Reply to Anonymous Referee #3

General comments

As far as I can tell the trajectory model itself has not changed, so this article does not describe development of a model, but of a new user interface to an existing model. While there are novel aspects in the functionality of the tool, the article seemed much too long for describing them. It reads more like a mix of review and detailed user guide, rather than an exposition of new scientific development. I recommend a major revision to trim down to a more concise article focussing on the new capabilities and science opportunities offered by the new front end to LAGRANTO, and moving the syntax and instructions to a system user guide, which perhaps could be linked to in supplementary material. For example, Section 3.4 has some clever ideas but the paragraphs are full of script-based commands that interrupt the flow of the discussion and make the article difficult to read. I believe that the command language would be better described in systematic user guide documentation, rather than within text discussion.

Lagranto, as expressed by the last two letters of the acronym, has always been designed as a tool, user-friendly and versatile, in which the "core model", i.e., the actual computation of the trajectories, is only a relatively minor part. This paper clearly reflects this "tool character" by describing in some detail how the user can work with Lagranto and use its functionalities to do innovative research. We think, supported by the feedback of the other referees, that GMD is a journal that also allows the description of tools, i.e., of technical achievements beyond the core model development. We therefore decided to shorten the paper only slightly (some paragraphs that read more like a user guide have been omitted). We also acknowledge that section 3.4 is rather technical, but this section in particular reflects very nicely the concept and rationale of Lagranto.

In the introduction paragraph to section 3.4 we removed the discussion of the different output options (boolean list and list of trajectory numbers). We think that its description takes too much space given the extra value added. Hence, it makes the technical section 3.4 a little shorter. Of course, the remainder of section 3.4 is still rather extensive. On the other hand, we regard LAGRANTO's powerful selection criteria as a particularly valuable feature. It allows many sensitivity experiments to be performed easily, without making any changes to, e.g., Fortran codes. In this sense, in our view it's worthwhile to provide a glimpse at the main selection features of LAGRANTO. The benefit becomes even more apparent, if the full reference guide for the select command is considered (see supplementary material at initial submission, or the web resource in the revised version). Indeed, it's lengthy and very technical style can make it a little intimidating, and a concise summary of the key features, section 3.4 of the manuscript, makes it more accessible.

In section 4.2 we leave out the reference to the trajectory quickview tool (L543-547). This implies that Figure 6 in the original manuscript is removed, and only one of the two panels is later shown in section 5.3 of the revised manuscript. Of course, the text of section 5.3 is acorrdingly adapted. The reviewer is perfelctly right that this is rather technical and can reasonably be omitted. Furthermore, we now think that it's also too technical to list the first few lines of the spherical polygon file (L587-594 in the original manuscript). We remove this part, hence further shortening the section on orographic flows. All the other parts we would like to keep in the section, because they discuss different and important aspects of LAGRANTO's capabilities.

Finally, we decided to shorten also section 4.4. Here we introduced the simple trajectory calculation tool 'tracal' which allows to perform simple arithmetic operations on the trajectory files. The tool is still mentioned in Table 3 and of course some examples are given in the detailed reference guide.

Specific comments

1) l.10: Not all these models solve the trajectory equation (1) iteratively. They all solve it numerically and perhaps with substeps as in Runge-Kutta schemes, but these are not iterative.

We have replaced 'iteratively' with 'numerically'. Of course, there are many numerical schemes which are not iterative, e.g., the Runge-Kutta scheme. We are aware of this and, actually, the wording was unfortunate. With 'iteratively' we did not mean the details of the numerical scheme itself, but the basic 'nature' of a trajcetory calculation. It starts with a starting position, then proceeds to a new position, and continues to do so in the course of the calculation. In this sense, we understood the term 'iteratively, but avoid this confusion now by using 'numerically' instead.

2) Eqn(1): Important to note that u(x,t) since if the wind field were steady (time-independent) then the trajectories could be integrable using a streamline method.

Thank you, this is a very important point, which we also considered when redrawing the schematic Fig. 3.

3) l.13: It is also not true that these trajectory models all use data in pressure coordinates and integrate vertical position using omega. Some use alternative vertical velocities depending upon the input data level type.

