<u>LATE</u> REQUEST FOR A SPECIAL PROJECT 2018–2020

MEMBER STATE: Germany

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Project Title:

Integrated Simulations of the Terrestrial System over the European CORDEX Domain

If this is a continuation of an existing project, please state the computer project account assigned previously.	**SP** DE KOLL	
Starting year: (A project can have a duration of up to 3 years, agreed at the beginning of the project.)	2018	
Would you accept support for 1 year only, if necessary?	YES ☒	NO ☐

Computer resources required for the years: (To make changes to an existing project please submit an amended version of the original form.)		**2018**	**2019**	**2020**
High Performance Computing Facility	(SBU)	10.000.000		
Accumulated data storage (total archive volume)[2]	(GB)	60.000		

An electronic copy of this form must be sent via e-mail to: *special_projects@ecmwf.int*

Electronic copy of the form sent on (please specify date):

17.05.2018

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 an annual progress report of the project's activities, etc.

[2] 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.

Principal Investigator: Stefan Kollet

Project Title: Integrated Simulations of the Terrestrial System over the European CORDEX Domain

Extended abstract

The objective of this study is to **identify and quantify feedback pathways of human water use on the atmospheric circulation** using a Lagrangian particle dispersion model and high-resolution fully coupled aquifer-to-atmosphere simulations over the European CORDEX domain.

Recent studies indicate that anthropogenic impacts on the terrestrial water cycle and the atmospheric circulation lead to a redistribution of water resources in space and time, can trigger land-atmosphere feedbacks, such as the soil moisture-precipitation feedback, and potentially enhance convection and precipitation. Yet, these studies do not consider the full hydrologic cycle from the bedrock to the atmosphere or apply simplified hydrologic models, neglecting the connection of irrigation to water withdrawal and groundwater depletion. Moreover, these simplified approaches assume an unlimited supply of water (Thiery et al., 2017, Leng et al., 2017) and thus neglect emerging issues of water scarcity and continental drying. Thus, there is a need to incorporate water resource management in 3D hydrologic models coupled to climate models. In our previous studies, realistic estimates of human interactions in the terrestrial water cycle, i.e. groundwater abstraction and irrigation (Wada et al., 2012, 2016; Siebert and Döll, 2010; Siebert et al., 2010), were considered in simulations with the integrated Terrestrial Systems Modeling Platform, TerrSysMP, consisting of the three-dimensional surface-subsurface model ParFlow, the Community Land Model CLM3.5 and the numerical weather prediction model COSMO of the German Weather Service (Shrestha et al., 2014, Gasper et al., 2014). The simulations were performed at the ECMWF within the special project SPDEKOLL 2016-2017, over the European CORDEX domain in 0.11° resolution (Keune et al., 2016; Keune et al., 2018).

This late request for a special project proposes an ensuing study, in which the feedback pathways of human water use are identified. We apply the Lagrangian particle dispersion model FLEXPART (Stohl et al., 1998) to trace atmospheric water vapour. This application facilitates the identification of moisture sources, which lead to precipitation, and allows to quantify a) local precipitation recycling rate, and b) remote feedback pathways, thereby addressing moisture recycling governance (Keys et al., 2017; Figure 1). Precipitation recycling is defined as the contribution of land surface evapotranspiration from a specific region (control volume, watershed) to precipitation in that same region (control volume, watershed) (Brubaker et al., 1993). It is an important land-atmosphere feedback process, which can intensify or alleviate droughts, and significantly affect water resources. In the context of the current study, particle tracking allows us to identify the human impact on precipitation recycling, i.e. how and where irrigation supplies water for rainfall. The simulations are evaluated using the moisture source attribution methodology of Sodemann et al. (2008). Figure 1 shows a sketch of the remote land-atmosphere feedbacks simulated by TerrSysMP. FLEXPART allows to disentangle the feedback processes and identify feedback pathways. A sketch of such a pathway is shown in Figure 2.

