Convocatorias 2017
Proyectos EXCELENCIA y Proyectos RETOS
AGENCIA ESTATAL DE INVESTIGACIÓN

Parte A: RESUMEN DE LA PROPUESTA/SUMMARY OF THE PROPOSAL

INVESTIGADOR PRINCIPAL 1 (Nombre y apellidos)**:**

Carlos Pérez García-Pando

INVESTIGADOR PRINCIPAL 2 (Nombre y apellidos)**:**

María Gonçalves Ageitos

TÍTULO DEL PROYECTO: CuaNtificación de la aportación presente y fUTuRa de hIErro biodispoNible de la aTmósfera al océano

ACRÓNIMO: NUTRIENT

RESUMEN Máximo 3500 caracteres (incluyendo espacios en blanco):

La productividad del océano depende del hierro biodisponible para la fotosíntesis, la respiración y la fijación de nitrógeno, lo que hace que el ciclo biogeoquímico del hierro module la capacidad del océano para absorber el CO_2 atmosférico. La aportación de hierro a la superficie del océano está dominada por el polvo mineral atmosférico emitido desde las superficies áridas y semiáridas del planeta. El polvo mineral contiene principalmente hierro insoluble, pero éste se transforma parcialmente en biodisponible durante el transporte atmosférico a través de diferentes mecanismos de disolución tales como la disolución ácida. Los aerosoles de combustión representan una pequeña fracción del hierro total, pero éste es más soluble que el hierro contenido en el polvo mineral. Siguen existiendo grandes incertidumbres sobre la aportación absoluta y relativa al hierro biodisponible tanto de las fuentes antropogénicas y naturales como de los mecanismos atmosféricos de disolución.

NUTRIENT tiene como objetivo mejorar nuestra comprensión de la aportación de hierro biodisponible al océano. El proyecto desarrollará y ajustará el ciclo del hierro atmosférico en el modelo climático EC-Earth, lo cual permitirá en el futuro simulaciones acopladas que tengan en cuenta el efecto de la deposición de hierro biodisponible en los ciclos del carbono y el nitrógeno. Nuestro principio rector será encontrar un equilibrio entre complejidad, eficiencia computacional y acuerdo con las observaciones. Esta pregunta es de interés para toda la comunidad de modelización que debe elegir el nivel adecuado de complejidad en sus propios modelos. NUTRIENT pondrá énfasis en aspectos novedosos tales como el papel de la mineralogía del polvo y de las fuentes antropogénicas de polvo en la deposición de hierro soluble.

El polvo mineral es una mezcla de diferentes minerales, cuyas abundancias relativas, distribución de tamaños, forma y estado de mezcla influyen en su efecto climático. Su contenido de hierro, especiación y habilidad para disolverse dependen de su mineralogía. Además, las reacciones químicas heterogéneas en su superficie que promueven la disolución ácida del hierro dependen de su composición mineralógica. En este sentido, NUTRIENT aportará avances en la representación de la mineralogía del polvo y sus efectos sobre el ciclo del hierro (1) proponiendo extensiones a la teoría de la fragmentación por fragilidad para describir adecuadamente la distribución de tamaños de los minerales del polvo al ser emitidos, e (2) investigando su influencia sobre la química heterogénea del polvo. NUTRIENT también cuantificará las contribuciones naturales y antropogénicas a la deposición de hierro soluble. En particular, proponemos cuantificar por primera vez la contribución de la fracción de polvo antropogénico (agrícola). El polvo emitido desde regiones agrícolas es potencialmente importante ya que hay evidencia de su composición es distinta de la que proviene de fuentes naturales.

Por último, exploraremos la deposición de hierro soluble en diferentes climas mediante la comparación de simulaciones de tiempo presente y final de siglo. Nuestra hipótesis es que las proyecciones futuras de hierro soluble dependerán en gran medida de los cambios proyectados en las emisiones antropogénicas (a través de cambios en la emisión de aerosoles de combustión y en la acidez atmosférica) y de las emisiones futuras de polvo.

PALABRAS CLAVE: hierro soluble, mineralogía del polvo atmosférico, aerosoles de combustión, modelización climática, química atmosférica

TITLE OF THE PROJECT: QuaNtifying the present and fUTure atmospheric deliveRy of bIoavailablE iroN to The ocean

ACRONYM: NUTRIENT

SUMMARY Maximum 3500 characters (including spaces):

Ocean productivity relies upon bioavailable iron (Fe) for photosynthesis, respiration and nitrogen fixation, which makes the Fe biogeochemical cycle a key modulator of the ocean's ability to uptake atmospheric CO2. The supply of Fe to the surface of the open ocean is dominated by soil dust aerosol created by wind erosion of arid and semi-arid surfaces. The emitted dust particles consist primarily of insoluble Fe that is partly transformed into bioavailable Fe species during atmospheric transport through a variety of dissolution mechanisms, for example acidic dissolution. Combustion sources account for a small fraction of the total Fe but it is considerably more soluble than dust Fe. Large uncertainties remain on both the absolute and relative contributions of anthropogenic and natural sources, and the atmospheric Fe dissolution mechanisms that determine the bioavailable Fe supply from the atmosphere to the ocean.

NUTRIENT aims to improve our understanding of the atmospheric delivery of bioavailable Fe to the ocean. The project will develop and constrain the atmospheric Fe cycle in the EC-Earth Earth System model, which will ultimately allow fully coupled simulations that account for the effect of bioavailable Fe variations upon the carbon and nitrogen cycles. Our guiding principle will be to find an optimum balance among complexity, computational efficiency and agreement to observations. This question is of interest to the broader modeling community who must choose the appropriate level of complexity in their own models. NUTRIENT will

emphasize on novel aspects such as the role of dust mineralogy and anthropogenic dust sources in the deposition of soluble Fe.

Soil dust aerosols are mixtures of different minerals, whose relative abundances, particle size distribution, shape and mixing state influence their effect upon climate. The dust Fe content, speciation and ability to dissolve depends upon mineralogy. Also, the rates of heterogeneous chemical reactions on the dust surface that promote acidic Fe dissolution depend on the dust mineralogical composition. NUTRIENT will advance the representation of dust mineralogy and its effects upon the Fe cycle by (1) proposing extensions to brittle fragmentation theory that better constrain the emitted size distribution of dust minerals and (2) by accounting for its influence upon dust heterogeneous chemistry. NUTRIENT will also quantify the natural and anthropogenic contributions to the soluble Fe deposition. In particular, we propose to understand, constrain and quantify for the first time the present-day anthropogenic (agricultural) dust fraction contribution to the soluble Fe deposition. Dust from cultivated regions is potentially important for the Fe cycle; there is evidence that it has a distinct composition from that arising from natural sources.

Finally, we will explore the soluble Fe deposition in different climates by comparing time-slice simulations for the present-day and future climate and emission scenarios. We hypothesize that projections will largely depend upon projected changes in anthropogenic emissions (through changes in the burden of combustion aerosols and in atmospheric acidity) and assumptions regarding future dust emissions.

KEY WORDS: soluble iron, aeolian dust mineralogy, combustion aerosols, climate modelling, atmospheric chemistry

Parte B: INFORMACIÓN ESPECÍFICA DEL EQUIPO

B.1. FINANCIACIÓN PÚBLICA Y PRIVADA (PROYECTOS Y/O CONTRATOS DE I+D+I) DEL EQUIPO DE INVESTIGACIÓN (repita la secuencia tantas veces como se precise hasta un máximo de 10 proyectos y/o contratos).

1. Investigador del equipo de investigación que participa en el proyecto/contrato (nombre y apellidos): Carlos Pérez García-Pando, Sara Basart, María Gonçalves
   Referencia del proyecto: AXA Chair 2015
   Título: AXA Chair on Sand and Dust Storms
   Investigador principal (nombre y apellidos): Dr. Carlos Pérez García-Pando
   Entidad financiadora: AXA Research Fund
   Duración (fecha inicio - fecha fin, en formato DD/MM/AAAA): 01/10/2016-30/08/2031
   Financiación recibida (en euros): 1 587 906,57€ (+ intereses de la dotación)
   Relación con el proyecto que se presenta: está muy relacionado
   Estado del proyecto o contrato: concedido

2. Investigador del equipo de investigación que participa en el proyecto/contrato (nombre y apellidos): Carlos Pérez García-Pando, Sara Basart, María Gonçalves
   Referencia del proyecto: ERC Consolidator Grant 2017
   Título: "*FRontiers in dust minerAloGical coMposition and its Effects upoN climaTe*" FRAGMENT
   Investigador principal (nombre y apellidos): Dr. Carlos Pérez García-Pando
   Entidad financiadora: Comisión Europea – Programa ERC Consolidator
   Duración (fecha inicio - fecha fin, en formato DD/MM/AAAA): 2018-2022
   Financiación recibida (en euros): 2 149 523€
   Relación con el proyecto que se presenta: está muy relacionado
   Estado del proyecto o contrato: pendiente de resolución (1ª fase: propuesta evaluada favorablemente, 2ª fase: entrevista personal en Octubre de 2017)

3. Investigador del equipo de investigación que participa en el proyecto/contrato (nombre y apellidos): Dr. Carlos Pérez García-Pando
   Referencia del proyecto: DoE DE-SC00671
   Título: *Improving the representation of soluble iron in climate models*
   Investigador principal (nombre y apellidos): Dr. Carlos Pérez García-Pando
   Entidad financiadora: US Department of Energy
   Duración (fecha inicio - fecha fin, en formato DD/MM/AAAA): 2011-2014
   Financiación recibida (en euros): 750 000$ (≈ 657 150 €)
   Relación con el proyecto que se presenta: está muy relacionado
   Estado del proyecto o contrato: concedido

4. Investigador del equipo de investigación que participa en el proyecto/contrato (nombre y apellidos): Dr Carlos Pérez García-Pando
   Referencia del proyecto: NASA ROSES
   Título: *Contribution to radiative forcing and climate by anthropogenic sources of dust aerosol*
   Investigador principal (nombre y apellidos): Dr. Ron Miller, Dr. Carlos Pérez García-Pando (co-PI)
   Entidad financiadora: NASA ROSES Modeling, Analysis and Prediction Program NASA
   Duración (fecha inicio - fecha fin, en formato DD/MM/AAAA): 2014-2016
   Financiación recibida (en euros): 1 020 000$ (≈ 893 620€)
   Relación con el proyecto que se presenta: está muy relacionado
   Estado del proyecto o contrato: concedido

5. Investigador del equipo de investigación que participa en el proyecto/contrato (nombre y apellidos): Dr Carlos Pérez García-Pando
   Referencia del proyecto: NGGPS

Título: *Implementation and testing of dust models for regional and global forecasting*
Investigador principal (nombre y apellidos): Dr. Paul Ginoux (NOAA GFDL), Dr. Carlos Pérez García-Pando (co-PI)
Entidad financiadora: R2O Initiative for the Next Generation Global Prediction System National Oceanic and Atmospheric Administration (US)
Duración (fecha inicio - fecha fin, en formato DD/MM/AAAA): 01/01/2015-30/09/2016
Financiación recibida (en euros): 200 000$ (≈ 175 225 €)
Relación con el proyecto que se presenta: está muy relacionado
Estado del proyecto o contrato: concedido

