Barcelona Supercomputing Center
Centro Nacional de Supercomputación

RED ESPAÑOLA DE SUPERCOMPUTACIÓN

AECT-2017-1-0008 Photochemical modelling to attribute emission sources and source regions to high particulate matter concentration in urban areas in Spain

1. General Information

Activity Id
AECT-2017-1-0008

a) Activity Title
Photochemical modelling to attribute emission sources and source regions to high particulate matter concentration in urban areas in Spain

b) Area
Astronomy, Space and Earth Sciences

2. Research Project Description

a) Is this a Test Activity?
No

b) Is this a Long Term Activity that will extend over several application periods?
Yes

c) Brief description of the Project
This activity takes place in the framework of several national and international projects (all ongoing or funded): PAISA, funded by the Ministry of Economy and Competitiveness (MINECO), the AXA Chair on Sand and Dust Storms, funded by the AXA Research Fund; the Forum for Air quality Modelling (FAIRMODE), which is an international initiative in which

the applicant is deeply involved.
The PAISA project ("Photochemical modelling to attribute emission sources and source regions to high particulate matter concentration in urban areas in Spain", Jan. 2017 - Dec. 2019: lead by M.T. Pay) aims to providing an integrated framework to diagnose the origin of air pollution with high spatial and temporal resolution over Spanish urban areas. The results will allow discriminating the contribution from regions (urban, regional, national, long-range), sources (natural or anthropogenic) and even further from fuel type (e.i., diesel and gasoline) for on-road traffic and residential combustion activity sectors which are the main sources of PM10 and NOx in urban areas. The outcomes of PAISA will determine to what extent the urban PM concentrations in Spain are controlled by specific anthropogenic sources and/or regional or transboundary contributions, allowing better information to policymakers in the application of the Air Quality Directive. We, therefore, expect the results obtained to be of high impact and to be of interest to scientific communities concerned with air pollution management, as well as critical input to support the Clean Air Policy Package for Europe. PAISA will include the state-of-the-art in emission, meteorological and air quality modelling based on the CALIOPE air quality system for Spain (?CALIdad del aire Operacional Para España?, www.bsc.es/caliope) developed at the Earth Sciences Department of the Barcelona Supercomputing Center (ES-BSC) to forecast air pollution (O3, NO2, SO2, PM10 and PM2.5) over Europe and Spain.
The AXA Chair on Sand and Dust Storms (2015-2025, lead by C. Pérez-García Pando) program will enable new knowledge, cutting-edge technology and capabilities to understand better and predict sand and dust storms and their effects, and manage their impacts upon society and economy. This research will allow a better quantification of the effects of dust upon climate, the development skilful model predictions, and the implementation of risk assessment and mitigation strategies in key sectors, including health, energy production, agriculture and transportation. The air quality modelling systems developed at ES-BSC will strongly benefit of the research conducted in the AXA Chair.
Finally, the FAIRMODE aim is to bring together air quality modellers and users to promote and support the harmonised use of models by the EU Member States, with emphasis on the model application under the European Air Quality Directives. The applicant M.T. Pay is the member of the Forum in which source apportionment stands a priority for decision making. PAISA's outcomes will contribute to the FAIRMODE initiatives on the assessment, best practices, and technology transfer in the use of source apportionment techniques to apply the Air Quality Directive.
The present project aims at covering the common desire of the all the aforementioned projects which is to integrate the state-of-the-art physical and chemical processes in an air quality modelling system to support the air pollution management and decision making, advocating the Clean Air Policy Package for Europe, that largely rests on the use of high-performance computing. The first phase of the project is to quantify the robustness of CALIOPE. The second phase of the project will be devoted to quantifying the

contribution from regions, sources and even further from fuel type (e.i., diesel and gasoline) to air pollution in Spain. The results of this project will improve the air quality management efforts in the design of emission abatements and guide researchers on future model developments to optimise resources, and reduce uncertainty and response time. This will be possible thanks to the combination of a profound knowledge of atmospheric chemistry, a compilation of air pollutant observation, an air quality model instrumented with unique air quality response tools, and the use of cutting-edge computational resources.
Source apportionment studies is a highly challenging objective that only a few centres in the world can afford to tackle. The BSC is one of them, thanks to the expertise in developing emission modelling and the unique alchemy of technical and scientific knowledge on the development of air quality models, and the efficient use of the major computational resources available. Considering source attribution to urban air pollution as an urgent need to improve the quality of the air we breathe in Spain: it is necessary to keep the air quality management and Spain in the forefront of air quality research for the next years.

