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)**:**

Mario César Acosta Cobos

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

TÍTULO DEL PROYECTO: Optimización de Modelos del sistema Terrestre en el camino a la nueva generación de Sistemas "Exascale" de alto rendimiento.

ACRÓNIMO: OEMES

RESUMEN Máximo 3500 caracteres (incluyendo espacios en blanco):

La computación de altas prestaciones (High Performance Computing, HPC) es ahora una pieza clave en el futuro de la ciencia, industria y la sociedad. Su aplicación para métodos matemáticos y algoritmos computaciones será esencial para producir aplicaciones robustas, que sean capaces de aprovechar las futuras arquitecturas de alto rendimiento conocidas como “exascale platforms”, haciendolo de una forma eficiente, sin malgastar los recursos y reduciendo el consumo. La modelización del sistema terrestre para la predicción del clima y del tiempo, es uno de los campos benificiados con la aplicación de HPC, sin embargo, aunque en la última década se han hecho grandes progresos en la comprensión del cambio climático, quedan aun muchas incertidumbres que desconocemos. Por ejemplo, se desconocen los niveles exactos de aerosoles y gases de efecto invernadero emitidos y, en consecuencia, todavía existen muchas incertidumbres en su grado de impacto en el calentamiento global. Resolver esta y otras cuestiones está fuertemente ligada a la cantidad de cómputo disponible y a la habilidad para usarlo, debido a que resolver estas incertidumbres pasará por mejorar la modelización con experimentos más complejos, como incrementos de resolución espacial, experimentos más largos en el tiempo, complejidad mayor en la modelización del sistema terrestre, y un mayor número de experimentos para cubrir diversos escenarios. Esto refleja la necesidad vital que existe de HPC si se quiere predecir la evolución del clima y responder a preguntas clave para la sociedad relacionadas con el impacto del calentamiento global.

El objetivo de OEMES es adaptar los modelos del sistema terrestre (“Earth System Models”, ESMs) a máquinas con mayor capacidad de cómputo, adaptando estos modelos para que puedan ser más paralelos, escalables y robustos. HPC está experimentando grandes cambios debido a los nuevos sistemas que se están desarrollando para los próximos años

("exascale systems"). Estos nuevos sistemas supondrán grandes retos, desde cómo reducir en un orden de 100 el consumo energético de los mismos, hasta el desarrollo de nuevos modelos de programación, los cuales permitirán dividir la ejecución en millones de elementos de computación. Más importante, es tener en cuenta que estos retos no pueden superarse por mera extrapolación de las técnicas usadas en el pasado, sino que hará falta innovar radicalmente en la tecnología y metodología a desarrollar. Teniendo en cuenta esto, OEMES pretende superar tres principales retos: (1) Cómo analizar los principales cuellos de botella de un ESM cuando se aplican métodos de paralelización másiva, (2) Cómo explotar arquitecturas de alto rendimiento, reduciendo el consumo energético de estos modelos a través de nuevos métodos matemáticos y algoritmos computacionales y (3) Cómo evaluar si la ejecución masiva en paralelo reduce la calidad de los experimentos o hace perder reproducibilidad de los mismos. El objetivo final de OEMES es mejorar la capacidad y exhaustividad de los modelos del sistema terrestre, para así recrear escenarios incluso más realistas y con mayor detalle que permitan reducir las incertidumbres que aun permanecen en nuestros estudios de predicción de clima. OEMES explorará estos retos en el marco de proyectos dentro del H2020, con el objetivo de adaptar los modelos europeos del sistema terretre a la nueva era.

PALABRAS CLAVE: Modelización del Sistema Terrestre, Computación de Altas Prestaciones, Predicción Climática, Optimización, Exascale

TITLE OF THE PROJECT: Optimization of Earth system Models in the path to the new generation of Exascale high performance computing Systems

ACRONYM: OEMES

SUMMARY Maximum 3500 characters (including spaces):

High Performance Computing (HPC) has gained recently more recognition as a key technology for the future of science, industry and society and it is widely accepted that the digital economy will heavily benefit from HPC. Its application use for mathematical methods and computational algorithms will be essential in order to produce robust applications that can leverage future high-performance exascale architectures and reach the goal of improving energy efficiency. Earth System Modelling for weather and climate prediction is one of the fields benefited by the symbiosis with HPC. However, though in the last decade our understanding of Climate Change has increased, there remain uncertainties. While there is dubiety about the levels of greenhouse gas emissions and aerosols likely to be emitted, there are perhaps more significantly uncertainties on the degree of warming and the likely impacts. This question is strongly linked to the amount of computing power and the ability to be used since the scientific community ask for increased model resolution, large numbers of experiments, increased complexity of Earth system models (ESMs), and longer simulation periods compared to the current state of climate models. This means that there is a vital need for high performance computing in order to predict the future evolution of the climate and answer key societal questions about the impact of global warming.

The aim of OEMES is to adapt ESMs to more powerful machines, becoming more parallel, scalable and robust, and to optimise for data locality on architectures with deepening and heterogeneous memory hierarchies. HPC is currently undergoing a major change as the next generation of computing systems ('exascale systems') is coming. These new systems pose numerous challenges, from a 100-fold reduction of energy consumption to the development of programming models for computers that host millions of computing elements. These challenges cannot be met by mere extrapolation but require radical innovation in several computing technologies. OEMES focuses on three main challenges: (1) How to analyse the main bottlenecks of an ESM when a massive parallelization is used, (2) How to exploit high-end architectures efficiently, reducing the energy consumption of these models through novel

mathematical methods and computational algorithms and (3) How to check if the massive parallel execution of the model reduce the quality of the simulations or lose reproducibility. The final goal of OEMES is to increase the capability and comprehensiveness of 'the whole Earth system' models in order to represent an ever-increasing realism and detail of new scenarios of our future climate, which is the only way to reduce these latter uncertainties. OEMES will explore these challenges in the framework of H2020 in order to adapt the European Earth System Models to the new era.

KEY WORDS: Earth System Modelling, High Performance Computing, Exascale computing, Climate change, Optimization, Exascale

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): Mario Acosta, Eleftheria Exarchou, Kim Serradell
   Referencia del proyecto: PRIMAVERA, GA 641727
   Título: PRocess-based climate sIMulation: AdVances in high resolution modelling and European climate Risk Assessment
   Investigador principal (nombre y apellidos): Francisco Doblas Reyes (Coordinator Malcolm Roberts, Met Office)
   Entidad financiadora: H2020
   Duración (fecha inicio - fecha fin):01/11/2015-31/10/2019
   Financiación recibida (en euros): 1.277.425€ (total budget 14.967.970€)
   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): Mario Acosta, Kim Serradell
   Referencia del proyecto: ESiWACE GA 675191
   Título: Centre of Excellence in Simulation of Weather and Climate in Europe
   Investigador principal (nombre y apellidos): Kim Serradell (coordinator Das Deutsche Klimarechenzentrum)
   Entidad financiadora: H2020
   Duración (fecha inicio - fecha fin): 01/09/2015-31/08/2019
   Financiación recibida (en euros): 269.750€
   Relación con el proyecto que se presenta: está muy relacionado
   Estado del proyecto o contrato: concedido

3. Investigador del equipo de investigación que participa en el proyecto/contrato (nombre y apellidos): Eleftheria Exarchou, Kim Serradell
   Referencia del proyecto: SPECS, GA 308378
   Título: Seasonal-to-decadal climate Prediction for the improvement of European Climate Services
   Investigador principal (nombre y apellidos): Francisco Doblas Reyes (Also coordinator)
   Entidad financiadora: FP7
   Duración (fecha inicio - fecha fin):01/11/2012-31/01/2017
   Financiación recibida (en euros): 1.615.305,75€ (total budget 8.224.862€)
   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): Mario Acosta, Kim Serradell
   Referencia del proyecto: IS-ENES2-312979
   Título: Infrastructure for the European Network for Earth System modelling –Phase 2
   Investigador principal (nombre y apellidos): Kim Serradell (coordinator CNRS-IPSL)
   Entidad financiadora: FP7
   Duración (fecha inicio - fecha fin): 01/04/2013-31/03/2017
   Financiación recibida (en euros): 77.967€ (total budget 125.800€)
   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):
   Referencia del proyecto: ITT Ref: C3S_51

Título: QA4Seas-Quality Assessment Strategies for Multi-Model Seasonal Forecasts
Investigador principal (nombre y apellidos): Francisco Doblas Reyes
Entidad financiadora: ECMWF (Copernicus Climate Change Service)
Duración (fecha inicio - fecha fin): 01/07/2016-30/09/2018
Financiación recibida (en euros): 731.214,40€ (total funding budget 1.681.760€)
Relación con el proyecto que se presenta: está algo relacionado
Estado del proyecto o contrato: concedido