6. Investigador del equipo de investigación que participa en el proyecto/contrato (nombre y apellidos): Sara Basart
Referencia del proyecto: ERA4CS joint call 2016 (Topic B)
Título: Dust Storms Assessment for the development of user-oriented Climate Services in Northern Africa, Middle East and Europe (DustClim)
Investigador principal (nombre y apellidos): Dr. Sara Basart
Entidad financiadora: European Research Area for Climate Services (ERA4CS)
Duración (fecha inicio - fecha fin, en formato DD/MM/AAAA): 01/09/2017 - 30/09/2020
Financiación recibida (en euros): 319 125€ (2 133 640€ total)
Relación con el proyecto que se presenta: está muy relacionado
Estado del proyecto o contrato: concedido/pendiente de resolución

7. Investigador del equipo de investigación que participa en el proyecto/contrato (nombre y apellidos): Sara Basart
Referencia del proyecto: 654169
Título: Aerosols, Clouds, and Trace gases Research InfraStructure (ACTRIS-2)
Investigador principal (nombre y apellidos): Dr. Gelsomina Pappalardo
Entidad financiadora: H2020 European Comission
Duración (fecha inicio - fecha fin, en formato DD/MM/AAAA): 01/05/2015-30/04/2019
Financiación recibida (en euros): 90 000€ (9 541 215€ total)
Relación con el proyecto que se presenta: está muy relacionado
Estado del proyecto o contrato: concedido

8. Investigador del equipo de investigación que participa en el proyecto/contrato (nombre y apellidos): Carlos Pérez García-Pando (como colaborador externo) Sara Basart, María Gonçalves
Referencia del proyecto: CGL-2013-46736-R
Título: Aerosol forecasting and assessment of radiative forcing on weather and climate applications with the online NMMB/BSC-CTM model
Investigador principal (nombre y apellidos): Dr. Oriol Jorba
Entidad financiadora: MINECO
Duración (fecha inicio - fecha fin, en formato DD/MM/AAAA): 01/01/2014 - 31/12/2016
Financiación recibida (en euros): 170 610€
Relación con el proyecto que se presenta: está muy relacionado
Estado del proyecto o contrato: concedido

9. Investigador del equipo de investigación que participa en el proyecto/contrato (nombre y apellidos): Sara Basart, María Gonçalves, Carlos Pérez García-Pando
Referencia del proyecto: 157/PC08/3-12.0, 357/2007/2-12.1, 441/2006/3-12.1
Título: CALIOPE: Sistema de Calidad del aire operativo para España
Investigador principal (nombre y apellidos): Dr. Jose Baldasano
Entidad financiadora: Ministerio de Medio Ambiente
Duración (fecha inicio - fecha fin, en formato DD/MM/AAAA): 01/01/2006 - 01/07/2010
Financiación recibida (en euros): 1 189 285 €
Relación con el proyecto que se presenta: está muy relacionado
Estado del proyecto o contrato: concedido

10. Investigador del equipo de investigación que participa en el proyecto/contrato (nombre y apellidos): Sara Basart

  Referencia del proyecto: N/A

  Título: Convenio para la gestión y mantenimiento del Centro Regional para el Norte de África, oriente Próximo y Europa del Sistema de Evaluación y Aviso de Tormentas de Polvo y Arena de la OMM. Sand and Dust Storms – Warning Advisory System (SDS-WAS)

  Investigador principal (nombre y apellidos): Dr. Francisco Doblas-Reyes

  Entidad financiadora: AEMET

  Duración (fecha inicio - fecha fin, en formato DD/MM/AAAA): 02/05/2016-01/05/2018

  Financiación recibida (en euros): 133 044€

  Relación con el proyecto que se presenta: está algo relacionado

  Estado del proyecto o contrato: concedido

B.2. RELACIÓN DE LAS PERSONAS NO DOCTORES QUE COMPONEN EL EQUIPO DE TRABAJO (se recuerda que los datos de los doctores del equipo de trabajo y de los componentes del equipo de investigación no se solicitan aquí). Repita la siguiente secuencia tantas veces como precise.

N/A

MINISTERIO
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MEMORIA CIENTÍFICO-TÉCNICA DE PROYECTOS INDIVIDUALES (TIPO A o B)

Parte C: DOCUMENTO CIENTÍFICO. Máximo 20 páginas.

C.1. PROPUESTA CIENTÍFICA

1   Background and state of the art

Our incomplete understanding of the supply of bioavailable iron to the ocean

Approximately one quarter of the carbon dioxide (CO_2) emitted since the industrial revolution has been taken up by the ocean (Ciais *et al.*, 2013). Therefore, understanding how oceanic uptake of CO_2 will be modified this century is crucial to project future climate. Ocean productivity relies on enzymatic iron (Fe) for photosynthesis, respiration and nitrogen fixation. This makes the Fe biogeochemical cycle a key modulator of the ocean's ability to uptake atmospheric CO_2, where increased Fe can potentially act as a large negative feedback on the climate system (Martin, 1990; Jickells *et al.*, 2005).

Fluvial and glacial particulate Fe are the major sources of Fe reaching the ocean, but their influence is mostly limited to near-coastal areas (Poulton and Raisewell, 2002). The dominant external input of Fe to the surface of the open ocean is soil dust aerosol transported from arid and semi-arid regions, with an estimated present-day contribution of ~95%; combustion sources of Fe account for the remaining ~5% (Luo *et al.*, 2008). Nonetheless, ocean productivity depends specifically upon the Fe bioavailable fraction. Fe in soil dust is mostly insoluble when emitted from source regions, but it is hypothesized to be partly transformed into bioavailable Fe species during atmospheric transport through a variety of dissolution mechanisms. Combustion Fe, while a much smaller source, is considerably more soluble than dust Fe and may contribute up to 50% of the bioavailable Fe deposition (Luo *et al.*, 2008; Mahowald *et al.*, 2009; Ito, 2015; Winton *et al.*, 2015).

Large uncertainties remain on both the absolute and relative contributions of anthropogenic and natural sources, and the atmospheric Fe dissolution mechanisms that determine the bioavailable Fe supply from the atmosphere to the ocean. The lack of a universally accepted method to determine the soluble Fe fraction together with the scarcity of observations for constraining models additionally challenge the estimation of the bioavailable fraction (Ravelo-Pérez *et al.*, 2016). NUTRIENT aims to improve our understanding of the atmospheric delivery of bioavailable Fe to the ocean. A major goal of the project is to develop and constrain the atmospheric Fe cycle in the Earth System model (ESM) co-developed by the Barcelona Supercomputing Center (BSC). This will ultimately allow fully coupled simulations that account for the effect of bioavailable Fe variations upon the carbon and nitrogen cycles.

Constraining atmospheric Fe processing in models

The definition of bioavailable Fe is unclear because how organisms utilize Fe is not well understood (Jickells *et al.*, 2005). Bioavailable Fe is typically considered to be dissolved Fe in the ferrous (Fe(II)) oxidation state but ocean organisms have been observed to utilize Fe in different forms (Barbeau *et al.*, 1996). (For simplicity this proposal will use indistinctly the terms "bioavailable" and "soluble".) Soil dust aerosols created by wind erosion of arid and semi-arid surfaces make the largest contribution to the global aerosol load (Andreae, 1995; Textor *et al.*, 2006) and represent ~95% of the total Fe deposition to the ocean. The average Fe abundance in soils is ~3.5% (Duce and Tindale, 1991), which primarily consists of insoluble ferric Fe (Fe(III)) (Zhu *et al.*, 1997); Fe solubility in soils is less than ~0.1% (Fung *et al.*, 2000). However, much higher solubility is reported for atmospheric aerosols (e.g., Siefert *et al.*, 1999; Johansen *et al.*, 2000; Baker *et al.*, 2006a; b). Observations, modelling and laboratory studies suggest that dust Fe is modified downwind of their source (e.g., Zhuang *et al.*, 1992; Desboeufs *et al.*, 2001). A major mechanism leading to an increase of Fe solubility is acidic (proton-promoted) dissolution, with low pH conditions in aerosol water favoring Fe dissolution through the weakening of Fe-O bonds of Fe oxides, Fe hydroxides and aluminosilicates in dust (Johnson and Meskhidze, 2013). During atmospheric transport, dust undergoes heterogeneous chemical reactions with acidic trace gases of natural and anthropogenic origin, leading to the formation of coatings, such as sulfate and nitrate, and to other chemical transformations on the surface of the dust particles (Usher *et al.*, 2002; Cwiertny *et al.*, 2008). The balance between the acidic species, basic mineral compounds or

other basic substances present, such as ammonia, determines the pH of the aqueous solution coating the dust particles. However, proton-promoted Fe processing is likely to work in conjunction with other physical and chemical mechanisms such as <u>photochemical reduction and organic ligand processing</u> (e.g., Pehkonen *et al.*, 1993). Oxalate, the oxidation product of oxalic acid, can act as an organic ligand, enhancing Fe dissolution in aqueous solutions under moderately acidic conditions (Cornell and Schindler, 1987; Xu and Gao, 2008; Solmon *et al.*, 2009; Paris *et al.*, 2011). Laboratory studies have demonstrated that Fe(III)-oxalate complexes can be photo-reduced to Fe(II) forms, increasing the fraction of dissolved Fe. The oxalate-mediated mechanisms for Fe(II) formation depend upon the availability of oxalic acid or oxalate compounds, which have mostly an anthropogenic origin, and are largely dependent on sunlight, having special relevance during daytime.

Different levels of model complexity have been employed to simulate atmospheric Fe dissolution: from simple schemes including first order rate processing constants applied to a globally uniform 3.5% of Fe in dust (e.g., Luo *et al.*, 2008), to more complex ones allowing different types of acidic species to interact with dust that account for mineral-specific dissolution rates and oxalate processing (Meskhidze *et al.*, 2005; Johnson and Meskhidze, 2013; Ito and Xu, 2014; Ito, 2015; Myriokefalitakis *et al.*, 2015; Ito and Shi, 2016). <u>The comparison of different modeling studies indicates that complexity, and therefore increased computational expense, does not necessarily imply a better match to available observations.</u> In a recent study co-authored by the PI of this proposal, an intermediate-complexity Fe dissolution scheme was proposed, implemented and tested in the NCAR Community Earth System Model (CESM; Scanza et al., 2017; Figure 1). The scheme includes basic features of more complex mechanisms but uses simplifications to represent pH regimes and mineral-specific dissolution rates that can be used with standard (mass-based) aerosol schemes available in most ESMs.
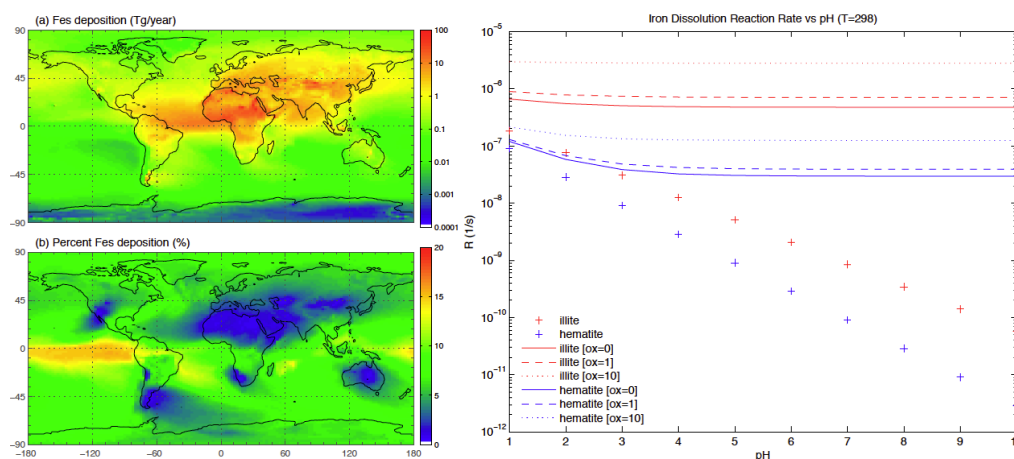
Figure 1. Left panel: Spatial distribution of annually averaged soluble Fe deposition from both dust and combuson in Tg/year (a). Spatial distribution of annually averaged fractional Fe solubility from dust and combustion (%) (b). Right panel: Fe dissolution rates for illite and hematite. + indicates proton-promoted dissolution; solid, dashed and dotted lines are the addition of proton-promoted and oxalate-promoted dissolution rates. From Scanza et al. (2017).