d) Grant References

CGL2016-75725-R CGL2013-46735-R Axa Chair on Sand and Dust Storms

e) Brief description of the Project (if this Activity takes place in the context of a Technology or Industrial Project)

Not applicable

f) Specific Activity proposed

The impact of urban air pollution is a significant factor in human health worldwide. The PAISA project aims to diagnose the origin of air pollution in Spanish urban areas using source apportionment techniques. PAISA will discriminate the contribution from regions (urban, regional, national, long-range), sources (natural or anthropogenic) and even further from fuel type (e.i., diesel and gasoline) for on-road traffic and residential combustion activity sectors which are the main sources of PM10 and NOx in urban areas.
PAISA will base on the CALIOPE system which has been widely evaluated against observations, used to assess air pollution effects on health, and as a support material to Spanish TV news during air pollution episodes over Europe and Spain. CALIOPE consists of a set of models: the Weather Research Forecast (WRF) meteorological model; the High-Elective Resolution Modeling Emissions System (HERMES) emission model, the BSC-DREAM8b natural dust model, and the Community Multiscale Air Quality Model (CMAQ). At urban scale, the results obtained using CALIOPE have demonstrated that high-resolution (1-4 km) and precise description of emissions are key points to simulate air quality levels over urban/suburban areas affected by traffic or industrial emissions. In this

sense, the HERMES model developed by the ES-BSC is a key and unique asset of the CALIOPE system. Furthermore, several scientific projects (e.g. CGL2008-02818/CLI, CGL2013-46735-R, coordinated by O. Jorba, and the AXA Chair on Sand and Dust Storms, lead by C. Pérez) are improving CALIOPE through the integration of an in-house chemical transport model, named NMMB/BSC-CTM, in the current operational system. The NMMB/BSC Chemical Transport Model is a chemical weather prediction system which includes the atmospheric chemistry that allows considering air quality studies involving from global to local scale processes in just one run, making a better use of the computational resources and reducing the simulation time. Furthermore, the NMMB/BSC-CTM enables to study further mesoscale processes associated with air pollution and its interactions with meteorology. Developing the NMMB/BSC-CTM is a strategic goal of the ES-BSC because it will allow the Department to better control the scientific and technical improvement in the model and enhance the model skills as desired in the future. The NMMB/BSC-CTM is providing an operational forecast to the Barcelona Dust Forecast Center and the Sand and Dust Storm Warning Advisory and Assessment System for North Africa, Middle East and Europe Regional Centers of the World Meteorological Organization.

Many efforts have been made to improve the CALIOPE system at regional and urban scale. The introduction of desert dust aerosol from the Sahara desert and the sea salt emissions have been identified as key points[1]. CALIOPE evaluations[2,3] showed that organic and inorganic aerosols present the highest underestimations partly due to the state-of-the-science concerning the secondary formation pathways and uncertainties in ammonia emissions. Currently, several actions devoted to improving aerosol mechanism have been implemented in the new CMAQ version [4], but they have not been evaluated within the CALIOPE system so far.

Besides the recent updates in the science within CMAQ, the model has been instrumented with algorithms allowing for the estimation of source contribution in just one run, named ISAM-CMAQ[5,6]. This is an advantage, because before source apportionment was performed by a brute-force method zeroing out sources one by one, but this becomes computationally prohibitive if many emitters are of interest and they not able to take into account non-linearities in chemical processes. Although more efficient, ISAM-CMAQ still requires high computational and storage resources, as well as skilled professionals to analyse the results. PAISA will integrate ISAM within the CALIOPE system, which includes the state-of-the-art atmospheric chemistry for gas and aerosol pollutants within CMAQ.

This project will cover three successive 4-month periods: evaluation and improvement of the CALIOPE system (Period 1), quantification of the origin of high levels of PM (Period 2) and ozone (Period 3) at high spatial and temporal resolution over Spain. We document below our planned procedure for the first four months (Period 1) but also present our longer-term strategy for consistency.

Period 1. Evaluation and improvement of the CALIOPE system. It will be devoted to run the experiments that allow quantifying the uncertainty of the CALIOPE system in comparison

with the state-of-the-art air quality models (benchmark) and test necessities of improvement (sensitivity tests) to end up with an improved CALIOPE configuration for source apportionment studies. By demonstrating the potency of CALIOPE system as air quality forecast models compared with COPERNICUS European Earth Observation products will open the possibilities of the CALIOPE system to be involved in the next COPERNICUS services in future calls, a strategic objective of the Earth Sciences Department.

