REQUEST FOR A SPECIAL PROJECT 2018–2020

MEMBER STATE:	Germany
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Project Title:	Copernicus Atmospheric Monitoring Service – Air Quality and Composition – Regional Component (CAMS_50)

If this is a continuation of an existing project, please state the computer project account assigned previously.	SP DEFRIU		
Starting year: (Each project will have a well defined duration, up to a maximum of 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 2015-2017: (The maximum project duration is 3 years, therefore a continuation project cannot request resources for 2017.)		2018	2019	2020
High Performance Computing Facility	(units)	3,500,000	4,200,000	4,200,000
Data storage capacity (total archive volume)	(gigabytes)	7,500	9,000	9,000

An electronic copy of this form **must be sent** via e-mail to:

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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. October 2013 Page 1 of 6 This form is available at:

http://www.ecmwf.int/about/computer_access_registration/forms/

Principal Investigator:

Project Title:

Hendrik Elbern

Copernicus Atmospheric Monitoring Service – Air Quality and Composition – Regional Component (CAMS_50)

Extended abstract

Preliminary remark:

The aim of this special project is to develop and operate the applicant's EURopean Air pollution Disperion - Inverse Model (EURAD-IM) as a member of the Copernicus Atmospheric Monitoring Service ensemble of regional air quality models in CAMS_50. Despite an installation of a home based back-up copy simulation, compute resources are requested at ECMWF, because super computer accessible at Research Centre Jülich have job scheduling schemes, which do not grant regular day time dependent launch of jobs. Rather, queuing rules are imposed without priority of regular submission schedules.

Motivation:

The Copernicus Atmosphere Monitoring Service (CAMS, atmosphere.copernicus.eu) is establishing the core global and regional atmospheric environmental service delivered as a component of Europe's Copernicus program. CAMS provides continuous data and information on atmospheric composition. The service describes the current situation, forecasts the situation a few days ahead, and analyses consistently retrospective data records for recent years. CAMS has been developed to support policymakers, business and citizens with enhanced atmospheric environmental information. These services, which achieved an operational status in 2015, are the result of more than ten years of pilot and active research projects (GEMS, MACC, MACC-III, MACC-III).

CAMS_50

The CAMS_50 service aims at delivering the operational European-scale air quality component of CAMS. The delivery of the European-scale air quality data is based upon a geographically distributed ensemble of 7 individual models under the lead of Meteo France. RIUUK provides a member of this ensemble with its comprehensive chemistry transport model EURAD-IM (Elbern et al., 2007). RIUUK plays an active role in sub-project CAMS_50. Three data streams are provided:

- on a daily basis, hourly analyses for the previous day and forecasts up to + 96 h;
- with a delay of a few weeks (in order to maximise the number of observations) interim re-analyses are produced daily with systems frozen in their configuration of January 1st every year;
- with a delay of up to 2 years (due to the delay in getting fully validated data), re-analyses are processed with frozen systems, which are only updated every few years.

An important component of CAMS 50 is the further development of the individual air quality forecast models and of the data assimilation systems.

Development of the EURAD-IM Regional System (CAMS_5020)

These activities aim at further developing the EURAD-IM regional services that are operated by RIUUK for the nearreal-time (NRT) daily production and for the reanalyses of CAMS_50. These activities are mainly to improve the quality of the EURAD-IM forecasts, analyses and reanalyses, to improve the reliability of the chains and to develop new products. Another aspect of the work is to keep the chains up-to-date with respect to the input datasets (meteorological data, emission inventories, etc.). The planned developments for EURAD-IM are thus intended to improve the CAMS_50 service.

Some new products out of the EURAD-IM chains will be developed. The EURAD-IM NRT analyses will be extended to all 8 levels (the same as for the forecasts), for all 10 requested species. Besides, a pollen emission scheme for ragweed will be developed, based on previous research & development activities done at FMI.

Other actions will aim at improving the reliability of the NRT EURAD-IM production chain. In the current operational EURAD-IM model chain, meteorological input data from IFS, chemical boundary values from C-IFS, and wildfire emission data from GFAS are extracted from MARS. We will seek to treat these dataflows in an operational manner after the operational upgrade in autumn 2017, to improve the reliability of the EURAD-IM productions.

Currently SMS (Supervisor Monitor Scheduler) is used for the scheduling of the EURAD-IM forecast, analysis, and interim reanalysis chains. In future operational upgrade, ecFlow will be used for the scheduling of at least one of these model chains.