The results show that while the model is not able to capture all of the observational variability, it is within range of the observational mean. The scheme performs as well as some of the computationally intensive methods in matching available observations of soluble Fe and is computationally efficient, which allows for multi-decadal to centennial simulations. The balance among complexity, accuracy and computational efficiency is crucial in Earth System modelling. <u>In NUTRIENT we propose to implement and constrain a Fe processing mechanism in an ESM building upon our previous work and taking into account recent experimental results. One of our goals is to better represent the observational variability. Our guiding principle will be to find an optimum balance among mechanistic representation, complexity, computational efficiency and agreement to observations. This question is of interest to the broader modeling community who must choose the appropriate level of complexity in their own models.</u>

Accounting for dust mineralogy

ESMs typically assume that dust aerosols have a globally uniform composition, neglecting the known local and regional variations in the mineralogical composition of the sources (Claquin *et al.*, 1999; Nickovic *et al.*, 2012; Journet *et al.*, 2014). Modeling efforts have focused on constraining dust sources (e.g., Ginoux *et al.*, 2001), emission (e.g., Cakmur *et al.*, 2006) and particle size distribution (PSD, e.g., Mahowald *et al.*, 2014). In reality, dust aerosols are a mixture of different minerals, whose relative abundances, PSD, shape, surface topography and mixing state influence their effect upon climate (Scheuvens and Kandler, 2014; Kiselev et al., 2016). The Intergovernmental Panel on Climate Change (IPCC) has identified dust mineralogy as a key uncertainty in the overall contributions of aerosols to radiative forcing (Boucher *et al.*, 2013; Myhre *et al.*, 2013). Two examples are the absorption of solar radiation by dust that is strongly related to the presence of Fe oxides (e.g., Wagner *et al.*, 2012); and the key role of K-feldspar in ice nucleation (e.g., Atkinson *et al.*, 2013).

The atmospheric Fe cycle is affected by dust mineralogy in multiple ways. The atmospheric lifetime of dust depends upon hygroscopicity, which increases during transport and depends on mineralogy (e.g., Hatch *et al.*, 2014). The rates of heterogeneous chemical reactions on the dust surface that form coatings of sulfate and nitrate promoting acidic Fe dissolution depend on the dust mineralogical composition (Usher *et al.*, 2003; Krueger *et al.*, 2004; Al-Hosney *et al.*, 2005, Rubasinghege *et al.*, 2013). For example, the uptake of sulfur dioxide by calcite exceeds by at least an order of magnitude uptake by quartz, feldspar and hematite (e.g., Harris *et al.*, 2012; Kong *et al.*, 2014). Finally, the dust Fe content, speciation and ability to dissolve depends also upon mineralogy (Journet *et al.*, 2008; Shi *et al.*, 2011). Fe in dust is mostly in the form of Fe oxides/hydroxides, mainly hematite and goethite, and in the crystalline structures of aluminosilicate minerals. Fe associated with micrometer-sized hematite and goethite is tightly bound as Fe oxides/hydroxides and its dissolution even under very acidic conditions is slow. Conversely, ferrihydrite, nano-sized Fe oxides, and heterogeneous inclusions of nano-Fe grains in aluminosilicates (e.g., illite, smectite, and chlorite) follow rapid dissolution owing to their high surface area (Shi *et al.*, 2011; Ito and Xu, 2014; Ito and Shi, 2016). Some studies also consider that Fe within aluminosilicate mineral lattices may be appreciable sources of soluble Fe (Journet *et al.*, 2008).

Modelling the global dust mineralogical composition poses key challenges. The most significant ones are related to constraining the emission of the different minerals and their PSD (Perlwitz *et al.*, 2015a; b; Scanza *et al.*, 2015; Pérez García-Pando *et al.*, 2016). The first difficulty is that soil mineralogy atlases for dust modelling are derived by massively extrapolating an inhomogeneous and limited set of mineralogical analyses of soil samples that are particularly scarce in the arid and semi-arid areas that contain the dust sources (e.g., Claquin *et al.*, 1999). The second one is that these atlases are based upon measurements following wet sieving, a technique that disperses (breaks) the mineral aggregates found in the undisturbed parent soil, replacing them with a collection of smaller particles (e.g., Chatenet *et al.,* 1996; Shao, 2001; Laurent *et al.*, 2008). During emission, the original, undisturbed aggregates are fragmented, but only partially. This results in differences in the PSD, mineralogy and mixing state between the emitted particles derived from the undisturbed soil versus the disturbed (wet-sieved) soil (Figure 2; Pérez García-Pando *et al.*, 2015).

In recent studies co-authored by the PI of this proposal (Perlwitz *et al.*, 2015a; 2015b; Pérez García-Pando *et al.*, 2015; Pérez García-Pando *et al.*, 2016), it was shown that Brittle Fragmentation Theory (BFT) (Kok *et al.*, 2011) provides a valuable framework to predict the emitted PSD in terms of its
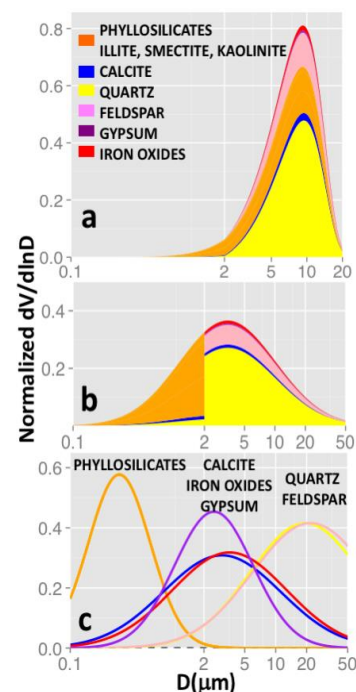
Figure 2. Example of (a) emitted PSD and mineralogy by BFT; (b) average soil dispersed PSD and mineral fractions; (c) proposed extension of BFT by fitting mineral-specific PSDs.

constituent minerals. BFT predicts that the emitted PSD (Figure 2a) is shifted toward larger diameters compared to the PSD of the dispersed soil (Figure 2b). That is, the fragmentation of mineral aggregates, specially phyllosilicates, during saltation preserves a greater fraction of mass at silt sizes compared to the breaking of aggregates during dispersion of the soil prior to analysis. The colored areas in Figure 2b are an example of the bulk mineral fractions within the clay size range (0-2 μm) and the silt size range (2-50 μm) derived from a global atlas and fitted to a monomodal PSD based upon measurements of a disturbed soil. Despite the crude size-dependence of the mineral fractions derived from the soil type atlas, the emitted PSD derived using BFT (Figure 2a) significantly improves our ability to predict global measurements of the dust mineral composition (Perlwitz *et al.*, 2015b). Recent Fe modelling studies co-authored by the PI (Scanza *et al.*, 2017) and other groups (Ito and Shi, 2016) include BFT to describe the emitted PSD of individual minerals. In NUTRIENT we will further advance on better representing both dust mineralogy (Figure 2c) and its effects upon the Fe cycle in ESMs by extending BFT and by accounting for its influence upon heterogeneous chemistry.

**Constraining natural and anthropogenic contributions**

Both natural and anthropogenic aerosols and gases contribute to the burden of soluble Fe. Current models estimate the deposition of soluble Fe to be a factor of ~2 higher for current climate compared to the preindustrial era (Myriokefalitakis *et al.*, 2015; Ito and Shi, 2016; Scanza *et al.,* 2017). These results account for the large increases in emitted Fe from industrial combustion sources along with the increased acidity of the atmosphere enhancing dust Fe dissolution over the past 100 years. In the study co-authored by the PI of NUTRIENT (Scanza *et al.*, 2017), also dust (and therefore dust Fe) emission was considered to be a factor of ~2 higher for current climate compared to the preindustrial era based on paleodata. Indeed, a doubling of global dust deposition during the 20th century has been inferred from ice core, lake sediment and coral records by Mahowald *et al.* (2010).

The observed contrast in dust emissions between the industrial era and the present day had to be forced in the model of Scanza *et al.* (2017). Current models are not able to simulate the large measured variations in deposition based solely on variations in meteorology that control dust emission, transport, and removal. This implies that there have been significant changes in the spatial extent of dust sources, an aspect that is not properly treated in current models. The problem is challenging since changes in dust source strength may have resulted from changes in land-use (due to cultivation and grazing associated with the increasing global population), as well as natural and anthropogenic changes in lake extent that expose fine sediment to wind erosion (Ginoux *et al.*, 2012a). The anthropogenic dust fraction is potentially important for the Fe cycle; there is evidence that dust aerosols created by human activity have a distinct composition from dust arising from natural sources. Ginoux *et al.* (2012b) show that anthropogenic dust sources are coincident with high levels of atmospheric ammonia. Ammonia is a precursor to heterogeneous chemical reactions associated with the uptake of nitrate aerosols and ammonium salts onto the surface of dust particles (Bauer *et al.*, 2007). Cultivated regions are enriched in ammonium precursors due to the use of fertilizers and large number of livestock (Beusen *et al.*, 2008), both of which are expected to increase in the coming century as the demand for food security increases with population. Cultivated sources are also expected to be enriched in Fe-bearing minerals including hematite and clays. This is because agriculture is practiced in regions where soil moisture is present during at least part of the year, and this moisture chemically weathers silicate minerals, creating clays along with Fe oxides and hydroxides like hematite and goethite.

