Coupling the Stochastic Particle-Resolved Aerosol Model PartMC-MOSAIC with WRF

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Introduction

The recently developed particle-resolved aerosol box model PartMC-MOSAIC (Riemer et al., 2009) has allowed unprecedented insight into the evolution of aerosol mixing state. So far, while resolving the aerosol composition on a per-particle level, PartMC-MOSAIC has lacked detail on a spatial scale. To overcome this limitation, we have now coupled PartMC-MOSAIC with the Weather Research and Forecast model (WRF) to allow transport of aerosol particle populations and gas species concentrations. In this study, PartMC-MOSAIC has been coupled with the WRF Single Column Model, resulting in a fully-coupled 1D atmospheric-dynamics/aerosol-particle model that not only resolves the particle mixing state on a per-particle level but also resolves the vertical structure of the atmosphere.

Stochastic Aerosol Transport

Transport processes such as turbulent diffusion are modeled using appropriate probabilities for the aerosol particles to move from one grid cell to another. These probabilities result from a finite-volume discretization of the governing 1D diffusion equation:

$$\frac{\partial \psi}{\partial t} = \frac{\partial}{\partial z}\left(K \frac{\partial}{\partial z}\psi\right), \tag{1}$$

where K is eddy diffusivity, and ψ is the particle concentration. For vertical atmospheric treatments this equation must be modified so that it is mixing ratio that is transported, rather than concentration. For simplicity, here we will describe the discretization of (1), as the extension to the atmospherically-relevant diffusion equation is straightforward.

This equation can be discretized as:

$$\psi_i(t+\Delta t) = \psi_i(t) + \underbrace{\frac{\Delta t}{\Delta z_i \Delta z_{i+\frac{1}{2}}} K_{i+\frac{1}{2}}}_{p_{i,i+1}} (\psi_{i+1}(t) - \psi_i(t)) - \underbrace{\frac{\Delta t}{\Delta z_i \Delta z_{i-\frac{1}{2}}} K_{i-\frac{1}{2}}}_{p_{i,i-1}} (\psi_i(t) - \psi_{i-1}(t)),$$

where $p_{i,j}$ can be interpreted as the probability of a particle moving from grid cell i to grid cell j. Rearranging gives:

$$\psi_i(t+\Delta t) = \psi_i(t) - \underbrace{p_{i,i+1}\psi_i(t)}_{\ell_{i,i+1}} - \underbrace{p_{i,i-1}\psi_i(t)}_{\ell_{i,i-1}} + \underbrace{p_{i-1,i}\psi_{i-1}(t)}_{g_{i-1,i}} + \underbrace{p_{i+1,i}\psi_{i+1}(t)}_{g_{i+1,i}},$$

where $\ell_{i,j}$ and $g_{i,j}$ are the mean loss and gain from grid cell i to grid cell j.

To account for the variable-sized grid cells that are encountered in vertical coordinate systems, we have that:

$$\frac{g_{i,j}}{\ell_{i,j}} = \frac{p_{j,i}}{p_{i,j}} = \frac{\Delta z_i}{\Delta z_j},$$

for the gain and loss terms from cell i to cell j.

For a set of particles Π_i in grid cell i, we obtain the loss and gain subsets $L_{i,j}$ and $G_{i,j}$ using binomial samples with means $\ell_{i,j}$ and $g_{i,j}$, given by

$$L_{i,j} \sim \mathrm{Binom}(\Pi_i, p_{i,j}) \text{ and } G_{i,j} \sim \mathrm{Binom}(L_{i,j}, \Delta z_i/\Delta z_j) \text{ if } \Delta z_i < \Delta z_j$$
$$G_{i,j} \sim \mathrm{Binom}(\Pi_i, p_{j,i}) \text{ and } L_{i,j} \sim \mathrm{Binom}(G_{i,j}, \Delta z_j/\Delta z_i) \text{ if } \Delta z_i > \Delta z_j,$$

where $\mathrm{Binom}(\Pi, p)$ is a binomial sample from the particle set Π with probability p of selecting each particle. Both loss (or gain) terms $L_{i,i+1}$ and $L_{i,i-1}$ for cell i are sampled collectively as a multinomial sample with the probabilities above, giving the correct individual binomials.

Model Verification with Analytical Solution

The particle sampling algorithm solution was compared to an exact solution to equation (1) for an instantaneous area source. Figures 1 and 2 show the convergence to the analytical solution.

