GMD manuscript #2020-404: replies to the reviews

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First, let us thank all three reviewers for their valuable critique and feedback. Below, we provide point-by-point replies to all comments. Quoted text of the reviews is typeset in teal and with larger margins.
A revised manuscript with changes automatically highlighted using the latexdiff tool is enclosed with additions marked with blue color and deleted text in red. Additions to the bibliography are not color-highlighted, but all references to new bibliography items are within blue-underlined blocks in the text.
The key change in the manuscript is the introduction of an entirely new section (numbered 3 in the revised manuscript) covering two-dimensional simulations in which one of the dimension corresponds to the particle size and the other to vertical displacement in a column of air. These simulations feature coupling between particle growth and ambient supersaturation dynamics. This addresses the main point of all three reviews of overly simplified test case employed.

comments by Josef Schröttle, 24 Feb 2021

> This study introduces a new Python library for advection of geophysical flows with the MPDATA scheme. More specifically, it concentrates on the broadening of cloud droplet distributions due to advection and compares those distributions to analytically derived functions. It is based on previous work by the authors in a C++ library and numerous studies that have been conducted since the 1980s up to now. The paper is clearly written in the introduction, the methodology, and results sections. The reader would profit from a more fluent overview of the background literature in this work (in section 1.2),

Several correction to punctuation, the usage of articles and sentence shortening has hopefully improved Section 1.2.

> ... as well as a brief motivation why this is such important work especially in the context of clouds. A short suggestion of how to incorporate this is given by the reviewer. Also, a brief description of the software for interested users would be very helpful. Overall, this work is unique in its focus on comparing 2-3 advection

> schemes in the context of cloud dynamics and could be a basis for many future applications after major revision.
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> First general comments from my side:
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> •To give a brief motivation, why your work is so important, I would refer to clouds in climate research, e.g.: Climate goals and computing the future of clouds, Nature Climate Change volume 7, pages 3–5 (2017) or a more recent publication

The background section was extended following the reviewer's suggestion including a reference to the Schneider et al. 2017 paper.

> •How do your simulations evolve in time? Besides the cloud distributions you show in Fig. 1ff, I would like to see Hovmoeller diagrams of cloud distributions of selected experiments to see their temporal evolution.

The new section covering two-dimensional simulations features two figures addressing this point. The newly introduced Figure 11 depicts the temporal evolution of the spectral width parameter d, while the new Figure 10 depicts actual binned size spectra at each level of the vertical grid conveying analogous information as a Hovmöller spectral-temporal diagram.

> •Have you tried more advection schemes besides: upwind, mpdata 2, mpdata 3?

A comparison with other techniques, in particular with the Lagrangian (moving-sectional, particle-reolved) representation is planned for a follow up study. The concept for this paper is to constitute a guide across different aspects of the MPDATA algorithm which need to (or can optionally) be, taken into account while addressing the particular problem of particle condensational growth.

> •You should point out the clear improvement of MPDATA compared to upwind scheme.

The newly introduced Fig. 12 aptly highlights this improvement depicting the robustness in which application of even a single corrective iteration of MPDATA basically halves the spectral width of the simulated droplet spectra.

> •What are the initial conditions in your simulation? What noise do you use?

The initial condition has been specified in section 1.5, in particular through the equation 1.6 (initial particle spectrum) and the numerical parameters given below (timestep, grid layout). No noise considered.

> •Please provide a comparison for the plot of mixing ratios versus Rd (Fig. 9) to observations from nature or experiments. Again, state explicitly in the caption of Fig. 9, what Rd symbolizes: Radius of ...

R_d symbolizes the analytical-to-numerical ratio of the values of the droplet spectral width d. The misleading R_{disp} vs. R_d naming has been unified and the figure cation includes the definition now instead of a reference to an equation.
The discussion of the newly introduced Figure 11 features a reference to observations.

> - The error overview plots Fig. A1ff are a very interesting way to compare advection schemes and experiments, efficiently. Why do you not pull those into the results section for selected experiments? Is the truth for computing the error the analytical model?

Yes, the error measure is based on the analytical solution (as indicated in eq. A1). The highlight of the polar plots presented in the appendix is the Courant number dependence of the rate of convergence. It is of importance when devising case study setups or developing adaptive timestepping criteria - both relevant, yet of secondary relevance to the storyline of the paper, hence presented in an appendix.

> - You should - point out in the conclusion, that this study can be a basis for future work.

The last paragraph of the conclusions now outlines the path towards four-dimensional MPDATA solver capable of integrating bin microphysics dynamics in 3D CFD framework.

> I am looking forward to providing more detailed comments in the next iteration of this manuscript. For now, some technical comments:
>
> (a) Fig.1:... those are cloud droplet distributions, right? Please state this, explicitly.

It is now clarified in the caption that the plot depicts particle number densities.

> (b) Fig.1: Can you provide the analytical functions for the distributions & its derivations?

It is given with an outline of derivation when introducing eq. 2.5, with reference to the .

