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## Original software publication

## TROVA: TRansport Of water VApor



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## ARTICLE INFO

ABSTRACT

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Keywords: Moisture sources Precipitation Python FLEXPART FLEXPART-WRF Evaporation The TRansport Of water VApor (TROVA) software, developed in Python and Fortran for the study of moisture sources and sinks, is presented here. TROVA includes the main Lagrangian methodologies established in the literature, using outputs from the global FLEXible PARTicle dispersion model and the regional FLEXPART-WRF model at different spatial resolutions. TROVA will benefit users investigating the physics of the atmosphere and fields associated with this branch in the study of current and future changes in source–sink moisture relationships and their link with mean and extreme precipitation. © 2022 The Author(s). Published by Elsevier B.V. This is an open access article under the CC BY-NC-ND

1. Motivation and significance

There is considerable research interest in the meteorology and

hydrology communities on understanding the origin of moisture

and precipitation that occurs over a given region, due to the

dependence of life on water resources [1]. There are different

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#### Code metadata

Current code version	1.0
Permanent link to the code/repository used for this code version	https://github.com/ElsevierSoftwareX/SOFTX-D-22-00100
Permanent link to reproducible capsule	https://github.com/tramo-ephyslab/TROVA-master/blob/main/Inputs/
Legal code license	GNU General Public License (GPL)
Code versioning system used	Git
Software code languages, tools, and services used	Python, Fortran, and MPI
Compilation requirements, operating environments, and dependencies	Linux operating system
If available, link to the developer documentation/manual	
Email support for questions	l.gimeno@uvigo.es

#### Software metadata

Current software version	1.0
Permanent link to executables of this version	https://github.com/tramo-ephyslab/TROVA-master
Legal Software License	GNU General Public License (GPL)
Computing platforms/Operating Systems	Python, Fortran and MPI/Linux
Installation requirements & dependencies	Python3, numpy1.16+, mpi4py3+, scipy1.2+
If available, link to user manual - if formally published include a reference to	
the publication in the reference list	
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approaches to studying moisture transport, for example, several authors have implemented classical Eulerian [2]. Lagrangian [3.4]. and stable isotope approaches [5], as well as new sophisticated and robust methods such as Eulerian mesoscale tracer tools [6]. However, the Lagrangian approach has advantages over other methods as it provides details regarding the origin of the air mass and the mechanism of moisture fluctuations (increases and decreases) in the particles along the trajectories affecting the moisture in the target region [7]. Recently, the accuracy and robustness of this approach have facilitated the assessment of the average values for moisture sources in various climatic regions [7]. The original Lagrangian method developed by Stohl and James [4] facilitated the determination of the moisture source of precipitation over a given area and the sinks associated with a given moisture source; a more sophisticated method based on the previously cited study [4] was developed by Sodemann et al. [8] to determine specific moisture sources. Then, these methodologies were modified to obtain finer results but with the disadvantage of being more computationally expensive and requiring a larger volume of data. For example, Sun and Wang [9] introduced areal source receptor attribution to the methodology of Stohl and James [4], and Keune et al. [10] presented a unified framework to estimate the origins of atmospheric moisture (and heat) as a derivation of Sodemann et al. [8], including the possibility of performing bias correction based on source-receptor relationships.

In general, all these methods calculate the difference of Evaporation (E) and Precipitation (E) (E-P) to quantify the transport based on particle trajectories. In these analyses, a moisture source and sink are considered when E-P < 0 and E-P > 0, respectively. This E-P computation can be applied to the outputs of Lagrangian particle dispersion models, such as those from the FLEXible PARTicle dispersion model (FLEXPART [11–14], its regional version FLEXPART-WRF [15], or by using the online trajectory module (version 1.0) for the model COSMO [16], or to trajectories from the LAGRANTO model [17]. These models are normally forced with reanalysis data, such as ERA-Interim (ERA-I, [18]), ERA5 [19] or earlier versions, or the outputs of a regional model such as Weather Research and Forecasting System (WRF-ARW) [20] forced with different reanalysis or climatic data or using COSMO model outputs [21].

The values of E and P for a vertical air column are determined from humidity changes in water vapor particles that crossed the column along their trajectories over a predefined time period [22]. The trajectories are obtained from outputs of the dispersion models mentioned above, and the usual time to track them is around 8–10 days, the mean atmospheric water vapor residence time (WVRT) [23,24]. However, calculating the E-P field representation from the outputs of these models is very cumbersome, both in the post-processing phase and in application of the aforementioned methodologies. This is due to the large volume of data under consideration, which depends on the number of particles analyzed, number of days to track them, and the spatial and vertical resolutions.

