## Answer to Referee 1

We wish to thank to this referee for his/her very useful comments, which have helped us to improve the manuscript, and have been addressed as follows:

## General comments:

1. The paper presents an algorithm for the integration of air parcel trajectories in three dimensions and the computation of the function M for the analysis of Lagrangian transport, and it is applied to atmospheric reanalyzed data for the study of the Antarctic stratospheric vortex. The paper is clearly written, and visualization of the Lagrangian geometry of the stratospheric vortex shows potential. However, the paper lacks of new scientific results. While I cannot recommend publication, I encourage the authors to address my concerns below and resubmit.

We have clarified in the new version of the article the major goal, as maybe this was not sufficiently clear in the original manuscript. In the new version we state very clearly that the goal is to describe 3D Lagrangian structures on the stratosphere. To this end we have described in more detail (Section 2) what kind of 3D Lagrangian structures are expected in the stratosphere and we list specifically what are the new scientific results in this regard in the Abstract, Section 5 and the Conclusions.

- 2. Regarding the first part, the authors state in the abstract "The present paper introduces an algorithm for the visualization, analysis and verification of transport and mixing processes in three-dimensional atmospheric flows". While sections 2 and 3 present the methodology in a very clear and concise way, I do not a find significant novelty in this part of the paper.
- Neither the reanalysis data processing, nor the parcel trajectory methods are new (the way they handle the singularity at the poles in geographical coordinates seems identical to that published by some of the co-authors in De la Camara et al. 2012).
- The authors have published multiple articles analyzing transport in oceanic and atmospheric flows using the function M to highlight the Lagrangian geometry of such flows. The extension to 3D, while interesting, does not constitute a new advance from a methodological point of view since the authors have already introduced it in at least a couple of studies (Mancho et al. 2013, Lopesino et al. 2017). Besides, the function M is conceptually defined for n-dimensional fields (Mancho et al. 2013).

The referee is right. The algorithm is not new, and that sentence has been modified. The previous applications of the function M to 3D flows are summarised between lines 19 and 25 in the Introduction. Regarding the algorithm, what is new is its implementation for analysing 3D atmospheric data sets as stated in line 36 of the Introduction. We mantain the section describing the implementation of the algorithm (Section 3) because it may be useful to other researchers interested in applying this tool for similar purposes.

3. I do not quite understand the verification part of the study. Section 4.1 visually compares maps of the function M obtained from 2D isentropic calculations and from full 3D calculations (Fig 1). But, if I am not mistaken, the authors use the same set of equations (5) for both the 2D and 3D calculations; the only difference is that in 2D the

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vertical velocity w is zero. Does this mean the authors verify their 3D integration code against itself?

The 2D calculation is done on constant potential temperature surfaces which in general are surfaces which are time dependent and do not coincide with spherical shells. The velocity fields on these surfaces are also downloaded from ERA-interim. The 3D calculation is done in the 3D space with 3D velocity fields downloaded from ERA-interim and processed as explained in the article. Section 4 now discusses these issues and has been extended to include calculations showing cases in which the 3D calculation on spherical shells and the 2D calculation on the constant potential temperature surfaces coincide (upper stratosphere) and where they do not (upper troposphere).

**4.** Figure 2 does a much better job at verifying the function M code by comparing maps of M with geopotential height and potential vorticity (PV) fields. Sadly, the authors do not discuss this figure at all (see lines 16-20). Why is the anticyclone that we see in the height field not visible in the PV or M fields? What are the expected differences between PV and M? What about the tongue of high PV (red colors) wrapping around the vortex? Why is there no equivalent structure in the M map?

Also, it is rather confusing to analyze maps of these three diagnostics, each using different vertical coordinates. I recommend the authors to interpolate the data to a common horizontal surface.

Figure 2 (now figure 3) has been thoroughly explained in Section 4. The issues rised by the referee have been addressed including a new figure.

The different vertical coordinates used for each map are standard in atmospheric sciences and we are plotting for each one the value which is in correspondence to their partners. We do not think that differences in the units is a problem.

5. It is argued throughout the paper that stratospheric motions are basically isentropic for timescales of 10 days. While I understand the authors choice of an integration time of 5 days in Fig. 1 to compare against isentropic trajectories, why using again tau = 5 days in section 4.2 to analyze the 3D Lagrangian geometry of the vortex? Are the results not practically identical to 2D isentropic calculations if the trajectories are integrated over time periods when the isentropic assumption is valid? A way of checking this point would be to perform isentropic calculations at different vertical levels in the stratosphere, and plot similar figures 3-8 (longitude versus height).

