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DATA NOTE

REVISED Ocean Lagrangian Trajectories (OLTraj): Lagrangian analysis for non-expert users

[version 2; peer review: 2 approved]

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Abstract

Lagrangian analysis is becoming increasingly important to better understand the ocean's biological and biogeochemical cycles. Yet, biologists and chemists often lack the technical skills required to set up such analyses. Here, we present a new product of pre-computed ocean Lagrangian trajectories (OLTraj) targeting non-expert users, and demonstrate how to use it by means of worked examples. OLTraj is based on satellite-derived geostrophic currents, which allows one to directly compare it with other in-situ or satellite products. We anticipate that OLTraj will foster a new interest in Lagrangian applications in ocean biology and biogeochemistry.

Keywords

Lagrangian analysis, geostrophic currents, non-expert users, satellite data, ocean colour, in-situ measurements

Open Peer Review

Approval Status ✓ ✓

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version 2 (revision) 15 Nov 2021	✓ view	
version 1 30 Sep 2021	? view	✓ view

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2. **Joan Llort**, University of Tasmania, Hobart, Australia

Any reports and responses or comments on the article can be found at the end of the article.

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REVISED **Amendments from Version 1**

We thank both reviewers for the time they took to read and comment on our paper. We are glad that both reviewers considered positively our work. As requested by Reviewer 1 we have added (i) links to the code for the examples in the text, (ii) a new figure to demonstrate how satellite-based trajectories can match more closely the features observed by other satellite sensors than modelled trajectories, as well as (iii) references that the describe in more detail the limitations of the geostrophic approximation.

Any further responses from the reviewers can be found at the end of the article

Introduction

To analyse how the properties of a moving fluid evolve as a function of time, we can proceed in two different ways. We can study the fluid as it flows in front of us (e.g., by using a moored set of instruments), which is known as an analysis in a Eulerian reference frame. Or we can imagine to be moving with a particular parcel of the fluid and study how the properties of this parcel evolve with time (e.g., by collecting measurements from a surface drifter): this is called an analysis in a Lagrangian frame of reference (or "Lagrangian analysis"). Thus, while variations observed within a Lagrangian reference frame are purely temporal (i.e. occurring within a given water parcel as it flows along its trajectory), those observed in a Eulerian reference frame are not, because they are also due to the variations between the different water parcels that flow through the fixed point of observation.

In the ocean, these two types of analyses can generate significantly different results, depending on the strength of the currents relative to the size of the geographic area under exam, the duration of the study, and the strength of the local spatial gradients of the property being investigated. When current speeds are slow with respect to the ratio of the spatial to the temporal scales of the study, and the horizontal gradients are weak (i.e. small variations between the area of observation and its surrounding), Eulerian and Lagrangian approaches are expected to deliver similar results. Conversely, when the speed of the water masses is comparable to or greater than the ratio of the spatial to temporal scales of the investigation, and the gradients are strong (i.e. large variations within the area of observation), results from Lagrangian and Eulerian analyses will, in principle, differ.

For example, given a surface water mass with a typical velocity υ = 5 cm/s (Lumpkin & Johnson, 2013), and strong variations of a water property over horizontal scales of 100 km, one could ask the question "If I want to analyse the evolution of the properties of this water mass over a temporal scale τ = 1 month, should I be considering a Lagrangian approach?". Since during such a study the water mass would move by a distance $\sigma = \upsilon/\tau \approx 130$ km (which is larger than the spatial scale of the horizontal gradients), the above reasoning will lead us to conclude that a Lagrangian approach would be appropriate. Indeed, with a Eulerian approach, our observations would also include the variations induced by the advection of water masses with different properties from the original one. In more energetic regions, with υ = 25 cm/s, the distance traveled by the water parcel would increase to > 650 km, and hence a Lagrangian approach would be required even in presence of weaker horizontal gradients. Naturally, this rule of thumb should be used as a very first-order indicator to decide the reference frame in which the analysis should be implemented.

Although Lagrangian analyses have been traditionally applied by physical oceanographers to investigate ocean circulation and tracer dispersion (e.g., Blanke *et al.*, 2001; Döös, 1995), in recent years they have also emerged as an important tools for biological and biogeochemical studies. Lagrangian analyses can be used to determine the source and fate of a water mass sampled from a ship or by an autonomous platform, thus providing a dynamic framework for interpreting in-situ data and optimising field campaigns (e.g., d'Ovidio *et al.*, 2015) or to follow the evolution of biogeochemical properties detected in satellite data while separating changes due to advection from those due to biological processes (Jönsson *et al.*, 2009; Lehahn *et al.*, 2011). Furthermore, Lagrangian analyses can be used to infer how spatially-separated components of a basin are connected by currents and how this connectivity impacts the life cycles of crucial ecosystem components (Falcini *et al.*, 2020; Raitsos *et al.*, 2017). These are only some examples of a vast array of applications. However, so far, Lagrangian analyses have been restricted to "expert users", who can convert velocity fields into Lagrangian trajectories.