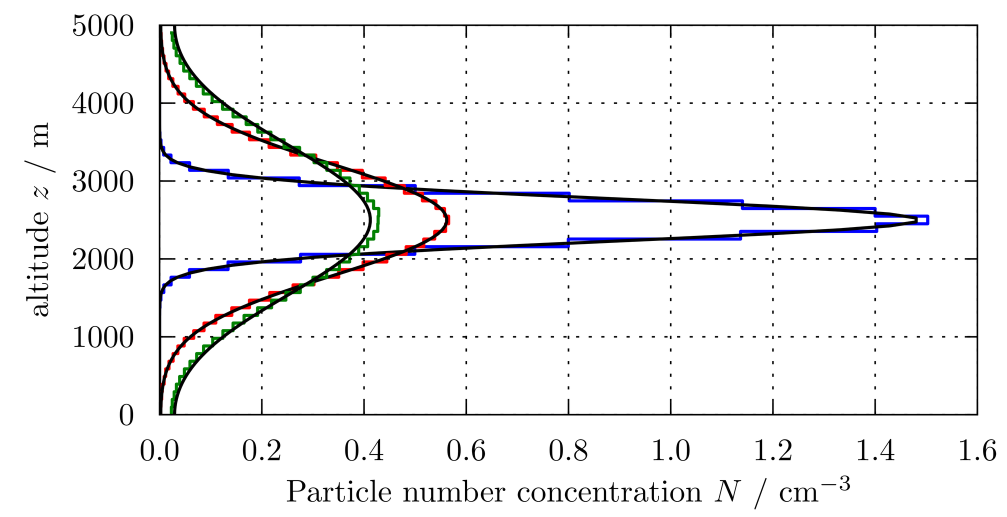

Figure 1: Simulation of an instantaneous area source released in the center of the domain at $t = 0$. The results of the stochastic simulation (51 grid cells and 100,000 particles, colored lines) represent the number concentration in each grid cell and is compared to the corresponding analytical solution (black lines) for $t = 1$ h (blue), $t = 6$ h (red), and $t = 12$ h (green).

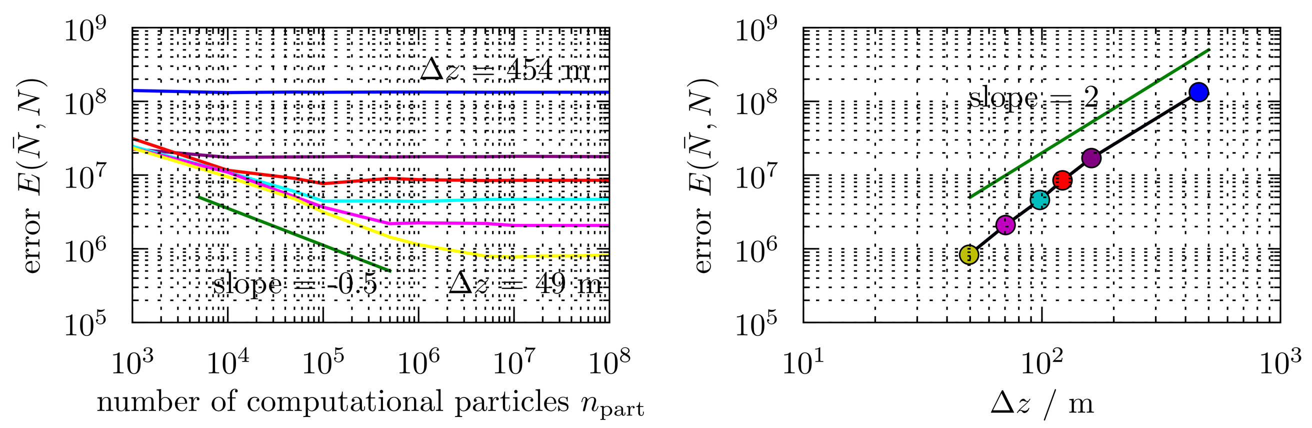

Figure 2: Left: Convergence of the stochastic solution $\bar{N}$ to the analytical solution N of the 1D diffusion equation. Right: Convergence of the error as a function of Δz for $n_{\text{part}} \to \infty$. Lines in green represent the expected slopes. The error is $E(\bar{N}, N) = \sqrt{\sum_{i=1}^{m} (\int_{z_i}^{z_{i+1}} \bar{N}_i dz - \int_{z_i}^{z_{i+1}} N(z) dz)^2}$.