> (c) A better description of the Python library is required for interested readers to repeat your experiments. You can do that either in README file on github or in a section of this paper.

The PyMPDATA README file has undergone significant expansion including addition of new examples and inclusion of sample code in Julia and Matlab. The public API of the library is now published along with annotations at `https://atmos-cloud-sim-uj.github.io/PyMPDATA`. Submission of a short paper to the Journal of Open Source Software outlining the package features is planned.

comments by Anonymous Referee #2, 01 May 2021

> This study examined performance of various MPDATA variants in solving drop size distribution evolution by condensation. The authors reviewed many previous studies in the context of improving MPDATA and showed that MPDATA with three anti-diffusive iterations, third order term, infinite gauge, and the non-oscillatory option reduces the numerical diffusion to roughly a tenth compared to that of the upwind scheme, although it requires ~ 10 times longer than the upwind scheme.

The computational cost footprint is now highlighted in the abstract to clarify that the increased accuracy comes at a trade off.

> Although this study examined the performance of MPDATA variants systematically, I would raise two serious problems this study bears. At the current stage, my recommendation is to reject the manuscript for publishing on GMD, and encouraging the authors to improve the manuscript accordingly.
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> 1. Somewhat outdated
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> I can find several recent papers closely related to the topic this study focuses on: Morrison et al. (2018, doi: 10.1175/JAS-D-18-0055.1), Pardo et al. (2020, doi:10.1175/JAS-D-20-0099.1), and Lee et al. (2021, doi:10.1175/JAS-D-20-0213.1). All those papers already pointed out that drop condensation itself can be sufficiently converged with better schemes or better designed grids, but it is the condensation w/ vertical advection or w/ collision-coalescence that causes serious problems. Furthermore, those studies utilized LES model results in explaining their results, whereas this study only showed the box model results. This study clearly exhibited the performance of MPDATA variants in solving drop condensation, but only the convergence test in solving drop condensation is somewhat outdated compared to the studies I mentioned. I strongly suggest the authors to improve their study by including vertical advection, collision-coalescence, and/or something we do not know its effects.

The newly added section featuring single-column case study involves vertical advection. All three recent papers mentioned are now referenced commented on.

> 2. Experimental setting
>
> In the authors' experimental setting, supersaturation is fixed so the liquid water content increases up to 10 g kg–1, which is almost unrealistic except for tropical cyclones. I strongly suggest the authors to modify the experimental setting so the results become more realistic. For example, Morrison et al. (2018) and Lee et al. (2021) fixed the vertical velocity to be 1 m s–1 for 20 min rather than fixed the supersaturation.

The newly added single-column test case features supersaturation dynamics coupling with the particle growth.

The original box model setup was kept as is. Despite somewhat unrealistic range of liquid water content it allows for performing the convergence analysis across a wide range of grid- and timesteps.

comments by Anonymous Referee #3, 04 May 2021

> This manuscript examines the fidelity of various flavors of the MPDATA advection scheme for solving condensation of the drop size distribution. The writing style is clear and concise, the historical review of bin scheme and MPDATA development was illuminating, and the figures were simple and easy to understand. That said, the study suffers from a few key flaws that lead me to suggest the paper be rejected.
>
> First, the authors recognize that the difficulty of numerically modeling condensation/evaporation is that drop growth processes (in the mass dimension) are fundamentally coupled to spatial advection. Yet the test case, which if I understand correctly was chosen because a reference analytical solution can be obtained, either did not include a spatial advection component or this was not discussed. Morrison et al. (2018) and Lee et al. (2021) both point out that satisfactory solutions can be obtained by a number of schemes in the absence of transport; it is when they are coupled that special consideration must be taken.

The newly added section (number 3 in the revised manuscript) addresses this point by considering a two-dimensional problem with both the spectral and spatial transport considered simultaneously.

> Secondly, the physical feasibility of the test case is dubious; in any warm cloud, a mass mixing ratio of 10 g/kg is nigh impossible.

The choice of the test case for the box model simulations was motivated partly by the aim of performing the convergence analysis presented in the appendix which covers a wide range of grid- and timesteps.

> Finally, another important aspect (in particular, of Lee et al., 2021) was not covered: the effect of refining grid spacing vs. refining algorithm formulation.

This point is addressed in the analysis presented in the newly introduced Fig. 12 where results with different number of MPDATA iterations are presented for an array of Δt, Δr and Δz settings.

> These three factors combined leave me with the impression that this study, while rigorous, is not relevant to the current state of the field.
>
> I strongly encourage the authors to reconsider the paper by formulating a test case that would demonstrate the relevance of the algorithms tested in dynamical models, and evaluating the trade-off of increased algorithmic accuracy versus refined size grid.

We have followed the request introducing the single-column test case which covers both the vertical transport aspect as well as the supersaturation dynamics coupling.

Let us close this reply by expressing again our thanks for the reviewers' feedback what is also expressed in the acknowledgments section in the revised text.