Here, we present a new product of pre-computed ocean Lagrangian trajectories (OLTraj) that should allow non-expert users to more easily implement Lagrangian analyses. Below we describe how OLTraj was derived and we demonstrate how to use it by providing three practical examples.

Data and methods

Input velocities

The Ocean Lagrangian Trajectory product (OLTraj) was computed using reprocessed global daily multi-mission altimeter-based surface geostrophic velocities obtained from the Copernicus Marine Services archive from January 1998 to December 2019, gridded at 0.25° × 0.25° resolution (Copernicus). This period was selected to overlap with the years of the available satellite ocean-colour observations.

Calculation of trajectories

OLTraj was generated using the LAgrangian Manifolds and Trajectories Analyser (LAMTA), originally developed by d'Ovidio *et al.* (2004) and subsequently described in van Sebille *et al.* (2018). See section Software availability. The LAMTA code has been previously applied in support of in-situ Lagrangian experiments (d'Ovidio *et al.*, 2015; Nencioli *et al.*, 2011) as well as satellite-based studies (e.g., to track Agulhas rings, Nencioli *et al.*, 2018). In OLTraj, trajectories are computed using a fourth-order Runge-Kutta scheme with an integration time step of six hours. During the integration, the geostrophic velocity fields are bi-linearly interpolated in space and linearly interpolated in time. For each day, we computed

trajectories at a resolution of 1/8th of a degree in both latitude and longitude. Each trajectory extended backward and forward in time for 29 days.

How Lagrangian trajectories are stored

The OLTraj product is stored in daily NetCDF-4 files. Each file contains the variables `trajlat` and `trajlon` that are the coordinates of the Lagrangian trajectories (latitude and longitude, respectively). `trajlat` and `trajlon` have three dimensions: `lat`, `lon` and `time`. `time` is of length 59, and its central time element (`time(30)`, hereafter t_0) is the time from which the Lagrangian trajectories are computed forward (from t_0 to t_0 + 29 days) and backward (from t_0 to t_0 − 29 days). t_0 corresponds to the time reported in the file name. `lat` and `lon` are the starting locations of the trajectories at t_0 (before backward or forward advection). Hence, at t_0 `trajlat=lat` and `trajlon=lon`. Elements 1 to 29 along the `time` dimension of `trajlat` and `trajlon` contain the coordinates of the backward trajectory. Thus, `trajlat` at `time(29)` contains the latitude values of the trajectory at t_0 − 1 day, at `time(28)` that at t_0 − 2 days, and so on until `time(1)` corresponding to t_0 − 29 days, i.e., the last day of the backward trajectory. In the same way, the latitude values of the forward trajectory are stored in the `trajlat` elements 31 to 59. Similarly, the longitude values of the trajectory are stored in `trajlon`.

How to access the OLTraj product

The OLTraj files were deposited as version 2.2 in open-access format at the UK Centre for Environmental Data Analysis (CEDA) archive. All files can be freely downloaded, but due to their relatively large sizes (~850 Mb each), we recommend accessing and subsetting them using the provided THREDDS data server (see README file).

Examples

To demonstrate how to use the OLTraj product, we provide three practical examples as jupyter notebooks. These require the user to clone a publicly available repository and follow the instructions provided in the README file (see Software availability). The link to the Binder Launcher for each example is added next to the titles of the following sections.

Example 1: Plotting trajectories around a fixed-point station. (Binder Launcher) The objective of this first example is to extract and plot the surface trajectories of the water masses sampled at a fixed-point station (e.g., the Bermuda Atlantic Time Series). These trajectories can be used to better understand the origin of the water masses sampled at the station and hence better interpret the variability observed in the time series. The coordinates of the station are used to extract OLTraj trajectories during each month of the year. Figure 1 presents the result of this example showing how surface water masses move differently during the year.

Example 2: Extracting and plotting backward and forward trajectories along a cruise track (Binder Launcher). The objective of this example is to plot the surface trajectories of the water masses sampled during a hypothetical research expedition. This information is particularly important because it can be used to better interpret the station-to-station variability measured during the expedition. The time and coordinates of the stations sampled during the expeditions are read from a text file and are then used to read and subset the corresponding OLTraj trajectories. Figure 2 presents the result of this example showing how different water masses along the expedition moved before and after they were sampled.

