Project scope and plan

Project name	eFRAGMENT2: eFRontiers in dust minerAloGical coMposition and its Effects upoN climaTe, phase 2
Research field	PE10_1 Atmospheric chemistry, atmospheric composition, air pollution PE10_3 Climatology and climate change

Principal Investigator (PI)

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1 Key scientific/societal/technological contribution of the proposal (200 words max.)

Soil dust aerosols are mixtures of different minerals, whose relative abundances, particle size distribution (PSD), shape, surface topography and mixing state influence their effect upon climate. However, Earth System and Chemical Transport Models typically assume dust aerosols to have a globally uniform composition, neglecting the regional variations in the mineralogy of the source. The omission of mineralogy impedes further understanding of the dust role in the Earth system. An on-going ERC Consolidator Grant entitled FRAGMENT attempts to fill in this gap. FRAGMENT combines field campaigns, new theory, remote spectroscopy and modeling to understand the global mineralogical composition of dust along with its effects upon climate.

eFRAGMENT2 is designed to tackle the modelling activities of FRAGMENT during the 2nd year of the project. It will produce and analyze 1) dust data assimilation experiments with an ensemble-based dust data assimilation system using 2D and 3D observations, 2) global runs including dust radiative effects that account for the currently known regional variations in soil mineralogical composition, and 3) global runs including heterogeneous chemistry in dust surfaces. Such experiments would not be possible without appropriate access to tier-0 computing resources and the associated support by PRACE.

2 Detailed proposal information (Maximum 14 pages, graphs and tables included)

2.1 Justification for the importance of the scientific problem and the requested resources (~2 pages)

Soil dust aerosols created by wind erosion of arid and semi-arid surfaces are amongst the largest contributors to the global aerosol mass load and dominate climate effects over large areas of the Earth; these effects depend fundamentally upon physical and chemical properties of dust. Indeed, dust aerosols are mixtures of a variety of minerals, whose relative abundances, particle size distribution (PSD), shape, surface topography and mixing state influence their effect upon climate. The Intergovernmental Panel on Climate Change (IPCC) has identified **dust mineralogy as a key uncertainty** in the overall contributions of aerosols to radiative forcing[1]:

- Dust perturbs the **energy and water cycles by direct radiative forcing**. The absorption of solar radiation by dust is strongly related to the presence of iron oxides[2]. Thermal radiation is also sensitive to mineralogy, specifically to abundance of phyllosilicates (clays), quartz and carbonates[3].
- Dust influences **cloud formation and the associated indirect radiative forcing** by providing nuclei for liquid and ice clouds. The ice nucleation properties of dust depend upon its surface defects. Recent studies have revealed that K-feldspar is the key mineral for ice nucleation[4]. The droplet nucleation properties of dust depend upon hygroscopicity, which increases during transport and depends on mineralogy.
- Dust undergoes **heterogeneous chemical reactions** during transport that increase its hygroscopicity, while altering its optical properties, and the associated radiative forcing. The rates of heterogeneous chemical reactions on the dust surface that form coatings of sulfate, nitrate, chloride, or organics depend strongly on the dust mineralogical composition[5]. Dust composition also affects the partitioning of semi-volatile inorganic compounds, altering their burden and radiative forcing.

- Dust minerals containing **bioavailable iron deposited into ocean waters** catalyze photosynthesis by ocean phytoplankton, increasing carbon dioxide uptake and influencing the global carbon cycle. The iron content and potential solubility of dust, along with the chemical processes that increase iron bioavailability during atmospheric transport, depend strongly upon mineralogical composition.

In spite of the potential importance of mineralogy, Earth System and Chemical Transport Models typically assume that dust aerosols have a globally uniform composition, neglecting the known local and regional variations in the mineralogical composition of the sources[6-8]. Modeling efforts have focused on constraining dust sources, emission and PSD. While this minimal representation has allowed significant advances in dust and climate research over the past decade, the omission of dust mineralogy impedes further understanding of the dust role in the Earth system.

The PI of **eFRAGMENT2** has been awarded with an ERC Consolidator Grant to advance the representation of dust mineralogy in models. The project, so-called FRAGMENT (FRontiers in dust minerAloGical coMposition and its Effects upoN climaTe), **aims to generate integrated and quantitative knowledge of the role of dust mineralogy in dust-radiation, dust-chemistry and dust-cloud interactions based on modeling experiments constrained with theoretical innovations and field measurements.** FRAGMENT officially started in October 1st 2018 and will have a duration of five years. eFRAGMENT2 is designed to tackle the modelling activities of FRAGMENT during the 2nd year of the project.

The project will be carried out by the Earth Sciences Department of the Barcelona Supercomputing Center (BSC-ES henceforth) using the Multiscale Online Non-hydrostatic AtmospheRe CHemistry model[9-19](MONARCH; previously known as NMMB/BSC-CTM), which is described in detail in the following sections. eFRAGMENT2 will focus on three key experiments necessary to advance towards the goals set in FRAGMENT. First, we will run and evaluate simulations using our Local Ensemble Transform Kalman Filter (LETKF) data assimilation system using 2D and 3D aerosol observations (~8.2 M-core hours). Second, we will run multiple simulations to calculate the radiative effects of dust accounting for regional variations in mineralogy through currently available soil mineralogical atlases (~12.3 M-core hours). Third, we will perform multiple simulations to explore the effect of heterogeneous chemistry at the surface of dust particles upon the burdens of precursor gases, dust, nitrate, sulfate, and ammonium (~12.3 M-core hours).

Such an ambitious exercise requires appropriate access to tier-0 computing resources and the associated support offered by PRACE. A total of 35 Mcore-hours are requested in this proposal, including a ~10% overhead to account for failing jobs that will need to be repeated. The detailed justification of this amount is presented in Sections 2.2 and 2.6.

2.2 Overview of the project (~4 pages)

2.2.1 Goals

The overarching goal of FRAGMENT is to understand, constrain and calculate the global mineralogical composition of dust along with its effects upon climate. **FRAGMENT will fundamentally advance the treatment of dust mineralogy by fulfilling the following objectives:**

Objective 1: We will contribute new fundamental understanding to reduce the large uncertainties in the emitted dust PSD by evaluating and extending current theoretical paradigms, based on an unprecedented ensemble of coordinated measurement campaigns and laboratory analyses. We will also address for the first time both experimentally and theoretically the size-resolved mineralogy of dust at emission and its relationship with the parent soil.

Given the paucity and incompleteness of measurements, and the apparent contradiction among theories, field observations and wind tunnel experiments, FRAGMENT is conducting field campaigns in distinct source regions to measure the size-resolved dust emission for a range of meteorological and soil conditions in conjunction with an extensive analysis of the underlying soil characteristics. Our aim is to improve our quantitative understanding of the emitted dust PSD.

Objective 2: Precise knowledge of dust mineral content requires more detailed and widespread measurements of soil mineralogy. We will evaluate and use airborne and spaceborne hyperspectral imaging to improve global atlases of soil mineralogy for dust modelling. Our new methods and understanding will help retrieving soil mineralogy through high-quality spaceborne hyperspectral measurements.

Modeling of dust aerosol mineralogy is based upon maps of soil type and the relation of this variable to soil mineralogy. This relation is inferred using massive extrapolation from a limited amount of soil mineralogical analyses, ancillary information on soil texture and color, and a number of additional assumptions[8]. This limited knowledge together with our incomplete understanding of the emitted dust PSD and its relationship with the PSD of the parent soil precludes accurate assessment of the effects of dust upon climate. To address this challenge, FRAGMENT will help improving current estimates of soil-surface mineralogy for dust modelling using spaceborne spectroscopy. FRAGMENT members, including the PI, are part of the science team of EMIT, a NASA funded mission that will sample the surface mineral composition of Earth dust sources at very high spatial resolution using hyperspectral imaging spectroscopy from the International Space Station (ISS) in 2021. EMIT will provide large spectral range (410 to 2450 nm), high signal-to-noise ratio (SNR), high-resolution spatial sampling (60 m), and comprehensive near-term coverage of most mineral dust sources. EMIT will supersede current space multispectral measurements from Landsat, ASTER, and SENTINEL, and create a paradigm shift by allowing the production of a near-global database of surface mineralogy that exceeds, by six orders of magnitude, the mineralogical analyses that underpin the current mineralogical atlases.

