PPM+W, an improved version of the Piecewise Parabolic Method advection scheme
Description, evaluation and implementation in the CHIMERE model.

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Outline

Excess diffusion : a problem for the representation of sharp plumes in chemistry-transport models

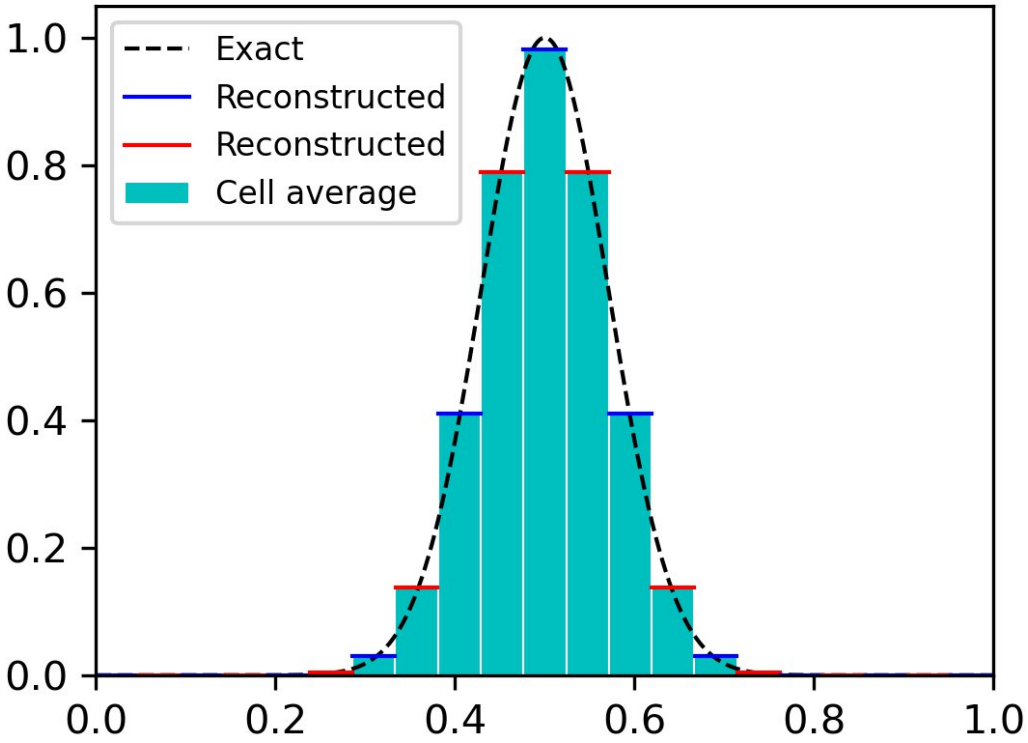
- For plumes with non-existent chemistry, excess of numerical diffusion will affect the location/structure of the plume but not its mass. On the contrary, for plumes with non-linear chemistry (volcanic + wildfire plumes), excess dilution of the plume will affect chemistry (including the mass of compounds).

- Excessive **vertical diffusion** of the plumes has been identified as a major cause of excess dilution. This problem has been clearly identified and there is an ongoing effort to solve it (e.g. Zhuang et al., 2018, Emery et al., 2011). Recent results obtained at LMD show promising output, by going back and forth between academic tools and real-cases studies.

References:

1. Colette, A., Alsac, N., Bessagnet, B., Biaudet, H., Chiappini, L., Favez, O., Frejafon, E., Gautier, F., Godefroy, F., Haeffelin, M., Leoz, E., Malherbe, L., Meleux, F., Menut, L., Morille, Y., Papin, A., Pietras, C., Ramel, M., and Rouil, L.: Assessing in near real time the impact of the April 2010 Eyjafjallajökull ash plume on air quality, Atmos. Env., doi: 10.1016/j.atmosenv.2010.09.064, 2010
2. Emery, C., Tai, E., Yarwood, G., and Morris, R.: Investigation into approaches to reduce excessive vertical transport over complex terrain in a regional photochemical grid model, Atmospheric Environment, 45, 7341 – 7351, doi: 10.1016/j.atmosenv.2011.07.052, 2011
3. Zhuang, J., Jacob, D. J., and Eastham, S. D.: The importance of vertical resolution in the free troposphere for modeling intercontinental plumes, Atmospheric Chemistry and Physics,doi: 10.5194/acp-18-6039-2018, 2018.