Currently, some tools based on the methodology of Sodemann et al. [8], such as WaterSip [25], identify moisture sources based on a considerable number of thresholds applied to particle behavior along their trajectories, or the adaptation thereto as Heat And MoiSture Tracking (HAMSTER) framework, [10], which applies a bias-corrected source-receptor by adjustment of certain meteorological fields. However, the current online-version of HAMSTER only supports grids of one degree for the whole run configuration (for defining the target region (mask), the reference data (FLEXPART forced with ERA-I), and outputs).

Here, we present a software that facilitates the use of the methodologies of Stohl and James [4] and Sodemann et al. [8]

using FLEXPART and FLEXPART-WRF outputs, with the possibility of considering different grid resolutions for both input and output data and masks used for the moisture sources or sinks: the TRansport Of water VApor (TROVA) software. In addition, the versatility of TROVA for use with different types of numerical outputs from FLEXPART or FLEXPART-WRF will be useful for studies on future changes associated with moisture sources and sinks using outputs from these forced models under future climate scenarios. TROVA has already been used to study moisture sources and sinks with different approaches. Specifically, using the methodology of Stohl and James [4], numerous publications have been made in several regions worldwide, some of them could be consulted at https://ephyslab.uvigo.es/moisturetransport/index.php/ Publications. However, recent research, based on the study by Sodemann et al. [8], has been conducted using this tool to determine moisture sources for precipitation associated with major hurricanes in the North Atlantic basin [26,27]. Examples for moisture sources and sinks are presented in Section 3.

#### 2. Software

#### 2.1. Software architecture

TROVA is a software with the main algorithm written in Python, using libraries such as numpy, netCDF4, scipy, mpi4py, and other basic python libraries [28] (https://github.com/tramoephyslab/TROVA-master). However, the calculations of greater time and computational requirements are carried out with functions developed in Fortran, improving the efficiency of the tool. This software was developed and tested on the Linux operating system, and we believe that it is fully compatible with any system supporting Python 3. In addition, it has been used in high performance computing CESGA (Centro de Supercomputación de Galicia) with different core numbers (https://github.com/tramoephyslab/TROVA-master/tree/main/run\_example\_HPC). Finally, a configuration input file is used that allows the user to modify fields depending on the problem to be solved, without modifying the tool itself. TROVA outputs correspond to the E-P field for each day analyzed and its integrated sum for these days (output file in NetCDF, ASCII, and npy format). In addition, it saves the humidity changes for all particles in the analyzed time interval.

For a more detailed understanding of TROVA, Fig. 1 presents a flowchart explaining the general algorithm of the software. The first step to be performed is the configuration of the input file where the parameters of the run are set. The second step is to run the model forward or backward in time to determine the moisture sources or sinks, respectively. The tracking mode is defined in the input file. In the third step, the files needed to track the particles should be indicated, and then the calculations of the moisture changes of the particles are performed using the functions developed in Fortran. This will allow for greater computational efficiency and decrease the execution time. The fourth step is the calculation of the E-P field, from the Stohl and James (2005) equation, on the user-defined output grid. Finally, TROVA saves the outputs in the user-defined format, which can be NetCDF, ASCII, and npy.

#### 2.2. Software functionalities

TROVA allows the study of moisture sources and sinks based on calculation of the E-P fields, using the main methodologies of Stohl and James [4] and Sodemann et al. [8]. In addition, TROVA provides the advantage of using different numerical outputs from FLEXPART and FLEXPART-WRF at different spatial resolutions, ensuring better representation of the E-P field to be obtained. The Table 1 shows a comparison of the TROVA with WaterSip and HAMSTER in which the main differences/advantages can be observed.



Fig. 1. Flowchart the TROVA software structure/processes.

#### Table 1

TROVA comparison with WaterSip [25] and HAMSTER [10]. Main differences/advantages.