Example 3: Following the evolution of a water mass over time (Binder Launcher). The objective of this example is to demonstrate how the temporal evolution of the properties of a given surface water mass can be tracked in a Lagrangian framework. Specifically, the example focuses on demonstrating how the chlorophyll concentration (chl) measured at a given location evolved before and after the initial observation as the water masses moved. We start by assuming we have observed a chl feature in a given image (Figure 3). We now want to understand how this feature evolved before and after our initial observation at time 2006-01-15. To do so, we first extract the OLTraj product at that date and then select the starting points (`trajlat` and `trajlon` at `time(30)`) for the trajectories that overlap with the feature (red squares in Figure 4). We then interpolate the chl data in time and space over the OLTraj Lagrangian trajectories in order to extract the chl values at the locations that the water mass occupied before and after the initial observation. We can finally plot the values of chl along the Lagrangian trajectories (Figure 5 top) and compare them with the values of chl we would have obtained by extracting time series of chl from the locations of the initial observation (Eulerian time series, Figure 5 bottom). The example also generates an interactive figure where the location of the Lagrangian parcels can be visualised over the corresponding chl image at any date for 29 days before and after the initial observation.

Dataset validation

Advantages

OLTraj was created to encourage, when needed, non-expert users to interpret in-situ and satellite observations by taking into account that surface water masses move. OLTraj provides pre-computed Lagrangian trajectories, which allow non-experts to skip this computing step and focus on analysing their data in a Lagrangian framework. Furthermore, we provide Python examples to demonstrate how to use OLTraj in practical and common applications. A final but important advantage of OLTraj is that it is based on satellite-derived geostrophic velocities. Thus, OLTraj has better spatio-temporal coherence with other satellite products, such as ocean colour and sea-surface temperature, than modelled velocities (see example in Figure 6).

Limitations

We do not intend to promote OLTraj as the ultimate tool for Lagrangian analysis. Many other state-of-the-art methods

