REQUEST FOR A SPECIAL PROJECT 2015–2017

MEMBER STATE: Germany

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Project Title: Monitoring Atmospheric Composition and Climate - Phase 3 (MACC-III)

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.)	2015	
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.)	**2015**	**2016**	**2017**
High Performance Computing Facility (units)	2,420,000	2,600,000	2,800,000
Data storage capacity (total archive volume) (gigabytes)	3,300	4,300	4,500

*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): .....

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: Hendrik Elbern

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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 member of the ensemble of regional air quality models in MACC-III and the Atmosphere Service envisaged to form part of Copernicus Operations later on. 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 overall objective of MACC-III (Monitoring Atmospheric Composition and Climate – Phase 3) is to function as the bridge between the on-going project MACC-II and the Atmosphere Service envisaged to form part of Copernicus Operations and expected to start in 2015. MACC-III will sustain the current pre-operational atmosphere activities until March 2015 in order to avoid any interruption in the critical handover phase between the pre-operational and fully operational service. Thus, at least in 2016 and 2017 this special project will be devoted to the fully operational Copernicus Atmosphere Service.

So far the scientific plan of this special project is fully based on the corresponding concept of MACC-III, 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 MACC-II.

The Rhenish Institute for Environmental Research at the University of Cologne (RIUUK) is leading subproject EDA (*Data assimilation for European air quality*) and takes an active part in sub-projects ENS (*Ensemble air quality forecasts for Europe*), EVA (*Validated Assessments of air quality for Europe*), and GRG (*Global reactive gases*) of MACC-III. Each of these sub-projects will entail a matching set of activities undertaken by partners responsible for seven nationally-developed regional air-quality models and associated data assimilation systems that combine to form a multi-model ensemble forecasting system. These common activities will be supported and extended by specific additional activities carried out by individual partners.

The seven models in the ensemble will use a common forecasting protocol (i.e. common start-times, common domain, common boundary conditions from the global system, common archiving, common display and common verification), so that the ensemble can sample the uncertainties arising from model formulation. In addition MACC-III will continue to undertake systematic assessments where the seven participating models will use validated data to provide reanalyses of atmospheric pollutant fields; this requires systematic re-runs several months after measurements are taken. This concerted effort represents a major step forward in validated assessments for air quality, combining sophisticated data assimilation techniques and the ensemble approach to provide the most realistic representation of air-pollution fields.

Of the three sub-projects, EDA undertakes essential development of data assimilation, including for the improved estimation of emissions.

ENS will focus primarily on the delivery and verification of the prototype operational European-scale regional NRT air-quality services. The individual forecasts will use ECMWF operational meteorological forecast data, the regional air quality assimilation systems developed and tested within EDA, and the chemical and aerosol boundary conditions provided by MACC-III sub-project GDA (*Global data assimilation*). The data assimilation and forecast systems will also be used for building up the *a posteriori* validated assessment services provided by EVA.

The EVA sub-project has the objective of further developing and implementing an operational process dedicated to the yearly production of European air quality assessment reports. These reports will be based on utilising MACC-III's assimilation and modelling capacities. They will describe the state and the 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). Validated observation and modelling data will be combined in reanalysis maps and numerical fields, to provide optimal estimates of air pollutant concentration fields for a given spatial resolution.

1. Data Assimilation for European Air Quality (EDA)

As its general objective the sub-project "Data assimilation for European air quality" (EDA) aims to ensure an optimal exploitation of information contents from all available in situ or space born observations. Within MACC-III EDA's products are primarily tailored to serve the objectives of subprojects ENS and EVA. This proposal for EDA in MACC-III seeks to extend the suite of data from sensors, which were not considered so far for assimilation by RIUUK.

Building on previous work in MACC-II, EDA's permanent 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 use in MACC-III subprojects ENS and EVA.

The scope of MACC-III applications includes (1) data assimilation improving daily forecasts, which highest demand in Near Real Time delivery characteristics, (2) slightly delayed analyses, producing hourly sequences as monitoring measure, and (3) assimilation products with non-operational data for science mode, where the two former are part of the operational service portfolio.

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) generalise 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.

EDA 1 Satellite data assimilation

The work package "Satellite data assimilation" for the troposphere will be prepared for prototype operational and case study use in data assimilation, with emphasis on efficient data processing, applying most recent error estimates from retrievals, and balancing with in-situ data. RIUUK will focus on IASI CO making use of the EUMETSAT CO retrievals of Klonecki et al. (2012). Furthermore AOD from MODIS will be integrated in the data stream and used to update particulate matter values. The related adjoint AOD observation operator will be developed and integrated in the DA algorithm.