The PPM+W advection scheme : better performance for (almost) the same cost

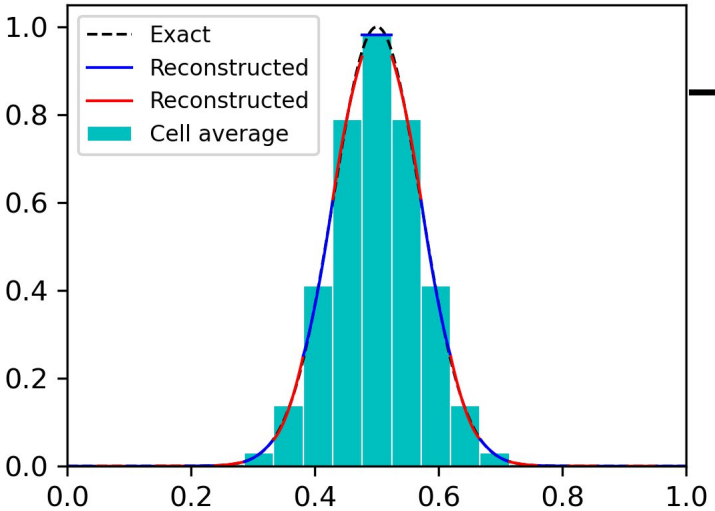


Flux-form advection schemes:

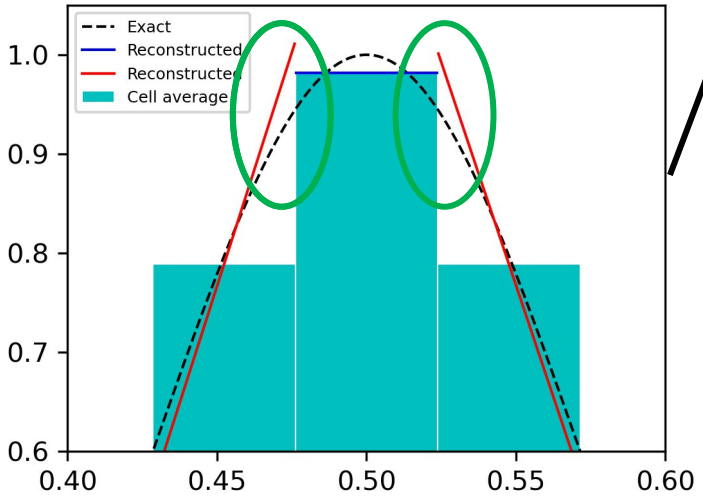
- From the cell-averaged values, reconstruct the mixing ratio within each cell
- This reconstructed mixing ratio permits to estimate the fluxes through cell-boundaries during each time step
- From these fluxes, the field of mixing ratio at the next time step can be constructed.

The simplest possible reconstruction: assume that the mixing ratio is equal to its cell-averaged value everywhere. Simple but...Very inaccurate and diffusive.

The PPM+W advection scheme : better performance for (almost) the same cost



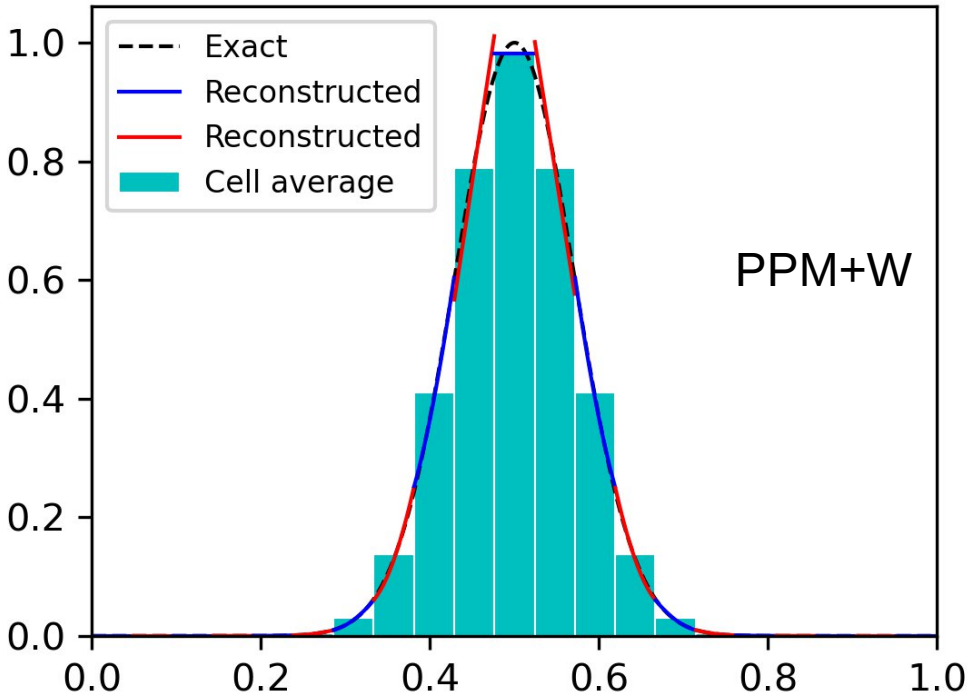
Colella (1984): PPM: high-order reconstruction away from extrema