Objective 3: While the impact of dust mineralogy upon climate is potentially large, the interconnection of mechanisms has been neglected in the few models that represent mineral variations. We will generate integrated and quantitative knowledge regarding the influence of dust mineral composition upon atmospheric radiation, chemistry and clouds based on modelling experiments constrained with our theoretical innovations and field measurements.

In this context, **eFRAGMENT2** is designed to tackle the modelling activities (Objective 3) of FRAGMENT during the 2nd year of the project. eFRAGMENT2 is a continuation of eFRAGMENT1 in which we tackled a first set data assimilation runs and implemented and run the global dust cycle with the inclusion of mineralogical variations based on current mineralogical atlases.

2.2.2 Hypotheses and key scientific questions

Emitted dust is transported throughout the atmosphere where it affects the energy and water cycles by radiative interactions and interacts with both warm and mixed-phase clouds. Dust radiative forcing in nearly all global models varies with environmental properties like surface albedo, along with the dust PSD, but excludes the effect of regional variations in forcing resulting from source variations in soil mineral composition. For particles of a given size, absorption at short wavelengths is most sensitive to the presence of iron oxide minerals within the dust particle, and at long wavelengths to the presence of phyllosilicates, calcite and quartz. Dust also affects the partitioning of inorganic aerosol components and undergoes heterogeneous chemical reactions with acidic trace gases that result in the formation of coatings on the dust particle surface, including sulfate and nitrate[1]. These interactions affect cloud droplet formation by changing both the burden of soluble material and by increasing the hygroscopicity of dust. We aim to address a number of questions including: What is the impact of our new mineral abundance and emitted PSD constraints upon the effects of dust? How large are the effects of regional variations in mineralogy relative to the effect of globally uniform particles? What is the radiative forcing of dust? What is the minimal representation of minerals that needs be considered by Earth System Models to incorporate the largest impacts of dust?

2.2.3 Specific experiments in eFRAGMENT2

The plan is to enable and evaluate a multiscale atmosphere-chemistry modelling system that includes state-of-the-art dust capabilities with unprecedented constraints on the composition-resolved dust emitted PSD. In eFRAGMENT2 we will focus on three key experiments necessary to advance towards the goals set in FRAGMENT.

Data assimilation: we want to minimize the errors in the spatial and temporal variability of the simulated total dust fluxes through data assimilation. Our goal is to allow a (more) independent test of the mineral abundance maps and the emitted PSDs. Indeed, data assimilation methods can be used not only to correct dust loading, but also to constrain (correct) dust emission[20-23]. In later stages, we plan use a fixed-lag Kalman smoother based on our LETKF data assimilation system, which is in essence a Kalman filter that iteratively estimates emissions, allowing for retrospective corrections of emissions from observations later in time. As a preliminary step, in eFRAGMENT1, we ran and evaluated simulations with our LETKF data assimilation system (without the smoother) using dust optical depth observations from MODIS Deep Blue at 10 km resolution. In eFRAGMENT2, we will run and evaluate simulations using other 2D and 3D dust products (MODIS Dark target, VIRS, CALIPSO-based LIVAS dust product).

Dust radiative effects: in eFRAGMENT1 we ran and evaluated the first simulations with individual dust mineral tracers using available soil mineralogical atlases. In eFRAGMENT2 we want to further run and evaluate multiple simulations that include sub-regional perturbations of the relative fractions and emitted PSD of each mineral within an estimated range of uncertainty. In addition to transporting mineral species, we will implement and calculate their effect upon radiation. In further stages of FRAGMENT this methodology will be enhanced by using a more advanced soil mineralogical atlas and emitted PSD methods derived from the experimental campaigns that will happen during the first two years of the project. For dust particles of a given size, absorption at solar wavelengths is most sensitive to the presence of iron oxide minerals. Because iron oxides contribute only a small fraction of the particle mass, their evaluation in models based upon direct measurements of dust composition are subject to greater uncertainty, compared to more abundant minerals like clays and quartz. Because of the strong influence of iron oxides upon shortwave absorption, radiance measurements by satellites and ground-based measurements offer a complementary means for evaluating and constraining the model. We will specifically evaluate our representation of iron oxide minerals using radiance measurements from multiple instruments.

Dust heterogeneous chemistry: we will explore and evaluate the effects of mineralogy upon the partitioning of semi-volatile inorganic compounds and dust heterogeneous chemistry, along with the associated changes in the burdens of precursor gases, dust, nitrate, sulfate, and ammonium. For this task, only minor model developments will be required. We will complement the model with the full set of (known) dust heterogeneous reactions (including the uptake of sulfure dioxide, HNO_3, H_2SO_4, N_2O_5, NO_3, NO_2, O_3, H_2O_2, HO_2, and OH), using the Kinetic PreProcessor (KPP) package[24] available within our model infrastructure. In this case, we will also include sub-regional perturbations of the relative fractions and emitted PSD of each mineral within an estimated range of uncertainty.

We will focus on the production of 10-year simulations of 20-member ensembles for the dust data assimilation experiment, 5-year simulations of 60-member ensembles for the radiative effect experiment, and 5-year simulations of 60-member ensembles for the dust heterogeneous chemistry experiment. The period of simulation will be 2007-2016 and 2011-2016, respectively. Table 1 summarises the experiments planned, which will run by chunks of 1 year. A simulation of one year for one member is expected to require a wallclock time of ~40 hours using 1032 cores.

Table 1: Cost of the experiments proposed.

Run type	# Runs	# Steps/Run	Walltime/Step	# CPU cores	Total core hours
Data assimilation	200	365	0,11	1032 (1024+8)	8.286.960
Dust radiative effects	300	365	0,11	1032 (1024+8)	12.430.440
Dust heterogeneous chemistry	300	365	0,11	1032 (1024+8)	12.430.440
TOTAL					33.147.840

By the end of eFRAGMENT2, we have the ambition of providing first estimates of global dust direct radiative effects and effects upon heterogeneous chemistry accounting for regional variations in mineralogical composition. At the same time the model will be prepared to allow more refined simulations using constraints of the emitted PSD from the ongoing field campaigns and of the surface mineralogical composition from EMIT.

eFRAGMENT2´s expected outcomes and impacts are:

-help understanding to what extent dust warms or cools the planet

-supporting major international scientific assessments such as the IPCC

-increase confidence in climate projections by advancing our understanding of dust effects

-contribute to the success of a NASA space-borne mission

2.3 Validation, verification, state of the art (~2 pages)

2.3.1 Validation

For validation of the radiative effect experiments we will use (1) AERONET, which provides PSD and single scattering albedo (ssa) at several wavelengths; (2) recent PARASOL retrievals, which provide ssa at 550 nm, effective radius and variance for two modes; (3) OMI OMAERUV, which provides ssa near the ultraviolet wavelengths, where hematite is an especially strong absorber. In order to avoid contamination by other aerosols, we will screen for dust using high AOD, a large fraction of non-spherical particles, the spectral dependence of ssa and the PSD.

For the evaluation of the dust heterogeneous chemistry experiments, we will use measurements available at regions near or downstream of dust sources. The evaluation will also include data from the Clean Air Status and Trends Network (CASTNet), the Interagency Monitoring of Protected Visual Environments network (IMPROVE), and the European Monitoring and Evaluation Programme (EMEP).

2.3.2 Verification

Our on-line monitoring of simulations directed at key diagnostics allows detecting errors in the experiment setup or numerical instabilities. This will ensure the best use of computational resources as problematic experiments are stopped as soon as a problem is detected. Some examples of on-line checks are the grid cell tracer mass concentration, air temperature, radiative fluxes, or the numerical convergence of the chemistry solver.