EDA 2 Aerosol data assimilation

In aerosol data assimilation, typically, the information is available as integrated parameter, such as particulate matter with integration over size and types PM10 in most cases, or as AOD with extinction along the radiative path. On the other hand, air quality models typically have a very detailed multi-component aerosol chemistry and dynamics module. These facts render the aerosol data assimilation as markedly ill-posed. Therefore a regularisation of the aerosol components will be introduced by a constraining function to assure realistic portions of aerosol components.

EDA 3 Bias correction scheme

As part of a permanent commitment to performance feedback, the bias correction scheme will account for typical time dependent model biases as found by EVA and ENS evaluation. Any model modification or new insight due to extended analysis records or assimilation of novel data types will engender a new evaluation for bias correction. This process will continue to be formalised.

EDA 4 4D-var CO_2 emission inversion

An emission source data inversion procedure based on 4D-var will be applied to identify emission correction factors, for RIUUK following the method outlined in Elbern et al. (2007), but using the MACC grid configuration. While so far reactive emitted species are considered, the task will now be extended to regional CO_2 source and sink optimisation.

EDA 5 A posteriori validation

In this work package the overall validation of the data assimilation algorithm is performed. The two test episodes selected in MACC-II will be further extended to analyse the performance of the assimilation systems. The expanded data set, now to comprise the period from 7. July to 5. August 2010, and 15. January to 18. February 2012. Observations, 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 3rd party sources, and additional remote sensing data. These include ceilometer data and MAXDOAS data, IAGOS-ERI and radio sonde data.

EDA 6 Mineral dust, volcano, and fire data assimilation

Aim of this task is the evaluation of developments achieved in MACC-II. Since our assimilation algorithm uses a BLUE, a "compromise" between an a priori from the forecast and measurements is analysed. However, with observational evidence from unpredicted events like mineral dust outbreaks, volcanic emissions and wild fires, a priori data are to be considered fairly unskilled, to avoid a degraded assimilation result, biased toward the "no-event" case. Addressing this problem, 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 experiences in Europe through the Eyjafjöll and Grimsvötn eruption, volcanic emissions.

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

The ENS sub-project is one of the sub-projects dedicated to regional air-quality services for Europe. ENS primarily focuses on the delivery and verification of the operational European-scale regional NRT air-quality services. Since the end of MACC-II, this service follows operational procedures except that it is not monitored 7/7day 24/24h because full monitoring is not funded at this stage. Thus the word 'operational' should be understood in this subproject as such. In direct continuation from MACC and MACC-II, this service is based upon an ensemble of forecasts performed at seven centres in Europe, recognised for their continuing experience in providing routine operational forecasts at the scale of Europe for several years.

Every day, forecasts for each hour out to 96h ahead and analyses for the day before will be produced by the seven designated centres. The results will be processed centrally for computing ensemble and verification and will be displayed on the regional NRT products MACC-III web platform.

The transition to operations of the ENS production chains (in demonstration mode) was achieved at the end of MACC-II. In each of the regional production centres and at the central production center, improvements/upgrades to the first operationalisation setup will be done in MACC-III. The feasibility of an operational service certification (ISO 9001) studied in MACC-II will be further assessed.

ENS 1 Model development including extension to CO_2 modeling

ENS 1 is devoted to the continuous development of models and regular update of the description of each individual suite. Regular model enhancements (resolution, parameterizations, emissions updates, use of boundary conditions, etc.) are indeed key to steady progress of service quality. It includes also a research component on Air Quality forecasting (process-oriented studies, developing and testing new ensemble methodologies…) and new developments on regional carbon dioxide modelling, in view of potential future high-resolution surface CO_2 fluxes inversion products over Europe. Due to the high variability in space and time of CO_2 fluxes over Europe, it is *a priori* interesting to investigate potential new regional services, complementing the ones provided for the global scale by GHG. Also, many users of ENS services, as national environment agencies, face increasingly the need to consider pollutants and greenhouse gas jointly (for instance to see combined effects of emission-abatement strategies), which further substantiate the interest of such an activity. In MACC-III effort and ambitions will be limited to direct CO_2 modelling (but including both anthropogenic and biogenic surface fluxes), regional-model intercomparisons and confrontation with the global models from GHG. The added value of a regional modelling CO_2 activity and expected benefits of developing new corresponding services beyond MACC-III (ENS but also and maybe primarily EVA) will be assessed. Additionally, preliminary RTD activities on CO_2 flux inversion over Europe will be done in EDA by only a limited number of regional models.