This point was also commented by another reviewer. We remove the explicit reference to 'pressure' in the revised manuscript. This should make clear that at this place of the manuscript we don't want to discuss all the technical details of the trajectory calculation, but only its basic 'nature'.

4) In Section 3.1 it is mentioned that different vertical coordinates can be used within LAGRANTO including hybrid-pressure and isentropic coordinates. The second paragraph in Section 3.1 appears to indicate that even if the input data is given on alternative vertical levels that LAGRANTO still integrates (1) in pressure coordinates using omega. Is this true, or does LAGRANTO v2 support the use of different vertical velocities, such as theta-dot (heating) in isentropic coordinates?

At the moment, all trajectory calculation with LAGRANTO v2 are done using pressure as vertical coordinate (or height for the COSMO version). However, we see the value of different vertical velocities and intend to implement this in a future extension of LAGRANTO. Especially heating rates will be of interest if problems in stratospheric dynamics are considered. By providing a web page to LAGRANTO (www.lagranto.ethz.ch) and distributing the code by means of a SVN repository, we hope that further extensions to LAGRANTO can easily be installed by the LAGRANTO user community.

5) l.26: Although it may be true that LAGRANTO v2 offers the user a ready-made tool that can combine selection criteria and enable efficient calculation, it should be noted that the same calculations could be performed (and have been in the literature) using other existing trajectory models, perhaps with less user friendly methods of selecting trajectories.

Of course, one can do very clever trajectory selections with the output of any trajectory model. However, the point is, that the idea of flexibly and iteratively selecting trajectory subsets, based upon physical and/or geometrical criteria, is a central point of the design of the Lagranto tool – and that any user can use this functionality very efficiently without investing in code development. To the best of our knowledge this is a unique feature of our tool.

6) Para 3, Intro: The review here misses the use of trajectory calculations in the stratosphere which was has been extensive since the 1980s. In particular, the long-time integration of trajectories was tested quantitatively using balloons in the MATCH experiment.

The reviewer is correct that our writing did not appropriately reflect the many trajectory applications in the stratosphere. We therefore have changed the sentence as follows and included references to three pioneering trajectory studies in the stratosphere:
"Since the late 1970s – using now wind fields from reanalyses or model simulations – trajectories have been frequently used for investigating different types of atmospheric flow phenomena including extratropical cyclones (e.g., Whitaker et al., 1988; Kuo et al., 1992), orographic flows (e.g., Buzzi and Tibaldi, 1978; Steinacker, 1984), stratosphere–troposphere exchange (e.g., Buzzi et al., 1984; Vaughan et al., 1994; Newman and Schoeberl, 1995), and transport and mixing in the stratosphere (e.g., Austin and Tuck, 1985; Schoeberl et al., 1992; Bowman, 1993)."

References

- Austin, J. and Tuck, A. F.: The calculation of stratospheric air parcel trajectories using satellite data, Q. J. Roy. Meteor. Soc., 111, 279-307, 1985.
- Bowman, K. P.: Large-scale isentropic mixing properties of the Antarctic polar vortex from analyzed winds, J. Geophys. Res., 98, 23013-23027, 1993.
- Schoeberl, M. R., Lait, L. R., Newman, P. A., and Rosenfield, J. E.: The structure of the polar vortex, J. Geophys. Res., 97, 7859-7882, 1992.

7) l.25: "to identify objectively"

done

8) end section 1: The authors state that "possibilities are further increased due to the novel features of LAGRANTO v2". However, I am not convinced that this is true. LAGRANTO v2 appears to make it easier for new investigators to conduct novel investigations along similar lines to those that have been published, but it seems to me that they could achieve this without the v2 front end if they had the required know how.

See reply to comment 5. For Lagranto, it does not make sense to talk about the v2 model and the v2 front end – Lagranto is a tool with the front end as an essential component. The remark that an experienced user who has the required know how can do without a specific tool is true generally, but, in our opinion does not diminish the value of a tool at all. It is exactly the aim of a tool to make things easier, more flexible and more appealing for a wider group of users.

9) Section 2: The authors have chosen to develop a command line interface to LAGRANTO v2 which could work well with a script approach to designing experiments. However, I imagine that it would be possible instead to develop a widget/button driven user interface with the same functionality. This is the reason why I think the specifics of using the interface need to be in a separate user guide. However, the authors could comment on the rationale for the approach they have taken.