The contribution of (anthropogenic) land use dust emission in the present day remains still subject to debate, with values ranging from 10% (Tegen *et al.*, 2004) to at least 50% (Tegen et al., 1996; Mahowald et al., 2004). Ginoux *et al.* (2012a) used high-resolution MODIS radiances to identify sources where the atmospheric column is frequently dusty. Sources were attributed to cultivation according to a land use atlas (Goldewijk, 2001). Maps of both natural and cultivated sources were introduced into a dust transport model; the anthropogenic fraction of present-day dust emission was estimated to be ~25 %. The calculated anthropogenic fraction is very sensitive to assumptions in the threshold of wind erosion in cultivated regions. Ginoux *et al.* (2012a) prescribe a uniform threshold for

anthropogenic sources that is higher than the natural source threshold: a heuristic representation of elements that inhibit wind erosion in cultivated environments, including higher soil moisture and more extensive vegetation that shields the soil from the force of the wind. In a recent project funded by NASA, where the PI of this proposal participated, the same dust source maps were introduced into the NASA Goddard Institute for Space Studies (GISS) Earth System ModelE2 (Miller *et al.*, 2014). The assumed threshold increases with soil moisture for both natural and anthropogenic sources, so that this inhibition was explicitly modeled, but the effect of contrasts in vegetation were omitted between the two source types. The derived anthropogenic fraction was estimated to be twice as large as the estimate of Ginoux *et al.* (2012a).

In NUTRIENT, we argue that differing treatments of the threshold wind speed between models is a key impediment to reducing the uncertainty of the anthropogenic fraction of dust emission (and the corresponding climate effect). In this sense, we are currently developing a new parameterization of the wind speed threshold for global models, including its dependence upon vegetation (Ginoux *et al.*, 2015; Pérez García-Pando *et al.*, 2017). The parametrization accounts for the partitioning of the force of the wind between the erodible soil particles and non-erodible roughness elements. The parameterization calculates a correction factor (f_R) that decreases as the surface gets rougher, so that a stronger wind (or more precisely, a higher wind stress) is needed to mobilize soil particles (Figure 3). NUTRIENT will quantify the natural and anthropogenic contributions to the soluble Fe deposition. In particular we propose to understand, constrain and quantify for the first time the present-day anthropogenic dust fraction contribution to the soluble Fe deposition based on our new parameterization.
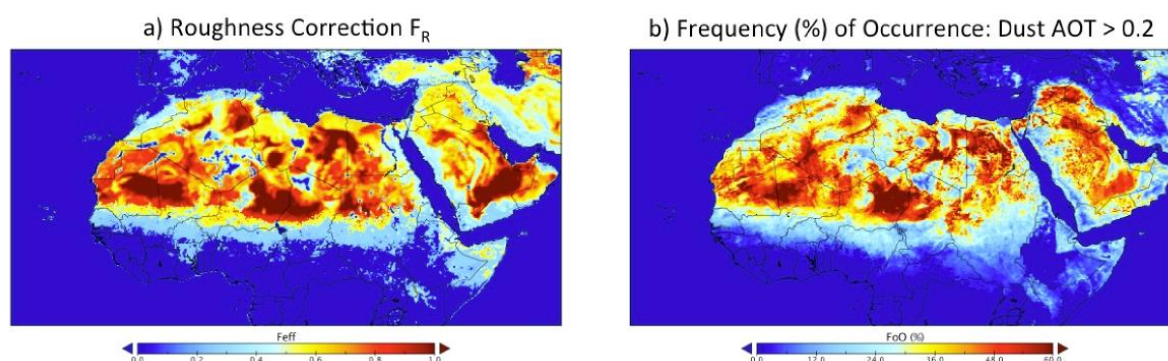

Figure 3. The threshold correction f_R (that increases the wind threshold for emission based upon topographic roughness and vegetation) strongly resembles the frequency of occurrence of dust optical thickness greater than 0.2. This suggests that prolific dust sources correspond to where the emission threshold is low, and that ESMs must represent variations in this threshold and its contrast between natural and anthropogenic sources. From Pérez García-Pando *et al.* (2017).

Earth System modelling at the Barcelona Supercomputing Center

EC-Earth is a state-of-the-art ESM collaboratively developed by European research centers from 10 different countries including BSC (Hazeleger *et al.*, 2012; Figure 4). EC-Earth integrates the Integrated Forecast System (IFS) coupled with the general ocean circulation model Nucleus for European Modelling of the Ocean (NEMO version 3.6, Madec 2008). Sea ice processes are represented by the Louvain-la-Neuve sea ice model (Vancoppenolle et al. 2012, LIM3) and marine biogeochemistry through PISCES (Aumont *et al.*, 2015) as part of the NEMO system. The Tracer Model 5 (TM5) allows for interactive simulation of atmospheric chemistry and transport of aerosols and reactive gas species (De Brugh *et al.*, 2011; Van Noije *et al.*, 2014). The LPJ-Guess dynamic vegetation model (Smith *et al.*, 2001), which considers the phenological cycle of natural vegetation, is coupled to the land surface model in IFS, H-TESSEL (Balsamo *et al.*, 2009). The OASIS-MCT software handles synchronized exchanges of information and interpolation between the different models. Early versions of EC-Earth contributed to the Coupled Model Intercomparison Project Phase 5 (CMIP5), provided information for downscaling exercises at regional scale, and have been used to study further feedbacks on the climate system and climate predictability. The latest model upgrades are oriented towards the CMIP6 exercise. In this context, our group is

contributing to the AerChemMIP experiments, which aim to quantify the climate impacts of aerosols and chemically reactive gases within CMIP6.
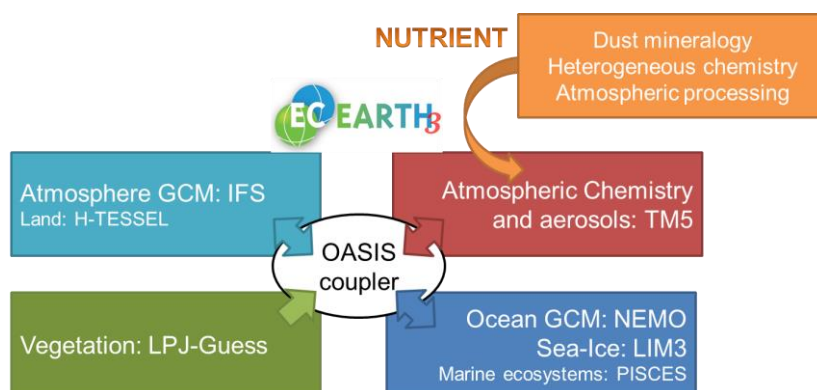
Figure 4. Main components of EC-Earth and developments proposed in NUTRIENT.

NUTRIENT will undertake the proposed developments and research within EC-Earth. All our developments will be implemented into the atmospheric chemistry component (TM5). One of the main outcomes of NUTRIENT will be the provision of online bioavailable Fe fluxes to the marine biogeochemistry component of the model (PISCES).

2   Objectives, hypotheses and key scientific questions addressed by NUTRIENT

The overarching goal NUTRIENT is to **improve our understanding and quantify the atmospheric supply of bioavailable Fe to the ocean**. The specific objectives are:

1) To develop and implement an atmospheric Fe lifecycle module into the EC-Earth ESM:

To achieve this objective we will build upon our previous studies and take into account recent experimental results. We hypothesize that 1) both dust and combustion aerosols are the major sources of bioavailable Fe to the ocean and therefore need to be properly described in the model; 2) accounting for the effect of dust mineralogy upon heterogeneous chemistry and Fe dissolution will produce a better match to observations; 3) parameterization complexity does not necessarily imply better results.

Our guiding principle will be to find an optimum balance among mechanistic representation, complexity, computational efficiency and agreement to observations. We will constrain the present-day soluble Fe deposition based on a thorough evaluation with available observations.

2) To improve and implement dust mineralogy in EC-Earth based on extensions of brittle fragmentation theory (BFT) and an updated soil mineralogy dataset:

We plan to apply improvements in the representation of the emitted PSD of dust minerals building upon our previous work. We hypothesize that approximate knowledge of the characteristic PSDs of each mineral in the dispersed soil is key to constraining the global mineralogical composition. Based on the bulk content of each mineral in the clay and silt size ranges and on several assumptions, we recently fitted mineral-specific dispersed PSDs (Figure 2c shows an example for one soil type). Our fitting matches qualitatively the expected soil particle sizes for each mineral. For example, feldspar and quartz feature larger median diameters in the soil than other silt minerals such as calcite. Extending BFT with this new dependence upon soil PSD is expected to improve our representation of the lifecycle of dust minerals and therefore the Fe cycle as well.

3) To advance in our understanding of the relative role of the natural versus anthropogenic sources of soluble Fe and of the different atmospheric dissolution mechanisms:

Because the distinction between dust and combustion aerosols has been assessed in previous studies, NUTRIENT will emphasize on the distinct impact upon soluble Fe from the natural and anthropogenic sources of dust, an aspect that has never been tackled before. We will quantify the present-day anthropogenic dust fraction contribution to the soluble Fe

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deposition using a source map derived from satellite and land use data together with our new wind threshold parameterization to represent dust emission (Figure 3). <u>Our questions include</u>: Do anthropogenic sources make a significant contribution to soluble Fe (compared to natural sources)? Does this reflect differences in the composition of parent soils of anthropogenic and natural dust sources?

4) <u>To quantify present-day and project future changes (end of the century) in the soluble Fe deposition to the ocean</u>

To see the effect of soluble Fe processing in different climates, we will carry out time-slice experiments for the present-day and future climate and emission scenarios. <u>We hypothesize</u> that projections will largely depend upon projected changes in anthropogenic emissions (through changes in the burden of combustion aerosols and in atmospheric acidity) and assumptions regarding future dust emissions.

3   Relevance, adequacy and challenge addressed

NUTRIENT aims to constrain the deposition of soluble Fe, which is crucial for marine productivity and the carbon and nitrogen cycles. NUTRIENT is therefore aligned with the research priorities defined by the World Climate Research Program (WRCP) from the World Meteorological Organization (WMO) and IPCC. WRCP identifies the characterization of *carbon feedbacks in the climate system* as one of the <u>7 Grand Challenges,</u> where emphasis in scientific research, modelling, analysis and observations has to be put in the coming decade. Climate-carbon cycle model assessments within AR5 identified the Southern Ocean as a key place for oceanic carbon uptake. However "*the variability of that sink and its response to future changes remain very poorly assessed and represented in models*". In this region, little changes on atmospheric soluble Fe inputs may have a disproportionately large global impact (Jickells *et al.*, 2005). Although carbon-climate feedbacks were considered in the AR5 temperature projections, other biogeochemical feedbacks (e.g., related to dust) were not. The quantification of the risk of large biogeochemical-climate feedbacks is one of the knowledge gaps where attention has to be focused, according to the "*IPCC 5th Assessment Report (AR5): Lessons Learnt for Climate Change Research and WCRP*" workshop report (WRCP, report nº 5/2015). Thus, methods have to be developed to allow full consideration of biogeochemical-climate feedbacks within ESMs, and NUTRIENT will provide insights on how to deal with the atmospheric Fe cycle influencing them.

NUTRIENT will provide better understanding of this research problem, whereby matching the premises of the challenge "*6.4.5. Reto en acción sobre el cambio climático y eficiencia en la utilización de recursos y materias primas"*, as defined in the "*Plan Estatal de Investigación Científica y Técnica y de innovación 2013-2016*", and in particular those of the sub-items *I. Cambio Climático* (i) and (viii) dealing with *"investigación aplicada al desarrollo de las técnicas de análisis y modelización de datos"*. Likewise, the objectives and expected outcomes of NUTRIENT tightly follow the H2020 societal challenge "*Climate action, environment, resource efficiency and raw materials*", since the project will increase European competitiveness in Earth System Modelling; this advance is assembled through the priority line "*Fighting and adapting to climate change*". NUTRIENT, through the improvement and implementation of a dust mineralogy in an ESM, will also provide valuable input to the short-term mineral dust modelling community. NUTRIENT outcomes will be shared within the framework of the Sand and Dust Storm Warning and Assessment System (SDS-WAS) of WMO, which gathers meteorological services and agencies from different countries, including the Agencia Estatal de Meteorología (AEMET). NUTRIENT also contributes to the objectives defined by the *"Estrategia Española de Ciencia y Tecnología y de Innovación 2013-2020"* promoting the formation of new research personnel, the collaboration with national and international research institutions, and the development of cutting-edge technologies.