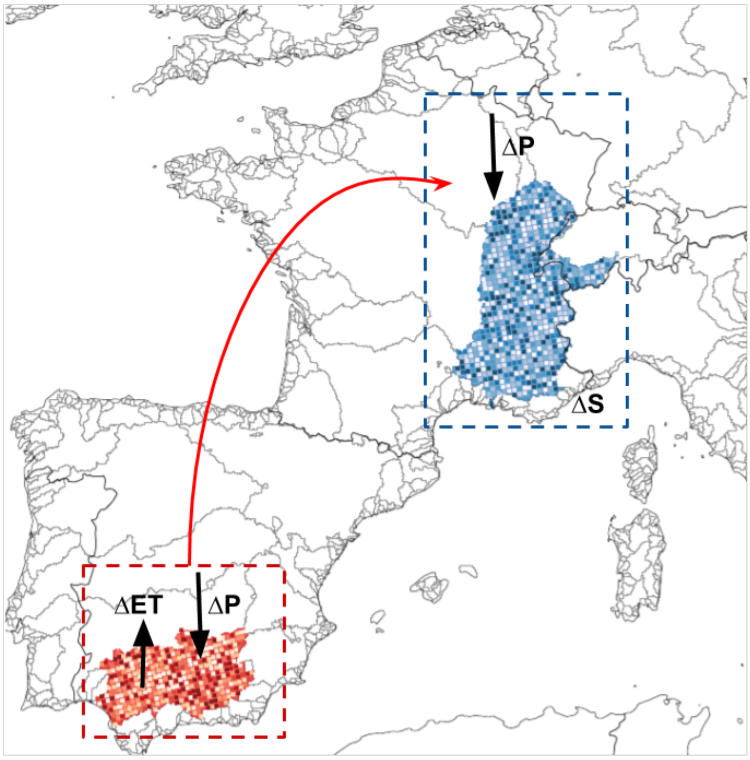

Figure 1. Sketch of a one-way remote land-atmosphere feedback pathway between two watersheds as simulated with TerrSysMP. Here, human water use leads to changes of evapotranspiration (ΔET) and precipitation (ΔP) in one watershed; but also affects atmospheric water vapor transport and impacts precipitation in another, remote watershed. These remote feedbacks furthermore contribute significantly to changes of groundwater storage (ΔS) and hence illustrate the remote impact of human water use (Keune et al., 2018).

Scientific plan

While FLEXPART has been applied in numerous global water vapor studies (e.g., Gimeno et al., 2015; Gimeno et al., 2013; Drumond et al., 2017; Winschall et al., 2014; Sodemann et al., 2007; Sodemann and Stohl, 2013), its application on regional domains and within integrated modeling systems, such as TerrSysMP, is new. We plan to

1. **Design simulation experiments with FLEXPART for TerrSysMP**
2. **Perform FLEXPART-TerrSysMP simulations over the European heat wave in 2003**

in order to quantify moisture recycling feedback pathways.

FLEXPART-TerrSysMP has already been setup, but an ideal experiment design has not been found yet. The study is divided into two parts: Step 1 includes the testing of a) the number of particles required to yield reliable results; and b) to find the most effective computational setup. A minimum of 8.5 Million particles is assumed to be required to cover the European CORDEX domain in 0.11° resolution. In step 2, FLEXPART will be applied to the TerrSysMP simulations from Keune et al. (2018), which comprise one natural reference simulation and four human water use scenarios. The comparison of the natural reference simulation to the four human water use scenarios allows us to identify human water use induced feedback pathways and their uncertainty.

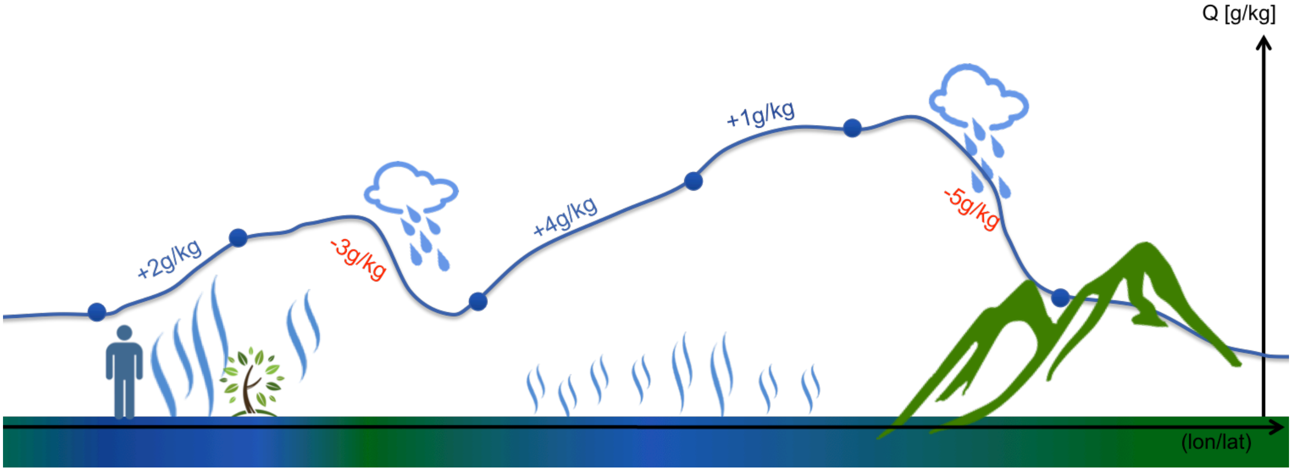

Figure 2. Sketch of a sample output trajectory from FLEXPART. The trajectory depicts specific humidity changes ΔQ [g/kg] in space and time (indicated along particle positions on the blue trajectory), which allows to attribute moisture sources for precipitation events. In our study, we will assess how human water management impacts local evapotranspiration (ΔQ>0) and (remote) precipitation (ΔQ<0). To account for model parameterizations and uncertainties, the moisture source attribution methodology from Sodemann et al. (2006) is applied.

