Answer to Dr. Hilary Weller 10.5194/gmd-2023-78-RC3 on the manuscript "**An improved version of the Piecewise Parabolic Method advection scheme: description and performance assessment in a bidimensional testcase with stiff chemistry in toyCTM v1.0.**"

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Oct. 2023

We are grateful to Dr. Wellerfor her careful reading and insightful comments on our manuscript.

Contents

1 Comments by Dr. Weller

1.1 General comments

This is a very nice paper that describes evaluation of tracer transport using a signature function, as well as the improved PPM scheme mentioned in the title. The signature function gives a lot of information about the evolution of transport errors without the need for an analytic solution. I like it and I am surprised that it is not already widely used.

I have two main comments which the authors may argue is beyond the scope, but these comments, I think, would make the paper even more convincing.

1. A new advection scheme is introduced - PPM+W. The results of your test cases look good but you are comparing against some old advection schemes using a non-standard test case. Please include results using a standard test case so that you can refer to other papers that include results of exactly the same test cases and the reader can easily compare errors.

2. You propose a new test case. There isn't enough evidence presented to demonstrate that a new test case is needed.

1.2 Minor comments

1. "Non-monotonic" rather than "non-monotonous".

2. The section heading 2.2 "Flux description" is not well named. This is really "Definition of Test Case".

3. It is not clear why the test case described in sections 2.2.1-2.3 is not exactly the same as LeVeque (1996). Using dimensioned rather than non-dimensional variables does not constitute an effective change.

4. Line 147. Replace with "PPM (Colella and Woodward, 1984)" as that is how you refer to it elsewhere.

5. The errors of van Leer and PPM are not obvious in figures 3 and 4. These schemes look better than the +W schemes. Would it be possible or helpful to compare the scheme cell averages with the exact cell averages?

6. Is it usual for chemistry schemes to violate machine precision conservation? Provide references.

7. You often start a new paragraph where there shouldn't be a new paragraph. Eg line 224 and 259. Note that any blank line in LaTeX will create a new paragraph. So don't put blank lines around equations unless you want a new paragraph.

8. Equations 9 and 10 need u to be displayed as a vector and equation 10 needs a dot between u and grad.

2 Answer to the General comments

We are very grateful of the consideration and positive appreciation given by Dr. Weller on our work.

1. "A new advection scheme is introduced - PPM+W. The results of your test cases look good but you are comparing against some old advection schemes using a non-standard test case. Please include results using a standard test case so that you can refer to other papers that include results of exactly the same test cases and the reader can easily compare errors."

Answer We agree that much work has been done on advection schemes since the design of the Van Leer [1977], Colella and Woodward [1984] and Walcek [2000] schemes. In this sense it is fair to say that we compare PPM+W to "some old advection schemes". This is why we are not able to claim (and we don't) that the PPM+W scheme represents an improvement over the latest state-of-the art regarding advection schemes. Most likely, it doesn't. However, as we argue, the PPM scheme [Colella and Woodward, 1984] is widely used in state-of-the-art geophysical models. Such models include oceanic models – see Gibson et al. [2017], Dietze et al. [2020], air quality models includeing the very popular models CMAQ, CAMx and Geos-CHEM. Atmospheric models such as GFDL [Harris et al., 2021] and Meso-NH [Lac et al., 2018] also use PPM.

This widespread use of the PPM scheme is probably due to the fact that, in the wording of Harris et al. [2021], it can be considered as "highly accurate and efficient enough to be useful", meaning that for some geophysical application it represents a good compromise between accuracy and computational cost. The recent paper of Cao et al. [2023] shows how PPM is being adapted to the latest technological evolution in order to optimize its good numerical efficiency in new architectures.

As a summary regarding PPM, while we are aware of the existence of higher-order or alternative approaches with improved accuracy, we think that PPM is still very used as a good and robust compromise between accuracy and numerical precision, so that any improvement to this scheme (in our case, improving accuracy without degrading efficiency) is potentially relevant, not as a novelty in the quest for more accurate advection schemes, but as a possible practical improvement in the fields of geophysics where PPM seems to be one of the best compromises between accuracy and cost, and PPM+W might further improve this balance by improving accuracy without increasing the cost.

We agree that the use of the other schemes we present as benchmarks, Van Leer [1977] and Walcek [2000] have become less frequent nowadays. Both these schemes are among the available options in the CHIMERE chemistry-transport model along with PPM [Menut et al., 2021], and Walcek is the advection scheme retained in the LOTOS-EUROS chemistry-transport model [Timmermans et al., 2022].

✓ In the introduction of the revised version we will include references to higher-order schemes, with Prather [1986] and Waruszewski et al. [2018] as examples, and mention explicitly the fact that PPM is hconsidered as a good balance between accuracy and computational efficiency–Harris et al. [2021].

Regarding the choice of the test case, we have worked with the swirling rotational flow exactly as defined in LeVeque [1996], we do not know if this can be qualified as a "standard" test case, most standard test cases we know of are designed on the sphere [Lauritzen et al., 2014], which is not adapted for applications to regional models. One of the test cases presented by Lauritzen is adapted from the LeVeque [1996] swirling rotational flow, which we decided to use for our study. It has several advantages that suit our purpose:

- The flow is non-constant in time which makes it both more realistic (compared to the real conditions in a chemistry-transport model), and a more challenging test of the correctness of the implementation.
- The flow is sheared, making it challenging by stretching the plumes into filaments.
- The flow is contained within a square box, preventing the need for a boundary condition and allowing to check mass conservation (unlike, *e.g.*, solid rotation).