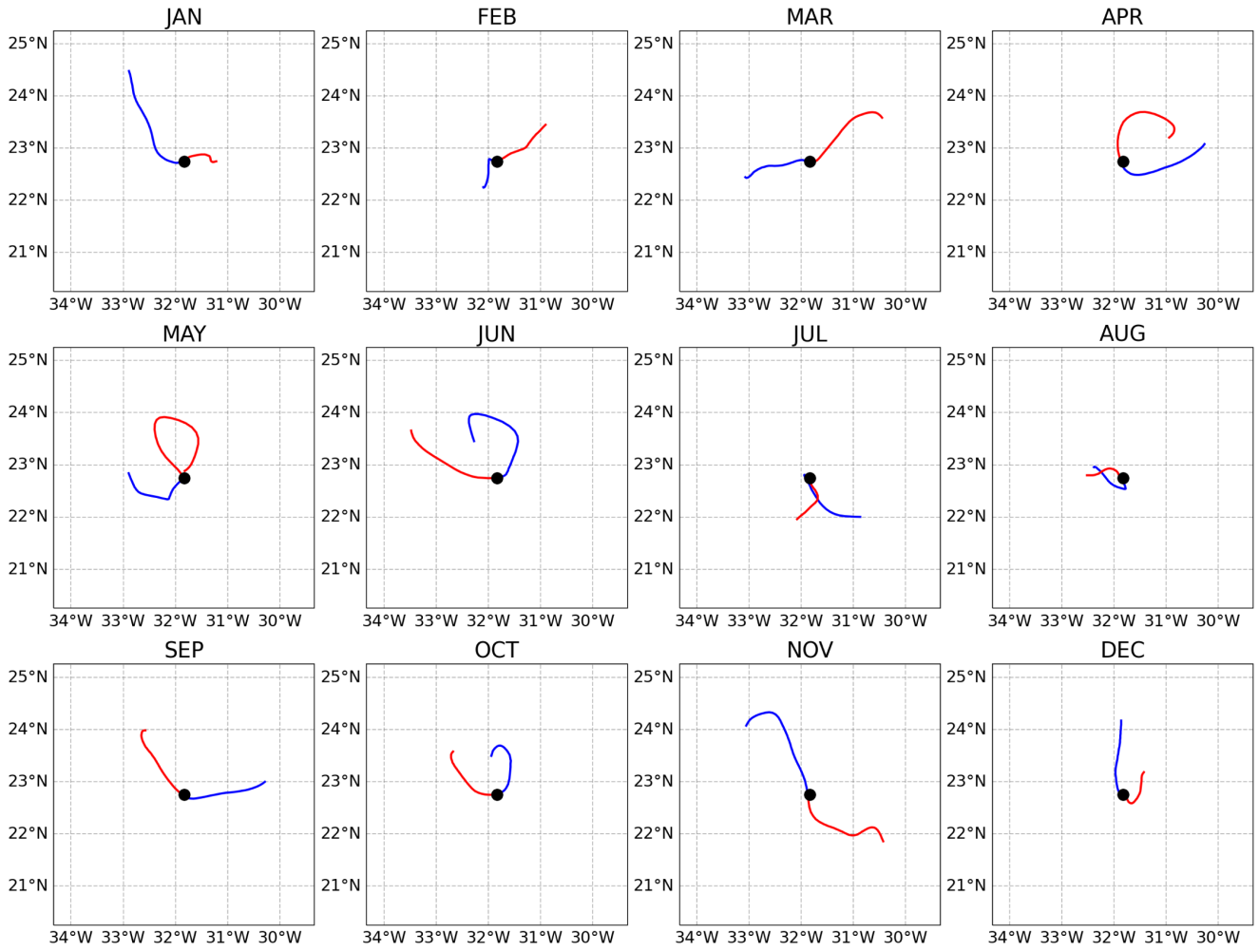


Figure 1. Backward (blue lines) and forward (red lines) trajectories of the water masses sampled at the fixed-point Bermuda Atlantic Time Series (BATS) station (black circles) during different months of year 2018 (presented in the different subplots). Each trajectory extends for 29 days backward and 29 days forward. The trajectories were extracted from the central day of each month.

are available (van Sebille *et al.*, 2018). Instead, the focus of OLTraj is to broaden the application of Lagrangian analysis to non-physical oceanographers. As such, OLTraj has several limitations.

One of the main limitations is inherent in its nature. Being a set of pre-computed trajectories, OLTraj has pre-defined spatial resolution (1/8°) and temporal extent (±29 days). These spatial and temporal characteristics were defined based on a trade off between the number and length of the trajectories computed and the size of the dataset produced that consists of daily files spanning over 22 years (the current overall size is approximately 6.3 Tb). To reduce the burden of storing the entire dataset in a local machine, we have exploited the UK CEDA THREDDS server, which allows users to subset the data before downloading them. Access via the THREDDS server is however necessarily slower than reading files stored on a local machine. We therefore encourage the users to assess if local or THREDDS access is needed for any specific analysis. The overall length of the dataset (1998–2019) was decided based on the extents of i) the satellite ocean-colour record and ii) of the reprocessed gridded geostrophic velocity product when the OLTraj product was computed.

The pre-defined length of the OLTraj product (±29 days) could potentially be seen as another limitation. Yet, methods

could be devised to combine multiple OLTraj files and estimate longer Lagrangian trajectories.

OLTraj trajectories are as good as the velocities from which they are derived. Although accurate in the open ocean, the gridded geostrophic velocities used to compute OLTraj have limitations near the coast (i.e., within ~50 km from the shore; e.g., Bouffard *et al.*, 2010; Nencioli *et al.*, 2011; Volkov *et al.*, 2007). These are in part due to technical limitations of satellite altimeters near the coast (Vignudelli *et al.*, 2019), and in part due to the methodologies used to grid the multi-satellite along-track observations which, although recently improved in the coastal region, are optimized for the open ocean (Taburet *et al.*, 2019). For these reasons, OLTraj should be used with caution in coastal regions.

Finally, the current version (v2.2) of the OLTraj product is derived from satellite-based geostrophic velocities and therefore only accounts for the mesoscale (i.e. O(100 km)) currents resulting from the balance between the pressure gradient and the Coriolis force (Isern-Fontanet *et al.*, 2017). Additional non-geostrophic currents are not included in the CMEMS surface velocities and hence nor in OLTraj. These currents are i) currents due to wind stress on the surface ocean (such as Ekman currents and near-inertial oscillations (d'Ovidio *et al.*, 2015; Rio *et al.*, 2014)), ii) tidal currents (Stammer *et al.*, 2014), iii) currents induced by waves (stokes drift, Onink *et al.*, 2019), iv) inertial oscillations (Elipot *et al.*, 2010), and v) the currents associated with ageostrophic processes typically occurring at scales of O(≤10 km) (McWilliams *et al.*, 2019).