Results: Aging of Black Carbon

The results are based on a 24-h simulation, starting at 6 am local time, and using the gas phase and particle emissions from the urban plume case described in Riemer et al. (2009). The aerosol emissions from combustion of gasoline and diesel (black carbon and primary organic carbon) and from meat cooking (primary organic carbon) persisted for the first 12 hours of simulation. Initial background aerosols were constant with height, contained no black carbon and were represented with 5000 computational particles per grid cell. During the day the black carbon concentration was about 1.2 μg m^{-3} near the ground and decreased with height as expected for a particle type emitted at the ground. In the evening, black-carbon-containing particles were emitted into the stable boundary layer where they accumulated similarly to the primary gas emissions.

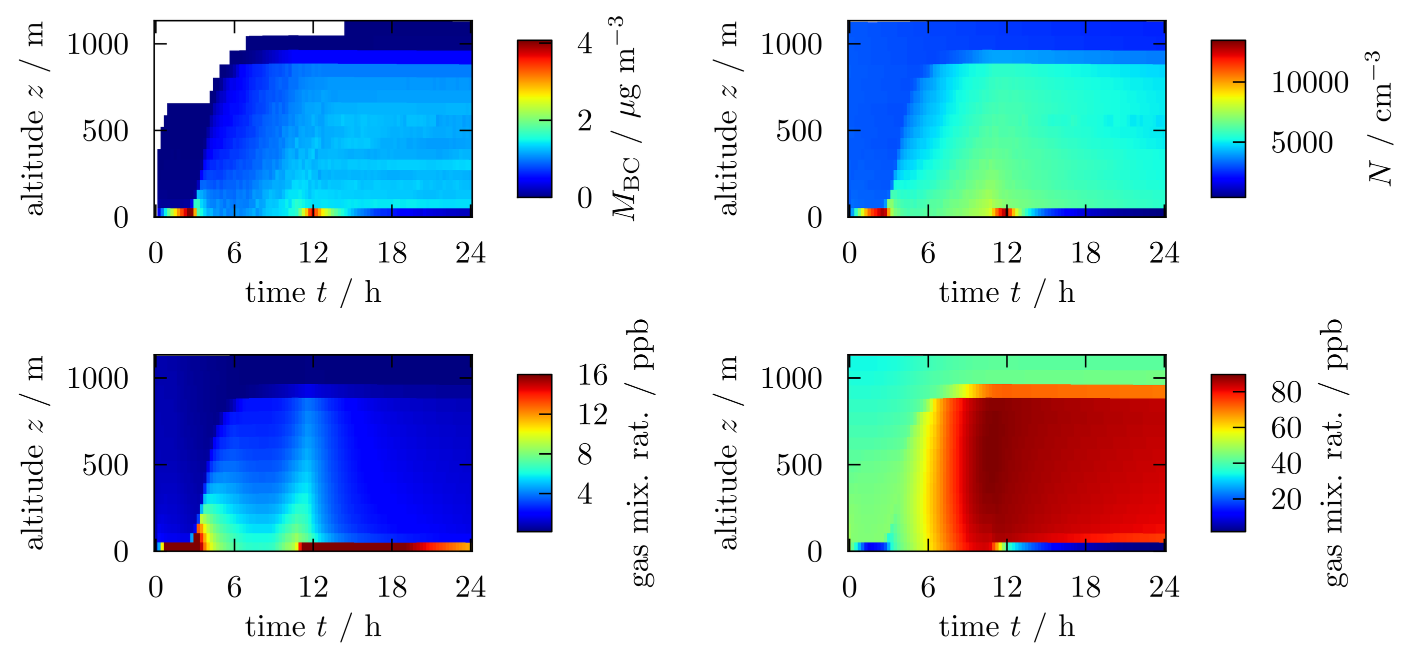

Figure 3: Time-height sections showing concentrations of black carbon (top left), aerosol number (top right), NO_2 (bottom left) and ozone (bottom right).

