Review of “Explicit stochastic advection algorithms for the regional scale particle-resolved atmospheric aerosol model WRF-PartMC (v1.0)” by Jeffrey H. Curtis, Nicole Riemer, and Matthew West

Summary

The paper presents a stochastic advection algorithm for particle-based models and its implementation in the particle-resolved atmospheric aerosol model WRF-PartMC. The algorithm is verified in a series of test cases of increasing complexity, starting from 1D advection in a periodic domain, and culminating in a three-dimensional simulation driven by realistic meteorology. Enabling regional simulations in WRF-PartMC is a significant model advancement. Therefore, the paper is suitable for publication in GMD after my minor comments and questions are addressed.

General comments

The proposed scheme is based on interpreting the fluxes coming from a numerical advection scheme as probabilities. This is valid only if the “probability” given by (14) is between 0 and 1. However, this may not always be the case. It seems to me that (14) will usually be very close numerically to the local Courant number. Some advection schemes are stable with Courant numbers greater than 1. This includes the WRF schemes used in this paper. Interestingly, in 1D the same condition that guarantees the probability to be less than 1 ($\frac{\Delta t}{\Delta x} f_{i+1/2} < n_i$) also guarantees positivity preservation. Yet, most advection schemes aren’t positivity-preserving without additional limiting. Can the authors comment on this ? In the provided reproducibility notebook for the 1D test case there is code that clips the probability value, but there is no mention of this in the paper. Was this necessary and was a similar limiter used in the other test cases ?

The authors show that the stochastic transport algorithm injects energy at high spatial frequencies and analyze this process in considerable detail, including an approximate Fourier analysis. This analysis is very similar to von Neumann stability analysis of finite-difference schemes. Based on this the authors say that odd-order advection schemes are preferable, as they damp high spatial frequencies. I am wondering if a stronger statement could be made: that the stochastic algorithm based on even-order energy-conserving advection schemes is unconditionally unstable in a periodic domain, since it leads to unbounded growth of energy ? In general, are the stochastic algorithms less stable than their finite-volume base schemes ?

One of the motivations for using the proposed stochastic transport algorithm instead of Lagrangian advection is computational performance. Would it be possible to add to the article some performance numbers showing how much slower the stochastic algorithm is compared to its base finite-volume scheme ?

Specific comments

- Line 157 “However, we now have three different probabilities for each boundary, …” : If I understood the extension to three dimensions correctly, this sentence can be misleading. Maybe it would be better to say: “However, we now have three different probabilities, one for each boundary, …”
- Line 161: I think it is not (16), but a multi-dimensional extension of it, that needs to be used in three-dimensional simulations.
- Section 2.5: Please provide more information on the new monotonic third-order advection scheme. There are many approaches to constructing limiters for advection schemes. If the approach is something standard, like FCT, then I don’t think it is necessary to provide every detail, but indicating which method was used and adding a citation would be helpful.
- Subsection 2.8 feels out of place to me in Section 2, since it details the computation of error metrics in numerical experiments. Maybe put it at the beginning of Section 3 ?
- In all numerical examples: Please indicate which experiments used the monotonic versions of the schemes and which the unlimited ones.
- Figure 2 caption: “at T = 2” should be “at t = 2”

- Lines 304-305 “The initial number concentration is given as …”: In subsection 2.6 it is stated that `q` refers to the mixing ratio. Figures 6 and 7 are also labeled as mixing ratios. I realize that in this simple advection example the values are probably numerically equal. However, a similar issue is present in the subsequent realistic meteorology test case, where the text sometimes refers to the number concentration field, but, according to their labels, the figures are showing mixing ratios. For example, in line 328. It would be good if the language was consistent with the symbols and labels.
- Section 3.4 (WRF meteorology test case) : It would be helpful to provide more information about the setup of this test case. At which geographic location was the computational domain centered ? What was the time step ? What were the boundary conditions ?
- (E10): Shouldn't the conditions on the right be $A_k < 0$ and $A_k = 0$ since a in (E7) corresponds to $\exp(A_k)$?