We have compared isentropic calculations and 3D calculations in the new Figures 2 and 3 in Section 4 and it is shown when they coincide or not. We also discuss the effect of the integration period  $\tau$  on M. Additionally we have explained more clearly what new insights are brought by our results. Indeed, the 3D calculations allow to perform slices in directions perpendicular to plane of motion and those sections highlight the structure of normally hyperbolic invariant objects whose vertical structure cannot be visualized otherwise. To our knowledge such visualisation is described for the first time in this article.

**6.** • I strongly encourage the authors to increase tau to explore the full potential of 3D calculations. Is there a value of tau over which the Lagrangian geometry from 2D (isentropic) and 3D significantly and 3D diverge?

We have done this in Section 4.

7. Besides, one problem of using the wind field in geometrical height coordinates is that it is difficult to assess what part of the vertical motion is due to the vertical displacement of isentropic surfaces. To prove the added value of the 3D calculations, I recommend using the velocity field in potential temperature surfaces (the vertical velocity would therefore be the heating rate, see Diallo et al 2012 ACP).

The wind field in geometrical coordinates is useful to integrate equations (7). The integration of this system has allowed us to describe 3D Lagrangian structures in the stratosphere. In particular we describe to our knowledge for the first time the following issues: vertical extension of the stratospheric polar vortex and its lower limit and its tilted character. We have identified the boundary between troposphere and stratosphere. We have identified lagrangian structures, fully 3D, showing strong mixing into the troposphere. We have discussed the vertical structures of two counterrotating vortices, (the polar vortex and a new emerging one) and identified an invariant structure separating them and have related this to the presence of a normally hyperbolic invariant curve. For all this purposes our approach has shown to be sufficient and consistent with other results, thus we do not think it is necessary to repeat calculations within another approach. To address the issues regarding transport across potential temperature surfaces is a very interesting question feasible also within our approach (just calculating M on the time dependent potential temperature surfaces) but out of the scope of the current manuscript.

- 8. 2) I do not see any new insights into the dynamics or transport of the polar vortex.
- The description of the evolution of the stratospheric flow during the spring season is, as the authors acknowledge, basically the same as that given in much earlier studies. What have we learned from the analysis of the function M? Is this description richer from that offered by dynamically relevant fields such as geopotential height or PV? I am afraid not

We have explained in the current version very clearly what are the novel insights on the stratosphere provided by our work. It might be that our discussions in the first version were too much focused in addressing consistency with previous findings, and our findings were not sufficiently emphasized. For this reason we have rewritten the manuscript to address these issues. A list of specific new insights are described in the 7th bullet point, and further discussion about the comparison with the geopotential height and PV is given in the new version.

9. One needs a very trained eye to see the geometrical structures that the authors highlight in Figs. 7 and 8 (hyperbolic trajectories and invariant manifolds). How are these structures identified? How is its hyperbolic nature assigned? Also, those structures seem to be located in the outer side of the westerly jet, just in the region where Joseph and Legras (2002 JAS), with similar tools, described a region of chaotic motions. I think this paper does not offer new significant insights into the nature of this region. The fact that the authors identify vertical transport barriers (hardly seen by untrained eyes) does not mean that the motions responsible for those structures are three-dimensional. Again, a detailed comparison between 3D and isentropic calculations is needed.

We have introduced a new Section 2 which introduces and mathematically describes the type of 3D Lagrangian structures expected in the stratosphere. A relevant example is introduced. We have added extra arrows in current figures 8 and 9 to highlight the geometrical structures we are interested in and those are linked with the example described in the new Section 2.

Figure 9 a) is similar to the projections performed by Josep and Legras, although in that article they do not discuss the event we address in this figure about the boundary separating two counterrotating vortices present in the atmosphere. The advantage of the used tools with respect to the FSLE used by Joseph and Legras is that the M function highlights simultaneously manifolds and coherent structures related to elliptic regions.

On the other hand figures showing the vertical structure across the stratosphere are new and to our knowledge have not been described before.

Figure 8 address the invariant character of structures related to sharp changes in the color code of M. This is done by tracking a particle trajectory and observing that during its evolution, its position stays on a line with an abrupt change in the M color code.

A detailed comparison between 3D and isentropic calculations is addressed now in figures 3 and 4.