REQUEST FOR A SPECIAL PROJECT 2012–2014

MEMBER STATE: Germany

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Project Title: Monitoring Atmospheric Climate and Composition – Interim Implementation (MACC-II)

If this is a continuation of an existing project, please state the computer project account assigned previously.	**SP** _____	
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 ☒

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)	2,250,000	2,250,000	2,250,00
Data storage capacity (total archive volume) (gigabytes)	14,600	14,600	14,600

*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): 29.4.2011

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.

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Extended abstract

Preliminary remark:

This special project is exclusively devoted to develop and operate the applicant's EURopean Air pollution Disperion - Inverse Model (EURAD-IM) as element of the regional ensemble air quality models in MACC-II. 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. However, during MACC-II a backup system will be installed at Research Centre Jülich for achieving utmost operational stability.

Motivation:

MACC-II (Monitoring Atmospheric Composition and Climate – Interim Implementation) is proposed as an interim stage in the development of the GMES Atmosphere Service. Its overall institutional objective is to function as the bridge between the developmental precursor project MACC and the Atmosphere Service envisaged to form part of GMES Operations for 2014-2020. MACC-II will provide continuity and refinement of the atmospheric services provided by MACC. In addition, MACC-II will respond promptly when needed to supply specific products related to major events involving atmospheric constituents such as volcanic ash and pollutants from major fires, especially in cases of particular importance to the area of the European Union.

The scientific plan of this special project is fully based on the corresponding concept of MACC II, as it is detailed below for the individual work elements, and the Description of Work in more comprehensive terms. The justification of the computer resources is a conservative estimate of the operational needs, based on the experiences made in GEMS and MACC-II. As mentioned above, all computations outside the diurnal assimilation and forecasting schedule (except final preoperational tests) are separated and performed on RIUUK's and Research Centre Jülich's facilities.

The assemblage of code consists as EURAD-IM numerical kernel, on an operator split solver of the reaction-advection-diffusion equation and its adjoint. This is linked with WRF as meteorological driver.

The Rhenish Institute for Environmental Research is leader of subproject EDA (*Data assimilation for European air quality*) and takes an active part in subprojects ENS (*Ensemble air quality forecasts for Europe*), EVA (*Validated Assessments of air quality for Europe*), and GRG (*Global reactive gases*) of MACC-II.

1. Data Assimilation for European Air Quality (EDA)

Building on developments of R-EDA in MACC, EDA's principal objective is to assure increasing and skilful use of new trace gas and aerosol measurements or retrievals, within a scenario of changing earth observation data compositions, retrieval versions and model configurations. These developments will be provided for prototype operational use in MACC-II sub-projects ENS and EVA.

While in MACC R-EDA activities laid the foundations for prototype operational chemical data assimilation procedures, with primary focus on *in situ* data, this proposal aims to (i) improve the regional DA system with respect to an extended or partly novel set of remote sensing data and *in situ* observations, (ii) generalize and refine the core data assimilation capacities of individual air-quality models in terms of operational stability, accuracy, and reliability, (iii) validate the assimilation system with refined methods and algorithms, and (iv) provide for validity of the data assimilation in case of extraordinary geophysical or atmospheric events.

The organization of work follows the four identified objectives, and is detailed below.

EDA 1 Satellite data assimilation

Establishment of an extended suite of data to be assimilated from **space-borne** sensors:

- IASI data assimilation module for ozone
- MODIS, MSG/SEVIRI AOD data assimilation module

In addition, further ingestion of *in situ* data is planned. These are collected by EEA EIONET, comprising constituents under EU directive rule, including particulate matters in the limits of PM10 and PM2.5 and IAGOS-ERI aircraft data, which provide profiles over some major European cities.

EDA2 Assimilation algorithm extension
This work package introduces a couple of improvements of the assimilation algorithm, which will substantially extend its applicability, while improving robustness, and stability. The work is made in the frame of "Making minor improvements to existing production systems to maintain performance".

