REQUEST FOR A SPECIAL PROJECT 2012–2014

MEMBER STATE: Germany

Principal Investigator[1]: Olaf Stein

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Project Title:

Global Atmospheric Chemistry Modelling

If this is a continuation of an existing project, please state the computer project account assigned previously.	**SP**DEACM	
Starting year: (Each project will have a well defined duration, up to a maximum of 3 years, agreed at the beginning of the project.)	2012	
Would you accept support for 1 year only, if necessary?	YES ☐	NO X☐

Computer resources required for 2012-2014: (The maximum project duration is 3 years, therefore a continuation project cannot request resources for 2014.)	**2012**	**2013**	**2014**
High Performance Computing Facility (units)	610000	610000	610000
Data storage capacity (total archive volume) (gigabytes)	30000	35000	40000

*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): 2011-04-29

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.

Principal Investigator: Martin Schultz

Project Title: Global Atmospheric Chemistry Modelling

Extended abstract

The main aim of this special project is the integration of gas-phase chemistry from the global chemistry transport model MOZART-3 (Kinnison et al. 2007) into the IFS model, a work which has begun during the EU projects GEMS and MACC and will be continued in the MACC-II project (2012-2014). The special project is a continuation of the SPDEACM project, which ends in 2011. Continuation of the SPDEACM work is essentially needed after the end of the MACC project in October 2011 in order to ensure the evolution of the MACC system into a fully operational forecast system by 2014. Therefore ECMWF computer resources are foreseen to be continuously needed after October 2011.

The project work is split into three major parts: First, new model developments and updates in the model input fields will be implemented and tested with the offline model MOZART (version 3.5). Second, the coupled model IFS-MOZART will be further developed and the MACC-II forecasts and reanalysis operated by ECMWF will be supported. Third, the IFS with integrated chemistry (C-IFS) will be developed in close collaboration with ECMWF. Simulations from all three work streams will be validated extensively by FZ Juelich and the MACC-II project partners.

MOZART-3

The global CTM MOZART3.5 includes of a comprehensive tropospheric and stratospheric chemistry reaching also up to the mesosphere. Since it is still a scientific challenge to correctly simulate stratospheric chemistry and transport further model studies will be needed to improve the model simulations, particularly for the ozone hole region (Flemming et al. 2011). New model input data fields for photochemistry and model boundary conditions need to be adapted, tested and validated. A major source of uncertainty is expected to be found in the emission inventories and the deposition fluxes. Several model sensitivity studies will be carried through to overcome these uncertainties. The standard configuration of MOZART3 in T63L60 resolution is typically using 3 nodes of c1a and a standard simulation consumes about 30,000 BU per simulation year together with stored netcdf data on ecfs of up to 800 GB. MOZART simulations with enhanced resolution T106L60 use 4 nodes of c1a, the estimated computational costs are 270,000 BU per simulation year and netcdf data storage of about 2,400 GB. The major part of the required computer resources will be used by these simulations which will also foster the development of the coupled model IFS-MOZART and the C-IFS. As already done in MACC, the MOZART model output is stored at ecfs and will be validated extensively by the MACC-II project partners. In turn, the MOZART model will support the further development of novel emission data sets also coming from MAC-II partners.

IFS-MOZART

The coupled model IFS-MOZART (Flemming et al. 2009) has been first implemented during the GEMS project. In MACC this model has been updated to digest the novel emission inventories, particularly the biomass burning emissions with high temporal resolution. The model will be continually employed for the quasi-operational forecasts and a MACC-II reanalysis. These simulations are operated by ECMWF, but all MOZART related code changes and scripting work will be initiated form this special project. Additional MOZART offline simulations will accompany the ECMWF operations whenever needed.

C-IFS

The integration of modules for chemistry, emissions, and deposition into the IFS module has begun during the MACC project. In the long term this model is intended to take over from IFS-MOZART for operational forecasts of the global chemical state of the atmosphere. MOZART is one out of three chemistry modules initially chosen for C-IFS and is currently being build into the IFS. This major scientific development will continue for the next three years at least. In close collaboration with ECMWF (J. Flemming) the new chemistry module will be developed based on the existing CTM routines. Experience form related CTMs and GCMs (MOZART-4, ECHAM6-HAMMOZ) will be incorporated into the new chemistry module. This

needs extensive testing of the module components both with the C-IFS prototype version and with standalone MOZART simulations. Additionally, the possible usage of the kpp chemistry solver instead of the MOZART solver will be investigated. Another important issue are the optimization of the various interfaces to the aerosol chemistry modules, which are currently not properly defined. Most of the C-IFS simulations will be operated by ECMWF, but several simulations will be done from this special project during the development phase.

Estimated resources

The yearly estimations (2012-2014) for the simulation runs which are necessary in the MACC-II project are as follows:

8 years MOZART sensitivity runs in standard resolution T63L60	240000 BU
1 year MOZART sensitivity runs in enhanced resolution T106L60	270000 BU
simulations with the fully coupled chemistry transport model C-IFS:	100000 BU

Total: 610000 BU and ca. 5000 GB new data storage on ecfs per year

References:

Flemming, J., Inness, A., Flentje, H., Huijnen, V., Moinat, P., Schultz, M. G., and Stein, O.: Coupling global chemistry transport models to ECMWF's integrated forecast system, Geosci. Model Dev., 2, 253-265, 2009.

Flemming, J., Inness, A., Jones, L., Eskes, H. J., Huijnen, V., Schultz, M. G., Stein, O., Cariolle, D., Kinnison, D., and Brasseur, G.: Forecasts and assimilation experiments of the Antarctic Ozone Hole 2008, Atmos. Chem. Phys. 11, 1961-1977, doi:10.5194/acp-11-1961-2011, 2011.

Kinnison, D. E., Brasseur, G. P., Walters, S., Garcia, R. R.,. Marsh, D. R , Sassi, F., Harvey, V. L., Randall, C. E., Emmons, L., Lamarque, J. F., Hess, P., Orlando, J. J., Tie, X. X., Randel, W., Pan, L. L., Gettelman, A., Granier, C., Diehl, T., Niemeier, U. and Simmons, A. J.: Sensitivity of Chemical Tracers to Meteorological Parameters in the MOZART-3 Chemical Transport Model. J. Geophys. Res, 112, D03303, doi:10.1029/2008JD010739, 2007