6. Investigador del equipo de investigación que participa en el proyecto/contrato (nombre y apellidos): Mario Acosta, Kim Serradell
   Referencia del proyecto: Mont-blanc 2 610402
   Título: Mont-Blanc 2, European scalable and power efficient HPC platform based on low-power embedded technology
   Investigador principal (nombre y apellidos): Filippo Mantovani (coordinator BSC)
   Entidad financiadora: FP7
   Duración (fecha inicio - fecha fin): 01/10/2013- 31/01/2017
   Financiación recibida (en euros): 1.808.660€ (total funding budget 2.168.841€)
   Relación con el proyecto que se presenta: está algo relacionado
   Estado del proyecto o contrato: concedido

7. Investigador del equipo de investigación que participa en el proyecto/contrato (nombre y apellidos):
   Referencia del proyecto: PoP GA 676553
   Título: Performance Optimisation and Productivity
   Investigador principal (nombre y apellidos): Judtih Giménez (coordinator BSC)
   Entidad financiadora: H2020
   Duración (fecha inicio - fecha fin): 01/10/2013- 31/01/2017
   Financiación recibida (en euros): 749.125€
   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):
   Referencia del proyecto: DEEP-EST GA 754304
   Título: DEEP - Extreme Scale Technologies
   Investigador principal (nombre y apellidos): Viçenc Beltrán Querol (coordinator Forschungszentrum Julich Gmbh)
   Entidad financiadora: H2020
   Duración (fecha inicio - fecha fin): 01/07/2017- 30/06/2020
   Financiación recibida (en euros): 1.076.250€
   Relación con el proyecto que se presenta: está algo relacionado
   Estado del proyecto o contrato: concedido

9. Investigador del equipo de investigación que participa en el proyecto/contrato (nombre y apellidos):
   Referencia del proyecto: EuroEXA 754337
   Título: Co-designed Innovation and System for Resilient Exascale Computing in Europe: From Applications to Silicon
   Investigador principal (nombre y apellidos): Paul Mattew Carpenter (coordinator Institute Of Communication And Computer Systems (Greece))
   Entidad financiadora: H2020
   Duración (fecha inicio - fecha fin): 01/09/2017- 01/02/2021
   Financiación recibida (en euros): 1.259.937,50€
   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):
Referencia del proyecto: NEXTGenIO GA 671591
Título: Next Generation I/O for Exascale
Investigador principal (nombre y apellidos): Antonio Cortés (coordinator The University of Edinburgh (UK))
Entidad financiadora: H2020
Duración (fecha inicio - fecha fin): 01/10/2015- 31/03/2019
Financiación recibida (en euros): 404.625€
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.

No aplicable

Parte C: DOCUMENTO CIENTÍFICO. Máximo 20 páginas.

C.1. PROPUESTA CIENTÍFICA

1. Introduction and state-of-the-art

In the last decade, our understanding of climate change has increased (Merchant et al, 2017), as the societal has need for pulling through to advice and policy. However, whilst there is a great confidence in the fact that climate change is happening, there remain uncertainties (Doblas-Reyes et al, 2013). For example, the levels of greenhouse gas emissions and aerosols likely to be emitted, or perhaps even more significantly uncertainties on the degree of warming and the likely impacts (Mudryk et al, 2017). Another example in Figure 1 (Flato et al, 2013) shows three main sources of uncertainty (global temperature) in projections of climate of the fifth phase of the Coupled Model Intercomparison Project (CMIP5): due to future emissions (scenario uncertainty, green), due to internal climate variability (orange), and due to inter-model differences (blue). The figure shows that the spread between RCP scenarios is the dominant source of uncertainty at the end of the century, but internal variability and inter-model uncertainty are more important for the near-term. Increasing the capability and comprehensiveness of 'whole Earth system' models, in order to represent an ever-increasing realism and detail of new scenarios for our future climate, is the only way to reduce these latter uncertainties (Palmer, 2014).

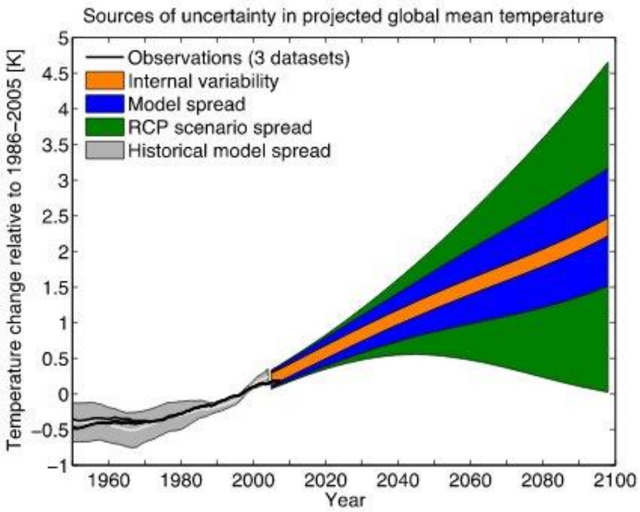

Figure 1. The sources of uncertainty in global decadal temperature projections, expressed as a 'plume' with the relative contribution to the total uncertainty colored appropriately. The shaded regions represent 90% confidence intervals.

This means that, even though the scientific community has little doubt that climate is sensitive to mankind's activity, many questions remain unsolved at the quantitative level (Stevens et al, 2013; Liu et al, 2015). There is a need to better qualify and quantify uncertainty of the predictions, estimate the probability of extreme events and regional impacts, quantify the feedbacks between climate and biogeochemical cycles such as carbon dioxide and methane, and therefore identify the impacts of climate change on marine and terrestrial ecosystems and on societies (Lenton et al, 2003; Doblas-Reyes et al, 2013; Flato et al 2013; Hartman et al, 2013; Mauristsen et al, 2013). These are some of the reasons why **the final goal of OEMES is to increase the capability and comprehensiveness of 'the whole Earth system' models, in order to represent an ever-increasing realism and detail of new scenarios for our future climate, being the only way to reduce these latter uncertainties in the future.**

However, the increase of the capability of ESMs is strongly linked to the amount of computing power and data storage capacity available. The scientific community ask for increased model resolution, large numbers of experiments, increased complexity of ESMs, and longer simulation periods compared to the current state of climate models (Palmer, 2014). It is also important to perform coordinated ensembles of simulations using different forcing to ensure the robustness of the model results (Reuser et al, 2015; Li et al, 2014). For example, Prodhomme et al (2016) showed the benefits when the horizontal resolution of a global ESM is increased for seasonal climate prediction. This proves that there is a vital need for high performance computing in order to predict the future evolution of the climate and answer key societal questions about the impact of global warming on human activities (Palmer 1999; Palmer 2014). Actually, sustained computing power of the order of 1 Pflop/s or more is already required today for Europe to maintain its scientific weight in climate change research worldwide.

HPC has evolved in the last years from a technology crucial to the academic research community to a point where it is acknowledged as a key piece of the numerical modelling (Casanova et al, 2011), being its application a real need for Earth System Modelling (Bastoul et al, 2004). HPC is currently undergoing a major change as the next generation of computing systems ('exascale systems') is being developed to be ready in a near future (Broekema et al, 2012). These new systems pose numerous challenges, from a 100-fold reduction of energy consumption to the development of programming models for computers that host millions of computing elements, while addressing the data challenge presented by the integration of both observational and simulation/modelling data (Alexandrov et al, 2014; Palmer, 2015). These challenges cannot be met by mere extrapolation but require radical innovation in several computing technologies and numerical algorithms.

Most applications targeting exascale machines require some degree of rewriting to expose more parallelism, and many face severe strong-scaling challenges if they are effectively to progress to exascale, as it is demanded by their science goals. There is an on-going need of support for software maintenance, tools to manage and optimise workflows across the infrastructure, and visualisation. Support for the development and maintenance of community code bases is recognised as enhancing research productivity and take-up of HPC (Palmer, 2014). There is an urgent need for algorithm and software development to be able to continue to exploit high-end architectures efficiently to meet the needs of science, industry and society. **This project aims (as starting hypothesis) at figuring out how to increase the computational performance of ESMs and how to adapt them for the new generation of supercomputers, when the increase of computer power will be mandatory to reduce the uncertainties of climate simulations.** This proposal is split into the following sections:

1. Earth System Modelling and the path to exascale challenge in Europe
2. The path to exascale challenge for EC-Earth, the European ESM
3. Societal challenges
4. Objectives
5. Background of the work team and other groups working on it
6. Methodology and planning
7. Technical resources
8. Human resources

1. Earth System Modelling and the path to exascale challenge in Europe

Weather, Climatology and Earth Sciences (WCES) encompass a wide range of disciplines ranging from the study of the atmosphere to the oceans. They are all part of Earth system sciences or geosciences. Earth system sciences address many important societal issues, from weather prediction to air quality, ocean prediction and climate change to natural hazards such as seismic, volcanic and tsunami hazards. The development and the use of high performance computing plays a crucial role to accomplish these societal issues, allowing the execution of numerical models with the computer power needed to obtain useful results (Stocker et al, 2013; Taylor et al, 2013; Li et al 2014).