MONARCH has been tested for reproducibility on MN4. We use restart files that allow bit reproducibility when the number of cores and MPI configurations are maintained. This will be the case for this project as all experiments will be performed with the same configuration.

2.3.3 Sensitivity analysis and uncertainty quantification

Our methodology includes running and evaluating multiple simulations with sub-regional perturbations of the relative abundance and emitted PSD of each mineral within our best estimates of ranges of uncertainty. To reduce the number of runs, perturbations will be generated based latin hypercube sampling (LHS)[25] within the most prominent dust sources only. LHS samples across a multi-dimensional parameter uncertainty space while retaining good coverage within any single parameter uncertainty range. The evaluation of these simulations with available mineral fraction observations and observations described in sections 2.3.1 will provide further constraints in the mineral abundances and emitted PSDs of each mineral.

2.3.4 Comparison with state of the art

The effect of dust mineralogy upon radiation and dust heterogeneous chemistry has received little attention so far. To our knowledge, in addition to MONARCH only one model (CESM) includes the capability of accounting for regional mineralogical variations when calculating radiative effects. On the other side, current models that include dust heterogeneous chemical reactions omit variations in dust mineralogy.

The PI has proposed novel approaches to represent the emission and global distribution of mineral aggregates[26,27,28]. His novel methods have remedied many important deficiencies of previous implementations in comparison to observations. On the basis of these results the PI obtained the ERC Consolidator grant (FRAGMENT). His results also granted him an invitation to be part of the Science Team of EMIT which has been selected by the NASA Earth Venture Instrument-4 program to sample the surface mineral composition of Earth dust sources by sending a hyperspectral imaging spectrometer to the International Space Station (ISS). In this sense, eFRAGMENT2 and future follow-up PRACE projects are uniquely positioned to tackle the effect of dust upon climate using the latest advances in the field.

2.4 Software and Attributes (~2 pages)

2.4.1 Software

We will use MONARCH[9-19], a model designed and developed by the PI and his research group at BSC, in close collaboration with partners at other institutions such as NOAA, NASA and University of California, Irvine. The model provides regional daily dust forecasts for Northern Africa, Middle East and Europe through the WMO Regional Centers for dust prediction hosted by BSC, and contributes with global forecasts to the International Cooperative for Aerosol Prediction (ICAP) Multi Model Ensemble. MONARCH is a multi-scale model that can be applied on a global or regional domain with telescoping nest capability. MONARCH contains advanced chemistry and aerosol packages, and is coupled online with the Non-hydrostatic Multiscale Model (NMMB), which allows for running either global or high-resolution (convection allowing) regional simulations. In recent projects, the dust-cycle component of MONARCH was upgraded with (1) a global-scale 10 km resolution mapping of dust sources based on MODIS Deep Blue (2) multiple choices for the dust emission scheme, (3) a drag partition correction for the wind speed threshold for dust emission, (4) the ability to run the model with separate mineral tracers using a soil mineralogy atlas, (5) a flexible treatment of atmospheric chemistry, and (5) a dust (and aerosol) data assimilation system based on the Local Ensemble Transform Kalman Filter (LETKF).

2.4.2 Particular libraries

A single executable needs to be built for MONARCH as well as an executable for the Local Ensemble Transform Kalman Filter (LETKF). The MONARCH model fully supports a parallel environment. For configuring and building the model executables, FORTRAN 77/90/95 complaint compiler with pre-processing capabilities and NetCDF-4 are needed. The simulations will require MPI libraries and runtime facilities (ESMF, wgrib, makedep90, bacio, sigio, sp), data handling tools, such as HDF4, HDF5, NETCDF3, NETCDF4, GRIB_API, R, CDO, NCO and general configurations tools, such as PERL, PYTHON, AUTOCONF and AUTOMAKE.

MONARCH is a coupled model constructed over the Earth System Modelling Framework (ESMF) coupling library; this implies that in between the execution of each module (dynamics, physics, chemistry, aerosol) the model performs a coupling step to exchange information. The numerical methods employed within the model 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. Additionally, the chemistry module applies a Euler-Backward Iterative scheme to solve the ordinary differential equations of the stiff system of gas-phase chemistry.

2.4.3 Parallel programming

MONARCH subdivides the domain of operation into horizontal tiles and assigns them to computational units. Thus, the parallelization is addressed on a subdomain basis approach. Since the global latitude-longitude grid deforms toward the pole region, the nodes closer to the poles perform an additional filtering step using fast Fourier transform (FFT) to be applied to keep the integration stable using a time step of decent size.

MONARCH is parallelised in the space dimension by using MPI. Currently, some components of MONARCH are being ported to the GPUs to take advantage of new heterogeneous architectures. Splitting the computation of chemical reactions in individual threads of the GPU has shown a speed-up of x12 in some subroutines compared with the CPU version. Similar computation time in the GPU is found for cases with 100 up to 10.000 chemical reactions.

2.4.4 I/O requirements

The I/O strategy of MONARCH is designed for the setup of dedicated writing nodes. This results in an asynchronous partition between computational and I/O nodes so the read and write of the model doesn't penalize the computational part. The writing nodes are balanced with the computational nodes to assure an efficient use of the resources. A single run of MONARCH reads 68 inputs files with a total size of 1 GB depending on the model grid resolution, and outputs one single NetCDF4 file of 16

GB with the model results and one single NetCDF4 file of 2GB as restart file. The output file is being filled during the execution time with a constant rate by the writing nodes and the restart files is written at the end of the model run. The model doesn't have a restart overhead, both initialization and restart steps require similar amount of time.

MONARCH experiments will include multiple members that either should or could be run at the same time. In this sense MONARCH is coupled with the Autosubmit software which is the BSC-ES workflow manager that ensures a uniform and optimal use of the resources. The jobs will be managed, and packed in groups in a single big job by Autosubmit to better manage the I/O system while maximising the use of the machine. The output will be transferred to the BSC-ES local storage as soon as each chunk of simulation is completed, which implies that data transfer will be part of the experiment workflow and be continuously active. Transfer rates between Marenostrum4 and the BSC local archive of up to 5 TB per day have been reached. The data storage and data transfer can be organised to require a space of 200 TB in the scratch file system. This required scratch space is motivated by the large amount of output to be generated.

2.5 Data: Management Plan, Storage, Analysis and Visualization (~1 page)

2.5.1 Data Management Plan covering

The type of simulations conducted during the eFRAGMENT2 project requires hosting a set of gridded satellite aerosol observations in order to conduct data assimilation (i.e. 23 GB per year of simulation) as well as the global meteorological input data files used as initial meteorological conditions and boundary conditions at intervals of 6 h (i.e. 250 GB per year of simulation considering ERA-5 reanalysis). Around 50 GB of space will be required to host the code. Hence the total disk space required hosting the input data and the code amounts to 2.6TB. Such dataset will be placed in a backup partition of the HPC file system (i.e., *home or projects*).

Two types of simulation will be conducted in eFRAGMENT2: (1) Data assimilation runs using 20 ensemble members, and (2) Mineralogy experiments including radiative effects and heterogeneous chemistry using 60 members. The simulations will be executed in chunks of one year to properly manage the data produced. After one year is produced, the post-process will be run in the HPC and the final data uploaded to the BSC storage system. One year of simulation will require a temporal disk space of (1) 58 TB and (2) 130 TB. Considering that the two types of simulations will run at the same time, the experiment requires around 190 TB of temporal working space in scratch or projects. After the post-process this amount of data will be reduced by a factor of 20 and Autosubmit will proceed with the upload to the BSC archive system and the cleaning of temporal files in the HPC. From our previous experience with Marenostrum4, a transfer rate between Marenostrum4 and the BSC local archive of up to 5 TB per day can be achieved, which should fit the plan mentioned. To account for maintenance activities in the BSC local storage or an increase in the line traffic that might temporarily lower the transfer rate, the space requested for handling the output data is increased to 200 TB, which offers a buffer for post-processing of 10 TB.