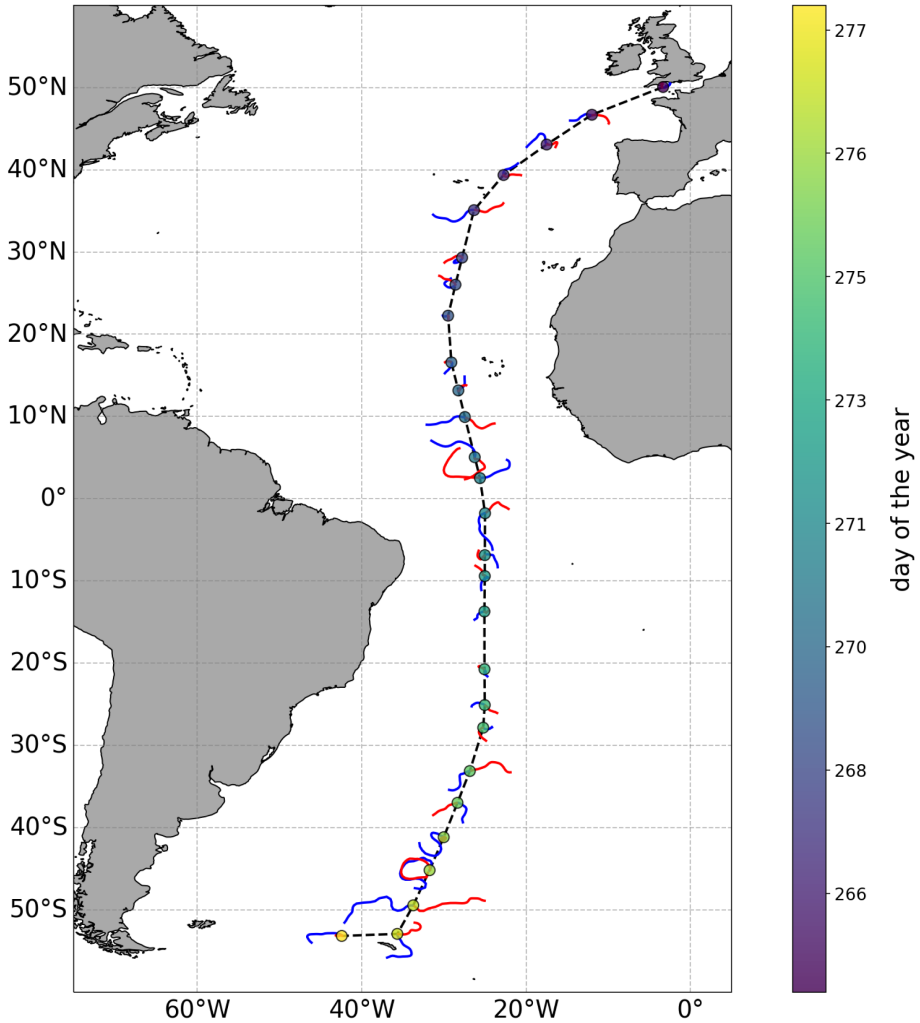


Figure 2. Backward (blue lines) and forward (red lines) trajectories of the water masses sampled at selected stations (circles, colour indicates the day of the year of each station) along the track (black dashed line) of a research expedition. Each trajectory extends for 29 days. Longer trajectories indicate that the sampled water masses were moving faster than those with shorter trajectories.

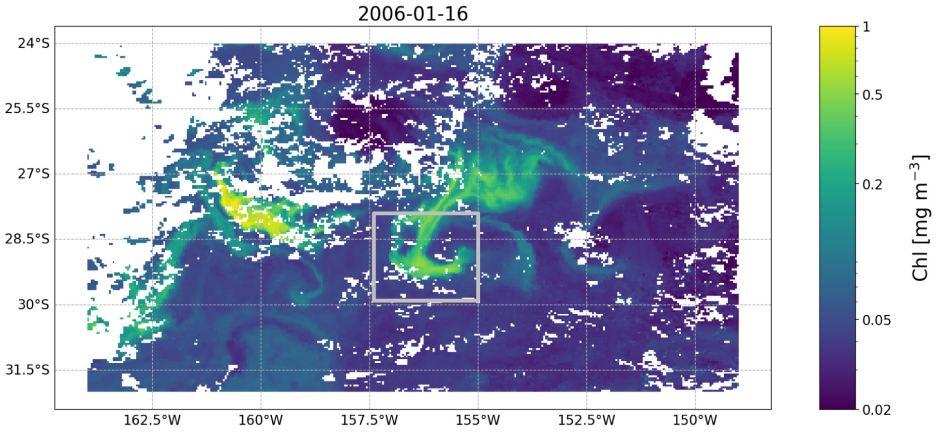


Figure 3. Satellite image of chlorophyll concentration (from the European Space Agency's Ocean Colour Climate Change Initiative project) taken on 2006-01-16 south east of Madagascar and containing the feature we focus on in Example 3. The feature is the relatively high chlorophyll (i.e., > 0.2 mg m^{-3}) patch within the silver rectangle. White patches are clouds obscuring the image.