Research in the fields of weather, climatology and Earth sciences is of key importance for Europe. Obviously, one of the main concerns for Europe is the climate change. Increasing the capability and comprehensiveness of 'whole Earth system' models that represent in ever increasing realism and detail scenarios for our future climate, is the only way to reduce the current uncertainties (Palmer, 2014). A further challenge is to provide more robust predictions of regional climate change at the decadal, multi decadal and centennial timescales to underpin local adaptation policies. In many regions of the world, there is still considerable uncertainty in the model predictions of the local consequences of climate at different timescales and model resolution plays therefore a key role. A dual track approach should be considered involving multi member multi model comparisons at the current leading edge model resolution (about 20 km, limited to a few decades) alongside the longer term, aiming to develop a global convective resolving model (down to 1 km resolution). Reducing these uncertainties in climate projections requires a coordinated set of experiments, taking advantage of existing and new HPC platforms (Alexandrov et al, 2014).

Modelling the climate system is a challenge because it requires the simulation of a myriad of interacting and complex processes as well as their analysis at different time and spatial scales. Climate system modelling requires furthermore sophisticated numerical models, due to the inherently non-linear governing equations (Randall et al, 2007). In addition, huge computational resources are needed to solve billions of individual equations describing the physical processes at different scales. Indeed, model simulations are required to represent both, the modification of the larger scale, global state (inside which extreme events are developing) and the fine temporal scale and spatial structure of such events (storms, cyclones, intense precipitation, etc.).

Currently, global climate models running in an efficient way (from a computational point of view) have typical grid spacing of 100–200 km and are limited in their capacity to represent processes such as eddies, clouds, orography effects, small scale hydrology, etc. The latest generation of models, under development or just starting to be used, have grid spacing in the 20-50 km range, and there are evidences that a number of important climate processes are better represented at this resolution (Prodhomme et al, 2016) (e.g. aqua planet, ENSO, satellite validation, blocking, tropical storm numbers, etc.). A priority for **OEMES is then to continue the development of coupled models at such high resolution and to use them in ultra-high resolution experiments (1-5 km range) focused on key climate processes.**

Very high resolution global models are expected to improve our predictions and understanding of the effect of global warming on high impact weather events on seasonal, decadal and century timescales (Zhang et al, 2015). Another issue is related to the simulation of regional scale climate features, of crucial importance for assessing impacts on society and economic activities (farming, fisheries, health, transportation, etc.) and for which improved regional models, embedded in global climate models, are necessary.

Increasing model resolution down to 1 km requires increases by factors of at least 100 to 1,000 in computing power compared to the current state. It should be noted that each increase of the spatial resolution by a factor 2 in each direction mandates at least an eightfold increase in computing power, depending on the time step length that needs to be decreased with increasing resolution. More computing power means more resources of a supercomputing used in parallel. However, the more resources in parallel are used, the more overhead is introduced to achieve the parallelization. **One of the main goals of OEMES is for instance to achieve the good scalability of the models, when the parallelization will be extreme.**

Climate models fundamentally scale with difficulty on supercomputers because the problems they represent are connected, physically and algorithmically (Broekema 2012). This requires significant communication results in an increasing overhead with increasing domain decomposition (Irony et al, 2004). Both capability and capacity computing are therefore important for Earth system modelling (Pavel et al 2014). Capability is needed given the long timescales every coupled model configuration needs to spin up to a stable state. For example, paleo studies in particular, also require relatively long runs and therefore capability. In both cases, this will be true as long as no technique of parallelisation by the time is available. Higher resolution simulations, of course, also strongly benefit from capability. However, to carry out control and transient multi member ensemble runs (same experiment with slight differences in the initial conditions) dealing with modern climate and based upon the above mentioned stable state is a typical capacity problem (Rauser et al, 2015). For example, producing the set of experiments for CMIP6, requires running of a high number of simulations (typically, one centre running all experiment for all MIPs would cumulate 50000 simulated years) and certainly asks for capacity, as all of these runs must be considered as being part of the same experiment. These capacity demanding ensemble type runs with high resolution models are generally done most efficiently on central HPC systems and not in a distributed manner. There are applications for which distributed systems would provide good performance (Dongarra et al, 2014), but these cases generally depend on models with very good portability and with relatively low input/output volumes, criteria that are not fulfilled in general by ESMs. So systems especially suited to ESM high performance computing applications need to provide both capability and capacity with a good balance between computer power and energy efficiency (Pavel et al, 2014).

One of these ESMs, which need urgently the improvement of his capability and capacity in the path to exascale, is EC-Earth. EC-Earth is one of model chosen by mostly of meteorological and other research institutes around Europe, including Spain. This model is used to provide information to address the regional impacts of climate change, and determine appropriate adaptation and mitigation measures on a more regional basis (Hazeleger, 2007).

2. The path to exascale challenge for EC-Earth, the European ESM

EC-Earth is a project, a consortium and a model system. The EC-Earth consortium consists of 24 academic institutions and meteorological services from 11 different countries in Europe, including the “Agencia Estatal de Meterología” (AEMET). EC-Earth is used in many EU FP7 and H2020 projects, including IS-ENES2, ESiWACE, PRIMAVERA and others.

ESMs, such as EC-Earth, are currently the only way of providing information on the future climate to society (Hazeleger et al, 2007). EC-Earth generates reliable in-house predictions and projections of global climate change, which are a prerequisite to support the development of national adaptation and mitigation strategies. EC-Earth is developed as part of a Europe-wide consortium thus promoting international cooperation and access to wide knowledge and data base. It further enables fruitful interactions between academic institutions and the European climate impact community. EC-Earth makes successful contributions to international climate change projections such as CMIP5 or the future CMIP6 (Taylor et al, 2015; Stocker et al 2013; Zhang et al, 2015). The development by the consortium will ensure more reliable projections, which can be offered to decision and policy makers at regional, national and international levels.

EC-Earth can be used for predictions across time scales, ranging from weather to climate. EC-Earth can be used to study climate feedbacks, which govern the global and regional response. The scientific questions at stake include the dynamics of both, the atmosphere and the ocean, at all spatial and temporal scales, with the many interactions between the various scales, which are significant from an energetic and/or transport points of view (Palmer et al, 2008). This includes progressing in the numerical simulation at higher spatial resolution, so that the effects of unresolved scales can be made as small as possible. However, this increase in the resolution of the grids involves the use of thousands of parallel resources of a supercomputer. The execution of these models are complex, and the lack of scalability of the multi component (including the simulation at the same time of the atmosphere, ocean, land, coupler, etc.) climate models is just one reason why they have not been run often on complex machines with good energy efficiency. EC-Earth is one of the ESMs, which has this kind of problems, preliminary studies proved that the improvement of the energy efficiency of EC-Earth is mandatory before thinking in the execution of ultra-high resolution experiments, where the computer power needed will increase dramatically (Yepes et al, 2016).

The EC-Earth model is a global, coupled climate Earth Model that consists of three main components: IFS for the atmospheric model, NEMO for the ocean model and the coupling between them using OASIS3-MCT. It has other sub-components: LIM for the sea ice, XIOS for NEMO’s input/output, and Run-off mapper for freshwater distribution (rivers, ice …) to the ocean. A brief description of the main components and their main computational challenges follow as:

2.1. IFS atmospheric component - Weather forecasting

The Integrated Forecasting System (IFS) as atmosphere model: this is an operational global meteorological forecasting model developed and maintained by the European Centre of Medium-Range Weather Forecasts (ECMWF). The dynamical core of IFS is hydrostatic, two-time-level, semi-implicit, semi-Lagrangian and applies spectral transformations between grid-point space and spectral space.

Weather forecasting applications such as IFS, cannot be run globally for climate because of the prohibitive cost of associated computing resources and limits in model scalability. The climate community's first 'grand challenge' in the longer term is therefore to develop global climate models that resolve convective scale motions (nominally around 1 km horizontal resolution) and represent better orographic effects.

Improve convective scale resolution is necessary for reliable predictions of some important aspects of regional climate change (Shepherd et al, 2014). Developing such very high resolutions will require developing scalable and more efficient dynamical cores and resolve explicitly physical processes, whose modelling still today relies on phenomenological parametrisations.

2.2. NEMO ocean component – Ocean modelling

The Nucleus for European Modelling of the Ocean (NEMO) as ocean model: NEMO is a state-of-the-art modelling framework for oceanographic research, operational oceanography seasonal forecast and climate studies. It discretizes the 3D Navier-Stokes equations, being a finite difference, hydrostatic model, with a free sea surface and a non-linear equation of state.

In ocean applications such as the NEMO model, the progress is intricately linked to the computing power and energy efficiency available due to the need for increasingly higher model resolutions, many more simulations, and greater complexity in ocean system models. Operational oceanography is a new and rapidly growing sector, providing key assessments for coastal water quality, fisheries and marine ecosystems, offshore, military, transport, etc. Yet the subsurface and deep ocean remains drastically under sampled. We must therefore assimilate available data into models and make sure that those models account for the key ocean physical and biogeochemical processes to be able to predict the evolution of ocean characteristics and of marine ecosystems at all relevant scales (Prodhomme et al, 2016). A key concern in the ocean, such as in the atmosphere, is eddies. This key concern can be addressed only by building upon recent advances in ocean modelling to construct more accurate, high resolution models.