Walcek (2000) :flux-adjustments in the vicinity of extrema

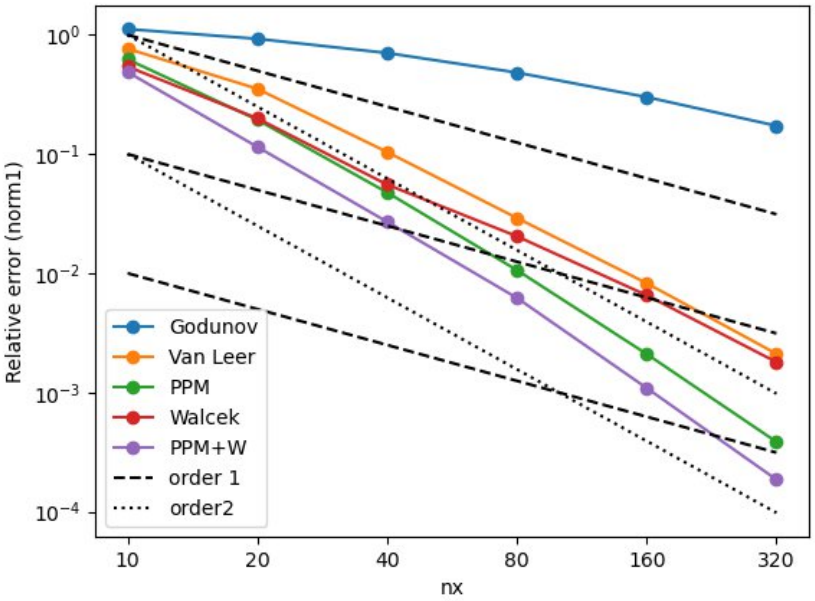
Idea:

Perform the same flux corrections than Walcek (2000) but in the PPM scheme (instead of Van Leer) ?



PPM+W (2023) : Piecewise Parabolic Method with Walcek Flux Adjustments

The PPM+W advection scheme : better performance for (almost) the same cost



Norm-1 convergence plot for the schemes mentioned so far, ***including PPM+W***

Scheme	Execution time
Godunov	5.8 ns
Van Leer	12.2 ns
Walcek	14.9 ns
PPM + W	30.3 ns
PPM	32.4 ns

Computation time for one execution of the scheme for the schemes mentioned so far.

Better accuracy

Similar cost

compared to the largely-used PPM scheme (CMAQ, CAMx, CHIMERE etc.)

PPM+W has better accuracy and similar cost w.r.to PPM

The PPM+W advection scheme : better performance for (almost) the same cost

Partial conclusions

- We have developed a **new advection scheme** suited for chemistry-transport models
- This scheme merges the **high-order characteristic**s of PPM with the **antiffusive properties** of Walcek
- **Better accuracy** than both PPM and Walcek
- **Computation time is not longer** than PPM

More questions (and some answers)

- Does PPM+W keep an edge on other schemes in 2d cases ?
- How to evaluate advection schemes in the presence of active (non-linear) chemistry ?
- What is the impact of resolution on the comparative performance of these schemes ?