The data stored in the BSC local archive will be managed and curated by the Data and Diagnostics Team of BSC-ES. They have developed a framework to store all the simulations and the observational data required by the BSC-ES researchers that offers access to all the data with a strict documentation, organisation and, of course, formatting. The data produced in eFRAGMENT2 will be made accessible via the BSC-ES THREDDS server. The terms of access will be fully public and accept commercial use of the data to better link to the future activities within the Copernicus programme, which is arguably one of the most efficient ways to link to a wide range of climate data users.

Both the data disseminated and the publications originated from them will appropriately acknowledge PRACE and will follow the criteria set by the EC for open data access.

2.5.2 Project workflow

Thanks to the well-defined workflow structure and the use of an adapted workflow manager like Autosubmit (see Sec. 2.5.3), the data produced by each simulation will be transferred to the permanent storage using a dedicated transfer node. The analysis of results is run locally as soon as the post-processing of a chunk is completed, which should happen on average around 3 hours after the chunk started running, although this time depends on the queue capacity for the different types of jobs. In this context, a standard two-week delay between the end of the project and the closing of the PRACE accounts is more than enough for the team members to clean the HPC repositories.

2.5.3 Software workflow solution

The Autosubmit software[29] is adopted to manage the workflow and ensure a uniform and optimal use of the resources. Autosubmit was developed by and is maintained at BSC. It is a python-based tool to create, manage and monitor experiments by using Computing Clusters, HPC's and Supercomputers remotely via ssh. It has support for experiments running in more than one HPC and for different workflow configurations. The jobs will be managed, and packed in groups in a single big job whenever required, by Autosubmit to better manage the I/O system while maximising the use of the machine.

2.5.4 I/O requirements

Most of the analysis will be run locally after the transfer of output is completed. Only limited post-processing is performed on the supercomputer to diagnose the correct functioning of the experiment. For this reason, we do not have any special I/O requirements related to analysis and visualization of results.

2.5.5 Associated Fenix infrastructure resources

Does not apply

2.6 Performance of Software (Maximum 3 pages)

2.6.1 Testing of your code on the requested machine

MONARCH has been tested and extensively used in production in MareNostrumIV for previous tier-0 PRACE calls under projects "eDUST" (July 2017 - March 2018) and "eFRAGMENT1" (October 2018 - September 2019), as well as Spanish Supercomputing Network (Red Española de Supercomputación, RES) calls under projects AECT-2019-3-0001 and AECT-2018-3-0012. In the last PRACE project where MONARCH model was used, eFRAGMENT1 (PI: C. Pérez García-Pando), ensemble runs of 12 members using simultaneously 18000 cores were successfully conducted with a sustained production rate.

BSC-ES has also expertise in analysing parallel programming model codes using cutting-edge tools. This allows continuously carrying out performance analyses to reach the optimum configurations for MONARCH. Several performance analyses have been conducted during the last years. Figure 1 illustrates an example of such performance analyses. These are two different views as shown by the Paraver tool of the execution of one routine (exch4) of MONARCH with one and two threads respectively. Paraver uses different types of plots to represent the values stored in a trace file. A trace file is a file holding information of an execution to perform a subsequent analysis. When we use more and more cores for the execution of an application, the communication can be more complicated. Moreover, many scientists agree that when we double the number of the cores, a new bottleneck is observed. That's why we tried to decrease the communication cost for a stencil communication routine called exch4. In the example, the speedup is 1.76 which means that when we doubled the number of the cores the communications routine was improved by 1.76 times.

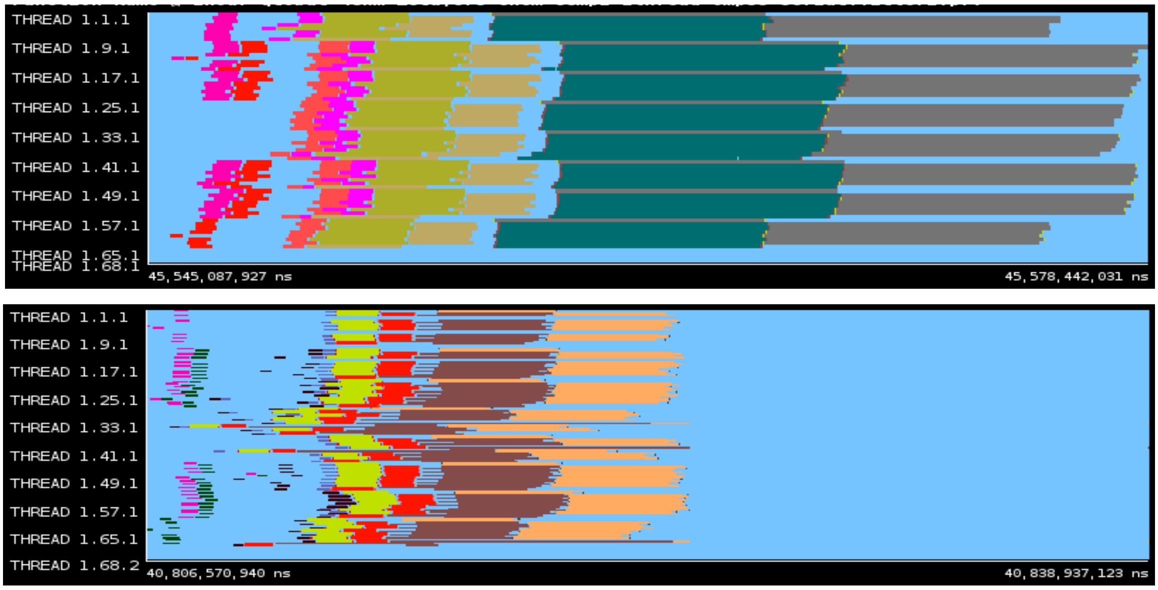


Figure 1. Executing exch4 routine of MONARCH with one thread (top) and two threads bottom.

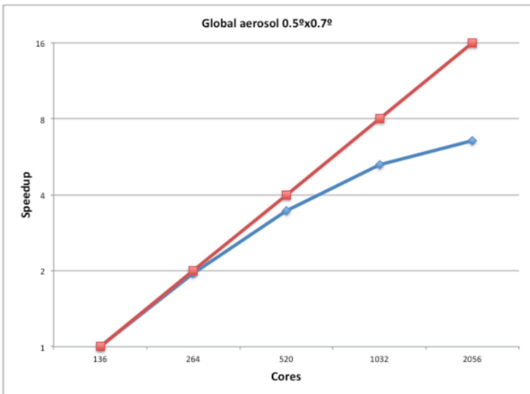
2.6.2 Quantify the HPC performance of your project

2.6.2.1Strong and weak scalability

For Earth System applications, weak scalability metrics are not applicable since the problem to solve is fixed in space (i.e. surface of the earth in the horizontal dimension and height of the atmosphere in the vertical dimension) and therefore only strong scaling metrics are used. MONARCH model can run with at least 4 computing cores and 1 writing core. Our experiments are constrained by time and memory usage, which are highly dependent to the configuration of the model (horizontal and vertical resolution, and complexity of the model physical schemes). With the configuration proposed in this project, global domain at 50 km horizontal resolution and 48 vertical layers, the model requires at least 3 nodes. With less, it fails due to memory limits in Marenostrum4 (maximum of 2GB per node).

Figure 2 shows the strong scalability test starting at 128 (computing) + 8 (writing) cores up to 2048 (computing) + 8 (writing) cores. MONARCH scales reasonably well up to 512 - 1024 computing cores.