High Resolution (O (10 km) grid) experiments have now begun to capture eddy processes in the subtropics and mid latitudes (with strong effects, for example, on the Gulf Stream), but much higher resolution is needed to achieve comparable progress in the subpolar and polar oceans. Yet it remains a challenge to run realistic global or regional ocean/sea ice models at resolutions high enough to ensure dynamical consistency over a wide range of resolved scales.

2.3. OASIS3-MCT coupler - Coupling among Earth System components

The OASIS3-MCT coupler is a coupling library to be linked to the component models, whose main task is to interpolate and exchange the coupling fields between them (using the same or different grids).

In ESMs, a climate model is the assembly of different numerical models, which can be independently developed, interacting in a coupled way. This is a complex process of coupling among different components that can all run on different grid configurations, supporting a variety of spatial resolutions and time scales and exchanging boundary data with each other through the coupler (Palmer, 2014).

This process of coupling among components is not a trivial task and can be computational expensive, where the atmosphere and ocean components continuously exchange several quantities such as momentum, heat or freshwater.

The huge computational cost comes because some of the variables must be coupled in a conservative way so that the total flux or energy in the source and target grids must be the same, increasing the complexity of the coupling algorithm. These issues represent serious practical implications for the numerical implementation and the computational expense of the coupling. The main problem will come when higher resolutions are used, where thousands of cores have to communicate the information of the coupling, converting this in a bottleneck.

2.4. Robustness and validation of Earth System Models

Finally, an important aspect to be addressed is robustness for EC-Earth. Robustness has several aspects including: fault resilient algorithms which enable them to run on large and error-prone systems, reproducibility of numerical results and numerical stability of algorithms, and accuracy and validation of the results compare to observational data (Palmet et al, 2008; Reichler and Kim, 2008). Additionally, robustness enables many opportunities to trade performance for accuracy and reproducibility, which makes it possible to consider approximate computing scenarios where the exactitude of some computations can be turned to maximise compute or memory access performance, whilst keeping the results' quality within an acceptable margin.

Taking into account the computational challenges to increase the main components of EC-Earth (the atmospheric model, IFS, the ocean model, NEMO, the coupling between them, OASIS3-MCT and the robustness of the Earth System) using more computing power with massive parallel platforms. And considering that these challenges cannot be met by mere extrapolation but that require radical innovation in several computing technologies, **OEMES focuses on three specific challenges for EC-Earth:**

(1) Analysing the main bottlenecks of the atmospheric, ocean and coupling components when an extreme parallelization is used.

(2) Trying to exploit high-end architectures efficiently, reducing the energy consumption of these models through novel mathematical methods and computational algorithms.

(3) Evaluating if massive parallel execution and the new methods implemented could impact the quality of the simulations or lose reproducibility.

3. Societal challenges

Once the main challenges for Earth System Modelling to remove the actual uncertainties in climate prediction have been addressed, by using for this the computing power provided by the future exascale platforms, the related societal challenges will be explained.

The interdisciplinary character of the actors involved in Earth System Modelling in Europe (Weather and climate prediction, numerical modelling, computer science and HPC) requires comprehensive solutions that include technological development, structural changes (e.g. optimisation of infrastructures to achieve exascale computing) and the adaptation of scientific models which are not evolved in the last decades. OEMES can provide this interdisciplinary framework to evolve finally these ESMs in order to do the ultra-high resolution experiments, which could solve the future evolution of the weather and climate and answer key societal questions about the impact of global warming.

All in all, OEMES's results are expected to provide better scientific understanding of climate change in Spain and Europe, whereby matching the premises of one challenge in the "Plan Estatal de Investigación Científica, Técnica y de Innovación 2013-2016": '5º Reto en acción sobre el cambio climático y eficiencia en la utilización de recursos y materias primas', in particular with the topic "I. Cambio Climático" by means the following sub-items:

(iii) Investigación aplicada a la evaluación de impacto, vulnerabilidad y adaptación al cambio climático en ámbitos como: zonas de alta biodiversidad, costas, bosques, agricultura, pesca y ecosistemas marinos, recursos hídricos, suelos, salud, turismo, transporte, industria y energía.

(iv) Investigación en ciencias sociales y humanidades asociada a la adaptación y la mitigación del cambio climático, en particular centrada en procesos de adaptación ambiental, económica, tecnológica y social relevantes para España y para Europa; (v) estimación y el seguimiento de las emisiones de gases de efecto invernadero en España y desarrollo de modelos de proyección

incluyendo análisis de incertidumbre y el coste beneficio de las distintas opciones de mitigación en España

OEMES will help to enhance the quality of the results of EC-Earth, contributing to the two sub-items specified, through the ability to exploit high-end architectures efficiently, reducing the energy consumption of EC-Earth in the simulation of ultra-high resolution experiments. These experiments will contribute to the reduction of uncertainties around the climate change study.

OEMES is also tightly following the H2020 societal challenge "**Climate action, environment, resource efficiency and raw material**", via its specific objectives "Climate action", "Resource efficiency" and "Earth Observations". In the interdisciplinary space, it is also related to the H2020 call in "**Future and Emergent Technologies for High Performance Computing**". In particular, "**FETHPC-02-2017: Transition to Exascale Computing**", whose specific challenge is **to take advantage of the full capabilities of exascale computing**, in particular through high-productivity programming environments and new mathematics and algorithms for extreme scale HPC systems for existing or visionary applications, in scientific areas such as physics, chemistry, biology, life sciences, materials, **climate**, geosciences, etc.

To complete these tasks, several European projects born under the H2020 framework, related to achieve the required exascale computing for ESMs with different societal challenges. OEMES follows the same goals that the next European projects and it will contribute to their finalization:

ESiWACE, this H2020 project aims at "building a critical mass and expertise to increase the weather and climate community impact on hardware development towards the extreme scale and create international ExaScale initiatives". OEMES will contribute to enhance this goal with the methodology to highlight the computational problems of ESMs and substantially improve efficiency and productivity of numerical weather and climate simulations on high-performance computing platforms. Other goal of ESiWACE is to establish demonstrator simulations, which will be run at highest affordable resolutions (target 1-5 km) to estimate the computability of configurations that will be sufficient to address key scientific challenges in weather and climate prediction. OEMES will contribute again to make this possible with the profiling and optimizations of EC-Earth and the development of the ultra-high resolution experiments for EC-Earth.

ESCAPE, this H2020 project is aware of the fact that "the socio-economic impact of disasters given that climate change is likely to be escalating because of their increasing frequency and severity and the growing vulnerability of human societies". One of the ESCAPE goals is "Future improvements in predictive skills for both, weather and climate that will eventually originate from enhanced spatial resolution, the better representation of more complex physical and chemical processes, from the coupling between atmosphere, land surface and oceans, cryosphere and biosphere, and from better characterization of forecast uncertainty through ensembles". This is also one of the OEMES goals, in particular with the improvement of the ocean and atmospherical components of EC-Earth and the coupling between them.

PRIMAVERA, this H2020 project is in charge of "simulating and predicting regional climate with unprecedented fidelity, for the benefit of governments, business and society in general". *PRIMAVERA* stands for "Process-based climate simulation: Advances in high-resolution modelling and European climate risk assessment". It aims at developing a new generation of advanced and well-evaluated high-resolution global climate models. This is also one of the goals of OEMES, optimizing in an efficient way EC-Earth in order to lunch ultra-high resolution simulations and prepare the models for the new exascale platforms.

OEMES framework contributes also to the objectives defined by the ***"Estrategia Española de Ciencia y Tecnología y de Innovación 2013-2020"*** promoting the formation of new research personnel and the stabilization of the BSC staff, the collaboration with national and international research institutions, and the developments of cutting-edge technologies.

4. Objectives

The overal scientific objective of OEMES is to <u>optimize the energy efficiency of EC-Earth, one of the main European Earth System Model, to take advantage of future exascale computers in a efficient</u>

way. The final goal is to use EC-Earth to simulate ultra-high resolutions experiments, increasing the capability and comprehensiveness of 'the whole Earth system' model, in order to to produce ever-increasing realism and detail scenarios for the future climate and reduce the uncertainties in climate change simulation.

This goal will be achieved through four complementary objectives, which define the project's methodological approach and cover all the possible optimizations for EC-Earth:

-Developing a profiling method to highlight numerical and computational problems of numerical models, executed in extreme parallel platforms. (WP1)
-Achieving a method to validate and reproduce the results of Earth System Models, taking into account a trade-off among accuracy, reproducibility and performance. (WP2)
-Being ready to take advantage of future exascale computers. To accomplish this, next sub-goals are needed (WP3-4-5):
    -Preparing ultra-high resolution experiments for extreme parallelization.
    -Improving energy efficiency of the main components of EC-Earth:
        -The atmospheric component of EC-Earth, IFS. (WP3)
        -The ocean model of EC-Earth, NEMO. (WP4)
        -The coupling among Earth System Components, OASIS. (WP5)
-Developing a method to optimize the execution and throughput of the model in exascale supercomputers. (WP6)

The completion of OEMES's scientific objectives is expected to make a leap forward in our understanding of weather and climate predictions. The developments within OEMES are expected to be key in the energy efficiency improvement of the ESMs. There are different EU-wide strategies designed to accomplish the main goal of several European projects, in order to move ESMs to exascale platforms in the future, trying to reduce the thousands and thousands of hours that these models spend in our supercomputers. OEMES project will contribute greatly to this goal.