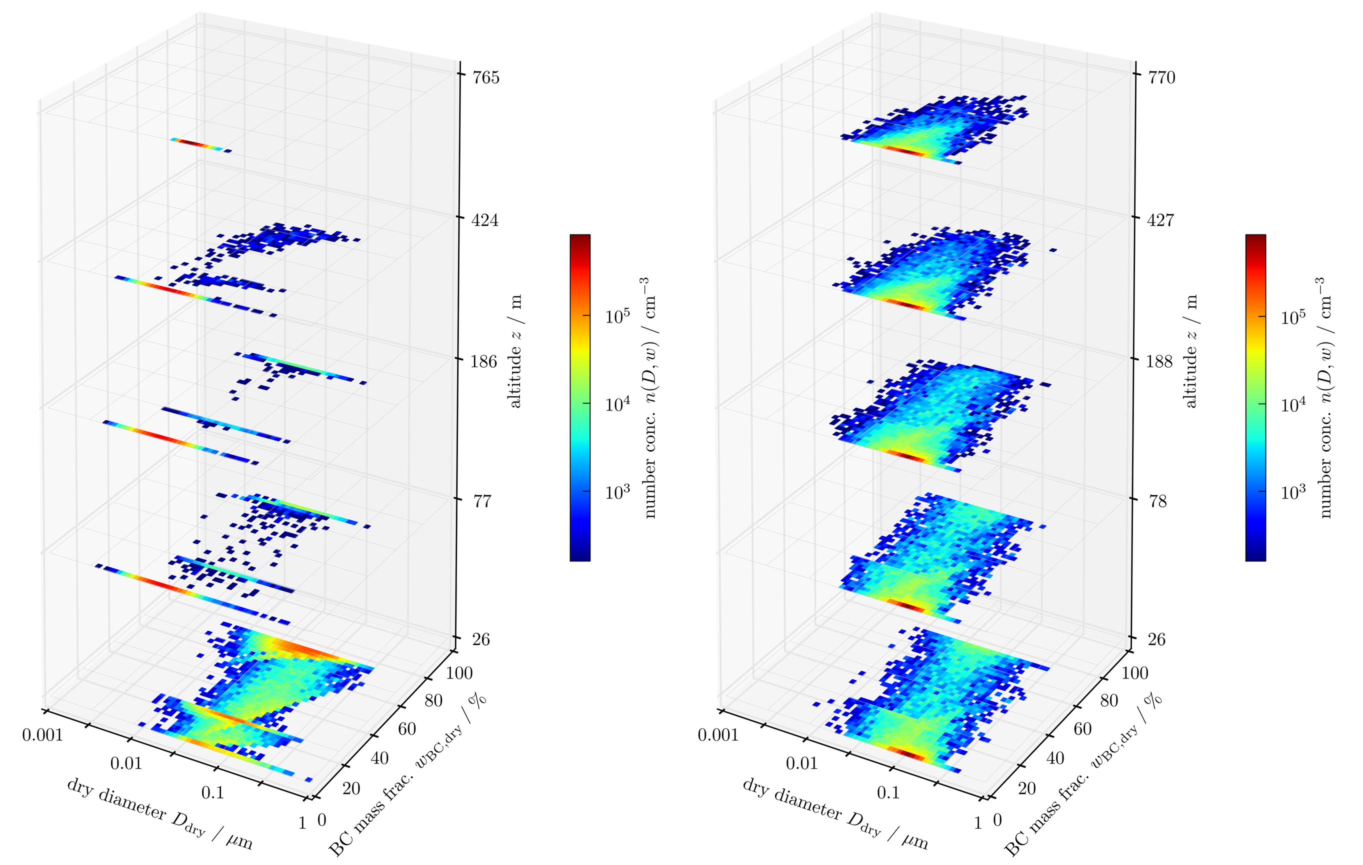

Figure 4: The mixing state of black carbon at 5 selected levels in the boundary layer at 2 h (left) and 7 h (right) into the simulation.

Conclusions

- We coupled the particle-resolved aerosol model PartMC-MOSAIC to the 1D version of WRF.
- The stochastic particle transport algorithm for diffusion converges to an analytical solution.
- Initial results for black carbon aging show that while black carbon particles become well mixed in the boundary layer with time, fresh black carbon particles exist in only the lowest layers.

References

N. Riemer, M. West, R. A. Zaveri, and R. C. Easter. Simulating the evolution of soot mixing state with a particle-resolved aerosol model. *J. Geophy. Res.*, 114:D09202, 2009. DOI: 10.1029/2008JD011073.