# nodes	#cores	Time 24h (s)	Speedup	Ideal speedup	% of scalability
3	136	2123	1	1	
6	264	1091	1,945921173	2	97,30
11	520	612	3,468954248	4	86,72
22	1032	402	5,281094527	8	66,01
43	2056	324	6,552469136	16	40,95



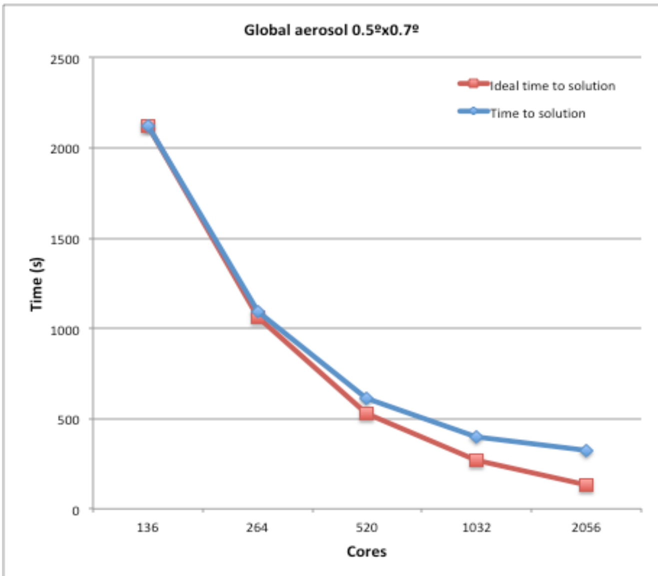


Figure 2. Scalability for the global aerosol configuration.

2.6.2.2 Precision reported

All operations will be carried out with mixed precision.

2.6.2.3 Time-to-solution

We provide the requested metrics for a 24-hour run of MONARCH configured on a global domain with 360 x 514 x 48 grid cells (8881920). The number of iterations for this run is 960 using a fundamental timestep of 90 seconds. Times to solution using 520 and 1032 cores are 612 and 402 seconds, and time per iteration 0,6375 and 0,41875 seconds.

Ti*_520 = 0,6375 x 520 / 8881920 = 3,73E-5

Tf*_520 = 612 x 520 / 8881920 = 3,58E-2

Ti*_1032 = 0,41875 x 1032 / 8881920 = 4,86E-5

Tf*_1032 = 402 x 1032 / 8881920 = 4,67E-2

2.6.2.4 System scale

Results were measured on full-scale system.

2.6.2.5 Measurement mechanism

Performance measurements were carried out through the usage of timers.

2.6.2.6 Memory usage

We will need full access to each occupied node's memory (2GB per core in Marenostrum4).

2.6.2.7 OPTIONAL: Percentage of available peak performance

Not reported

3 Milestones (quarterly basis) (Maximum 1 page)

3.1 Gantt Chart

Table 2. Schedule of the activities. Milestones are indicated in the corresponding month with an "M".

Simulations	M1	M2	M3	M4	M5	M6	M7	M8	M9	M10	M11	M12
Data assimilation experiment (~8Mcore-hour)				M1								
Radiative effect experiment (~12Mcore-hour)									M2			P1
Heterogeneous chemistry experiment (~12Mcore-hour)											M3	P2

To monitor the resource management a number of milestones have been considered and added to Table 2:

- M1: Completion of the data assimilation experiment
- M2: Completion of the radiative effects experiment
- M3: Completion of the dust heterogeneous chemistry experiment

3.2 Communication plan

At least two publications (P1 and P2 in the Gantt Chart) in international peer-reviewed journals will be prepared summarizing the results. The first article will summarise the results of the dust radiative effect experiment and the second article should provide new insights about the effect of dust mineralogy upon dust heterogeneous chemistry. The results of eFRAGMENT2 will be widely presented in scientific conferences and will be submitted for presentation in the PRACEdays event of the years in which the project is active. eFRAGMENT2 will additionally benefit from the communications channels of FRAGMENT, EMIT, and the WMO Sand and Dust Storm Warning Advisory and Assessment System (SDS-WAS) Regional Center hosted by BSC.

4 Personnel and Management Plan (~1/2 page)

Activities within eFRAGMENT2 will be carried out by the PI together with a team of researchers already part of the BSC-ES. These are:

Dr. Oriol Jorba is the Co-group leader of the Atmospheric Composition group of the BSC-ES and one of the main developers of the MONARCH model. He has wide experience in PRACE projects (2010PA0419, 2010PA0627, EHRRDRBE, GG1CCS, and HRERS) and has participated in projects funded by the European Commission on air quality, specifically in aerosols, (APPRAISAL, EARLINET, FIELD-AC, ACTRIS1, ACTRIS2) and in the application of atmospheric modeling in HPC (IS-ENES, IS-ENES2, RETHINK big). He has been the supervisor of two Marie Skłodowska-Curie Individual Fellowship in the call H2020-MSCA-IF-2015 and H2020-MSCA-IF-2016. He will act as co-PI of eFRAGMENT2 and supervise the most of the technical aspects of the proposal and he will be in charge of the heterogeneous chemistry experiments (M3).

Dr. Enza Di Tomaso has a degree in Physics from the University of Bologna in Italy, and a PhD in Engineering Mathematics from the University of Bristol in UK. She has worked at the European Centre for Medium-Range Weather Forecasts. At BSC she has expanded her interest to atmospheric chemistry, and in particular to aerosol data assimilation, implementing a scheme to ingest satellite observations into MONARCH. She will be in charge of the data assimilation experiments (M1).

Dr. Jeronimo Escribano has a degree in Civil Engineering, and a MSc on Meteorology and Climate from the Universidad de Chile, and a PhD in Enviromental Sciences from the Université Pierre et Marie Curie. He is an expert on data assimilation and will support the data assimilations experiments (M1).

Dr. Maria Gonçalves is Chemical Engineer by the University of Santiago de Compostela (2004) and holds a PhD in Environmental Engineering by the Technical University of Catalonia -UPC- (2009). She has collaborated in a range of national and international projects and initiatives focusing on atmospheric models development and evaluation (e.g. CALIOPE, NMMB-MONARCH) or regional climate modelling (e.g. ESCAT, MedCORDEX) and more recently Earth System Modelling (e.g. EC-Earth, AerChemMIP). She will in charge of the radiative effect experiments (M2).

Dr. Sara Basart received a degree in Physics from the University of Barcelona (UB). She studied a Masters in Meteorology and Climatology at the University of Barcelona (UB). Dr Basart obtained her PhD degree in Engineering Environmental (Degree of European Doctor) at Technical University of Catalonia (UPC). She is the scientist in charge of the WMO Sand and Dust Storm Warning Advisory and Assessment System (SDS-WAS) Regional Center for Northern Africa, Middle East and Europe, and the Barcelona Dust Forecast Center (BDFC), hosted in BSC. She will be in charge of the validation activities in eFRAGMENT2.

Dr. Martina Klose is holding a doctoral degree (Dr. rer. nat.) in Meteorology obtained at the University of Cologne, Germany. She is currently a Marie-Skłodowska-Curie Fellowship (DUST.ES, H2020-MSCA-IF-2017 789630). She is an expert on dust emission processes and she will contribute to the creation of the ensemble perturbations for the assimilation experiment (M1).

Mr Kim Serradell is currently the leader of the Computational Earth Sciences (CES) group of the BSC-ES. The group is a multidisciplinary team of 19 members with different IT profiles that interacts closely with all the other groups of the BSC-ES. Kim Serradell is the PI of the ESIWACE H2020 project that focuses on porting and optimising codes at the highest-resolution possible on a range of platforms. He will contribute with this expertise to eFRAGMENT2.

Mr Miguel Castrillo is an expert in performance profiling and optimisation applied to NEMO and EC-Earth with a strong experience in software development. He is coordinator of the Models and Workflows team in the BSC-ES. He has experience in deploying and running the NEMO ocean model on several platforms. He is a member of the Technical Issues Working Group of EC-Earth and a member of the NEMO model HPC Working Group. He will be in charge of the updates of the workflow manager used in the project (autosubmit).

Mrs Francesca Macchia, Mr Carles Tena and Mr. Gilbert Montané are Research Engineers whose work will be to further improve the performance of MONARCH model and the data assimilation, and support the project runs and their verification. Miss Elisa Bergas is a PhD student who will contribute to M2

5 Previous Allocations and Results (~1/2 page)

BSC-ES members are involved in a range of projects in the broad spectrum of climate sciences. These efforts have been supported by PRACE computing resources in previous calls. For instance, members of the department have led PRACE projects: "HiResClim", "HiResClim2", "HiResSIR", "LSIHP", " Glob15km", "HiResNTCP" and “eDust” over the past 6 years, each including a handful of publications and/or reports acknowledging PRACE. The PI of this proposal has led PRACE project “eFRAGMENT1” from which three publications are under preparation.