The LeVeque [1996] study itself does not provide quantitative results in terms of reproducible metrics. More generally, we did not find a suitable test-case with a simplified but stiff chemistry in a square area (well-suited to the test of the advections schems tested here, which are designed for cartesian geometry).

Producing another test-case as suggested would have made the study very tedious. However, in the revised version, we have made two improvements in this direction:

- ✓ we perform a convergence test to compare the selected advection schemes across a range of resolutions, confirming that PPM+W performs consistently better than PPM even when resolution increases (Section 3.1.4, Fig. 5 and Table 2 in the revised version);
- ✓ we provide results from a higher resolution simulation of the same test case (Table 6 in the revised version). These results confirm a generally better performance of PPM+W compared to other schemes, but the edge over PPM is more reduced and one species is better reproduced by PPM at this high resolution.

Also, in the conclusion of the revised version, we insist more on the fact that we have not tested this new scheme in realistic conditions, and that we have not tested the full range of Courant numbers and of possible tracer patterns.

2. You propose a new test case. There isn't enough evidence presented to demonstrate that a new test case is needed.

See above, we did not find a standard test case designed for a chemistry-transport problem in cartesian geometry, which is why we have designed our own test case build a ultra-simplified –but stiff– system representing tropospheric chemistry, and a flow (which is exactly the swirling deformational flow of LeVeque [1996]), that has the desirable properties listed above.

The initial formulation ("This flow is defined from the ideas of LeVeque [1996].") was leading the reader to understand that we have defined a new flow, that would be "almost" the swirling deformation flow of LeVeque [1996], while we actually used *the exact flow* of LeVeque [1996].

✓ **in the revised version, this sentence has been changed to:**
The flow we use in this study is the swirling deformational flow introduced by LeVeque [1996] (their Eqs. 9.5-9.6): ...

3 Answers to the Minor comments

1. "Non-monotonic" rather than "non-monotonous".
✓ . We have also replaced two more occurences of "monotonous" by "monotonic'

2. The section heading 2.2 "Flux description" is not well named. This is really "Definition of Test Case".
✓ . The section has been renamed as suggested.

3. It is not clear why the test case described in sections 2.2.1-2.3 is not exactly the same as LeVeque (1996). Using dimensioned rather than non-dimensional variables does not constitute an effective change.
✓ The flow is actually exactly the same as LeVeque [1996] (but with dimensioned variables). The fact that this is exactly the same flow has been clarified in the revised version..

4. Line 147. Replace with "PPM (Colella and Woodward, 1984)" as that is how you refer to it elsewhere.
✓ THis has been changed accordingly.

5. The errors of van Leer and PPM are not obvious in figures 3 and 4. These schemes look better than the +W schemes. Would it be possible or helpful to compare the scheme cell averages with the exact cell averages?

The Van Leer and PPM schemes look better than the "+W" schemes in this figure because they are an actual polynomial (degree-1 for Van Leer and degree-2 for PPM) reconstruction of the exact flow, which the Walcek-corrected slopes are not. As said in the manusript, the idea of the Walcek slope modifications is to intentionnally overestimate the fluxes into the cell with the maximum mixing ratio in order to better maintain this maximum value. Therefore, the Walcek reconstruction departs more strongly from the exact mixing ratio than the Van Leer or PPM schemes because it is not a polynomial reconstruction of the exact mixing ratio. Hawever, as shown by Walcek [2000], this intentional departure from the polynomial reconstruction brings added skill to the scheme in resolving the advection equation.

It would not be helpful to compare the cell averages with the exact cell averages, becaus in all gthese schemes, by construction, the cell-average of the reconstructed concentration is equal to the exact cell average.

6. Is it usual for chemistry schemes to violate machine precision conservation? Provide references.
This is usual, unfortunately. It is not frequent that authors discuss this problem explicitly in their publications. For example, Brasseur and Jacob [2017] in their chapter 6 on numerical methods for chemical systems only allude very briefly to this issue ("Mass is not fully conserved by the Jacobi and Gauss–Seidel iterative procedures"). Cariolle et al. [2017] (cited line 197 of the initial manuscript) does discuss this issue in some detail however in their Section 2.1, giving more precision on the reason for this lack of mass conservation: the scheme itself (Eq. 6 in our initial manuscript) is mass conservative, however "the mass conservation can only be obtained if a good convergence of the solution is reached".

✓ **We have added a new reference to Cariolle et al. [2017] at the point when we explain why perfect mass conservation is not obtained**

7. You often start a new paragraph where there shouldn't be a new paragraph. Eg line 224 and 259. Note that any blank line in LaTeX will create a new paragraph. So don't put blank lines around equations unless you want a new paragraph.

✓ We have checked and corrected these undesirable new paragraphs around equations, we hope there is none left in the revised version.

8. Equations 9 and 10 need u to be displayed as a vector and equation 10 needs a dot between u and grad.

✓ This has been fixed, thanks.

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