REQUEST FOR AN EMI R&D PROJECT 2027–2029

Country/ Organisation:	Austria
Principal Investigator[1]:	Sophie Scharinger
Affiliation:	University of Vienna, Department of Meteorology and Geophysics
Address:	UZA II Josef-Holaubek-Platz 2 1090 Vienna
Other researchers:	Andreas Stohl, Michael Blaschek, Marina Dütsch, Ioanna Evangelou, Seyed Omid Nabavi, Anjumol Raju, Martin Vojta, Sophie Wittig, Alina Reininger, Rakesh Subramanian
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.)	2027	
Would you accept support for 1 year only, if necessary?	YES ☒	NO ☐

Computer resources required for project year:		**2027**	**2028**	**2029**
High Performance Computing Facility	[SBU]	2M	2M	2M
Graphics Processing Unit Cluster-A	[GBU]	/	/	/
Graphics Processing Unit Cluster-B	[GBU]	/	/	/
Accumulated data storage (total archive volume)[2]	[GB]	4000	5000	6000

[1] The Principal Investigator will act as contact person for this EMI R&D 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.

EWC resources required for project year:		2027	2028	2029
Number of vCPUs	[#]	20	20	20
Total memory	[GB]	50	50	50
Storage	[GB]	5000	5000	5000
Number of vGPUs[3]	[#]	/	/	/

Continue overleaf.

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Extended abstract

All EMI R&D 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 EMI R&D 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 EMI R&D 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; Bakels et al, 2024) is a widely used atmospheric transport and dispersion model that is under continuous development at the University of Vienna. 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 previous project SPATVOJT, FLEXPART has been used to, among other things, convert the Eulerian reanalysis ERA5 into a Lagrangian reanalysis (Bakels et al., 2025), to quantify European SF_6 emissions using inverse modeling (Vojta et al., 2025) and to estimate global emissions of atmospheric microplastics (Evangelou et al., 2026).

In order to simulate the movement of gases and particles in the atmosphere, FLEXPART relies on gridded meteorological data, including winds, temperature, pressure, and humidity. For most applications, 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 the ERA5 and ERA6 reanalyses, the CERA-20C reanalysis, and the operational data archive. The software package Flex_extract is used to retrieve and prepare this data for use as input to FLEXPART (Tipka et al., 2020).

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.

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.

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.

Modelling of pyroCb emissions

Major wildfire events in recent years have produced wildfire-driven thunderstorms (pyroCbs) that have emitted large quantities of smoke into the stratosphere. The impact of some of these events has been shown to be comparable to moderate volcanic eruptions (Peterson et al., 2025). FLEXPART is used to investigate the dynamics, long-range transport and global impact of pyroCb emissions. To accurately model these plumes, a parameterisation of the radiatively driven self-lofting that occurs in major stratospheric smoke plumes is being developed.

Computational resources

The requested HPC resources will be used to run FLEXPART, which may require between 1000 and 200000 SBUs per run, depending on the application. Additionally we're planning to use the European Weather Cloud (EWC) to run interactive jobs. Users will be able to launch FLEXPART jobs through a graphical user interface and directly plot the output. For these runs we will use the parallel version of FLEXPART with up to 20 OpenMP threads. An EMI R&D project furthermore provides the means to retrieve and pre-process data using Flex_extract. In the past years, this pre-processing was limited to continuously updating the dataset available to FLEXPART as ERA5 data was released. However, with the expected rollout of ERA6 in the next years, we anticipate a higher demand for this use case, since the entire historical dataset will be processed.

References

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