Members of the proposing team are regularly involved in a number of PRACE activities. For instance, Mr Castrillo gave the presentation “Making Global coupled simulations possible” at the most recent PRACEDays event in Poland. Besides, the BSC-ES is responsible for the annual organisation of the PRACE Advanced Training Course “Earth Sciences Simulation Environments”, which is held at the BSC. Several members of the proposing team have given lectures there (Dr. Di Tomaso and Dr. Jorba).

6 References (Maximum 30)

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2) Moosmüller, H., Engelbrecht, J. P., Skiba, M., Frey, G., Chakrabarty, R. K., & Arnott, W. P. (2012). Single scattering albedo of fine mineral dust aerosols controlled by iron concentration. Journal of Geophysical Research: Atmospheres, 117, D11210.
3) Di Biagio, C., Formenti, P., Balkanski, Y., Caponi, L., Cazaunau, M., Pangui, E., Journet, E., Nowak, S., Caquineau, S., Andreae, M. O., Kandler, K., Saeed, T., Piketh, S., Seibert, D., Williams, E., and Doussin, J.-F. (2017) Global scale variability of the mineral dust long-wave refractive index: a new dataset of in situ measurements for climate modeling and remote sensing, Atmos. Chem. Phys., 17, 1901–1929,
4) Atkinson, J. D., Murray, B. J., Woodhouse, M. T., Whale, T. F., Baustian, K. J., Carslaw, K. S., ... & Malkin, T. L. (2013). The importance of feldspar for ice nucleation by mineral dust in mixed-phase clouds. Nature, 498(7454), 355-358.
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8) Journet, E., Balkanski, Y., & Harrison, S. P. (2014). A new data set of soil mineralogy for dust-cycle modeling. Atmospheric Chemistry and Physics, 14(8), 3801-3816.
9) Pérez, C., Haustein, K., Janjic, Z., Jorba, O., Huneeus, N., Baldasano, J. M., ... & Perlwitz, J. P. (2011). Atmospheric dust modeling from meso to global scales with the online NMMB/BSC-Dust model–Part 1: Model description, annual simulations and evaluation. Atmospheric Chemistry and Physics, 11(24), 13001-13027.

10) Haustein, K., Pérez, C., Baldasano, J. M., Jorba, O., Basart, S., Miller, R. L., ... & Washington, R. (2012). Atmospheric dust modeling from meso to global scales with the online NMMB/BSC-Dust model Part 2: Experimental campaigns in Northern Africa. Atmospheric Chemistry and Physics, 12(L03812), 2933-2958.
11) Jorba, O., Dabdub, D., Blaszczak-Boxe, C., Pérez, C., Janjic, Z., Baldasano, J. M., ... & Gonçalves, M. (2012). Potential significance of photoexcited NO2 on global air quality with the NMMB/BSC chemical transport model. Journal of Geophysical Research: Atmospheres, 117, D13301.
12) Spada, M., Jorba, O., Pérez García-Pando, C., Janjic, Z., & Baldasano, J. M. (2013). Modeling and evaluation of the global sea-salt aerosol distribution: sensitivity to size-resolved and sea-surface temperature dependent emission schemes. Atmospheric Chemistry and Physics, 13(23), 11735-11755.
13) Spada, M., Jorba, O., García-Pando, C. P., Janjic, Z., & Baldasano, J. M. (2015). On the evaluation of global sea-salt aerosol models at coastal/orographic sites. Atmospheric Environment, 101, 41-48.
14) Spada, M. (2015). Development and evaluation of an atmospheric aerosol module implemented within the NMMB/BSC-CTM. PhD thesis, available online at: http://hdl.handle.net/10803/327593.
15) Badia, A., & Jorba, O. (2015). Gas-phase evaluation of the online NMMB/BSC-CTM model over Europe for 2010 in the framework of the AQMEII-Phase2 project. Atmospheric Environment, 115, 657-669.
16) Gama, C., Tchepel, O., Baldasano, J. M., Basart, S., Ferreira, J., Pio, C., ... & Borrego, C. (2015). Seasonal patterns of Saharan dust over Cape Verde - a combined approach using observations and modelling. Tellus B, 67.
17) Basart, S., Vendrell, L., & Baldasano, J. M. (2016). High-resolution dust modelling over complex terrains in West Asia. Aeolian Research, 23, 37-50.
18) Badia, A., Jorba, O., Voulgarakis, A., Dabdub, D., Pérez García-Pando, C., … & Janjic, Z. (2016) Description and evaluation of the Multiscale Online Nonhydrostatic AtmospheRe CHemistry model (NMMB-MONARCH) version 1.0: gas-phase chemistry at global scale, Geosci. Model Dev., accepted.
19) Di Tomaso, E., Schutgens, N. A. J., Jorba, O., & Pérez García-Pando, C. (2016) Assimilation of MODIS Dark Target and Deep Blue observations in the dust aerosol component of NMMB/BSC-CTM version 1.0, Geosci. Model Dev., accepted.
20) Dubovik, O., Lapyonok, T., Kaufman, Y. J., Chin, M., Ginoux, P., Kahn, R. A., & Sinyuk, A. (2008). Retrieving global aerosol sources from satellites using inverse modeling. Atmospheric Chemistry and Physics, 8(2), 209-250.
21) Escribano, J., Boucher, O., Chevallier, F., & Huneeus, N. (2016). Subregional inversion of North African dust sources. Journal of Geophysical Research: Atmospheres, 121(14), 8549-8566.
22) Huneeus, N., Chevallier, F., & Boucher, O. (2012). Estimating aerosol emissions by assimilating observed aerosol optical depth in a global aerosol model. Atmospheric Chemistry and Physics, 12(10), 4585-4606.
23) Schutgens, N., Nakata, M., & Nakajima, T. (2012). Estimating aerosol emissions by assimilating remote sensing observations into a global transport model. Remote Sensing, 4(11), 3528-3543.
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26) Perlwitz, J. P., Pérez García-Pando, C., & Miller, R. L. (2015). Predicting the mineral composition of dust aerosols–Part 1: Representing key processes. Atmospheric Chemistry and Physics, 15(20), 11593-11627.
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28) Pérez García-Pando, C., Miller, R. L., Perlwitz, J. P., Rodríguez, S., & Prospero, J. M. (2016). Predicting the mineral composition of dust aerosols: Insights from elemental composition measured at the Izaña Observatory. Geophysical Research Letters, 43(19), 10520–10529.
29) Manubens-Gil, D., Vegas-Regidor, J., Prodhomme, C., Mula-Valls, O., and Doblas-Reyes, F.J., "Seamless management of ensemble climate prediction experiments on HPC platforms," 2016 International Conference on High Performance Computing & Simulation (HPCS), Innsbruck, 2016, pp. 895-900. doi: 10.1109/HPCSim.2016.7568429

Appendix 1: Track Record of the PI

Curriculum vitae and list of publications of the Principal Investigator

Dr. Carlos Pérez García-Pando

Birth date: 25 June 1977 in Barcelona, Spain

Institution: Barcelona Supercomputing Center

Address: C/ Jordi Girona 29, 08034 Barcelona, Spain

Telephone: +34 93 413 77 22

Email: carlos.perez@bsc.es

SCOPUS: 55928817500

ORCID: 0000-0002-4456-0697

G Scholar: http://bit.ly/perez_scholar

Web sites: http://bit.ly/perez_bsc_team

http://bit.ly/perez_axa_chair

Languages: Spanish and Catalan - Native

English and French – Fluent

CURRENT POSITIONS

10/2016– Head of the Atmospheric Composition Group

AXA Professor on Sand and Dust Storms

Ramon y Cajal Researcher

Earth Sciences Department, Barcelona Supercomputing Center (BSC), Spain

PREVIOUS POSITIONS

2011-2016 Associate Research Scientist

NASA Goddard Institute for Space Studies, New York

Department of Applied Physics and Applied Math, Columbia University, New York

2009-2011 Earth Institute Fellow

The Earth Institute at Columbia University, New York

NASA Goddard Institute for Space Studies, New York

International Research Institute for Climate and Society, New Jersey

2009 Visiting Scientist (5 months)

NOAA National Centers for Environmental Prediction, Camp Springs, Maryland

2006-2009 Research Scientist and Mineral Dust Group Leader

Earth Sciences Department, Barcelona Supercomputing Center, Spain

2005	Visiting Scientist Mediterranean Centre on Insular Coastal Dynamics. University of Malta (Malta)
2002-2005	Research Assistant and PhD. Candidate. Polytechnic University of Catalonia, Environmental Modelling Laboratory, Barcelona.