Of course, there are many ways how a user can interact with a trajectory model. The reviewer suggests a widget/button driven user interface, whereas we see more value in a basic command-driven one. Certainly, the first approach offers one key advantage: it's very intuitive and can be run without learning mnemonic LAGRANTO commands. On the other hand, we see also some disadvantages compared to the more basic approach chosen for LAGRANTO:

i) Whereas it would be very convenient to have a graphical user interface for the calculation of single or few trajectory calculations, it becomes increasingly cumbersome if the number of trajectories becomes larger. We have run many trajectory calculations which cover more than 30 years, resulting in millions of trajectory calculations. In our experience it turns out that a command-driven interface can easily be embedded into standard Unix/Linux shell scripts and make the handling of these huge calculations very stable. In fact, only by embedding LAGRANTO in shell scripts, with its many powerful tools, LAGRANTO could be optimally used.

ii) Of course, one could argue that a suitable graphical interface for extensive calculations, as described in i), could easily be developed, e.g. by asking for starting and ending dates. Indeed, special graphical interfaces to LAGRANTO are currently developed at our institute or are already published. One is used for radisonde analysis, the other for flight planning. In both cases, the developers relied on LAGRANTO as the underlying trajectory model, but designed a graphical user interface that meets specifically their needs. In short, we think that it would be difficult to develop a graphical interface that suits well the requirements of all potential users of LAGRANTO. Therefore, we prefer to keep a command-driven interface, which offers a lot of versatility and can readily be included in more specialized user interfaces. In some sense, our approach is very similar to existing chess playing programs. They also clearly distinguish between a chess playing machine, and a graphical chessboard with the possibility to interact with the machine. In our view, LAGRANTO offers the machine, but it's up to the users to develop more convenient user interfaces, if needed.

iii) LAGRANTO is developed and run on Unix/Linux platform. We follow its basic philosophy in providing many little tools, accessible from a command terminal, to build more powerful tools. A graphical user interface, on the other hand, would come more like a 'monolithic' tool which defies exactly this principle. Furthermore, if we consider current trends in scientific computing, new programing languages (e.g., Python) are becoming more important. It would be relatively easy to integrate LAGRANTO in such a new setting because of its simple user interface.

In summary, we would strongly prefer to keep the command-driven interface of LAGRANTO, based on our personal and on other researchers' experience. In the same line, we think that the specific commands should remain in the manuscript. They provide a flavor of how it is to work with LAGRANTO. If all specific commands are missing or moved into a separate user guide, it would become rather difficult to grasp the essentials of LAGRANTO. To formulate it in still another way: trajectory calculations are actually rather trivial, just interpolation and forward time-stepping; it's the specific interface that makes the tool very useful. In the case of LAGRANTO, it's a command-driven interface.

10) Section 3.1: "vertically de-staggered" is not a standard use of English. Suggest re-wording and explaining a little.

We replaced 'de-staggered' with 'unstaggered', which to our knowledge is often used in the NWP community.

11) Eqns (2)-(4): Although the scheme described here is the same as in LAGRANTO v1, it requires some justification. There are several other alterative numerical methods that would be higher order and therefore more accurate when the wind field is sufficiently smoothly varying. It is similar to the midpoint, or second order Runge-Kutta method. A key point with

the basic (first order) forward scheme is that it is unstable even for simple flows such as circling around a steady vortex (trajectories spiral outwards). Is the LAGRANTO scheme stable (like the midpoint scheme)?

Of course, stability is a key issue when dealing with numerical schemes. In the manuscript we only mention the iterative Euler scheme, or Petterssen scheme, without discussing its numerical stability. Since this scheme has been used in the previous version of LAGRANTO (LAGRANTO v1) very extensively, it has been tested for stability during the development of LAGRANTO v1, and because the new version of LAGRANTO is based on exactly the same numerical scheme, we refrained from repeating the stability tests. However, we fully agree with the reviewer that additional tests are very valuable to confirm this absolutely essential aspect.