Task 1.1. Benchmarking for a reference year. This task will run an annual air quality simulation over Europe using the WRF-CMAQ and NMMB/BSC-CTM models within the CALIOPE system to quantify the model uncertainty and identify necessities of improvement. The relevance of these calculations to the research project is twofold. First, to assess the performance of the WRF-CMAQ against NMMB/BSC-CTM to forecast air pollution over Europe. The WRF-CMAQ has been successfully used in the CALIOPE system, meanwhile the NMMB/BSC-CTM is the new fully on-line coupled chemical weather prediction system for research applications and experimental forecasts. Second, the annual air quality simulation using WRF-CMAQ and the NMMB/BSC-CTM will provide a benchmark to compare with COPERNICUS products on air quality [7], specifically with the regional air quality analysis performed by the Atmosphere Monitoring Service[8]. The benchmark will integrate the full year 2015, which is the most recent years with a validated European inventory (e.g., EMEP, European Monitoring and Evaluation Programme), experimental campaigns (e.g., EMEP or CSIC) and validated measurements from the European Environmental Agency (EEA). The modelling domain of study will cover the whole Europe[9] with 12-km horizontal resolution. The number of grid cells of this domain is 480 x 400 with 38 to 48 vertical levels up to 50hPa. The ERA-Interim global reanalysis (with a resolution of 0.8º) of the European Center for Medium-Range Forecasts will be used for meteorological initial and boundary conditions, and COPERNICUS global products (1.1º x 1.1º) for the reactive gases and aerosols. The emissions of pollutants will be computed with the HERMES model which provides hourly emission fluxes for Europe based on the EMEP inventory.

Task 1.2 Sensitivity studies to improve the CALIOPE system. This task will run several sensitivity tests devoted to improving background concentration of PM crustal material which is a major component of PM10 and inorganic aerosols over Europe. This task will set the optimal model configuration that allows improving the necessities of improvement detected for PM modelling in Task 1.1. Tests will analyse the model performance to simulate air pollutants by means of the comparison between model and observations (e.g. intensive experimental campaign, EMEP, EEA). Previous studies have pointed out the necessity of exploring the contribution of wind-blown dust emissions from arid areas[10], the contribution of forest fires in PM and ozone[11], and the sensitivity of aerosol to ammonia emissions[12].

Task 1.3. Annual simulation with the improved air quality modelling. A full 2015 European air quality simulation will be run using an improved version of the CALIOPE system. The

annual simulation will be performed with the WRF-CMAQ because CMAQ is one of the few models including source apportionment algorithms. Future research in the NMMB/BSC-CTM will devote to enhance the model with source apportionment approaches, but it is out of the scope of the present project. This annual simulation will use the set-up described in Task 1.1 and include the identified improvements in Task 1.2. This simulation will be an essential milestone for the PAISA project to calculate high-resolution background concentrations of ozone and aerosol which are required inputs to quantify the contribution of sources at higher resolution (4 km) over Spain.
Period 2 (a detail implementation plan will be submitted if the Period 2 is granted). The second period of the project will quantify the contribution of the large variety of natural and anthropogenic sources and source regions to the PM concentrations at high resolution over Spain using highly resolution emission from the HERMES model. This activity will be crucial to determining to what extent the urban PM concentrations in Spain are controlled by specific anthropogenic sources and/or regional or transboundary contributions, allowing better information to policymakers in the application of the Air Quality Directive.
Period 3 (a detail implementation plan will be submitted if the Period 3 is granted). There is an urgent need for action plans at the national and international level to reduce ozone levels[13]. These plans should accounts for non-linearities in ozone chemistry, transboundary transport of pollutants, and climate and air quality impacts. The third period of the project will provide a unique modelling study for ozone using CALIOPE which aims at providing a quantitative estimation of the contribution of national sources to high ozone episodes in Spain for the design of future ozone reduction plans.
References: https://docs.google.com/document /d/1EikWm_iWtqh0FNSDRzGpzyKUgyzll4wyS8IFn2xM4xk/edit?usp=sharing

g) Computational algorithms and codes outline

The air quality models used in the present projects are the CMAQ-WRF system and the NMMB/BSC-CTM. The CMAQ programs are optimised for use on computers running a version of the Linux operating system. Its distribution package includes utilities and libraries for setting up the model for multiprocessor computing. The stencil exchange code library (STENEX) is a module that CMAQ uses to control the communication between processors in a multiprocessor computing environment. CMAQ uses the parallel I/O (PARIO) code library to synchronise the reading and writing of information among multiple processors. The CMAQ programs are the Meteorology-Chemistry Interface Processor, the Initial Condition Processors, the Boundary Conditions Processor, the Photolysis Rate Processor, and the CMAQ Chemical Transport Model. The CMAQ chemistry is based on the CB05 and the aerosol module includes multicomponent aerosol schemes solving dust, sea salt, black carbon, organic aerosol and secondary inorganic aerosols. The horizontal and vertical advection module is the piecewise parabolic method. The vertical diffusion is represented by the Asymmetric Convective Method. There are three options for solving

