Research Networking Programmes

Short Visit Grant ☒ or Exchange Visit Grant ☐

(please tick the relevant box)

Scientific Report

The scientific report (WORD or PDF file – maximum of eight A4 pages) should be submitted online within one month of the event. It will be published on the ESF website.

Proposal Title: Future development in testing environments and wet deposition parameterisation for the Lagrangian particle dispersion model FLEXPART

Application Reference N°: 6677

1) Purpose of the visit

The aim of this short research visit was to further discuss and plan my doctoral thesis project at the University of Vienna. Generally, my research topic is about improvements to the Lagrangian particle dispersion model FLEXPART. Since most of the main developers of FLEXPART I want to work with are stationed at NILU (Norwegian Institute for Air Research) in Kjeller/Norway, I was invited for a short research stay.

One of the purposes was to introduce my ideas and to discuss and plan the best way of co-operating and benefiting from each other. The improvements that I am planning to develop in my doctoral project are divided into the revision of the wet deposition and the development of a testing environment.

For the wet deposition we wanted to discuss and exchange ideas in the current work of improving the wet deposition parameterisation in FLEXPART and where there are the biggest problems and the best chances for a successful improvement. We want to be able to continuously bring together our independent development paths of the physical and numerical approaches so that we can benefit of each others work and bring the wet deposition in FLEXPART to a better level of accuracy. To show the improvements of

results in the work on wet deposition, I am going to develop a proper test with several test cases.

Since FLEXPART is being used by more than 35 groups in 14 different countries and is applied for research and operational work (e.g. CTBTO), there is a need for continuously working to improve the program. These improvements are carried out under challenging conditions: a number of scientists at different locations are involved, workign on several different foci. A consistent evaluation and validation of the model performance is therefore quite important.

For future work with, and especially future developments of the model, a more uniform way of assessing validity, performance, and quality is needed. For this purpose, a general testing environment needs to be built. This should assist all developers of FLEXPART as they can then easily test all relevant aspects after any model change.

To ensure an optimum result for this testing environment, it is essential to discuss and plan my project with other developers and users of FLEXPART in order to include all the different perspectives. For a better commitment of the community it is essential to include their ideas in building the testing environment.

2) Description of the work carried out during the visit

During my stay at NILU, the release of the latest FLEXPART version 9.2 was prepared. Over some months FLEXPART developers at NILU had merged together a couple of changes, added some new features, modified the performance and corrected some bugs. Eventually, the latest release of the ECMWF data extraction software for FLEXPART (ECMWFDATA V6.0), was used for providing FLEXPART 9.2 input data. My presence during this week was helpful since I could assist in implementing the algorithms for reading the input data in FLEXPART from ECMWFDATA v6.0. This was because of my involvement in testing and evaluating the ECMWFDATA software version 6. Hence, I could give some hints to use ECMWFDATA in version 6, too.

During the week at NILU we discussed and planned the general part of the testing environment for FLEXPART. First of all we started to change the tree structure for FLEXPART, so it is more understandable for users and easier to run automatic tests. Then we discussed some suggestions on how developers from all different countries and institutes could be motivated to use our subversion system so everyone can benefit from new features in FLEXPART. If correctly applied, developers and users can keep track of all of the modifications with ease. We want to create a short guideline for this so everyone is using the same method in development. Also, one of the first things we need is to implement some standard tests to guarantee that FLEXPART is running. This includes for example a test for reading the input data correctly and finishing the simulation with the “congratulations” line at the end of the standard output. To start with the testing environment, we did a local installation of the continuous integration system “Jenkins” at NILU and described some test cases. We used Jenkins to run an automated batch script every time the trunk or one of the branches in our svn system were updated.

A further purpose of the short research stay was to talk to another PhD Student who is currently working on wet deposition in FLEXPART. After some first statistics, we found that the deposition is too strong. Thus, we talked about the possibilities and our different approaches for improving the wet deposition numerically and physically. An adaption of the below-cloud scheme including the dependence on aerosol size distribution as well as the integration of cloud liquid water content (clwc) and cloud ice water content (ciwc) for defining the cloud mask in FLEXPART were discussed. Besides these possible changes we discussed the current interpolation and disaggregation of the precipitation and cloud cover fields. There is definitly a wide scope for improvement of the deposition by changing the interpolation routine in addition to the adaption of physical behaviour.

3) **Description of the main results obtained**

One outcome of my stay at NILU was my contribution on the official release of the latest FLEXPART 9.2 beta version for developers. This was a very urgent release since developers are constantly implementing new features to severeal different and older versions of FLEXPART. It is very likely that the integration into newer versions is much more complicated and accompanied by compatibility problems than implementing new features with the method of "continuous integration". This means that all developers are going to merge their developments continously with the main FLEXPART release. The decision to release just a beta version for developers was made because full testing of this version is still going on. Users should get only very detailed tested releases.

The development process with testing and adaptations of features from older versions to the latest version showed precisely why I want to create an automated testing environment. The generation of test cases and searching for problems and bugs are very time consuming. Hence, an automated testing environment can save a lot of time in verification of correctness. Moreover, we will not discover development errors and compatibility problems during (operational) application but in the development and testing phase. Furthermore, FLEXPART can gain more quality because of a comprehensive spectrum of test cases (collection of standard test cases for the general simulation of FLEXPART and some detailed cases for testing the behaviour of explicite features and properties) which are repeated after every change in the subversion system. We found out that Jenkins is the perfect tool for our needs to start the testing process automatically after a change in the subversion system. Therefore we will set up a local testing environment on a server of the University of Vienna and install the continuous integration system Jenkins. We will continue to work on a guideline for our version of the branch-when-needed subversion system and publish it at flexpart.eu. We also started to describe some basic test cases and to change the tree struktur of the FLEXPART tarball. To build an automatic testing environment, memory allocation in FLEXPART has to be changed to guarantee a fully automatical testing

For the wet deposition problem, we came to the conclusion that we will continue to pursue work on two different approaches. We will investigate the utility of a new horizontal interpolation and disaggregation scheme for precipitation fields as well as an adaption in the distribution of cloud fields in the horizontal and vertical. We also want to investigate the utility of using the CLWC and CIWC. Continuously, we will discuss our

progress and merge our developments to guarantee a useful improvement in both ways, numerically and physically.

4) **Future collaboration with host institution (if applicable)**

Both sides declared that it was a very helpful exchange of information and ideas. All parties are interested in further research stays and close co-operation in developing a testing environment and improvements in wet deposition – but also in other aspectes concerning FLEXPART (e.g. the development platform http://flexpart.eu, the creation of guidelines for several cases like the usage of the flexpart.eu ticket system and how to release new FLEXPART versions). NILU is going to contribute to the testing environment with suggestions and ideas for useful tests as well as data for basic test cases, input data and measurement data. We strive to merge both development paths of wet deposition together, regularly. We think that this will give us a better wet deposition parameterization, especially because of we will review each others work and use different approaches for improvement.

5) **Projected publications / articles resulting or to result from the grant *(ESF must be acknowledged in publications resulting from the grantee's work in relation with the grant)***

There are a couple of long-term publication plans. We want to publish at least one article with respect to the new wet deposition parameterization in FLEXPART. Additionally, the documentation of the testing environment should be submitted to the journal of Geoscientific Model Development (GMD). A couple of other documentations or guidelines for FLEXPART might result out of the co-operation with NILU.

6) **Other comments (if any)**

The personal meeting with the FLEXPART developer group at NILU was very efficient and helpful. Thus, a long-term benefit for FLEXPART, an important tool for the simulation of the transport of various atmospheric trace substances, can be expected.