Several actions are also planned to improve the performance of EURAD-IM analyses above surface. EURAD-IM has established ability to assimilate in situ aircraft measurements. The related forward and backward observation operators were successfully applied to MOSAIC (Measurement of Ozone and Water Vapour on Airbus in-service Aircraft) measurements. This ability of EURAD-IM will be applied to IAGOS (In-service Aircraft for a Global Observing System) measurements of O3, CO, NOx, and aerosols. IAGOS measurements are provided in shortly delayed time (a few days), thus they can be implemented in the EURAD-IM interim reanalysis and 'validated' reanalysis. The added value of the assimilation of the upper-air observations with regards to surface measurements will be assessed and reported.

Furthermore, the EURAD-IM system will be augmented by the 3d-var assimilation of SO2 column retrievals. Near Real time SO2 column retrievals are provided by the AURA/OMI and MetOp/GOME-2 instruments. The assimilation of these retrievals has been successfully applied in the EURAD-IM system to volcanic SO2 emissions. MOPITT CO data has been repeatedly assimilated in the EURAD-IM CAMS_50 reanalysis. MOPITT CO data will be deployed in near-real time via the NASA LANCE system. This opportunity will be used to develop and assess the assimilation MOPITT CO retrievals also in EURAD-IM.

In continuation of the developments, the ability of EURAD-IM to assimilate MODIS AOD data will be further developed, with the aim to assimilate the MODIS AOD products over land. The assimilation of the MODIS Aerosol Optical Depth Land and Ocean of MOD04_L2 retrieval was successfully applied to mineral dust episodes in 2013 and 2016.

During evaluation of EURAD-IM in 2016, a relatively weak performance of the ozone forecast became evident. Particularly in spring and autumn the EURAD-IM ozone forecast shows a large positive bias. The following plan has been devised: in order to understand and reduce this bias first hypotheses will be tested. As a preparatory action, the specific situations with most significant failures will be identified, and further used for the following analyses:

1. The sensitivity of the EURAD-IM photolysis module with respect to the stratospheric ozone column will be investigated. EURAD-IM uses a constant value that appears to be too low.

2. The cloud optical thickness appears to be too low on average. Therefore, the performance of EURAD-IM with respect to different cloud input data (IFS and different WRF cloud microphysics schemes) will be investigated.

In case of unsatisfying results and failure to identify causes, for comparison reasons only another model will be implemented and operated independently, yet with the conventions given for CAMS_50 ENSEMBLE. Critical episodes will be re-analysed by both models, differences will be evaluated and comparisons will be made to identify reasons behind the differences.

Other possible developments:

Additionally to the assimilation of MODIS AOD data, the application of sentinel-3 SLSTR AOD retrievals will be investigated.

A bias correction scheme will be further upgraded and tested, in order to lower the bias in the background before assimilation. If the scheme is able to improve the skill of analyses, it is planned to apply it on the operational EURAD-IM analysis upon the regular update.

The EURAD-IM forecast and analysis system will be prepared for the increase of horizontal resolution from 15 km to 10 km. Input fields e.g. anthropogenic emissions will be prepared with increased horizontal resolution. The impact of the resolution increase on the computing time will be investigated. It is planned to put the increase of model resolution from 15 to 10 km into effect with an operational upgrade in 2018.

Distributed Regional Production (CAMS_5030)

The objective of WP5030 is to provide to both CRPUs (METEO-FRANCE for NRT analyses and forecasts, INERIS for interim and 'validated' re-analyses), the results of the 7 operational models. As a general principle, upgrades of individual productions are carried out once a year. They require important preparation and monitoring efforts. Some extra upgrades are also necessary at a regular basis to test and take into account changes regarding input datasets (IFS, C-IFS, etc.).

The main activities of this work-package will be the operational implementation of the complete datasets for NRT analyses (except pollens) and of a set of changes tested and validated by WP5020, as well as the settings related to the best use of EIONET observations.

Two upgrades per operational model are anticipated for the year: The first one, mainly dedicated to the provision of all species (except pollens) at all levels for NRT analyses, will take place by the end of June 2017. The yearly upgrade will

take place in November. Both upgrades will be supported by the e-suite and will be documented with one Request for Change per operational model.