Such supporting research and development activities are vital for maintaining Copernicus atmosphere regional products at the highest international standards.

ENS 2 Air-quality forecasts

This task corresponds to the prototype operational provision of forecasts for key air-quality compounds with the seven individual model suites, including EURAD-IM. Forecasts, up to 96h will be provided for a range of molecules and vertical levels in GRIB2 and netCDF format. Core products (forecasts of O_3, NO_2, SO_2, CO, $PM_{2.5}$, PM_{10}), and additional products (forecasts of NO, PANs, total NMVOCs, NH_3) will be provided as part of the operational service at the surface and at 50, 250, 500, 1000, 2000, 3000, and 5000 m height. The core products will be regularly verified at the surface. The list of additional species implemented in test mode in MACC-II, will be assessed by interaction with key users to confirm usefulness.

ENS 3 Pollen forecasts

Biogenic particulate matter (pollen grains, enzymes and other material released by plants, spores, etc.) contribute significantly to primary particulate matter mass, affect its size distribution, and interact with other pollutants. Due to their seasonal character, they affect also the temporal variation of primary PM in the atmosphere. The introduction of bio-aerosols as intrinsic components of particulate matter in Europe is expected to improve significantly the forecast of PM in the region. Also, it is recognised that it is necessary to consider exposure to both pollutants and bio-aerosols in health impact studies.

Traditionally, pollen forecasts have been based solely on local observations and do not consider transport of pollens from other regions, while measurements have shown evidences of transport of some bio-aerosols over thousands of kilometres. Within MACC and MACC-II a modelling component of primary biogenic aerosol particles (PBAP) has been developed first for Birch pollen. Further developments have been carried out focusing on three new species affecting importantly health in Europe: grass, olive and ambrosia.

Within the MACC-III timeframe and thereafter, this WP will proceed with implementation and evaluation of the PBAP source terms for grass, olive and ambrosia. Priority will be given to the operational production of birch forecasts for the 2015 season and its evaluation.

ENS 4 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 continuously developed further during MACC-III, including

EURAD-IM. Hourly analyses for the previous day will be delivered at a daily basis. The objectives of this WP are the provision of hourly analyses in quasi-near real-time for key air quality observed species as well as the assessment of the quality of unobserved species in analyses against observation and background.
Throughout MACC-III, RIUUK will continue research activity on the impact of assimilating some species on the forecast of these species and of other non-assimilated species. Joint work will allow to evaluate how robust are conclusion depending upon the assimilation technique employed and the background/forecast model used.

ENS 5 Operation upgrade

The project will be devoted to consolidate and upgrade the operational status reached at the end of MACC-II. A task will be to further investigate the opportunity and feasibility of a certification (ISO9001) of the regional service, and document the steps and effort needed. At this stage, it is believed that service certification will be of benefit to the regional service production quality, compensating for the fact that the regional services are effectively based upon a network of collaborating centres.

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

The objectives of the EVA sub-project are the development and the implementation of an operational process dedicated to the yearly production of air quality assessment reports that describe air quality in Europe.
MACC-III/EVA is the straightforward follow-up of the EVA subproject in MACC-II, with substantial improvements of the service, to facilitate future transition to operations. Experience from MACC-II and feedback from the users are taken into account to improve EVA products, not only on a scientific point of view, but also to comply with operational needs (especially policy applications).

In MACC, in-situ data available in the AIRBASE European database were mainly used for in the assessment reports, for both re-analyses and model evaluation. However in some cases, satellite information was considered for deeper investigation of some particular air pollution episodes (dust outbreaks, forest fires, etc...). For its pre-operational stage, it is necessary to consider broadened sets of observation data, including both satellite observation and in-situ data from research networks (that are supposed to monitor more physic-chemical variables than regulatory networks).
The idea is to account for some observation data that cannot be assimilated in the models in an operational way, although they have a clear interest for the yearly air quality assessment produced in delayed-mode. For the year 2013, observation data sources will be investigated that can be of interest for the assessment report. In particular field campaigns that held during this period will be carefully considered as the datasets available when critical pollution episodes arose in the target year.

MACC and MACC-II allowed covering the 2007-2012 period with validated assessment reports. They have been used by involved modelling teams to develop the re-analysis chains as well as to improve their processes (as well as the scientific quality of the model results) and to deal with operational and QA/QC requirements. Model performances are quite satisfactory, but some improvements are still needed to make operational chains more robust.