EDA.2.1 Aerosol data assimilation
The special problem in aerosol data assimilation is that the information is available as integrated particulate matter, PM_{10} in most cases, or as AOD. On the other hand, air quality models typically have a very detailed multi-component aerosol chemistry and dynamics module. The aerosol data assimilation is either introduced or refined to address the following issues:

- The observation-minus-model differences in AOD will be adjusted not simply by a suitable factor applied to all components. Rather, the adjustment is introduced according to the height dependent forecast error variances. Further

- A regularization of the aerosol components is introduced by a constraining function to assure realistic portions of aerosol components.

EDA.2.2 Bias correction scheme
The bias correction scheme will account for typical time-dependent model biases as found by EVA and ENS evaluation.

EDA.2.3 Dynamic covariance evolution
This work task focuses on the optimal exploitation of background/forecast information from ensemble runs and the related formulation as covariance. The forecast/background error covariance matrix will be made flow dependent. This is done either by application of the "NMC"-method or by exploitation of the ENS model ensemble.

EDA.2.4 4d-var emission inversion
The emission data inversion procedure based on the 4d-var will be applied to identify emission correction factors. Emission factors to be improved comprise observed species in the first place, but also not observed, yet influenced by chemical coupling. The continued inversion of the model with respect to emissions should provide emission factors, which are able to improve forecast quality even in a free model run.

EDA.3 A posteriori validation
This work package uses the state-of-the-art approaches of *a posteriori* validation of data assimilation algorithms. While testing of developments for individual components of other work tasks are part of the related work packages, the overall validation of the data assimilation algorithms is performed in this work package.

EDA.3.1 χ^2-validation regionally and seasonally resolved
Models perform with different skill levels in regions with different emission impact, seasons or weather conditions. Likewise, the observation representativity may vary. The χ^2 testing activities will ensure a proper balance between the observation and forecast error covariance matrices, based on pertinent related performance statistics of models and observations.

EDA3.2 Case study analyses with non-NRT data
Two test episode types, a standard case and special event cases (biomass burning, mineral dust, volcanic emissions) will be selected and analyzed with the prototype operational data assimilation algorithm. However, an expanded data set, the observations of which are not available in NRT, will be taken for a more comprehensive control. These data comprise scientific *in situ* data of opportunity, as made available by partners from most probably national or other third-party sources, and additional remote sensing data. These include EARLINET lidar, CALIPSO, IAGOS-ERI (as long as not available in NRT) and TES.

EDA.4 Mineral dust, volcano and fire data assimilation
This work package comprises the development of measures to address data assimilation modifications for special transient atmospheric conditions. These include biomass burning, mineral dust events, and, based on recent experience in Europe due to the Eyjafjallajökull eruption, volcanic emissions.

2. Ensemble Air-Quality Forecasts for Europe (ENS)

ENS primarily focuses on the delivery and verification of the prototype operational European-scale regional NRT air-quality services. In direct continuation from MACC, this service is based upon an ensemble of forecasts performed at seven centers in Europe, including RIUUK. The individual forecasts will use ECMWF operational meteorological forecast data, the regional air quality assimilation systems developed and tested within EDA, as well as the chemical boundary conditions provided by GDA. Every day, forecasts for each hour out to 96h ahead and analyses for the day before of key atmospheric pollutants in the form of maps and numerical data will be produced.

The main work packages in which RIUUK plays an active role are detailed below.

ENS.2 Model development including extension to CO_2 modeling

ENS.2 is devoted to the continuous development of models and regular update of the description of each individual suite. Regular model enhancements (resolution, area covered, parameterizations, emissions updates, use of boundary conditions, etc.) are key to steady progress of service quality.
A new development on regional CO_2 modeling will be initiated within MACC-II. The objective is to build up regional-scale greenhouse gas services, such as CO_2 flux inversion. In MACC-II effort and ambitions will be limited to direct CO_2 modeling (but including both anthropogenic and biogenic surface fluxes), regional-model intercomparisons and confrontation with the global models from MACC-II sub-project GHG.