Justification of computer resources requested

The setup of FLEXPART has not been tested at ECMWF yet. However, test simulations were performed on a comparable CRAY machine. From these test simulations we learned that the ideal setup for FLEXPART over the European CORDEX domain is expected to require about 1.6 Million SBU for a one-year simulation (cf. Table 2). Adding the estimated compute time for pre-processing and post-processing (0.4 Million SBU, this sums up to approx. 2 Million SBU, and to 10 Million SBU for a total of 5 simulations.
FLEXPART model output is approx. 650 MB/hour (15 GB/day), and accumulates to 2.8 TB for one simulation for one year. The five simulations in this study require 14TB of data storage. This is added to our current storage of the TerrSysMP simulations, which are input to FLEXPART (56TB). A total storage of 60TB is thus needed to perform this study. Thus, **we kindly request a total of 10.000.000 SBU and 60TB for the accounting period 2018.**

Table 1. Input and output fields and formats for FLEXPART-TerrSysMP. The file size refers to single time step output of a FLEXPART-TerrSysMP simulation over the European CORDEX domain (0.11° resolution, domain size: 424x412x50) with approx. 8.73 Million particles (cf. scaling study).

DATA	TYPE	FORMAT	FILE SIZE
INPUT			
2D fields	p, tcc, u_10m, v_10m, sh, le, taux, tauy, hgt, mask, hgt_std, t_2m, td_2m, p_ls, p_con	netcdf	182 MB
3D fields	u, v, w, t, q	netcdf	128 MB
OUTPUT			
2D fields	grid concentration	netcdf	18 MB
particle information	lon, lat, z, q, t, pblh	binary	601 MB

Table 2. Required compute time for an idealized FLEXPART-TerrSysMP setup over the European CORDEX domain (cut down to 436x424 grid points with 50 vertical levels) with approx. 8.73 Million particles.

TEST SIMULATIONS					
	Cores (total tasks)	**Simulation period [h]**	**Wall clock time [s]**	**Core-hours [h]**	**SBU**
Test-1	16	1 h	2520	11.2	180.4
Test-2	16	24 h	60480	268.8	4330.4
ESTIMATES FOR A 1 YEAR SIMULATION					
	Cores (total tasks)	**Simulation period [h]**	**Wall clock time [s]**	**Core-hours [h]**	**SBU**
Estimate	16	8760 h (1 year)	22075200	98112	1580584

Technical characteristics of FLEXPART

FLEXPART is a 3-dimensional Lagrangian particle dispersion model by Stohl et al. (2005), originally developed to trace dispersion of air pollution. FLEXPART simulates the long-range atmospheric mesoscale transport through trajectories of a large number of particles. Particle releases are prescribed and transported with the mean velocity field, to which a stochastic turbulent component is added (Stohl et al., 2005; Seibert and Frank, 2004). FLEXPART allows to determine source-receptor relationships in forward or backward mode, where the backward mode is computationally advantageous for small scale problems (Seibert and Frank, 2004). Over time, FLEXPART evolved to an open-source model, to which multiple communities contribute (https://www.flexpart.eu/). This opened the field for further atmospheric transport studies, allowing e.g. for a more detailed analysis of the terrestrial water cycle (e.g., Stohl et al. 2008; Winschall et al., 2014; Gimeno et al., 2016; Miralles et al., 2016).

The **standard global FLEXPART model** (version 9.02) is driven by analysis or reanalysis fields from the European Centre for Medium Range Weather Forecast (ECMWF). This model version has been adapted to regional domains, using output from the non-hydrostatic numerical weather prediction model COnsortium for Small-Scale MOdeling (COSMO; Baldauf et al., 2001; Doms and Schaettler, 2002) from the German Weather Service (DWD) and is hereafter called **FLEXPART-COSMO** (Henne et al., 2016). The two models mainly differ in the vertical grid representation and the convective transport parameterization (Henne et al. 2016). The terrain-following coordinates with constant level depths from the standard FLEXPART have been adapted to the height-based hybrid coordinate system in COSMO (Gal-Chen and Somerville, 1975). Analogously, the Tiedke convection scheme (Tiedke, 1989) replaces the Emanuel-type convection scheme (Emanuel and Živković-Rothman, 1999; Forster et al., 2007) in FLEXPART-COSMO. Other minor changes include e.g., the use of the lowest level temperatures instead of 2m temperatures to calculate planetary boundary layer (PBL) heights, in order to reduce positive PBL height biases. Additional technical changes include the integration of a netcdf-option for reading and writing input and output fields, respectively.