5. Background of the research team and other groups working in the topic

Experience of the PI: During his PhD, Dr Acosta contributed greatly to HPC applied to ESMs and therefore developed expertise in this field. The general knowledge acquired was to improve the computational efficiency of existing computational dynamic fluids models to address the study of circulation, transport and mixing of water components, obtaining the results in an efficient way. This expertise includes wide knowledge in numerical models (governing equations, numerical algorithms and computational implementation) and how to adapt them efficiently to actual and new HPC resources. He has moved to BSC two years ago. Dr Acosta's research lines are well embodied in those related to HPC applied to ESMs in the BSC-Es. He is leading the performance team inside the department, being the supervisor of one PhD student and one master student, who are developing theses in the HPC topic. Only during the last year, Dr Acosta has collaborated in the submission of five peer-reviewed papers (two accepted), five oral communications, four posters in international conferences and four technical memoranda, all within the framework of five H2020 and FP7 projects. He has also several formal collaborations with international institutions, the Centre Européen de Recherche et de Formation Avancée en Calcul Scientifique (CERFACS, OASIS developers), and the ECMWF (IFS developers), where Acosta did a post-doctoral visit (Severo Ochoa mobility grant) of two months in 2017. During his career, the applicant has participated in 9 national and international projects. He is author of 4 peer-reviewed articles in international journals. He presented his work at 11 congresses and workshops, and reviewed some manuscripts for peer-review journals. He is part of the group of experts of European eXtreme Data and Computing Initiative: Weather, Climatology and Solid Earth Sciences (EXDCI/WCES). The group is responsible of the reviewing of deliverables related to Earth Sciences, produced by the coordination and support action EXDCI project, to coordinate the development and implementation of a common strategy for the European HPC Ecosystem.

Experience of Eleftheria in the Research Group: Dr. Eleftheria Exarchou is currently a postdoctoral scientist in the Climate Prediction (CP) group within the Earth Sciences Department. She has a strong background in physical oceanography and in ocean and climate modeling. She has experience in seasonal/decadal forecasting and climate projections, with a particular focus on ocean dynamics. She is involved in the EC-Earth Ocean working group, which, among other tasks, coordinates the tuning of the ocean model component of EC-Earth. She has investigated the model biases of the coupled EC-Earth climate model in the Tropical Atlantic within the PREFACE project.

Experience of Kim in the Research Group: He is the manager of the CES group at the Earth Sciences department in the BSC. In the last years, he has been in charge for the system administration of all the computational resources of the department and he was also responsible of supervising the operational runs of the NMMB/BSC-Dust model and CALIOPE Air Quality System in the HPC infrastructures of the BSC. In that sense, he was also involved in the analysis of the models to improve their performance and developed strong skills of compilation and scripting. In March 2014, he wrote his Master Thesis in the "Analysis, Developments and optimizations on the NMMB/BSC model", focusing his research on applying many different techniques to improve the model performance in an HPC environment. Furthermore, he's focused on deploying ESMs (dust transport, climate or weather forecast) required by the department in a wide range of HPC architectures. He succeeds in porting these models in next HPC architectures like Montblanc cluster (ARM Based). He applied with success these skills in projects like IS-ENES (1 & 2), ESiWACE, SDS-WAS or BDFC or CONSOLIDER. He also teaches in different HPC schools oriented to the Earth Sciences and Climate Model as PRACE Advanced Training Centres Course for Introduction to simulation environment for Earth Sciences (2012 to 2016) and the IS-ENES Summer Schools (2014, 2016).

At national level, several research groups work using EC-Earth, among them:

-Earth Science department at Barcelona Supercomputing Centre (BSC-ES). The department was granted several H2020, FP7, Copernicus, ESCAPE European projects, apart from other projects funded by the Ministerio de Economía y Competitividad (MINECO), all related to Earth System Modelling researching. During that same period, BSC-ES also participated in 21 RES and 4 PRACE projects. The BSC-ES has participated in climate services initiatives like the Climate Services Partnership (CSP). Members of the BSC-ES participate in committees of the World Climate Research Programme (WCRP), such as the CLIVAR Scientific Steering Group or the Working Group on Seasonal to Interannual Prediction (WGSIP). Two research groups work using EC-Earth, the Computational Earth Science (CES) and the Climate Prediction (CP) groups, both of them in the Earth Science department.

CES group provides expertise and guidance to the other scientists in the technical issues and develops a framework for the most efficient use of HPC applied to ESMs. The performance area aims at providing feedback on model efficiency to modellers around Europe. Many of these activities are related to EC-Earth. Some members of CES (including Mario Acosta, Pablo Echeverria and Kim Serradell) are part of the technical working group of EC-earth and NEMO consortium. There is also an official collaboration with the main developers of IFS, the ECMWF. CES group is also taking part in different H2020 European projects related to the goals of OEMES for HPC. These projects are ESiWACE, IS-ENES2, Montblanc or PRIMAVERA, and participating in new proposals as ESCAPE2.

On the other hand, CP group undertakes advanced research to forecast climate variations from one month to several years into the future (also known as seasonal-to-decadal predictions) and from regional to global scales. Many of the activities in modelling and prediction are based on research, development and predictions with the EC-Earth climate forecast system. CP has contributed to CMIP5, which is one of the key datasets used to produce the UN Intergovernmental Panel on Climate Change (IPCC) Fifth Assessment Report (AR5), global climate research activities of this group enabled production of historical global climate reconstructions and initial conditions for the EC-Earth community. This group is already active in the planning of the next phase of Coupled Climate Model Intercomparison project, CMIP6, and is preparing to make core contributions including the ground-breaking high-resolution global climate simulations with EC-Earth. Moreover, the group is also contributing to H2020 European projects, planning a set of experiments using exascale platforms for the future, with horizontal spacing close to 1km for the atmosphere and ocean for PRIMAVERA project.

The environment of the department provides a unique opportunity where experts from both groups can collaborate together, pursuing the same goal. The expertise in climate prediction will be needed to prepare ultra-high resolution experiments, in order to take advantage of the future exascale platforms to simulate patters which cannot be possible using the actual computer power. The expertise in HPC will be needed to improve the energy efficiency of these experiments and obtain results in a logical time. The team formed by the PI, Dra. Eleftheria and Mr. Kim provide an interdisciplinary and complimentary expertise beyond the computer science, HPC and climate modelling backgrounds. As a consequence, this project will make advantage of this knowledge, and therefore ensure the application of novel HPC techniques for these kind of numerical models, the only way to take advantage of the new platforms and adapt the needs of the scientists in the computational algorithms at the same time.

-La Agencia Estatal de Meteorología (AEMET). They work actively using EC-Earth, their main goal is to build a fully coupled Atmosphere-Ocean- Land-Biosphere system model, usable from seasonal to decadal climate prediction and climate projections.

At international level, many different research centres and universities departments work on the topic (EC-Earth consortium is compound by 24 universities and institutions around Europe, all of them use EC-Earth actively). Listed below are the most relevant ones for the project:

-The European Centre for Medium-Range Weather Forecasts (ECMWF), they develop the atmospheric model (IFS) used by EC-Earth.

-The University of Exeter, they are one of the main developers of the ocean model (NEMO) used by EC-Earth.

-The Centre Européen de Recherche et de Formation Avancée en Calcul Scientifique (CERFACS), they develop the coupling library (OASIS) used by EC-Earth.

-The Swedish Meteorological and Hydrological Institute (SMHI). They are one of the main developers of EC-Earth.

-The Royal Netherlands Meteorological Institute (KNMI). They are one of the main developers of EC-Earth.

The Working Group includes six PhD researchers from the international groups commented. Dr. Nils Wedi is the head of Earth System Modelling at the ECMWF. Dr. Kristian Mogensen is a senior researcher at the ECMWF, in the same division. Their expertise includes all aspects of scientific and computational performance related to weather prediction (Dr. Nils) and ocean coupling for IFS (Dr. Kristian). Dr. Sophie Valcke is the leader of the OASIS code coupler development team at the CERFACS. His expertise includes the knowledge on high-resolution atmosphere-ocean-ice coupled modelling. Dr. Martin Schreiber is a proleptic lecturer at the University of Exeter (UK), in the Mathematics Department. His expertise includes the knowledge of performance analysis and optimization of ocean models on HPC architectures. Dr. Uwe Fladrich is a scientific software developer at the SMHI, in the Rossby Centre. His expertise includes the knowledge on efficient software development processes and numerical aspects of climate models. Dr. Philippe Le Sager is a research software engineer at the KNMI. His expertise includes the development of ESMs and the implementation of Fortran codes for CMIP6, and for PRIMAVERA and CRESCENDO projects.