4   Background of the group, role of the PIs and other groups working in the topic

Principal Investigator 1. Dr. Carlos Pérez García-Pando´s research focuses on understanding the physical and chemical processes controlling atmospheric aerosols, and on evaluating their effects upon climate, ocean biogeochemistry, air quality and health. After 8 years as a researcher at NASA and Columbia University, he joined the BSC in October 2016

as Head of the Atmospheric Composition group (AC-BSC). He also holds an AXA Chair (Cátedra AXA) on Sand and dust storms generously funded by the AXA Research fund, with which he will be developing a unified and cross-disciplinary dust research program at BSC over the next 15 years. He also recently obtained the Ramon y Cajal fellowship after being ranked first by the Earth Sciences panel. His group is composed of 12 people including senior researchers, postdocs, PhD students and technical support staff.

Dr. Pérez García-Pando has led recent contributions to basic, applied and cross-disciplinary aspects in the field of dust aerosols that are relevant to this proposal (see CVA for details). In a collaborative project between Columbia University, NASA and Cornell University funded by the US Department of Energy and led by Dr. Pérez García-Pando, 1) he proposed novel methods to represent the emitted PSD of dust minerals (Perlwitz *et al.*, 2015a, 2015b; Pérez García-Pando *et al.,* 2016), and 2) contributed to the development of an intermediate complexity Fe dissolution scheme in the NCAR Earth System model. Together with his NASA colleagues he also contributed to further understanding of the mechanisms by which dust affects global and regional climate. Through other projects funded by NASA and NOAA Dr. Pérez developed the parameterization of threshold wind speed to constrain the anthropogenic fraction. All these results are the starting point of the work proposed in NUTRIENT. We note that Dr. Pérez recently submitted an ERC Consolidator Grant entitled: "FRontiers in dust minerAloGical coMposition and its Effects upoN climaTe (FRAGMENT)" that has passed to Step 2 in the evaluation process (Interview in Brussels in October). He is also part of the Science Team of the "Earth surface Mineral dust source InvesTigation (EMIT). EMIT is under review within the NASA Earth Venture Instrument-4 program, and proposes to send a hyperspectral imager to the International Space Station (ISS) during a 12- month mission to measure the global soil mineralogical composition. Other members of the team include: Robert O. Green, JPL (PI); Natalie M. Mahowald (Deputy PI), Cornell Roger Clark, PSI; Paul Ginoux, NOAA; Olga Kalashnikova, JPL; Ron Miller, NASA; Greg Okin, UCLA; Bethany Ehlmann, Caltech; Luis Gaunter, DLR. Dr. Pérez García-Pando will be the coordinator of NUTRIENT and PI1 in charge of WP1 and WP3 (see methodology section).

Principal Investigator 2. Dr. María Gonçalves brings in her strong background on atmospheric emissions and atmospheric chemistry modelling. She has experience in defining new processes within air quality and emission models (e.g., Gonçalves *et al.*, 2009a; 2012) and quantifying the contribution of different processes to pollution episodes (Gonçalves *et al.*, 2009b). She has been involved in numerous model development and evaluation activities, for air quality (e.g., Pay *et al.*, 2010; Gonçalves *et al.*, 2008; 2009b; 2012), global atmospheric gas-phase chemistry (Badia *et al.*, 2017) and regional climate models (e.g., Barrera *et al.*, 2014; Gonçalves *et al.*, 2014). She is currently working with the EC-Earth ESM and she will be involved in the ES-BSC contribution to the AerChemMIP project, including a DECK simulation with coupled atmosphere-ocean and full-chemistry and a shorter run using atmospheric chemistry with prescribed SSTs to assess the effect of doubling mineral dust emissions. Dr. María Gonçalves will act as PI2 in NUTRIENT and will be in charge of WP2.

Dr. Sara Basart is a postdoctoral researcher at BSC. Her research covers mineral dust modelling, air quality and aerosols. She is a major contributor to the WMO Sand and Dust Storm Warning Advisory and Assessment System Regional Center for Northern Africa, Middle East and Europe, and the Barcelona Dust Forecast Center (BDFC), hosted by AEMET and BSC. She has participated in a number of national and international projects and co-authored more than 30 peer reviewed publications, mostly on dust modeling and observations. Dr. Sara Basart has a very strong background on aerosol model evaluation and she will contribute in all model evaluation activities within NUTRIENT (WP1 and WP2).

Dr. Jack Ogaja holds a doctoral degree in Natural Sciences from Brandenburg University of Technology (BTU, Cottbus-Senftenberg) in Germany, awarded in 2016. His doctoral thesis was funded by the German Weather Service (DWD) under the topic 'Towards Conservative Dynamical Core for COSMO model'. From 2010 he actively participated in the development of the COSMO model. Since 2016, he has worked on the computational performance of the new schemes and prepared the new schemes for NWP application by DWD under a postdoctoral fellowship before joining BSC in June 2017. Dr. Ogaja is currently working as Model Developer at BSC. He he will contribute to the development of the soluble Fe scheme (WP2).

In addition to the Research Group described above, NUTRIENT will count with a very strong Working Group composed of four world-class researchers in the field: **Dr. Ron Miller (NASA, US), Dr. Jan Perlwitz (NASA, US), Dr. Paul Ginoux (NOAA GFDL) and Dr. Yves Balkanski (IPSL, France)**. All of them are collaborators of Dr. Pérez García-Pando and have co-authored novel contributions in recent years in many of the aspects tackled in NUTRIENT. Their contribution is highlighted in the methodology section.

Other groups: To our knowledge, at national level there are no other modelling groups working specifically on developing soluble Fe schemes within ESMs. However, there are many strong experimental groups working on global and regional biogeochemistry that may benefit from our work. We highlight the group of Dr. Josep Peñuelas, who is the PI of a ERC Synergy grant tackling the Phosphorus Cycle (Imbalance-P). At the international level, we highlight the modelling contributions of Akinori Ito (Japan Agency for Marine-Earth Science and Tech.), Maria Kanakidou (University of Crete), Stelios Myriokefalitakis (Utrecht University), Natalie Mahowald (Cornell U.) and Nicholas Meskhidze (North Carolina State U.). We note that while the list is not exhaustive, it samples well the state-of-art in soluble Fe modelling for ESMs.

5   Methodology

To achieve the proposed objectives, we have organized NUTRIENT into four work-packages (WP). **WP1** will focus on the development, implementation and evaluation of the anthropogenic and natural Fe and mineral sources and emissions in the model. **WP2** will be devoted to the development, implementation and evaluation of a mineral-dependent soluble Fe mechanism, and to the assessment of the impact of mineralogy upon dust heterogeneous chemistry and acidity. **WP3** will quantify the deposition of soluble Fe to the ocean both in the present-day and the future, along with the relative contributions to soluble Fe of natural dust, anthropogenic dust and combustion aerosols. **WP4** will ensure the appropriate management of the project and broadly disseminate the outputs throughout its duration.

Model: All our developments will be implemented in the CMIP6 version of EC-Earth (EC-Earth v3.2) at the standard atmosphere-chemistry resolution: T255L91 (~0.75º) for IFS (atmosphere) and 3ºx2º for TM5 (chemistry). TM5 includes many advanced features that will facilitate the success of our Fe dissolution scheme. Gas-phase tropospheric chemistry is solved through the Carbon Bond 5 (CB05) chemical mechanism. TM5 also accounts for some aqueous chemistry reactions, and the heterogeneous chemistry of dinitrogen pentoxide to produce nitric acid. Aerosol microphysics are handled through the M7 scheme, which defines 7 modes characterized by log-normal size distributions with pre-defined geometric standard deviations: 4 soluble and 3 insoluble. Black carbon, organic carbon, sulfate, sea salt and dust are internally mixed and each mode is characterized by the mass of each component and the total particle number. Nucleation of sulfate droplets, water uptake, and particle growth through condensation or coagulation are considered within M7. A scheme to parametrize Secondary Organic Aerosols (SOA) has been recently included in the model. The EQSAM thermodynamic equilibrium model represents the aerosol-gas partition of semi-volatile inorganic species, such as nitrate-nitric acid or ammonium-ammonia.

WP1. Mineral and Fe anthropogenic and natural emission

WP1 will implement and constrain the natural and anthropogenic soil dust emission for the present-day (Task 1.1), dust mineralogy (Task 1.2), and combustion and dust Fe emissions (Task 1.3) in EC-Earth/TM5. A thorough evaluation with available observations will be performed in all tasks. Dr. Pérez García-Pando will be the PI in charge of this WP.

Task 1.1 Natural and anthropogenic dust emission for the present-day

We will implement the natural and cultivated dust source map of Ginoux *et al.* (2012a) along with separate tracers for natural and anthropogenic dust in the model, and we will constrain their contributions to the total dust burden. Because environmental contrasts between natural and cultivated regions are large, we need a physically based model of the threshold that accounts for these differences. We will implement and calibrate a new parameterization of the wind speed threshold that accounts for the partitioning of the force of the wind between the erodible soil particles and non-erodible roughness elements (Perez García-Pando *et al.*,

2017). The latter includes pebbles, rocks, local topography and vegetation that reduce the force of the wind on the erodible soil particles. This shielding can be represented by a reduction in the surface wind stress. Alternatively, the threshold for emission can be increased (Figure 3a). Our approach is to assume that the roughness is controlled predominately by variables that are related to satellite retrievals with high spatial resolution: namely, a static aerodynamic roughness length for arid regions (Prigent *et al.*, 2012) along with a time varying contribution roughness related to monthly variations of vegetation derived from MODIS leaf area index.

Evaluation: For comparison with observations, our model winds will be nudged toward observed (reanalyzed) values so that the circulation and aerosol transport resemble the actual conditions. Our simulations will cover the quantitative satellite era, i.e., from year 2000 to the present-day. First, we will constrain the global emission in the model by bringing the dust cycle into optimal agreement with a worldwide array of measurements including aerosol optical depth (AOD) retrieved by MODIS and AERONET (Cakmur *et al.*, 2006). Our optimization is also subject to size distribution retrieved by AERONET and standard measurements of surface concentration and deposition. This constraint is necessary because the coefficient of proportionality between wind speed and the emitted mass of dust must be determined empirically, and optimization provides an explicit and reproducible criterion for adjustment. Note that only the global emission is adjusted with this approach. Comparison of regional (and seasonal) variations in the dust cycle with satellite and AERONET retrievals remains an independent test of the quality of the model. Previous comparisons have typically emphasized climatological values. However, a key additional constraint for the calibration of our scheme will be the frequency of occurrence that different thresholds of dust optical depth (taken from MODIS Deep Blue retrievals) are exceeded (Ginoux *et al.*, 2012a; Figure 3b). Frequency of Occurrence is an especially appropriate constraint upon the wind speed threshold that determines how often the winds are strong enough to mobilize dust.