We set up a little numerical experiment to test the stability of the iterative Euler scheme. Motivated by the systematic approach taken by Seibert (1993), we chose a purely rotational flow. The vortex centre is placed at 0°E, 45°N and the wind speed is assumed to be constant (10 ms^{-1}). Furthermore, the wind is stationary, i.e., it is not evolving in time. This last assumption implies that the air parcel trajectories must be closed circles and any deviation from this clearly indicates a numerically unstable setting. The flow setting is shown in the figure below with wind arrows. Forward trajectories are then started from four starting positions: (0°E, 10°N), (0°E, 20°N), (0°E, 30°N) and (0°E, 40°N) and run 648 hours forward in time. The outermost trajectory (in blue) just completes a full circle and the final position after these 1296 time steps (taken the default 30 min time step in LAGRANTO) coincides/overlaps very well with the initial position of the air parcel (blue dot). In summary, for such a long forward integration (27 days) the accuracy of the trajectory is indeed not limited by numerical issues, but by several other sources of uncertainty related to trajectory calculations, e.g., the chaotic nature of the flow field itself or the unresolved scales of the wind fields.
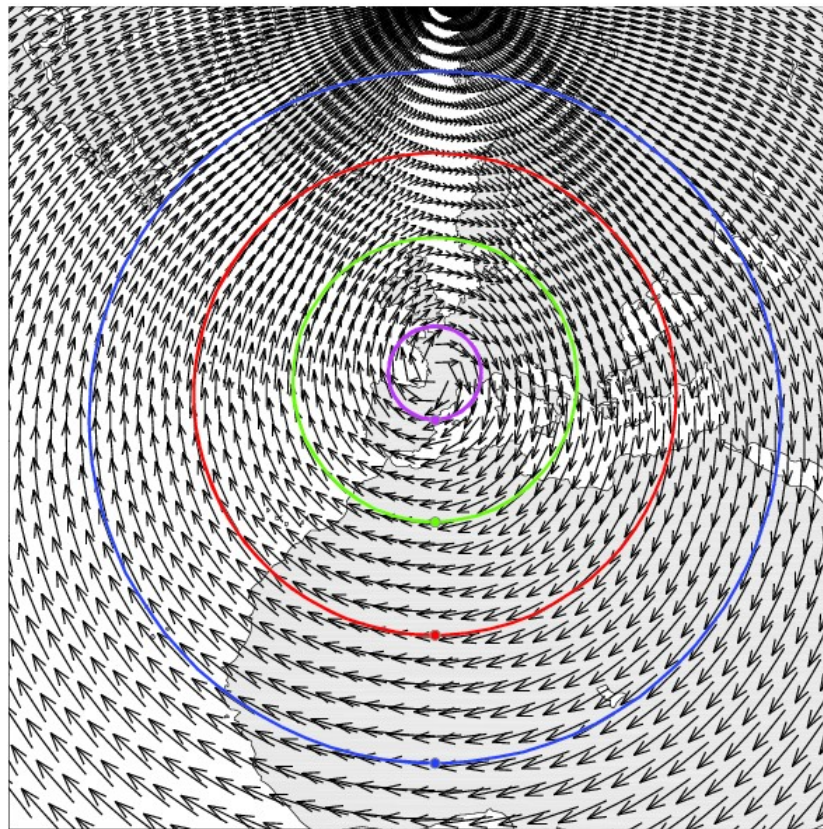
For the other starting positions (red, green, magenta) the outcome is very similar: all circles are nearly perfectly closed. Note that for the innermost trajectory, the constant wind speed of 10 ms^{-1} and the long forward integration time implies that actually 6.5 circles are completed at the end of the test. This can be most easily captured from the following figure, which shows the latitude as a function of the 6-h time intervals. Any instability would become discernible in a change of the amplitude of the oscillations as time increases.
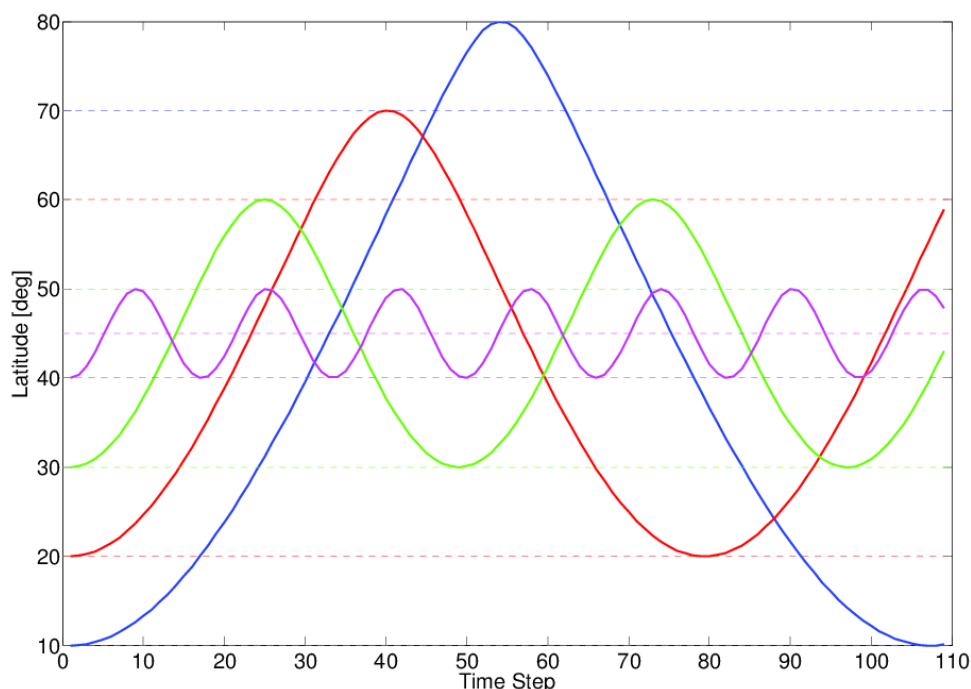
Finally, it is worthwhile to mention that LAGRANTO includes a 2nd order Runge-Kutta scheme, but it is not used in the default setting.