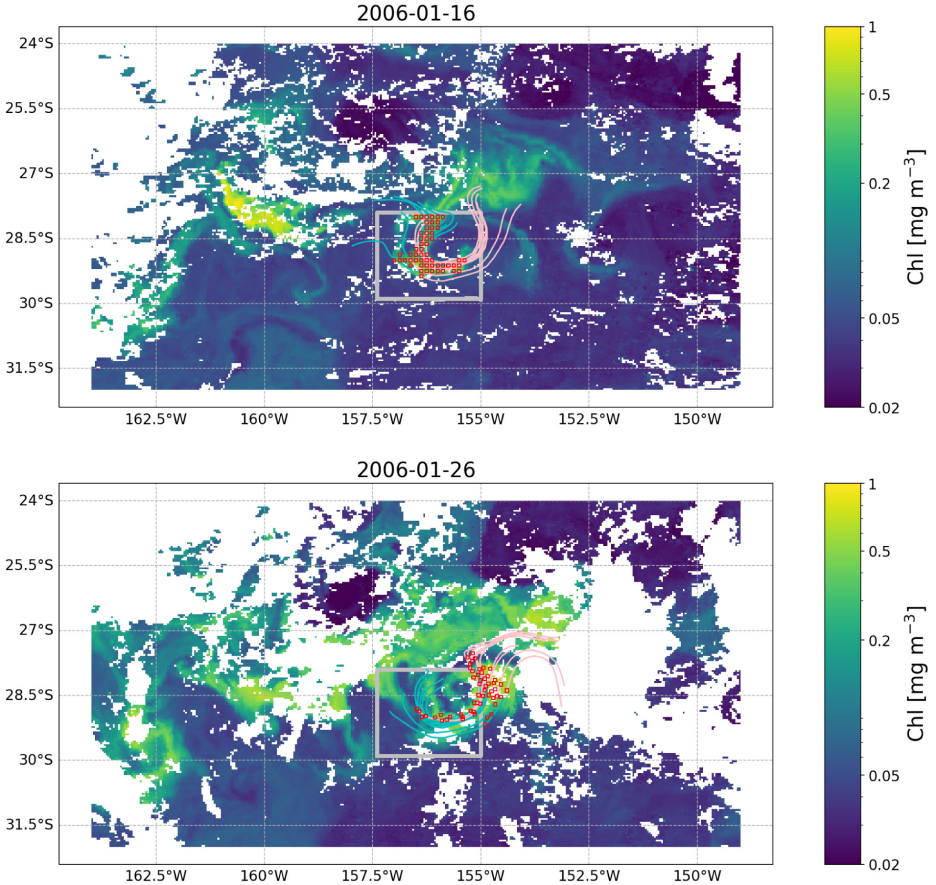


Figure 4. OLTraj product (red squares) matching in time and space the feature observed in the image of Figure 3 on 2006-01-16 (top) and 2006-01-26 (bottom). Some of the backward (cyan lines) and forward (pink lines) Lagrangian trajectories are plotted for each snapshot. Each trajectory extends for 15 days. White patches are clouds obscuring the image.