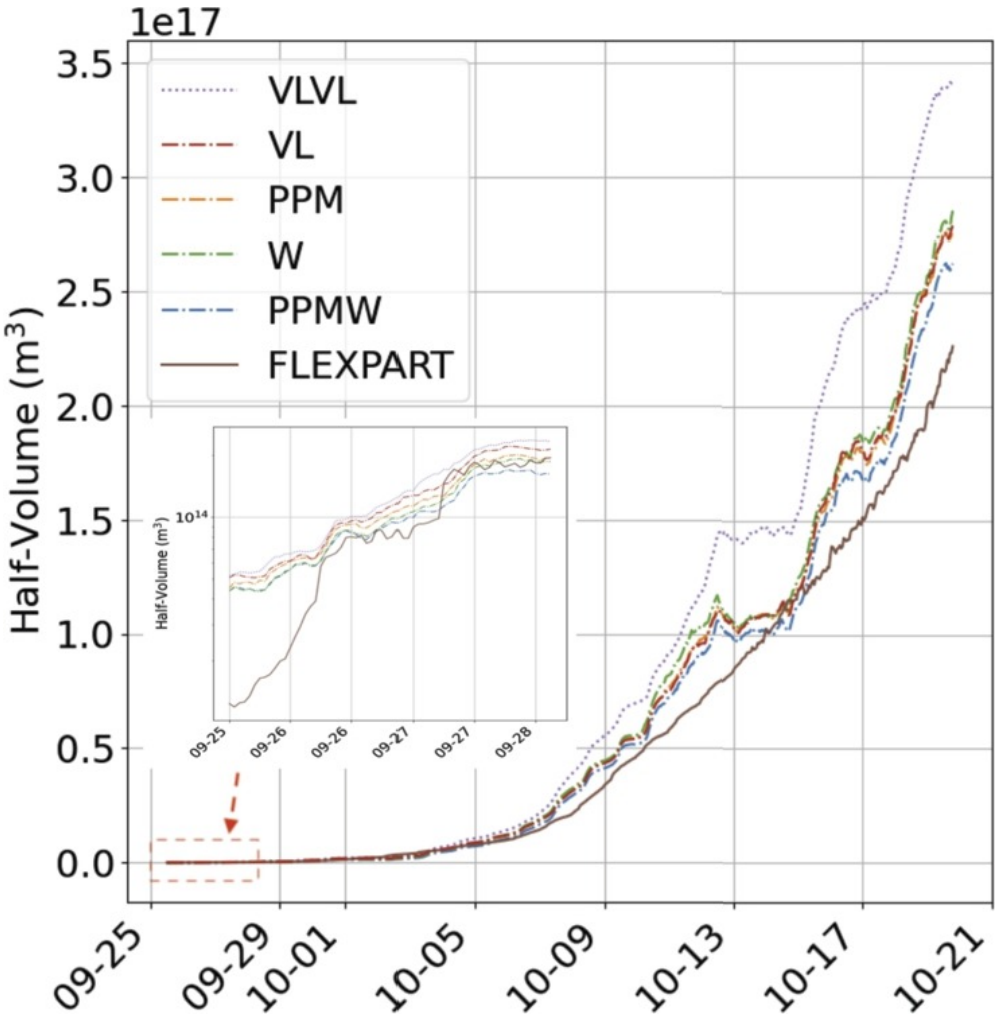
See: Mailler, Pennel, Menut and Cholakian, Geosci Model Dev. (2023), doi: 10.5194/gmd-16-7509-2023

More results in our GMD paper...

Implementation in the CHIMERE chemistry-transport model

- Following the above results, **the PPM+W scheme has been implemented in the last version of CHIMERE**. See:
  The CHIMERE chemistry-transport model v2023r1, **Laurent Menut** et al., Geosci. Model Dev. Discuss., 2024
  doi: 10.5194/gmd-2024-20

- We have tested this scheme in a real case of accidental tracer dispersion, and shown that the use of PPM+W **reduces model diffusion and makes it closer to a Lagrangien model**. See:
  Lagrangian and Eulerian modelling of ^{106}Ru atmospheric transport in 2017 over northern hemisphere. **Leo Adenis** et al., J. Environ. Rad., 2024.
  doi: 10.1016/j.jenvrad.2024.107416



Comparison between the PPM+W and other schemes in CHIMERE, and modelling in FLEXPART. Half-volume is an indicator of plume diffusion. ***Adenis et al., 2024***

Conclusions and perspectives

- We have developed a **new advection scheme** suited for chemistry-transport models
- This scheme merges the **high-order characteristics** of PPM with the **antiffusive properties** of Walcek
- This scheme is now available in **Chimere v2023**.
- Standalone code for the advection schemes presented here including PPM+W are available at:
  doi: 10.5281/zenodo.7937121
- Apart from horizontal diffusion, it is important and difficult to reduce vertical diffusion. See **Using the Després and Lagoutière (1999) antidiffusive transport scheme: a promising and novel method against excessive vertical diffusion in chemistry-transport models.** *Geosci. Model Dev.*, 2021 .doi: 10.5194/gmd-14-2221-2021
- **We think the approaches presented here (PPM+W in the horizontal and Després-Lagoutière in the vertical direction) could benefit other geoscientific models: chemistry-transport, atmosphere, ocean. Implementation is easy (<20 lines of code) and effect is strong, particularly in the vertical direction.**

These approaches are available to all the Geoscientific modelling community