FLEXPART-TerrSysMP, refers to the latest version of FLEXPART-COSMO, which has been adapted to output from TerrSysMP. FLEXPART-TerrSysMP is currently setup with COSMO version 5.1 coupled to CLM3.5. In this version, land surface fluxes of energy, moisture and momentum are simulated by CLM3.5 and determine atmospheric boundary layer characteristics and turbulence intensity in FLEXPART.

FLEXPART is coded in Fortran 95 and has been tested with several compilers (gfortran, Absoft, Portland Group) under different operating systems (Linux, Solaris, Mac OS X, etc.) and is optimized for run-time performance (Stohl et al., 2005; Stohl et al., 2010 The numerical core of FLEXPART-COSMO is parallelized and allows for an efficient allocation of resources. Table 1 shows the results of a 24 hour simulation of FLEXPART-TerrSysMP over the European CORDEX domain at 0.11° (approx. 12.5 km) resolution and with 424x412 grid cells and 50 vertical levels. This corresponds to an ideal setup with 8.73 Million initial particle releases and a boundary release of approx. 175.000 particles per time step (which is approx. the number of particles that leave the domain per time step).

The workflow of FLEXPART-TerrSysMP is illustrated in Figure 3. First, the TerrSysMP simulation results are pre-processed for the use in FLEXPART (bash-based scripts; https://github.com/jkeune/cclm4flexpart). The FLEXPART simulations are started and the single time-step particle positions (binary output, cf. Table 1) are post-processed into particle trajectories (https://github.com/jkeune/flexpart-utils, using python and GNU R; parallelization possible). In the final step, the trajectories are filtered with respect to the analysis objective and evaluated using e.g. the moisture source attribution methodology from Sodemann et al. (2008) (using python and GNU R).

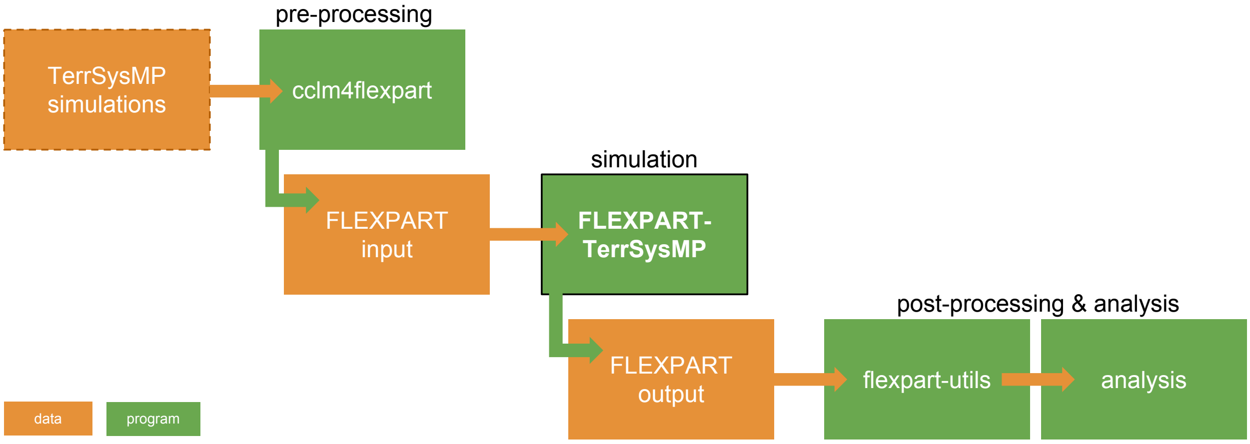

Figure 3. Diagram of the workflow for the FLEXPART-TerrSysMP simulations, assuming that the TerrSysMP simulations have already been performed: the raw model output is pre-processed using the newly developed cclm4flexpart tools, which create input files for FLEXPART-TerrSysMP. FLEXPART-TerrSysMP simulations are started and post-processed using flexpart-utils, which is currently being developed, and creates and filters particle trajectories for analyses, including e.g. a moisture source attribution according to Sodemann et al. (2008).

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