Comment on gmd-2021-382

Anonymous Referee #1

Referee comment on "Massive-Parallel Trajectory Calculations version 2.2 (MPTRAC-2.2): Lagrangian transport simulations on graphics processing units (GPUs)" by Lars Hoffmann et al., Geosci. Model Dev. Discuss., https://doi.org/10.5194/gmd-2021-382-RC1, 2022

The manuscript contains the matter of two articles. The first Is a thorough description of the new version of the MPTRAC trajectory code and the second one is the description of the parallelization of this code using GPU which is an excellent example of the application of modern programming methods that is more general that MPTRAC. I accept the choice of the author to group these two works but it would have made sense to make two separate articles to reach a wider audience, at least for the second one.

The manuscript contains very useful material, in particular in the second part where it demonstrates how a complex simulation code can be moved to a GPU system using the high level library OpenACC with relatively small effort (compared to the full rewriting required by direct use of CUDA low level libraries). This is an important and inspiring contribution.

I only have a few comments to be accounted in the revised version

In regard of the sophistication of the rest of the code, the treatment of the vicinity of the pole appears very crude and inaccurate. There has been possibly few concern in the applications of MPTRAC so far but this is a point that should be corrected in the next version.

The convective parameterization is based on the assumption of CAPE relaxation and an important parameter is the CAPE threshold that should deserve some discussion. The manuscript says that a global value is used but CAPE accumulates much more over the continents than over the ocean, leading to much more intense storms in continental regions. Therefore a single threshold value will probably produce excessive mixing over the continents and too small mixing over the oceans. More generally, it is recognized by all experts in convective parameterization that CAPE alone is a bad predictor of convective

onset. As the ERA5 archive the upward and downward convective fluxes resulting from its state of the art parameterization of convection, why not using these data instead of a very crude representation of convection. Again, this might be considered in the next version.

The manuscript fails to quote this work "optimization of atmospheric transport models on HPC platforms, de la Cruz et al., Computers & Geosciences, 2016, doi: 10.1016/j.cageo.2016.08.019" which addresses very similar issues.

Figure 10 made from screen copies is not readable, either on print or on the screen.

Other minor comments

- 185: pressure is not the best choice of vertical transport for Lagrangian transport in the stratosphere as well where many models use instead the potential temperature and heating rates instead of pressure tendencies.
- 205: I guess the authors meant linear in log pressure.
- 770: The results from OpenMP parallelization may vary a lot according the scheduling strategy. This should be mentioned.
- 896: I do not see any fluctuations but a regular increase in fig. 11.