Group contributions: Sara Basart (evaluation), Ron Miller (global optimization), Paul Ginoux (dust source mapping), IT1 (technical support for implementation in EC-Earth and evaluation)

Task 1.2 Dust mineralogy

In our previous work on modelling dust mineralogy (e.g., Pérez García-Pando *et al.*, 2016) we used the soil mineralogical dataset of Claquin *et al.* (1999). In NUTRIENT, we will implement the most recent dataset available that characterizes the clay (0-2 μm) and silt (2-63 μm) size ranges of FAO soil types (units) in terms of abundance of 12 key minerals important for dust-climate interactions, i.e., quartz, feldspar, illite, smectite, kaolinite, chlorite, vermiculite, mica, calcite, gypsum, hematite and goethite (Journet *et al.*, 2014). This dataset represents a substantial improvement compared with previous versions. We will improve and apply our extended version of brittle fragmentation theory (BFT) to this updated dataset to represent the emitted PSD of each mineral in each grid cell of the model (Figure 2). Our new approach requires fitting mineral-specific dispersed PSDs by combining the mineralogical dataset and a soil texture dataset that provides the fractions of clay and silt in the soil. Global characterization of soil types will be based on Harmonized World Soil Database v1.2, which provides a characterization of soil units according to the FAO classification. We will develop a customizable dataset of the emitted PSD for each mineral that is flexible enough to be used by different models and resolutions.

In this case, we will also implement separate tracers for each mineral in the model. The emission of each mineral will be calculated by combining the total emission (constrained in Task 1.1) and the normalized emitted mineral PSDs derived from the application the extended BFT.

Evaluation: We will perform nudged simulations from 2000 to present-day including mineral tracers and using the dust sources and emission constrained through Task 1.1. We will use the evaluation framework for minerals that is thoroughly described in one of our recent contributions (Perlwitz *et al.*, 2015b). Our compilation of observations gathers data from more than sixty studies and includes information on size and fractional mineral abundance (Table 1 and Figure 1 in Perlwitz *et al.*, 2015b).

Group contributions: Sara Basart (evaluation), Yves Balkanski (provision of updated soil mineral dataset), Jan Perlwitz (support with BFT), IT1 (technical support for implementation in EC-Earth and evaluation), PD1 (proposing and testing extensions of BFT).

Task 1.3 Combustion and dust Fe emissions

EC-Earth/TM5 already includes the new annual data set of historical anthropogenic reactive gases, aerosols, and aerosol and ozone precursor compounds up to 2014 for use in CMIP6 (Community Emission Data System, CEDS; Hoesly *et al.*, 2017) and that will be used in NUTRIENT. Open biomass burning emissions will be based on GFASv1.2. To calculate the Fe emitted from combustion sources we will use and compare two different approaches (Luo *et al.*, 2008 and Wang *et al.*, 2015). Luo *et al.* (2008) provides fractional emission factors for submicron and supermicron aerosols for fossil fuels, industrial processes, biofuels, waste and biomass burning. This method has been used to estimate combustion Fe emissions in previous studies. We will also test a more sophisticated approach proposed by Wang *et al.* (2015), where the emission of Fe is calculated based on the Fe content in each type of fuel, the partitioning of Fe between residue ash, cyclone ash and fly ash, the size distribution of Fe-contained particles, and the efficiency of removal by different types of control device. The implementation of the second approach will be facilitated by Yves Balkanski, a collaborator of NUTRIENT and co-author in Wang *et al.* (2015). Dust Fe content will be calculated based on standard chemical formulas for each mineral as in Pérez García-Pando *et al.* (2016).

Evaluation: Present-day nudged simulations including combustion Fe and dust Fe will be evaluated with available compilations of total Fe deposition and concentration measurements (Mahowald *et al.,* 2009; Wang *et al.*, 2015). Fe measurements are provided either by point source stations, which may have relatively long term records, or by cruise specific campaigns, which extend through different time-periods, but usually do not allow deriving climatologically representative data. The model output, whenever possible, will be subsampled to match the timing and geographical location of the observations. The skill of each model at simulating total Fe will depend on the accuracy of combustion Fe emissions and the dust cycle along with the prescribed mineral content at the source. For total Fe we will mostly use globally distributed measurements of deposition and surface concentration compiled by Mahowald *et al.* (2009). We will assess whether the explicit simulation of mineral content by the models improves the estimation of total Fe downwind of sources compared to the common assumption of a global constant mineral content and Fe fraction, and which of the approaches to estimate combustion Fe emissions better matches the available observations.

Group contributions: Sara Basart (evaluation), Yves Balkanski (support in applying Wang et al., 2015), IT1 (technical support for implementation in EC-Earth and evaluation)

WP2. Fe processing in the atmosphere

In WP2 we will implement and evaluate an updated mineral-dependent Fe processing mechanism based on our previous work and recent experimental studies (Task 2.1). We also aim to understand whether mineralogy substantially affects acidic Fe processing through its influence upon the partitioning of semi-volatile inorganic compounds and dust heterogeneous chemistry (Task 2.2). A thorough evaluation with available observations will be performed in all tasks. Dr. Maria Gonçalves will be the PI in charge of this WP.

Task 2.1. Mineralogy-dependent dust Fe processing and combustion Fe processing

We will first implement a baseline Fe dissolution scheme developed in previous work (Figure 1; Scanza et al., 2017) into EC-Earth/TM5. The scheme was designed to be both computationally fast for ESMs and relatively straightforward to implement. The acidic processing scheme considers three types of Fe species linked to mineralogy; it is based on laboratory experiments by Shi *et al.* (2011) and the dissolution framework proposed by Ito and Xu (2014). The Fe pools considered are readily-released Fe (Fe_{RR}), medium-soluble Fe (Fe_{med}) and slow-soluble or refractory Fe (Fe_{slow}), where Fe_{RR} is assumed to come mostly from ferrihydrite (calculated as a fraction of illte), and nanohematite (calculated as a fraction of smectite); Fe_{med} is the remaining Fe in illite and smectite; and Fe_{slow} comes from hematite.

The Fe dissolution is represented as a kinetic process depending on the pH, mineral-dependent Fe species, reactivity of Fe species, ambient temperature, and degree of solution saturation. A number of simplifications are applied in our case in comparison to Ito and Xu (2014), including: 1) a portion of Fe_{RR} is assumed to be soluble at emission, 2) the change in the dissolution rate with variation from equilibrium is neglected, 3) the pH is parameterized based the concentration of calcite and sulfate, and 4) the temperature-dependent reaction coefficients are assumed to be equal for certain minerals. For combustion aerosol, 4 % of its total Fe content is assumed to be soluble at emission, and the Fe_{med} dissolution rate is applied for the processing of the remaining combustion Fe during transport. A constant oxalate-promoted dissolution rate with time (no dissolution kinetics) is applied to illite and hematite based on the experimental work of Paris et al. (2011). Because the production of atmospheric oxalate is complex, uncertain and computationally expensive (it would involve solving more than 40 additional aqueous phase reactions; Myriokefalitakis *et al.*, 2011), a simple scheme is used to estimate oxalate concentrations at cloudy grid boxes based on the concentration organic carbon (OC) and secondary organic aerosol (SOA).

In a second step we will update the Fe dissolution scheme and compare it with our baseline. The updates will account for the recent experimental study by Ito and Shi (2016), who have further examined how inorganic and organic ligands in solution affect Fe dissolution rates in mineral dust. Ito and Shi (2016) propose the kinetic mechanism to be extended to oxalate-promoted and quasi-photo-reductive Fe dissolution. Our plan is implement these extensions while proposing and thoroughly evaluating simplifications suitable for ESMs. With these simplified extensions, our final model is expected to represent more realistically the observational variability compared to Scanza *et al.* (2017) without compromising computational efficiency.

Evaluation*:* We will test, evaluate and compare a number nudged model experiments with the baseline and updated schemes using measurements of soluble Fe. Using observations of soluble Fe for model evaluation is complicated due to the variety of collection methods, differences in the filter sizes and solvents used for extraction, and the ambiguous definition of what form of Fe is actually soluble. We will therefore compare our model to observations of labile Fe only, which is the dissolved Fe in either the ferrous or ferric oxidation state. In comparison to total Fe, substantially less data are available showing the distribution of labile Fe. We have compiled observation datasets (e.g., Mahowald e*t al.*, 2009) that will be complemented further within this task, adding for instance new relevant data on aerosol and rain composition and deposition associated to the Surface Ocean Low Atmosphere Study (SOLAS) Project.

Group contributions: Carlos Pérez García-Pando (liaison with WP1 and advice on Fe dissolution mechanisms); Sara Basart (evaluation), Jack Ogaja (implementation of Fe dissolution scheme), Yves Balkanski (advice on Fe dissolution mechanisms), IT1 (technical support for implementation in EC-Earth and evaluation).

Task 2.2 Mineralogy-dependent dust heterogeneous chemistry

In contrast to Scanza *et al.* (2017) it will not be necessary to assume simplifications in the calculation of the pH as TM5 already includes the EQSAM thermodynamic equilibrium model that provides the pH of aerosol water. Indeed, we aim to understand how important are the effects of mineralogy upon the partitioning of semi-volatile inorganic compounds and dust heterogeneous chemistry (and therefore on Fe dissolution rates), a novel aspect that hasn't been tackled before. We will complement the M7 aerosol microphysics and EQSAM thermodynamic equilibrium model with the full set of (known) dust heterogeneous reactions (including the uptake of SO_2, HNO_3, H_2SO_4, N_2O_5, NO_3, NO_2, O_3, H_2O_2, HO_2, and OH). EQSAM calculates the gas/liquid/solid equilibrium partitioning of semi-volatile inorganic compounds, where K, Ca, Mg, and Na are considered as chemically active components and assumed to exist in the form of mineral salts. The amount of these individual crustal species will be obtained at each model grid box from the elemental composition of each mineral weighted by mineral amount. For the heterogeneous chemistry, the mineral-specific uptake coefficients will be taken from the literature (e.g., Crowley *et al.*, 2010).

Evaluation: We will perform nudged simulations and compare the enhanced model relative to a configuration where the dependencies on composition are neglected. We will explore the relative importance of partitioning and heterogeneous chemistry upon the results, and study

the role of each mineral with the goal of proposing a minimal representation if it turns out that the effects are not negligible. For the evaluation, in addition to the comparison with soluble Fe observations, we will use chemistry measurements available at regions near or downstream of dust sources (e.g., Topping *et al.,* 2004; Kim and Park, 2012; Rodríguez *et al.*, 2011) and 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).

Group contributions: Carlos Pérez García-Pando (liaison with WP1 and advice on heterogeneous chemistry); Sara Basart (evaluation), Jack Ogaja (liaison with Task 2.1), Jan Perlwitz (advice on mineral-heterogeneous chemistry interactions), IT1 (technical support for implementation in EC-Earth and evaluation), PD1 (exploration of the effects of mineralogy upon heterogeneous chemistry)

WP3. Quantification, contributions and projections

Using our best model configuration, WP3 will quantify the present-day deposition of soluble Fe to the ocean along with the separate contributions from different sources and mechanisms (Task 3.1), and compare time-slice experiments of the present-day and future climates (Task 3.2). Dr. Pérez García-Pando will be the PI in charge of this WP.