Description of activities of CAMS_5030

• Task 5031: Daily NRT European air quality analyses

For each of the 7 operational modelling teams, this task consists in providing NRT analyses every day to METEO-FRANCE (CRPU), for the required species and levels. METEO FRANCE will then make these analyses available to users no later than 12 UTC. The NRT data effectively assimilated each day will be reported quarterly, per model; their impact on analyses will be reported.

• Task 5032: Daily NRT European air quality forecasts

For each of the 7 operational modelling teams, this task consists in providing NRT forecasts every day to METEO-FRANCE (CRPU), for the required species and levels. METEOFRANCE will then make these forecasts available to users no later than 8UTC (0-48h) and 10 UTC (49-96h). The NRT forecasts effectively delivered each day will be reported.

• Task 5033: European air quality interim reanalyses

For each of the 7 operational modelling teams, this task consists in providing interim re-analyses on time to INERIS (CRPU), for the required species and levels.

• Task 5034: European air quality 'validated' reanalyses

For each of the 7 operational modelling teams, this task consists in providing annual re-analyses on time to INERIS (CRPU), for the required species and levels.

Because the tasks 5033 and 5034 are less time critical, the compute resources of the Research Centre Jülich will be used for the production of interim and validated re-analyses with EURAD-IM.

4. Technical description of code

The model used for the computational work is the EURAD-IM model system. This model system consists of 5 major parts: the meteorological driver WRF (version 3.5), the pre-processors EEP and PREP for preparation of anthropogenic emissions and observation data, the emission model EEM, and the chemistry transport model EURAD-IM. The data flow of the EURAD-IM system is depicted in Figure 4.1. EURAD-IM is a mesoscale- α chemistry transport model involving transport, diffusion, chemical transformation, wet and dry deposition, and sedimentation of tropospheric trace gases and aerosols. EURAD-IM allows for three-dimensional variational data assimilation (3d-var) and for optimization of chemical initial values and/or emission factors using the four-dimensional variational data assimilation (4d-var) method.

For the execution of the daily pre-operational AQ forecast and analysis, EURAD-IM is controlled by SMS software on ECMWF's compute platforms. This proved to be a stable and efficient set-up during the recent period.



Figure 4.1: Flowchart of the EURAD-IM model system consisting of the meteorological driver WRF, the pre-processors EEP and PREP, the emission model EEM, and the chemistry transport model EURAD-IM (input parameters are shaded in blue, output parameters are shaded in light yellow and procedural parts are shaded in green).

On ECMWF's compute server, WRF and the EURAD-IM are using 288 CPUs each. MPI is used for parallelisation.

5. Justification of requested computer resources

The scientific plan of this special project is fully based on the corresponding concept of CAMS_50 and the operational service envisioned thereafter, as it is detailed in the Description of Work of this project. Compute resources are requested at ECMWF, because super computer at Research Centre Jülich are using scheduling schemes, which do not grant regular time dependent launch of jobs. There, queued jobs are executed without any priority of submission schedules. Hence, provision of regular forecasts, which are dependent of predefined exact times of day, cannot be rendered.

The assessment of the computer resources rests on an exact estimate of the operational needs, based on the experiences made in previous projects. All computations outside the diurnal assimilation and forecasting schedule (except final pre-operational tests) are separated and performed on RIUUK's and Research Centre Jülich's facilities.

The computer resources requested are mainly due to the following tasks:

5.1 Air quality forecasts

The operational air quality forecast for Europe has been set up using the EURAD-IM system with 15 km resolution. A 96h forecast is regularly delivered. Computing resources needed are 1,100 SBU's per day for the meteorological driver WRF and about 4,400 SBU's per day for the chemistry transport model EURAD-IM. This results in an amount of about 2,000 kSBU's per year.

5.2 Air quality analyses

Daily 3d-var air quality analyses for Europe are provided with 15 km horizontal resolution. This task needs about 350 SBU's per day for the meteorological driver WRF and about 1500 SBU's per day for the chemistry transport model EURAD-IM, which results in an amount of about 675 kSBU's per year.

To our estimate, about 2,800 kSBU's per year are probably sufficient to fulfil the requirements of Task 5031 and Task 5032.

The CAMS_50 development plan includes an increase of the horizontal resolution of the EURAD-IM forecast and analysis to 10 km. We expect that this resolution increase will take place mid of 2018 and that about 50% more computing time will be needed to fulfil this requirement.

References

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