EDUCATION

12/2005	PhD in Environmental Engineering Polytechnic University of Catalonia, Environmental Modelling Laboratory, Barcelona, Spain Summa Cum Laude (Unanimity)
2001	Industrial Engineer - Environmental Option Polytechnic University of Catalonia, Industrial Engineering School, Barcelona, Spain
2001	Ingénieur des Arts et Manufactures École Centrale Paris, France

FELLOWSHIPS AND PRIZES

2017	**Agustín de Betancourt y Molina prize**. Awarded by the Spanish Royal Academy of Engineering for my contributions in the field of environmental risks, and in particular, in the field of mineral aerosols.
2016- 2020	**Ramon y Cajal fellowship (ranked #1 by the Earth Sciences Panel)**. Awarded by the Ministry of Economy, Industry and Competitiveness, Spain. Amount: EUR 210,000
2014	**Co-author of the Best Publication of 2014 at NASA Goddard Institute for Space Studies**
2014	**Best Science Brief of 2014 at NASA Goddard Institute for Space Studies**
2009– 2011	**Earth Institute Fellowship** (~5% success rate). Earth Institute at Columbia University, New York. Amount: $110,000.
2009	**Mobility grant José Castillejo to visit NOAA/NCEP**. Awarded by the Ministry of Science and Innovation, Spain. Amount: EUR 20,000
2001– 2005	**PhD Thesis fellowship awarded by the Polytechnic University of Catalonia, Spain**.
2007	**Poster presentation prize** at the 11th International Conference on Harmonisation within atmospheric dispersion modelling for atmospheric purposes.
1998– 2000	**EU Fellowship to obtain the double Spanish-French Engineering degree** at the École Centrale Paris, France

SCIENCE TEAM MEMBER OF A NASA INSTRUMENT MISSION

2018 – 2023 **Earth surface Mineral dust source InvesTigation (EMIT)**

NASA Earth Venture Instrument-4 (EVI-4) program

EMIT will sample the surface mineral composition of Earth dust sources using hyperspectral imaging spectroscopy from the International Space Station (ISS).

Role: Science team member / Co-I.

The other members of the Science Team are: Robert O. Green, NASA JPL (PI); Natalie M. Mahowald (Deputy PI), Cornell U.; David Thompson (Co-I), NASA JPL); Roger Clark (Co-I), PSI; Paul Ginoux (Co-I), NOAA; Olga Kalashnikova (Co-I), NASA JPL; Ron Miller (Co-I), NASA GISS; Greg Okin (Co-I), UCLA; Bethany Ehlmann (Co-I), Caltech; Thomas Painter (Co-I), NASA JPL; Vincent Realmuto (Co-I), NASA JPL; Greg Swayze (Co-I), USGS.

Budget: ~$ 50 Million

CURRENT GRANTS AS PI

2018– 2023 ***FRontiers in dust minerAloGical coMposition and its Effects upoN climaTe (FRAGMENT)*. ERC CONSOLIDATOR GRANT (2017)**.

Budget: EUR 2 Million.

2016– 2030 ***AXA Chair on Sand and Dust Storms.***

AXA CHAIR (2015) awarded by the AXA Research Fund.

Budget: EUR 1.7 Million.

2018– 2021 *Development and improvement of the products and services provided by the WMO Dust Regional Prediction Centers at the Barcelona Supercomputing Center***.**

SERVICES ENTRUST (Encomienda de Servicios) by Agencia Estatal de Meteorología. Budget: EUR 500,196.

2018– 2020 *QuaNtifying the present and fUTure atmospheric deliveRy of bIoavailablE iroN to The ocean (NUTRIENT).*

PROYECTO RETOS (2017) awarded by Agencia Estatal de Investigación.

Budget: EUR 72,600.

2017– 2018 *Dust forecast System for Kuwait Phase 1 (K-Dust Phase 1).*

Funded by the Kuwait Institute for Scientific Research.

Budget: EUR 140,999

PREVIOUS GRANTS AS PI OR CO-PI

2015 – 2016 *Implementation and testing of dust models for regional and global forecasting*

R2O Initiative for the Next Generation Global Prediction System (NGGPS), NOAA Collaborative project between Columbia University, NASA and NOAA GFDL

Role: Co-PI (PI: Paul Ginoux)

Budget: $200,000.

2014 – 2016 *Contribution to radiative forcing and climate by anthropogenic sources of dust aerosol*

NASA ROSES Modeling, Analysis and Prediction Program. Co-I's from NASA, Columbia University, NOAA GFDL and Princeton University.

Role: Co-PI (PI: Ron Miller)

Budget: $1,020,000

2011 – 2014 *Improving the representation of soluble iron in climate models.*

Department of Energy (DoE DE-SC00671). Collaborative Project between Columbia University, NASA and Cornell University

Role: Project Director and Institutional PI

Budget: $750,000.

2010 – 2015 *Atmospheric aerosol impacts on health in sub-Saharan Africa*.

Earth Institute Cross-Cutting Initiative (CCI).

Role: PI

Budget: $45.000.

2006 – 2009 *Improvement of the Dust Regional Atmospheric Model (DREAM) for prediction of Saharan dust events in the Mediterranean and the Canary Islands.*

Ministry of Science and Technology, Spain. Contract CGL2006-11879/CLI.

Role: PI.

Budget: EUR 98,000.

ORGANISATION OF SCIENTIFIC MEETINGS

2019 Co-Convener of the American Geophysical Union Session Dust in a changing climate: from small-scale insights to large-scale understanding. December 2019.

2019 Local Organizer of the AEROCOM meeting in Barcelona. September 2019

2018 Member of the Scientific Committee of the 9th International Workshop on Sand/Duststorms and Associated Dustfall 22-24 May 2018 Tenerife, Spain

2018 Chair of Session on dust, radiation and clouds at the the 9th International Workshop on Sand/Duststorms and Associated Dustfall 22-24 May 2018 Tenerife, Spain

2018 Chair of the Special Session on dust and air quality at the 11th International conference on Air Quality – Science and Application, Barcelona, Spain, 12-16 March 2018

2017 Chair of Session. 5th International Workshop on Sand Dust Storms, 23-25 Oct. 2017, Istanbul.

2012 Workshop Organizer, "Dust, climate and Health in sub-Saharan Africa" sponsored by the Earth Institute, International Research Institute for Climate and Society, New York

2011 Co-Chair, WMO SDS-WAS/GESAMP Expert Workshop on Modelling and Observing the Impacts of Dust Transport and Deposition on Marine Productivity, Malta

2007 Member of the Steering Committee and local organizer, "WMO/GEO Expert Meeting on an International Sand and Dust Storm Warning System", Barcelona, Spain

COMMISSIONS OF TRUST

2019 Member of the Expert Committee for the evaluation of the Laboratoire Interuniversitaire des Systèmes Atmosphériques (UMR CNRS 7583). Creteil, France.

