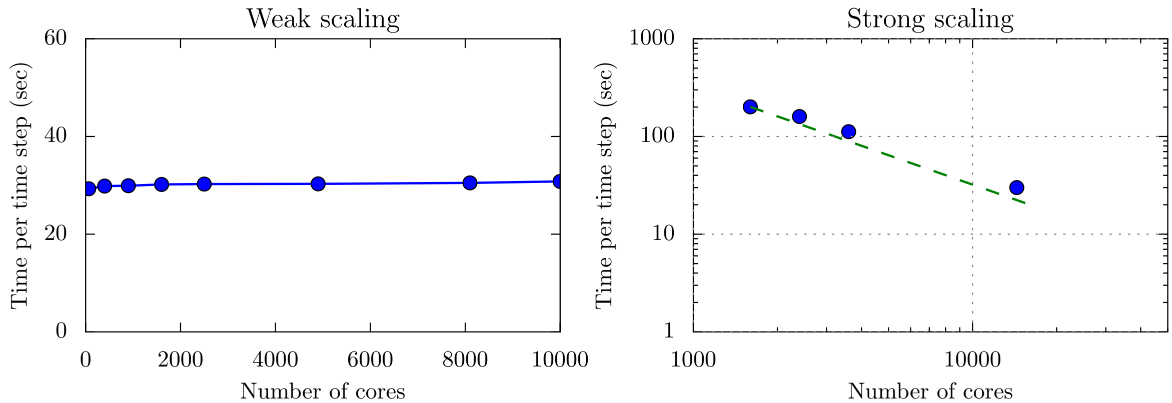

Figure 1: Scaling properties of the 3D particle-resolved WRF-PartMC-MOSAIC on Blue Waters on XE nodes. Left: Data shows the weak scaling properties in terms of wall clock time per model time step. Each core was used to simulate a 1 × 1 × 60 subdomain with 10 000 computational particles per grid cell. Right: Strong scaling performance using 10 000 computational particles per grid cell and an initial domain size of 120 × 120 × 60. The problem size per core ranged from 3 × 3 × 60 to 1 × 1 × 60.

3 Publications and products

- Scaling results and model performance on Blue Waters were presented as a poster at the Department of Energy 2016 Atmospheric Radiation Measurement/Atmospheric System Research (ARM/ASR) PI Meeting May 2 - 6, 2016 titled "A 3D Particle-resolved Model to Quantify the Importance of Aerosol Mixing State for CCN Activity".

References

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Stocker, T. F., et al., (Eds.), 2013: *Summary for Policymakers*, chap. SPM, 1–30. Cambridge University Press, doi:10.1017/CBO9781107415324.004.

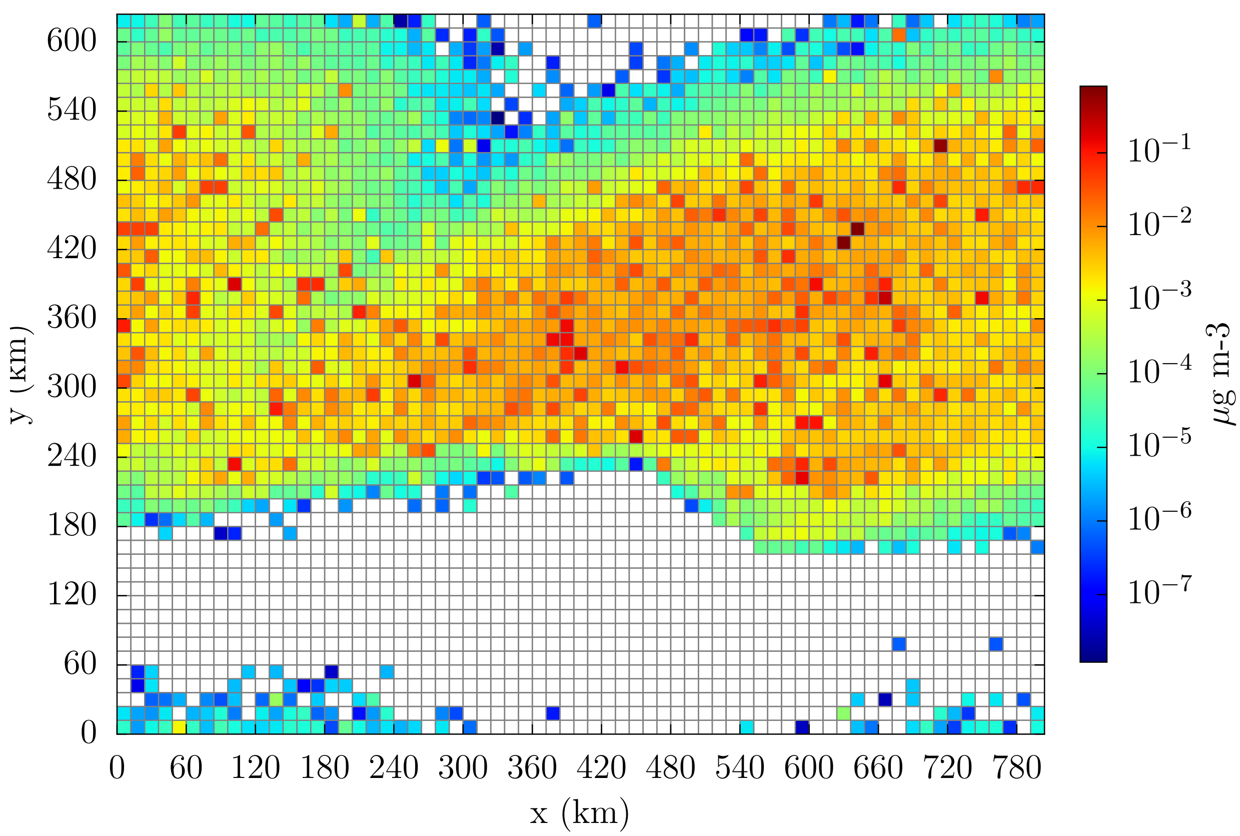

Figure 2: Black carbon mass concentration for a North Carolina domain after 12 hour as simulated on Blue Waters.