gas-phase chemical transformations: the Rosenbrock solver, the Euler Backward Iterative (EBI) solver, and the Sparse Matrix Vectorized GEAR solver.
The NMMB/BSC-CTM is a parallel MPI application designed to run on both regional and global domains. It subdivides the domain of operation into horizontal tiles and assigns them to computational units. Thus, the parallelization is addressed on a sub-domain basis approach. Its I/O strategy is designed through the set-up of dedicated writing nodes. This results in a partition between computational and I/O nodes. The NMMB/BSC-CTM is a set of programs: the Non-hydrostatic Multiscale Model on the B grid (NMMB) for meteorology and the BSC Chemical Transport Model (BSC-CTM) for pollutants. The programs are coupled with the Earth System Modeling Framework software which implies that in between the execution of each module the model performs a coupling step to exchange information. The NMMB/BSC-CTM resolves gas?aerosol?meteorology interactions using the CB05 mechanism that account for the aqueous phase. The schemes employed are the Adams-Bashforth scheme for horizontal advection, the Crank-Nicholson scheme to compute vertical advection tendencies, the forward-backward scheme for horizontally propagating fast waves, and an implicit scheme for vertically propagating sound waves. It uses the EBI solver to compute these concentrations and rates at each time step. Benchmarks using CMAQ and NMMB/BSC-CTM have been performed in MareNostrum, CURIE and Minotauro. The NMMB/BSC-CTM has scaled up to 8000 cores for a mid-resolution domain in CURIE, and it is routinely used for mineral dust forecast at Mare Nostrum using 512 cores. The CALIOPE system is regularly executed in Marenostrum using 256 cores.

3. Software and Numerical Libraries

Software components that the project team requires for the activity.

a) Applications + Libraries

HDF5, NETCDF, R, OPENMPI, WRF, NCO

b) Compilers and Development Tools

GCC, TOTALVIEW, INTEL

c) Utilities + Parallel Debuggers and Performance Analysis Tools

CMAKE, PERL, PYTHON, GNUPLOT, IMAGEMAGICK, NCVIEW, NCL, AUTOCONF, PARAVER

d) Other requested software

CMAQ, NMMB/BSC-CTM, HERMES

e) Proprietary software

not applicable

4. Research Team Description

a) Personal Data

Name of Team Leader	Maria Teresa Pay Pérez
Institution	Barcelona Supercomputing Center
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Phone	+34 93 41 34038
Nationality	Spain

b) The employment contract of the activity leader with the research organisation is valid at least 3 months after the end of the allocation period.

Yes

c) Curriculum Vitae of the Team Leader

Dr. Maria Teresa was born in Murcia, Spain, April 20th, 1982. She got her B.S. in Chemical Engineering (University of Murcia, Jun 2006) and PhD in Environmental Engineering with the Degree of European Doctor and the Special Doctoral Award (Technical University of Catalonia, Nov 2011). During her PhD, She developed profound skills on air quality chemistry and modelling atmospheric processes at regional and urban scale. Her work contributed to implement an air quality forecast system at high spatial and temporal resolution over Spain, the CALIOPE system. From 2013 to 2015 she worked as a postdoc researcher at École Polytechnique in the ?Laboratoire de Météorologie Dynamique? in Palaisaeu (France) where she got experience in the use of different chemical transport model and the association of synoptic circulation patterns to air quality dynamics over Spain. Being a visiting Scientist at U.S. EPA, she got experience in the use of the source apportionment techniques (ISAM-CMAQ). Now, she is a researcher at the Earth Sciences Department at the Barcelona Supercomputing Center and where she coordinates the air quality activities on the evaluation of air quality models for their improvements and to perform environmental impact assessment to support policies. She is a scientific expert on the Forum for Air Quality Modelling (FAIRMODE) and in the Task Force on Measurement and Modelling (TFMM) under the EMEP and the United Nations - Economic Commission for Europe (UNECE). She was a Marie Curie fellow under the Beatriu de Pinós competitive programme (BP-DGR 2011, 2013-2016). She has participated in 8 national and