Some constrains related to the availability of validated regulatory observation data from the AIRBASE database maintained by the European Environment Agency (EEA), appeared to be an issue for the publication of the EVA reports within a period shorter than two years. MACC-III will give the opportunity to assess the feasibility of the publication of “interim reports” in a shorter time. Such assessments would be based on “non-fully validated” observation data (in the sense of the air quality directive reporting process) quickly available to be assimilated in the assessments. Several options will be considered

Comparison of air quality re-analyses based on validated data with those based on “un-validated” data will be achieved for the year 2013.

Beyond the yearly production, with the availability of a number of re-analysed years (since 2007 with MACC) further policy-related studies related to the evolution of air pollution in Europe will be proposed.

4. Technical description of code

The model used for the computational work to be done in the work packages of MACC-III 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.

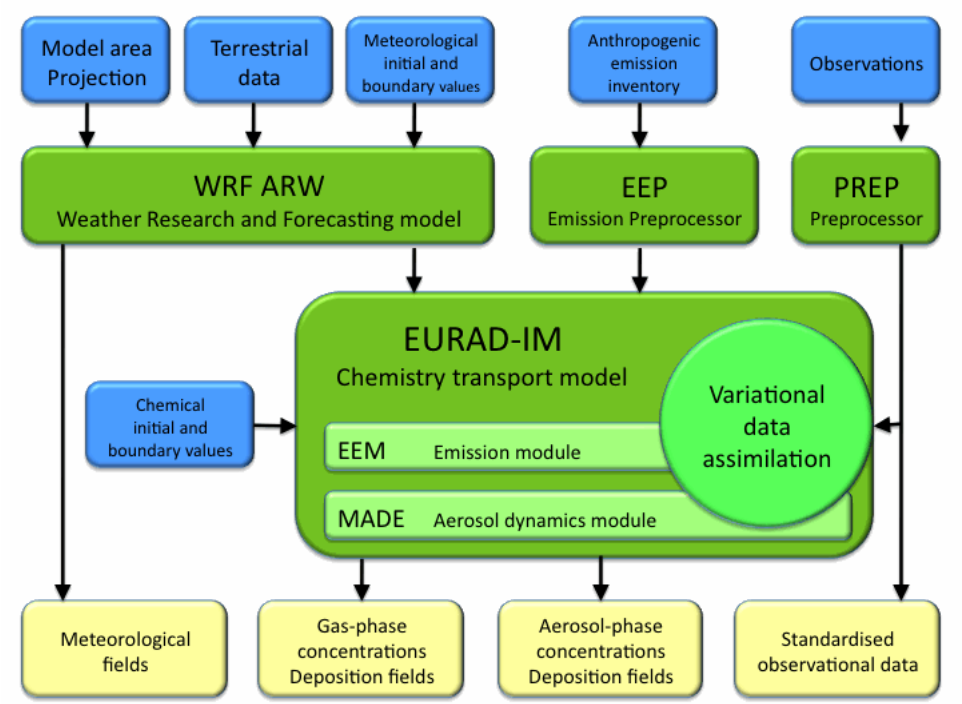

Figure 4.1: Flowchart of the EURAD-IM model system consisting of the meteorological driver WRF, the pre-processors EEP and PREP, the emission model EEM, and the chemistry transport model EURAD-IM (input parameters are shaded in blue, output parameters are shaded in light yellow and procedural parts are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

On ECMWF's compute server, WRF and the EURAD-IM are using 120 and 121 CPU's, respectively. 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 MACC-III 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 MACC-II. 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 pre-operational air quality forecast for Europe has been set up using the EURAD-IM system with 15 km resolution, and 10 km after 2015. A 96h forecast is regularly delivered. Computing resources needed are 960 SBU's per day for the meteorological driver WRF and about 4050 SBU's per day for the chemistry transport model EURAD-IM. This results in an amount of about 1,500 kSBU's per year.

5.2 Air quality analyses

Daily 3d-var air quality analyses for Europe are provided with 15 km horizontal resolution, and 10 km after 2015. This task needs about 230 SBU's per day for the meteorological driver WRF and about 1470 SBU's per day for the chemistry transport model EURAD-IM, which results in an amount of about 620 kSBU's per year.

To our estimate, about 2,100 kSBU's per year are probably sufficient to fulfil the requirements of sub-projects ENS and EVA. An overhead of about 15 % is expected to be necessary to test new developments.

References

Elbern, H.,Strunk, **A**., Schmidt and Talagrand, O., Emmision rate and chemical state estimation by 4-dimensional variational inversion, *Atmos. Chem. Phys*., **7**, 3749-3769, 2007

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