REQUEST FOR A SPECIAL PROJECT 2024–2026

MEMBER STATE:	Austria
Principal Investigator[1]:	Marina Dütsch
Affiliation:	University of Vienna, Department of Meteorology and Geophysics
Address:	UZA II Josef-Holaubek-Platz 2 1090 Vienna
Other researchers:	Katharina Baier, Lucie Bakels, Silvia Bucci, Ioanna Evangelou, Seyed Omid Nabavi, Andreas Plach, Anjumol Raju, Andreas Stohl, Rakesh Subramanian, Daria Tatsii, Martin Vojta, Sophie Wittig
Project Title:	FLEXPART transport simulations and inverse modelling of atmospheric constituents

To make changes to an existing project please submit an amended version of the original form.)

If this is a continuation of an existing project, please state the computer project account assigned previously.	**SPATVOJT**	
Starting year: (A project can have a duration of up to 3 years, agreed at the beginning of the project.)	2024	
Would you accept support for 1 year only, if necessary?	YES ☒	NO ☐

Computer resources required for project year:		**2024**	**2025**	**2026**
High Performance Computing Facility	[SBU]	2000000	2000000	2000000
Accumulated data storage (total archive volume)[2]	[GB]	40000	50000	60000

EWC resources required for project year:		**2024**	**2025**	**2026**
Number of vCPUs	[#]	20	20	20
Total memory	[GB]	50	50	50
Storage	[GB]	5000	5000	5000
Number of vGPUs[3]	[#]	0	0	0

Continue overleaf.

[1] The Principal Investigator will act as contact person for this Special Project and, in particular, will be asked to register the project, provide annual progress reports of the project's activities, etc.
[2] These figures refer to data archived in ECFS and MARS. If e.g. you archive x GB in year one and y GB in year two and don't delete anything you need to request x + y GB for the second project year etc.
[3]The number of vGPU is referred to the equivalent number of virtualized vGPUs with 8GB memory.

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Extended abstract

All Special Project requests should provide an abstract/project description including a scientific plan, a justification of the computer resources requested and the technical characteristics of the code to be used. The completed form should be submitted/uploaded at https://www.ecmwf.int/en/research/special-projects/special-project-application/special-project-request-submission.

Following submission by the relevant Member State the Special Project requests will be published on the ECMWF website and evaluated by ECMWF and its Scientific Advisory Committee. The requests are evaluated based on their scientific and technical quality, and the justification of the resources requested. Previous Special Project reports and the use of ECMWF software and data infrastructure will also be considered in the evaluation process.

Requests exceeding 5,000,000 SBU should be more detailed (3-5 pages).

Introduction

The Lagrangian particle dispersion model FLEXPART (Stohl et al., 2005, Pisso et al., 2019) is a widely used atmospheric transport and dispersion model. It can simulate the long-range transport of various atmospheric constituents, such as water vapour, greenhouse gases, volcanic ash, radioactive materials, or microplastics. Within the framework of the special project SPATVOJT, FLEXPART has been used to quantify the role of atmospheric transport for El Niño-Southern Oscillation Teleconnections (Baier et al., 2022), to improve emission estimates of greenhouse gases (Vojta et al., 2022), and to study the influence of particle geometry on transport of microplastics (Tatsii et al., in review). FLEXPART is under active development at the University of Vienna, and a new version will be released soon (Bakels et al., in prep.).

To simulate the movement of gases and particles in the atmosphere, FLEXPART relies on gridded meteorological data, including winds, temperature, pressure, and humidity. Typically, these fields are provided by atmospheric (re)analyses. In this project, we plan to (continue to) run FLEXPART with the products from the European Centre for Medium-Range Weather Forecasts (ECMWF). Specifically, we plan to use the ERA5 reanalysis, the CERA-20C reanalysis, and the operational data archive.

Applications

Inverse modelling of greenhouse gases

Inverse modelling is a powerful tool for verifying greenhouse gas emissions with atmospheric observations using Bayesian statistics. We use this approach to improve *a priori* emission estimates of greenhouse gases like sulfur hexafluoride and methane. This is achieved by running FLEXPART in backward mode to produce the relationship between changes in atmospheric mixing ratios and fluxes. The so-called source-receptor relationship is then used in the Bayesian inversion system FLEXINVERT (Thompson and Stohl, 2014) to obtain *a posteriori* emissions. This helps to identify important greenhouse gas sources and to provide a better estimate of the contribution of different countries to observed concentrations of greenhouse gases.

Interpretation of ice core data

Atmospheric transport simulations help to interpret the deposition of species found in ice core records. We run FLEXPART in backward mode, releasing particles from ice core sites to identify potential emission sources, and in forward mode, releasing particles from known or suspected emission sources, to identify ice core sites at which most deposition occurred. This provides insight into the atmospheric pathways the deposited particles took, and helps to identify the most important emission sources of different species in the past.

Transport of microplastics in the atmosphere
There is increasing evidence that microplastic particles transported in the atmosphere have harmful effects on the ecosystem and human health (e.g., Baldwin et al., 2016; Cox et al., 2019). We use FLEXPART to simulate the transport of microplastic particles emitted from different regions (e.g., the ocean or deserts) to quantify the impact of different sources on the atmospheric distribution of microplastics and their redistribution over the ocean and land. In this context we also work on improving the gravitational settling scheme in FLEXPART to more accurately simulate the transport and removal of microplastic particles with different shapes.

Lagrangian moisture source diagnostic
By tracking the moisture content of air parcels as they move through the atmosphere, Lagrangian moisture source diagnostics provide insight into the contributions of different moisture sources to precipitation or drought events. We diagnose moisture uptakes along FLEXPART trajectories to identify moisture sources for different regions, e.g., the Amazon rainforest or the Arctic, under different weather conditions. This helps to improve our understanding of regional water cycles, predict changes in precipitation patterns, and assess the vulnerability of ecosystems to changes in moisture availability.

Computational resources

Typical FLEXPART runs for these applications require between 1000 and 200000 SBUs. We plan around 100 jobs per user per year, which amounts to 2000000 SBUs in total for the HPC resources. In addition to the HPC resources, we would also like to use the European Weather Cloud (EWC). The plan is to run interactive jobs on the EWC, where users can launch FLEXPART jobs through a graphical user interface and directly plot the output. For these runs we would use the newly developed parallel version of FLEXPART with up to 20 OpenMP threads.

References

Baier, K., Dütsch, M., Mayer, M., Bakels, L., Haimberger, L., & Stohl, A. (2022). The Role of Atmospheric Transport for El Niño-Southern Oscillation Teleconnections. Geophysical Research Letters, 49(23). doi.org/10.1029/2022GL100906

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Cox, K. D., Covernton, G. A., Davies, H. L., Dower, J. F., Juanes, F., & Dudas, S. E. (2019). Human consumption of microplastics. Environmental Science and Technology, 53:7068–7074.

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