Task 3.1 Quantification and contributions from different sources and mechanisms

We will quantify the total and fractional soluble Fe deposition in the different ocean basins for the present-day, along with the relative contribution of different Fe sources and mechanisms. Experiments will be carried out for periods of 5 years applying atmospheric nudging. A simulation including all the sources and mechanisms will provide the total quantification. To assess the contributions of sources and mechanisms, simulations where a source and/or mechanism is neglected will be compared to the full simulation. Our analysis will assess the contributions from anthropogenic (cultivated) dust Fe, natural dust Fe, and combustion Fe, and the relative importance of proton-promoted, oxalate-promoted and quasi-photo-reductive Fe dissolution.

Group contributions: María Gonçalves (running experiments), Jack Ogaja (analyzing results of experiments), PD1 (contributions of processes and sources), Working Group (discussion).

Task 3.2 Time-slice experiments of the present-day and future climates

To see the effect of soluble Fe processing in different climates, we propose to carry out time-slice experiments for present-day (2000-2010) and future conditions (2090-2100). For the present-day run sea surface temperature (SST) and sea ice concentrations will be prescribed using observed data. For the late 21st century run, SST and sea ice will be taken from a coupled ocean-atmosphere transient simulation carried out for IPCC AR6. Changes in the soluble Fe fraction during transport depend upon atmospheric processes that adjust quickly (within a few months) and to changes in climate associated with decadal trends in atmospheric composition. Thus, decadal simulations are sufficiently long to see the effect of a changed climate on atmospheric Fe processing. Our goal is to understand and compare the responses and regional variations of soluble Fe deposition under different periods and with different anthropogenic emissions affecting the Fe solubility. Greenhouse gas concentrations, emissions of reactive species and aerosols other than dust (including combustion aerosols) will be based on the inventory prepared for the CMIP6 (see Task 1.3). For the future run we will use the Shared Socio-economic Pathway (SSP) scenario SSP3-7.0, in accordance with the AerChemMIP experiments (Collins *et al*., 2017). The SSP3-7.0 is characterized by "Regional Rivalry" without climate policy and weak air quality control measures (Fujimori *et al*., 2017).

The attribution of anthropogenic dust sources by Ginoux *et al.* (2012a) benefits from high resolution and consistency with satellite retrievals of dust optical thickness. This makes the source distribution a valuable tool for studying the effect of anthropogenic dust on the present-day climate. However, there are many compelling questions about the role of anthropogenic dust in future climates, where the sources due to cultivation may be different. Projecting the anthropogenic area fraction in future climate is beyond the scope of NUTRIENT. Instead we will carry out an additional future sensitivity simulations where we perturb the emission from cultivated areas assuming a distribution similar to present-day.

Group contributions: María Gonçalves (running experiments), Jack Ogaja (analyzing results of experiments), PD1 (changes between present and future), Working Group (discussion).

WP4. Project management and dissemination.

WP4 will ensure the appropriate management of the project and broadly communicate and disseminate the outputs throughout its duration. It will be feasible thanks to project management support at the host institution (BSC) and the communication support from the Earth System Services group of the Department of Earth Sciences (www.bsc.es/ESS). WP4 will monitor the progress of the project, and ensure timely preparation of scientific reports through milestones and deliverables (see schedule below) and outreach activities (see Section C.2). It will also facilitate communication among the Research and Working group members' institutions (BSC, NASA, NOAA GFDL and IPSL) and organize quarterly project meetings that will be followed remotely by the Working Group members. There will be several 1-week visits by each member of the Working group to discuss the aspects highlighted in WPs 1 to 3.

Managing risks: The proposal is ambitious and tackles several themes. However, we have not identified substantial risks, besides potential occasional delays with the milestones/deliverables. There is substantial and novel work done previously by the group on all those themes. Our hypotheses are based on evidence, and the formulation of the objectives and the methodology has been designed according to the ample competences of the group in the field. In addition, all the modeling tools and datasets needed are available. Progress will be tracked through the project meetings and the achievement of milestones. If any task is delayed because of unexpected setbacks, the PIs of NUTRIENT will discuss and implement alternatives and/or simplifications in a way to ensure that the specific delay in one task does not compromise other tasks.

List of milestones
M1: Natural and anthropogenic dust in the model implemented and evaluated
M2: Dust mineralogy in the model implemented and evaluated
M3: Total Fe content implemented and evaluated
M4: Role of mineral-dependent heterogeneous chemistry assessed
M5: Final Fe dissolution scheme implemented and ready for assessments
M6: Deposition of soluble Fe and contributions for present-day assessed
M7: Future changes in soluble Fe deposition assessed

List of deliverables
R1-R3: Yearly Reports for the Ministry
D1- New global dataset on emitted PSDs of each mineral
D2- New model developments committed to the EC-Earth repository
D3- Model estimates of present and future soluble Fe available for public use

6 Schedule

	Res. Group	Work Group	Hired	YEAR 1				YEAR 2				YEAR 3			
				Q1	Q2	Q3	Q4	Q5	Q6	Q7	Q8	Q9	Q10	Q11	Q12
WP1	CP														
T1.1	CP, SB	PG, RM	IT1												
T1.2	CP, SB	YB, JP	PD1, IT1												
T1.3	CP, SB	YB	IT1												
WP2	MG														
T2.1	MG, CP, SB, JO	YB	IT1												
T2.2	MG, CP, SB, JO	JP	PD1,IT1												
WP3	CP														
T3.1	CP, MG, JO	ALL	PD1												
T3.2	CP, MG, JO	ALL	PD1												
WP4	CP, MG														
Comm.	ALL		PD1												
Dissem.	ALL		PD1				DIS1		DIS2		DIS3	DIS4			DIS5 & 6
Milestones	ALL		PD1				M1	M2	M3		M4	M5		M6	M7
Deliverables	CP, MG						R1	D1			R2	D2			R3, D3
Meetings	ALL	ALL	ALL	KO, PM	PM	PM	PM	PM	PM	PM	PM	PM	PM	PM	PM

CP: Dr. Carlos Pérez García-Pando (principal investigator 1); MG: Dr. María Gonçalves (principal investigator 2); SB: Dr. Sara Basart; JO: Dr. Jack Ogaja; PG: Dr. Paul Ginoux (GFDL); RM: Dr. Ron Miller (NASA); JP: Dr. Jan Perlwitz (NASA); YB: Dr. Yves Balkanski (IPSL); PD1: requested Post-doctoral scientist; IT1: requested computational support engineer; ALL means all members of the respective group.

The schedule of the tasks is presented in the chronogram above, which is organized into quarters. Each quarter represents a 3-month period, where Q1 represents the first quarter of the project and Q12 is the last (36 months total). All milestones (Ms), deliverables (Ds) and Rs) and project meetings (PM) will happen at the end of the indicated quarter. KO stands for kick-off meeting, which will happen at the beginning of Q1. We also indicate where the members of the Research and Working groups, and the requested new hires will participate. DISs stand for dissemination actions, which are described in section C.2.2.

7 Justification of human resources needed

The contribution of all the Research and Working group members to the each of the proposed tasks is highlighted in the methodology section. We request 3 years of support for a Post-doctoral researcher (PD1) and 2 years of support for an experienced computational support engineer (IT1).

PD1 will ensure the successful achievement of the tasks linked to dust mineralogy (Task 1.2 and Task 2.2) and contribute to the analysis of the impact of processes and sources to the soluble Fe deposition (Task 3.1) along with its change in the future (Task 2.2). In Task 1.2, PD1´s main role will be to propose additional theoretical extensions to BFT. Mineralogy affects all aspects of the dust interaction with climate. Devoting a full time post-doc to this specific problem will timely advance our knowledge and provide the Earth System modeling community with satisfactory methods to represent mineralogy in models. In Task 2.2, PD1 will analyze the impact of mineralogy upon heterogeneous chemistry, an aspect that hasn't been tackled in a model before. Finally, PD1 will contribute to the analysis of soluble Fe deposition in the present and the future. All in all, the coherence and framework proposed will provide the candidate an excellent opportunity to thrive and publish in high impact journals. The candidate should hold a PhD in Atmospheric Sciences with a solid background in atmospheric chemistry.

IT1 will assist the project team in programming and software development tasks as well as, in model compilation, execution, and computational efficiency in different HPC platforms. As such, his/her support will be needed during the first 2 years of the project, when there will be more intensive technical developments (WP1 and WP2). She/he will provide support for the implementation in EC-Earth of the anthropogenic and natural dust tracers (Task 1.1), the mineralogical tracers (Task 1.2), and the combustion tracers (Task 1.3). She/he will be the technical backbone for the generation of a customizable emitted mineral PSD dataset (D1). In WP2, IT1 will provide the necessary assistance to optimize the parameterizations implemented in terms of computational efficiency.

8 Infrastructure

The BSC-CNS constitutes a reference center in High Performance Computing nationally and internationally, since its inception in 2005. All the center computational resources will be available for NUTRIENT to carry out the simulations described in Tasks 1.1, 1.2, 2.1, 2.2, 3.1 and 3.2. BSC hosts the MareNostrum Supercomputer, which has been upgraded for the fourth time since it was installed to achieve a peak performance of 13.7 Petaflops/s. It counts on 165888 Intel Xeon v5 processors, distributed in 3456 nodes, and a central memory of 390 Terabytes. An EC-Earth coupled atmosphere-chemistry simulation, with prescribed SST, at standard resolution: T255L91 for IFS and 3ºx2º for TM5, has an average computational time of 2 simulated years per day using 256 cpu. The computational time for the experiments planned is likely to increase due to the foreseen modifications of the code (larger number of tracers to be transported; increased number of reactions and aerosols' processing), but the new facilities in place will certainly improve the computational performance with respect to MareNostrum3. As part of the EC-Earth consortium, the research team has access to the latest model developments, as all the upgrades included in the code are shared within the community. Moreover, ECMWF grants access to emissions, initial conditions and reanalysis data to the EC-Earth community.

However, additional equipment is required for a successful implementation of the work plan. Model outputs, observation data, and restart files for reproducibility, have to be stored and preserved during the project and after its closure. To that end, it is necessary to extend the storage capacity available for the group, and it is highly desirable to have a specific storage

unit solely devoted to NUTRIENT. Considering that some of the evaluation activities will require increased temporal resolution of the output, with respect to standard monthly frequency in EC-Earth, and the increased number of tracers (i.e. 12 minerals, explicit Fe tracers), as well as the total duration of the simulations, we estimate the additional storage needs in 120 Tb. This extension could be covered with a suite of 40 disks of 3 Tb of storage capacity and a JBOD disk cabinet to mount them. NUTRIENT considers hiring a post-doc (PD1), who will intensively contribute to Tasks 1.2 and 2.2 and WP3 (see schedule), and a technician (IT1), who will support the team in WP1 and WP2 activities. Therefore, to provide them with suitable tools to develop their work, two workstations are required. Finally, to facilitate attending to conferences and project meetings, a UNIX laptop will be needed.