2 European research projects. She has led two projects with Spanish Regional Governments on the design of air quality networks (Generalitat de Catalunya and Gobierno de Canarias). Currently, she is PI on a MINECO project (PAISA, CGL2016-75725-R). She has co-authored 3 chapters in books, two technical reports, and 21 papers in international scientific journals (17 publications within the Q1, an 8 h-index and 244 citations). She has supervised one PhD Thesis (Technical University of Catalonia), and she is an assistant professor at the University of Barcelona (Department of Statistics, Faculty of Biology). She co-authored over 60 communications to International conferences. She has acted as a reviewer of several international journals and as a jury member two PhD defences.

d) Names of other researchers involved in this activity

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Laura Cifuentes Fontanals | Barcelona Supercomputing Center | laura.cifuentes@bsc.es

e) Relevant publications

Pay, M.T., Martínez, F., Guevara, M., Baldasano, J.M., 2014. Air quality forecasts at kilometer scale grid over Spanish complex terrains. Geosci. Model Dev., 7, 1979?1999. 3363-3392. doi: 10.5194/acp-12-3363-2012. Impact Factor (2010 JCR Science Edition): 5.309/Quartil: Q1/Area: Meteorology and Atmospheric Sciences.

Guevara, M., Pay, M.T., Martínez, F., Soret, A., Denier van der Gon, H.A.C., Baldasano, J.M., 2014. Inter-comparison between HERMESv2.0 and TNO-MACC-II emission data using the CALIOPE air quality system (Spain). Atmos. Environ., 98, 134-145

Valverde, V., M.T. Pay and J.M. Baldasano, 2016. Ozone attributed to Madrid and Barcelona on-road transport emissions: characterization of plume dynamics over the Iberian Peninsula. Scienc. Tot. Environ, 543, 670-682

Badia, A., O. Jorba, A. Voulgarakis, D. Dabdub, C. Pérez García-Pando, A. Hilboll, M. Gonçalves, Z. Janjic, 2016. Gas-phase chemistry in the online multiscale NMMB/BSC Chemical Transport Model: Description and evaluation at global scale. Geosci. Model Dev., 7, 1979-1999

Badia, A. and Jorba, O., 2015. Gas-phase chemistry in the online multiscale NMMB/BSC Chemical Transport Model: Description and evaluation at global scale, Geosci. Model Dev. Discuss., doi:10.5194/gmd-2016-141, in review, 2016.

5. Resources

a) Estimated resources required for the Activity for the current Application Period

Requested machine	Finis Terrae II ((BULL with 7712 cores Intel Haswell 2680v3, Infiniband Fat-Tree FDR, 44TB memory, 1 PB disk)
Interprocess communication	Null

Typical Job Run				
Number of processors needed for each job		128.00		
Estimated number of jobs to submit		1095.00		
Average job durations (hours) per job		2.00		
Total memory used by the job (GBytes)		20.00		
Largest Job Run				
Number of processors needed for each job		128.00		
Estimated number of jobs to submit		1095.00		
Average job durations (hours) per job		2.00		
Total memory used by the job (GBytes)		20.00		
Total disk space (Gigabytes)	**Minimum**	2000.00	**Desirable**	5000.00
Total scratch space (Gigabytes)	**Minimum**	500.00	**Desirable**	1000.00
Total tape space (Gigabytes)	**Minimum**	0.00	**Desirable**	0.00
Total Requested time (Thousands of hours)		300.00		

If this activity is asking for more than 2Million CPU hours, you need to justify the amount of resources requested for the activity. (max 1000 characters)

INFORMATION: The estimated cost of the requested hours, considering only the electricity cost, is 3429 euros.

The architectures selected for the requested resources are only a suggestion. If no hours in this machine/these machines are available, please grant resources in any other similar architecture where the codes used for the application may run efficiently.

** this option implies that if no hours in this machine/these machines are available, the acces committee will reject the full application.

b) Estimate of the total resources that the Activity will require until it is completed (including the present and all the following Application Periods)

Number of application periods expected to complete this Activity

3

Total Requested Time (thousands of hours) expected to complete this Activity

1900.00

6. Abstract for publication

Air pollution remains a major health risk factor in Europe. Only with a precise knowledge of air pollution origin, effective actions to reduce its impacts can be designed. This long-term activity will provide a robust estimate of the contribution from different source classes (activities and regions) to the air pollution in Spanish urban areas using the CALIOPE air quality system. This activity will combine a profound knowledge of atmospheric chemistry, available air quality measurements, and an advanced chemical transport model into a framework of high-performance computing. This activity will contribute to improving the air quality management efforts in the design of emission abatements and guide researchers on future model developments to optimise resources and reduce model uncertainty

7. Contact with CURES during last year

Information about the RES Users Committee (CURES).

a) User has contacted the CURES during last year

No

b) If not, indicate why you have not contacted the CURES

Because I have not needed it.