In summary, we can confirm that LAGRANTO v2 is numerically stable and the accuracy of the trajectories are determined not by numerical, but by physical processes (atmospheric chaos, unresolved scales of driving winds). With respect to the manuscript, we think that no detailed discussion of these stability checks must be included. However, we mention shortly that stability checks have been performed and turned out to be successful. We added the following sentences in section 3.3:

"The stability of the numerical scheme was tested in a rotational flow setting (see Seibert, 1993) for 648-h forward trajectories. No hint for any numerical instability could be discerned for these rather long trajectories."

Reference:

Seibert, P. (1993): Convergence and Stability of Numerical Methods for Trajectory Calculations. Journal of Applied Meteorology, Vol. 32, pp. 558-566.

12) Section 3.3, l.15: It does seem a weakness that trajectories can cross below ground. This is avoided by design in some models by using the lower boundary condition on vertical velocity when interpolating velocity to particle locations. It is possible to do this in pressure or hybrid (eta) coordinates.

We fully agree that this is a weakness and during the last years, we made several attempts to solve this problem when using vertical winds in pressure coordinates on model levels.
So far, all our attempts have been unsuccessful, and a detailed discussion of this issue is included in our COSMO online trajectory paper (Miltenberger et al., 2013, section 2.2). We discussed this issue also with John Methven, and in his trajectory code the problem does not occur when using eta-dot as the vertical velocity on half-levels. However, the problem that trajectories go below ground also occurs in his code when using pressure coordinates. We therefore, at the moment, do not see an alternative to the frequently used "solution" of reinserting surface-intersecting trajectories above the ground, and agree with the referee that more attention should be paid to this issue in the future.

13) INPOLYGON: what does a "spherical polygon" mean? It seems like an inappropriate description to me since a sphere has only one curved face.

We agree that the term 'spherical polygon' might not be well known. It refers to "a closed geometric figure on the surface of

a sphere which is formed by the arcs of great circles" (see http://mathworld.wolfram.com/SphericalPolygon.html). We changed the footnote in the following way to make the definition more clear: "The INPOLYGON field relies on spherical polygons, i.e., closed geometric figures on the sphere formed by arcs of great circles. For LAGRANTO they are specified as a list of longitude/latitude vertices and a single latitude/longitude point inside the polygon."

14) Section 4.4: For back trajectories it is also necessary to read the input wind records in reverse order as well as rotating the wind vectors by 180deg.

done

15) Figure 6 caption: "All panels . . ."

Figure 6 is removed in the revised version of the manuscript, and combined with Figure 8.