2017 – Member of the Steering Committee, World Meteorological Organization Sand and Dust Storm Warning System Regional Center for North Africa, Europe and Middle East

2016 – Scientific Advisor, World Meteorological Organization Sand and Dust Storm Warning System Regional Center for North Africa, Europe and Middle East. http://sds-was.aemet.es/

2014 – 2015 Evaluator of Research proposals, NERC, UK / Department of Energy, US

2014 Member of the expert panel on extreme events for "The Impacts of Climate Change on Human Health in the United States: A Scientific Assessment", as part of the President's Climate Action Plan, US Global Change Research Program (USGCRP)

2012 Principal Science Advisor, Atmospheric dust module of the COMET Program, University Corporation for Atmospheric Research (UCAR) and NOAA National Weather Service.

2008 – 2011 Spanish Representative, Meningitis Environmental Risk Information Technologies (MERIT), World Health Organization, Geneva, Switzerland

2007 – 2010 Member of the Steering Committee, World Meteorological Organization Sand and Dust Storm Warning System Regional Center for North Africa, Europe and Middle East

2007 Member of the Writing team, Implementation Plan for an International Sand and Dust Storm Warning System of the World Meteorological Organization

2007 Editor, Book of proceedings "WMO/GEO Expert Meeting on an International Sand and Dust Storm Warning System", IOP Conference Series: Earth Environmental Science

2004 Reviewer: Science Advances, Scientific Reports, Nature Geoscience, Biomedcentral Infectious Diseases, Journal of Climate, Geoscientific Model Development, Atmospheric Chemistry and Physics, Tellus B, Theoretical and Applied Climatology, Atmospheric Environment, Geophysical Research Letters, Journal of Geophysical Research, and other

SELECTED PUBLICATIONS

1. Guevara, M., Tena, C., Porquet, M., Jorba, O., and Pérez García-Pando, C. (2019) HERMESv3, a stand-alone multiscale atmospheric emission modelling framework – Part 1: global and regional module, Geosci. Model Dev.(accepted)

2. Benavides, J., Snyder, M., Guevara, M., Soret, A., Pérez García-Pando, C., Amato, F., Querol, X., and Jorba, O.: CALIOPE-Urban v1.0: Coupling R-LINE with a mesoscale air quality modelling system for urban air quality forecasts over Barcelona city (Spain), Geosci. Model Dev. (accepted)

3. Querol, X., Tobias, A., Perez, N., Karanasiou, A., Amato, F., Stafoggia, M., Perez Garcia-Pando, C., Ginoux, P., Forastiere, F., Gumy, S.P., Mudu, P., Alastuey, A. (2019) Monitoring the impact of desert dust outbreaks on air quality for health studies (accepted)

4. Xian, P., Reid, J.S., Hyer, E.J., Sampson, C.R., Rubin, J.I., Ades, M., Asencio, N., Basart, S., Benedetti, A., Bhattacharjee, P., Brooks, M.E., Colarco, P.R., Da Silva, A., Eck, T.F., Guth, J., Kouznetsov, R., Kipling, Z., Lu, S., Sofiev, M., Perez Garcia-Pando, C., Pradhan, Y., Tanaka, T., Wang, J., Westphal, D.L., and Zhang, J. Current State of the global operational aerosol multi-model

ensemble: an update from the International Cooperative for Aerosol Prediction (ICAP). Quarterly Journal of the Royal Meteorological Society (accepted)

5. Scanza, R. A., Hamilton, D. S., Perez Garcia-Pando, C., Buck, C., Baker, A., and Mahowald, N. M. (2018) Atmospheric processing of iron in mineral and combustion aerosols: development of an intermediate-complexity mechanism suitable for Earth system models, Atmos. Chem. Phys., 18, 14175-14196.

6. Gkikas, A., Obiso, V., Pérez García-Pando, C., Jorba, O., Hatzianastassiou, N., Vendrell, L., Basart, S., Solomos, S., Gassó, S., and Baldasano, J. M. (2018) Direct radiative effects during intense Mediterranean desert dust outbreaks, Atmos. Chem. Phys., 18, 8757-8787.

7. Badia, A., O. Jorba, A. Voulgarakis, D. Dabdub, C. Pérez García-Pando, A. Hilboll, M. Gonçalves, and Z. Janjic, 2017: Description and evaluation of the Multiscale Online Nonhydrostatic AtmospheRe CHemistry model (NMMB-MONARCH) version 1.0: Gas-phase chemistry at global scale. Geosci. Model Dev., 10, 609-638, doi:10.5194/gmd-10-609-2017.

8. Di Tomaso, E., N.A.J. Schutgens, O. Jorba, and C. Pérez García-Pando, 2017: Assimilation of MODIS Dark Target and Deep Blue observations in the dust aerosol component of NMMB-MONARCH version 1.0. Geosci. Model Dev., 10, 1107-1129, doi:10.5194/gmd-10-1107-2017.

9. Pérez García-Pando, C., R.L. Miller, J.P. Perlwitz, S. Rodríguez, and J.M. Prospero, 2016: Predicting the mineral composition of dust aerosols: Insights from elemental composition measured at the Izaña Observatory. Geophys. Res. Lett., 43, no. 19, 10520-10529, doi:10.1002/2016GL069873.

10. Perlwitz, J.P., C. Pérez García-Pando, and R.L. Miller, 2015: Predicting the mineral composition of dust aerosols — Part 1: Representing key processes. Atmos. Chem. Phys., 15, 11593-11627.

11. Perlwitz, J.P., C. Pérez García-Pando, and R.L. Miller, 2015: Predicting the mineral composition of dust aerosols — Part 2: Model evaluation and identification of key processes with observations. Atmos. Chem. Phys., 15, 11629-11652.

12. Pérez García-Pando, C., M.C. Stanton, P.J. Diggle, S. Trzaska, R.L. Miller, J.P. Perlwitz, J.M. Baldasano, E. Cuevas, P. Ceccato, P. Yaka and M.C Thomson, 2014. Soil dust aerosols and wind as predictors of seasonal meningitis incidence in Niger. Environmental Health Perspectives. doi:10.1289/ehp.1306640

13. Miller, R.L., G.A. Schmidt, L.S. Nazarenko, N. Tausnev, S.E. Bauer, A.D. Del Genio, M. Kelley, K.K. Lo, R. Ruedy, D.T. Shindell, I. Aleinov, M. Bauer, R. Bleck, V. Canuto, Y.-H. Chen, Y. Cheng, T.L. Clune, G. Faluvegi, J.E. Hansen, R.J. Healy, N.Y. Kiang, D. Koch, A.A. Lacis, A.N. LeGrande, J. Lerner, S. Menon, V. Oinas, C. Pérez García-Pando, J.P. Perlwitz, M.J. Puma, D. Rind, A. Romanou, G.L. Russell, Mki. Sato, S. Sun, K. Tsigaridis, N. Unger, A. Voulgarakis, M.-S. Yao, and J. Zhang 2014. CMIP5 historical simulations (1850-2012) with GISS ModelE2. Journal of Advances in Modeling Earth Systems, doi: 10.1002/2013MS000266.

Prior allocation history in PRACE, national calls, as well as international programs such as INCITE of the US DoE

2018 – 2019 eFRontiers in dust minerAloGical coMposition and its Effects upoN climaTe, phase 1 (eFRAGMENT1). PRACE access. 34 Million cpu hours in Marenostrum IV Supercomputer

Participation by team members in other European Commission (EC) actions, such as ERC or Marie Skłodowska-Curie EC grants, etc.

ERC Consolidator Grant: Carlos Pérez García-Pando (FRAGMENT)

Marie Skłodowska-Curie: Martina Klose (DUST.ES)

Marie Skłodowska-Curie (CO-FUND) STARS program: Jerónimo Escribano

Previous presentations at PRACEdays

Basart et al. (2019) High Resolution Regional Dust Reanalysis based on Ensemble Data assimilation techniques (eDUST). PRACEdays19 - Euro HPC Summit Week – 13 – 17 May, Poznan, Poland.

Castrillo et al. (2019) Making Global coupled simulations possible. PRACEdays19 - Euro HPC Summit Week – 13 – 17 May, Poznan, Poland.

Serradell et al. (2017) Software stack deployment for Earth System Modeling using Spack. PRACE days17 - - Euro HPC Summit Week – 17 May, Barcelona, Spain.