6. Methodology and planning

As envisaged from its conception, OEMES has been designed with the aim of tailoring the objectives, the Research Group's background, the Working Group's expertise and the facilities of the host institution, in order to ensure its successful completion. The work plan reflects this idea, where the scientific program can be implemented from head-to-tail and in autonomy. The project is divided in seven work packages (WP): one for research (WP1), five for research and development (WPs2-6) and one for management and dissemination (WP7).

WP1: Develop a profiling method to highlight numerical and computational problems of numerical models executed in extreme parallel platforms.

Mario Acosta, PhD (20%) Kim Serradell (20%)
Eleftheria Exarchou, PhD (20%) Pablo Echeverria (00%)

The goal of this WP is to create a profiling methodology personalized for ESMs. This methodology will be used for WPs from 2 to 5. Moreover, the new methodology could be used for scientists in other ESMs to facilitate the effort in order to improve the energy efficiency of the models, using a methodology oriented to improve this kind of models for platforms with thousands of cores. It comprises task 1.1 and will be monitored by M1, M3 and D1.

Task 1.1. Creation of a profiling method specific for ESMs

In the ESMs case, an in-depth performance analysis can lead to feasible and productive solutions that do not require a full rewrite of the code while effectively improving the performance of the model. Preliminary studies proved that an exhaustive profiling analysis of EC-Earth will be useful to improve its performance (Yepes et al, 2017). Knowing the understanding of the computational behaviour of applications, running in HPC systems, is not straightforward, this task will develop a methodology to undertake this analysis, with the aim of helping scientists to cope with this issue.

The methodology proposed in this task intends to be useful to scientists that are running EC-Earth on HPC systems and are willing to understand its computational performance, uncovering issues that are potentially hindering its efficiency. This methodology will be specific for the needs of weather and climate models. For this purpose, the next methodology will be extended to study each of the components of EC-Earth.

1) Mathematical study
2) Computational study
3) Profiling study applied to ESMs
4) Identification of main bottlenecks

The interdisciplinary environment of the research group will provide the basis to complete the three first steps from different point of views, including the requirements of each field. The third step will be completed taking into account ESMs and computational metrics, following a novel path that foresees to revolute the profiling analysis for ESMs.

The main outcome of this task will be to highlight problems not previously identified, explaining the reasons for their occurrence and propose optimizations to substantially improve the computational performance of the model.

WP2: Achieving a method to validate and reproduce the results of Earth System Models, taking into account a trade-off among accuracy, reproducibility and performance.

Mario Acosta, PhD (10%) Kim Serradell (00%)
Eleftheria Exarchou, PhD (20%) Pablo Echeverria (10%)

The goal of this WP is to prove that the optimizations developed for the different components of EC-Earth do not reduce the accuracy and reproducibility of the results. We will propose a specific methodology for ESMs, taking into account the chaotic nature of weather and climate models and the round off errors introduced by parallel executions. This new methodology could be used by scientists in other ESMs and environments in order to prove that new optimizations for exascale computing do not affect the quality of the results. It comprises tasks 2.1 and will be monitored by M2-M3 and D2.

Task 2.1. Creation of a validation and reproducibility method to evaluate computational optimizations

This task will develop a method to evaluate all the possible optimizations for EC-Earth, taking into account the chaotic nature of ESMs and the introduction of round off errors produced by parallel computing. The methodology will use statistical methods to evaluate ensemble experiments (same experiment run several times with small perturbations in the initial conditions) and compare the results when the optimizations are included or not.

The main goal of this task is to create a novel methodology which could be used by both climate and computer scientists to evaluate the accuracy and reproducibility of the results. To achieve this, the process will compare automatically the results among ensemble experiments and between different parallel executions. The comparison will include data from CMIP5 to evaluate the accuracy of the simulations. The computational performance of each experiment, including some optimizations on a different scale of aggressiveness will be also evaluated. The final result will be to achieve a trade-off among accuracy (comparing to CMIP5 data), reproducibility (comparing different parallel executions) and performance (using performance metrics among executions).

WP3: Improving energy efficiency of the atmospheric component of EC-Earth (IFS), to take advantage of future exascale computers in an efficient way. Preparing ultra-high resolution experiments for extreme parallelization.

Mario Acosta, PhD (20%)	Computer Engineer (30%)
Eleftheria Exarchou, PhD (20%)	Nils Wedi, PhD
Kim Serradell (10%)	Uwe Fladrich, PhD
Pablo Echeverria (30%)	

The goal of this WP is to improve the energy efficiency of the atmospheric model used by EC-Earth, IFS, in order to adapt the model for exascale platforms with thousands and thousands of cores, where the parallel overhead in the algorithms could be a handicap. Preliminary work proved that a profiling analysis for IFS can localize some bottlenecks of the model (Acosta et al, 2017). This work , which has started in collaboration with ECMWF, it will follow through two tasks: 3.1 Highlight the main bottlenecks of the model using the methodology proposed in WP1, and 3.2, where some novel optimizations will be implemented in order to improve the energy efficiency and accomplish the climate and weather requirements of the modelization at the same time. It comprises tasks 3.1-3.2 and will be monitored by M4-M6 and D3.

Task 3.1. Profiling methodology applied to IFS

This task will create the profiling evaluation of IFS, using the methodology developed in the task 1.1, explicitly oriented to atmospheric models. The goals for this task will be to understand perfectly the mathematical and computational algorithm used by the model in order to evaluate if the implementation is optimal and which numerical methods could be changed. The profiling tools will be used to highlight the main bottlenecks of the model for the parallel execution using a large number of resources and ultra-high resolution grids, pointed out with parts of the code should be optimized before running experiments with ultra-high resolution grids and exascale platforms.

Task 3.2. Energy efficiency optimization of IFS

This task includes the development and configuration of ultra-high resolution grids for IFS and the application of the profiling methodology, which will help to disentangle the main bottlenecks of the code and deal with them accordingly. This task will develop different optimizations in order to improve the scalability of the model when ultra-high resolution grids and supercomputers with thousands of cores are used. Preliminary tests proved that IFS has different areas of the code which could be improved. Some of the strategies that can be developed and tested for IFS are:

- Overlapping communications and calculations for the transposition and transformation stages. This could reduce the communication process in parallel executions after the calculations phases. A novel technique which could be used here is the use of Ompss (a BSC tool to automatize the parallelization of tasks, https://tools.bsc.es/) to do this process, which could improve the performance of the model dramatically.
- Optimizing the access memory during the calculations phases, reducing the cache misses. The optimization will be done taking into account the architecture of big supercomputers.
- Optimizing the shared memory implementation (OpenMP), taking into account the architecture of big supercomputers.
- Using heterogeneous computation to share the computational calculations among the resources available such as CPUs, GPUs…

- Optimizing the domain decomposition of the model during the calculation phases to reduce the unload balance in the parallel execution.

WP4: Improving energy efficiency of the ocean component of EC-Earth (NEMO), to take advantage of future exascale computers in an efficient way. Preparing ultra-high resolution experiments for extreme parallelization

Mario Acosta, PhD (20%)	Computer Engineer (30%)
Eleftheria Exarchou, PhD (20%)	Martin Schreiber, PhD
Kim Serradell (10%)	Uwe Fladrich, PhD
Pablo Echeverria (20%)	

The goal of this WP is to improve the energy efficiency of the ocean model used by EC-Earth, NEMO, similar to WP3 but for the ocean component. Preliminary work proved that optimizations for NEMO can increase the computational performance (Tintó et al, paper accepted). This work, which has started in collaboration with the NEMO consortium, it will follow the same strategy that WP3, with similar tasks. It comprises tasks 4.1-4.2 and will be monitored by M4-M6 and D4.

Task 4.1. Profiling methodology applied to NEMO

This task will create the profiling evaluation of NEMO, using the methodology developed in the task 1.1, explicitly oriented to ocean models. The strategy is similar to Task 3.1 but for NEMO.

Task 4.2. Energy efficiency optimization of NEMO

Apart from the creation of the ultra-high resolution grids for NEMO, the profiling methodology will reveal the main bottlenecks of the code, similar to the strategy explained in task 3.2. Preliminary tests proved that NEMO has different areas of the code which could be improved. Some of the strategies that can be developed and tested for NEMO are:

- A novel technique for ESMs which could be used here is the reduction of the accuracy of the variables from double to single precision. This task will determine which computational phases of NEMO can use single precision and whether this process could be automatize to be used in others similar ocean models.
- Optimizing the shared memory implementation (OpenMP), taking into account the architecture of big supercomputers.
- Using heterogeneous computation to share the computational calculations among the resources available such as CPUs, GPUs…
- Optimizing the domain decomposition of the model during the calculation phases to reduce the unload balance in the parallel execution.

WP5: Improving energy efficiency of coupling among Earth System components when ultra-high resolution experiments are used for extreme parallelization

Mario Acosta, PhD (20%)	Computer Engineer (30%)
Eleftheria Exarchou, PhD (20%)	Sophie Valcke, PhD
Kim Serradell (10%)	Kristian Mogensen, PhD
Pablo Echeverria (20%)	Uwe Fladrich, PhD

The goal of this WP is to improve the energy efficiency of the coupling library used by EC-Earth, OASIS, similar to WP3 and WP4, but for the coupler. Preliminary analysis proved that a correct configuration for OASIS can increase the computational performance (Acosta et al, 2016). This work, which has started in collaboration with CERFACS, it will follow the same strategy that WP3 and WP4, with similar tasks. It comprises tasks 5.1-5.2 and will be monitored by M4-M6 and D5.