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C.2. IMPACTO ESPERADO DE LOS RESULTADOS

1. Social, economic, scientific and technical impact

The last IPCC Assessment Report acknowledges discrepancies on the impact of atmospheric Fe deposition on ocean fertilization, and thus CO_2 uptake, derived from different models and modelling approaches. NUTRIENT aims to constrain the atmospheric Fe cycle and quantify the natural and anthropogenic contribution to soluble Fe deposition over the ocean, thus contributing to address the aforementioned uncertainties, and provide relevant knowledge to the Earth System Modelling Community. The implementation of NUTIRENT will also benefit to the short-term forecast communities, particularly those involved in mineral dust modelling and its effects.

NUTRIENT will contribute to the EC-Earth modelling community, by introducing improvements and efficient schemes for the atmospheric aerosols' characterization and chemical processing focusing on the Fe cycle. As such, the advances included are expected to be part of Coupled Models Intercomparison Experiments (CMIP) in the future, which constitute the basis for the IPCC Assessment Reports. In this sense NUTRIENT contributes to the strategic goals of the H2020 work program for the 2018-2020 period, which identifies as a major priority "*Building a low-carbon, climate resilient future*", to materialize the COP21 Paris Agreement objectives, and clearly states that "*science is needed to underpin the next cycle of IPCC reports (2018-2022) that will contribute to the UNFCCC Global Stocktake process*".

Through the EC-Earth consortium the model improvements and project results will impact recognized Spanish and European research teams and institutions, such as the Spanish Meteorological Agency (AEMET), the Department of Research and Development of Weather and Climate models of the Royal Netherlands Meteorological Institute (KNMI), the Department of Physical Geography and Ecosystem Science of the Lund University, or the research team working at BSC on ocean biogeochemistry.

From a broader perspective, NUTRIENT will also positively impact the climate change and climate prediction scientific communities at the national and international level. A better reproduction of the soluble Fe deposition to the ocean will allow improving the carbon cycle representation in the next generation of fully coupled Earth System Models, thus aiding national and international research teams focusing on climate change projections, impacts assessment and decision makers involved in the definition of mitigation and adaptation strategies. It would constitute also a step forward towards the evaluation of controversial geoengineering strategies that are under discussion nowadays.

2. Dissemination, exploitation and communication, of results

NUTRIENT will devote specific resources to the communication, dissemination and exploitation of results, with the aim of maximizing the impact and knowledge transfer of the research conducted. Dissemination will tailor different audiences, including the scientific community, key stakeholders, such as decision makers and private companies, and the general public. The strategy is aligned with the European Commission's policy on open data and open access to scientific results.

Dissemination: NUTRIENT will include dissemination activities oriented towards the scientific community. The project will make available new knowledge and science discoveries through

the publication of at least 6 open-access <u>articles in internationally recognized journals of high impact</u> (DIS 1 to 6 in the schedule). The <u>presentation of project progress and results in national and international scientific forums</u> (AGU, EGU conferences, SDS-WAS workshops, AEROCOM meetings) has the twofold objective of disseminating new scientific advances and foster the exchange of knowledge within the scientific community, receiving feedback from experts in the field. The active involvement of the research team members <u>in national and international scientific committees</u> (i.e., EC-Earth consortium, ICAP, SDS-WAS) ensures the projection of NUTRIENT outcomes. In the framework of the WMO regional center SDS-WAS, the BDFC, and under the umbrella of the AXA Chair on Sand and Dust Storms held by Dr. Carlos Pérez García-Pando at BSC, the center hosts several events that will constitute valuable forums to spread the project scientific advances. Particularly, the conference on dust that will be organized in Barcelona next year constitutes an excellent forum to share the project results with the mineral dust scientific community. Also, a series of <u>training courses and seminars</u> that target operational meteorologists from National Meteorological and Hydrological Services from Northern Africa and Middle East, but which are also open to interested PhD students and post-doctoral researchers, are periodically organized, with specific sections devoted to the dust cycle and its impacts, as well as dust modelling. Relevant aspects of NUTRIENT to be discussed there include the definition of dust mineralogy and dust ageing, as well as its impacts. Other stakeholders', decision makers and private actors, will be targeted through a specific section on the BSC-CNS <u>website.</u>

<u>Exploitation:</u> Once scientifically exploited, the project results will be made available to the public, following the aforementioned EC open-access science strategy. To increase the impact of the project on different sectors: (1) the new global dataset on emitted PSDs of each mineral will be shared with the scientific community (D1), (2) model developments will be committed to the EC-Earth development portal (D2), (3) model estimates of present and future soluble Fe will be made available for public use making use of appropriate data standards and associated comprehensive metadata, and will be maintained and stored up to 5 years after the project is finished, so that they can be used by different modelling communities (i.e. the biogeochemical impacts assessments) and other potential stakeholders.

<u>Communication and outreach:</u> Outreach activities are crucial to increase public awareness and understanding of science and, at the same time, to show the payback of national investment in I+D+i. NUTRIENT will target the general public through the preparation of specific materials that will make use of a language understandable by non-specialists and with an appealing format. To this end, we foresee the creation of a wiki page with a team-restricted access area and an open access area to publish: main project results (open access articles, presentations, reports, other project deliverables), dissemination materials and general public tailored products (i.e. leaflets, videos, press releases, etc.). The project will also take advantage of the BSC presence in social media (Facebook and twitter accounts with more than 2500 followers) to spread further the project results. BSC has a media communication manager, a communication team, and an in-house designer.

C.3. CAPACIDAD FORMATIVA DEL EQUIPO SOLICITANTE

The Earth Sciences Department of BSC offers the opportunity for prospective PhD students to work in an international multidisciplinary scientific environment. In the context of this project we would like to recruit and enroll a PhD student in the Environmental Engineering doctoral program (https://doctorat.upc.edu/ca/programes/enginyeria-ambiental) of the Technical University of Catalonia (UPC), which was recognized with MEC Excellence Mention from 2004 to 2013 (MCD2004-00394, MEE2011-0335), and it is currently registered in the VERIFICA process of the ANECA evaluation agency (RUCT: 5600080).

The PhD student will count on the direct supervision and advice of the PIs of NUTRIENT, who will guide him/her to develop a <u>Research and Training Plan</u> within the first academic year, considering both the training goals and the student needs. The training plan will be oriented towards the acquisition of competences in climate modelling, atmospheric chemistry and the atmospheric Fe cycle. The student will be involved in the research group activities, including periodical internal and external seminars, journal clubs, and invited speaker conferences held at BSC. In addition, he/she will have the opportunity to share the results of his/her research in different national and international scientific forums and he/she will be

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encouraged to co-author scientific research articles of high impact. Complementary skills required for efficient research execution and communication will be fostered through the student participation on multiple training activities offered by BSC.

The Earth Sciences Department has a long record of supervising PhD theses in the Environmental Engineering program of the UPC. In the last 10 years 14 PhD theses were developed and 7 are currently ongoing within the Department. In particular, Dr. Carlos Perez García-Pando has co-supervised 3 PhD thesis, and Dr. María Gonçalves Ageitos is part of the faculty of the Environmental Engineering program of the UPC and acts as a tutor for 3 ongoing PhD students within the Department. Additionally, BSC has a specialized Education and Training Team, dedicated to establish a curriculum based on cutting-edge scientific research on software tools for HPC and application areas. BSC offers a personalized professional development plan to each member, according to their profile and objectives. Thanks to this approach, BSC has been awarded with the _Human Resources Excellence in Research_, recognizing the alignment of its human resources policies to the principles set out in the EU Charter and Code for Research.

PhD Thesis defended (last 10 years, list is not exhaustive, the total is 14)

1. Víctor Manuel Valverde Morales. "_Characterization of atmospheric pollution dynamics in Spain by means of air quality modelling_". 08/04/2016. Publications: Valverde et al. (2015, _Int. J. Clim.)_; Valverde et al. (2016a, 2016b, _Sci.Total Env._); **2. Robert Banks**. "_Assessment of planetary boundary-layer schemes with advanced remote sensing instruments and air quality modelling_". 04/04/2016. Publications: Banks et al. (2015, _Bound.-lay. Meteorol._); Banks and Baldasano (2016, _Sci.Total Env._); Banks et al. (2016, _Atm. Res._); **3. Michele Spada**. "_Development and implementation of a fully coupled global aerosol model within the chemical non-hydrostatic multiscale model (NMMB/BSC-CHEM)_". 23/11/2015. Publications: Spada et al. (2013, _Atm.Chem.Phys._); Spada et al. (2015, _Atm. Env._); **4. Alba Badia Moragas**. "_Implementation and development of a gas-phase chemical mechanism within the global/regional atmospheric model chemical non-non-hydrostatic multiscale model (NMMB/BSC-CHEM)_". 12/12/2014. Publications: Badia and Jorba (2015, _Atm. Env._); Badia et al. (2017, _Geosc. Model Dev._); **5. Marc Guevara Vilardell**. "_Desarrollo de un modelo para la estimación de las emisiones atmosféricas en España orientado a la modelización de la calidad del aire_". 17/12/2014. Publications: Guevara et al. (2014a, _Atm. Env._); Guevara et al. (2014b, _Atm. Env._); **6. Simone Marras**. "_Variational Multiscale Stabilization of finite and spectral elements for dry and moist atmospheric problems_". 10/12/2012. Publications: Marras et al. (2012a, 2012b, _J. Comp. Phys._); Marras et al. (2013, _J. Comp. Phys._); **7. Karsten Haustein**."_Development of an atmospheric modeling system for regional and global mineral dust prediction_". 31/01/2012. Publications: Haustein et al. (2012, _Atm. Chem. Phys_); **8. Sara Basart Alpuente**."_Mineral dust model validation through ground based and satellite observation in North Africa and Europe_" 30/01/2012. Publications: Basart et al. (2009 _Atm. Chem. Phys._), Basart et al. (2012 _Atm. Chem. Phys._), Basart et al. (2012 _Tellus_); **9. María Teresa Pay Pérez**. "_Regional and urban evaluation of an air quality modelling system in the European and Spanish domains_". 22/11/2011. Publications: Pay et al. (2010ab, _Atm. Env._), Pay et al. (2011, _Atm. Env._), Pay et al. (2012, _Atm. Env._).

Profesional and scientific careers of graduated PhDs from the group

Pedro Jiménez - Associate professor at Universidad de Murcia (Departamento de Física); **María Gonçalves** - Associate professor at Universitat Politènica de Catalunya (Departamento de Proyectos de Ingeniería); **María Teresa Pay** - Assistant professor at Universitat de Barcelona (Departamento de Genética, Microbiología y Estadística); **Karsten Hausetin** - Researcher at Univesity of Oxford (School of Geography and the Environment); **Simone Marras** - Associate Researcher at US Naval Research Laboratory (Monterey), now Associate Researcher at Stanford University (Department of Geophysics); **Angel Alberto Rincon** - Associate professor at Universidad del Pacífico Paraguay (Facultad de Ingeniería); **Alba Badia** - Research Associate at University of East Anglia (School of Environmental Sciences); **Robert Banks** - Researcher at Delft University of Technology (Department of Geoscience and Remote Sensing); **Victor Valverde** - Researcher at Joint Research Center.

C.4. IMPLICACIONES ÉTICAS Y/O DE BIOSEGURIDAD

N/A