ENS.3 Air-quality forecasts

This task corresponds to the prototype operational provision of forecasts for key air-quality compounds with the seven individual model suites, which are developed and constantly updated within ENS.1. Forecasts, up to 96h (an extra 24h forecast compared to the situation in MACC is necessary to accommodate users' needs that require to have 72h of forecasts just after 00 UTC daily, in practice too early for the new daily forecast to be available) will be provided for a range of molecules and vertical levels in GRIB2 and netCDF format. Core product are forecasts of O_3, NO, NO_2, SO_2, $PM_{2.5}$, PM_{10}, CO at the surface level and at 500, 1000, and 3000 m height. These core products will be verified at the surface on a daily NRT basis.

ENS.4 Pollen forecasts

Primary biogenic particulate matter (pollen grains, enzymes and other genetic material released by plants, spores, etc.) contributes significantly to primary particulate matter mass and affect its size distribution. Due to their seasonal character, they affect also the temporal variation of primary PM in the atmosphere. The introduction of primary biogenic PM as intrinsic component of particulate matter in Europe is expected to improve significantly the forecast of PM in the region.

ENS.5 Air-quality analyses

This task corresponds to the prototype operational provision of analyses for key air-quality compounds (O_3, NO, NO_2, SO_2, $PM_{2.5}$, PM_{10}, CO) with the seven assimilation suites (developed within EDA), including EURAD-IM. Hourly analyses for the previous day will be delivered daily. At first, this will be done once per day in the early morning with a reduced set of observations to provide improved initial values for the subsequent forecast. A second analysis for the previous day will be set up in the early afternoon, which includes as many as possible observations from all available NRT instruments.

ENS.8 Transition to operations

ENS.8 is a new component compared to MACC: it is aimed at specifically organizing the transition from prototype operational to fully operational services, which requires end-to-end analysis for the seven individual production lines and for central processing of the NRT regional core services for the atmosphere.
The first year of MACC-II will be devoted to the analysis of the existing procedures set up by the different regional partners: the 8 production chains (7 individual models, central processing and ENS platform) will be described in full detail, assessing the level of operationality of each step and the corresponding risks for failure. In particular, these activities will establish operationalization plans, compatible with the timing and resources of MACC-II.
The rest of the project will be devoted to the implementation of these operationalization plans, with the objective of being ready for full operational status at the end of MACC-II. During the last year, a task will study the opportunity of a certification (ISO9001) of the regional services, and document the steps and effort needed at each of the partners.

3. Validated Assessments of Air Quality for Europe (EVA)

In MACC-II, the objectives of the EVA sub-project are the development and implementation of an operational process dedicated to the yearly production of European air quality assessment reports. These reports will be based on the MACC-II assimilation and modeling capacities, and will provide the state and evolution of background concentrations of air pollutants in Europe, according to a number of indicators relevant for policy use (regulatory indicators) and impact assessment (health and ecosystems exposure oriented).

Seven regional state-of-the-art compliant air quality models, including EURAD-IM, that run within the MACC-II prototype operational process and are proving their capacities and operationality, are involved in the service production. Each modeling team is responsible for upgrading model capacity and for the quality of the results this provides.
An increasing amount of available observation data is expected up to 2015, especially through the GMES *in situ* and satellite data coordination. The wealth of data currently available and expected in the near future should be considered in the operational products as they go along. Moreover, the continuous improvement of models and data-assimilation techniques (including ensemble approaches) will be taken into account for an overall improvement of the EVA products. Work to be done by each involved modeling team includes

- Assimilating new types of observational data in their reanalysis chain.
- Producing individual model re-analyses for the years 2010 to 2013.
- Evaluating model performance.

4. Justification of Computer Resources and Technical Description of Code

The system for the computational work to be done in the work packages of MACC-II is the EURAD-IM model system. The EURAD-IM model system consists of 5 major parts: the meteorological driver MM5 (version 3), the pre-processors EPC and PREP for preparation of meteorological fields and observation data, the EURAD-IMEmission Model EEM and the chemistry transport model EURAD-IM. The data flow of the EURAD-IMsystem is depicted in figure 1. The 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.