Comparison parameters	Softwares				
	TROVA	WaterSip	HAMSTER		
Input data	Outputs of the FLEXPART and FLEXPART-WRF models forced with reanalysis (ERA-Interim and ERA5) or climatic scenarios	Outputs of the FLEXPART and Lagranto models forced with ERA-Interim	Outputs of the FLEXPART model forced with ERA-Interim		
Input data spatial resolution	Several (e.g. 1°, 0.5°, 0.25°, and 0.18°)	1°	1°		
Output data spatial resolution	Several (e.g. 1°, 0.5°, 0.25°, and 0.18°)	1°	1°		
Lagrangian methodologies implemented	Stohl and James [4] and Sodemann et al. [8]	Sodemann et al. [8]	Sodemann et al. [8] including the possibility of performing bias correction based on source-receptor relationships		
Use for related studies with future changes in moisture sources and sinks	Yes	No	No		
Parallelization	Yes	Yes	No		
Adapted for High-performance computing	Yes	Yes	No		

#### 2.3. Software validation

TROVA software has been validated by Perez-Alarcon et al. [26, 27] in the analysis of tropical cyclone moisture sources for the North Atlantic basin using the methodology of Sodemann et al. [8]. In these studies, the outputs of FLEXPART with ERA-I ( $\sim$ 1° of spatial resolution) were used as input data. Currently, a TROVA evaluation has been carried out using the methodology of Stohl and James [4] for studies of the sources that contribute to humidity on the Iberian Peninsula and for sinks associated with the sources of the North Atlantic Ocean and the Mediterranean Sea [29]. In this study, FLEXPART is used with ERA5 ( $\sim$ 0.5° and 1°) and ERA-I ( $\sim$ 1°) and FLEXPART-WRF is forced with outputs of the WRF model (forced with ERA5 at 0.25°) at a resolution of 0.18°.

#### 3. Illustrative examples

To demonstrate the use of TROVA software, several examples of its application for two target regions (masks, Fig. 2b–f) in the North Atlantic Ocean are presented. In addition, some examples to determine moisture sources and sinks for these case studies are shown. It is important to note that different outputs of FLEXPART forced with reanalysis data from ERA-I, ERA5, and FLEXPART-WRF (also forced with ERA5) were used. We also present results using different spatial resolutions (1°, 0.5°, and 0.18°, respectively) for these input data to showcase TROVA's ability. The data available for testing with TROVA is available at the link: https://doi.org/10. 5281/zenodo.6490365.

Fig. 2b-c represents the moisture sources associated with a tropical cyclone (red circle in Fig. 2a) using the methodology of Sodemann et al. [8] for October 17, 2014, at 18 UTC. These



**Fig. 2.** Pattern representation of moisture sources and sinks associated with a TC and NATL. The patterns correspond to numerical outputs of the dispersion models: FLEXPART ( $\sim 0.5^{\circ}$ ) [c, f], FLEXPART ( $1^{\circ}$ ) [b, e] and FLEXPART-WRF ( $\sim 0.18^{\circ}$ ) [d]. ERA5 and ERA-I are the reanalyses used for forcing. The masks for the TC and NATL-source are represented in pink and blue, respectively [a].

results have been published by Perez-Alarcon et al. [26,27] for case studies or climatological analyses of all tropical cyclones (TCs) in the North Atlantic basin. In addition, Fig. 2d–f shows the moisture sinks associated with a target position over the North Atlantic Ocean, the so-called NATL moisture source (blue area in Fig. 2a), for the period from January to March 2014 (boreal winter). In this case, the methodology of Stohl and James [4] was used. These results show similarity with the pattern found by Gimeno et al. [22].

In these two examples, two types of masks have been used, one that is mobile for tracking a TC (regional), changing position as the TC moves (in this case only one position is shown) and another fixed for the NATL (global), allowing correct representation of the pattern to be achieved in each example. The WVRT for these examples was considered as 10 days. The number of days considered in the TROVA runs is an adjustable parameter, depending on the number of days used for the residence of the water vapor. This facilitates the use of optimal integration times determined by Nieto et al. [30] globally and thus provides a better representation in the pattern of moisture sources. It is necessary to clarify that the differences in the patterns for the same case study are related to differences in input data. These differences are associated with the differences in the configurations of FLEX-PART and FLEXPART-WRF models and not related to the TROVA software.

## 3.1. Sensitivity analysis of TROVA

Below is a sensitivity analysis of the software in which the input data corresponding to FLEXPART-WRF with a spatial resolution of  $\sim 0.2^{\circ}$  was considered constant, but the spatial resolution of the TROVA output mesh was varied to analyze the sensitivity of this software for different resolutions in the representation of the E-P pattern. The period considered corresponds to the months of January to March 2014 (boreal winter). It is important to note that different FLEXPART or FLEXPART-WRF input data were not considered for this analysis (as shown in Fig. 2), since these data present differences related to the configuration of each model, which influences the representation of the moisture budget. Therefore, differences in the E-P pattern cannot be directly associated with TROVA.