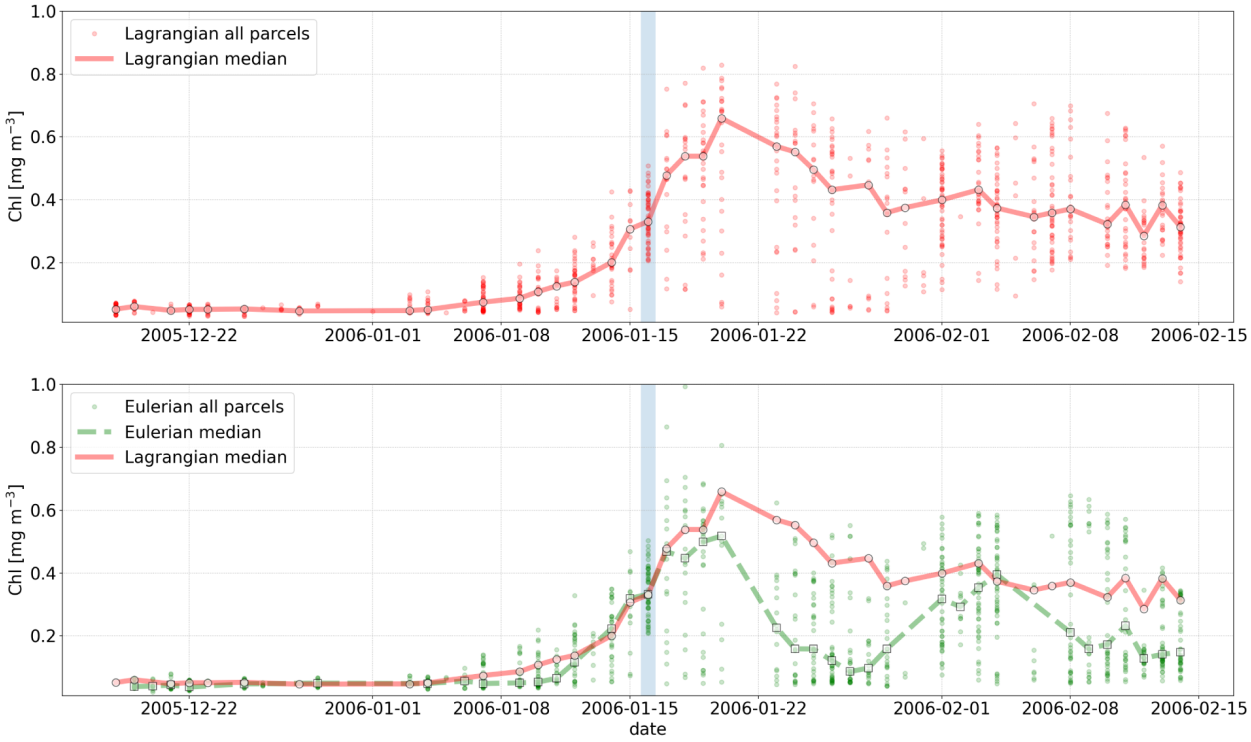


Figure 5. Comparison of chlorophyll concentrations extracted from the Lagrangian (top plot) vs. Eulerian (bottom plot) time series. Small red circles and continuous line represent the chl values extracted along the Lagrangian trajectory of each water parcel and their median (also marked with larger red circles), respectively. Green small circles and dashed line represent the Eulerian time series, i.e., chl values extracted at the location of the initial observation (light blue vertical bar) and their median (also marked with larger green squares), respectively. For both time-series, medians were computed for a given date only if at least 10 of the 54 points were associated with valid chlorophyll observations (i.e. not with cloud pixels). The bottom plot demonstrates the differences in the median Eulerian (green dashed line) and Lagrangian (red continuous line) time series.

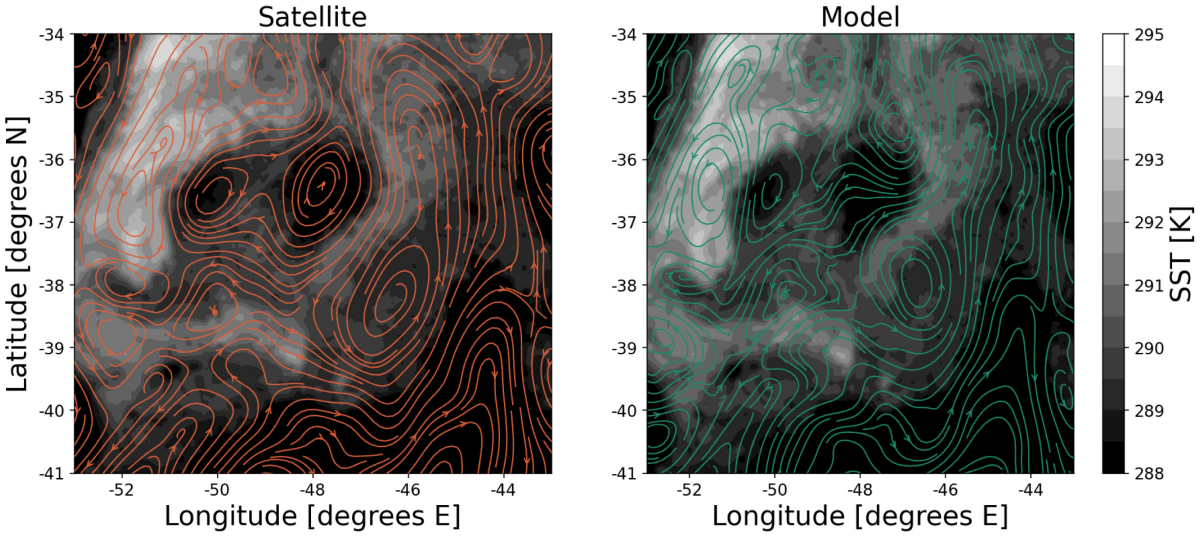


Figure 6. Example of a comparison of satellite-based streamlines from geostrophic currents (left plot, orange lines, from AVISO product) and streamlines from modelled currents (right plot, green lines, from COPERNICUS 1/12 degree reanalysis), superimposed on sea-surface temperature product (grey colours, GHRSST) for the south-west Atlantic on Oct. 4th, 2018. The locations of cold-core eddies (dark grey areas in the centre of the plot) in the centre of the image agree with the AVISO streamlines, but not with the model-reanalysis streamlines.

Data availability

Underlying data

The original Copernicus data (January 1998 - December 2019) is available from: https://resources.marine.copernicus.eu/product-detail/SEALEVEL_GLO_PHY_L4_REP_OBSERVATIONS_008_047/INFORMATION

CEDA: Global ocean Lagrangian trajectories based on AVISO velocities, v2.2.

http://doi.org/10.5285/5c2b70d069cb467ab73e80b84c3e395a

This dataset contains the following underlying data:

- Daily files from 1998-01-01 to 2019-12-31.

This dataset is available under the terms of the Creative Commons Attribution 4.0 International license (CC-BY 4.0).

Software availability

Source code to compute OLTraj available from: https://github.com/grgdll/OLTraj

Archived source code at time of publication: https://doi.org/10.5281/zenodo.5082983

The repository for the examples is: https://github.com/grgdll/OLTraj_examples

Archived source code at time of publication: https://doi.org/10.5281/zenodo.5518531

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Publisher Full Text

Open Peer Review

Current Peer Review Status: ✔ ✔

Version 2

Reviewer Report 17 November 2021

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✔ **Alice Della Penna**
University of Auckland, Auckland, New Zealand

I appreciate the edits that the authors I've put together. I'm very happy to encourage you to accept this Data Note as ready for indexing.