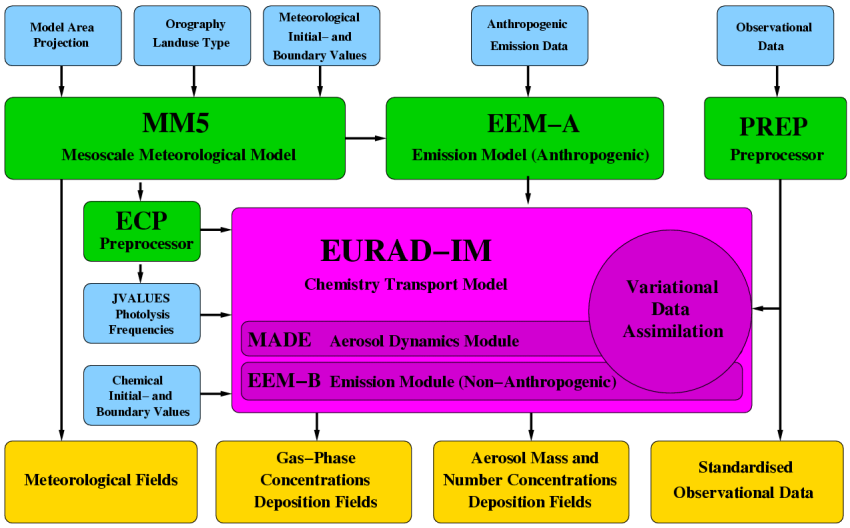

Figure 1: Flowchart of the EURAD model system containing the meteorological driver MM5, the pre-processors ECP and PREP, the emission model EEM and the chemistry transport model EURAD-IM (input parameters are shaded in blue, output parameters are shaded in yellow and procedural parts are shaded in green or magenta).

On ECMWF's compute server c1a, the EURAD-IM uses 121 CPU's with are parallelised with MPI. MM5 is currently parallelised with the OMP interface using 64 CPU's. Later on a changeover to the Weather Research & Forecasting Model (WRF) is planned. WRF will be parallelized using MPI.

The Supervisor Monitor Scheduler (SMS) is used to control the pre-operational air quality forecast as well as the analysis of the air quality of the previous day.

Computer resources requested are mainly due to the following work packages:

EDA.2.4 4d-var emission inversion

The EURAD-IM forecasting system will be used to study the capabilities of the 4d-var emission inversion to improve the quality of air quality forecasts. Computing resources needed for this purpose are hardly determined at current stage

of the project but because of the very high demand of computing time for 4d-var applications, a yearly requirement of about 500 kSBU's per year is expected.

ENS.3 Air quality forecasts

The pre-operational air quality forecast for Europe, based upon the 12:00 IFS operational meteorological forecast, has been set up using the continental-to-local scale chemical data assimilation system EURAD-IM with 15 km resolution. A 96h forecast of O_3, NO, NO_2, CO, SO_2, $PM_{2.5}$, and PM_{10} is regularly delivered. Chemical initial and boundary values are provided by the pre-operational 3d-var analysis for the previous day and MACC-II sub-project GDA, respectively. Computing resources needed are 860 SBU's per day for the meteorological driver MM5 and about 2300 SBU's per day for the chemistry transport model EURAD-IM. This results in an amount of about 1,200 kSBU's per year.

ENS.5 Air quality analyses

Using the system developed and tested within sub-project EDA, daily pre-operational 3d-var air quality analyses based upon the 00:00 IFS operational forecast are provided for Europe with 15 km resolution. For this purpose near real time surface in-situ measurements of O_3, NO_2, NO, SO_2, CO, and PM_{10} as well as satellite derived NO_2 column retrievals from OMI, GOME-2, and SCIAMACHY are hourly assimilated using the intermittent 3d-var method. This task needs about 210 SBU's per day for the meteorological driver MM5 and about 1,300 SBU's per day for the chemistry transport model EURAD-IM, which results in an amount of about 550 kSBU's per year.