Table 2 shows the calculated statistics in the representation of the moisture sources contributing to the precipitation in the Iberian Peninsula (IP, in Fig. 2a) in winter. In general, it is observed a smoothing of the E-P pattern as the spatial resolution of the output grid decreases, as shown by the mean, the extreme values, and the standard deviation. This result is related to the method of calculating the humidity changes (dq/dt, [4]) at the nodes of the output grid; for each point of the grid, when the resolution is low, many particles showing dq/dt<0 or dq/dt>0 are added and a smoothing of the final dq/dt value is obtained. However, when a higher resolution is considered, the sum of dq/dt values at the nodes considers fewer particles, and the pattern shows higher values. This does not imply errors in TROVA, simply that the user must know the resolution at which he/she wishes to work and thus obtain a more homogeneous pattern or one with greater variation.

To corroborate the above, we analyzed the changes in the structure of the E-P pattern that can be observed for the different gridded resolutions. For this, the Structural Similarity Index (SSIM, Wang et al. [31]) was used. The SSIM is perfect when the value is 1 and shows the greatest difference when it approaches -1. For this analysis, the images in Fig. 3 of the moisture sources for 0.2, 0.25, 0.5, and 1 degrees of spatial resolution were used. Fig. 3a is considered as the reference image as it has input data at ~0.2°, therefore its representation should be the most perfect. In general, it is verified that there is a smoothing of the pattern as the spatial resolution decreases, but the structure is shown to be very similar between all resolutions, as shown by a SSMI with values  $\geq$  0.85. Therefore, it is suggested to use a resolution for TROVA very similar to that of the FLEXPART-WRF or FLEXPART input data.

### 4. Impact

The moisture transport from ocean sources to the continents forms the link between evaporation from the ocean and precipitation over the continents, thus establishing the moisture source–sink relationship [32]. In the context of climate change, a change in moisture transport is associated with the moisture increase derived from the increment of temperature [33, 34]. Therefore, the study of moisture transport is crucial for a better understanding of the observed changes and those derived Table 2

Resolution	Statigraphs (mm/day)			Structural similarity	
	Mean	Maximum	Minimum	Standard deviation	SSIM
0.2°	0.12	2.00	0.0	0.15	_
0.25°	0.10	1.85	0.0	0.13	0.86
0.5°	0.08	1.25	0.0	0.11	0.85
1.0°	0.07	1.10	0.0	0.10	0.86



Fig. 3. Moisture sources pattern (E-P>0) that contributed to precipitation over the Iberian Peninsula (IP) calculated from TROVA using different spatial resolutions: (a) 0.2, (b) 0.25, (c) 0.5 and (d) 1 degrees.

from projections of future climate data [1,32]. Therefore, it is important to have a set of tools for Lagrangian post-processing of different model outputs. Specifically, TROVA enables the user community to post-process these model outputs in present and future times to understand changes in the hydrological cycle. In addition, TROVA allows for the two main Lagrangian methodologies established in literature to be integrated into a single tool, thus facilitating comparison of the results obtained and proposing more conclusive results for the scientific community.

#### 5. Conclusions

In this study, TROVA software is presented with its use in the analysis and modeling of atmospheric moisture transport. We anticipate that TROVA will benefit a wide range of users of this scientific field and help understand future changes in the hydrological cycle, thus predicting changes in precipitation over certain regions. In addition, the software will enable the study of future changes in moisture sources and sinks for climatological analysis, specific local events, extremes, or meteorological phenomena.

## **CRediT authorship contribution statement**

**José C. Fernández-Alvarez:** Conceptualization, Methodology, Software, Writing – original draft, Writing – review & editing, Data curation, Formal analysis. **Albenis Pérez-Alarcón:** Data curation, Software, Methodology, Formal analysis. **Raquel Nieto:** Conceptualization, Writing – review & editing, Investigation, Supervision. **Luis Gimeno:** Conceptualization, Writing – review & editing, Investigation, Supervision.

#### **Declaration of competing interest**

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

#### Data availability

Data will be made available on request.

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## Appendix A. Supplementary data

Supplementary material related to this article can be found online at https://doi.org/10.1016/j.softx.2022.101228.

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