Competing Interests: No competing interests were disclosed.

I confirm that I have read this submission and believe that I have an appropriate level of expertise to confirm that it is of an acceptable scientific standard.

Version 1

Reviewer Report 27 October 2021

https://doi.org/10.21956/openreseurope.15238.r27802

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✔ **Joan Llort**
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The data note "Ocean Lagrangian Trajectories (OLTraj): Lagrangian analysis for non-expert users" by Dall'Olmo and co-authors provides an easy-to-use toolbox for analysing surface water-mass trajectories in the ocean.

The note is well written, provides three different and illustrative examples that can be run online thanks to Juptyer Notebooks and MyBinder and clearly details all the data sources and limitations of the approach. The goal of this tool is to allow the general community on oceanography to incorporate Lagrangian trajectories analysis in observations works. As stated in the introduction of the note, Lagrangian analyses are of great help to interpret ocean observations, particularly for studies focusing on phytoplankton and ocean biogeochemistry. These methods have been used several times in the past for a number of cruise surveys but so far, they required at least one or two experts in physical oceanography and satellite data to implement them. OLTraj breaks this barrier by simplifying the implementation of the approach so any researcher with minimal programming skills can apply it to its own zone/period of interest.

I strongly support the indexing of this note in its current version.

Is the rationale for creating the dataset(s) clearly described?
Yes

Are the protocols appropriate and is the work technically sound?
Yes

Are sufficient details of methods and materials provided to allow replication by others?
Yes

Are the datasets clearly presented in a useable and accessible format?
Yes

Competing Interests: No competing interests were disclosed.

Reviewer Expertise: Ocean biogeochemistry, Physical oceanography, Observations, (sub)mescoscale circulation

I confirm that I have read this submission and believe that I have an appropriate level of expertise to confirm that it is of an acceptable scientific standard.

Author Response 03 Nov 2021

Giorgio Dall'Olmo

We thanks Dr Llort for their positive review.

Competing Interests: No competing interests were disclosed.

Reviewer Report 15 October 2021

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This *Data Note* provides good information for an exciting dataset that is aimed at encouraging non-specialists to work with Lagrangian re-analyses of satellite altimetry. I think tools like this are very valuable for interdisciplinary research and I also think this could be a good tool for teaching – exposing students to these approaches early in their studies. Overall, this is a very positive review. I only have a few small comments that I think could be helpful.

1. Most of the potential users of this dataset are likely to have limited experience in Python so I think it's great that Python notebooks for the examples are made available. My suggestion is to include the links to each notebook individually in the text and not only at the end of the manuscript (and in the heading paragraph of the examples section) so that a reader can potentially look at them in parallel while reading the text. So, for example, just after "*Example 1: Plotting trajectories around a fixed-point station"* I would recommend including the link to the notebook – even if is already mentioned at the end of the manuscript.

2. In the "Advantages" section, I do understand the point the authors are making about how using altimetry-based currents makes matches with biogeochemical data more accurate compared to models. And I totally agree. However, I'm not sure that many readers who are not familiar with this kind of analyses would understand exactly what that means. Would there be any reference with an example of a mismatch the authors could include? Or could they add a figure showing an example where a model shows a mismatch but not the altimetry? Perhaps just a schematic showing a possible scenario?

3. In the "Limitations" section, I think the authors do a good job at describing the ageostrophic components. I recommend adding some references for readers who might want to read more about each different component and mention that previous studies that have incorporated estimates of ageostrophic components have increased the accuracy of the near-surface currents (e.g. d'Ovidio *et al*., 2015).

References

1. d'Ovidio F, Della Penna A, Trull T, Nencioli F, et al.: The biogeochemical structuring role of horizontal stirring: Lagrangian perspectives on iron delivery downstream of the Kerguelen Plateau. *Biogeosciences*. 2015; **12** (19): 5567-5581 Publisher Full Text

Is the rationale for creating the dataset(s) clearly described?

Yes

Are the protocols appropriate and is the work technically sound?

Yes

Are sufficient details of methods and materials provided to allow replication by others?
Yes

Are the datasets clearly presented in a useable and accessible format?
Yes

Competing Interests: No competing interests were disclosed.

Reviewer Expertise: My area of expertise encompasses the use of Lagrangian re-analyses. In particular, I have been using tools such as the ones described in this Data Note to interpret oceanographic observations, understand the relationship between tracked animals and their environment, and designed tools to aid the spatial planning for Marine Protected Areas.

I confirm that I have read this submission and believe that I have an appropriate level of expertise to confirm that it is of an acceptable scientific standard, however I have significant reservations, as outlined above.

Author Response 03 Nov 2021

Giorgio Dall'Olmo

We thanks Dr Della Penna for their positive and constructive review. In the revised version of the manuscript we have addressed all suggestions, which we believe have improved the manuscript.

Competing Interests: No competing interests were disclosed.