Task 5.1. Profiling methodology applied to coupling between components using OASIS

This task will create the profiling evaluation of coupling, using the methodology developed in the task 1.1, explicitly oriented to the coupling using OASIS. The strategy is similar to Task 3.1 but for the coupler.

Task 5.2. Energy efficiency optimization of coupling between components using OASIS

In analogy to previous tasks, the application of the profiling methodology will help to address some problematic points within the code, similar to the strategy explained in Task 3.2. Preliminary tests proved that coupling between EC-Earth components has different areas of the code which could be improved. Some of the strategies that can be developed and tested for the coupling used by EC-Earth are:

- Optimizing the load balance between components. A process to optimize the synchronization of the execution time of each component executed in parallel will improve the performance of the coupled model.
- Exploring the different methods for the conservative methods available, in order to determine the best one for EC-Earth, taking into account a trade-off among accuracy, reproducibility and energy efficiency.
- Exploring two different methods for the execution and interaction of Earth components, comparing in parallel executions two different paradigms. Comparing the Multiple Program, Multiple Data paradigm used by OASIS (CERFACS) and the Single Program, Multiple Data (SPMD) paradigm used by ECMWF institution.

WP6: Optimizing throughput of complex experiments for supercomputers. Optimizing affinity process and thread of ESMs

Mario Acosta, PhD (10%)
Eleftheria Exarchou, PhD (00%)
Kim Serradell (50%)
Pablo Echeverria (20%)
Computer Engineer (30%)
Uwe Fladrich, PhD
Philippe Le Sager, PhD

The goal of this WP is to optimize the execution of large experiments using supercomputers with thousands of cores. This WP will provide a plan which can follow the scientists to optimize the throughput of large parallel executions, where workflow managers and parallel schedulers are needed. It comprises tasks 6.1 and will be monitored by M5-M7 and D6.

Task 6.1. Optimizing throughput of large experiments in supercomputers

The goal of this task is to enhance the throughput of ESM workflows by developing an algorithm that deals with the execution of large experiments. On the one hand, it will use a formula to find a trade-off between computational performance and efficiency to set the right amount of processes for each part of the experiment (known as chunk). On the other hand, the algorithm will be able to predict the queue waiting time by learning from the past experiments.

Then, using these two inputs, the algorithm developed in this task would be able to launch new simulation chunks dynamically, setting their amount of resources and adjusting their wall-clock time to maximize the whole throughput of the workflow. In addition, the algorithm could also have into account the budget of available execution hours to fit the experiment and be able to finish it.

<u>WP7. Project management and dissemination of results.</u>

This work-package will ensure the appropriate management of the project and broadly disseminate the outputs throughout its duration. It will be feasible thanks to the Project Management Department at the host institution (BSC) and the strong group of “Earth System Services” established at the department level (BSC-ES). WP7 will monitor the progress of the project, ensure timely preparation of scientific reports (milestones and deliverables) and outreach activities, facilitate communication among the Research, Working Group members’ institutions (BSC, ECMWF, KNMI, SMHI, CERFACS, Lexeter University) and organize the project meetings. There will be three annual meetings organized by BSC within the OEMES project to ensure that action items are under way [Me1-Me3]. These project meetings are not intended to be internal symposiums but open conferences, in which researchers not directly involved in OEMES, e.g. from other scientific groups using EC-Earth, the last project meeting will be also used to communicate and ensure the exploitation of the new version of EC-Earth by all the institutions interested. There will be visits to ensure the collaboration and communication with the Working Group members [V1-V7], to discuss the results [V1-V2-V5], plan additional analysis [V2-V3-V4] and ensure the exploitation of the results by all the institutions interested [V6-V7]. Under WP7, the project will also undertake a final report that, in addition to the summary of the scientific achievements, will identify priority research lines to enhance the energy efficiency of EC-Earth in the path to take advantage of exascale platforms [D7].

Planning

Further details are provided bellow about the methodology plan, including milestones (Ms), deliverables (Ds) and visits (Vs). Note that the expected date is indicated in terms of the corresponding month, thereafter *pm*. The schedule of the tasks described above is presented in the following chronogram.

Project month (PM)		1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
WP1	T1.1																		
WP2	T2.1																		
WP3	T3.1																		
	T3.2																		
WP4	T4.1																		
	T4.2																		
WP5	T5.1																		
	T5.2																		
WP6	T6.1																		
WP7	Comm												C1						
	Dissem						Dis1						Dis2						
	Explot												E1						
Milestones							M1						M2	M3					
Deliverable							D1						D2						
Meeting													Me1						
Visit								V1					V2						

Project month (PM)		19	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34	35	36
WP1	T1.1																		
WP2	T2.1																		
WP3	T3.1																		
	T3.2																		
WP4	T4.1																		
	T4.2																		
WP5	T5.1																		
	T5.2																		
WP6	T6.1																		
WP7	Comm												C2						C3
	Dissem		Dis3				Dis4						Dis5						Dis6
	Explot												E2						E3
Milestones													M4					M5	M6
Deliverable													D3	D4	D5			D6	D7
Meeting													Me2						Me3
Visit			V3						V4				V5				V6		V7

List of milestones (tracking progress)

- M1- Profiling methodology for ESMs
- M2- Reproducibility methodology for parallel execution of ESMs
- M3- First project meeting
- M4- New optimized version of EC-Earth
- M5- ESM throughput optimization for exascale platforms
- M6- Second project meeting

List of deliverables (tracking achievements)

- D1- Assessment of profiling methodology for ESMs
- D2- Assessment of reproducibility methodology for ESMs
- D3- Assessment of profiling and optimization work for IFS
- D4- Assessment of profiling and optimization work for NEMO
- D5- Assessment of profiling and optimization work for coupling of OASIS3-MCT
- D6- Assessment of work for throughput efficiency of ESMs
- D7- Final scientific report and recommendations

List of deliverables (tracking achievements)

- V1- 1 two-day visit of Lexter University and KNMI at BSC for the kick-off meeting
- V2- 1 five-day visit at ECMWF
- V3- 1 two-day visit of ECMWF and CERFACS for the 2nd project meeting
- V4- 1 two-month visit at SMHI
- V5- 1 five-day visit at CERFACS
- V6- 1 day visit at AEMET
- V7- 1 two-day visit of SMHI and KNMI at BSC for the final meeting

7. Technical resources

OEMES will have access to the BSC high performance computing facilities to run the experiments in all WPs. The simulations will require a large number of resources for each test and WP. WP3-4-5 and 6 will require a big numbers of cores in order to do the tests to evaluate the energy efficiency and optimizations developed for each of the EC-Earth components. This means that more than 20,000 cores are needed per tests. However, mostly of these tests will not require long period of simulations. Only reproducibility tests will require experiments of at least 100 years of simulation in order to evaluate the accuracy and reproducibility of the results. Thanks to the computational resources of BSC, with the new MareNostrum IV (165,888 cores, 11.15 PetaFlops) the tests will be possible though it will be demanding. However, the completion of the OEMES would be ensured thanks to the use of Marenostrum IV. Moreover, MareNostrum IV is formed of clusters of three different technologies. These are technologies currently being developed in the US and Japan to accelerate the arrival of the new generation of pre-exascale supercomputers. Marenostrum IV includes a cluster which consists of IBM POWER9 processors and NVIDIA Tesla GPUs (1.5 PetaFlops), a cluster made up of Intel Knights Hill (KNH) processors (0.5 PetaFlops) and a cluster formed of 64 bit ARMv8 processors in a prototype machine (0.5 Petaflops). This structure presents a unique opportunity to fulfill the OEMES goal related to optimizations for heterogeneous platforms.

Additional infrastructure is needed for a successful implementation of OEMES. Due to the unusually large data needed to do the profiling analysis and evaluate the parallel execution of the model, additional local storage will be needed. The profiling results are expected to generate files with a size of 300 Gb per execution. The output of ultra-high resolution grids (for the reproducibility experiments) should be also taken into account, from 250 GB to 500 GB per experiment. For the amount of data that the project is expected to generate, we need around 120 TB of raw space. That will require the acquisition of 60 4TB disks. Additionally, the project would need a workstation (PC) for the new Computer Engineer demanded to work in autonomy. Finally, and in order to facilitate an efficient execution/development of the activities in missions outside the host institution, e.g. attendance to meetings, OEMES would require a laptop with an UNIX-based OS.

8. Human resources

The need for a Computer Engineer for the optimal achievement of the tasks in WP3, WP4, WP5 and WP6 is justified by the evaluation of the model performance and the implementation of different optimizations that contribute to the improvement of each of the components of EC-Earth (IFS, NEMO and OASIS). There are three complex components (an atmospheric model, an ocean model and a coupler) which require being analyzed and optimized at the same time (from pm 13 to pm 30). This requires enough human resources, not only to analyze test results or develop the optimizations, but also to do all the scalability and reproducibility tests and take the results, namely the preparation and execution of hundreds of tests which can be automatized only partially. Though Pablo Echeverria can fulfill this support tasks for WP1 and WP2 alone, the additional computer engineer will help the scientists of the Research and Working Group towards a better completion of these objectives, taking over the preparation, execution and analysis of the tests, developed for three components of EC-Earth in parallel. At the same time, he/she will benefit from the support of another dedicated Computer Engineer (**Pablo Echevarria**) at BSC. The candidate should be a recent master graduate in computer science, physical or mathematical, preferably with a background in HPC.

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C.2. IMPACTO ESPERADO DE LOS RESULTADOS

National and international impacts: scientific, social and economic. [See attached letters of support]

Increasing the capability and comprehensiveness of 'whole Earth system' models, in order to represent an ever-increasing realism and detail of new scenarios for our future climate, is the only way to reduce the uncertainties in the study of climate. However, the numerical models that scientifics are using are not ready for the massive parallel platforms which are coming to allow these studies. OEMES will help to evaluate and optimize one of the most important Earth System Model in Europe, EC-Earth, for these exascale platforms. This will allow the obtention of ultra-high resolution global simulations which will be used for several socio-economic activities as well in Spain as in the rest of Europe, providing society with information on the future climate and generating reliable in-house predictions and projections of global climate change. Something which is a prerequisite to support the development of national adaptation and mitigation strategies. The EC-Earth consortium consists of 24 academic institutions and meteorological services from 11 different countries in Europe. In Spain, AEMET and BSC are two important institutions witch will benefit from the OEMES results, producing a new optimized version of EC-Earth, being AEMET and BSC research groups both users.

In this sense, OEMES will help to improve the application of HPC to Earth System Modelling, promoting the synergies between different scientific groups (modellers, mathematics and computer scientists), meteorologists and governments. With this framework, OEMES agrees with some European projects in H2020 as ESiWACE and ESCAPE that highlights the necessity of improving our actual numerical models in order to adapt them to the new generation of exascale computers.

The main impacts derived from OEMES, which meets the priorities of the European community are:

1. The increase of the knowledge of relevant information to improve the parallel execution of the numerical models, which were developed several years ago, following a determined methodology which allow to highlight the real problems of the model to scale in an easy way.

2. The increase of the knowledge of relevant information to evaluate the accuracy and reproducibility of ESMs, when HPC optimizations are implemented, following a determined methodology to automatically evaluate the simulations of several experiments and determine if the improvement in the energy efficiency of the model affects to the accuracy and reproducibility.

3. The improvement of the quality of the simulation results of weather and climate prediction, using ultra-high resolution grids to reduce the uncertainty presented in ESMs. Large and complex experiments such as PRIMAVERA or CMIP6 will benefit of a new version of EC-Earth. The new optimized version will allow to 1) take advantage of platforms with much more computing power, 2) achieve a reasonable energy efficiency and 3) take the results in a reasonable time, producing results impossible until now.

4. The improvement of the performance of the computational execution of the three main components of EC-Earth (IFS, NEMO and OASIS). The computational study and optimization of all of them will allow to the Spanish and European community to take advantage of massive parallel supercomputers, presenting a good scalability in the execution.

5. The increase of the knowledge of launching huge Earth System simulations in massive parallel platforms, determining the best way to manage the execution and resources of these experiments and optimize the production and post processing of the results.

6. Weather and climate community awareness on the HPC requirements for ESMs in order to be ready for exascale computing.

7. The promotion of the real need of interdisciplinary expertise, helping in the formation of new PhDs researchers who will be able to adapt the requirements of both computational and climate worlds for ESMs.

8. The promotion of the synergies between scientific groups, meteorology institutions and governments.

Summarizing, OEMES fosters the integration of advanced HPC techniques specifically oriented for the assessment and modelling of weather and climate predictions with the idea of testing innovative technological options and strategies to improve our climate prediction. OEMES will cause a step forward in the development of numerical models for massive parallel platforms and its application to produce ultra-high resolution simulations, transferring knowledge on a short, medium and long-term to scientific community and environmental institutions.

Communication, dissemination and exploitation

OEMES is committed to (1) share the methods and novelties implemented in the project with the scientific community; (2) promote the methodology, best practices and knowledge to private and institutional stakeholders (3) allow the execution of ultra-high resolution experiments.

Communication. The achievements in HPC oriented to Earth System Modelling are currently not communicated to the community in an effective and engaging way. In this sense, 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. OEMES activities will be communicated using a language that can be understood by non-specialists using appealing communication formats such as leaflets [C1-C3], explaining the real need for these ultra-high resolution experiments and models developed by HPC experts which are able to scale in massive parallel platforms in an efficient way.

Dissemination. The results will be presented in top international scientific conferences and meetings [Dis1-Dis6] with the idea of engaging the target scientific community and getting new ideas and feedback. Planned European conferences and meetings to attend are: the EC-Earth meetings (one a year), the OpenIFS workshop supported by ECMWF, the coupling workshop supported by CERFACS and NEMO meeting supported by the NEMO consortium. Furthermore, it is foreseen to publish four articles in relevant peer-reviewed scientific journals following the European Commission's policy on open-access for research articles. The description of the project and main outcomes will be disseminated through the website of the Earth System Department. Finally, three open-project meetings organized by the BSC are planned with the aim to present the state and progress of the project to the local scientific staff, BSC collaborators, national and European institutions. The continuous presence and coordinating role of the Working Group members and the BSC-ES scientists will ensure the dissemination of the OEMES's outcomes.

Exploitation. OEMES will produce a new version of EC-Earth which will be available for the community in order to produce ultra-high resolution experiments using massive parallel platforms. Different institutions have manifested their interest for this new version. From Spain, BSC and AEMET (see recommendation letter) will use the results of this project. At European level, all the external collaborator institutions (ECMWF, SMHI, KNMI, Lexeter University and CERFACS) have manifested their complete support and interest for the future use of the optimized version. These results can be exploited in different ways by the national and international meteorological institutions. OEMES also plans to send annual newsletters [E1, E2] to institutions and the target, as well as a technical report [E3] that ensures a detailed communication and understanding of the project results.

The project will take advantage from the BSC's dissemination infrastructure (i.e., Media communication manager, communication team, in-house designer, BSC website, BSC social media accounts with >2,500 followers, MareNostrum open day events with >5,000 visitors per years, etc.) to enhance the spread of the results derived from research activities among the general public, companies (e.g. automotive or gas companies) and the international scientific community.

C.3. CAPACIDAD FORMATIVA DEL EQUIPO SOLICITANTE

Since its goals are clearly stated, the methodology is precise and the technical support to undertake the research is considerable (see Research Group), OEMES is very adequate for the formation of young researchers. Considering the complex problem for achieving the requirements of both computational and climate fields, where both communities agree on the missing processes that take place in the development of the models and the adaptation to parallel platforms. Training young experts on this interdisciplinary research will reinforce the Spanish position in the global framework. The background of the PI (supervisor of one PhD thesis and one master thesis), the experience of other PhD in the Research Group and the head of the computational group provides a great opportunity for training new experts (see CVs attached for more research information). The PhD student will also benefit from interacting with the Working Group as well as with the large amount of scientist visiting BSC-ES. Hence, OEMES provides a highly stimulating scenario for carrying a PhD thesis. It could be the continuation of the work of the PhD student in the group directed by the PI (including a paper accepted by the PhD student related to the topic during his first year).

OEMES will be developed within the BSC-ES Department which has a long record of supervising PhD theses in the doctoral programme Environmental Engineering (UPC) with MEC Excellence Mention from 2011 (MEE2011-0335), with 21 dissertations completed during the last 10 years and available in the following link: http://www.bsc.es/earth-sciences/phd-thesis). BSC-ES has also experience in organizing/hosting conferences and workshops. Additionally, BSC has a specialized Education and Training Team, dedicated to establish a curricula based on cutting-edge scientific research on HPC and application areas targeting research communities and industry with HPC needs. E.g., BSC-ES offers the course "Earth Sciences Simulation Environments at BSC" every year funded by PRACE ("Partnership for Advance Computing in Europe"). During last 5 years (2012-2016), BSC-ES was granted 9 EU H2020 projects, 5 EU FP7 projects, 5 EU Copernicus projects, 7 projects funded by the Ministerio de Economía y Competitividad (MINECO), 2 projects funded by the European Space Agency, 1 project funded by the French Ministry of Sciences and 1 project from ERA-NET. During that same period, BSC-ES also participated in 21 RES and 4 PRACE projects. BSC-CNS has been awarded with the Severo Ochoa's Centre of Excellence project of the Spanish government since its first call (2011). BSC provides professional development plan for each member according to their profile and objectives. In this sense, BSC has been awarded with the Human Resources Excellence in Research due to its progress in aligning their human resources policies with the principles set out in the EU Charter and Code for Research.

C.4. IMPLICACIONES ÉTICAS Y/O DE BIOSEGURIDAD

Not applicable